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DarcyTools, Version 2.1 User´s guide

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March 2004

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Preface

The User's Guide for DarcyTools V2.1 is intended to assist new users of DarcyTools. The Guide is far from complete and it has not been the ambition to write a manual that answers all questions a user may have.

The objectives of the Guide can be stated as follows:

- Give an overview of the code structure and how DarcyTools is used.
- Get familiar with the "Compact Input File", which is the main way to specify input data.
- Get familiar with the "Fortran Input File", which is the more advanced way to specify input data.

Table of content

1 Introduction

1.1 Background

DarcyTools is a computer code for simulation of flow and transport in porous and/or fractured media. The fractured media in mind is a fractured rock and the porous media the soil cover on the top of the rock; it is hence groundwater flows, which is the class of flows in mind.

DarcyTools is developed by a collaborative effort by SKB AB (The Swedish Nuclear Waste Management Company AB) and CFE AB (Computer-aided Fluid Engineering AB). It builds upon earlier development of groundwater models, carried out by CFE AB during the last ten years. In this earlier work the CFD code PHOENICS (Spalding, 1981) was used as an equation solver. DarcyTools is based on a solver called MIGAL (Ferry, 2002). It has however been carefully evaluated that the two solvers produce very similar solutions and the earlier work is thus still valid as a background for DarcyTools.

The present report will focus on the software that constitutes DarcyTools. Two accompanying reports cover other aspects:

- Concepts, Methods, Equations and Demo Simulations (Svensson et al. 2004) (Hereafter Report 1).
- Verification and Validation (Svensson, 2004) (Hereafter Report 2).

Two basic approaches in groundwater modelling can be identified; in one we define grid cell conductivities (sometimes called the continuum porous-medium (CPM) approach, Jackson et al., 2000), in the other we calculate the flow through the fracture network directly (DFN approach). Both approaches have their merits and drawbacks, which however will not be discussed here (for a discussion, see Sahimi, 1995). In DarcyTools the two approaches are combined, meaning that we first generate a fracture network and then represent the network as grid cell properties. Further background information is given in the two reports mentioned.

1.2 Objective

The main objective of this User's Guide is to introduce and explain all parts of DarcyTools that a user needs to be concerned with.

1.3 Intended use and user

Commercially available computer codes often have a well structured way to specify input data. This may make the code easy to use and control. However, normally it also introduces a limit in the generality (in terms of applications) of the code. It may for example not be possible to add new source and sink terms, as formulated by the user. For a commercial code it may be necessary to limit the access to the source code, as “well meant improvements” by users will make user support impossible.

DarcyTools is not a commercial code and it is intended for a small group of users. The user will therefore have access to the source code needed for more “advanced” modifications. The user accessible parts are however well separated from the main codes and are also “as small as possible” (perhaps 1-2% of the total code); this to simplify the task for the user. For most problems it will however suffice to specify the input by way of data statements (details later).

The intended user is thus assumed to have a general knowledge about advanced computer codes and be able to take the right decisions about possible additions to the code.

1.4 Outline

After a few introductory sections (Sections 1 to 3), the Compact Input File (CIF) is described. This is the main mode of input specification. If the CIF commands do not suffice (for example if complex transient boundary conditions need to be specified) a Fortran input file (fif.f) is used. The fif.f gives a user significantly more control, but also requires deeper understanding of the code and, of course, also the skill of programming in Fortran. Similarly if the advanced option for fracture network representation is used, a Fortran file called prpgen.f (for property generation) needs to be considered. After these sections a DemoCase is discussed. A deeper understanding of the code structure can be obtained by studying the Appendices.

2 What DarcyTools does

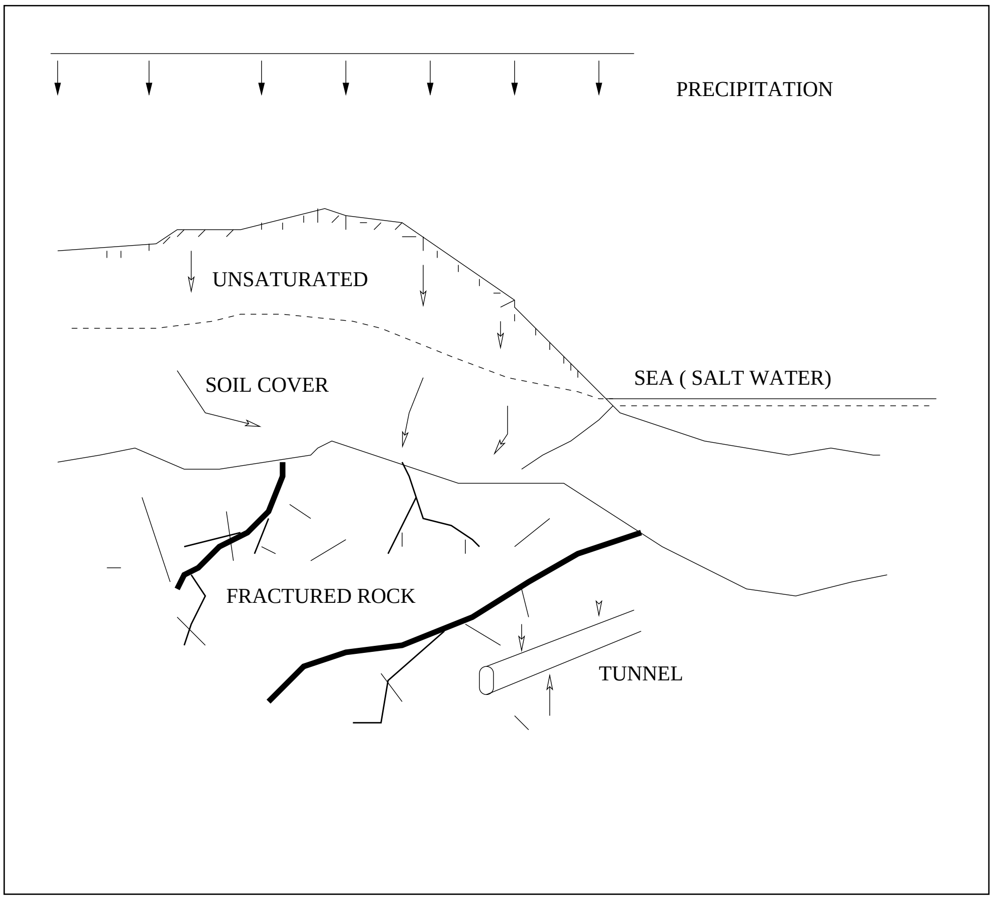
2.1 Situation in mind

As the name indicates DarcyTools is based on the concept of Darcian flow, i.e. the general momentum equations can be reduced to the Darcy equation. This class of flow includes flow in porous media and fractured rock, see Figure 2-1. In order to give a brief description of the physical processes involved, let us assume that it is of interest to analyse the origin of the water that leaks into the tunnel (Figure 2-1, top). Two possible sources are precipitation and seawater. To track the precipitation water, the simulation model must include descriptions of flow in the unsaturated zone, flow in the porous media and in the fractured rock. The groundwater table determines, largely, the pressure gradients in the porous media (and may influence conditions deep into the rock) and it is thus essential to calculate the groundwater table correctly. Seawater may be saline which introduces density effects (affects the pressure distribution). To handle this situation one needs to solve the coupled pressure-salinity problem and also consider dispersion processes. The complexity is hence greatly increased, when density effects come into play.

If a non uniform temperature distribution is present this will also affect the density. DarcyTools can handle also the temperature-salinity-pressure coupling.

If transport of a substance (salt, radionuclide, etc) is to be analysed, it is necessary to consider processes on the mm scale, see Figure 2-1 (bottom). A number of processes, on a range of time and space scales, contribute to the dispersion of a substance as it travels with the flow. The processes on the mm scale are often very significant and DarcyTools includes a novel subgrid model, called FRAME, to deal with these processes.

Hopefully this brief introduction has indicated the scope of DarcyTools. For a complete account, see Report 1.



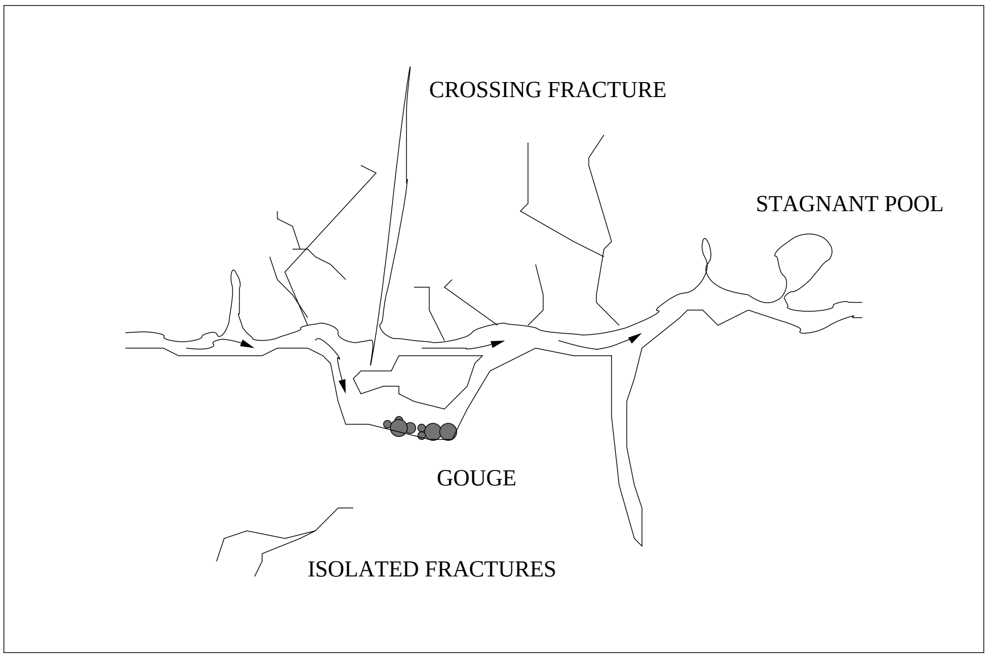


Figure 2-1. *Illustration of processes that can be analysed with DarcyTools. The large scale view (top) and the mm scale view.*

2.2 Key features

Another type of characterisation of the scope and content of DarcyTools can be obtained by listing the key features of the code:

- **Mathematical model.** DarcyTools is based on conservation laws (mass, heat, momentum and mass fractions) and state laws (density, porosity, etc.). The subgrid model utilises the multi-rate diffusion concept and the fracture network (resolved and subgrid) is based on fractal scaling laws.

- **Continuum model.** Even if a fracture network forms the basis of the approach, DarcyTools should be classified as a continuum porous-medium (CPM) model.

- **Fractures and fracture network.** Fractures and fracture zones are idealised as conductive elements, to which properties (conductivity, porosity, flow wetted surface, etc.) are ascribed. Empirical laws are used for the determination of these properties. The fracture network is based on fractal scaling laws and statistical distributions (random in space, Fisher distribution for orientation, etc).

- **GEHYCO.** This is the algorithm, based on the intersecting volume concept (see Report 1), that transforms the fracture network (with properties of conductive elements) to grid cell properties.

- **FRAME.** Subgrid processes are parameterised as "diffusive exchange with immobile zones". FRAME uses the multi-rate diffusion model and fractal scaling laws, to formulate a simple and effective subgrid model.

- **SOLVE.** When the continuum model is generated, effective CFD-methods are used to solve the resulting finite-volume equations. DarcyTools uses the MIGAL-solver, which is a multigrid solver with the capability to solve coupled problems (like pressure and salinity) in a fully coupled way.

- **PARTRACK.** This particle tracking algorithm is fully integrated with DarcyTools and uses the same basic concepts as FRAME. PARTRACK can handle Taylor dispersion, sorption and matrix diffusion simultaniously in large 3D grids ($> 10^6$ cells).

- **Verification and validation.** A set of verification and validation studies is presented (see Report 2).

A full description of features is given in Report 1.

2.3 Limitations

All models that intend to simulate flow and transport have limitations and so also DarcyTools. Many advanced features have been introduced, but few applications have so far, for obvious reasons, been carried out. The main limitation is hence immaturity. More applications are needed in order to identify shortcomings and bugs. Another way to express this point is to state that the process of confidence building has only started.

3 How DarcyTools operates

3.1 Introduction

It was mentioned in Section 1.1 that the approach adopted in DarcyTools is "to first generate a fracture network and then represent the network as grid cell properties in the continuum model". The adopted approach also governs the general structure and working of DarcyTools. The first step is to generate a grid and a fracture network. When grid cell properties have been generated the continuum problem is solved, as the second step. The final step is the postprocessing of the output.

3.2 General structure

DarcyTools is not one computer program, but a suite of "main codes" and a number of auxiliary ones. Figure 3-1 gives the relationship between the various components of DarcyTools. The figure also indicates the typical work process, as one normally "works from left to right in the diagram". A first introduction to the various programs will now be given.

FRACGEN

This is the set of programs that generates material properties, i.e. conductivity, flow wetted surface, diffusivity and porosity fields, for the media. The name GEHYCO was first introduced for conductivity fields (GEnerate HYdraulic COnductivity). GEHYCO was later generalised to also calculate other property fields, but the name was kept. Perhaps it could be interpreted as GEnerate HYdraulic COnditions. The code that encapsulates the GEHYCO algorithm is called FRACGEN.

GRIDGEN

As the name indicates this is the program that generates the grid coordinates. Presently three types of grids can be used with DarcyTools: Cartesian, General Body-Fitted Coordinates (BFC) and a simplified version of BFC (BFC:s).

PROPGEN

This small auxiliary program is used to modify the properties generated by FRACGEN. This is useful if, as an example, the conductivity of the soil cover is to be established in a calibration process. The execution of FRACGEN may take hours in complex simulations, while PROPGEN will perform its task in a minute or two.

SOLVE

This is the program that solves the differential equations for pressure, salinity and other scalars. SOLVE hence contains subroutines for the formulation of the finite volume equations, boundary and source terms, etc. A key element in SOLVE is the solver of the linear equation system, MIGAL.

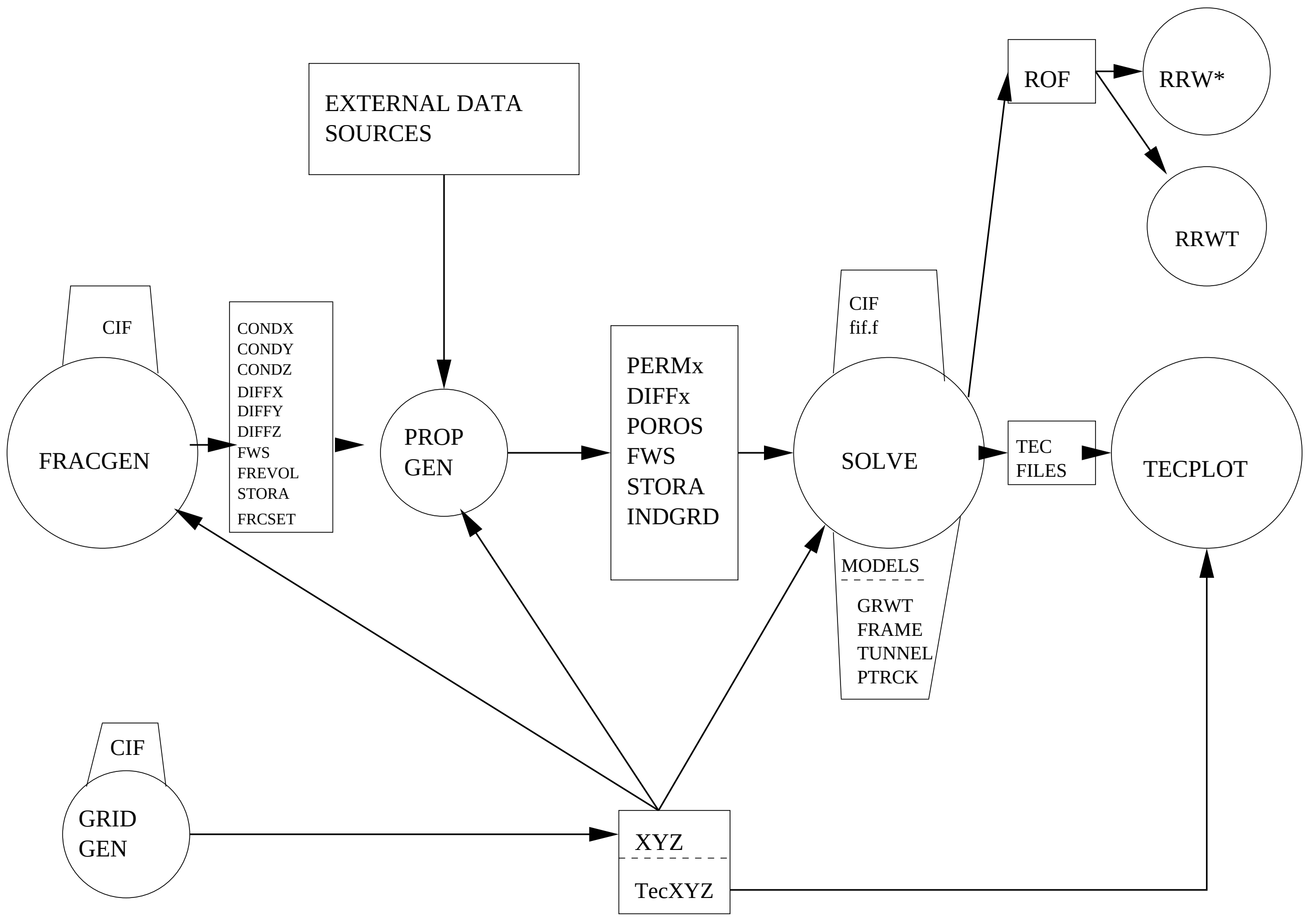


Figure 3-1. *How DarcyTools operates. Circles indicate a program, while squares indicate data files.*

MODELS

This is a file containing subroutines that handle various physical and chemical processes (so far no chemical processes have been included). Examples of tasks for these subroutines are the specification of the skin factor applied around a tunnel and the determination of the groundwater table. Both these tasks are coupled with the pressure solution and can hence not be given as input parameters.

RRW* and RRWT

The Result Output File is called ROF. In ROF all data necessary for a restart are stored. Also intermediate data, for example a time series, can be stored, if so specified by the user. It is anticipated that a non-DarcyTools user may like to explore the simulation results stored in ROF, maybe using a postprocessor like Tecplot. The small program RRW* (Read ROF Write for some postprocessor) is intended to fulfil this need. RRWT is a small program that writes output files that can be viewed in Tecplot.

POSTPROC, Tecplot

As described above, (RRW*), DarcyTools prepares for the user to use the postprocessor he/she may prefer. However, Tecplot has been selected as the “standard” postprocessor for DarcyTools. From the input files a user can specify the content of Tecplot files, which are then generated by DarcyTools.

3.3 Mathematical Model

DarcyTools computes fracture network flows using a continuum model in which the mass conservation equation is associated to several mass fraction transport equations for the salinity and/or particle mass concentrations, and to a heat transport equation.

Conservation of mass:

$$\frac{\partial \rho\theta}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = Q \qquad (3\text{-}1)$$

where ρ is fluid density, θ porosity, u, v and w Darcy velocities and Q a source/sink term. The coordinate system is denoted x, y, z (space) and t (time).

Mass fraction transport equation:

$$\begin{aligned}\frac{\partial \rho\theta C}{\partial t} &+ \frac{\partial}{\partial x}\left(\rho u C - \rho\gamma D_x \frac{\partial C}{\partial x} \right) \\ &+ \frac{\partial}{\partial y}\left(\rho v C - \rho\gamma D_y \frac{\partial C}{\partial y} \right) \\ &+ \frac{\partial}{\partial z}\left(\rho w C - \rho\gamma D_z \frac{\partial C}{\partial z} \right) = QC + Q_C\end{aligned} \qquad (3\text{-}2)$$

where C is transported mass fraction, D_x, D_y and D_z the normal terms of the diffusion-dispersion tensor and Q_c a source/sink term. When C is salinity, the source term represents the exchange with immobile zones and Q_c is determined by the subgrid model FRAME. Note that the diffusion coefficients are the effective coefficients that include the porosity, see further explanation in connection with Equation (3-10) below.

Conservation of heat:

$$\begin{aligned}\frac{\partial\left(\rho\theta c_p + (1-\theta)c \right)T}{\partial t} &+ \frac{\partial}{\partial x}\left(\rho u c_p T - \lambda_x \frac{\partial T}{\partial x} \right) \\ &+ \frac{\partial}{\partial y}\left(\rho v c_p T - \lambda_y \frac{\partial T}{\partial y} \right) \\ &+ \frac{\partial}{\partial z}\left(\rho w c_p T - \lambda_z \frac{\partial T}{\partial z} \right) = Q\,c_p T + Q_T\end{aligned} \qquad (3\text{-}3)$$

where λ_x, λ_y and λ_z are the normal terms of the equivalent (i.e. rock with fluid) thermal conductivity tensor, c is the rock thermal capacity and c_p the specific heat of the fluid and Q_T a source/sink term. We are hence only solving for one temperature, assuming thermal equilibrium between the rock and the water.

The mass conservation equation is turned into a pressure equation under the well known Darcy's assumption:

$$\rho u = -\frac{K_x}{g}\frac{\partial P}{\partial x}$$

$$\rho v = -\frac{K_y}{g}\frac{\partial P}{\partial y} \tag{3-4}$$

$$\rho w = -\frac{K_z}{g}\frac{\partial P}{\partial z} - K_z(\rho - \rho_0)$$

where K_x, K_y and K_z are the local hydraulic conductivities in *x*, *y* and *z* direction, *g* the gravity acceleration, ρ_0 a reference fluid density and *P* the dynamic fluid pressure relative to the reference hydrostatic pressure.

$$P = p + \rho_0 g z \tag{3-5}$$

where *p* is the total pressure. The hydraulic conductivity, *K*, is related to the permeability, *k*, by the relation.

$$K = \frac{\rho g k}{\mu} \tag{3-6}$$

where μ is dynamic viscosity.

The fluid properties like the dynamic viscosity, μ, the density, ρ, and the specific heat, c_p, are given by state laws:

$$\mu = \mu_0\left[1 + a_1\left(T - T_\mu\right) + a_2\left(T - T_\mu\right)^2\right]^{n_\mu} \tag{3-7}$$

$$\rho = \rho_0\left[1 + \alpha_1 S + \alpha_2 S^2 - \beta_1\left(T - T_\rho\right) - \beta_2\left(T - T_\rho\right)^2\right] \tag{3-8}$$

$$c_p = c_{p0}\left(1 + b_1\, S + b_2\, S^2\right) \tag{3-9}$$

while the porosity, θ, and the compaction, γ, of the matrix are given the following dependencies:

$$\theta = \theta_0\, \gamma \tag{3-10}$$

$$\gamma = 1 + (\sigma/\theta_0)\,(P - P_0)/\rho g \tag{3-11}$$

In the above formulas S represents the salinity (salt mass fraction), θ_0 a reference porosity field given for a reference pressure field P_0 and σ the specific storativity field. n_μ, a_i, b_i, α_i, β_i, μ_0, ρ_0, $C_{\rho 0}$, T_μ and T_ρ are constants.

In the advection/diffusion equation (3-2), it is common to write the diffusion coefficient as θD_{mol}, where D_{mol} is the molecular diffusion coefficient. In DarcyTools we choose to write the term as $\theta D_{mol} = \theta_0 \gamma D_{mol} = \gamma D$, where D is now the effective diffusion coefficient. The reason is that it is the effective diffusion coefficient that is specified for a conductive element and the GEHYCO-algorithm will hence deliver effective diffusion coefficients for cell walls. When a porous media case is simulated and the diffusion coefficients are specified, one thus needs to remember that it is the effective coefficients that should be given.

3.4 Finite volume equations and solver

CFD (Computational Fluid Dynamics) methods transform the differential equations into algebraic ones, which can be solved by a computer and a computer program. DarcyTools uses the so-called finite volume method, which can be thought of as having three well-defined stages:

1) Discretize the computational domain into a number of cells, which fill entirely the domain.

2) Integrate each differential equation for each cell, to yield an algebraic equation.

3) Solve the resulting set of algebraic equations.

The differential equations were given in the previous section. After the integration, step 2 above, an algebraic equation of the following type results:

$$a_P \Phi_P = a_W \Phi_W + a_E \Phi_E + a_S \Phi_S + a_N \Phi_N + a_B \Phi_B + a_T \Phi_T + S_\phi \qquad (3\text{-}12)$$

where Φ denotes the variable in question, a coefficients and S_ϕ source terms. For further details see Report 1.

It is equations of type (3-12) that are solved by the solver MIGAL (see Report 1, Appendix A); in fact MIGAL can solve linked systems of this kind of equations, a feature that is used for the pressure-salinity coupling in the present set of equations.

3.5 Grid arrangements

DarcyTools can only work with structured grids. Within this class, the following grids can be employed:

- BFC (Body Fitted Coordinates, sometimes called curvilinear grids). This is the most general type of grid. It is not generally used in practical applications, as it requires significant computer resources and a further limitation is that GEHYCO can not generate properties for this kind of grids.

- BFC:s (BFC simplified). In this grid "all vertical lines remain vertical and the horizontal grid is cartesian, while the horizontal layers are allowed to float". It is hence the grid to use to describe topography. This is the main grid used in DarcyTools for real world applications.
- Cartesian. In this grid, the grid coordinates can be specified as depending on only one coordinate, i.e. $z\ (i, j, k)$ is only a function of k.
- Embedded grids. DarcyTools can employ embedded grids in several levels (see Report 1). Also mixed types, i.e. a Cartesian grid embedded in a BFC:s grid can be handled.

The four grid types are illustrated in Figure 3-2.

A further characterisation of the grid system concerns the variable locations. DarcyTools uses a so called node-centred arrangement, which means that variables (pressure, salinity, etc) are located at grid cell centres.

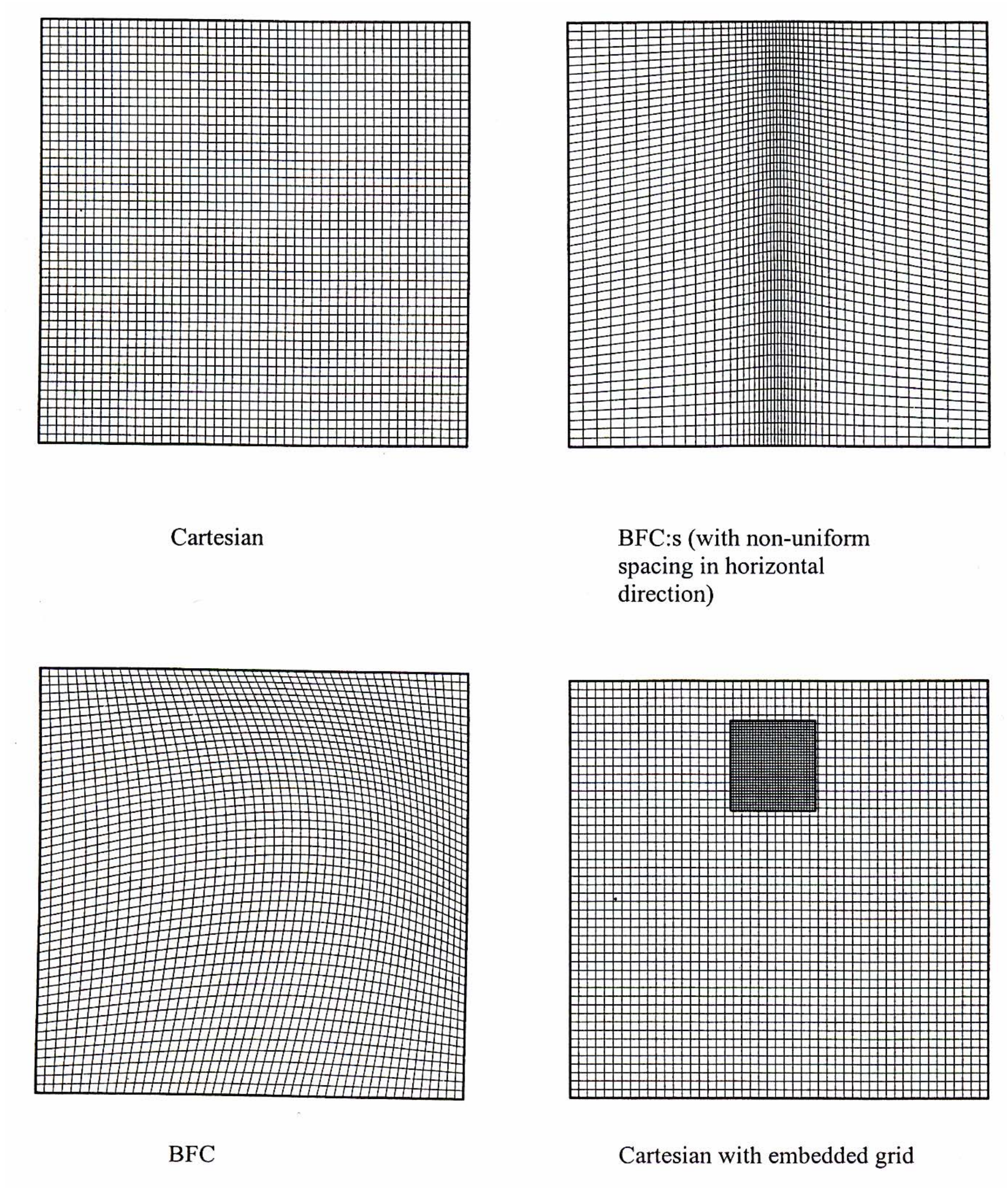

Cartesian
BFC:s (with non-uniform spacing in horizontal direction)
BFC
Cartesian with embedded grid

Figure 3-2. *The four grid types used in DarcyTools. Top-right grid only valid as a vertical section.*

3.6 Hardware, OS, etc

DarcyTools is written in Fortran90, although some parts are restricted to Fortran77 (parts that non-DarcyTools user may need like the RRW* feature discussed above).

The following points give the currently favoured working environment:

- A PC/Workstation with as much power (processor, ram, disk space, graphics, etc) as possible.
- Red Hat LINUX, as operating system (8.0, 9,0 or enterprise 3.0)
- Intel Fortran Compiler 8.0 for LINUX
- Tecplot 10 for postprocessing

DarcyTools requires very little disk space (about 2MB), and calculations can be performed on a laptop. The concepts built into DarcyTools assume however a high resolution grid (more grid cells $\Rightarrow$ more accurate simulation) and practical simulations can hence be quite demanding for the computer.

3.7 Directories, files and scripts

This section describes how to run DarcyTools and the recommended directory structure. It is assumed that the user has created this directory structure and copied files from the delivery CD.

The recommended directory structure is outlined in Figure 3-3. In the DT21 (for DarcyTools V2.1) directory, three subdirectories are found:

<u>bin:</u> contains runscripts and libraries

RUNSLV	for running	SOLVE
RUNGGN	for running	GRIDGEN
RUNFGN	for running	FRACGEN
RUNSBR	for running	SUBROF generation
RUNTRT	for running	Tecplot rotation

These scripts can be launched from the user's directory, as the PATH to bin should be specified in *.bash_profile*.

libdtslv.a	library for SOLVE
libdtggn.a	library for GRIDGEN

project: contains user files.
All files needed to start a new application, or project, are stored in this directory. A new project thus starts by copying all files in this directory to the new project directory (called MyProject in Figure 3-3). This directory contains scripts for building local RUNSLV and RUNGGN, which are called RUNMYSLV and RUNMYGGN. When the fortran input file (*fif.f*) is used, it is necessary to compile *fif.f* and create a new executable. The scripts will do this. Note that the new executables are launched by ./RUNMY ***, as we now have to point to the working directory.

VerCase: contains verification cases; see Report 2 for a full description.

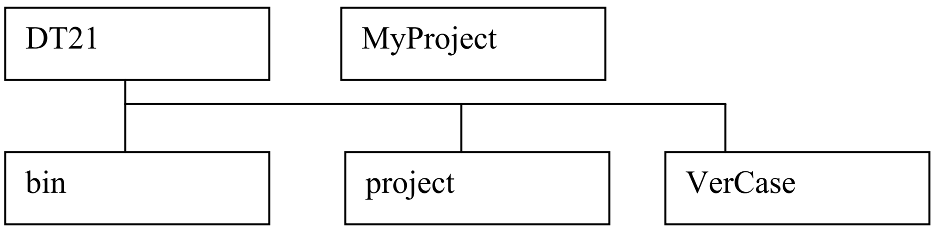


Figure 3-3. *Recommended directory structure.*

4 Compact Input File (CIF)

4.1 Introduction

The main input specification to DarcyTools is by way of a Compact Input File (CIF). The CIF is a free formatted file that contains both comment and command lines. The comment lines are defined as being any empty line or a line whose first character is the '*' or 'c' character. The command lines are defined as being all other lines. Each command line starts with an integer value representing the command identification number. The data follow this integer ID according to the specified format of the command.

A list of all CIF commands is given in Figure 4-1. The page number, where a full description of the command is found, is also provided.

The group of commands, 1 to 99, corresponds to commands that affect the memory allocation, the F-array, while commands starting from 100 have to be called after the F array allocation. Commands for special tasks (GRIDGEN, FRACGEN, TECROT and SUBROF) have their individual command group numbers, as can be seen in Figure 4-1.

Further information related to the CIF commands can be found in the Notation, Section 9, and examples of use are given by the thirty verification cases. Four of these cases are listed in Appendix C.

In the following all CIF commands will be described, in the order as they appear in the CIF. After the command line a line with data statements will follow. The only purpose of this line is to illustrate the command; the actual numbers have no significance.

