A
User's Guide
to
I3ELVIS
in Subduction and Collision setup

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1 Physics

1.1 Basic physical principals

1.1.1 The continuity equation

The continuity equation describes the conservation of mass, while it is displaced in a continuous medium. In its Lagrangian form it reads the following,

$$\frac{D\rho}{Dt} + \rho\nabla \cdot \vec{v} = 0, \tag{1.1}$$

where ρ denotes material density, $\vec{v}$ denotes displacement velocity and $\frac{D}{Dt}$ denotes the Lagrangian time derivative.

For many geological media like the crust or the mantle, where temperature and pressure are not too large and no phase changes occur, which would lead to larger volume changes, one can assume the following *incompressibility condition*,

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \vec{v}\nabla\rho = 0, \tag{1.2}$$

which means that the density of material points does not change in time.

This leads us to the following *incompressible continuity equation*, which is the same in its Eulerian and Lagrangian form,

$$\nabla \cdot \vec{v} = 0, \tag{1.3}$$

The *incompressible continuity equation* very widely used in numerical geodynamic modelling, although it is often a rather strong simplification.

1.1.2 The Navier-Stokes Euqation

The Navier-Stokes equation of motion in its full form reads the following,

$$\frac{\partial\sigma'_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_i} + \rho g_i = \rho\frac{Dv_i}{Dt}, \tag{1.4}$$

where σ_{ij} is the strain-rate and $\vec{g} = (g_x, g_y, g_z)$ is the gravity vector.

In highly viscous flows the right-hand side of (1.4), the inertial forces $\rho\frac{Dv_i}{Dt}$, is much smaller compared to the gravitational force and therefore, be neglected. This leads to the *Stokes equation for creeping flow*,

$$\frac{\partial\sigma'_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_i} + \rho g_i = 0. \tag{1.5}$$

Under Boussinesq approximation the density is assumed to be constant, except in the buoyancy force term, where temperature and volatile content play an important role (Gerya and Yuen, 2003). Taking into account the Boussinesq approximation, density $\rho(T, P, c)$ in the buoyancy term ρg_i may vary locally as a function of temperature T, pressure P and composition c,

$$\frac{\partial\sigma'_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_i} = -\rho(T, P, c)g_i. \tag{1.6}$$

1.1.3 Heat conservation equation

The heat conservation equation, also called temperature equation, describes the heat balance in a convective medium, taking into account changes due to internal heat generation, advection and conduction. The Lagrangian heat conservation equation reads as follows,

$$\rho C_p \left(\frac{DT}{Dt}\right) = -\nabla\cdot\vec{q} + H_r + H_a + H_s + H_L, \tag{1.7}$$

with $\vec{q} = -k(T, p, c)\nabla T$, where thermal conductivity $k(T, P, c)$ depends on temperature, pressure and rock composition c. H_r, H_a, H_s, H_L denote radioactive, adiabatic, shear and latent heating.

Adiabatic and shear heating have shown to be important in many tectonic situations, which is why they are not taken as constant.

$$H_r = const. \tag{1.8a}$$

$$H_a = T\alpha\vec{v}\nabla P \tag{1.8b}$$

$$H_s = \sigma'_{ij}\left(\dot{\epsilon}'_{ij} - \dot{\epsilon}_{ij(elastic)}\right) \tag{1.8c}$$

$$H_L = const. \tag{1.8d}$$

The resulting set of the above equations, together with equations (1.6) and (1.8), is called the extended Boussinesq approximations.

1.1.4 Rheology

Equation of State

$$\rho = \rho_r \left[1 + \beta \left(P - P_r\right)\right] \times \left[1 - \alpha \left(T - T_r\right)\right] \tag{1.9}$$

where ρ_r is the reference density given separately for each rock type, $P_r = 1.0\,bar$ is the reference pressure, $T_r = 298.15\,K$ is the reference temperature, α is the thermal expansion and β is the compressibility.

Viscosity

Plastic yield strength

$$\sigma_{yield} = C + sin(\phi_{dry})(1 - \lambda)P \tag{1.10}$$

where σ_{yield} denotes the shear stress limit after which plastic yielding occurs, C is the cohesion, ϕ_{dry} is the effective internal friction angle in dry rock, $\lambda = 1 - \dfrac{P_{fluid}}{P_{solid}}$ is the pore fluid pressure factor and $P = P_{solid}$ is the mean stress of the solid.

Peirl's creep (Katayamo & Karato, 2008)

$$\dot{\epsilon}_{II} = A_{Peirl}\sigma_{II}^2 exp\left\{-\frac{E_a + PV_a}{RT}\left[1 - \left(\frac{\sigma_{II}}{\sigma_{Peirl}}\right)^k\right]^q\right\} \tag{1.11}$$

For I3ELVIS, elasticity has not yet been implemented, thus the implemented rheology in three dimensions is visco-plastic (time of writing: December 14, 2020). For I2ELVIS, a visco-elasto-plastic rheology is employed, with the deviatoric strain-rate $\dot{\epsilon}'_{ij}$ being composed of the following components,

$$\dot{\epsilon}'_{ij} = \dot{\epsilon}'_{ij(viscous)} + \dot{\epsilon}'_{ij(elastic)} + \dot{\epsilon}'_{ij(plastic}, \tag{1.12}$$

where

$$\dot{\epsilon}'_{ij(viscous)} = \frac{1}{2\eta}\sigma'_{ij}, \tag{1.13a}$$

$$\dot{\epsilon}'_{ij(elastic)} = \frac{1}{2\mu}\frac{D\sigma'_{ij}}{Dt}, \tag{1.13b}$$

$$\dot{\epsilon}'_{ij(plastic)} = \chi\frac{\partial G}{\partial \sigma'_{ij}} = \chi\frac{\sigma'_{ij}}{2\sigma_{II}} \quad \text{for } G = \sigma_{II} = \sigma_{yield}. \tag{1.13c}$$

where η denotes viscosity, σ'_{ij} denotes the deviatoric stress tensor, μ denotes the shear modulus, G is the plastic potential, σ_{yield} is yield strength, $\sigma_{II} = \sqrt{\frac{1}{2}\sigma'^2_{ij}}$ is second deviatoric stress invariant and χ is plastic potential. Generally the strain tensor ϵ_{ij} can be defined as a function of displacement $\vec{u} = (u_x, u_y, u_z)$,

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{x_i}\right). \tag{1.14}$$

and the second strain rate invariant is given by $\dot{\epsilon}_{II} = \sqrt{\frac{1}{2}\dot{\epsilon}'^2_{ij}}$

The viscosity η is defined as follows,

$$\eta = \left(\frac{2}{\sigma_{II}}\right)^{(n-1)}\frac{F^n}{A_D}exp\left(\frac{E+PV}{RT}\right), \tag{1.15}$$

where A_D, E, V and n are experimentally defined flow parameters, R is the gas constant and F is a dimensionless factor depending on the type of experiment (triaxial compression, simple shear).

The viscous constitutive relationship relates stress σ_{ij} with strain ϵ_{ij},

$$\sigma'_{ij} = 2\eta\dot{\epsilon}'_{ij} + \delta_{ij}\eta_{bulk}\dot{\epsilon}_{kk}, \tag{1.16}$$

where σ'_{ij} is the deviatoric stress, $\dot{\epsilon}'_{ij}$ is the deviatoric strain-rate, $\dot{\epsilon}_{kk}$ is the bulk strain-rate, and η and η_{bulk} are shear and bulk viscosity.

1.1.5 Impact treatment

The actual impact is not part of the model. The model only starts after the intrusion of the impactor into the parent body. Processes like crater excavation, redistribution of impactor and parent body material around the planet or decompression melting are not considered. A simplified model takes into account the thermal anomaly created by the impactor. A region called the isobaric core, of uniform temperature increase and shock pressure around the impactor can be found (Senshu et al., 2002).

$$R_{ic} = 3^{\frac{1}{3}} r_{imp} \tag{1.17}$$

where R_{ic} is the radius of the isobaric core and r_{imp} is the radius of the impactor.

Thermal anomaly in the isobaric core has been approximated by Monteux et al. (2007) in the following way,

$$\Delta T = \frac{4\pi}{9} \frac{\psi}{F} \frac{\rho_P G R_P^2}{c_P} \tag{1.18}$$

where ψ is the efficiency of conversion of kinetic energy to thermal energy and in this thesis assumed to be 0.3.