			Page
1	SETTITLE	: title	19
2	SETGRDF	: fname	19
3	SETLICM	: licence, path	20
4	SETNBVAR	: nx	20
5	SETCPL	:	21
6	SETSTEP	: dt, nstep, iorder	21
7	SETTIME	: t1,t2,nstep1,nstep2	22
8	SETARRAY	: name, igrd, length	23
9	SETF0	: name, igrd, value	24
10	SETFLUB	: id, i1, i2, j1, j2, k1, k2, igrd	24
11	SETCST1	: g	25
12	SETLAW1	: rho0, Trho, alpha1, alpha2, beta1, beta2	25
13	SETLAW2	: visc0, a1, a2, Tvisc, n	26
14	SETLAW3	: cp0, a1, a2	26
15	SETFRM	: nalint, alphl, alphh, frmk, bettot	27
16	SETGWT	: grlx, facmin	27
17	SETTUN1	: fname	28
18	SETTUN2	: isec, iaction, sink, skin, skmin, skmax, rlx	28
19	SETYIELD	: deltsy, vlfrsy, betasy	30
20	SETSLV1	: ivar, igrd, relin, resfac, liter	31
21	SETSLV2	: ivar, igrd, relax, nbrelax, ipreco	32
22	SETSLV3	: ivar, igrd, igmres, nbgrid, icycle, nbprer, igms	33
23	SETSLV4	: iusolv	34
25	SETPTK1	: igrd, method, fname	34
26	SETPTK2	: is1, is2, js1, js2, ks1, ks2, nps, ts1, ts2, pfsta1, pfsta2, pfsta3	35
27	SETPTK3	: ie1, ie2, je1, je2, ke1, ke2	35
28	SETPTK4	: nalint, alphl, alphh, ak, bettot, fxdift, retmob, nmobst, naintn	36
29	SETPTK5	: tsteph, wnstph1, wnstph2, wnstph3	36
30	SETPTK6	: seed	37
31	SETPTK7	: nbtrj, ntrjfr, lentrj	37
32	SETPTK8	: nolond, iadsorp	38
33	SETPTK9	: fname	38
34	SETPTK10	: form, fname	39
35	SETPTK11	:	39
109	SETNITG	: nitg	40
110	SETSWEEP	: nsweep, ivar1, ivar2	40
111	SETITC1	: nitc1, ivar3, ivar4	41
112	SETITC2	: nitc2, ivar5, ivar6	41
115	SETTOP	: ssea, tsea, tland	42
117	SETINDG	: igrd, form, fname	42
118	SETF1	: name, igrd, value	43
119	SETF2	: name, igrd, value, i1, i2, j1, j2, k1, k2	43
120	SETF3	: name, igrd, form, fname	44
121	SETSPT	: s1, t1, s0, t0, dwt, dsdz, dtdz, i1, i2 j1, j2, k1, k2	45

Figure 4-1. *CIF commands, with page number, where a full description of the command can be found.*

122 SETBOSS	: ivar, igrd, itype, i1,i2,j1,j2,k1,k2,it1,it2, qsrc, qphi	48
123 SETTECF	: fname, title, isbin	49
124 SETTECZ	: ifile, igrd, i1, i2, ifr, j1, j2, jfr, k1, k2, kfr	49
125 SETTECB	: ifile, vname, iaction, value	50
126 SETTEC1	: ifile, isgrd	51
127 SETTEC2	: ifile, it1, it2, itfr	51
128 SETTEC3	: ifile, ivar	52
129 SETPRECO	: precdif	52
130 SETSTORE	: name, igrd	53
131 SETRST	: irst	53
132 SETROF1	: istep1, istep2, istepfr	54
133 SETF4	: name, igrd	54
134 SETFLUX	: igrd, iflu	55
135 SETHIST1	: i, j, k, igrd, iv, title	55
136 SETHIST2	: igra, vname, label	56
137 SETSERV	: iport	56
1001 GRGTEC	: fname, title, isbin	57
1002 GRGFILE	: fname	57
1003 GRGTOP	: fname	58
1004 GRGPCOS	: icosp	58
1005 GRGXDIS	: x0, x1, x2, x3, nx1, nx2, nx3	59
1006 GRGYDIS	: y0, y1, y2, y3, ny1, ny2, ny3	59
1007 GRGZDIS	: z3, z4, z5, nz1, nz2, nz3, nz4, nz5	60
1008 GRGEMBG	: icos, ifac, jfac, kfac, ip, i1, i2, j1, j2, k1, k2	61
1009 GRGZTOP	: ztop	62
1010 GRGROC	: fname	62
1011 GRGDROC	: dmin	63
1012 GRGZROC	: zroc	63
2001 FRGGRD	: igrd, fname	64
2002 FRGSEED	: seed	64
2003 FRGWKD	: wkdivh1, wkdivh2, wkdivh3	65
2004 FRGNRD	: nxrd, nyrd	65
2005 FRGNLD	: nld	66
2006 FRGOFN	: id, fname	66
2007 FRGKNWF	: fname	67
2008 FRGKNW	: inhomf, htknsf, frevolf, fwsrff, storaf, conduf, diffuf	68
2009 FRGRANF	: fname	69
2010 FRGRAN1	: igenf, lfl, lfh, thknsf, frevof, storaf, diffuf, fwsrff	70
2011 FRGRAN2	: iset, tcsta, tcstb, tcstc, tcstd, lreff, expidf, idreff, lambdf1, lambdf2, lambdf3	71
3001 TKRIN	: fname	72
3002 TKROUT	: fname	72
3003 TKRTRF	: dx, dy, degree	73

***Figure 4-1.** Cont.*

4000 SBRTITLE	: title	73
4001 SBRGIN	: fname	74
4002 SBRGOUT	: fname	74
4003 SBRRIN	: fname	75
4004 SBRROUT	: fname	75
4005 SBRPDEF	: icos, ifac, jfac, kfac, ip, i1, i2, j1, j2, k1, k2	76
4006 SBRTEC	: fname, title, isbin	76

Figure 4-1. *Cont.*

4.2 Commands

1 SETTITLE

* 1 SETTITLE : *title*

1 'Taylor Dispersion'

This command defines a title for the current run. The title will appear on the Monitor screen and in various output files.

The title string must be less than 256 characters long. The default string is an empty string.

2 SETGRDF

* 2 SETGRDF : *fname*

2 'xyz'

The grid is specified in the unformatted file 'xyz', where xyz is a user chosen name that may be up to 256 characters long.

The default grid is a Cartesian grid with $ni = nj = nk = 10$ and $dx = dy = dz = 1$.

Usually the file is generated by a set of CIF commands, see commands starting with number 1001, perhaps reading in a topography file.

3 SETLICM

```
* 3 SETLICM : licence,     path
       3        'bx / yXz'   ‘ ‘
```

This command sets the unlocking string for the MIGAL solver. When MIGAL is protected by a software license manager the path defining the license log-file must also be set. When MIGAL is protected by a hardware key (dongle) the path name must be an empty string.

4 SETNBVAR

```
* 4 SETNBVAR:          nx
       4               3
```

This command fixes the number of variables contained in the *X* sub-array. The default value is 3 since the salinity and the temperature are always used to compute the fluid properties. In case of fixed properties, the salinity and the temperature will be present in X sub-array but not solved for. In the same way, when computing transport of a scalar quantity only, the pressure must be stored to define the mass fluxes. Hence, the first variable of the X sub-array will always be the pressure, the second variable the salinity and the third variable the temperature. Users should note that, when the pressure or the salinity or the temperature is fixed, they have the opportunity not to solve them by setting adequate loop indexes via SETSWEEP, SETITC1 and SETITC2.

5 SETCPL

```
* 5 SETCPL :

          5
```

This command switches ON a coupled solution for the pressure and salinity variables. Since the default setting is the segregated algorithm this routine has to be called only when the coupled solution is desired. The command has no dummy arguments. When switched ON, the coupled solution is set for every grid of the domain.

6 SETSTEP

```
* 6 SETSTEP :  dt,         nstep,       iorder

          6      10.         100          1
```

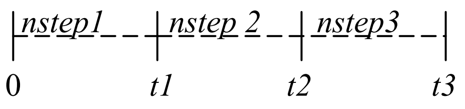
This command defines the time integration loop as well as an initial time step. It also set the default ROF output control parameters and should be called before SETROF1. The default values are those of a stationary case: $nstep = 1$, $iorder = 0$ and dt not used. $iorder$ = 1 gives a Euler first order implicit scheme while $iorder$ = 2 gives a second order scheme, see Report 1.
A variable dt can also be specified; see command 7 SETTIME

7 SETTIME

```
* 7 SETTIME :  t1,        t2,         nstep1,        nstep2

           7       10.        20.         10             20
```

A variable time step can be specified with this command. This command should be considered together with SETSTEP, as information in both specifies the time step distribution.



where: $nstep3 = nstep - nstep1 - nstep2$

$$t3 = t2 + dt \times nstep3$$

The tree parts give a uniform, expanding/contracting (hyperbolic tangent distribution) and uniform time step.

The default values are $t1 = t2 = 0$ and $nstep1 = nstep2 = 0$, which means that the specification in SETSTEP governs the distribution.

8 SETARRAY

* 8 SETARRAY :	*name,*	*igrid,*	*length*
8	‘VAR1’	1	10 000
8	‘VAR2’	1	10 000

It is possible to define user declared variables by this command. The name can be up to ten characters long and must differ from the following reserved names:

DT, XyP, XyS, XyT, XyCxx, RESP, RESS, REST, RESCxx, A, E, S, R, W, W2, W3, M1, M2, M3, PME, B, XV, YV, ZV, ZC, PERMz, DIFFz, TCONDz, POROS, STORA, PREF, CAPA, FLUBz, DARCY-U, DARCY-V, DARCY-W.

Where y=1->3, xx=1->99, z=1->9 and n=1->2

The length is calculated as $ni \times nj \times nk$.

It is expected that the main use of user defined variables is related to coding in *fif.f*. The variables are stored in the F-array and it is possible to use the same techniques as for other variables, when working with the F-array. Also the routines for output to Tecplot accept the user defined variables.

9 SETF0

* 9 SETF0 : v*name*, *igrid,* *val*

9	‘POROS‘	1	1.E - 3
9	‘PERM3‘	1	1.E - 9

This command declares the array named *‘vname’* as being 1 element long on the given grid *igrd* and fills its unique value with *val*. This facility allows memory saving when a property is uniform in the whole domain. It applies only to the following arrays: POROS, STORA, PREF, CAPA, TCONDx, PERMx and DIFFx with x=1…9.

See also commands 118 → 120, which give alternative ways of array specification.

10 SETFLUB

* 10 SETFLUB : *id, i1, i2, j1, j2, k1, k2, igrid*

10	4	10	20	10	30	5	15	2

This command declares the array named *FLUBid* as being 1 element long (instead of 0) and set the footprint command for the flux balance definition on the given grid *igrid*. *id* should remain between 0 and 9. When no footprint index is null FLUBid contains the mass fluxes balance on the given footprint. When one index is null (e.g. *j2*) FLUBid contains the mass fluxes sum through the footprint of the corresponding plane (*j=j1*). The fluxes are then east, north or top fluxes of the cells (*i,j1,k*). Only one index may be null at a time. When no index is null the footprint index can vary from 2 to nbcells-1. When one index is null the corresponding footprint index can vary from 1 to nbcells-1 (*nj*-1) and the other indexes from 1 to *nbcells*.

The mass flux balance is usually used for convergence monitoring. It may also be useful if the flux through the domain, in a certain direction, is of interest.

11 SETCST1

```
* 11  SETCST1  :  g

          11         9.81
```

The default value of the acceleration of gravity is 9.81 and this command does not normally need to be set. It may be used if a problem is scaled in some way or if gravitational forces are not considered. However, for the latter case command 12 SETLAW1 is often used.

12 SETLAW1

```
* 12  SETLAW1  :  rho0,  Trho,  alpha1,  alpha2,  beta1,  beta2

          12          1000.  0.0    0.008    0.0      0.0     0.0
```

This command sets the density state law parameters. The default values are:

$r_0 = 1000.$
$T_0 = 0.0$
$a_1 = 0.008$
$a_2 = 0.0$
$b_1 = 0.0$
$b_2 = 0.0$

They represent the constants of the following law:

$$\rho = r_0\left(1 + a_1 S + a_2 S^2 - b_1(T - T_0) - b_2(T - T_0)^2\right)$$

For complex situations, with non-linear and coupled relations, it is left to the user to specify the constants that fit the problem best.

13 SETLAW2

```
* 13  SETLAW2  :  a0,   a1,   a2,   T0,   n
              13          1.E-3       0.0   0.0   10.      1
```

This command sets the dynamic viscosity state law parameters. The default values are:

$$a_0 = 1.78E-3$$
$$a_1 = 0.0$$
$$a_2 = 0.0$$
$$T_0 = 0.0$$
$$n = -1$$

They represent the constants of the following law:

$$\mu = a_0\left(1 + a_1(T - T_0) + a_2(T - T_0)^2\right)^n$$

It is left to the user to specify the constants that fits the problem at hand. Note that a certain pressure effect may also need to be considered when choosing the optimum constants.

14 SETLAW3

```
* 14  SETLAW3  :  a0,       a1,       a2
               14           4182.   - 0.13      - 0.0001
```

This command sets the fluid specific mass heat state law parameters. The default values are:

$$a_0 = 4182.$$
$$a_1 = 0.13$$
$$a_2 = -0.0001$$

They represent the constants of the following law:

$$C_p = a_0\left(1 + a_1 S + a_2 S^2\right)$$

where S is salinity.

15 SETFRM

* 15 SETFRM :	*nalint,*	*alph1,*	*alph2,*	*frmk,*	*bettot*
15	10	1.E-8	1.E-3	2.0	10.

This command activates the subgrid model FRAME, as applied to the salinity equation. The meaning of the variables are

nalint = number of alpha intervals.

alph1 = low alpha limit.

alph2 = high alpha limit.

frmk = FRAME – *k*, where *k* is late time slope of a breakthrough curve.

bettot = global value of volume ratio (immobile/mobile)

The reader is referenced to Report 1 for a background to this model and its parameters.

16 SETGRWT

* 16 SETGRWT :	*grlx,*	*facmin*
16	0.2	1.E - 3

This command activates the Ground Water Table calculation. The two parameters are:

grlx = under relaxation parameter.

facmin = minimum property reduction factor.

See Report 1 for further background.

17 SETTUN1

* 17 SETTUN1 : *fname*

```
     17        'tunfile'
```

This command activates the TUNNEL model and reads the tunnel section definitions in the file named ‘fname’.

The file should be a formatted file, giving the location of the tunnel sections in grid space. Each tunnel cell should hence be listed and it should further be specified which grid and tunnel section it belongs to.

Format:

nbcells

i j k igrd isection

Where *nbcells* is the number of tunnel cells (hence the number of lines to follow).

Note also that all tunnel cells should be specified in the INDGRD-array. See the Demo Case (Section 7) for an example.

* 18 SETTUN2 :	*isec,*	*iaction,*	*sink,*	*skin,*	*skmin,*	*skmax,*	*rlx*
18	1	1	0.	0.001	1.E-10	1.E10	.1
18	2	2	1.	0.001	1.E-10	1.E10	.1

Once the TUNNEL model has been activated, this command sets the appropriate action *iaction* and its parameters to the specified section *isec*. The default action is *0* which means *'no action'* i.e. the routine TUNNEL ignores the section.

Meaning of parameters:

isec .... section index
iaction ..... type of action to apply: 0 = no action
1 = skin given
2 = sink given
skin .... fixed skin factor (iaction=1)
sink .... mass rate withdrawal of the section (kg/s)
skmin ....minimum skin factor
skmax ......maximum skin factor
rlx .... relaxation factor

* 19 SETYIELD :	*deltsy,*	*vlfrsy,*	*betasy*
19	50.	0.2	0.0

Once the Ground Water Table model has been activated, this routine sets the appropriate specific yield parameters and creates the GWT_VSY sub-array. The default values correspond to zero specific yield.

Meaning of parameters:

deltsy .... time constant for delayed response
vlfrsy .... volume fraction that contains the yield water
betasy ....immobile to mobile volume fraction

Note that two alternative ways of specifying the specific yield volume are supported. Only one can be active; the other should be given a value of 0.0.

See Report 1 for details.

20 SETSLV1

* 20 SETSLV1 :	*ivar,*	*igrd,*	*relin,*	*resfac,*	*liter*
20	2	1	1.	0.1	2

This command defines for each grid and each variable to solve, the first level of the MIGAL solver parameters. When setting a null index for the grid or the variable, the parameters are set to all the grids or all the variables respectively. When a coupled solution is performed, only the salinity values are taken into account for the pressure-salinity couple. These parameters are in relation with the quality of the solution to perform during a sweep. RELIN is the relaxation parameter applied to the solution from one sweep to the next one. RESFAC fixes the residual reduction level which stops MIGAL, and LITER fixes the maximum number of sweeps allowed when RESFAC is not reached. Defaults values are:

relin = 1.

resfac = 0.1

liter = 2

Meaning of parameters:

ivar .... index of variable
igrd .... index of grid
relin .... relaxation parameter of final MIGAL's solution
resfac ...... ending condition: stop when RMS residuals are reduced by the factor resfac
liter .... maximum number of cycles allowed

21 SETSLV2

* 21 SETSLV2 :	*ivar,*	*igrd,*	*relax,*	*nbrelax,*	*ipreco*
21	0	0	.95	3	1

This command defines for each grid and each variable to solve, the second level of the MIGAL solver parameters. When setting a null index for the grid or the variable, the parameters are set to all the grids or all the variables respectively. When a coupled solution is performed, only the salinity values are taken into account for the pressure-salinity couple. These parameters are in relation with the effort imposed to the MIGAL smoother in order to reduce the residuals during iterations (cycles). RELAX fixes the relaxation parameter of the ILU smoother, NBRELAX fixes the number of post-prolongation relaxations and IPRECO the number of multi-grid cycles preconditioning the GMRES iterations. Defaults values are:

relax = .95

nbrelax = 3

ipreco = 1

Meaning of parameters:

ivar .... index of variable
igrd .... index of grid
relax .... relaxation parameter for multi-grid smoother
nbrelax .... number of relaxation for each smoother run
ipreco ...... number of multi-grid cycles for each gmres iteration

22 SETSLV3

* 22 SETSLV3 :	*ivar,*	*igrd,*	*igmres,*	*nbgrid,*	*icycle,*	*nbprer,*	*igms*
22	1	1	-1	0	0	1	0

This command defines for each grid and each variable to solve, the third level of the MIGAL solver parameters. When setting a null index for the grid or the variable, the parameters are set to all the grids or all the variables respectively. When a coupled solution is performed, only the salinity values are taken into account for the pressure-salinity couple. These parameters set a more precise tuning of the solver for difficult cases. In particular, IGMRES and IGMS fix the size of the Krylov-Subspace for the global and the grid level GMRES solvers. ICYCLE sets the kind of multi-grid cycles (i.e. V or W) and NBPRER the number of pre-restriction relaxations on each grid level. Default values are:

igmres = -1

nbgrid = 0

icycle = 0

nbprer = 1

igms = 0

igmres = - 1 means that *igmres* is automatically set to *liter* before calling MIGAL.

Meaning of parameters:

ivar	index of variable
igrd	index of grid
igmres	size of the krylov subspace
nbgrid	number of grid levels used in multi-grid (0=auto)
icycle	type of multi-grid cycle: 0 = V cycle
	1 = W cycle
nbprer	number of prerestriction relaxations
igms	size of the Krylov subspace of the smoother

23 SETSLV4

```
* 23  SETSLV4  :  ivar,        igrd,        iusolv

            23          0            0            6
```

This command defines for each grid and each variable to solve, the output file for the residuals printings. When setting a null index for the grid or the variable, the parameters are set to all the grids or all the variables respectively. When a coupled solution is performed, only the salinity values are taken into account for the pressure-salinity couple. Defaults value is:

iusolv = 6

Meaning of parameters:

```
ivar ......... index of variable
igrd ......... index of grid
iusolv ....... MIGAL output unit  ( 0 = no output)
                                  (-1 = solve.log)
                                  ( 6 = screen   )
```

25 SETPTK1

```
* 25  SETPTK1  :  igrd,   method,   fname

            25          1        2            ' '
```

This command sets the PARTRACK method parameters for the given grid. It is this routine that switches ON the PARTRACK feature. When a restart is made a valid file name must be set in *fname*. Hence, during the last time step, the particles positions and states will be saved. Then the file *fname* will have to be specified again for proceeding to the restart of PARTRACK. Nevertheless it is also possible to start or suspend PARTRACK for the restart computations.

Meaning of parameters:

```
igrd .........    index of grid
method ....... PARTRACK method (1 or 2)
fname ........  PARTRACK restart file name
```

26 SETPTK2

```
* 26  SETPTK2  : is1,   is2,  js1,   js2,    ks1,    ks2,  nps,  ts1, ts2,  pfsta1,  pfsta2,  pfsta3
             26      1     2     10    20      5     10    100  0.    0.  0.5       0.5       0.5
```

This command sets the footprint in which the PARTRACK particles are initially spread out. Since the footprint refers to the PARTRACK grid the routine SETPTK1 must have been called before. The particles are spread out along the unrolled index array of the footprint.

Meaning of parameters:

is1, is2 ...... span of the starting footprint in x-direction
js1, js2 ...... span of the starting footprint in y-direction
ks1, ks2 ..... span of the starting footprint in z-direction
ts1, ts2 ...... span of the starting footprint in time-direction
nps .... number of particles
pfsta1 .... initial relative x position in cells [0,1]
pfsta2 .... initial relative y position in cells [0,1]
pfsta3 .... initial relative z position in cells [0,1]

27 SETPTK3

```
* 27  SETPTK3  :  ie1,     ie2,       je1,       je2,         ke1,       ke2
             27         25      25         50         50           40         40
```

This command sets the footprint in which the PARTRACK particles are captured. Since the footprint refers to the PARTRACK grid the routine SETPTK1 must have been called before. The particles arriving in this footprint are removed and counted in the variable PTK_NPC while the number of particles leaving through the grid boundary is given by (PTK_NPO - PTK_NPC). The default values are *ie1=ie2=je1=je2=ke1=ke2=0* and disable the capturing feature.

Meaning of parameters:

ie1, ie2 ...... span of the arriving footprint in x-direction
je1, je2 ...... span of the arriving footprint in y-direction
ke1, ke2 .....span of the arriving footprint in z-direction

28 SETPTK4

* 28 SETPTK4 : *nalint*, *alphl*, *alphh*, *ak*, *bettot*, *fxdift*, *retmob*, *nmobst*, *naintn*

```
28          100     1.E-9      1.E-3  2.0   10.       1.E-5    1.5       5          100
```

This routine sets the PARTRACK multi-rate model parameters. The default values disable this model.

Meaning of parameters:

nalint .... number of alpha intervals (= naintt)
alphl .... low aplha limit
alphh .... high aplha limit
ak .... late time slope of breakthrough curve
bettot .... global value of volume ratio (immobile/mobile)
fxdift .... uniform cross diffusion coefficient
retmob ..... retardation mobile
nmobst ..... number of a/d states in the mobile zone
naintn ...... number of a/d states in the immobile zone

The reader is referred to Report 1 for further details and a general background.

29 SETPTK5

* 29 SETPTK5 : *tsteph*, *wnstph1*, *wnstph2*, *wnstph3*

```
29          1.       0.1        0.1        0.1
```

This command sets the PARTRACK parameters when the first method is specified (method=1 in SETPTK1). The default values are:

tsteph = 10.

wnstph1 = *wnstph2* = *wnstph3* = 0.1

Meaning of parameters:

tsteph .... velocity freezing time [s]
wnstph1 ...... x displacement limit for velocity freezing
wnstph2 ...... y displacement limit for velocity freezing
wnstph3 ...... z displacement limit for velocity freezing

30 SETPTK6

* 30 SETPTK6 : *seed*

```
        30        0.4391
```

This command sets the PARTRACK random generator initialisation seed. By default this parameter is set from the clock time of the computer (i.e. seconds and milliseconds).

31 SETPTK7

* 31 SETPTK7 : *nbtrj*, *ntrjfr,* *lentrj,*

```
        31        100     1          1000
```

This command sets the number of PARTRACK trajectories and their time definition in terms of time step frequency and maximum length. When the number of trajectories is less than the total number of particles, the selected particles are spread out in the particles array. Hence, during a restart, the total number of particles and trajectories must remain identical. The trajectories are stored in the F sub-arrays named PTK_TRJX, PTK_TRJY, PTK_TRJZ and PTK_TRJT. In the same way that the density of particles PTK_DEN, the trajectories can be outputted in a TECPLOT file by using SETTECB with the name PTK_TRJ. Nevertheless, it is recommended to output the trajectories in a devoted TECPLOT file. The trajectories are saved in the PARTRACK restart file when this file has been specified in SETPTK1. By default no trajectories are produced.

Meaning of parameters:

nbtrj .... number of trajectories
ntrjfr .... time step frequency for trajectory outputs
lentrj .... lentgh of trajectories in time steps

32 SETPTK8

```
* 32  SETPTK8  :  nolond,          iadsorp

              32          1                   0
```

This command sets the PARTRACK longitudinal diffusion and adsorption triggers. The default values are:

nolond = 1

iadsorp = 0

Meaning of parameters:

nolond .... longitudinal diffusion (1=no, 0=yes)
iadsorp ...... adsorption (1=yes, 0=no)

See Report 1 for details about *nolond.*

33 SETPTK9

```
* 33  SETPTK9  :  fname

              33          'pdata'
```

This command specifies the filename of a file where startpositions of particles are given. The format of the data is the same as for command 26. However, the first line of the file should specify the number of specifications that follow, i e the number of lines.

34 SETPTK10

* 34 SETPTK10 : form, *fname*

34 'unformatted' 'fquo.dat'

This command activates the F-quotient calculation and also specify the name and form of the result file. Note that only method = 1 is allowed for calculation of F-quotients. When the unformatted option is used, which may be advisable for large files, a small code is required to read the file and perfom required further development of the results (for example statistics).

35 SETPTK11

* 35 SETPTK11 :

35

The free volume in each cell, required by PARTRACK, is by default calculated from the porosity field. This command activates an alternative specification by the array PTK_FREVOL, where the free volume in each cell is given.

109 SETNITG

```
* 109  SETNITG  :  nitg

            109          5
```

This command defines the number of iterations that the program must accomplish during each time step to solve the interaction between the different grid solutions. The default value is:

nitg = 1

110 SETSWEEP

```
* 110  SETSWEEP  :  nsweep,     ivar1,     ivar2

            110            10          1          3
```

This command defines the number of sweeps to perform per time step, on each grid. It also defines the variables to solve in this iteration loop. Defaults values are:

nsweep = *ivar1* = *ivar2* = 1

Meaning of parameters:

nsweep ...... number of coupling iterations
ivar1 ...... lower limit of the loop on variables
ivar2 .... upper limit of the loop on variables

111 SETITC1

```
* 111  SETITC1  :  nitc1,     ivar3,     ivar4

           111       2           3           3
```

This command defines the number of iterations to perform per time step, on each grid for coupling the variables ivar3 to ivar4 inside the sweep loop. Defaults values are:

nitc1 = 0

ivar3 = 0

ivar4 = 0

Meaning of parameters:

nitc1 ...... number of coupling iterations
ivar3 .... lower limit of the loop on variables
ivar4 ..... upper limit of the loop on variables

112 SETITC2

```
* 112  SETITC2  :  nitc2,     ivar5,     ivar6

           112       2           4           4
```

This command defines the second number of iterations to perform per time step, on each grid for coupling the variables ivar5 to ivar6 outside the sweep loop. Defaults values are:

nitc2 = 0

ivar5 = 0

ivar6 = 0

Meaning of parameters:

nitc2 ...... number of coupling iterations
ivar5 .... lower limit of the loop on variables
ivar6 ..... upper limit of the loop on variables

115 SETTOP

* 115 SETTOP :	*ssea,*	*tsea,*	*tland*
115	1.0	5.	10.

This command sets the the top boundary conditions (*k=nk)*. The top boundary is considered as being land where *z(nk+1)>0* or *PME(i,j)* differs from zero. Elsewhere the top boundary is considered as being sea bottom. *PME* is an array containing the precipitation minus the evaporation velocity, which can be set using the routines SETF1, SETF2 or SETF3. Besides adding the *PME* mass source term, the command fixes in *k=nk* the salinity to *zero* on land and *ssea* on sea bottom, the temperature to *tland* on land and to *tsea* on sea bottom and the pressure to:

$$P_{sea} = z_{c(nk)} g \left(\rho_0 - \rho_{(S_{sea},T_{sea})} \right)$$

Meaning of parameters:

ssea .... salinity of the sea (z<0)
tsea .... temperature of the sea (z<0)
tland .... temperature of the land (z>0)

117 SETINDG

* 117 SETINDG :	*igrd,*	*form,*	*fname,*
117	1	'FORMATTED'	'INDFILE'

This command fills the INDGRD array associated with the grid *igrd* with the values read in the file *fname*. When form='FORMATTED' the file must be formatted but is read with free format. Any line starting with the character '*' is then considered as being a comment line. The values are read by the following statements:

Formatted files: *read(iu,*) (indgrd(i),i=1,ni*nj*nk)*

Unformatted files: *read(iu) (indgrd(i),i=1,ni*nj*nk)*

Where *ni, nj* and *nk* are the dimensions of the given grid.

Meaning of parameters:

igrd .... index of the grid
form ....form specifier of the file to open
fname ....name of the file containing the values

118 SETF1

* 118 SETF1 :	*vname,*	*igrd,*	*val*
118	'X1P'	2	1.E4

This command fills the entire sub-array named *vname* on the grid *igrd* with the value *val*.

119 SETF2

* 119 SETF2 :	*vname,*	*igrd,*	*val,*	*i1,*	*i2,*	*j1,*	*j2,*	*k1,*	*k2*
119	'X1S'	1	0.5	10	20	1	50	1	20

This command sets the value *val* into the specified footprint of the sub-array named *vname* on the grid *igrd*. The dimension of the given sub-array must be *(ni,nj,nk)* if the associated grid has $ni \times nj \times nk$ cells. Nevertheless when *i1* or *i2* etc equals zero the corresponding dimension is discarded. For example, filling a 2D (ni,nk) array can be achieved by setting $j1 = j2 = 0$.

Meaning of parameters:

vname	name of the variable
igrd	index of the grid
val	value to set in the footprint
i1, i2	setting's footprint x-definition
j1, j2	setting's footprint y-definition
k1, k2	setting's footprint z-definition

* 120 SETF3 : *vname*, *igrd*, *form*, *fname*

120 'X2P' 1 'UNFORMATTED' 'PINIVAL'

This command fills the entire sub-array named *vname* on the grid *igrd* with the values read in the file named *fname*. When the *form* of the file is specified as being the string 'FORMATTED', the file is read without any predefined format. Further, any line starting with the character '*' is considered to be a comment line as long as the first non comment line is encountered. Then the data are read with the following statement: *read(iu,*) (f(i),i=i1,i2),* with *i1* being the F sub-array location and *i2-i1+1* the sub-array length. When the *form* of the file is specified as being the string 'UNFORMATTED', the file does not contain comment lines and the reading statement is: *read(iu) (f(i),i=i1,i2).*

Meaning of parameters:

vname	name of the variable
igrd	index of the grid
form	form specifier of the file to open
fname	name of the file containing the values

```
* 121 SETSPT : s1,  t1,  s0   t0  dwt,  dsdz,    dtdz  i1,   i2,   j1, j2    k1,   k2
           121   0.    0.   1.   0.  0.    -2.E-3   0.    1     50    1   50    1     50
```

This command initializes the pressure, the salinity and the temperature fields on the very parent grid (*igrd* = 1). It also initializes all the embedded grids from the parent grids by calling the routine SETF4. Model constants and all grid coordinates must be previously defined. The vertical equilibrium is given by:

$$\frac{\partial P}{\partial z} = (\rho_0 - \rho) g \tag{1}$$

For the sake of efficiency the initialization procedure splits the domain into five zones. The zone 1 is located above the ground water table. In the land regions, the zone 2 is located under zone 1 and above the sea level $z = 0$ and the zone 3 is located under $z = 0$. The zone 4 is located under the sea regions. Finally the zone 5, which is not in the computational domain, represents the sea.

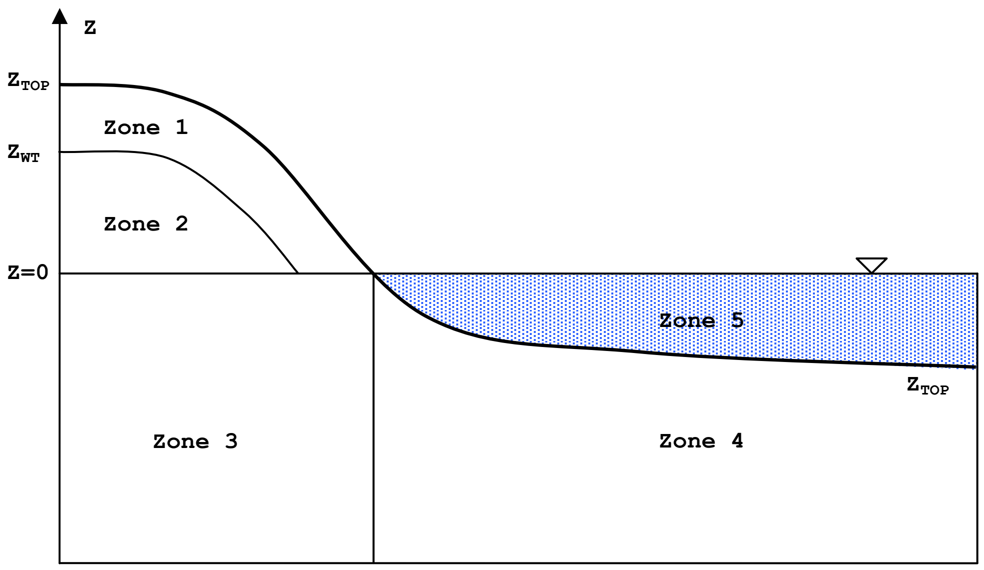


Figure 1 : SETSPT zone labelling

The initialization favours a smooth distribution in the bottom of the domain by setting a linear vertical profile for salinity and temperature and an equilibrium pressure in the zones 3 and 4. An approximated uniform distribution is assumed in zones 1 and 2.

Zone 1 & 2:
$$\begin{cases} S = S_1 \\ T = T_1 \\ P = \left(\rho_0 - \rho_{(S1,T1)}\right) g\,(z - z_{WT}) + \rho_0 g\, z_{WT} \end{cases} \tag{2}$$

Zone 3:
$$\begin{cases} S = S_0 + \dfrac{\partial S}{\partial z}\, z \\ T = T_0 + \dfrac{\partial T}{\partial z}\, z \\ P = \rho_{(S1,T1)}\, g\, z_{WT} - \rho_0 g\, f_0(z) \end{cases} \tag{3}$$

Zone 4:
$$\begin{cases} S = S_0 + \dfrac{\partial S}{\partial z}\,(z - z_{Top}) \\ T = T_0 + \dfrac{\partial T}{\partial z}\,(z - z_{Top}) \\ P = \left(\rho_0 - \rho_{(S0,T0)}\right) g\, z_{top} - \rho_0 g\, f_0(z - z_{Top}) \end{cases} \tag{4}$$

Zone 5:
$$\begin{cases} S = S_0 \\ T = T_0 \\ P = \left(\rho_0 - \rho_{(S0,T0)}\right) g\, z \end{cases} \tag{5}$$

with the function *f₀*, accordingly to the density state law, such as:

$$\begin{aligned} f_0(x) = x\, &\left(\alpha_1 S_0 + \alpha_2 S_0^2 - \beta_1 (T_0 - T_\rho) - \beta_2 (T_0 - T_\rho)^2\right) + \\ &\frac{x^2}{2}\left((\alpha_1 + 2\alpha_2 S_0)\frac{\partial S}{\partial z} - (\beta_1 + 2\beta_2 (T_0 - T_\rho))\frac{\partial T}{\partial z}\right) + \\ &\frac{x^3}{3}\left(\alpha_2 \frac{\partial S}{\partial z}^2 - \beta_2 \frac{\partial T}{\partial z}^2 \right) \end{aligned} \tag{6}$$

and where the ground water table altitude is given by the depth d_{WT} (>0) and the formula (10) so that setting a very large value for d_{WT} (e.g. 1.E20) fixes the ground water table at sea level z = 0.

$$z_{WT} = \max\left(0, z_{top} - d_{WT}\right) \tag{7}$$

z_{top} represents the altitude of the top boundary cell face center.

$$z_{Top} = \frac{1}{4}\left(z_{(i,j,nk+1)} + z_{(i+1,j,nk+1)} + z_{(i,j+1,nk+1)} + z_{(i+1,j+1,nk+1)}\right) \tag{8}$$

Finally, the routine SETSPT can partially initialize the salinity, pressure and temperature fields by specifying the footprint *i1, i2, j1, j2, k1, k2* on the very parent grid.

Meaning of parameters:

s1	salinity for z>0
t1	temperature for z>0
s0 ……	salinity for z = 0
t0 ……	temperature for z = 0
dwt …..	depth of the water table (>0) for z>0
dsdz	salinity gradient (<0)
dtdz ….	temperature gradient (<0)
i1, i2 …	setting's footprint x-definition
j1, j2 …	setting's footprint y-definition
k1, k2 …	setting's footprint z-definition

122 SETBOSS

* 122 SETBOSSS :	*ivar,*	*igrd,*	*itype,*	*i1,*	*i2,*	*j1,*	*j2,*	*k1,*	*k2,*	*it1,*	*it2,*	*qsrc,*	*qphi*
122	1	1	0	1	50	1	50	1	20	1	100	9.81*E*23	1*E*20
122	2	1	1	1	50	1	1	1	20	1	100	0	0

This command sets the automatic boundary/sink/source conditions which are implemented by DarcyTools. Those conditions concern the variable whose index in the X sub-array is *ivar* and apply to the specified footprint of the *igrd* grid. To operate with time dependent computations the footprint notion is extended to the time steps *it1, it2*. This routine implements two kinds of boundary/sink/source conditions. With the first kind, *itype=0*, the values *qsrc* and *qphi* are uniformly applied to the entire footprint. With the second kind, *itype=1*, the values *qsrc* and *qphi* are not used and Dirichlet boundary conditions are applied to the footprint in order to freeze the variable to its previous time step value. Boundary/sink/source conditions apply in the order of the SETBOSS calls. Hence, when overlapping, only the last definition applies to the footprint intersection.

Meaning of parameters:

ivar .... index of the variable in the X sub-array
igrd .... index of the grid
i1, i2 .... setting's footprint x-definition
j1, j2 .... setting's footprint y-definition
k1,k2 .... setting's footprint z-definition
it1, it2 ...... setting's footprint t-definition
qsrc .... qsrc value to apply in the footprint
qphi .... qphi value to apply in the footprint
itype .... type of condition 0 = uniform values
1 = fixed values in time

123 SETTECF

```
* 123  SETTECF  :  fname,      title,      isbin

            123        'TecOut'   ' '          1
```

This command creates a file named *fname* for saving a Tecplot data set. The file can be binary or ascii depending on *isbin*. The Tecplot files ID are associated to the SETTECF calling order, starting from one. If the *title* string is empty, the title of the run is applied to the file.

Meaning of parameters:

fname	name (including path) of the file to create
title	title of the data set
isbin	set to 1 for creating a binary file
	0 for creating an ascii file

124 SETTECZ

```
* 124  SETTECZ  :  ifile,  igrd,  i1,  i2,  ifr,  j1,  j2,  jfr,  k1,  k2,  kfr

            124      1      1      1     50    2     1     60    2     1     80    1
```

This command defines a zone that will be added to the Tecplot data set *ifile* previously created by a SETTECF call. Each zone is attached to a single grid and the data are exported from *n1* to *n2* with a *nfr* increment for allowing the extraction of lines, planes or partial domain data.

Meaning of parameters:

ifile	index of TECPLOT file
igrd	index of the grid associated to the zone
i1, i2, ifr	x-footprint and frequency for data extraction
j1, j2, jfr	y-footprint and frequency for data extraction
k1, k2, kfr ...	z-footprint and frequency for data extraction

* 125 SETTECB :	*ifile,*	*vname,*	*iaction,*	*value*
125	1	'X1P'	0	0.
125	1	'PERM1'	3	0.

This routine adds the sub-array named *vname* to the list of variables to be output in the Tecplot data set *ifile*. The added sub-array must be common to all the grids of all the zones defined in the data set.

Meaning of parameters:

ifile	index of TECPLOT file
vname	name of the variable to add in the data set
iaction	modifying action before output (0) no action
	(1) phi+value
	(2) phi*value
	(3) log10(phi)
	(4) ln(phi)
value	value for the action when needed

The *iaction* facility can be used when non-dimensional output is desired or when some other scaling is involved.

126 SETTEC1

* 126 SETTEC1 : *ifile*, *isgrd*

126 1 1

This command specifies the kind of mesh that is to be automatically included into the Tecplot dataset *ifile*. When *isgrid=0* no mesh is added. When *isgrid=1* only the mesh linking the cell centres (i.e. the DarcyTools variables location) is added. When *isgrd=2* a dummy zone containing the DarcyTools grid is added in first position before returning to the variables location mesh. The default setting is *isgrd=2*.

Meaning of parameters:

ifile .... index of TECPLOT file
isgrd ....kind of grid to be included
0 = no mesh
1 = only mesh linking the cell centres
2 = add a first zone with a mesh linking vertexes

127 SETTEC2

* 127 SETTEC2 : *ifile*, *it1*, *it2*, *itfr*

127 1 11 50 2

This command defines the time domain and increment for creating Tecplot zones. It allows reducing the number of zones and therefore the size of the produced Tecplot file. The defaults values are:

it1 = nstep

it2 = nstep

itfr = 1

A null value for *it1* means that a zone will be created for the initialization time.

Meaning of parameters:

ifile .... index of TECPLOT file
it1, *it2* ...... istep boundary for TECPLOT's zones creation
itfr .... istep frequency for TECPLOT's zones creation

128 SETTEC3

```
* 128  SETTEC3  :  ifile,    ivar

          128         1        2
```

This command sets up a trigger for creating a new Tecplot zone after each call of the routine SOLVE concerning the variable ivar on the grid associated to the zone. The default value is *ivar=0* and means that zones are only created at the end of each time step according to the frequency definition *it1, it2, itfr* from SETTEC2.

129 SETPRECO

```
* 129  SETPRECO  :  precdif

          129           0.
```

This command sets the automatic preconditioning artificial diffusion coefficient for the coupled correction operator. The default value is null and means that no preconditioning is applied. The automatic preconditioning is set by DarcyTools before calling USRPRECO so that users can add a second effect by programming. The automatic preconditioning technique consists in adding the value 7.2 × *precdif* to the central coefficient and the value *precdif* to the neighbour coefficients of the second equation of the correction operator.

130 SETSTORE

```
* 130  SETSTORE  :   name,          igrd

            130         'M1'            1
```

This command marks the sub-array named *name* associated to the grid *igrd* for intermediary output into the ROF file. The grid coordinates *xv*, *yv* and *zv*, as well as all the variables are automatically output into the ROF after the last time step and shouldn't be specified by this routine if not needed before.

131 SETRST

```
* 131  SETRST  :   irst

            131         1
```

This command switches ON a restarting computation from a previous ROF file. Since the default setting is "do not restart" this routine has to be called only when a restart is desired and has no dummy arguments. The parameter *irst* controls wheter the time-value should be reset to 0. or pick up the value from the restart file. *irst* = 1 reads the value from the restart file, while *irst* = 0 resets time to 0.0.

132 SETROF1

* 132 SETROF1 :	*istep1,*	*istep2*,	*istepfr*
132	10	100	10

This command sets the range and frequency of the ROF outputs. It should be called after SETSTEP since the default values are:

istep1 = nstep

istep2 = nstep

istepfr = 1

Meaning of parameters:

istep1	first istep value for ROF intermediary ouput
istep2	last istep value for ROF intermediary ouput
itfr	istep frequency for ROF intermediary ouput

133 SETF4

* 133 SETF4 :	v*name,*	*igrd*
133	'X1S'	2

This command sets, on the grid *igrd*, the value of the sub-array named *vname* from the array having the same name on the parent grid. This implies that *igrd* is an embedded grid and that *vname* is valid for both the embedded and the parent grid. No interpolation is performed. The parent values are considered to be uniform inside the parent grid cells.

134 SETFLUX

* 134 SETFLUX :	*igrd,*	*iflu*
134	3	1

This routine sets the kind of parent grid's boundary conditions that DarcyTools must implement for the specified embedded grid. When *iflu=1* the fluxes at parent footprint boundaries are set from the fluxes of the child (embedded) grid *igrd*. When *iflu=0*, the parent footprint boundaries values are fixed to the child grid mean local values. The default value is *iflu=0*.

135 SETHIST1

* 135 SETHIST1 :	*i,*	*j,*	*k,*	*igrd,*	*iv,*	*title*
135	10	20	30	1	0	'Spot Value'

This command defines a new graph for the real time DarcyTools visualization. When *i=j=k=0* the graph is for RESIDUALS. When *i=0* or *j=0* or *k=0* and only one of them, the graph is for PROFILES along the (*j,k*), (*i,k*) or (*i,j*) line. When none of *i, j* or *k* is null the graph is for SPOT VALUES and *i, j, k* represents the indexes of the point to plot. The graph is attached to the grid *igrd* and the writing in HISTxx files is trigged by solving the variable *iv* unless *iv=0*. In that case the writing occurs at the end of the time step.

Meaning of parameters:

i, j, k	position indexes
igrd	index of the grid
iv	index of the variable trigging the file writting
title	title of the graph (35 characters long)

136 SETHIST2

* 136 SETHIST2 :	*igra,*	*vname,*	*label*
136	1	‘X1P’	‘Pressure’

This routine adds a variable to the graph *igra* for being drawn. The variable is a sub-array defined both by its name *vname* and by the grid index associated to the graph. The number of variables per graph is limited to 10. This routine also assigns a label for the variable plot.

Meaning of parameters:

igra .... graph index in order of the creation via SETHIST1
vname .... name of variable associated to *igrid* of the graph
label .... a label for the variable (10 characters long)

137 SETSERV

* 137 SETSURV : *iport*

137

This routine sets the port ID of the darcytools-serv server for communication with the monitoring of HIST files. The default value is 0 and means that the server port has not been change during the installation process (i.e. 1961).

1001 GRGTEC

* 1001 GRGTEC : *fname,* *title,* *isbin*

```
             1001    'Tecgrid'   ' '      1
```

This command generates a Tecplot file, which can be used to check the grid before any simulations are attempted. The file can be ascii or binary depending on *isbin*. Default is no output.

1002 GRGFILE

* 1002 GRGFILE : *fname*

```
             1002    'xyz'
```

This command sets the file name *fname* for the grid data. Default is 'xyz'.

1003 GRGTOP

* 1003 GRGTOP : *fname*

1003 'topography'

This routine sets the file name *fname* for reading the topography.
Independently of the coordinate system of the very parent grid,
the topography files are UNFORMATED files, read as follows:

```
read(iu) ni,nj
do j = 1, nj + 1
do i= 1, ni + 1
read (iu) x (i, j), y (i, j), z (i, j)
enddo
enddo
```

When the very parent grid is BFC:s or CART the X and Y set are
respectively the lines x(i,nj+1) and y(ni+1,j). When the very
parent grid is CART the top Z value is z(ni+1,nj+1).

Default is no topography, i.e. *ztop* = 0. When the file name is 'user' or 'USER', no file is read but the user subroutine TOPOG, in *fif.f*, is called.

1004 GRGPCOS

* 1004 GRGPCOS : *icosp*

1004 3

This command sets the coordinate system of the very parent grid (1 = BFC, 2 = BFC:s and
3 = CARTESIAN).
Default is BFC:s.

1005 GRGXDIS

* 1005 GRGXDIS :	*x0,*	*x1,*	*x2,*	*x3,*	*nx1,*	*nx2,*	*nx3*
1005	0	10.	20.	50.	10	20	10

This command sets the *x* coordinate distribution.

The tree zones are: one expanding/contracting followed by a uniform grid size and finally an expanding/contracting part.

Meaning of parameters:

x0	west abscissa (node 1)
x1	west abscissa of zone 2 (node nx1+1)
x2	east abscissa of zone 2 (node nx1+nx2+1)
x3	east abscissa (node nx1+nx2+nx3+1)
nx1	number of cells in zone 1
nx2	number of cells in zone 2
nx3	number of cells in zone 3

Default: *x0 = x2 = x3 = 0. x1 = 10, nx1 = 10, nx2 = nx3 = 0.*

1006 GRGYDIS

* 1006 GRGYDIS :	*y0,*	*y1,*	*y2,*	*y3,*	*ny1,*	*ny2,*	*ny3*
1006	0	10.	20.	50.	10	20	10

This command sets the *y* coordinate distribution.

The tree zones are: one expanding/contracting followed by a uniform grid size and finally an expanding/contracting part.

Meaning of parameters:

y0	west abscissa (node 1)
y1	west abscissa of zone 2 (node ny1+1)
y2	east abscissa of zone 2 (node ny1+ny2+1)
y3	east abscissa (node ny1+ny2+ny3+1)
ny1	number of cells in zone 1
ny2	number of cells in zone 2
ny3	number of cells in zone 3

Default: *y0 = y2 = y3 = 0. y1 = 10, ny1 = 10, ny2 = ny3 = 0.*

```
* 1007 GRGZDIS :  z3,       z4,      z5,     nz1,    nz2,    nz3,    nz4,     nz5
*                 1         d1(1)
*                 ..        ..
*                 nz1       d1(nz1)

           1007   -100.     -200.    -500.   2       10      0       10       20
              +   1         5.
              +   2         8.
```

The *z*-distribution is specified according to a five zone partitioning.

zone 1: user given distribution by cell sizes ($d1$) from top and for *n1* cells. $d1(i) = z(n-i+1) - z(n-i)$ with $n = n1 + n2 + n3 + n4 + n5$

zone 2. (hyperbolic) tangent distribution of *n2* cells that fits a soil/rock surface at *z2* and the lower boundary of zone 1.

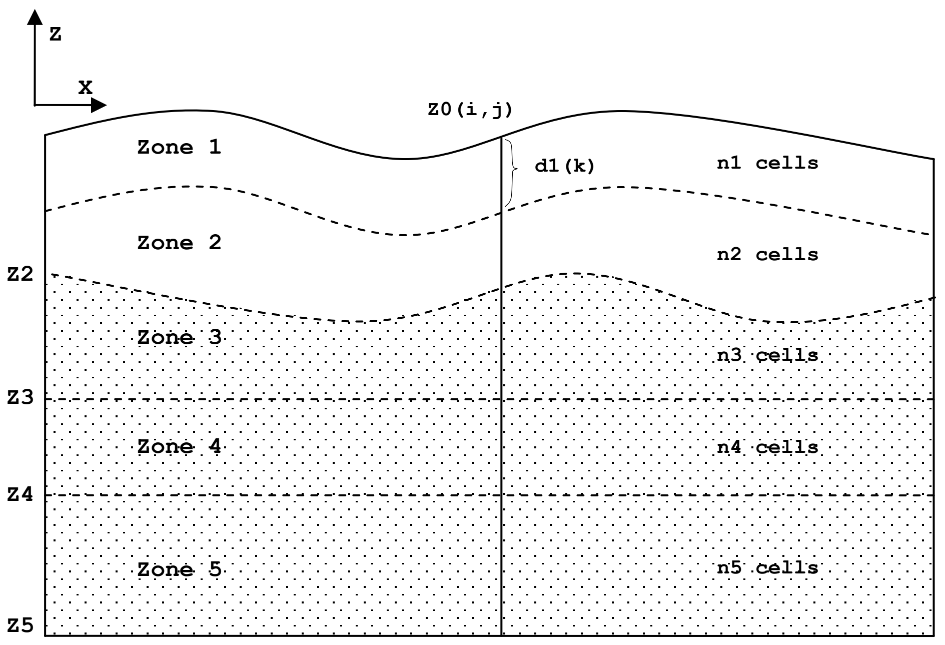
zone 3: (hyperbolic) tangent distribution with the first node coinciding to the last node of zone 2 and with last node such as $z\,(n4 + n5 + 1) = z3$.

zone 4: uniform distribution between the last node of zone 3 and *z4*. The last node is such as $z\,(n5 + 1) = z4$.

zone 5: (hyperbolic) tangent distribution with the first node ($n5+1$) coinciding to the last node of zone 4 and with last node such as $z(1) = z5$.

The total number of grid nodes along the z direction is $n = n1 + n2 + n3 + n4 + n5 + 1$.

n1, n2, n3, n4 or n5 may be null to discard the corresponding zone.



1008 GRGEMBG

* 1008 GRGEMBG :	*icos,*	*ifac,*	*jfac,*	*kfac,*	*ip,*	*i1,*	*i2,*	*j1,*	*j2,*	*k1,*	*k2*
1008	3	2	2	3	1	10	20	15	25	5	25

This command specifies an embedded grid.

Meaning of parameters:

icos .... kind of grid (1=BFC, 2=BFC:s, 3=CART)
ifac .... refining factor in i-direction
jfac .... refining factor in j-direction
kfac .... refining factor in k-direction
ip .... index of the parent grid
i1, i2 .... footprint definition on the parent grid
j1, j2 .... footprint definition on the parent grid
k1, k2 ....footprint definition on the parent grid

Default: no embedded grid.

1009 GRGZTOP

* 1009 GRGZTOP : *ztop*

```
1009      -450
```

This command sets the *z*-coordinate of the upper boundary. Default = 0.0

1010 GRGROC

* 1010 GRGROC : *fname*

```
1010     'SoilRock'
```

This command sets the file name for reading the soilrock topography. Regarding the file format, see command 1003 GRGTOP.

1011 GRGDROC

```
* 1011  GRGDROC  :  dmin

            1011        50.
```

It is not possible to let the soilrock surface reach ground level as the thicknesses of zones 1 and 2 would then be zero. By setting *dmin* to a suitable value the soilrock surface is "pressed down".

dmin: minimum distance between ground level and soilrock surface.

Note: GRIDGEN will print a warning when *dmin* is activated, in order to alert the user of the modified property specification.

1012 GRGZROC

```
* 1012  GRGZROC  :  zrock

            1012        -50.
```

This command sets a uniform value to the soilrock surface level.

2001 FRGGRD

* 2001 FRGGRD : *igrid*, *fname*

2001 1 'xyz'

This command sets the file name and the grid index for reading the grid coordinates.

2002 FRGSEED

* 2002 FRGSEED : *seed*

2002 0.917

This command sets the random number generator seed.

2003 FRGWKD

```
*  2003  FRGWKD  :   wkdivh1,     wkdivh2,      wkdivh3

                2003      100.           100.           100.
```

When isolated fractures or clusters are identified and removed the domain is subdivided, as part of the algorithm. The speed of the algorithm is affected by how the subdivision is made; *wkdivh*∗ is therefore accessible to specify the subdivision in the three coordinate directions.

It is recommended that *wkdivh*∗ is two to ten times the smallest fracture considered. A sensitivity study may give the optimum value.

Default values: 1500.   1500.   1500.

2004 FRGNRD

```
*  2004  FRGNRD  :  nxrd,          nyrd

                2004      100            100
```

Used for inhomogeneous fractures, see comments for command 2008.

Default values: 1000   1000

2005 FRGNLD

* 2005 FRGNLD : *nld*

```
        2005      1 000 000
```

An array dimension related to the total number of fractures generated. If an error print out related to *nld* is given, this number may need to be larger.

Default value. 1 000 000

2006 FRGOFN

* 2006 FRGOFN : *id*, *fname*

```
        2006
```

This command sets the output files names. The index ordering of the OFNAMES array is as follows:

1- FRCSETx.DAT
2- FREVOLx.DAT
3- FWSx.DAT
4- STORAx.DAT
5- CONDXx.DAT
6- DIFFXx.DAT
7- CONDYx.DAT
8- DIFFYx.DAT
9- CONDZx.DAT
10- DIFFZx.DAT

These names should not be modified.

* 2007 FRGKNWF : *fname*

```
            2007     'Fracdata'
```

This command reads the file *fname* and adds fractures to the list of known fractures.

```
* 2008  FRGKNW  :  inhomf,    htknsf,    frevolf,    fwsrff    storaf,    conduf,     diffuf
*                    x1,   y1,   z1,   x2,   y2,   z2,   x3,   y3,  z3
*                vkirf1, vkirf2, vkirf3, lewirf1, lewirf2, rcorrf, fsdevf, fwsdevf, ssdevf, csdevf, dsdevf
  2008           0    1.   0.005     20.   1.E-6    1.E-4   1.E-10
                 9.2      -1.        12.1    90.    101     -73    9.2    -1.      -6.
```

This three line command adds a known fracture to the list. If *inhomf* = 0 (meaning that the fracture is homogeneous) the third line does not need to be specified.

Meaning of parameters:

inhomf.........a homogeneous fracture is specified by 0, an inhomogeneous by 1
htknsf .... half thickness of fracture
frevolf.........fracture porosity (in %)
fwsrff...........flow wetted surface (m^2/m^3)
storaf..........specific storativity
conduf.........hydraulic conductivity
diffuf...........diffusion coefficient
x_i, y_i, z_i.......coordinates for the triangular fracture

An inhomogeneous fracture specification is activated by setting *inhomf* = 1. A number of additional parameters then need to be considered. The triangle is first divided into a number of equal rectangles by a rectangular grid. The length and width of the rectangles are specified by a parameter *lewirf*, with first index corresponds to length and second to width. A vector *vkirf*, with three indexes, specifies the orientation of the grid by the condition that the "length" sides of the rectangles shall be parallel to the orthogonal projection of *vkirf* onto the fracture plane.

A random number with a multivariate normal distribution is then generated, by the method described in Report 1, Appendix C. The correlation length of the random number field is denoted *rcorrf* and the correlation lengths in the fracture plane are obtained by multiplying *rcorrf* with the length and width of the rectangles.

The amplitude is controlled by the specification of the standard deviation, for the variable in question.

Thus:

vkirf∗	vector for orientation of anisotropy
lewirf∗	length and width of rectangles, covering the fracture plane
rcorrf	correlation length of random numbers
fsdevf	standard deviation of porosity
fwsdevf	standard deviation of flow wetted surface
ssdevf	standard deviation of storativity
csdevf	standard deviation of conductivity
dsdevf	standard deviation diffusivity

When specifying inhomogeneous fractures, command 2004 FRGNRD may need to be considered. *nxrd* and *ngrd* give the dimensioning of the arrays used for the rectangles described above. A error print out results if *nxrd* or *nyrd* are given to small values.

2009 FRGRANF

```
* 2009  FRGRANF  :  fname

            2009      'RANFRAC'
```

This command reads the file *fname* and adds its fractures to the list of random fractures.

* 2010 FRGRAN1 :	*igenf,*	*lfl,*	*lfh*	*thknsf,*	*frevof,*	*storaf,*	*diffuf,*	*fwsrff*
	1	10	10.1	0.01	1E-3	1E-6	1E-10	1

This command should always be used together with 2011, as this is the first part of the specification of random fractures.

Meaning of parameters:

igenf………if 1 the set is generated; 0 ignores the set
lfl ……..…..smallest size of the fractures in the set
lfh……… ....largest size of the fractures in the set
thknsf………thickness of fractures in the set
frevof………porosity of the fractures
storaf………specific storativity
diffuf………diffusion coefficient
fwsrff…….... flow wetted surface (m^2/m^3)

* 2011 FRGRAN2 : *iset, tcsta, tcstb, tcstc, tcstd, lreff, expidf, idreff, lambdf1, lambdf2, lambdf3*

1 1.E-4 0 1.E-4 0.2 500 -2.6 4.E-6 0. 0. 0.

This command should always be used together with 2010, as this is the second part of the specification of random fractures.

Meaning of parameters:

iset.........index to set; refers to the sets given in 2010

$\left.\begin{array}{l} tcsta \\ tcstb \\ tcstc \\ tcstd \end{array}\right\}$...........The relation between transmissivity, T, and length, L, is given by:

$$T = tcsta \times (L/100) \times\times (tcstb + ran \times tcstd)$$
$$\text{if } (T > tcstc) \; T = tcstc$$

where *ran* is a uniform random number in the interval -0.5 to 0.5.

lreff............a reference length in the power law
expidf..........exponent in the power law
idreff............intensity factor in the power law

$\left.\begin{array}{l} lambdf1 \\ lambdf2 \\ lambdf3 \end{array}\right\}$........... gives the position on the sphere for a Fisher-distribution. The length of the vector (given by the three components) gives the *kappa* in the Fisher-distribution.

3001 TKRIN

* 3001 TKRIN : *fname*

3001 ‘xyz’

This command specifies the input file, that is to be translated horizontally and rotated around a vertical axes.

3002 TKROUT

* 3002 TKROUT : *fname*

3002 ‘xyzrot’

This command specifies the output file, i e the file with translated and rotated coordinates.

3003 TKRTRF

```
* 3003  TKRTRF  :  dx,     dy,        degree

        3003        100.    10.        40.
```

The horizontal translation is given by *dx* and *dy*, and the rotation by degree (anticlockwise).

4000 SBRTITLE

```
* 4000  SBRTITLE  :  title

        4000          'NEWMODEL'
```

By default the SUBROF file has the same title as the parent grid. This command gives the opportunity to set a new title to the SUBROF file.

4001 SBRGIN

* 4001 SBRGIN : *fname*

4001 ‘xyz’

This command specify the input grid file.

4002 SBRGOUT

* 4002 SBRGOUT : *fname*

4002 ‘xyz.out’

This command specify the output grid file, generated by SUBROF.

4003 SBRRIN

* 4003 SBRRIN : *fname*

4003 ‘rof’

This command specify the input ROF file.

4004 SBRROUT

* 4004 SBRROUT : *fname*

4004 ‘rofout’

This command specify the output ROF file.

4005 SBRPDEF

* 4005 SBRPDEF :	*icos,*	*ifac,*	*jfac,*	*kfac,*	*ip,*	*i1,*	*i2,*	*j1,*	*j2,*	*k1,*	*k2*
4005	2	3	2	4	1	10	20	20	30	5	15

This command defines how the new ROF should be generated.

icos	kind of grid (1=BFC, 2=BFC:s, 3=CART)
ifac	refining factor in i-direction
jfac	refining factor in j-direction
kfac	refining factor in k-direction
ip	index of the parent grid
i1, i2	footprint definition on the parent grid
j1, j2	footprint definition on the parent grid
k1, k2	footprint definition on the parent grid

4006 SBRTEC

* 4006 SBRTEC :	*fname,*	*title,*	*isbin*
4006	'TecSBR'	' '	1

This command generates a Tecplot file, which can be used to check the generated ROF. The file can be ascii or binary depending on *isbin* (0 = ascii, 1 = binary).

5 Property Generation (*prpgen.f*)

The included property generation file is only an example. It is expected that this program will be further developed, as it should be the place where external data (RVS, SICADA, GIS, etc) is introduced and allowed to influence the property fields.

```
            PROGRAM PROPGEN
C
C-----This program generates property files for SOLVE.
C
C    --It reads the grid coordinates from XYZ
C    --It reads FRCPRP (Fracture properties) from GEHYCO
C    --It reads data from external data sources.
C    --It generates INDGRD, the index grid property file
C    --It generates the property files for SOLVE
C
*      Set the dimensions
*      ------------------

       parameter (ni=100, nj=100, nk=100)

       dimension xv(ni+1),yv(nj+1),zv(ni+1,nj+1,nk+1)
       dimension conduc(ni,nj,nk,3),diffus(ni,nj,nk,3)
       dimension frevol(ni,nj,nk),fwsurf(ni,nj,nk),storat(ni,nj,nk)
       dimension pme(ni,nj), poros(ni,nj,nk)



C   Read Grid coordinates from file  "XYZ"
C   ======================================
       WRITE(6,*) 'Read in grid'


C      Read in fracture properties from file "FRCPRP.dat"
C      =================================================
C
C Note: -frevol is free volume in cell, not porosity
       open (unit=80, file='condx1.dat', form='UNFORMATTED')
       open (unit=81, file='condy1.dat', form='UNFORMATTED')
       open (unit=82, file='condz1.dat', form='UNFORMATTED')
       open (unit=83, file='frevol1.dat', form='UNFORMATTED')
       do 160 k=1, nk
       do 160 j=1, nj
       do 160 i=1, ni
          read(83) frevol(i,j,k)
          read(80) conduc(i,j,k,1)
          read(81) conduc(i,j,k,2)
          read(82) conduc(i,j,k,3)
160    continue

       close (unit=60)
       WRITE(6,*) 'Read in Fracture properties'

C --Read in data from external sources
C   ==================================
       WRITE(6,*) 'Read in data from external sources'
```

Figure 5-1. *Example of prpgen.f*

```
C  --Modify properties and prepare arrays for SOLVE
C   =================================================
C




C-- Generate Conductivities,Scale  and convert to permeabilities
      do k=1,nk
      do j=1,nj
      do i=1,ni

        conduc(i,j,k,1)=conduc(i,j,k,1)*2.0387E-7+1.E-20
        conduc(i,j,k,2)=conduc(i,j,k,2)*2.0387e-7+1.E-20
        conduc(i,j,k,3)=conduc(i,j,k,3)*2.0387e-7+1.E-20

        poros(i,j,k)=frevol(i,j,k)/(1.*1.*1.)+1.E-10
      enddo
      enddo
      enddo


C


C--Generate property arrays to be read by SOLVE
C===============================================

C
      open (unit=61, file='PERMX', form='UNFORMATTED')
      open (unit=62, file='PERMY', form='UNFORMATTED')
      open (unit=63, file='PERMZ', form='UNFORMATTED')
      open (unit=64, file='POROS', form='UNFORMATTED')

      write(61) (conduc(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
     f ,(L-1)/ni/nj+1,1), L=1,ni*nj*nk)

      write(62) (conduc(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
     f ,(L-1)/ni/nj+1,2), L=1,ni*nj*nk)

      write(63) (conduc(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
     f ,(L-1)/ni/nj+1,3), L=1,ni*nj*nk)

      write(64) (poros(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
     f ,(L-1)/ni/nj+1), L=1,ni*nj*nk)

      close (unit=61)
      close (unit=62)
      close (unit=63)
      close (unit=64)

      WRITE(6,*) 'Generated arrays for SOLVE'


      end
```

***Figure 5-1.** Cont.*

6 Fortran Input File (*fif.f*)

6.1 Why needed?

The CIF-commands have been designed to handle most "standard" applications. It is however easy to find situations where it is impossible to handle the problem specification by this method:

- Transient source terms, that may be based on measured data (for example pumping in a borehole).
- Fluid properties that are a function of calculated variables (for example pressure effects on viscosity).
- Boundary conditions that need to be specified as a function of space and time coordinates.

DarcyTools provides a Fortran input file (*fif.f*), where more advanced problem specifications can be formulated.

6.2 How to use

First of all a word of warning may be in place. The *fif.f* offers great flexibility, but it also requires more skill and caution of the user. It is up to the user to check that the coding is correct.

The *fif.f* is visited after the CIF-commands have been interpreted and hence overwrites these. Some parts are also visited every time step or sweep, which needs to be considered when, for example, transient conditions are to be specified.

Probably the best way to learn how to use *fif.f* is by way of examples; such examples will be given later in this section together with explaining comments. A few general comments may however be useful:

- All variables are stored in a one-dimensional array called the F-array. When using or modifying a variable, one thus has to find its place in the F-array.
- To help the user, a number of "service routines" have been created. These will, for example, help the user to find a variable in the F-array or modify some fluid property.
- When *fif.f* has been modified, it is of course required that it is recompiled and a new executable is created.