Outside the isobaric core, for $r > R_{ic}$, the thermal anomaly ΔT is decaying exponentially, according to the following rule (Senshu et al., 2002; Monteux et al., 2007),

$$T(r) = \Delta T \left(\frac{R_{ic}}{r} \right)^{4.4} \tag{1.19}$$

1.1.6 Computation of crust

This algorithm is only implemented in the 3D code.

Silicate melt within a certain depth is positively buoyant ($d_{depthmelt} = 2e5$) and rises up to the surface (Golabek et al., 2011). Only markers with a melt fraction between 1% and 20% are considered, as this corresponds roughly to the pyroxene fraction in a fertile mantle (Golabek et al., 2011). Silicate melt on markers fulfilling these criteria now percolates upwards through the mantle and at the surface crust is formed by freezing of the silicate melt.

1.1.7 Phase transitions, melting and hydration reactions

Melting +20

Melting occurs a soon as the melt fraction is larger than 0. +20 is added to the type rock type (not for 11/13/31/33 and 19/20/21). A rock type >20 signifies that the material is partially molten.

Freezing -20

If the melt fraction becomes 0, -20 is subtracted from the type (not for 11/13/31/33 and 19/20/21). A rock type <20 signifies that the material is fully solid.

Hydrated Peridotite 11 -> 34 (-> 14) (and 31 -> 14)

Hydrated wet mantle peridotite (type 11) can be molten (type 34) and resolidified again to quenched dry mantle peridotite (type 14).

Hydrated, wet mantle peridotite (11) -> Molten Peridotite (34) -> Resolidified dry quenched mantle peridotite (14)

(31 -> 14)

Mantle hydration [9,10,12,14] -> 11

If water is present, lithospheric (type 9) and asthenospheric (type 10) peridotite as well as dry peridotite from the shear zone (type 12) and the resolidified quenched (type 14) peridotite are hydrated (type 11).

Crust hydration 5/6 -> 17/18

If water is present, continental upper (type 5) and lower (type 6) crust are hydrated (type 17+18).

Layered Sedimentation Sequence of 3,4,3,4,3,4,....

Formation of new crust -> 16

Antigorite weakening 13 -> 11 (11 -> 13)

Serpentinization of hydrated peridotite depending on Antigorite pressure and temperature field following (Schmidt and Poli, 1998)

Eclogitization No type change.

Happens for type 7/8 (upper/lower oc. crust) and 27/28 (molten upper/lower oc. crust).

1.2 I2ELVIS

To model two-dimensional creeping flow under extended Boussinesq approximation, with both thermal and chemical buoyancy, the conservative finite-difference code I2ELVIS (Gerya and Yuen, 2003, 2007) is used, which operates on a staggered grid and uses the moving marker technique. Silicate material is assumed to have temperature-, pressure-, strain-rate and melt

fraction-dependant visco-elasto-plastic rheology. Furthermore, impact heat, batch melting of silicates and phase changes have all been taken into account.

1.3 I3ELVIS

The 3D models have been carried out by the 3D numerical I3ELVIS (Gerya and Yuen, 2007) code which is also based on a conservative finite difference method with a marker-in-cell technique and multigrid solver (Gerya and Yuen, 2003, 2007). Additionally, the 3D code also features impact heat, batch melting of silicates and phase changes as discussed in Golabek et al. (2011) for the 2D case. The initial thermal-chemical model setup (including initial conditions, boundary condition and fluid/melt transport mechanism) and numerical approach are kept as similar as possible to the 2D models. Furthermore, the 3D code also features computation of the primordial crust from silicate melt.