The structure of the F-array and the utility routines are described in the Appendices.

An empty *fif.f* is given in Figure 6-1. As can be seen it consists of a number of subroutines and the user's task is to program one or several of these. In the comments the input and output variables are described. In most of the subroutines a declaration "dimension f (∗)" is found; this is the above mentioned F-array.

```
*=======================================================================*
*=======================================================================*
*=======================================================================*
*===========                                                ============*
*===========                                                ============*
*===========                  DARCYTOOLS                    ============*
*===========                                                ============*
*===========              solver's user section             ============*
*===========                                                ============*
*===========                                    2002-04-25  ============*
*===========                                                ============*
*=======================================================================*
*=======================================================================*
*=======================================================================*
*
*
*
*=======================================================================*
*                                                                       *
*     subroutine usrset()                                               *
*                                                                       *
*=======================================================================*
*
      subroutine usrset()

      end
*
*=======================================================================*

*                                                                       *
*     subroutine usrdt(dt)                                              *
*                                                                       *
*=======================================================================*
*                                                                       *
*     INPUT                                                             *
*     -----                                                             *
*                                                                       *
*     dt ......... current time step                                    *
*                                                                       *
*                                                                       *
*     OUPUT                                                             *
*     -----                                                             *
*                                                                       *
*     dt ......... new current time step                                *
*                                                                       *
*=======================================================================*
*
      subroutine usrdt(dt)

      end
```

Figure 6-1. *An empty fif.f.*

```
*=======================================================================*
*                                                                       *
*     subroutine usrmesh(igrd,icos,f,ni,nj,nk,nx,nt)                    *
*                                                                       *
*=======================================================================*
*                                                                       *
*     INPUT                                                             *
*     -----                                                             *
*                                                                       *
*     igrd ....... grid index                                           *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)                *
*     f .......... farray                                               *
*     ni ......... number of cells in the direction x                   *
*     nj ......... number of cells in the direction y                   *
*     nk ......... number of cells in the direction z                   *
*     nx ......... number of variables in the X sub-array               *
*     nt ......... number of time steps in the X sub-array              *
*                                                                       *
*                                                                       *
*     OUPUT                                                             *
*     -----                                                             *
*                                                                       *
*     xv ......... new x-coordinates of grid nodes                      *
*     yv ......... new y-coordinates of grid nodes                      *
*     zv ......... new z-coordinates of grid nodes                      *
*                                                                       *
*=======================================================================*
*
      subroutine usrmesh(igrd,icos,f,ni,nj,nk,nx,nt)

      dimension f(*)

      end
*
*=======================================================================*
*                                                                       *
*     subroutine usrini(igrd,icos,f,ni,nj,nk,nx,nt)                     *
*                                                                       *
*=======================================================================*
*                                                                       *
*     INPUT                                                             *
*     -----                                                             *
*                                                                       *
*     igrd ....... grid index                                           *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)                *
*     f .......... farray                                               *
*     ni ......... number of cells in the direction x                   *
*     nj ......... number of cells in the direction y                   *
*     nk ......... number of cells in the direction z                   *
*     nx ......... number of variables in the X sub-array               *
*     nt ......... number of time steps in the X sub-array              *
*                                                                       *
*                                                                       *
*     OUPUT                                                             *
*     -----                                                             *
*                                                                       *
*     x .......... X past values (i,j,k,n,2...)                         *
*                                                                       *
*=======================================================================*
```
Figure 6-1.*Cont.*

```
      subroutine usrini(igrd,icos,f,ni,nj,nk,nx,nt)

      dimension f(*)

      end
*
*======================================================================*
*                                                                      *
*     subroutine usrprop(ivar,igrd,icos,f,ni,nj,nk,nx,nt)              *
*                                                                      *
*======================================================================*
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*                                                                      *
*     ivar ....... variable index                                      *
*     igrd ....... grid index                                          *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)               *
*     f .......... farray                                              *
*     ni ......... number of cells in the direction x                  *
*     nj ......... number of cells in the direction y                  *
*     nk ......... number of cells in the direction z                  *
*     nx ......... number of variables in the X sub-array              *
*     nt ......... number of time steps in the X sub-array             *
*                                                                      *
*                                                                      *
*     OUPUT                                                            *
*     -----                                                            *
*                                                                      *
*     permea ..... new permeability field                              *
*     diffco ..... new diffusivity field                               *
*     poros ...... new porosity field                                  *
*     stora ...... new storativity field                               *
*     capa ....... new thermal capacity field                          *
*     etc.                                                             *
*                                                                      *
*======================================================================*
*
      subroutine usrprop(ivar,igrd,icos,f,ni,nj,nk,nx,nt)

      dimension f(*)

      end
```

Figure 6-1.*Cont.*

```
*
*=========================================================================*
*                                                                         *
*     subroutine usrboss(ivar,igrd,icos,f,qsrc,qphi,ni,nj,nk,nx,nt)      *
*                                                                         *
*=========================================================================*
*                                                                         *
*     INPUT                                                               *
*     -----                                                               *
*                                                                         *
*     ivar ....... variable index                                         *
*     igrd ....... grid index                                             *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)                  *
*     f .......... farray                                                 *
*     qsrc ....... automatic explicit source term                         *
*     qphi ....... automatic implicit source term S = Qsrc - Qphi*PHI     *
*     ni ......... number of cells in the direction x                     *
*     nj ......... number of cells in the direction y                     *
*     nk ......... number of cells in the direction z                     *
*     nx ......... number of variables in the X sub-array                 *
*     nt ......... number of time steps in the X sub-array                *
*                                                                         *
*                                                                         *
*     OUPUT                                                               *
*     -----                                                               *
*                                                                         *
*     qsrc ....... explicit source term                                   *
*     qphi ....... implicit source term S = Qsrc - Qphi*PHI               *
*                                                                         *
*=========================================================================*
*
      subroutine usrboss(ivar,igrd,icos,f,qsrc,qphi,ni,nj,nk,nx,nt)

      dimension f(*),qsrc(ni,nj,nk),qphi(ni,nj,nk)

      end
*
*=========================================================================*
*                                                                         *
*     subroutine usrslv(ivar,igrd,icos,nv)                                *
*                                                                         *
*=========================================================================*
*                                                                         *
*     INPUT                                                               *
*     -----                                                               *
*                                                                         *
*     ivar ....... variable index                                         *
*     igrd ....... grid index                                             *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)                  *
*     nv ......... trigger of coupling (1=uncoupled, 2=coupled)           *
*     /solve1/ ... default or user defined MIGAL's parameters             *
*                                                                         *
*                                                                         *
*     OUPUT                                                               *
*     -----                                                               *
*                                                                         *
*     /solve1/ ... new MIGAL's parameters                                 *
*                                                                         *
*=========================================================================*
```
Figure 6-1.*Cont.*

```
*
      subroutine usrslv(ivar,igrd,icos,nv)

      common /solve1/ icycle, nbgrid, liter, nbrelax, igmres, ipreco,
     &                iusolv, nbprer, igms, resfac, relax, relin

      end
*
*=======================================================================*
*                                                                       *
*     subroutine usrpreco(a,x,s,nt,nx,ni,nj,nk,nv,npts)                 *
*                                                                       *
*=======================================================================*
*                                                                       *
*     INPUT                                                             *
*     -----                                                             *
*                                                                       *
*     a .......... correction operator ready for MIGAL                  *
*     x .......... current X array                                      *
*     s .......... residuals (sources the correction operator)          *
*     nt ......... number of time steps in the X array                  *
*     nx ......... number of variables in the X array                   *
*     ni ......... number of cells in the direction x                   *
*     nj ......... number of cells in the direction y                   *
*     nk ......... number of cells in the direction z                   *
*     nv ......... trigger of coupling (1=uncoupled, 2=coupled)         *
*     npts ....... number of neighbors in the scheme                    *
*                                                                       *
*                                                                       *
*     OUPUT                                                             *
*     -----                                                             *
*                                                                       *
*     a .......... preconditioned operator                              *
*     s .......... preconditioned sources terms                         *
*                                                                       *
*=======================================================================*
*
      subroutine usrpreco(a,x,s,nt,nx,ni,nj,nk,nv,npts)

      dimension a(nv,nv,npts,ni,nj,nk),x(ni,nj,nk,nx,nt),s(nv,ni,nj,nk)

      end
```

Figure 6-1.*Cont.*

```
*
*=========================================================================*
*                                                                         *
*     subroutine usrout(ivar,igrd,icos,f,ni,nj,nk,nx,nt)                  *
*                                                                         *
*=========================================================================*
*                                                                         *
*     INPUT                                                               *
*     -----                                                               *
*                                                                         *
*     ivar ....... variable index                                         *
*     igrd ....... grid index                                             *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)                  *
*     f .......... farray                                                 *
*     ni ......... number of cells in the direction x                     *
*     nj ......... number of cells in the direction y                     *
*     nk ......... number of cells in the direction z                     *
*     nx ......... number of variables in the X sub-array                 *
*     nt ......... number of time steps in the X sub-array                *
*
*                                                                         *
*=========================================================================*
*
      subroutine usrout(ivar,igrd,icos,f,ni,nj,nk,nx,nt)
      dimension f(*)
      end

*
*=========================================================================*
*                                                                         *
*     subroutine setdomi(igr, gamma)                                      *
*                                                                         *
*=========================================================================*
*                                                                         *
*     INPUT                                                               *
*     -----                                                               *
*                                                                         *
*     igr ........ grid level from 1=fine to NBGRID=coarse                *
*     gamma ...... artificial diagonal dominance from MIGAL               *
*                                                                         *
*                                                                         *
*     OUTPUT                                                              *
*     ------                                                              *
*                                                                         *
*     gamma ...... artificial diagonal dominance Ap->Ap/gamma             *
*                  must be srtictly positive, gamma=1 => nothing done     *
*                                                                         *
*                                                                         *
*=========================================================================*
*
      subroutine setdomi(igr, gamma)

      gamma = 1.0 - 0.5**igr
      if(igr.eq.1) gamma = 0.95

      end
```

Figure 6-1.*Cont.*

```
*
*=================================================================*
*                                                                 *
*     subroutine setrelax(igr, nbrelax, relax)                    *
*                                                                 *
*=================================================================*
*                                                                 *
*     INPUT                                                       *
*     -----                                                       *
*                                                                 *
*     igr ........ grid level from 1=fine to NBGRID=coarse        *
*                    igr<0 <=> pre-restriction relaxations        *
*                    igr>0 <=> post-prolongation relaxations      *
*     nbrelax .... number of relaxations from MIGAL               *
*     relax ...... relaxation coefficient from MIGAL              *
*                                                                 *
*                                                                 *
*     OUTPUT                                                      *
*     ------                                                      *
*                                                                 *
*     nbrelax .... new number of relaxations to be done           *
*     relax ...... new relaxation coefficient                     *
*                                                                 *
*                                                                 *
*=================================================================*
*
      subroutine setrelax(igr, nbrelax, relax)

      end
*
*=================================================================*
*                                                                 *
*     subroutine topog(xv,yv,zv,ni,nj,nk,icos)                    *
*                                                                 *
*=================================================================*
*                                                                 *
*     INPUT                                                       *
*     -----                                                       *
*     xv,yv,zv ..... default grid coordinates for k=nk+1          *
*     ni,nj,nk ..... number of cells in each direction            *
*     icos ......... kind of grid (1=BFC, 2=BFC:s, 3=CART)        *
*                                                                 *
*                                                                 *
*     OUTPUT                                                      *
*     ------                                                      *
*     xv,yv,zv ..... users grid coordinates for k=nk+1            *
*                                                                 *
*                                                                 *
*     REMARK                                                      *
*     ------                                                      *
*     This routine allows users to modify the top plan of the very    *
*     parent grid when running GRIDGEN.The arrays xv, yv and zv are   *
*     the entire coordinates arrays but only the plan k=nk+1 must be  *
*     modified here. Beside setting a given topography, this routine  *
*     also gives the opportunity to set any x or y distribution. In   *
*     order to activate this routine, the topography file name must   *
*     be set to 'USER' or 'user' in the CIF command GRGTOP of GRIDGEN. *
*                                                                 *
*=================================================================*
```
Figure 6-1.*Cont.*

```
*
      subroutine topog(xv,yv,zv,ni,nj,nk,icos)

      end
*
*======================================================================*
*                                                                      *
*     subroutine soilroc(zv,ni,nj,icos)                                *
*                                                                      *
*======================================================================*
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*     zv ........... default soil/rock Z coordinates                   *
*     ni,nj ........ number of cells in x and y directions             *
*     icos ......... kind of grid (1=BFC, 2=BFC:s, 3=CART)             *
*                                                                      *
*                                                                      *
*     OUTPUT                                                           *
*     ------                                                           *
*     zv ........... users soil/rock Z coordinates                     *
*                                                                      *
*                                                                      *
*     REMARK                                                           *
*     ------                                                           *
*     This routine allows users to modify the soil/rock plan on the    *
*     very parent grid when running GRIDGEN.When icos=3 zv is a scalar *
*     value instead of a (ni+1,nj+1) array. In order to activate this  *
*     routine, the soil:rock file name must be set to 'USER' or 'user' *
*     in the CIF command GRGROC of GRIDGEN.                            *
*                                                                      *
*======================================================================*
*
      subroutine soilroc(zv,ni,nj,icos)

      end
*
*======================================================================*
```

Figure 6-1.*Cont.*

6.3 Examples of use

The five examples to be discussed are taken from the verification cases (see Report 2) and the user is hence advised to study the relevant cases to bring the coding into context. It may also be useful to have a look on the empty *fif.f* , Figure 6-1, in parallel in order to get the relevant comments about input and output parameters and the position of the subroutine in *fif.f.*

Subroutine usrmesh

Different grid options are tested in verification Case A4, from where the coding shown in Figure 6-2 is taken.

Comments:

- The routine *lfname* is used to get the position of the vertex coordinates in the F-array.
- The index for coordinate system, *icos*, is used to distinguish the BFC (*icos* = 1) from the BFC:s case (*icos* = 2).
- The do-loops and the *ijk*-index give the relevant F-array positions for the *x*-coordinates $(lxv+ijk)$, *y*-coordinates $(lyv+ijk)$ and the z-coordinates $(lzv+ijk)$.
- For the BFC:s case (*icos* = 2), the *x* and *y* coordinates are only a function of one index as the coordinate system is Cartesian in the horizontal plane.

Subroutine usrprop

In Case E2, dispersion coefficients that are a function of the local velocity are needed. This is clearly a situation that calls for *fif.f* coding, as we do not know the velocity field before hand. This subroutine, see Figure 6-3, is hence visited at every iteration sweep and the properties are updated.

Comments:

- As in the previous example we need the first location of variables in the F-array. M1 and M3 are mass-fluxes across *x* and *z* cell walls (the case is 2D) and X1S and X1T are the variable names for salinity and temperature respectively.
- We are only interested in dispersion coefficients for salinity, hence the statement "*if* (*ivar.eq.*2) *then* "
- Utility routines are used (fn_rho, get_poros, get_diff and set_diff). Details about these can be found in the Appendices.
- Some under-relaxation is used to change the dispersion coefficients smoothly during the iterations.

```
      subroutine usrmesh(igrd,icos,f,ni,nj,nk,nx,nt)

      dimension f(*)

      lxv=lfname('XV', igrd)
      lyv=lfname('YV', igrd)
      lzv=lfname('ZV', igrd)

      h=20.

       if(icos.eq.1) then
         do i=1,ni+1
         do j=1,nj+1
         do k=1,nk+1

          ijk=(i-1)+(j-1)*(ni+1)+(k-1)*(ni+1)*(nj+1)

          amplit=5.*h*sin(3.1416*float(i-1)/float(ni))*
     f               sin(3.1416*float(k-1)/float(nk))*
     f               sin(3.1416*float(j-1)/float(nj))

          xvloc=(i-1)*h+amplit
          yvloc=(j-1)*h+amplit
          zvloc=(k-1)*h+amplit
          f(lxv+ijk) = xvloc
          f(lyv+ijk) = yvloc
          f(lzv+ijk) = -1000.+zvloc
         enddo
         enddo
         enddo
       endif


       if(icos.eq.2) then
         do i=1,ni+1
          amplit=5.*h*sin(3.1416*float(i-1)/float(ni)*2)
          f(lxv+i-1) = (i-1) * h + amplit
         enddo

         do j=1,nj+1
          amplit=5.*h*sin(3.1416*float(j-1)/float(nj)*2)
          f(lyv+j-1)= (j-1) * h + amplit
         enddo

        do i=1,ni+1
        do j=1,nj+1
        do k=1,nk+1
          ijk=(i-1)+(j-1)*(ni+1)+(k-1)*(ni+1)*(nj+1)
          amplit=5.*h*sin(3.1416*float(i-1)/float(ni))*
     f              sin(3.1416*float(k-1)/float(nk))*
     f              sin(3.1416*float(j-1)/float(nj))
         f(lzv+ijk) = (k-1)*h + amplit-1000.
        enddo
        enddo
        enddo
      endif

      end
```

Figure 6-2. *Example of usrmesh-coding (from Case A4).*

```
      subroutine usrprop(ivar,igrd,icos,f,ni,nj,nk,nx,nt)

      dimension f(*)

      Ima1 = LFNAME('M1',1)
      Ima3 = LFNAME('M3',1)
      Isalt = LFNAME('X1S',1)
      Itemp = LFNAME('X1T',1)

*
*     Calculate dispersion terms
*     --------

      if(ivar.eq.2)then
      area=5.*5.
      do k=1,nk
      do i=1,ni
      ik=i+(k-1)*ni-1
      sloc=f(Isalt+ik)
      tloc=f(Itemp+ik)
      rholoc=fn_rho(sloc,tloc)
      porloc=get_poros(i,1,k,1)
      uvel=f(ima1+ik)/(rholoc*area*porloc)
      wvel=f(Ima3+ik)/(rholoc*area*porloc)
      absvel=sqrt(uvel**2+wvel**2+1.E-20)

      difnew=porloc*(2.*absvel+18.*uvel**2/absvel)
      difold=GET_DIFF(i,1,k,1,1)
      difset=0.1*difnew+0.9*difold
       call SET_DIFF(i,1,k,1,1,difset)

      difnew=porloc*(2.*absvel+18.*wvel**2/absvel)
      difold=GET_DIFF(i,1,k,1,3)
      difset=0.1*difnew+0.9*difold
       call SET_DIFF(i,1,k,1,3,difset)
      enddo
      enddo
      endif



      end
```

Figure 6-3. *Example of usrprop-coding (from Case E2).*

Subroutine usrboss

This is the place where complex boundary and source terms can be specified (***boss*** means ***bo***undary, ***s***ources and ***s***inks). Also this example, see Figure 6-4, is taken from Case E2, where the pressure at the top boundary is given a linear distribution.

Comments:

- We need the *x*-coordinates from the F-array.
- It is the pressure that is to be specified, hence " *if* (*ivar.eq.*1) *then*".
- "*Val*" is the prescribed pressure at the cell centre *xcc*.
- For "*qsrc*" and "*qphi*" settings, see Report 1 (Appendix A).

```
      subroutine usrboss(ivar,igrd,icos,f,qsrc,qphi,ni,nj,nk,nx,nt)

      dimension f(*),qsrc(ni,nj,nk),qphi(ni,nj,nk)

      Ixv  = LFNAME('XV',1)


C  Set pressure on top boundary
      if(ivar.eq.1) then
       do i=1,ni
         xcc=0.5*(f(Ixv+i-1)+f(Ixv+i))
         val=1.E5*(1.-xcc/900.)
         qsrc(i,nj,nk)=val*1.E20
         qphi(i,nj,nk)=1.E20
       enddo
      endif

      end
```

Figure 6-4. *Example of usrboss-coding (from Case E2).*

Subroutine usrout

As the name indicates this is the place where additional output is generated. In the example (Case E6), see Figure 6-5, output for comparison with an analytical solution is generated.

Comments:

- We need access to the mass fluxes (M1) and the *z*-coordinates (*zv*) in the F-array.
- Only one set of profiles is needed, hence the statement " *if* (*ivar.eq.1. and. istep.eq.nstep*)".
- The utility routine "*iufree*" is used to get a free logical unit number.
- Two commons are used to get access to "*isweep*" and "*nstep*".
- ijk gives the location of a scalar located at a cell centre, while *ijkv* gives the location of vertex coordinates (there is one more vertex value than scalar value in a coordinate direction).

```
      subroutine usrout(ivar,igrd,icos,f,ni,nj,nk,nx,nt)
      dimension f(*)

      common /const2/ nstep,nsweep,nvar1,nvar2,nitc1,
     &                nvar3,nvar4, nitc2,nvar5,nvar6,nitg
      common /const3/ istep,isweep,dum1,itc,dum2,itg,t


      lvu=lfname('M1', igrd)
      lzv=lfname('ZV', igrd)

      if(ivar.eq.1.and.istep.eq.nstep) then
      ifile=iufree()
      OPEN(unit=ifile,file='TWOFL.dat')
      j=1
      i=ni/2
      area=0.25*0.25
      do k=1,nk
      ijk=i-1+(j-1)*ni+(k-1)*ni*nj
      ijkv=i-1+(j-1)*(ni+1)+(k-1)*(ni+1)*(nj+1)
      zcord=0.5*(f(lzv+k-1)+f(lzv+k))
      uvel=-f(lvu+ijk)/1000./area
c--analytical solution
      perm=1.e-12
      drho=50.
      emu1=2.E-3
      emu2=6.E-3
      zsize=10.
      fact1=sin(3.14159*(zcord+5.)/zsize)
      fact2=alog((1.+fact1)/(1.-fact1))
      qzero=perm*drho*9.81/(emu1+emu2)
      uanl=qzero*fact2/3.14159
      write(ifile,*) zcord, uvel, uanl
      enddo
      endif
      end
```

Figure 6-5. *Example of usrout-coding (from Case E6).*

Subroutine topog

The coding, see Figure 6-6, is used in Case E5, where the top boundary is given the shape of a sinusoidal function.

Comments:

- As *zv* is given as a 3D array in the dimension statement, one can access the array by these indexes.

```
      subroutine topog(xv,yv,zv,ni,nj,nk,icos)
      dimension zv(ni+1,nj+1,nk+1)


C---GENERATE TOPOGRAPHY
        DO  j=1,nj+1
        DO  i=1,ni+1
        PId2=3.1416/2.
        amplit=(10.*sin(2.*3.1416*float(i-1)/
     f  float(ni)-PId2)+10.)-10.0
          zv(i,j,nk+1) =  amplit
        ENDDO
        ENDDO
      end
```

Figure 6-6. *Example of topog-coding (from Case E5).*

7 A SITE-LABORATORY-EXPERIMENTAL SCALE DEMO

7.1 Introduction

In Report 1 results from this Demo Case were presented and discussed. It was also noted that the Demo is generic, but share many features of a real world application.

Here the emphasis is on the set-up of the case in DarcyTools; the CIF and *fif.f* files, and other programs, will be presented and discussed.

In order to make the presentation self-contained some parts of the presentation of the case will first be repeated.

7.2 The situation studied

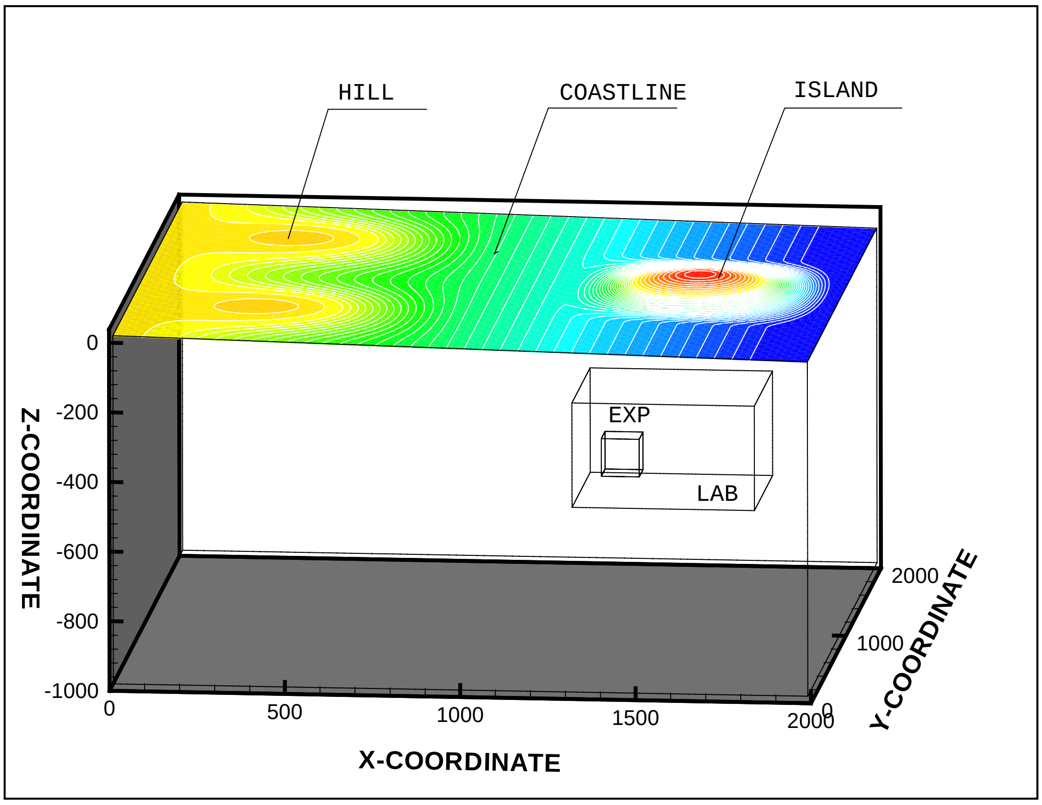
The situation studied is outlined in Figure 7-1. It is a coastal site, with seawater of a brackish nature (salinity of 1%). We assume a certain precipitation on land and we hence have a density stratification to take into account. Two hills give a certain topography on land. A tunnel, with a certain inflow, will be placed below the small island in the laboratory volume shown in the figure. The focus of the analysis will be on the effects of the tunnel. The situation has a clear resemblance with the Äspö region. The fracture system will however be much simpler in this demo, as compared to the detailed information available for Äspö HRL. Four major fracture zones, shown in Figure 7-1, are assumed to represent the deterministic system. Random fractures will be generated to build a working fracture network.

A summary of the problem specification is given in Table 7-1. It is not the intention to give a complete account of the input data; this is considered to be outside the scope (the specification of the fracture network would be lengthy, for example). A few comments may be needed as a complement to the key features in the table (see also Figure 7-1):

- Domains. The site model covers the whole domain, while the laboratory model is located below the island. The first of these two grids are of the BFC:s type (follows the topography), while the second grid is a cartesian one. The experimental model is placed in the laboratory model, but outside the tunnel area.

- Properties. Porosity is specified for each fracture and fracture zone. The diffusion coefficient is given a value of ten times the value for molecular diffusion for salt; this process is hence insignificant. Transmissivities, orientations, etc for the random fractures are set according to the values found appropriate for Äspö HRL.

- Random fractures. When the fracture network for the site domain is generated, random fracture in the interval 20 → 1000 metres are generated. Those random fractures that intersect the laboratory volume are imported as deterministic fractures to this domain. Random fractures in the interval 10 - 20 metres are then added. The same procedure is repeated for the experimental volume; now with all fractures larger than 10 metres as deterministic and random fractures in the interval 2 – 10 metres.



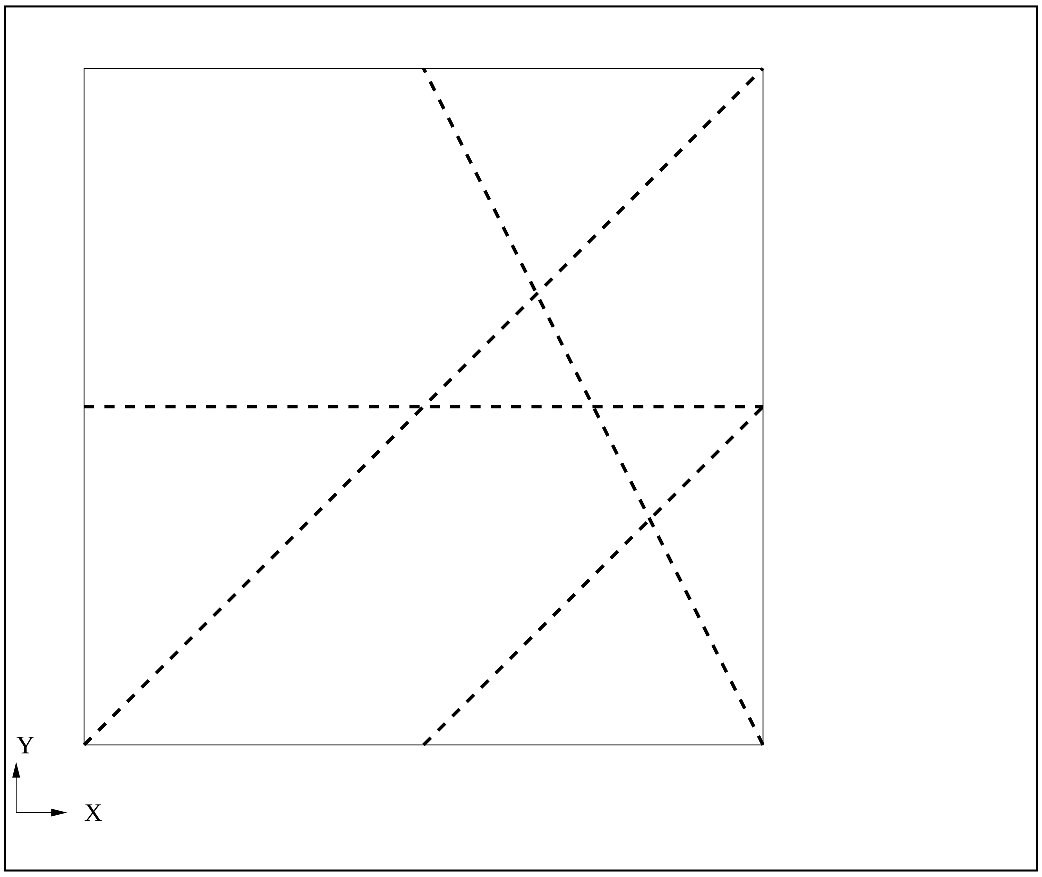


Figure 7-1. *Situation considered (top) and deterministic fracture zones.*

Table 7-1. Summary of problem specification.

Domains and grids	Site: $2 \times 2 \times 1$ km^3 NX = 100, NY = 100, NZ = 50, Δ =20 Laboratory: $500 \times 500 \times 300$ m^3 NX = 50, NY = 50, NZ = 30, Δ = 10 Experimental: $100 \times 100 \times 100$ m^3 NX = 50, NY =50, NZ = 50 Δ =2
Properties	- Deterministic zones according to Figure 7-1, Transmissivity = 10^{-5} m^2/s - Random fractures Site: $l = 20 \rightarrow 1000$ m Laboratory: $l = 10 \rightarrow 20$ m Experimental: $l = 2 \rightarrow 10$ m - Diffusion coefficients: 10^{-8} m^2/s, constant - Porosity: 10^{-3}, constant
Boundary conditions	Top: Precipitation on land , 50 mm/year Pressure and salinity fixed below sea Vertical boundaries: Zero flux when boundary on land, prescribed pressure and salinity when below sea. Fixed salinity at bottom boundary. Tunnel : Three tunnel sections are defined; two with a prescribed skin (= 0.01) and one with a prescribed inflow (= 1 l/s). Groundwater table: As part of the simulation the groundwater table is calculated. The specific yield feature is not activated as we are only considering the steady state.

7.3 The set-up

In this section the files that make up the Demo Case will be presented and commented. Only some of the settings will however be commented, as most settings are “standard” and are discussed in the previous chapters of this report.

CIF

The CIF is found in Figure 7-2.

Comments:

- 6 SETSTEP: A long integration time is needed in order to get a steady state salinity distribution. This long time step does however introduce some oscillation in the solution. Some steps with a smaller time step are required to damp the oscillations.
- 10 SETFLUB: We use this box to evaluate the overall mass balance; the mass flux into the tunnel should be equal to the mass flux over the boundaries of this box.
- 12 SETLAW: Only salinity is assumed to affect density.
- 17 SETTUN1: The file 'TUNNEL.dat' gives the cell index of the tunnel.
- 18 SETTUN2: The first two sections have a specified skin, while the third section has a specified inflow.
- 117 SETFINDG: This file is used to export the tunnel cells to Tecplot.
- 118 SETF1: The files for groundwater table calculations are initialized and the porosity × diffusion is put to $10.\times 10^{-3} \times 10^{-9} = 10^{-11}$.
- 120 SETF3: These files are generated in *prpgen.f.*
- 121 SETSPT: A linear salinity profile is specified, as an initial condition.
- 122 SETBOSS: ITYPE = 1 means that we freeze the initial conditions on some of the boundaries.
- 1003 GRGTOP: by putting 'USER' in *fname* we specify that the topography is given in *fif.f.*
- 1007 GRGZDIS: Five top layers are used, then ten cells are used to stretch the grid down to z = - 200 m, then a constant cell size is specified for 500 m and finally the grid is stretched down to 1000 m, using ten cells.
- 2007 FRGKNWF: deterministic fractures are specified by this command. Note the different number of files for different model domains (SITE, LAB, EXP).

fif.f

Only the topography is specified in *fif.f* for the DEMO Case. The subroutine *topog* is given in Figure 7-3.

fractools.f

This is a small program written for the Demo Case, see Figure 7-4. The main task for this program is to read input files, specifying fractures and zones, and write these on a format that can be read by DarcyTools. For the Demo Case, random fractures from a larger domain are specified as deterministic fractures for the next smaller domain; the main part of *fractools.f* is devoted to this task.

prpgen.f

A property generation program, *prpgen.f*, is written for each domain. In Figure 7-5, the *prpgen.f*, for the SITE domain is given. The comments in the program explain the different tasks of this program.

```
**********************************************************
*                                                        *
*                        DemoCase                        *
*                                                        *
*                     10 May  2003                       *
*                                                        *
**********************************************************

*   1 SETTITLE  :     title
        1         'DEMO CASE'

*   2 SETGRDF  : fname
        2        'xyz'

*   3 SETLICM  :      licence,             path
        3        'y]GCJ?HJAMTVlxHZmDa'     ''

*   6 SETSTEP  :     dt         nstep    iorder
*   Run 500 steps with dt=1.e7 and underrealaxtion 0.3, then make
*   a restart with dt=1.E5 and underrelaxation=0.1. This to damp
*   oscillations.
*        6            1.E7       500      1
        6           1.E5       200      1

*  10 SETFLUB  : id, i1, i2, j1, j2, k1, k2, igrd
        10       1   50   90 30  70  5   40   1

*  12 SETLAW1  : rho0, Trho, alpha1, alpha2, beta1, beta2
        12       1000.  0.   0.008      0.     0.     0.

*  13 SETLAW2  : visc0, a1, a2, Tvisc, n
        13        2.E-3 0.   0.   0.   1

*  16 SETGWT   : grlx, facmin
        16        0.8   0.001

*  17 SETTUN1  : fname
        17       'TUNNEL2.dat'

*  18 SETTUN2  : isec, iaction, sink, skin,   skmin, skmax, rlx
        18         1     1      0.    .01     1.E-10  1.E9    .1
        18         2     1      0.    .01     1.E-10  1.E9    .1
        18         3     2      1.    .05     1.E-10  1.E9    .1

*  20 SETSLV1  : ivar, igrd, relin, resfac, liter
        20        1      0    .1     0.00   6
        20        2      0    .1     0.00   6

* 110 SETSWEEP : nsweep,  ivar1,  ivar2
      110          1       1       2

* 115 SETBNDY  : ssea, tsea, tland
      115        1.0   0.0    0.0

* 117 SETFINDG : igrd,      form,       fname
      117         2   'unformatted'  'INDGRD_2'
```

Figure 7-2. *Demo Case, CIF.*

```
* 118 SETF1    :  name,     igrd,  value
       118       'GWT_FILL'  1    1.
       118       'GWT_GH'    1    0.
       118       'DIFF1'     3    10.E-12
       118       'DIFF2'     3    10.E-12
       118       'DIFF3'     3    10.E-12
       118       'DIFF1'     2    10.E-12
       118       'DIFF2'     2    10.E-12
       118       'DIFF3'     2    10.E-12
       118       'DIFF1'     1    10.E-12
       118       'DIFF2'     1    10.E-12
       118       'DIFF3'     1    10.E-12
       118       'DIFF4'     1    10.E-12
       118       'DIFF5'     1    10.E-12

* 120 SETF3    : name,  igrd, form,         fname
       120      'PME'    1    'UNFORMATTED' 'PREME'
       120      'POROS'  1    'UNFORMATTED' 'POROS1'
       120      'PERM1'  1    'UNFORMATTED' 'PERMX1'
       120      'PERM2'  1    'UNFORMATTED' 'PERMY1'
       120      'PERM3'  1    'UNFORMATTED' 'PERMZ1'
       120      'PERM4'  1    'UNFORMATTED' 'PERMX1'
       120      'PERM5'  1    'UNFORMATTED' 'PERMY1'
       120      'POROS'  2    'UNFORMATTED' 'POROS2'
       120      'PERM1'  2    'UNFORMATTED' 'PERMX2'
       120      'PERM2'  2    'UNFORMATTED' 'PERMY2'
       120      'PERM3'  2    'UNFORMATTED' 'PERMZ2'
       120      'POROS'  3    'UNFORMATTED' 'POROS3'
       120      'PERM1'  3    'UNFORMATTED' 'PERMX3'
       120      'PERM2'  3    'UNFORMATTED' 'PERMY3'
       120      'PERM3'  3    'UNFORMATTED' 'PERMZ3'

* 121 SETSPT   : s1, t1, s0, t0, dwt, dsdz, dtdz, i1, i2 j1, j2, k1, k2
         121       0.  0.  1.  0.  2.  -2.E-3  0.  1  100  1  100 1   50

* 122 SETBOSS  : ivar, igrd, itype, i1, i2, j1, j2, k1, k2, it1, it2, qsrc, qphi
      122          1    1     1     100 100 1   100 1   50   1   1000  0.    0.
      122          1    1     1     1   1   1   100 46  50   1   1000  0.    0.
      122          1    1     1     50  100 1   1   46  50   1   1000  0.    0.
      122          1    1     1     50  100 100 100 46  50   1   1000  0.    0.
      122          2    1     1     100 100 1   100 1   50   1   1000  0.    0.
      122          2    1     1     1   100 1   100 1    1   1   1000  0.    0.
      122          2    1     1     1   1   1   100 46  50   1   1000  0.    0.
      122          2    1     1     50  100 1   1   46  50   1   1000  0.    0.
      122          2    1     1     50  100 100 100 46  50   1   1000  0.    0.

* 123 SETTECF  :   fname,       title,  isbin
       123        'DEMO.dat'     ''      1

* 124 SETTECZ  : ifile, igrd, i1, i2, ifr, j1, j2, jfr, k1, k2, kfr
       124         1      1    1  100  1   1   100  1    1   50   1
       124         1      2    2   54  1   2   54   1    2   32   1
       124         1      3    2   56  1   2   56   1    2   56   1
```

***Figure 7-2.** Cont.*

```
* 125 SETTECB  : ifile, vname       action  value
       125         1    'GWT_FILL'   0        0
       125         1    'X1P'        0        0
       125         1    'X1S'        0        0
       125         1    'INDGRD15'   0        0
       125         1    'DARCY-U'    0        0
       125         1    'DARCY-V'    0        0
       125         1    'DARCY-W'    0        0
       125         1    'POROS'      0        0
       125         1    'PERM1'      0        0
       125         1    'PERM2'      0        0
       125         1    'PERM3'      0        0

* 130 SETSTORE : name,    igrd
        130      GWT_GH    1
        130      GWT_FILL  1

* 131 SETRST   :
       131

* 135 SETHIST : i   j   k   igrd  iv   title
       135      0   0   0    1     2   'Residuals'

       135      81 46  31    1     2   'Spot Values (81,46,31)'
       135      5   25  0    1     2   'Profile,  j=25  i=5'
       135      0   0   0    1     2   'Mass balance Grid 1'
       135      30 50   48   1     2   'Spot Values (30,50,48)'


* 136 SETHIST2 : igra  vname   label
       136        1    'RESP'  'Pressure'
       136        1    'RESS'  'Salinity'
       136        2    'X1P'   'Pressure'
       136        2    'X1S'   'Salinity'
       136        3    'GWT_FILL'  'Saturation'
       136        3    'X1P'   'Pressure'
       136        3    'X1S'   'Salinity'
       136        4    'FLUB1' 'Flub1'
       136        5    'X1P'  'Pressure'

**********************************************************
*                                                        *
*                GRIDGEN setting                         *

* 1001 GRGTEC  : fname,    title, isbin
        1001      'TecXYZ'    ''   1

* 1003 GRGTOP   : fname
        1003      'USER'

* 1004 GRGPCOS  : icosp
        1004       2

* 1005 GRGXDIS  : x0,   x1,     x2,    x3,   nx1,  nx2, nx3
        1005      0.    0.    2000.   2000.  0     100   0

* 1006 GRGYDIS  : y0,   y1,     y2,    y3,   ny1,  ny2, ny3
        1006      0.    0.     2000.  2000.  0     100   0
```

Figure 7-2. *Cont.*

```
* 1007 GRGZDIS  : z3,    z4,    z5,        nz1, nz2, nz3, nz4, nz5
       1007       -200. -700.  -1000.       5    10  0    25   10
+                 1, 2.
+                 2, 3.
+                 3, 4.
+                 4, 5.
+                 5, 6.

* 1008 GRGEMBG  : icos, ifac, jfac, kfac, ip, i1, i2, j1, j2, k1, k2
       1008        3     2     2     2    1   63  88  38  63  16 30
       1008        3     5     5     5    2   10  20  10  20  10 20

*********************************************************
*                                                       *
*                FRACGEN setting                        *

* 2001 FRGGRD   : igrd, fname
       2001         1   'xyz'

* 2002 FRGSEED   : seed
       2002         0.234

* 2007 FRGKNWF  : fname
      2007        'FRACSITE'
*      2007        'FRACLAB'
*      2007        'FRACEXP'

* 2010 FRGRAN1  : igenf, lfl,   lfh,  thknsf,  frevof,  storaf,  diffuf,  fwsrff
       2010        1      500.  1000.    5.      1.E-3    1.E-6    1.E-10    100.
       2010        1      200.   500.    2.      1.E-3    1.E-6    1.E-10    100.
       2010        1      100.   200.    1.      1.E-3    1.E-6    1.E-10    100.
       2010        1       50.   100.    0.5     1.E-3    1.E-6    1.E-10    100.
       2010        1       20.    50.    0.25    1.E-3    1.E-6    1.E-10    100.
       2010        0       10.    20.    0.10    1.E-3    1.E-6    1.E-10    100.
       2010        0        2.    10.    0.05    1.E-3    1.E-6    1.E-10    100.
       2010        1      500.  1000.    5.      1.E-3    1.E-6    1.E-10    100.
       2010        1      200.   500.    2.      1.E-3    1.E-6    1.E-10    100.
       2010        1      100.   200.    1.      1.E-3    1.E-6    1.E-10    100.
       2010        1       50.   100.    0.5     1.E-3    1.E-6    1.E-10    100.
       2010        1       20.    50.    0.25    1.E-3    1.E-6    1.E-10    100.
       2010        0       10.    20.    0.10    1.E-3    1.E-6    1.E-10    100.
       2010        0        2.    10.    0.05    1.E-3    1.E-6    1.E-10    100.
```

Figure 7-2. *Cont.*

```
* 2011 FRGRAN2  : iset, tcsta, tcstb, tcstc, lreff, expidf, idreff, lambdf1,
lambdf2,lambdf3
        2011       1    1.E-5   2.0   1.E-5   500.   -2.6   7.E-9    8.487
8.487     0.
        2011       2    1.E-5   2.0   1.E-5   500.   -2.6   7.E-9    8.487
8.487     0.
        2011       3    1.E-5   2.0   1.E-5   500.   -2.6   7.E-9    8.487
8.487     0.
        2011       4    1.E-5   2.0   1.E-5   500.   -2.6   7.E-9    8.487
8.487     0.
        2011       5    1.E-5   2.0   1.E-5   500.   -2.6   7.E-9    8.487
8.487     0.
        2011       6    1.E-5   2.0   1.E-5   500.   -2.6   7.E-9    8.487
8.487     0.
        2011       7    1.E-5   2.0   1.E-5   500.   -2.6   7.E-9    8.487
8.487     0.
        2011       8    1.E-5   2.0   1.E-5   500.   -2.6   3.E-9   -4.95
4.95      0.
        2011       9    1.E-5   2.0   1.E-5   500.   -2.6   3.E-9   -4.95
4.95      0.
        2011      10    1.E-5   2.0   1.E-5   500.   -2.6   3.E-9   -4.95
4.95      0.
        2011      11    1.E-5   2.0   1.E-5   500.   -2.6   3.E-9   -4.95
4.95      0.
        2011      12    1.E-5   2.0   1.E-5   500.   -2.6   3.E-9   -4.95
4.95      0.
        2011      13    1.E-5   2.0   1.E-5   500.   -2.6   3.E-9   -4.95
4.95      0.
        2011      14    1.E-5   2.0   1.E-5   500.   -2.6   3.E-9   -4.95
4.95      0.
```

Figure 7-2. *Cont.*

```
      subroutine topog(xv,yv,zv,ni,nj,nk,icos)

      dimension xv(ni+1),yv(nj+1),zv(ni+1,nj+1,nk+1)

      if(icos.ne.2) return

      XMIN = 0.
      YMIN = 0.
      DX = 20.
      DY = 20.

      xv(1)=XMIN
      DO 10 i=2,ni+1
       xv(i)=xv(i-1)+DX
  10  CONTINUE

      yv(1)=YMIN
      DO 20 j=2,nj+1
       yv(j)=yv(j-1)+DY
  20  CONTINUE

      DO 40 j=1,nj+1
      DO 50 i=1,ni+1
       slope=20.-40.*xv(i)/xv(ni+1)
       PI=4*ATAN(1.0)
       PId2=PI/2.
       hhill=10.
       hisla=50.
       if(i.le.50) then
c---two hills
       if(j.le.50) then
       SN=0.5*(sin(-PId2+PI*2.*yv(j)/yv(50))+1.)
       EW=0.5*(sin(-PId2+PI*2.*xv(i)/xv(50))+1.)
       htop=hhill*SN*EW
        slope=slope+htop
       else
       SN=0.5*(sin(-PId2+PI*2.*yv(j-50)/yv(51))+1.)
       EW=0.5*(sin(-PId2+PI*2.*xv(i)/xv(50))+1.)
       htop=hhill*SN*EW
        slope=slope+htop
       endif
c---island
       else
       if(j.gt.25.and.j.le.75.and.i.gt.60) then
       SN=0.5*(sin(-PId2+PI*2.*yv(j-25)/yv(50))+1.)
       EW=0.5*(sin(-PId2+PI*2.*xv(i-60)/xv(41))+1.)
       htop= hisla*SN*EW
       slope=slope+htop
       endif
       endif


       zv(i,j,nk+1)=slope
 50   CONTINUE
 40   CONTINUE

        end
```

Figure 7-3. *Demo Case, fif.f.*

```
C          PROGRAM FRACTOOLS
C
C-----This program reads and prepares fracture data for DEMO CASE
C     2003-05-10: The program is in a draft form.
C
C--- Declarations
C=================

      Parameter(nfd=20000,nfDET=4,nfLAB=46040,nfEXP=4456)
      dimension x(4,nfd),y(4,nfd),z(4,nfd)
      dimension pkvp(3,8,nfLAB),frevol(nfLAB),fwsurf(nfLAB)
      dimension storat(nfLAB),conduc(nfLAB)
      dimension diffus(nfLAB),thickn(nfLAB)


      OPEN(UNIT=70,FILE='frcset1.dat',form='unformatted')
      OPEN(UNIT=80,FILE='FRACLAB',form='unformatted')

      OPEN(UNIT=90,FILE='frcset2.dat',form='unformatted')
      OPEN(UNIT=91,FILE='FRACEXP',form='unformatted')

      OPEN(UNIT=71,FILE='zon.dat')
      OPEN(UNIT=72,FILE='FRACSITE',form='unformatted')

C---READ  FRACTURE DATA
C======================

c--deterministic
      do 11 ifr=1,nfDET
      read(71,*)
     f           x(1,ifr),y(1,ifr),z(1,ifr),x(2,ifr),y(2,ifr),
     f           z(2,ifr),x(3,ifr),y(3,ifr),z(3,ifr)

 11   continue
      close(unit=71)


c--PRINT DATA TO FILE (FOR INPUT TO DARCYTOOLS)
C==============================================

      do 10 ifr=1,nfDET

c---properties
       inhomf=0
       htknsf=10.
       frevlf=1.E-3
       fwsrff=1.
       storaf=1.E-6
       conduf=1.E-5/(2.*htknsf)
       diffuf=1.e-10

c--coordinates
       X1=x(1,ifr)
       X2=x(2,ifr)
       X3=x(3,ifr)
```

Figure 7-4. *Demo Case, fractools.f.*

```
        Y1=y(1,ifr)
        Y2=y(2,ifr)
        Y3=y(3,ifr)

        Z1=z(1,ifr)
        Z2=z(2,ifr)
        Z3=z(3,ifr)

c---write to file that can be read by FRACGEN (a triangle)
        write(72) inhomf, htknsf,frevlf,fwsrff,storaf,conduf,diffuf,
      f   X1,Y1,Z1, X2,Y2,Z2, X3,Y3,Z3,
      f   0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.
10     continue

       close(unit=72)

C--GENERATE AND PRINT TO FILE FRACTURES FOR LABORATORY VOLUME
C=============================================================
C-----This program CONVERTS FRACTURE GEOMETRY AS 4-POINTS TO
C       3-POINTS FOR INPUT TO DarcyTools

       nincl=0

       do 20 il=1,nfLAB
C---Read in data as 4-point specification
       READ(70) frevol(il),fwsurf(il),storat(il),conduc(il)
      f            ,diffus(il)
c  -first plane
        READ(70)pkvp(1,1,il),pkvp(2,1,il),pkvp(3,1,il)
        READ(70)pkvp(1,3,il),pkvp(2,3,il),pkvp(3,3,il)
        READ(70)pkvp(1,5,il),pkvp(2,5,il),pkvp(3,5,il)
        READ(70)pkvp(1,7,il),pkvp(2,7,il),pkvp(3,7,il)

c  -second plane
        READ(70)pkvp(1,2,il),pkvp(2,2,il),pkvp(3,2,il)
        READ(70)pkvp(1,4,il),pkvp(2,4,il),pkvp(3,4,il)
        READ(70)pkvp(1,6,il),pkvp(2,6,il),pkvp(3,6,il)
        READ(70)pkvp(1,8,il),pkvp(2,8,il),pkvp(3,8,il)

c-- calculate thickness
        x1p=pkvp(1,1,il)
        y1p=pkvp(2,1,il)
        z1p=pkvp(3,1,il)
        x2p=pkvp(1,2,il)
        y2p=pkvp(2,2,il)
        z2p=pkvp(3,2,il)
        thickn(il)=sqrt((x1p-x2p)**2+(y1p-y2p)**2+(z1p-z2p)**2)

c-- calculate coordinates for central plane
        x1=0.5*(pkvp(1,1,il)+pkvp(1,2,il))
        y1=0.5*(pkvp(2,1,il)+pkvp(2,2,il))
        z1=0.5*(pkvp(3,1,il)+pkvp(3,2,il))

        x2=0.5*(pkvp(1,3,il)+pkvp(1,4,il))
        y2=0.5*(pkvp(2,3,il)+pkvp(2,4,il))
        z2=0.5*(pkvp(3,3,il)+pkvp(3,4,il))
```

Figure 7-4. *Cont.*

```
       x3=0.5*(pkvp(1,5,il)+pkvp(1,6,il))
       y3=0.5*(pkvp(2,5,il)+pkvp(2,6,il))
       z3=0.5*(pkvp(3,5,il)+pkvp(3,6,il))

       x4=0.5*(pkvp(1,7,il)+pkvp(1,8,il))
       y4=0.5*(pkvp(2,7,il)+pkvp(2,8,il))
       z4=0.5*(pkvp(3,7,il)+pkvp(3,8,il))

c-- determine which fractures may be in contact with LAB-volume

c   fracture
       xmin=amin1(x1,x2,x3,x4)
       xmax=amax1(x1,x2,x3,x4)

       ymin=amin1(y1,y2,y3,y4)
       ymax=amax1(y1,y2,y3,y4)

       zmin=amin1(z1,z2,z3,z4)
       zmax=amax1(z1,z2,z3,z4)

       sizef=sqrt((xmax-xmin)**2+(ymax-ymin)**2+(zmax-zmin)**2)

       xccf=0.25*(x1+x2+x3+x4)
       yccf=0.25*(y1+y2+y3+y4)
       zccf=0.25*(z1+z2+z3+z4)

c   LAB-volume
       xmin=1250.
       xmax=1750.

       ymin=750.
       ymax=1250.

       zmin=-650.
       zmax=-250.

       sizeL=sqrt((xmax-xmin)**2+(ymax-ymin)**2+(zmax-zmin)**2)

       xccL=1500.
       yccL=1000.
       zccL=-450.

c    Distance
       dist=sqrt((xccf-xccL)**2+(yccf-yccL)**2+(zccf-zccL)**2)

c    If dist< 0.5*sizef+0.5*sizeL  include in file

       if( dist.le.(0.5*sizef+0.5*sizeL)) then
```

Figure 7-4. *Cont.*

```
       nincl=nincl+2
C---Print out as two 3-point fractures
c---properties
       inhomf=0
       htknsf=thickn(il)/2.
       frevlf=frevol(il)
       fwsrff=fwsurf(il)
       storaf=storat(il)
       conduf=conduc(il)
       diffuf=diffus(il)


c---write to file that can be read by FRACGEN (two triangles)
       write(80) inhomf, htknsf,frevlf,fwsrff,storaf,conduf,diffuf,
     f   X1,Y1,Z1, X2,Y2,Z2, X3,Y3,Z3,
     f   0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.

       write(80) inhomf, htknsf,frevlf,fwsrff,storaf,conduf,diffuf,
     f   X2,Y2,Z2, X3,Y3,Z3, X4,Y4,Z4,
     f   0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.
       endif

20    continue
      close(unit=80)
      close(unit=70)
      write(6,*) nincl,'triangular fractures in file FRACLAB'

C--GENERATE AND PRINT TO FILE FRACTURES FOR EXPERIMENTAL VOLUME
C==============================================================
C-----This program CONVERTS FRACTURE GEOMETRY AS 4-POINTS TO
C      3-POINTS FOR INPUT TO DarcyTools

      nincl=0

      do 30 il=1,nfEXP
c
C---Read in data as 4-point specification
      READ(90) frevol(il),fwsurf(il),storat(il),conduc(il)
     f           ,diffus(il)
c  -first plane
       READ(90)pkvp(1,1,il),pkvp(2,1,il),pkvp(3,1,il)
       READ(90)pkvp(1,3,il),pkvp(2,3,il),pkvp(3,3,il)
       READ(90)pkvp(1,5,il),pkvp(2,5,il),pkvp(3,5,il)
       READ(90)pkvp(1,7,il),pkvp(2,7,il),pkvp(3,7,il)

c  -second plane
       READ(90)pkvp(1,2,il),pkvp(2,2,il),pkvp(3,2,il)
       READ(90)pkvp(1,4,il),pkvp(2,4,il),pkvp(3,4,il)
       READ(90)pkvp(1,6,il),pkvp(2,6,il),pkvp(3,6,il)
       READ(90)pkvp(1,8,il),pkvp(2,8,il),pkvp(3,8,il)
```

Figure 7-4. *Cont.*

```
c-- calculate thickness
       x1p=pkvp(1,1,il)
       y1p=pkvp(2,1,il)
       z1p=pkvp(3,1,il)
       x2p=pkvp(1,2,il)
       y2p=pkvp(2,2,il)
       z2p=pkvp(3,2,il)
       thickn(il)=sqrt((x1p-x2p)**2+(y1p-y2p)**2+(z1p-z2p)**2)

c-- calculate coordinates for central plane
       x1=0.5*(pkvp(1,1,il)+pkvp(1,2,il))
       y1=0.5*(pkvp(2,1,il)+pkvp(2,2,il))
       z1=0.5*(pkvp(3,1,il)+pkvp(3,2,il))

       x2=0.5*(pkvp(1,3,il)+pkvp(1,4,il))
       y2=0.5*(pkvp(2,3,il)+pkvp(2,4,il))
       z2=0.5*(pkvp(3,3,il)+pkvp(3,4,il))

       x3=0.5*(pkvp(1,5,il)+pkvp(1,6,il))
       y3=0.5*(pkvp(2,5,il)+pkvp(2,6,il))
       z3=0.5*(pkvp(3,5,il)+pkvp(3,6,il))

       x4=0.5*(pkvp(1,7,il)+pkvp(1,8,il))
       y4=0.5*(pkvp(2,7,il)+pkvp(2,8,il))
       z4=0.5*(pkvp(3,7,il)+pkvp(3,8,il))

c-- determine which fractures may be in contact with EXP-volume

c   fracture
       xmin=amin1(x1,x2,x3,x4)
       xmax=amax1(x1,x2,x3,x4)

       ymin=amin1(y1,y2,y3,y4)
       ymax=amax1(y1,y2,y3,y4)

       zmin=amin1(z1,z2,z3,z4)
       zmax=amax1(z1,z2,z3,z4)


       sizef=sqrt((xmax-xmin)**2+(ymax-ymin)**2+(zmax-zmin)**2)

       xccf=0.25*(x1+x2+x3+x4)
       yccf=0.25*(y1+y2+y3+y4)
       zccf=0.25*(z1+z2+z3+z4)

c   Exp-volume
       xmin=1350.
       xmax=1450.

       ymin=850.
       ymax= 950.

       zmin=-500.
       zmax=-400.

       sizeL=sqrt((xmax-xmin)**2+(ymax-ymin)**2+(zmax-zmin)**2)
```

Figure 7-4. *Cont.*

```
       xccL=1400.
       yccL=900.
       zccL=-450.

c    Distance
       dist=sqrt((xccf-xccL)**2+(yccf-yccL)**2+(zccf-zccL)**2)

c    If dist< 0.5*sizef+0.5*sizeL  include in file

       if( dist.le.(0.5*sizef+0.5*sizeL)) then

       nincl=nincl+2
C---Print out as two 3-point fractures
c---properties
       inhomf=0
       htknsf=thickn(il)/2.
       frevlf=frevol(il)
       fwsrff=fwsurf(il)
       storaf=storat(il)
       conduf=conduc(il)
       diffuf=diffus(il)


c---write to file that can be read by FRACGEN (two triangles)
       write(91) inhomf, htknsf,frevlf,fwsrff,storaf,conduf,diffuf,
     f   X1,Y1,Z1, X2,Y2,Z2, X3,Y3,Z3,
     f   0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.

       write(91) inhomf, htknsf,frevlf,fwsrff,storaf,conduf,diffuf,
     f   X2,Y2,Z2, X3,Y3,Z3, X4,Y4,Z4,
     f   0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.
       endif

30    continue
      close(unit=90)
      close(unit=91)
      write(6,*) nincl,'triangular fractures in file FRACEXP'
      end
```

Figure 7-4. *Cont.*

```
          PROGRAM PROPGEN
C
C-----This program generates property files for DEMO Case,SITE
C
C    --It reads the grid coordinates from xyz
C    --It reads fracture properties as generated by FRACGEN
C    --It reads data from external data sources.
C    --It generates INDGRD, the index grid property file
C    --It generates the property files for SOLVE
C
*     Set  dimensions
*     ===============

      parameter (nid=100, njd=100, nkd=50)

      dimension xv(nid+1), yv(njd+1), zv(nid+1,njd+1,nkd+1)
      dimension conduc(nid,njd,nkd,3), diffus(nid,njd,nkd,3)
      dimension fwsurf(nid,njd,nkd), frevol(nid,njd,nkd)
      dimension storat(nid,njd,nkd),pme(nid,njd)
      dimension perm(nid,njd,nkd,3), poros(nid,njd,nkd)


C   Read Grid coordinates from file  "xyz"
C   ======================================

      open(unit=98,file='xyz',form='unformatted')
      ires= mesh_p(98,1,nii,njj,nkk,icos,ip,i1,i2,j1,j2,k1,k2)
      if(ires.ne.0) WRITE(6,*) 'GRID ERROR'
      ni=nii
      nj=njj

      nk=nkk
      ires = mesh_r(98,1,xv,yv,zv)
      if(ires.ne.0) WRITE(6,*) 'GRID ERROR'
      close(unit=98)
      WRITE(6,*) 'Read in grid'

C     Read in fracture properties from files
C     ======================================
C
C Note: -frevol is free volume in cell, not porosity
      open (unit=80, file='condx1.dat', form='UNFORMATTED')
      open (unit=81, file='condy1.dat', form='UNFORMATTED')
      open (unit=82, file='condz1.dat', form='UNFORMATTED')
      open (unit=83, file='frevol1.dat', form='UNFORMATTED')
      do 160 k=1, nk
      do 160 j=1, nj
      do 160 i=1, ni
         read(80) conduc(i,j,k,1)
         read(81) conduc(i,j,k,2)
         read(82) conduc(i,j,k,3)
         read(83) frevol(i,j,k)
160   continue

      close (unit=80)
      close (unit=81)
      close (unit=82)
      close (unit=83)
      WRITE(6,*) 'Read in Fracture properties'
```
Figure 7-5. *Demo Case, prpgen.f.*

```
C --Read in data from external sources
C   ===================================
      WRITE(6,*) 'Read in data from external sources'

C --Modify properties and prepare arrays for SOLVE
C   =============================================

C-- Generate Porosity and Permeabilities. Add min values.
      do k=1,nk
      do j=1,nj
      do i=1,ni
        vol=(xv(i+1)-xv(i))*(yv(j+1)-yv(j))*(zv(i,j,k+1)-zv(i,j,k))

      do idir=1,3
      con=conduc(i,j,k,idir)
      if(k.eq.50.and.con.lt.2.e-4) conduc(i,j,k,idir)=2.e-4
      if(k.eq.49.and.con.lt.2.e-5) conduc(i,j,k,idir)=2.e-5
      if(k.eq.48.and.con.lt.2.e-6) conduc(i,j,k,idir)=2.e-6
      if(k.eq.47.and.con.lt.2.e-7) conduc(i,j,k,idir)=2.e-7
      enddo

        perm(i,j,k,1)=conduc(i,j,k,1)*2.0387E-7+2.E-16
        perm(i,j,k,2)=conduc(i,j,k,2)*2.0387e-7+2.E-16
        perm(i,j,k,3)=conduc(i,j,k,3)*2.0387e-7+2.E-16

        poros(i,j,k)=frevol(i,j,k)/vol+1.E-6
      enddo
      enddo
      enddo

C--Fill pme array and Scale
      do j=1,nj
      do i=1,ni
         zsurf=0.25*(zv(i,j,nk+1)+zv(i+1,j,nk+1)+
     f         zv(i,j+1,nk+1)+zv(i+1,j+1,nk+1))
         rain=50.
         pme(i,j)=rain*1.E-3/(3600.*24.*365.)*1.
         if(zsurf.lt.0.) pme(i,j)=0.
      enddo
      enddo

      WRITE(6,*) 'Arrays for SOLVE ready'


C-- Generate property arrays to be read by SOLVE
C   ==========================================

      open (unit=61, file='PERMX1',  form='UNFORMATTED')
      open (unit=62, file='PERMY1',  form='UNFORMATTED')
      open (unit=63, file='PERMZ1',  form='UNFORMATTED')
      open (unit=64, file='POROS1',  form='UNFORMATTED')
      open (unit=65, file='PREME', form='UNFORMATTED')

      write(61) (perm(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
     f ,(L-1)/ni/nj+1,1), L=1,ni*nj*nk)
```

Figure 7-5. *Cont.*

```
       write(62) (perm(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
      f ,(L-1)/ni/nj+1,2), L=1,ni*nj*nk)



       write(63) (perm(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
      f ,(L-1)/ni/nj+1,3), L=1,ni*nj*nk)

       write(64) (poros(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1
      f ,(L-1)/ni/nj+1), L=1,ni*nj*nk)

       write(65) (pme(L-(L-1)/ni*ni,(L-1)/ni-(L-1)/ni/nj*nj+1)
      f , L=1,ni*nj*1)


       close (unit=61)
       close (unit=62)
       close (unit=63)
       close (unit=64)
       close (unit=65)

       WRITE(6,*) 'Generated arrays for SOLVE'

       end
```

Figure 7-5. *Cont.*

8 References

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9 Notation

Most variable names and parameters are defined in connection with the description of the related CIF command, see Section 4.

Some names are used internally (in the F-array) and thus have a special significance. For example, if a user defines an array it can not have one of these names. The reserved names are:

A, E, S, R, W, W2, W3, DT, XyP, XyS, XyT, XyCxx, RESP, RESS, REST, RESCxx, M1, M2, M3, PME, B, XV, YV, ZV, ZC, PERMz, DIFFz, TCONDz, POROS, STORA, PREF, CAPA, FLUXn, DARCY-U, DARCY-V, DARCY-W

where y=1,…,3 represents the time step index, xx=1,…,99 represents the index of the transported mass fraction, z=1,…,9 represents the properties' location and n=0,…,9 the fluxes balance indexes. When the GRWT, FRAME, TUNNEL or PARTRACK models are activated additional F sub-arrays are also automatically declared:

GWT_FILL, GWT_REF, GWT-GH, FRM_FWS, FRM_CCV, FRM_ALPHA, FRM_BETA, FRM_BETCLL, FRM_SUMC, TUN_REF, PTK_NPC, PTK_NPO, PTK_DEN, PTK_TRJX, PTK_TRJY, PTK_TRJZ, PTK_TRJT, PTK_FREVOL, PTK_FWS

These arrays are defined in Appendix B (pages 3-9), where also their position in the F-array is explained. For convinience, the major variables are summarized in Table 9-1.

It should also be pointed out that DarcyTools uses SI-units.

Table 9-1. Main variables, with explanation and units. Same notation ('*y*', '*xx*' and '*z*') as in main text is used.

Variable	Meaning	Unit
DT	the values of the present (1) and the previous (2…) time steps for time derivative evaluation when nt>0.	s
RES	the Log10 of the mean square residual of the variables. The names for accessing that array are RESP, RESS and RESxx according to the variable order.	-
X	the variables fields from 1 to nx for the present time (1) and the previous time steps (2…nt). The pressure index is fixed at 1 and the salinity index at 2. The names to access this array are X1P, X1S, X1T, X1Cxx, X2P, X2S, X2T, X2Cxx, X3P, X3S, X3T and X3Cxx, according to the numbers nx and nt.	-
M	the mass flux through the east (1), the north (2) and top (3) faces. The names to access this array are respectively M1, M2, M3.	kg/s
XV	the cell vertex X-coordinates.	m
YV	the cell vertex Y-coordinates.	m
ZV	the cell vertex Z-coordinates.	m
ZC	the cell center Z-coordinates for BFC:S case only.	m
PERMz	the permeability field defined at cell face centers. Kx-East (1), Ky-North (2) and Kz-Top (3) for all cases, Kx-Top (4) and Ky-Top (5) for BFC and BFC:s cases and Kx-North (6), Kz-North (7), Ky-East (8) and Kz-East (9) for BFC cases. The names to access this array are PERMz.	m^2
DIFFz	the diffusivity field defined at cell face centers in the same way as PERMx.	m^2/s
TCONDz	the equivalent (rock+fluid) thermal conductivity field defined at cell face centers in the same way as PERMx.	$W/m/^oC$
POROS	the porosity field.	%
PREF	the reference pressure for compaction effect.	N/m^2
STORA	the storativity field for compaction effect.	m^{-1}
CAPA	the rock thermal capacity field.	$J/kg/\,^oC$
PME	the precipitation minus evapo-transpiration on the very parent grid only.	m/s

Appendix A User Subroutines

Contents

User subroutines

Introduction

In order to provide users with programming capabilities the DarcyTools solver automatically calls some template subroutines named user's routines. All those routines are gathered into the User-Section and are initially empty. Depending on the case to run, users will be able to program one or several routines of this section.