Parameter	Symbol	Value	Unit
Radius of planetary body	R_{Mars}	3389	km
Radius of impactor core	r_{ic}	$232 - 500$	km
Radius of final core rel. to R_{planet}	r_{core}	0.5	%
Temperature of impactor core	T_{ic}	$1300 - 2300$	K
Temperature of protocore	T_p	$1300 - 2500$	K
Temperature of diapirs	T_d	$1300 - 2300$	K
Mean temperature of final core	$\bar{T}_c$	–	K
Mean temperature of silicate mantle	$\bar{T}_m$	–	K
Mean temperature of planetary body	$\bar{T}_{tot}$	–	K
Mean density of final core	$\bar{\rho}_c$	–	$kg\,m^{-3}$
Mean density of silicate mantle	$\bar{\rho}_m$	–	$kg\,m^{-3}$
Mean density of planetary body	$\bar{\rho}_{tot}$	–	$kg\,m^{-3}$
Volume fraction of iron (3D)	$f_{Fe,vol}$	0.1	%
Mass fraction of iron (3D)	$f_{Fe,mass}$	0.2	%
Gravitational acceleration	g	3.73	$m\,s^{-2}$

Table 1: **TODO: complete table** List of parameters

2 t3c files

2.1 file.t3c

The file 'file.t3c' contains only one number, which gives the number of the NEXT file to write. The number given here is the actual number of the file, if all files would be numbered from the beginning (including the initial file), starting with 0. The file name though can be different (and is given in the 'mode.t3c'-file) and can contain any different number.

2.2 init.t3c

Null-point is in the frontal upper left corner of the grid.

2.2.1 Grid parameter description

The first part of 'init.t3c' describes some basic grid parameters:

Parameter	Description	Initial value	Unit
xnumx	Number of nodes in x	$16N + 5$ (4 multi-grid levels)	-
ynumy	Number of nodes in y	$16N + 5$ (4 multi-grid levels)	-
znumz	Number of nodes in z	$16N + 5$ (4 multi-grid levels)	-
mnumx	Number markers per cell in x	-	-
mnumy	Number markers per cell in y	-	-
mnumz	Number markers per cell in z	-	-
xsize	Dimension of model in x	-	$[m]$
ysize	Dimension of model in y	-	$[m]$
zsize	Dimension of model in z	-	$[m]$
pxinit	x-coordinate of initial pressure cell	$(xnumx - 1)/2$	-
pyinit	y-coordinate of initial pressure cell	$(ynumy - 1)/2$	-
pzinit	z-coordinate of initial pressure cell	-	-
pinit	Initial pressure in initial pressure cell	-	$[Pa]$
GXKOEFF	Gravitational acceleration in x	-	$[m/s^2]$
GYKOEFF	Gravitational acceleration in y	-	$[m/s^2]$
GZKOEFF	Gravitational acceleration in z	-	$[m/s^2]$
timesum	Starting time	-	$[years]$
nonstab	number of random number generated	-	
xnonstab	maximum random displacement of markers in x direction	-	
ynonstab	maximum random displacement of markers in y direction	-	
znonstab	maximum random displacement of markers in z direction	-	
markers types file name Y(Name) N(0)	Number of initial output file	-	-
data output file name	Name of initial output file	name_0.prn	-
TYPE	type of data output	b (= binary), no other supported	-

Table 2: Grid parameter description

2.2.2 Rock type description

In the next part a table lists all possible types of material compositions together with their rheological properties.

Parameter	Description	Unit
rocknum	Rock number	-
markn0	Individual lower viscosity limit	-
markn1	Individual upper viscosity limit	-
marks0	Connate water content at surface and surface temperature	$[wt\%]$
marks1	Individual upper stress limit	-
Nu or marknu	Newtonian viscosity	$[Pa^{MM} * s]$
DE or markdh	Activation energy E_a	$[J]$
DV or markdv	Activation volume V_a	$[J/bar]$
SS or markss	dislocation-diffusion transition stress σ_{crit}	$[Pa]$
MM or markmm	Stress exponent for creep law	$(Power)$
LL or markll	Pore fluid pressure factor $1 - \lambda$ (see eq. 1.10)	$(koef)$
a0 or marka0	Cohesion before cohesion weakening (see eq. 1.10)	$[Pa]$
a1 or marka1	Cohesion after cohesion weakening	-
b0 or markb0	Sinus of effective internal friction angle in dry rock (see eq. 1.10)	[deg°]/[rad]
b1 or markb1	$\sin(\phi)$ after strain weakening	-
e0 or marke0	Amount of strain marking beginning of strain weakening	-
e1 or marke1	Amount of strain marking the end of strain weakening	-
RO or markro	Density	$[kg/M^3]$
bb or bRo or markbb	Thermal expansion α (see eq.1.9)	$[1/K]$
aa or aRo or markaa	Compressibility β (see eq.1.9)	$[1/kbar]$
CP or markcp	Heat capacity	$[J/kg]$
Kt or markkt	Thermal conductivity	$[Wt/(m * K)]$
Kf or markkf	Temperature dependency coefficient of conductivity	$[Wt/m]$
Kp or markkp	Pressure dependency coefficient of conductivity	$[1/bar]$
Ht	heat generation	$[Wt/kg]$

Table 3: Rock type parameters

Nr.	Description	Rheology
00	Air	-
01	Water	-
02	-	-
03	Sediments 2	WET QUARTZITE RANALLI 1995
04	Sediments 3	WET QUARTZITE RANALLI 1995
05	Upper Continental Crust	dry,felsic - WET QUARTZITE RANALLI 1995
06	Lower Continental Crust	dry,felsic - WET QUARTZITE RANALLI 1995
07	Upper Oceanic Crust	Basalts - WET QUARTZITE RANALLI 1995
08	Lower Oceanic Crust	Gabbro - An75 Ranalli1995
09	Lithospheric Mantle	dry peridotite - DRY OL Ranalli1995
10	Asthenospheric Mantle	dry peridotite - DRY OL Ranalli1995
11	Hydrated Mantle	wet peridotite - WET OL Ranalli1995
12	Shear Zone	dry mantle peridotite - WET OL Ranalli1995
13	Serpentinized Mantle	wet peridotite
14	Resolidified peridotite/ quenched mantle	dry peridotite
15	-	-
16	Newly formed crust	Basalt
17	Hydrated Upper Crust	felsic - Hydrated WET QUARTZITE RANALLI 1995
18	Hydrated Lower Crust	felsic - Hydrated WET QUARTZITE RANALLI 1995
19	-	
20	-	
21	-	
22	-	-
23	Partially molten Sediments 2	
24	Partially molten Sediments 3	
25	Partially molten Upper Continental Crust	felsic
26	Partially molten Lower Continental Crust	molten gabbro
27	Partially molten Upper Oceanic Crust	molten basalt
28	Partially molten Lower Oceanic Crust	molten gabbro
29	Partially molten Lithospheric Mantle	dry peridotite
30	Partially molten Asthenospheric Mantle	dry peridotite
31	-	-
32	Partially molten Shear Zone	dry peridotite
33	-	-
34	Partially molten Peridotite	
35	-	-
36	Partially molten Newly Formed Crust	molten basalt
37	Partially molten Hydrated Upper Crust	molten gabbro
38	Partially molten Hydrated Lower Crust	molten gabbro
+50	Water markers	
+100	External Composition	
NAN	Undefined composition	black

Table 4: Rock types

Compositions 0-19 are all solids (except air and water). 20-39 are the equivalent melts. 50-89 are fluid markers. 100-139 are external compositions of the equivalent type, waiting outside the boundary to come into the model. They have the same properties as their internal equivalents.

2.2.3 Boundary conditions

Boundary conditions are prescribed separately for each of the six faces of the cube. Boundary conditions on each face don't have to be homogeneous. Special 'open boundary conditions' can be prescribed, where e.g. the last marker gets 99% of the velocity of the second to last and so on.

Parameter	Description	Range of values
Val	BC type	P, Vx, Vy, Vz, T, X, Y, Z, M
m10	starting node position in x	
m11	ending node position in x	
m20	starting node position in y	
m21	ending node position in y	
m30	starting node position in z.	
m31	ending node position in z	
Const	boundary value	
Koef	multiplier for boundary velocity	[0,1]
nshiftx	determines which x-node is used to calculate value at next node	-1, +0 or +1
nshifty	determines which y-node is used to calculate value at next node	-1, +0 or +1
nshiftz	determines which z-node is used to calculate value at next node	-1, +0 or +1
Koef1		
nshiftx1	Ignored if Koef1 is 0	
nshifty1	Ignored if Koef1 is 0	
nshiftz1	Ignored if Koef1 is 0	
Koef2		
nshiftx2	Ignored if Koef2 is 0	
nshifty2	Ignored if Koef2 is 0	
nshiftz2	Ignored if Koef2 is 0	