The kernel of the setting is located into USRSET and is called at the beginning of each run. To support users in programming this routine, and because of the interdependence between some of the parameters, a Set-Section has been created that contains many routines dedicated to the parameters setting.

Several users' routines are also called during the run to provide users with a certain level of control on the computation. Those routines allow overwriting the initial parameters, the properties or the outputs.

UTIL-section

In order to help users with internal programming and data organization (i.e. with F array handling) a Util-Section gathers some utility routines that users should use for safely programming the User-Section routines.

LFNAME

This routine returns the F array index of the first element of the sub-array named *'name'* on the grid *igrd*. It allows user to safely access the any sub-array independently of the solver internal data ordering. It also applies to user's data defined by routine SETARRAY. When the sub-array is not defined on the given grid this routine returns 0.

```
*====================================================================*
*                                                                    *
*     function lfname(name,igrd)                                     *
*                                                                    *
*====================================================================*
*F90                                                                 *
*                                                                    *
*     INPUT                                                          *
*     -----                                                          *
*     name ......... array or user's variable name                   *
*     igrd ......... grid index                                      *
*                                                                    *
*====================================================================*
```

LENAME

This routine returns the length of the F sub-array named *'name'* on the grid *igrd*. In conjunction with the LFNAME routine it allows user to safely access the any sub-array independently of the solver internal data ordering. For example, the good practice for setting a property should be:

```
subroutine usrxxx(f,igrd,ni,nj,nk,...)
dimension f(*)

lstora = lfname('STORA',igrd)
nstora = lename('STORA',igrd)

if(nstora.eq.1) then

 f(lstora) = value

elseif(nstora.eq.ni*nj*nk) then

 do i=1,ni
 do j=1,nj
 do k=1,nk
  l = (i-1) + (j-1)*ni + (k-1)*ni*nj
  f(lstora+l) = val(i,j,k)
 enddo
 enddo
 enddo

else

 print *,'STORA is undefined on this grid'
 return

endif
.
.
.
end
```

When the sub-array is not defined on the given grid this routine returns 0.

```
*======================================================================*
*                                                                      *
*     function lename(name,igrd)                                       *
*                                                                      *
*======================================================================*
*F90                                                                   *
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*     name ......... array or user's variable name                     *
*     igrd ......... grid index                                        *
*                                                                      *
*======================================================================*
```

SET_xxxx

In order to save memory storage, users can store uniform properties into single element arrays instead of 3D arrays by calling the routine SETF0. Hence to free users from checking the array length when accessing properties the Util-Section implements routines with the pattern SET_xxxx where xxxx represents the property name (SET_POROS, SET_STORA, SET_PREF, SET_CAPA, SET_TCONDx, SET_PERMx, SET_DIFFx). For example, the good practice for setting a property could also be:

```
subroutine usrxxx(f,igrd,ni,nj,nk,...)
dimension f(*)

do i=1,ni
do j=1,nj
do k=1,nk
 call set_stora(i,j,k,igrd,val(i,j,k))
enddo
enddo
enddo
.
.
.
end
```

```
*======================================================================*
*                                                                      *
*     subroutine set_xxxx(i,j,k,igrd,value)                            *
*                                                                      *
*======================================================================*
* F90                                                                  *
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*     i,j,k ........ cell indexes                                      *
*     igrd ......... grid index                                        *
*     value ........ value to set                                      *
*                                                                      *
*======================================================================*
```

GET_xxxx

Like the routines SET_xxxx set properties values independently of the length of the corresponding sub-array length, the GET_xxxx functions retrieve the properties value of the cell *(i,j,k)* of the grid *igrd*. The name of those functions follows the pattern GET_xxxx where xxxx represents the property name (GET_POROS, GET_STORA, GET_PREF, GET_CAPA, GET_TCOND, GET_PERM, GET_DIFF). For example, the good practice for getting a property could be:

```
subroutine usrxxx(f,igrd,ni,nj,nk,...)
dimension f(*)

do i=1,ni
do j=1,nj
do k=1,nk
 value(i,j,k) = get_stora(i,j,k,igrd)
enddo
enddo
enddo
.
.
.
end
```

```
*==================================================================*
*                                                                  *
*     function get_xxxx(i,j,k,igrd)                                *
*                                                                  *
*==================================================================*
* F90                                                              *
*                                                                  *
*     INPUT                                                        *
*     -----                                                        *
*     i,j,k ........ cell indexes                                  *
*     igrd ......... grid index                                    *
*                                                                  *
*==================================================================*
```

When properties such as the conductivity, the permeability or the diffusivity fields are four dimensional array, the GET_xxxx function uses one argument more; namely the fourth index in the array (the x value of the names TCONDx, PERMx or DIFFx). In such a case the GET_xxxx function becomes.

```
*==================================================================*
*                                                                  *
*     function get_xxxx(i,j,k,igrd,lval)                           *
*                                                                  *
*==================================================================*
* F90                                                              *
*                                                                  *
*     INPUT                                                        *
*     -----                                                        *
*     i,j,k ........ cell indexes                                  *
*     igrd ......... grid index                                    *
*     lval ......... xxxx fourth index                             *
*                                                                  *
*==================================================================*
```

IUFREE

Since DarcyTools internally opens some logical units for input/output operations, the Util-Section implements a utility function that returns a free logical unit number (between 1 and 1000) for immediate use. Users are in charge of closing the logical unit after use. A good practice for reading a file should be:

```
subroutine usrxxx(f,igrd,ni,nj,nk,...)
dimension f(*)

iu = iufree()
if(iu.le.0) then
 print *,'No more free logical unit'
 return
endif

open(iunit=iu, fname='filename')
 read(iu,*) (val(i),i=1,ni)
close(iu)
.
.
.
end
```

IND_VAL

The DarcyTools INDGRD array contains encrypted data used for model programming and/or visual control of inputs. For each grid, INDGRD is a 3D array of indexes which break down into 9 positions (from 1 to 9). The value of each position is an integer between 0 and 9. The IND_VAL function parses any INDGRD value to extract the given position value.

```
*===================================================================*
*                                                                   *
*     function ind_val(number,ind_pos)                              *
*                                                                   *
*===================================================================*
*                                                                   *
*     INPUT                                                         *
*     -----                                                         *
*     number ....... INDGRD encrypted number                        *
*     ind_pos ...... index position                                 *
*                                                                   *
*                                                                   *
*===================================================================*
```

IND_SET

This routine encrypts the INDGRD array *(i,j,k)* index for the grid *igrd* by setting the value *ind_val* at position *ind_pos*. The validity of the routine arguments is not checked for efficiency reason and remain the responsibility of users.

```
*===================================================================*
*                                                                   *
*     subroutine ind_set(i,j,k,igrd,ind_pos,ind_val)                  *
*                                                                     *
*=====================================================================*
*F90                                                                  *
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     i,j,k ........ cell indexes of INDGRD array                     *
*     igrd ......... grid index                                       *
*     ind_pos ...... index position                                   *
*     ind_val ...... index value at position ind_pos                  *
*                                                                     *
*=====================================================================*
```

IND_GET

This function retrieves from the INDGRD array *(i,j,k)* index of the grid *igrd* the value of position *ind_pos*. The validity of the routine arguments are not checked for efficiency reason and remain the responsibility of users. Nevertheless, it returns -1 when the INDGRD array is not defined on the given grid.

```
*=====================================================================*
*                                                                     *
*     function ind_get(i,j,k,igrd,ind_pos)                            *
*                                                                     *
*=====================================================================*
*F90                                                                  *
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     i,j,k ........ cell indexes of INDGRD array                     *
*     igrd ......... grid index                                       *
*     ind_pos ...... index position                                   *
*                                                                     *
*=====================================================================*
```

USR routines

The user's routines form a set of template routines which are automatically called by the program to provide a user with control during a run. By convention all those routine names follow the pattern USRxxxxx. A first set of routines USRSET, USRINI and USRMESH are initialization routines. They are called to define the case to run. A second set of routines USRDT, USRBOSS, USRPROP, USRSLV, USRPRECO and USROUT are called from the iteration loops and give a user control all along the run. The user routines form the User-Level and are initially empty. They only need to be programmed when necessary, according to their calling sequence.

```
default setting
CIF setting
USRSET
USRMEH
USRINI
do istep = 1, nstep
   USRDT
   do itg = 1, nitg
   do igrd = lgrd,1,-1
      do sweep = 1, nsweep
         do ivar = nvar1, nvar2
            USRPROP
            build operator
            USRBOSS
            if coupled USRPRECO
            USRSLV
            solve operator
            USROUT
         enddo
         do itc = 1, nitc1
            do ivar = nvar3, nvar4
               USRPROP
               build operator
               USRBOSS
               if coupled USRPRECO
               USRSLV
               solve operator
               USROUT
            enddo
         enddo
      enddo
      do itc = 1, nitc2
         do ivar = nvar5, nvar6
            USRPROP
            build operator
            USRBOSS
            if coupled USRPRECO
            USRSLV
            solve operator
            USROUT
         enddo
      enddo
   enddo
   enddo
enddo
```

Figure 1: User's routines calling sequence

USRSET

This routine is the first user's routine called after the installation of the default setting by the main program. It is where users must define and specify the parameters of the case to run by calling several setting's routines of the Set-Section. This routine is called once and only once so that it is also the right place to declare and allocate user's arrays.

```
*======================================================================*
*                                                                      *
*     subroutine usrset()                                              *
*                                                                      *
*======================================================================*
```

USRINI

This routine is called after USRSET and USRMESH, and before starting the integration loops. It is called by the routine SETINI and dedicated to initialization. It is the place where users should overwrite the NULL field default initialization of variables. Only the previous time steps variables need to be defined here (e.g. X2P, X3P…). The current time step initial estimation is automatically set to the previous time step solution by the routine SETINI.

```
*======================================================================*
*                                                                      *
*     subroutine usrini(igrd,icos,f,ni,nj,nk,nx,nt)                    *
*                                                                      *
*======================================================================*
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*                                                                      *
*     igrd ....... grid index                                          *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)               *
*     f .......... farray                                              *
*     ni ......... number of cells in the direction x                  *
*     nj ......... number of cells in the direction y                  *
*     nk ......... number of cells in the direction z                  *
*     nx ......... number of variables in the X sub-array              *
*     nt ......... number of time steps in the X sub-array             *
*                                                                      *
*                                                                      *
*     OUPUT                                                            *
*     -----                                                            *
*                                                                      *
*     x .......... X past values (i,j,k,n,2...)                        *
*                                                                      *
*======================================================================*
```

USRMESH

This routine is automatically called from SETINI/SETMESH after the user settings. Its programming is necessary to define the grid vertex coordinates and to overwrite the default uniform Cartesian grid. These coordinates can be read from a file or computed in the routine. This routine is not called for embedded grids. The embedded grids are automatically interpolated from their parent grid by the routine EMBMESHx of Geom-Section. Therefore, if the embedded grids are needed outside of the DarcyTools solver, for example to define the property fields, users should use the same EMBMESHx routines to compute them. Because of the node-centered approach of the code, the control volumes are defined by grid cells and the number of vertexes in each direction equals the number of cells plus one. Depending on the coordinate system (icos) employed a good practice for coordinate access could be:

```
subroutine usrmesh(igrd,icos,f,igrd,ni,nj,nk,nx,nt)
dimension f(*)

lzv = lfname(‘ZV’,igrd)

if(icos.eq.3) then

 do k=1,nk+1
  f(lzv+k-1) = zv1(k)
 enddo

else

 do i=1,ni+1
 do j=1,nj+1
 do k=1,nk+1
  l = (i-1) + (j-1)*(ni+1) + (k-1)*(ni+1)*(nj+1)
  f(lzv+l) = zv3(i,j,k)
 enddo
 enddo
 enddo

endif
.
.
.
end
```

```
*=====================================================================*
*                                                                     *
*     subroutine usrmesh(igrd,icos,f,ni,nj,nk,nx,nt)                  *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*                                                                     *
*     igrd ....... grid index                                         *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)              *
*     f .......... farray                                             *
*     ni ......... number of cells in the direction x                 *
*     nj ......... number of cells in the direction y                 *
*     nk ......... number of cells in the direction z                 *
*     nx ......... number of variables in the X sub-array             *
*     nt ......... number of time steps in the X sub-array            *
*                                                                     *
*                                                                     *
*     OUPUT                                                           *
*     -----                                                           *
*                                                                     *
*     xv ......... new x-coordinates of grid nodes                    *
*     yv ......... new y-coordinates of grid nodes                    *
*     zv ......... new z-coordinates of grid nodes                    *
*                                                                     *
*=====================================================================*
```

USRDT

This routine is called at the beginning of every time step calculation and gives the opportunity to change the current time step during the integration process. The new value is saved into the F array and becomes the default value for next time steps.

```
*=====================================================================*
*                                                                     *
*     subroutine usrdt(dt)                                            *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*                                                                     *
*     dt ......... current time step                                  *
*                                                                     *
*                                                                     *
*     OUPUT                                                           *
*     -----                                                           *
*                                                                     *
*     dt ......... new current time step                              *
*                                                                     *
*=====================================================================*
```

USRBOSS

This routine is fundamental in that it fixes the boundary conditions and source/sink terms for each variable. It is called by VARSOL after the discretisation of the equations, the embedded grid exchange boundary conditions and the automatic source/sink terms computation. When no automatic boundary conditions are specified, not programming this routine leads to no particular boundary conditions and to the NULL field solution. The boundary and source/sink conditions are expected to take the following form $S=Q_{src}-Q_{phi}f$ where Q_{src} is added to the source term of the algebraic operator and Q_{phi} is implicated by addition to the central coefficient (f represents the current value of the variable). For stability reason, Q_{phi} must be a positive value. When boundary conditions are time dependent, the current time value can be retrieve from common /const3/.

```
*=====================================================================*
*                                                                     *
*     subroutine usrboss(ivar,igrd,icos,f,qsrc,qphi,ni,nj,nk,nx,nt)    *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*                                                                     *
*     ivar ....... variable index                                     *
*     igrd ....... grid index                                         *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)              *
*     f .......... farray                                             *
*     qsrc ....... automatic explicit source term                     *
*     qphi ....... automatic implicit source term S = Qsrc - Qphi*PHI  *
*     ni ......... number of cells in the direction x                  *
*     nj ......... number of cells in the direction y                  *
*     nk ......... number of cells in the direction z                  *
*     nx ......... number of variables in the X sub-array              *
*     nt ......... number of time steps in the X sub-array             *
*                                                                      *
*                                                                      *
*     OUPUT                                                            *
*     -----                                                            *
*                                                                      *
*     qsrc ....... explicit source term                                *
*     qphi ....... implicit source term S = Qsrc - Qphi*PHI            *
*                                                                      *
*======================================================================*
```

Default *(DEFBC)* and automatic boundary *(SETBOSS)* conditions are applied before calling this routine so that they can be overwritten. When programming USRBOSS the *F* sub-arrays *W* and *W2* must not be used since they temporarily contain Q_{src} and Q_{phi}.

USRPROP

This routine is dedicated to user's modifications of physical properties such as conductivity, porosity or diffusivity fields. It is called at the very beginning of the routine VARSOL so that the properties can be changed before forming the algebraic equations. Because properties sub arrays are either one element long or 3D arrays, a good practice consists in checking the sub-array length or in using the SET_XXXX routines of Util-Section.

```
*======================================================================*
*                                                                      *
*     subroutine usrprop(ivar,igrd,icos,f,ni,nj,nk,nx,nt)              *
*                                                                      *
*======================================================================*
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*                                                                      *
*     ivar ....... variable index                                      *
*     igrd ....... grid index                                          *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)               *
*     f .......... farray                                              *
*     ni ......... number of cells in the direction x                  *
*     nj ......... number of cells in the direction y                  *
*     nk ......... number of cells in the direction z                  *
*     nx ......... number of variables in the X sub-array              *
*     nt ......... number of time steps in the X sub-array             *
*                                                                      *
*                                                                      *
*     OUPUT                                                            *
*     -----                                                            *
*                                                                      *
*     permea ..... new permeability field                              *
*     diffco ..... new diffusivity field                               *
*     poros ...... new porosity field                                  *
*     stora ...... new storativity field                               *
*     capa ....... new thermal capacity field                          *
*     etc.                                                             *
*                                                                      *
*======================================================================*
```

USRSLV

This routine is called just before calling MIGAL and is dedicated to the adaptation of the solver parameters depending on the current solution, grid, or iteration. To transmit parameters to MIGAL the routine SOLVE first load the parameters contained in the PDEF array and resulting of default or initial user's setting. Then it calls USRSLV and retrieves the new parameters from the common /solve1/. The new parameters are not saved into the PDEF array so that they are only temporarily changed. Because some parameters like IGMRES or NBGRID influence the F array size, the new values will be retained only if they lead to less memory requirement than the initial values.

```
*======================================================================*
*                                                                      *
*     subroutine usrslv(igrd,ivar,nv,icas)                             *
*                                                                      *
*======================================================================*
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*                                                                      *
*     igrd ....... grid index                                          *
*     ivar ....... variable index                                      *
*     nv ......... trigger of coupling (1=uncoupled, 2=coupled)        *
*     icas ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)               *
*     /solve1/ ... default or user defined MIGAL's parameters          *
*                                                                      *
*                                                                      *
*     OUPUT                                                            *
*     -----                                                            *
*                                                                      *
*     /solve1/ ... new MIGAL's parameters                              *
*                                                                      *
*======================================================================*
```

USROUT

This routine is called by the main program before starting integration loops and after every MIGAL's call. It is the right place for saving solution or to printing out convergence progress. The very moment of its call can be retrieved by the analysis of the loop indexes of common /const3/. *Ivar* is null during the initialization call.

```
*======================================================================*
*                                                                      *
*     subroutine usrout(ivar,igrd,icos,f,ni,nj,nk,nx,nt)               *
*                                                                      *
*======================================================================*
*                                                                      *
*     INPUT                                                            *
*     -----                                                            *
*                                                                      *
*     ivar ....... variable index                                   *
*     igrd ....... grid index                                       *
*     icos ....... kind of grid (1=BFC, 2=BFC:s, 3=CART)            *
*     f .......... farray                                           *
*     ni ......... number of cells in the direction x               *
*     nj ......... number of cells in the direction y               *
*     nk ......... number of cells in the direction z               *
*     nx ......... number of variables in the X sub-array           *
*     nt ......... number of time steps in the X sub-array          *
*                                                                   *
*===================================================================*
```

USRPRECO

This routine is called by the VARSOL routine for the coupled algorithm after the construction and the automatic preconditioning of the correction operator and before the call of MIGAL. It provides users with the capability of preconditioning the operator before solving the correction fields.

```
*===================================================================*
*                                                                   *
*     subroutine usrpreco(a,x,s,nt,nx,ni,nj,nk,nv,npts)             *
*                                                                   *
*===================================================================*
*                                                                   *
*     INPUT                                                         *
*     -----                                                         *
*                                                                   *
*     a .......... correction operator ready for MIGAL              *
*     x .......... current X array                                  *
*     s .......... residuals (sources the correction operator)      *
*     nt ......... number of time steps in the X array              *
*     nx ......... number of variables in the X array               *
*     ni ......... number of cells in the direction x               *
*     nj ......... number of cells in the direction y               *
*     nk ......... number of cells in the direction z               *
*     nv ......... trigger of coupling (1=uncoupled, 2=coupled)     *
*     npts ....... number of neighbors in the scheme                *
*                                                                   *
*                                                                   *
*     OUPUT                                                         *
*     -----                                                         *
*                                                                   *
*     a .......... preconditioned operator                          *
*     s .......... preconditioned sources terms                     *
*                                                                   *
*===================================================================*
```

MIGAL routines

DarcyTools uses the MIGAL multi-grid solver to solve the successive algebraic sets of equations resulting from discretisation. Among its features this solver offers the possibility of programming several routines for efficiency control, namely SETRELAX and SETDOMI.

SETRELAX

This routine is called by MIGAL before any smoother's run on any grid level to give the opportunity to control the number of relaxations as well as the relaxation factor, depending on the grid level and on the kind of smoothing to proceed (i.e. pre-restriction or post-prolongation). For sharply varying conductivities or diffusivities, it is recommended to minimally reduce (even to 0) the number of pre-restriction relaxations.

```
*=====================================================================*
*                                                                     *
*     subroutine setrelax(igr, nbrelax, relax)                        *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*                                                                     *
*     igr ........ grid level from 1=fine to NBGRID=coarse            *
*                    igr<0 <=> pre-restriction relaxations            *
*                    igr>0 <=> post-prolongation relaxations          *
*     nbrelax .... number of relaxations from MIGAL                   *
*     relax ...... relaxation coefficient from MIGAL                  *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*                                                                     *
*     nbrelax .... new number of relaxations to be done               *
*     relax ...... new relaxation coefficient                         *
*                                                                     *
*                                                                     *
*=====================================================================*
```

SETDOMI

For sake of robustness and in order to increase its smoother (ILU0) efficiency MIGAL does not directly solve the operator but a defect correction operator with increased diagonal dominance:

$$(A_F + D)dx_F = S_F - A_F x_F \qquad (1)$$

where D is a diagonal matrix proportional to the central diagonal of the operator:

$$D_i = \left(\frac{1-g}{g}\right)a_{Pi} \qquad (2)$$

By default the parameter g equals relaxation parameter of the smoother. Nevertheless users can control the amount of artificial diagonal dominance by programming the routine SETDOMI. This routine is called once by MIGAL before the operator restriction.

```
*=====================================================================*
*                                                                     *
*     subroutine setdomi(igr, gamma)                                  *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*                                                                     *
*     igr ........ grid level from 1=fine to NBGRID=coarse            *
*     gamma ...... artificial diagonal dominance from MIGAL           *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*                                                                     *
*     gamma ...... artificial diagonal dominance Ap->Ap/gamma         *
*                  must be srtictly positive, gamma=1 => nothing done *
*                                                                     *
*                                                                     *
*=====================================================================*
```

GEOM routines

Some routines of the Geom-section are also of user interest for programming inside or outside the USRxxx routines. They are dedicated to grid generation and to read and write the mesh files when needed.

MESH_P

This function reads the specified grid *igrd* parameters on the open logical unit *iu*. It returns -1 when the reading operation fails or when the given grid does not exist in the file. This routine does not open nor close the file and firstly try to read from the current position before rewinding the file during grid finding operation. When the grid parameters are read, the current file index position is reset to the beginning of the parameters line in order to improve the efficiency of data reading when a call to MESH_P is followed by the corresponding MESH_R call for the retrieval of coordinates.

```
*=====================================================================*
*                                                                     *
*     function mesh_p(iu,igrd, ni,nj,nk,icos,ip,i1,i2,j1,j2,k1,k2)    *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     iu ........... open logical unit on grid file (unformatted)     *
*     igrd ......... grid index                                       *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ni,nj,nk ..... number of cells per direction                    *
*     icos ......... kind of grid 1=BFC, 2=BFC:s, 3=CART              *
*     ip ........... parent grid index                                *
*     i1,i2,.,k2 ... footprint on parent grid                         *
*     mesh_p ....... reading status  0 = ok                           *
*                                   -1 = error                        *
*                                                                     *
*=====================================================================*
```

MESH_R

This function reads the specified grid *igrd* on the open logical unit *iu* and fills the cell vertex coordinates arrays *Xv*, *Yv* and *Zv*. It returns -1 when the reading operation fails or when the given grid does not exist in the file. This routine does not open nor close the file and firstly try to read from the current position before rewinding the file during grid finding operation. No dimension checking is performed on the coordinate arrays. Hence users are in charge of the proper allocation e.g. by calling MESH_P before.

```
*=====================================================================*
*                                                                     *
*     function mesh_r(iu,igrd,xv,yv,zv)                               *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     iu ........... open logical unit on grid file (unformatted)     *
*     igrd ......... grid index                                       *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     xv,yv,zv ..... coordinates arrays                               *
*     mesh_r ....... reading status  0 = ok                           *
*                                   -1 = error                        *
*                                                                     *
*=====================================================================*
```

MESH_W

This function writes the specified grid *igrd* cell vertex coordinates arrays *Xv*, *Yv* and *Zv* on the open logical unit *iu*. It returns -1 when the writing operation fails. This routine does not open nor close the file.

```
*=====================================================================*
*                                                                     *
*     function mesh_w(iu,igrd,xv,yv,zv,ni,nj,nk,icos,ip,i1,i2,        *
*                     j1,j2,k1,k2)                                    *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     iu .......... open logical unit on grid file (unformatted)      *
*     igrd ........ grid index                                        *
*     xv,yv,zv ..... coordinates arrays                               *
*     ni,nj,nk ..... number of cells per direction                    *
*     icos ........ kind of grid 1=BFC, 2=BFC:s, 3=CART               *
*     ip .......... parent grid index                                 *
*     i1,i2,.,k2 ... footprint on parent grid                         *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     mesh_w ....... writing status  0 = ok                           *
*                                   -1 = error                        *
*                                                                     *
*=====================================================================*
```

IZN1

This function fills a 1D distribution array from *i=i1* to *i=i2* with a hyperbolic tangent distribution such that *s(i1)=s1*, *s(i2)=s2* and with initial steps that *d1=s(i1+1)-s(i1)* and *d2=s(i2)-s(i2-1)*. This function returns a status error which is negative when problems occurred during the distribution generation.

```
*=====================================================================*
*                                                                     *
*     function izn1(s,s1,s2,d1,d2,i1,i2)                              *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     s1 .......... first  abscissa                                   *
*     s2 .......... second abscissa                                   *
*     d1 .......... first  distance d1=s(i1+1)-s(i1)                  *
*     d2 .......... second distance d2=s(i2)-s(i2-1)                  *
*     i1 .......... index of first  point                             *
*     i2 .......... index of second point                             *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     s ........... abscissa array                                    *
*     izn1 ........ error status <0 when not converged                *
*                                                                     *
*=====================================================================*
```

IZN2

This function fills a one dimensional uniform distribution array from *i=i1* to *i=i2*. *s(i) = s1 + (s2-s1)*(i-i1)/(i2-i1)*. This function returns *-1* when *i2=i1*.

```
*=====================================================================*
*                                                                     *
*     function izn2(s,s1,s2,i1,i2)                                    *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     s1 ........... first  abscissa                                  *
*     s2 ........... second abscissa                                  *
*     i1 ........... index of first  point                            *
*     i2 ........... index of second point                            *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     s ............ abscissa array                                   *
*     izn2 ......... error status <0 when not ok                      *
*                                                                     *
*=====================================================================*
```

IZN3

This function fills a one dimensional distribution array from *i=i1* to *i=i2* with a hyperbolic tangent distribution such that *s(i1)=s1*, *s(i2)=s2* and with a initial step *d1=s(i1+1)-s(i1)*. This function returns a status error which is negative when problems occurred during the distribution generation.

```
*=====================================================================*
*                                                                     *
*     function izn3(s,s1,s2,d1,i1,i2)                                 *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     s1 ........... first  abscissa                                  *
*     s2 ........... second abscissa                                  *
*     d1 ........... first  distance d1=s(i1+1)-s(i1)                 *
*     i1 ........... index of first  point                            *
*     i2 ........... index of second point                            *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     s ............ abscissa array                                   *
*     izn3 ......... error status <0 when not converged               *
*                                                                     *
*=====================================================================*
```

IZN4

This function computes the geometrical ratio of the abscissa series from s1 to s3 such that *s(i+1)=s(i)+r*(s(i)-s(i-1))* with *s(i1)=s1*, *s(i2)=s2* and *s(i3)=s3*. Then it fills the s array from i1 to i3 with:

```
s(i) = s1 + (s3-s1) * (1-r**(i-i1)) / (1-r**(i3-i1))
```

```
*=====================================================================*
*                                                                     *
*     function izn4(s,s1,s2,s3,i1,i2,i3)                              *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     s1 ........... first  abscissa                                  *
*     s2 ........... second abscissa                                  *
*     s3 ........... third  abscissa                                  *
*     i1 ........... index of first  point                            *
*     i2 ........... index of second point                            *
*     i3 ........... index of third  point                            *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     s ............ abscissa array                                   *
*     izn4 ......... error status <0 when not converged               *
*                                                                     *
*=====================================================================*
```

IXDIST

This routine fills a one dimensional distribution array following three zones. The first zone sets a (hyperbolic) tangent distribution of n1 cells between x0 and x1. The expansion (contraction) is computed to fit an n1+1 cell size d=(x2-x1)/n2. When n2=0 the first zone is a uniform distribution zone. The second zone set n2 constant size cells between x1 and x2 when n1>0 and between x0 and x2 when n1=0. The third zone is a (hyperbolic) tangent distribution of n3 cells between x2 and x3 when n2>0. The expansion (contraction) is computed to fit an n1+n2 cell size d=(x2-x1)/n2. When n2=0 the third zone is a uniform distribution zone between x1 and x3 if n1>0 or between x0 and x3 if n1=0.

```
*=====================================================================*
*                                                                     *
*     function ixdist(x,x0,x1,x2,x3,n1,n2,n3)                         *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     x0 ........... west abscissa (node 1)                           *
*     x1 ........... west abscissa of zone 2 (node n1+1)              *
*     x2 ........... east abscissa of zone 2 (node n1+n2+1)           *
*     x3 ........... east abscissa (node n1+n2+n3+1)                  *
*     n1 ........... number of cells in zone 1                        *
*     n2 ........... number of cells in zone 2                        *
*     n3 ........... number of cells in zone 3                        *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     x ............ coordinate array                                 *
*     ixdist ....... error status =0 when ok                          *
*                                                                     *
*=====================================================================*
```

IZDIST

This routine fills a one dimensional $Zv_{ij}(k)$ distribution array following four zones. The first zone sets a user distribution of *n1* cells from top by cell sizes *d1* i.e. *d1(i)=z(n-i+1)-z(n-i)* with n=n1+n2+n3+n4. The second zone sets a (hyperbolic) tangent distribution of n2 cells between z(n-n1+1) and z2. The expansion (contraction) is computed to fit the n-n1+1 cell size and an n-n1-n2 cell size d=(z2-z3)/n3 when n3>0 or d=(z2-z4)/n4 when n3=0 and n4>0. When n1=0 or n3=n4=0 the expansion (contraction) is only one side constraint and when n1=n3=n4=0 the distribution is uniform between z0 and z2. The third zone is a uniform cell spacing zone of n3 cells between z(n-n2-n1+1) and z3. The fourth zone sets a (hyperbolic) tangent distribution of n4 cells between z(n-n1-n2-n3+1) and z4. The expansion (contraction) is computed to fit the n-n1-n2-n3+1 cell size when n1+n2+n3>0. The fourth zone is uniformly spanned between z0 and z4 when n1=n2=n3=0.

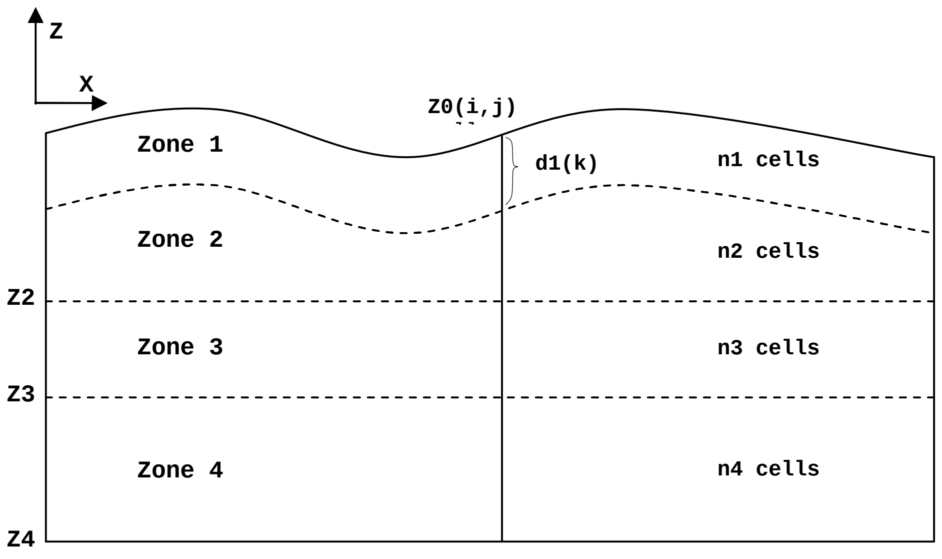

Figure 2 : IZDIST zone labelling

This function returns a status error which is negative when problems occurred during the distribution generation.

```
*=====================================================================*
*                                                                     *
*     function izdist(z,z0,n1,d1,n2,z2,n3,z3,n4,z4)                   *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     z0 ........... top abscissa (node n1+n2+n3+n4+1)                *
*     n1 ........... number of cells in zone 1                        *
*     d1 ........... array of cell sizes in zone 1 (when n1>0)         *
*     n2 ........... number of cells in zone 2                          *
*     z2 ........... abscissa of node n3+n4+1 (when n2>0)               *
*     n3 ........... number of cells in zone 3                          *
*     z3 ........... abscissa of node n4+1 (when n3>0)                  *
*     n4 ........... number of cells in zone 4                          *
*     z4 ........... bottom abscissa (node 1) (when n4>0)               *
*                                                                       *
*                                                                       *
*     OUTPUT                                                            *
*     ------                                                            *
*     z ............ z-coordinate array                                 *
*     izdist ....... error status <0 when not converged                 *
*                                                                       *
*=======================================================================*
```

DTDIST

This function computes discrete distribution t(*i*) of the variable t and returns the step size dt=t(*i+1*)-t(*i*) with *i* such as t(*i+1*)=t<t(*i*). The t distribution follows a three zone set. Inside the first zone when nt1>0 and t<t1 this function returns the value dt=t1/nt1 corresponding to a uniform distribution between 0 and t(n1+1)=t1. Inside the second zone, when nt2>0 and t<t2 the distribution is a (hyperbolic) tangent distribution of nt2 steps between t(n1+1) and t2. When n1>0 the expansion (contraction) is computed to fit t(n1+1)-t(n1)=t1/n1 and t(n1+n2+2)-t(n1+n2+1)=dt3. When n1=0 the expansion (contraction) is only one side constrained. In all the other cases this function returns dt3.

```
*=======================================================================*
*                                                                       *
*     function dtdist(t,t1,t2,nt1,nt2,dt3)                              *
*                                                                       *
*=======================================================================*
*                                                                       *
*     INPUT                                                             *
*     -----                                                             *
*     t ............ current time (begining of time step)               *
*     t1 ........... upper limit for zone 1                             *
*     t2 ........... upper limit for zone 2                             *
*     nt1 .......... number of time step in zone 1                      *
*     nt2 .......... number of time step in zone 2                      *
*     dt3 .......... default time setp (zone 3 or error in zone 1-2)    *
*                                                                       *
*                                                                       *
*     OUTPUT                                                            *
*     ------                                                            *
*     dtdist ....... time setp for time t                               *
*                                                                       *
*=======================================================================*
```

TEC routines

Beside the collection of routines SETxxxx of the Set-Section that users can apply for programming the user subroutines, some more specific and low level routines are also available for output purpose. Theses routines named TEC_xxx are gathered into the IO-Section and concern the creation of Tecplot data set files. They are written in Fortran 77 with no commons and can be used as an additional library for external post processing programs. To write a Tecplot data set files with the TEC_xxx routines one must call them in a specific order. The correct sequence is as follows:

```
TEC_INI
   TEC_ZNE
      TEC_BLK
      .
      .
      .
      TEC_BLK
   TEC_ZNE
      TEC_BLK
      .
      .
      .
      TEC_BLK
   TEC_ZNE
      TEC_BLK
      .
      .
      .
      TEC_BLK
   .
   .
   .
TEC_END
```

Figure 3 : TEC_xxx calling sequence

where the number of zones is not fixed and where the number of blocks must match the number of variables. To exchange data and to keep the history of the calling sequence the TEC_xxx routines use two INTEGER arrays namely FTEC and ZTEC and one REAL array BTEC, whose sizes need to be respectively 4 and 10 and 2.

FTEC(1)	iunit	locical unit number of the opened file
FTEC(2)	isgrid	kind of mesh (0=no mesh, 1=cell centers, 2=cell vertexes)
FTEC(3)	lastzone	last zone written in the file for duplicating information
FTEC(4)	isbin	format of output file (1=BINARY, 0=ASCII)

ZTEC(1)	nbcall	counter for zone naming
ZTEC(2)	i1	lower bound of the outputs in x direction
ZTEC(3)	i2	upper bound of the outputs in x direction
ZTEC(4)	ifr	increment value of outputs in x direction
ZTEC(5)	j1	lower bound of the outputs in y direction
ZTEC(6)	j2	upper bound of the outputs in y direction
ZTEC(7)	jfr	increment value of the outputs in x direction
ZTEC(8)	k1	lower bound of the outputs in z direction
ZTEC(9)	k2	upper bound of the outputs in z direction
ZTEC(10)	kfr	increment value of outputs in z direction
BTEC(1)	iaction	kind of action to be performed on data before output
BTEC(2)	vaction	parameter of the specified action if any

FTEC(3) as well as ZTEC(1) are internally maintained by the calling sequence. The former FTEC(3) doesn't need to be set by users while the latter ZTEC(1) should be initialize to 0.

The TEC_XXX routines call the TECXXX routines of the TECPLOT library when binary option is selected. Hence, any program using the TEC_XXX routines, must be linked either to the TECIO.LIB file (for windows) or to the TECIO.A file (for linux). Moreover, for compatibility reason, the TEC_XXX routines include a TECIO.FOR file provided with the TECPLOT package for windows. Under LINUX the TECIO.FOR file must be an empty file.

TEC_INI

When FTEC(4)=0 this routine opens a new ASCII file, given a free logical unit FTEC(1) and the file name *fname*. When FTEC(4)=1 this routine opens a new binary TECPLOT file given the file name *fname* and return the file TECPLOT index in FTEC(1). This routine also writes the title and variable names vlist strings in the opened file. When FTEC(2) differs from 0 the "X Y Z" names are automatically added first. The number of variables specified in the TEC_VAR arguments will have to correspond exactly to the number of TEC_BLK calls in the sequence. The file stays open during all the TEC_xxx calling sequence until TEC_END. The last zone value FTEC(3) is initialized to 0.

```
*=====================================================================*
*                                                                     *
*     subroutine tec_ini(ftec,fname,title,vlist,ierr)                 *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     ftec ......... file parameters                                  *
*     fname ........ name (including path) of the file to create      *
*     title ........ title of the data set (max 70 characters)        *
*     vlist ........ list of variable names separated by space        *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ierr ......... error indicator (0 when successful)              *
*                                                                     *
*=====================================================================*
```

TEC_ZNE

This routine first adds the TECPLOT zone statement to the data set. Then the TECPLOT XYZ mesh is automatically added or declared DUPLICATE when izne differs from FTEC(3). When FTEC(2)=1 the mesh is computed from xv, yv and zv to be located at cell centers. When FTEC(2)=2 the mesh coincides with the DarcyTools grid. Finally when FTEC(2)=0 no mesh is added after the zone statement. ZTEC(1) is incremented by one in this routine.

```
*=====================================================================*
*                                                                     *
*     subroutine tec_zne(izne,ftec,ztec,xv,yv,zv,w,ni,nj,nk,icos,ierr) *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     izne ......... index of zone                                    *
*     ftec ......... file parameters                                  *
*     ztec ......... zone parameters                                  *
*     xv,yv,zv ..... grid nodes coordinates                           *
*     w ........... work array at least (ni+1)*(nj+1)*(nk+1) long     *
*     ni,nj,nk ..... number of cells in x,y and z directions          *
*     icos ......... kind of grid (0=TRJ, 1=BFC, 2=BFC:s, 3=CART)     *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ierr ......... error indicator (0 if successful)                *
*                                                                     *
*=====================================================================*
```

This routine automatically names the zone with the following pattern Zxxx-yyyy, where xxx represents the zone index izne and where yyyy represents the nbcall=ZTEC(1) value for the zone.

When ICOS=0 the routine writes a “trajectory” zone statement to the data set. A trajectory statement is a I-ORDERED statement whose length is NI so that the mesh becomes a line whose points coordinates are given by xv(i), yv(i) and zv(i) with i=1 to i=ni. The trajectory zone statements are named following the pattern TRJ-xxxxxx.

TEC_BLK

This routine is in charge of writing a block of data to the TECPLOT data set. It must be called for each variable after a TEC_ZNE call in order to complete a zone description. Before outputs the data may be modified depending on the BTEC values. When BTEC(1)=0 no action is performed. When BTEC(1)=1 the value BTEC(2) is added to VAL. When BTEC(1)=2 the array VAL is multiplied by BTEC(2). When BTEC(1)=3 the decimal logarithm of VAL is outputted and BTEC(2) is unused. Finally when BETC(1)=4 the natural logarithm of VAL is outputted and BTEC(2) is unused.

```
*=====================================================================*
*                                                                     *
*     subroutine tec_blk(ftec,ztec,btec,val,w,ni,nj,nk,ierr)          *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     ftec ......... file parameters                                  *
*     ztec ......... zone parameters                                  *
*     btec ......... action parameters                                *
*     val .......... array to output                                  *
*     w ............ work array at least ni*nj*nk long                *
*     ni,nj,nk ..... array's dimensions                               *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ierr ......... error indicator (0 if successful)                *
*                                                                     *
*=====================================================================*
```

TEC_END

This routine closes the file and frees the logical unit FTEC(1) of ASCII files.

```
*=====================================================================*
*                                                                     *
*     subroutine tec_end(ftec,ierr)                                   *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     ftec ......... file parameters                                  *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ierr ......... error indicator (0 if successful)                *
*                                                                     *
*                                                                     *
*=====================================================================*
```

Example program

This section lists an example program written in Fortran 77 which demonstrates how to use of the TEC_xxx routines to write a Tecplot data set.

```
*======================================================================*
*======================================================================*
*======================================================================*
*===========                                              ============*
*===========                                              ============*
*===========                  DARCYTOOLS                  ============*
*===========                                              ============*
*===========              TEC writing sample              ============*
*===========                                              ============*
*===========                                              ============*
*======================================================================*
*======================================================================*
*======================================================================*
*
      program writetec

      parameter (ni=10, nj=10, nk=10, nx=3, nt=10, ns=11*nx)

      character *(ns) sname
      integer   ftec(4), ztec(10)
      dimension xv(ni+1), yv(nj+1), zv(nk+1), x(ni,nj,nk,nx,nt)
      dimension w(ni+1,nj+1,nk+1), btec(2)

*     prepare some data

      hx = 1.
      hy = 2.
      hz = 3.

      icos = 3

      do i=1,ni+1
       xv(i) = hx * (i-1)
      enddo

      do j=1,nj+1
       yv(j) = hy * (j-1)
      enddo

      do k=1,nk+1
       zv(k) = hz * (k-1)
      enddo

      do i=1,ni
      do j=1,nj
      do k=1,nk
      do l=1,nx
      do m=1,nt
       x(i,j,k,l,m) = i+j+k+l+m
      enddo
      enddo
      enddo
      enddo
      enddo

*     prepare the variable names string

      do i=1,nx
       j=1+(i-1)*11
       write(sname(j:j+10),'(A5,I5.5,A1)') 'MyVar',i,' '
      enddo

*     set the file unit

      ftec(1) = 15
```

```
*     set mesh as cell centered

      ftec(2) = 1

*     set an ASCII file

      ftec(4) = 0

*     open the file

      ierr = 1
      call TEC_INI(ftec,"MyFile.plt","The Title",sname,ires)
      if(ires.ne.0) goto 999

*     prepare one zone definition

      izone = 1

      ztec(1) = 0

      ztec(2)  = 1
      ztec(3)  = ni
      ztec(4)  = 1

      ztec(5)  = 1
      ztec(6)  = nj
      ztec(7)  = 1

      ztec(8)  = 1
      ztec(9) = nk
      ztec(10) = 1

*     prepare action on data

      btec(1) = 0
      btec(2) = 0

*     write data

      do it = 1,nt

       ierr = 2
       call TEC_ZNE(izone,ftec,ztec,xv,yv,zv,w,ni,nj,nk,icos,ires)
       if(ires.ne.0) goto 999

       do iv=1,nx

        ierr = 3
        call TEC_BLK(ftec,ztec,btec,x(1,1,1,iv,it),w,ni,nj,nk,ires)
        if(ires.ne.0) goto 999

       enddo

      enddo

*     close the file

      ierr = 4
      call TEC_END(ftec,ires)
      if(ires.ne.0) goto 999

*     errors printouts

      goto 1000
 999  write(*,*)
      write(*,*) '************************************************'
      write(*,*) '*                 FATAL ERROR                  *'
      write(*,*) '************************************************'
      write(*,*)
      if(ierr.eq.1)  write(*,*) 'TEC_INI failed :',ires
      if(ierr.eq.2)  write(*,*) 'TEC_ZNE failed :',ires
      if(ierr.eq.3)  write(*,*) 'TEC_BLK failed :',ires
      if(ierr.eq.4)  write(*,*) 'TEC_END failed :',ires
      write(*,*)
      stop

 1000 pause
      end
```

ROF routines

Beside the collection of routines SETxxxx of the Set-Section that users can apply for programming the user subroutines, some more specific and low level routines are also available for ROF reading and writing purposes.

```
ROF_INI


ROF_GRD
.
.
.
ROF_GRD


ROF_TIM
   ROF_NAM
   ROF_VAL
   .
   .
   .
   ROF_NAM
   ROF_VAL

ROF_TIM
   ROF_NAM
   ROF_VAL
   .
   .
   .
   ROF_NAM
   ROF_VAL

ROF_TIM
   ROF_NAM
   ROF_VAL
   .
   .
   .
   ROF_NAM
   ROF_VAL
.
.
.
```

Figure 4 : ROF_xxx calling sequence

Theses routines named ROF_xxx are gathered into the IO-Section and concern the data handling of the unformatted Result Output File (ROF). They are written in Fortran 77 with no commons and can be used as an additional library for external post processing programs. To read/write a ROF file with the ROF_xxx routines one must call them in a specific order. The correct sequence is depicted on Figure 4.

ROF_INI

This routine reads/writes the ROF header. This header tries to uniquely define the DarcyTools run by the DarcyTools version number, the date and time of the first execution, a title and the number of grids involved. This routine doesn't open the file but works on an unformatted file already open. The title is a 256 characters long string. The date is a 19 characters long string formatted as follows "yyy-mm-dd hh:mm:ss". The version is a 10 characters long string.

```
*=====================================================================*
*                                                                     *
*     subroutine rof_ini(io,iu,ierr,title,date,version,lgrd)          *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     io ........... read/write switch (0=read, 1=write)              *
*     iu ........... opened unformatted file unit                     *
*     title ........ title of the run (io=1)                          *
*     date ......... date of the run (io=1)                           *
*     version ...... DarcyTools version of the run (io=1)             *
*     lgrd ......... number of grids (io=1)                           *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ierr ......... error indicator (0 if successful)                *
*     title ........ title of the run (io=0)                          *
*     date ......... date of the run (io=0)                           *
*     version ...... DarcyTools version of the run (io=0)             *
*     lgrd ......... number of grids (io=0)                           *
*                                                                     *
*=====================================================================*
```

ROF_GRD

This routine reads/writes the grid definitions. A grid definition is an 11 integers long array organized as follows: (ni, nj, nk, icas, ip, i1, i2, j1, j2, k1, k2).

```
*====================================================================*
*                                                                    *
*     subroutine rof_grd(io,iu,ierr,igrdef)                          *
*                                                                    *
*====================================================================*
*                                                                    *
*     INPUT                                                          *
*     -----                                                          *
*     io ........... read/write switch (0=read, 1=write)             *
*     iu ........... opened unformatted file unit                    *
*     igrdef ....... grid definition array (io=1)                    *
*                                                                    *
*                                                                    *
*     OUTPUT                                                         *
*     ------                                                         *
*     ierr ......... error indicator (0 if successful)               *
*     igrdef ....... grid definition array (io=0)                    *
*                                                                    *
*====================================================================*
```

ROF_TIM

This routine reads/writes the time header statement. This statement contains the istep values of the data, the corresponding time as well as the number of variables that will follow. If this routine returns IERR=1 after a reading operation it means that the end of the file was reached.

```
*====================================================================*
*                                                                    *
*     subroutine rof_tim(io,iu,ierr,istep,t,nbvar)                   *
*                                                                    *
*====================================================================*
*                                                                    *
*     INPUT                                                          *
*     -----                                                          *
*     io ........... read/write switch (0=read, 1=write)             *
*     iu ........... opened unformatted file unit                    *
*     istep ........ step index (io=1)                               *
*     t ............ time (io=1)                                     *
*     nbvar ........ number of variable to follow (io=1)             *
*                                                                    *
*                                                                    *
*     OUTPUT                                                         *
*     ------                                                         *
*     ierr ......... error indicator (0 if successful)               *
*     istep ........ step index (io=0)                               *
*     t ............ time (io=0)                                     *
*     nbvar ........ number of variable to follow (io=0)             *
*                                                                    *
*====================================================================*
```

ROF_NAM

This routine reads/writes the variable header statement. This statement contains the name of the variable in a 10 characters long string, the index of the associated grid and the length of the sub-array.

```
*=====================================================================*
*                                                                     *
*     subroutine rof_nam(io,iu,ierr,vname,igrd,lenv)                  *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     io ........... read/write switch (0=read, 1=write)              *
*     iu ........... opened unformatted file unit                     *
*     vname ........ name of the variable array (io=1)                *
*     igrd ......... index of the grid associated with vname (io=1)   *
*     lenv ......... length of the variable array (io=1)              *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ierr ......... error indicator (0 if successful)                *
*     val .......... variable array  (io=0)                           *
*     vname ........ name of the variable array (io=0)                *
*     igrd ......... index of the grid associated with vname (io=0)   *
*     lenv ......... length of the variable array (io=0)              *
*                                                                     *
*=====================================================================*
```

ROF_VAL

This routine reads/writes a variable array. When reading: the length is known from ROF_NAM.

```
*=====================================================================*
*                                                                     *
*     subroutine rof_val(io,iu,ierr,lenval,val)                       *
*                                                                     *
*=====================================================================*
*                                                                     *
*     INPUT                                                           *
*     -----                                                           *
*     io ........... read/write switch (0=read, 1=write)              *
*     iu ........... opened unformatted file unit                     *
*     lenval ....... length of val                                    *
*     val .......... variable array (io=1)                            *
*                                                                     *
*                                                                     *
*     OUTPUT                                                          *
*     ------                                                          *
*     ierr ......... error indicator (0 if successful)                *
*     val .......... variable array  (io=0)                           *
*                                                                     *
*=====================================================================*
```

Example program

This section lists an example program written in Fortran 77 which demonstrates how to use of the ROF_xxx routines to read a ROF file.

```
*======================================================================*
*======================================================================*
*======================================================================*
*===========                                              ============*
*===========                                              ============*
*===========                  DARCYTOOLS                  ============*
*===========                                              ============*
*===========              ROF reading sample              ============*
*===========                                              ============*
*===========                                              ============*
*======================================================================*
*======================================================================*
*======================================================================*
*
      program readrof

      character *256  title
      character *10   vname,version
      character *19   date
      dimension igrdef(11), f(1000000)


      iures=6

*     open ROF file

      ierr=1
      open(unit=iurof, file='rof', form='unformatted', err=999)

*     read header

      write(iures,*)
      write(iures,*) 'Header'
      write(iures,*) '------'
      write(iures,*)

      ierr = 2
      call ROF_INI(0,iurof,ires,title,date,version,lgrd)
      if(ires.ne.0) goto 999

      do i=256,1,-1
       if(title(i:i).ne.' ') goto 5
      enddo

  5   write(iures,*) 'Version   = ',version
      write(iures,*) 'Date      = ',date
      write(iures,*) 'Title     = ',title(1:i)
      write(iures,*) 'NbGrids   =',lgrd


*     read grids' definition

      write(iures,*)
      write(iures,*) 'Grids'
      write(iures,*) '-----'

      do igrd=1,lgrd

       write(iures,*)
       write(iures,*) 'Grid no   =',igrd

       ierr = 4
       call ROF_GRD(0,iurof,ires,igrdef)

       write(iures,*) '     ni   =',igrdef(1)
       write(iures,*) '     nj   =',igrdef(2)
       write(iures,*) '     nk   =',igrdef(3)
       write(iures,*) '     icas =',igrdef(4)
       write(iures,*) '     ip   =',igrdef(5)
       write(iures,*) '     i1   =',igrdef(6)
       write(iures,*) '     i2   =',igrdef(7)
       write(iures,*) '     j1   =',igrdef(8)
```

```
         write(iures,*) '     j2   =',igrdef(9)
         write(iures,*) '     k1   =',igrdef(10)
         write(iures,*) '     k2   =',igrdef(11)
        enddo

*       read data

        write(iures,*)
        write(iures,*) 'Data'
        write(iures,*) '----'

   10   ierr = 5
         call ROF_TIM (0,iurof,ires,istep,t,nbvar)
         if(ires.eq.1) goto 20
         if(ires.ne.0) goto 999

         write(iures,*)
         write(iures,*) 'TIME istep =',istep
         write(iures,*) '     time  =',t
         write(iures,*) '     nbvar =',nbvar

          do iv=1,nbvar
           ierr = 6
           call ROF_NAM(0,iurof,ires,vname,igrd,lenv)
           if(ires.ne.0) goto 999
           write(iures,*) '     vname = ',vname
           ierr = 7
           call ROF_VAL(0,iurof,ires,lenv,f)
           if(ires.ne.0) goto 999
          enddo

         goto 10

   20   close(unit=iurof)

*       errors printouts

        goto 1000
 999    write(iures,*)
        write(iures,*) '*************************************************'
        write(iures,*) '*                 FATAL ERROR                   *'
        write(iures,*) '*************************************************'
        write(iures,*)
        if(ierr.eq.1)  write(iures,*) 'ROF openning failed'
        if(ierr.eq.2)  write(iures,*) 'ROF_INI reading error',ires
        if(ierr.eq.3)  write(iures,*) 'Wrong number of grids in ROF'
        if(ierr.eq.4)  write(iures,*) 'ROF_GRD reading error',ires
        if(ierr.eq.5)  write(iures,*) 'ROF_TIM reading error',ires
        if(ierr.eq.6)  write(iures,*) 'ROF_NAM reading error',ires
        if(ierr.eq.7)  write(iures,*) 'ROF_VAL reading error',ires
        write(iures,*)
        stop

 1000   pause
        end
```

Appendix B Structure of SOLVE

Contents

Structure of SOLVE

Introduction

When associated to the MIGAL library, the code is split in several sections and forms three accessibility levels. A top User level is made of template user's routines, a mid Developer level is made of the Main, Setting, Geometric, IO, Utilities, Physics, Models and Numerical Sections and a low "Not-Accessible" Level is made of MIGAL's subroutines. The different sections encapsulate the routines in the following way:

NUM-Section:	The numerical discretisation procedures SETOPx where x is 1 for BFC, 2 for BFC:S and 3 for Cartesian grids.
SET-Section:	The memory and setting management.
GEOM-Section:	The mesh generation facilities, metric calculations and the read/write format for grid files.
IO-Section:	The ROF and TEC input-output procedures.
PHYS-Section:	The physical fluid and rock laws encoding.
MOD-Section:	The special procedures for boundary and source/sink conditions or properties like GWRT, FRAME or TUNNEL and the PARTRACK routines.
UTIL-Section:	The utility routines for safe programming.
USER-Section:	Templates routines for user control.

The User-Section is a set of template routines automatically called by the program that the users can complete to define and control the calculations. Among those routines, whose names follow the pattern URSxxxxx, the USRSET routine is dedicated to case definition. To program the user's routine, a set of routines, whose names follow the pattern SETxxxxx is provided in the Set-Section.

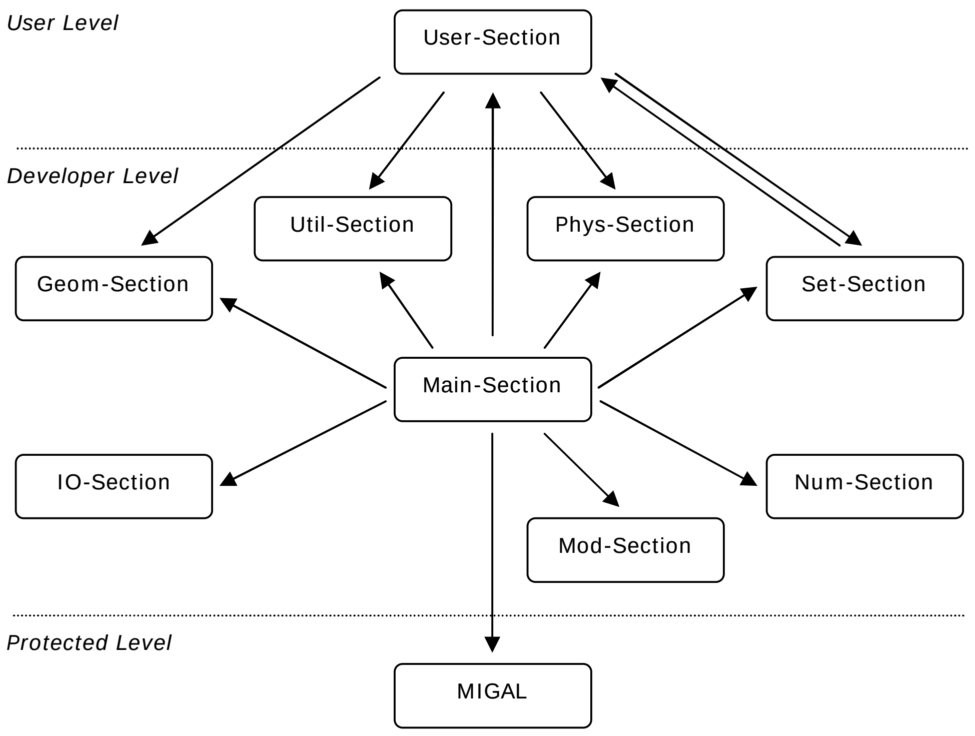

Figure 1 : Code structure and main dependencies

The Numerical, Geometrical and IO sections of the DarcyTools solver have been written in FORTAN 77 for sake of portability and maintenance. Only part of the upper level, concerned by memory management and user interface, is written in FORTRAN 90. In that case, mainly the pointers allocation capability feature is used.

Memory management

To enable various scenarios to run without compilation and manual adjustments DarcyTools uses a self adaptive memory management written in FORTRAN 90 and entirely located into the Setting Section of the program. This memory management is based on a single F array allocation technique for the numerical part of the program and on several annex arrays dedicated to the storage of the setting.

SNAME array

Each sub-array of F is uniquely defined by a name (10 characters long) stored into the array SNAME and the grid it is attached to.

```
SNAME(nbname)
```

The number of names NBNAME does not correspond to the total numbers of sub-arrays since a name may be shared by several sub-arrays on different grids. For example, the current pressure field has the same name 'X1P' on every grid. The SNAME array is dynamically allocated by the routine NOM during the user's array definition in SETARRAY and the F array's definition in DEFNAME. The following names are reserved names and should not be used for user's arrays:

```
A, E, S, R, W, W2, W3, DT, XyP, XyS, XyT, XyCxx, RESP, RESS, REST,
RESCxx, M1, M2, M3, PME, B, XV, YV, ZV, ZC, PERMz, DIFFz, TCONDz,
POROS, STORA, PREF, CAPA, FLUXn, DARCY-U, DARCY-V, DARCY-W
```

where y=1,…,3 represents the time step index, xx=1,…,99 represents the index of the transported mass fraction, z=1,…,9 represents the properties' location and n=0,…,9 the fluxes balance indexes. When the GRWT, FRAME, TUNNEL or PARTRACK models are activated additional F sub-arrays are also automatically declared:

```
GWT_FILL, GWT_REF, GWT-GH, FRM_FWS, FRM_CCV, FRM_ALPHA, FRM_BETA,
FRM_BETCLL, FRM_SUMC, TUN_REF, PTK_NPC, PTK_NPO, PTK_DEN, PTK_TRJX,
PTK_TRJY, PTK_TRJZ, PTK_TRJT, PTK_FREVOL, PTK_FWS
```

LNAME array

The F array's location and the length of each array are stored in the LNAME array dynamically dimensioned as follows.

```
LNAME(nbname,lgrd,nl)
```

where LGRD represents the number of grids and NL=3 the number of parameters that describe the sub-array. The first parameter contains the F array index of the sub-array, the second parameter contains its length and the third parameter is a trigger for storing the array on disk. To retrieve the index and length of a sub-array given its name and a grid index, it is highly recommended to use the functions LFNAME and LENAME defined in Util-Section.

F array

The first part of the F array contains the user arrays while a second part follows with the grid independent sub-arrays A, E, S, R, W and DT. The third part contains the variables, geometric quantities and properties sub-arrays for each grid: X, M, B, XV, YV, ZV… (see Figure 2). The sub-arrays dimensions and their locations into the F array are computed by the routine FARRAY and stored into a separated array called LNAME. The FARRAY subroutine is executed only once and its call is automatically launched by the first setting routines that need to write into the F array. During this call, some default values initialize the sub-arrays.

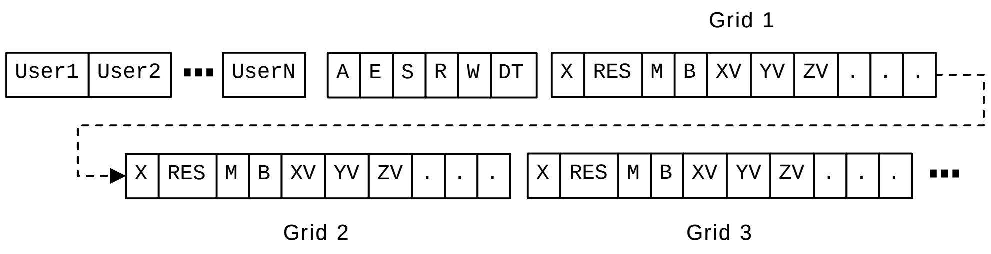

Figure 2 : F array's structure

The position of the different sub-arrays is not guaranteed. It depend of the name declaration ordering. Nevertheless users can be ensured that the mass flux array M is made of the three consecutive arrays M1, M2 and M3. In the same way the W2 and W3 arrays are sub-arrays of W such that W2(1)=W(N+1) and W3(1)=W(2*N+1) with N the largest value of (ni+1)*(nj+1)*(nk+1) on all grids. The length of W3 is at least N.

The dimensions of the grid independent sub-arrays are computed so that they can be used for any grid of the running case with the following definition:

```
A(nv,nv,npts,ni,nj,nk)
E(nv,ni,nj,nk)
S(nv,ni,nj,nk)
R(nv,ni,nj,nk)
W(ntrv)
DT(nt-1)
```

Those arrays are associated to every grid. The dimensions of the grid dependent sub-arrays depend on the kind of grid they refer to:

BFC	BFC:s	CART
`X(ni,nj,nk,nx,nt)`	`X(ni,nj,nk,nx,nt)`	`X(ni,nj,nk,nx,nt)`
`RES(nx)`	`RES(nx)`	`RES(nx)`
`M(ni,nj,nk,3)`	`M(ni,nj,nk,3)`	`M(ni,nj,nk,3)`
`B(31,ni,nj,nk)`	-	-
`XV(ni+1,nj+1,nk+1)`	`XV(ni+1)`	`XV(ni+1)`
`YV(ni+1,nj+1,nk+1)`	`YV(nj+1)`	`YV(nj+1)`
`ZV(ni+1,nj+1,nk+1)`	`ZV(ni+1,nj+1,nk+1)`	`ZV(nk+1)`
-	`ZC(ni,nj,nk)`	-

The parameters nv, nt and nx are grid independent and represent respectively the number of coupled variables (1 for the segregated approach, 2 for the coupled pressure-salinity approach), the number of time steps involved in the time discretisation and the number of variables contained in the X array (e.g 2 for a pressure-salinity problem).

The parameters npts, ni, nj and nk are grid dependent and represent respectively the width of the discretisation stencil (i.e. 7 for 3D, 5 for 2D and 3 for 1D), and the number of cells in x, y and z direction.

For memory storage saving, users can define uniform properties as being single element long sub-arrays via routine SETF0. The concerned sub-arrays are:

`PERMz, DIFFz, TCONDz, POROS, STORA, PREF, CAPA`

Finally, for top boundary condition facility a two dimensional sub-array is defined on the very parent grid only PME(ni,nj).

sub-arrays

DT	the values of the present (1) and the previous (2…) time steps for time derivative evaluation when nt>0.
RES	the Log10 of the mean square residual of the variables. The names for accessing that array are RESP, RESS and RESxx accordingly to the variable order.
A	the operator coefficients ordered for MIGAL.
E	a work array used to contain the estimation of the solution during MIGAL computation.
S	the operator source term for MIGAL.
R	a work array that contains the residual field returned by MIGAL. It also temporarily contains the cell centre z-coordinates in BFC:s case.
W	a work array for MIGAL. It also temporarily contains the Q_{src} and Q_{phi} arrays used for user's definition of boundary and sources/sinks terms.
X	the variables fields from 1 to nx for the present time (1) and the previous time steps (2…nt). The pressure index is fixed at 1 and the

	salinity index at 2. The names to access this array are X1P, X1S, X1T, X1Cxx, X2P, X2S, X2T, X2Cxx, X3P, X3S, X3T and X3Cxx, accordingly to the numbers nx and nt.
M	the mass flux through the east (1), the north (2) and top (3) faces. The names to access this array are repsectively M1, M2, M3.
B	the 31 metric coefficients of BFC case only.
XV	the cell vertex X-coordinates.
YV	the cell vertex Y-coordinates.
ZV	the cell vertex Z-coordinates.
ZC	the cell center Z-coordinates for BFC:S case only.
PERMx	the permeability field defined at cell face centers. Kx-East (1), Ky-North (2) and Kz-Top (3) for all cases, Kx-Top (4) and Ky-Top (5) for BFC and BFC:s cases and Kx-North (6), Kz-North (7), Ky-East (8) and Kz-East (9) for BFC case. The names to access this array are CONDx.
DIFFx	the diffusivity field defined at cell face centers in the same way as PERMx.
TCONDx	the equivalent (rock+fluid) thermal conductivity field defined at cell face centers in the same way as PERMx.
POROS	the porosity field.
PREF	the reference pressure for compaction effect.
STORA	the storativity field for compaction effect.
CAPA	the rock thermal capacity field.
PME	the precipitation minus evapo-transpiration on very parent grid only.

The three DARCY-U, DARCY-V and DARCY-W arrays are only alias names of the work arrays W, W2 and W3 temporarily used for outputs.

PDEF array

The PDEF array is in charge of storing all the needed parameters for the computation of any variable on any grid. To that respect, and in spite of today's redundancies, it has been designed as a three dimensional array.

```
PDEF(np,lgrd,nx)
```

Where np represents the total number of parameters (presently 28), lgrd the total number of grids defined by user and nx the number of variables.

Definitions

(1)	ni	number of cells in x-direction
(2)	nj	number of cells in y-direction
(3)	nk	number of cells in z-direction
(4)	nv	number of coupled variables (1 for segregated, 2 for coupled)

(5)	npts	width of stencil (7 for 3D, 5 for 2D, 3 for 1D).
(6)	-	undefined
(7)	iunit	opened logical unit for MIGAL’s printings
(8)	icycle	kind of MIGAL’s multi-grid cycle
(9)	nbgrid	depth of MIGAL’s multi-grid cycles
(10)	liter	maximum number of cycles for MIGAL
(11)	nbrelax	number of relaxations on each MIGAL’s multi-grid level
(12)	iform	kind of operator organization for MIGAL (always 0)
(13)	igmres	depth of GMRES sub-space
(14)	ipreco	number of GMRES preconditioning iteration
(15)	resfac	desired residual reduction before leaving MIGAL
(16)	relax	ILU0 relaxation factor for MIGAL
(17)	relin	relaxation factor applied to the MIGAL solution
(18)	ntv	number of time steps involved in time discretisation
(19)	nx	number of variables in X array
(20)	icas	kind of grid (1 for BFC, 2 for BFC:s, 3 for CART)
(21)	ip	index of the parent grid
(22)	i1	first parent cell index of the grid footprint in x-direction
(23)	i2	last parent cell index of the grid footprint in x-direction
(24)	j1	first parent cell index of the grid footprint in y-direction
(25)	j2	last parent cell index of the grid footprint in y-direction
(26)	k1	first parent cell index of the grid footprint in z-direction
(27)	k2	last parent cell index of the grid footprint in z-direction
(28)	iflu	embedded boundary conditions (1 fixed fluxes, 2 fixed values)
(29)	nbprer	number of pre-restriction relaxations for MIGAL
(30)	igms	depth of GMRES sub-space smoother for MIGAL

COMMONs

To simplify the user’s routines programming some parameters and variables are stored into commons. In principle, users are not allowed to change any values in the following commons:

```
      common /memor1/ f, pdef
      common /memor2/ lname,sname
      common /memor3/ bossdef, nboss
      common /memor4/ ftec,ztec,btec,stec,nftec,nztec,nbtec
      common /memor5/ tihist,vnhist,lphist,nbhist,nbvhist,nbphist
      common /memor6/ flubdef(7,10)
      common /memor7/ indgrd,lindg
      common /memor8/ fxdiff,vrm,vim,pfp,cumfac,alpha,volrp,
     &                pip,typep,adtypp,adstap
      common /iufile/ iures,iurof,iuhist
      common /server/ idport
      common /const0/ dtini,t1,t2,nt1,nt2
      common /const1/ g
      common /const2/ nstep,nsweep,nvar1,nvar2,nitc1,
     &                nvar3,nvar4, nitc2,nvar5,nvar6,nitg
      common /const3/ istep,isweep,igrd,itc,ivar,itg,t
      common /const4/ np,lgrd,nbname,nl,lf
      common /const5/ title, version, date
      common /const6/ hx,hy,hz
      common /const7/ precdif
      common /const8/ istep1,istep2,istepfr,irst
      common /const9/ grdfile
      common /defv1 / poros,stora,pref,capa,tcond(9),perm(9),diff(9)
      common /defv2 / iporos,istora,ipref,icapa,itcond(9),
     &                iperm(9),idiff(9)
      common /law1  / rho0, trho, alpha1, alpha2, beta1, beta2
      common /law2  / amu0, amu1, amu2, tmu, n_mu
      common /law3  / acp0, acp1, acp2
      common /tun/     itundef,tunsec,ntun_p,ntun_c,ntun_s,nsec_p
      common /frm   / nalint,alphl,alphh,frmk,bettot
      common /gwt   / grlx,facmin
      common /ptk01 / npd,nptk,method,igptk,ptkfile,nleave,narriv
      common /ptk02 / is1,is2,js1,js2,ks1,ks2
      common /ptk03 / ie1,ie2,je1,je2,ke1,ke2
      common /ptk04 / nalint,alphl,alphh,ak,bettot,fxdiff,retmob
     &                nmobst,naintn
      common /ptk05 / pfsta(3),tsteph,wnstph(3)
      common /ptk06 / seed
      common /ptk07 / nbtrj,ntrjfr,lentrj,ltrj
      common /ptk08 / nolond,adsorp
      common /bndy1 / ssea,tsea,tland
      common /bands / lbndp,lbndn,lbnds,lbnde,lbndw,lbndt,lbndb
      common /solve2/ licence, path, lenpath
```

Beside these and for simplicity, a common is also dedicated to the exchange of MIGAL's control parameters between the program and the user's routine USRSLV.

```
      common /solve1/ icycle, nbgrid, liter, nbrelax, igmres, ipreco
     &                iusolv, resfac, relax, relin
```

Definitions

/memor1/ contains the F and PDEF pointers
/memor2/ contains the sub-arrays locations and names
/memor3/ contains the setting for automatic boundary conditions

/memor4/	contains the setting for Tecplot outputs
/memor5/	contains the setting for history visualization
/memor6/	contains the setting for mass fluxes balances outputs
/memor7/	contains the INDGRD pointers
/memor8/	contains pointers on the internal PARTRACK work arrays
/iufile/	contains the logical unit for RESULT, ROF and HISTxx files
/server/	contains the monitoring server port ID
/const0/	contains the time step zoning parameters
/const1/	contains the gravity constant
/const2/	contains the loops definition of the algorithm
/const3/	contains the current index of the loops and the current time value
/const4/	contains some arrays dimensions
/const5/	contains the run definition strings
/const6/	contains the default grid dimensions
/const7/	contains the preconditioning parameter
/const8/	contains the ROF outputs definition and the RESTART trigger.
/const9/	contains the grid file name for reading the initial grid.
/defv1/	contains the initial value of properties.
/defv2/	contains properties parameters for SET_xx and GET_xx optimization
/law1/	contains the density state law parameters
/law2/	contains the viscosity state law parameters
/law3/	contains the specific heat state law parameters
/tun/	contains the setting for the TUNNEL model
/frm/	contains the setting for the FRAME model
/gwt/	contains the setting for the GRWT model
/ptk01/	contains the setting for the PARTRACK model
/ptk02/	contains the definition of the PARTRACK emission box
/ptk03/	contains the definition of the PARTRACK capturing box
/ptk04/	contains the setting for the PARTRACK multi-rate model
/ptk05/	contains the setting for the PARTRACK method 1
/ptk06/	contains the seed for PARTRACK random kernel
/ptk07/	contains the setting for PARTRACK trajectories
/ptk08/	contains the PARTRACK diffusion-adsorption triggers
/bndy1/	contains the setting for the top boundary conditions
/bands/	contains the band indexes for operator A array
/solve1/	contains MIGAL's parameters temporarily overwritten by user
/solve2/	contains the MIGAL unlocking information

Naturally, users can create other commons to exchange data between several user's routines, for example between the setting case routine URSSET and the boundary conditions routines USRBOSS.

Users should also note that all the reserved logical units are not present in the common /iufile/. Hence, it is highly recommended to use the routine IUFREE of Util-Section to get a free unit number when needed.

Algorithm

The DarcyTools algorithm is encapsulated into the Main Section of the program. It consists of several nested loops sequentially solving variables and/or groups of variables. The external loop is the time integration loop running from 1 to nstep. The second loop is the grid sequence loop running from the most embedded grid level lgrd to the largest grid level 1. For each time step and each grid, the computation of the nx variables is split in three groups defined by the nvar1 to nvar6 parameters.

MAIN

```
Setting & Initializations
DO istep = 1, nstep
    DO itg = 1, nitg
        DO igrd = lgrd, 1, -1
            DO isweep = 1, nsweep
                DO ivar = nvar1, nvar2
                    Solve variable ivar
                ENDDO
                DO itc = 1, nitc1
                    DO ivar = nvar3, nvar4
                        Solve variable ivar
                    ENDDO
                ENDDO
            ENDDO

            DO itc = 1, nitc2
                DO ivar = nvar5, nvar6
                    Solve variable ivar
                ENDDO
            ENDDO
        ENDDO
    ENDDO
ENDDO
```

Figure 3 : Main algorithm and loops nomenclature

Those three groups have been introduced to offer many possible non-linear coupling scenarios to users. For example, with the default loop definition nvar1=1, nvar2=2, nitc1=0 and nitc2=0 the program will compute only pressure and velocity once every sweep. A second example could be when a neutral scalar is transported by the flow. Then one can add its computation after that the salinity-pressure coupling is satisfied by setting nitc2=1, nvar5=4 and nvar6=4 (nvar=3 is reserved for the temperature). Alternatively, if the scalar influences the salinity one can introduce its computation into the SWEEP loop by setting nitc1=1, nvar3=4 and nvar4=4. Finally, when several scalars are coupled between them, the nitc values can be taken greater than one.

```
VARSOL

CALL properties user's routine
IF not pressure and not already available THEN
  | Build mass fluxes
ENDIF
Build discrete operator
IF embedded grid THEN
  | Set boundary conditions from parent grid solution
ENDIF
IF parent grid THEN
  | Set boundary conditions from ALL child grids solution
ENDIF
CALL automatic boundary conditions and source/sink terms
CALL boundary conditions and source/sink terms user's routine
IF not coupled or salinity THEN
  | Load MIGAL's parameters
  | CALL MIGAL's parameters user's routine
  | CALL MIGAL and update current variable
  | CALL output routines (tecplot, hist, usrout)
ENDIF
```

Figure 4 : VARSOL's algorithm

In the main algorithm (Figure 3) "Solve variable ivar" means: build the discrete operator and solve the resulting linear set of equations with MIGAL. This task is encapsulated in the VARSOL routine and calls user's routines such as definition of properties, boundary conditions and source/sink terms, overwriting of the MIGAL parameters and printings.

The ITG loop ensures the convergence of the mutual influence of the grid levels of cases running with embedded grids.

The mass fluxes are usually computed during the construction of the operator for pressure or after a pressure update. Nevertheless, if the pressure is a fixed input and one only uses DarcyTools for scalar transport, the mass fluxes are automatically built.

When the coupled pressure-salinity solution is selected, the VARSOL routine does not call MIGAL for the pressure but wait until the salinity is called to solve them together. Hence, there is a restriction in the ivar loops definition: when coupled, the pressure (ivar=1) must always immediately precede the salinity (ivar=2).

The routines PROPS and BOSS are respectively in charge of calling the model routines (TUNNEL, GRWT, FRAME…) of setting the default and automatic conditions stipulated by users and of calling the routines USRPROP and USRBOSS.

Before calling MIGAL, an opportunity is given to users of adapting the solver parameters depending on the current solution, grid, or iteration via the routine USRSLV. For coupled iterations, the opportunity to modify the preconditioned operator is also given via the routine USRPRECO.

Finally, after every MIGAL's run, the template routine USROUT is called for user's outputs. By checking the iteration variables in common /const3/ the user is informed of the very moment of this call. This routine is also called once per grid after initialization, just before starting the time integration loop. Then ivar is null and igrd represents the grid index (i.e. 1 for the largest grid, lgrd for the most embedded grid).

Setting and IO management

Beside the numerical calculations DarcyTools implements a user interface for setting and Input/Output purpose. Those additional features have been separated from the F array memory management for the sake of clarity. Three commons have been designed for this task, namely /memor3/, /memor4/ and /memor5/.

Automatic Boundary Conditions

The common /memor3/ is in charge of storing the automatic source/sink boundary conditions setting. It contains a two dimensional array BOSSDEF and the number NBOSS of automatic conditions stipulated by the user.

```
BOSSDEF(13,nboss)
```

BOSSDEF

This array is dynamically allocated by the routine SETBOSS and, for each boundary condition, stores the following information:

(1)	ivar	X array's index of the variable
(2)	igrd	index of the grid
(3)	i1	lower bound of the footprint in x direction
(4)	i2	upper bound of the footprint in x direction
(5)	j1	lower bound of the footprint in y direction
(6)	j2	upper bound of the footprint in y direction
(7)	k1	lower bound of the footprint in z direction
(8)	k2	upper bound of the footprint in z direction
(9)	it1	lower bound of the footprint in time
(10)	it2	upper bound of the footprint in time
(11)	qsrc	explicit part of the source term to apply to the footprint
(12)	qphi	implicit part of the source term to apply to the footprint
(13)	itype	type of source term condition (0 uniform, 1 fixed in time)

Given the array BOSSDEF, the routine BOSS will automatically apply the specified source/sink boundary condition to the specified footprint before calling the USRBOSS routine but after DEFBC which fixes the default top boundary conditions and the PME masse sources. This feature allows for example to repeat or change the boundary conditions from the initial ones during time integration.

Tecplot setting

The common /memor4/ is in charge of storing the user's commands relative to the Tecplot output facilities. It contains four two dimensional arrays FTEC, ZTEC, BTEC and STEC as well as the number NFTEC of files to create, the total number NZTEC of zone's definitions and the number NBTEC of block's definitions.

```
FTEC(4, nftec)
ZTEC(16,nztec)
BTEC(4, nbtec)
STEC(2, nbtec)
```

FTEC

The FTEC array is dynamically allocated by the routine SETTECF and stores the following information about the file created by DarcyTools to write the desired Tecplot data set.

(1)	iunit	locical unit number of the opened file
(2)	is_grid	kind of mesh (0=no mesh, 1=cell centers, 2=cell vertexes)
(3)	lastzone	last zone written in the file for duplicating information
(4)	isbinary	unused

ZTEC

The ZTEC array is dynamically allocated by the routine SETTECZ and stores the information relative to the zones extents.

(1)	nbcall	counter for zone naming
(2)	i1	lower bound of the outputs in x direction
(3)	i2	upper bound of the outputs in x direction
(4)	ifr	increment value of outputs in x direction
(5)	j1	lower bound of the outputs in y direction
(6)	j2	upper bound of the outputs in y direction
(7)	jfr	increment value of the outputs in x direction
(8)	k1	lower bound of the outputs in z direction
(9)	k2	upper bound of the outputs in z direction
(10)	kfr	increment value of outputs in z direction
(11)	it1	lower bound of the outputs in time
(12)	it2	upper bound of the outputs in time
(13)	itfr	increment value of outputs in time
(14)	ifile	index of the concerned file (in FTEC)
(15)	igrid	index of the associated grid
(16)	ivar	trigger variable index for writing activation

BTEC

The BTEC array is dynamically allocated by the routine SETTECB and stores the F sub-arrays name index of the values to write in the data set.

(1)	iaction	type of action to perform on the data before output
(2)	value	value for the action iaction
(3)	ifile	index of the concerned grid (in FTEC)
(4)	ivname	index of the sub-array name (in SNAME)

STEC

The STEC array is dynamically allocated by the routine SETTECF and stores the output file name and the title of the data set into 256 characters long strings.

(1)	filename	file name for output (including path)
(2)	title	index of the sub-array name (in SNAME)

Given all this information, DarcyTools automatically call the relevant routines TECxxx of the IO_section via the routine TECPLOT in order to create outputs data files directly readable by the post-processing software Tecplot.

History setting

The common /memor5/ is in charge of storing the user's commands relative to the history visualization facilities. It contains three arrays TIHIST, VNHIST and LPHIST, as well as the number NBHIST of files (graph) to create, the maximum number NBVHIST of plots allowed per graph and the number NBPHIST of parameters of the graph definition.

```
TIHIST(nbhist)
VNHIST(nbhist,nbvhist)
LPHIST(nbhist,nbphist)
```

TIHIST

The TIHIST array is in charge of storing the 35 characters long strings dedicated to the title of the graphs.

VNHIST

The VNHIST array is in charge of storing the 10 characters long strings that contain the label of every variable of the graph.

LPHIST

The LPHIST array is in charge of storing the curves definition of the graphs with the following convention:

(1-nbvhist)	sub-array indexes of the values to plot in plotting order.
(nbvhist +1)	I position index
(nbvhist +2)	J position index
(nbvhist +3)	K position index
(nbvhist +4)	index of the concerned grid
(nbvhist +5)	X index of the variable triggering the outputs
(nbvhist +6)	writing counter for abscise coordinate

Given all this information, DarcyTools automatically creates a HIST.HTM file and several HISTxx files via the routine HIST for real time history visualization via a web browser.

A HIST00 file is also automatically created which contains an ON/OFF trigger and the STEP and SWEEP current values. The ON/OFF trigger is periodically read by DarcyTools in order to know if it should stop or go on computing the next time step integration. Hence a visualization program can stop DarcyTools before its last time step by removing the file HIST00 or by setting the ON/OFF trigger (first line) to 0. Then DarcyTools terminates the current time step and saves all the required information like it would have done during the last time step.

ROF management

DarcyTools also implements in the subroutine ROF an automatic restart and an intermediary result storage facility.

In any case, DarcyTools creates an unformatted ROF file to store on disk, after the last time step, the minimum information to proceed to restart. If necessary, users may also use this ROF file to automatically store intermediary results for certain time steps. In that case, DarcyTools raises to 1 the third parameter in the LNAME array for the user selected sub-arrays, and stores the first, the last and the increment time steps indexes into the common /const8/.

When a restart is ordered DarcyTools raises to 1 the variable IRST of the common /const8/ and starts by reading the file ROF.

The IO low level ROF_xxx routines as well as the TEC_xxx routines have been gathered into an IO-Section to provide users with a library for post processing data. All those low level IO routines are written in Fortran 77.

Appendix C Four CIF-examples

```
**********************************************************
*                                                        *
*                 Test of grids, (Case A4)               *
*                                                        *
*                     26 December  2003                  *
*                                                        *
**********************************************************

*   1 SETTITLE  :     title
        1      'Test of Grids'

*   2 SETGRDF  : fname
        2      'xyz'

*   3 SETLICM  :      licence,             path
        3         'aa8vMYhrHd8VqPMWq3Lm'    ''

*   6 SETSTEP  :     dt         nstep    iorder
        6          0.31636E-2    100      1

*  12 SETLAW1  : rho0, Trho, alpha1, alpha2, beta1, beta2
       12         1000.  0.   0.008      0.     0.     0.

*  13 SETLAW2  : visc0, a1, a2, Tvisc, n
       13        2.E-3  0.  0.   0.    1

* 110 SETSWEEP : nsweep,  ivar1,  ivar2
       110          1       1       2

* 118 SETF1    :  name,   igrd,  value
       118       'PERM1'    1     2.E-4
       118       'PERM2'    1     2.E-4
       118       'PERM3'    1     2.E-4
*      118       'PERM4'    1     2.E-4
*      118       'PERM5'    1     2.E-4
*      118       'PERM6'    1     2.E-4
*      118       'PERM7'    1     2.E-4
*      118       'PERM8'    1     2.E-4
*      118       'PERM9'    1     2.E-4
       118       'DIFF1'    1    1.
       118       'DIFF2'    1    1.
       118       'DIFF3'    1    1.
*      118       'DIFF4'    1    1.
*      118       'DIFF5'    1    1.
*      118       'DIFF6'    1    1.
*      118       'DIFF7'    1    1.
*      118       'DIFF8'    1    1.
*      118       'DIFF9'    1    1.
       118       'POROS'    1    1.E-3


* 121 SETSPT : s1, t1, s0, t0, dwt, dsdz, dtdz, i1, i2 j1, j2, k1, k2
       121     0.  0.  1.  0.   0. -2.0E-3 0.   1   50 1   50  1   50

* 122 SETBOSS : ivar, igrd, itype, i1, i2, j1, j2, k1, k2, it1, it2, qsrc, qphi
       122         1     1     1   1   1   1   50  1   50  1    950   0.    0.
       122         1     1     1   50  50  1   50  1   50  1    950   0.    0.
       122         1     1     1   1   50  1   1   1   50  1    950   0.    0.
       122         1     1     1   1   50  50  50  1   50  1    950   0.    0.
       122         1     1     1   1   50  1   50  1   1   1    950   0.    0.
       122         1     1     1   1   50  1   50  50  50  1    950   0.    0.
       122         1     1     0   16  35   16  35  50  50  1   950 1.26839E7 0
       122         2     1     1   1   50   1   50  1   1   1   950   0.      0.
       122         2     1     1   1   50   1   50  50  50  1   950   0.      0.
       122         2     1     0   16  35   16  35  50  50  1   950   0.   1.E20

* 123 SETTECF  :   fname,      title,  isbin
       123       'A4.dat'       ''     1

* 124 SETTECZ  : ifile, igrd, i1, i2, ifr, j1, j2, jfr, k1, k2, kfr
       124        1      1    1   50   1   1   50   1   1   50   1
       124        1      2    2   34   1   2   34   1   2   34   1

* 125 SETTECB  : ifile, vname, iaction, value
       125         1    'X1P'     0      0.
       125         1    'X1S'     0      0.

* 131 SETRSRT :
*       131

* 135 SETHIST : i  j   k   igrd  iv   title
       135      0  0   0    1     2   'Residuals'
       135      25 25  25   1     2   'Spot Values (25, 25, 25)'
       135      25 25  0    1     2   'Profiles, i = j = 25'

* 136 SETHIST2 : igra  vname   label
       136        1    'RESP'  'Pressure'
       136        1    'RESS'  'Salinity'
       136        2    'X1P'   'Pressure'
       136        2    'X1S'   'Salinity'
       136        3    'X1P'   'Pressure'
       136        3    'X1S'   'Salinity'

**********************************************************
*                                                        *
*                GRIDGEN setting                         *

* 1004 GRGPCOS  : icosp
        1004       3

* 1005 GRGXDIS  : x0,   x1,     x2,    x3,        nx1,  nx2,  nx3
        1005      0.    0.      1000.  1000.      0     50    0

* 1006 GRGYDIS  : y0,   y1,     y2,    y3,        ny1,  ny2,  ny3
        1006      0.    0.      1000.  1000.      0     50    0

* 1007 GRGZDIS  : z3, z4,       z5,     nz1, nz2, nz3, nz4, nz5
        1007      0. -1000.  -1000.     0    0    0    50    0

* 1008 GRGEMBG  : icos, ifac, jfac, kfac, ip, i1, i2, j1, j2, k1, k2
        1008       3     3     3      3    1  20  30  20  30  35 45

**********************************************************************
* NOTE: BFC grid set in fif.f. A grid can not be combined with embedded
*       grid if set in fif.f
```

```
***********************************************************
*                                                         *
*          The salt dome problem ( Case E2)               *
*                                                         *
*                   30 December 2003                      *
*                                                         *
***********************************************************

*   1 SETTITLE  :     title
        1         ' The salt dome problem'

*   2 SETGRDF  : fname
        2       'xyz'

*   3 SETLICM  :      licence,             path
        3        'aa8vMYhrHd8VqPMWq3Lm'    ''

*   6 SETSTEP  :     dt          nstep    iorder
        6           2.E-4       5000      1

*  12 SETLAW1  : rho0, Trho, alpha1, alpha2, beta1, beta2
        12      1000.  0.    0.2      0.     0.     0.

*  13 SETLAW2  : visc0, a1, a2, Tvisc, n
        13      1.E-3  0.   0.   0.   1

* 110 SETSWEEP : nsweep,  ivar1,  ivar2
       110          1       1       2

* 118 SETF1    :  name,   igrd,  value
       118      'PERM1'    1    2.e-2
       118      'PERM3'    1    2.e-2
       118      'POROS'    1    0.2

* 121 SETSPT   : s1, t1, s0, t0, dwt,    dsdz,   dtdz, i1, i2 j1, j2, k1, k2
        121     0.  0.  0.  0.   0.    -0.00333  0    1   180 1  1   1  60

* 122 SETBOSS  : ivar, igrd, itype, i1, i2, j1, j2, k1, k2, it1, it2, qsrc, qphi
       122         2     1     0    60  120 1   1   1   1   1   15000 1.E20 1.E20
       122         2     1     0    1   180 1   1   60  60  1   15000 0.    1.E20

* 123 SETTECF  :   fname,       title,  isbin
       123        'E2.dat'        ''     1

* 124 SETTECZ  : ifile, igrd, i1, i2, ifr, j1, j2, jfr, k1, k2, kfr
       124         1      1    1  180  1    1   1   1    1  60   1

* 125 SETTECB  : ifile, vname,  action,  value
       125         1    'X1P'      0       0.
       125         1    'X1S'      0       0.
       125         1    'DARCY-U'  0       0.
       125         1    'DARCY-W'  0       0.
       125         1    'DARCY-V'  0       0.
       125         1    'DIFF1'    0       0.

* 131 SETRST  :
*   131

* 135 SETHIST : i  j   k   igrd  iv   title
       135      0  0   0    1     2   'Residuals'
       135      90 1   10   1     2   'Spot Values (90, 1, 10)'
       135      90 1   0    1     2   'Profiles, i = 90'

* 136 SETHIST2 : igra  vname   label
       136        1    'RESP'  'Pressure'
       136        1    'RESS'  'Salinity'
       136        2    'X1P'   'Pressure'
       136        2    'X1S'   'Salinity'
       136        3    'X1P'   'Pressure'
       136        3    'X1S'   'Salinity'

**********************************************************
*                                                        *
*                GRIDGEN setting                         *

* 1004 GRGPCOS  : icosp
        1004       3

* 1005 GRGXDIS  : x0,   x1,     x2,    x3,     nx1,  nx2,  nx3
        1005      0.    0.      900.   900.     0    180    0

* 1006 GRGYDIS  : y0,   y1,     y2,    y3,     ny1,  ny2,  ny3
        1006      0.    0.      5.     5.      0     1      0

* 1007 GRGZDIS  : z3, z4,    z5,     nz1, nz2, nz3, nz4, nz5
        1007      0. -300.  -300.     0    0    0   60    0

***********************************************************
*
*  NOTE: Problem scaled with a factor of 1.E13
```

```
**********************************************************
*                                                        *
*            The floating island  ( Case E5)             *
*                                                        *
*                    30 December 2003                    *
*                                                        *
**********************************************************
*   1 SETTITLE  :     title
        1         ' The floating island'

*   2 SETGRDF  :     fname
        2            'xyz'

*   3 SETLICM  :      licence,             path
        3         'aa8vMYhrHd8VqPMWq3Lm'    ''

*   6 SETSTEP  :     dt         nstep    iorder
        6           8.64E5        2000      1

*  12 SETLAW1  : rho0, Trho, alpha1, alpha2, beta1, beta2
        12       1000.  0.    0.0078    0.     0.     0.

*  13 SETLAW2  : visc0, a1, a2, Tvisc, n
        13       2.E-3  0.   0.   0.   1

*  16 SETGWT   : grlx, facmin
        16        0.8   0.001

* 110 SETSWEEP : nsweep,  ivar1,  ivar2
       110          1       1       2

* 115 SETTOP :  ssea,  tsea, tland
        115     1.0     0.    0.

* 118 SETF1    :  name,   igrd,  value
       118       'PERM1'    1    2.E-14
       118       'PERM3'    1    2.E-12
       118       'PERM4'    1    2.E-14
       118       'DIFF1'    1    1.E-12
       118       'DIFF3'    1    1.E-12
       118       'DIFF4'    1    1.E-12
       118       'POROS'    1    1.E-3
       118       'GWT_FILL' 1    1.
       118       'GWT_GH'   1    0.

* 119 SETF2    :  name, igrd,  value,   i1, i2, j1, j2, k1, k2
*       119        'PME'  1    3.17E-9   26  75  1   1   0  0
       119        'PME'  1     1.58E-9   26  75  1   1   0  0

* 121 SETSPT   : s1, t1, s0, t0, dwt, dsdz, dtdz, i1, i2, j1, j2, k1, k2
        121      0.  0.  1.  0.   0.   0.    0.   1   100  1  1  1    50

* 122 SETBOSS  : ivar, igrd, itype, i1, i2, j1, j2, k1, k2, it1, it2, qsrc, qphi
        122       2    1     1      1   100 1   1   1   1   1    20000 0.   0.

* 123 SETTECF  :   fname,    title,  isbin
       123        'E5.dat'      ''     0

* 124 SETTECZ  : ifile, igrd, i1, i2, ifr, j1, j2, jfr, k1, k2, kfr
       124          1      1    1  100  1   1   1   1    1   53   1
```

```
* 125 SETTECB  : ifile, vname,    action,   value
       125         1    'X1P'       0        0.
       125         1    'X1S'       0        0.
       125         1    'GWT_FILL'  0        0.
       125         1    'DARCY-U'   0        0.
       125         1    'DARCY-V'   0        0.
       125         1    'DARCY-W'   0        0.

* 131 SETRST   :
*        131

* 135 SETHIST : i  j   k   igrd  iv   title
       135      0  0   0    1     1   'Residuals'
       135      50 1   49   1     1   'Spot Values (50, 1, 49)'
       135      50 1   0    1     1   'Profile, i = 50'

* 136 SETHIST2 : igra  vname   label
       136        1    'RESP'  'Pressure'
       136        1    'RESS'  'Salinity'
       136        2    'X1P'   'Pressure'
       136        2    'X1S'   'Salinity'
       136        3    'GWT_FILL'  'Saturation'
       136        3    'X1S'   'Salinity'

**********************************************************
*                                                        *
*                GRIDGEN setting                         *

* 1001 GRGTEC   : fname,   title, isbin
        1001      'FItec'  'grid'   0

* 1003 GRGTOP  : fname
        1003     'USER'

* 1004 GRGPCOS  : icosp
        1004       2

* 1005 GRGXDIS  : x0,   x1,     x2,    x3,     nx1,  nx2,  nx3
        1005      0.    0.     1000.    1000.   0    100    0

* 1006 GRGYDIS  : y0,   y1,     y2,    y3,     ny1,  ny2,  ny3
        1006      0.  0000.     10.    00.     0      1    0

* 1007 GRGZDIS  : z3, z4,    z5,     nz1, nz2, nz3, nz4, nz5
        1007       -100. -500. -500.   4   0     9   40   0
+                 1, 1.
+                 2, 2.
+                 3, 3.
+                 4, 4.


**********************************************************

* NOTES :  * Analytical solution should be included ( see Case A1)
* -----
*          * Timestep is equal to 10 days

*          * Array-Lengths:  conref=ni*nj*nk*5  fill=ni*nj*nk gh=ni*nj
*            conref is the saturated conductivity, fill is the saturatio
*            level in a cell and gh is the groundwater level
*          * The coupled Pressure-Salinity solution should be tried.

*          * For rain=100 mm/year the fresh water lens reaches the bottom
*            boundary. May affect the simulation.
```

```
**********************************************************
*                                                        *
*                  Two-Fluid  problem  ( Case E6)        *
*                                                        *
*                  30 December  2003                     *
*                                                        *
**********************************************************

*   1 SETTITLE  :     title
        1         'Two Fluid Problem'

*   2 SETGRDF  :     fname
        2            'xyz'

*   3 SETLICM  :      licence,             path
        3         'aa8vMYhrHd8VqPMWq3Lm'    ''

*   6 SETSTEP  :     dt         nstep    iorder
        6          1.e2        100      1

*   9 SETF0:   vname,  igrd,    val
        9     'POROS'    1      1.
        9     'PERM1'    1      1.E-12
        9     'PERM3'    1      1.E-12
        9     'CAPA'     1      2.E6
        9     'TCOND1'   1      1.E-10
        9     'TCOND3'   1      1.E-10

*  12 SETLAW1:  rho0, Trho,  alpha1,  alpha2,  beta1,    beta2
        12      1000.  10.    0.00       0.    5.e-3      0.

*  13 SETLAW2  : visc0,  a1, a2, Tvisc, n
        13       2.E-3   0.2  0.   10   1

*  14 SETLAW3  : cp0,   a1, a2
        14       4200.  0.  0.

* 110 SETSWEEP : nsweep,  ivar1,  ivar2
       110          1       1       1

* 111 SETITC1  : nitc1,  nvar3, nvar4
       111          1       3       3

* 119 SETF2 : name,  igrid,  value, i1, i2, j1, j2, k1, k2
        119   'X2T'   1      10.    1    80  1  1   1   40
        119   'X2T'   1      20.    81  160  1  1   1   40

* 123 SETTECF  :   fname,         title,  isbin
        123      'E6.dat'          ''      1

* 124 SETTECZ  : ifile, igrd, i1, i2, ifr, j1, j2, jfr, k1, k2, kfr
        124        1      1    1  160  1    1   1   1    1  40   1

* 125 SETTECB  : ifile, vname     iaction   value
       125         1    'DARCY-U'    0        0.
       125         1    'DARCY-V'    0        0.
       125         1    'DARCY-W'    0        0.
       125         1    'X1T'        0        0.
       125         1    'X1P'        0        0.

* 135 SETHIST : i   j   k   igrd  iv   title
```

```
       135      0   0   0    1     3   'Residuals grid 1'
       135      80  1   10   1     3   'Spot Values (80, 1, 10)'
       135      80  1   0    1     3   'Profiles, i = 80'

* 136 SETHIST2 : igra  vname      label
       136        1    'RESP'     'Pressure'
       136        1    'REST'     'Temperature'
       136        2    'X1P'      'Pressure'
       136        2    'X1T'      'Temp'
       136        2    'DARCY-U'  'Darcy-U'
       136        3    'DARCY-U'  'Darcy-U'
       136        3    'X1T'      'Temp'

**********************************************************
*                                                        *
*                GRIDGEN setting                         *

* 1004 GRGPCOS  : icosp
        1004       3

* 1005 GRGXDIS  : x0,   x1,     x2,    x3,     nx1,  nx2,  nx3
        1005      0.    0.      40.    40.      0    160    0

* 1006 GRGYDIS  : y0,   y1,     y2,    y3,     ny1,  ny2,  ny3
        1006      0.  0000.     .25    .25     0      1    0

* 1007 GRGZDIS  : z3,   z4,    z5,     nz1, nz2, nz3, nz4, nz5
        1007       0.   -10.  -10.     0    0     0    40   0

**********************************************************
```