Table 5: Boundary condition parameters

P, Vx, Vy, Vz, T boundary conditions For all nodes in the given range $[m10, m11] \times [m20, m21] \times [m30, m31]$ the following boundary condition is applied:

$$A(x, y, z) = Const + Koef \cdot A(x + nshiftx, y + nshifty, z + nshiftz) \tag{2.1}$$

E.g. the following part in the *init.t3c* file:

```
/Left_Bondary
/Val___m10_m11___m20_m21___m30_m31___Const___Koef_dm1_dm2_dm3
```

Vx____0___0_____0___y–1___0___z–1___3e–10___0____0___0___0

translates into the following boundary condition:

$$V_x(x,y,z) = 3 \times 10^{-10} \quad | \; x = 0, y \in [0, y-1], z \in [0, z-1] \tag{2.2}$$

X, Y, Z coordinates definition For all nodes in the given range $[m10, m11] \times [m20, m21] \times [m30, m31]$ the following equation is applied, shown at the example of the x-grid:

$$X(x,y,z) = X(x-1,y,z) + Const + (Koef - Const) \cdot \frac{(x - m10)}{(m11 - m10)} \quad | \; Koef1 = 0 \tag{2.3a}$$

$$X(x,y,z) = X(x-1,y,z) + exp\left(log(Const) + log\left(\frac{Koef1}{Const}\right)\right) \cdot \frac{(x - m10)}{(m11 - m10)} \tag{2.3b}$$

M marker grid set to cell For all nodes in the given range $[m10, m11] \times [m20, m21] \times [m30, m31]$ additional markers are added. All parameters ($Koef$, $Koef1$, $Koef2$, $nshiftx$, $nshiftx1$,..,$nshiftz1$,$nshiftz2$) need to be set. $nshiftx$ gives the shift in x, $nshifty1$ gives the shift in y, $nshiftz2$ gives the shift in z and all other shift parameters are ignored. If $Koef$ is set, random nonstability is set on the new marker field in X in the following way:

$$markx = x + \frac{rand()\,\%\,(\lfloor Const \rfloor * 2 + 1) - \lfloor Const \rfloor}{Const} \cdot \frac{X(x+1,y,z) - X(x,y,z)}{nshiftx} \cdot Koef \tag{2.4}$$

Random nonstability is set in Y for $Koef1 > 0$ and in Z for $Koef2 > 0$ in the same way.

2.2.4 Box description

Arbitrary shapes of cubes are prescribed by setting the (x,y,z) coordinate of each of the 8 corners (Figure 1).

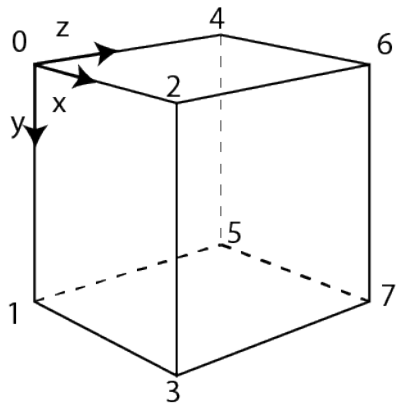

Figure 1: Illustration of the faces of the cube referred to in Tables 6 and 7.

Parameter	Description	Range of value
Type	Rock type	$0 - 140$
$[x_0, y_0, z_0]$	front upper left	
$[x_1, y_1, z_1]$	front lower left	
$[x_2, y_2, z_2]$	front upper right	
$[x_3, y_3, z_3]$	front lower right	
$[x_4, y_4, z_4]$	back upper left	
$[x_5, y_5, z_5]$	back lower left	
$[x_6, y_6, z_6]$	back upper right	
$[x_7, y_7, z_7]$	back lower right	

Table 6: Box parameters

Coordinates can be given either relative [0,1], or absolute [m0, mMAXSIZE], where MAXSIZE cannot be larger than the maximum domain size in this direction. With the leading 'm', the value is interpreted as an absolute value in meters.

e.g.

```
/Type=RockType
/Type__x0__y0__z0___x1__y1__z1_____x2__y2__z2_____x3__y3__z3
/_____x4__y4__z4___x5__y5__z5_____x6__y6__z6______x7__y7__z7
/Asthenosphere
10____0_m15000_0___0__1.1__0_____1.1_m15000_0_____1.1_1.1__0
______0_m15000_1___0__1.1__1_____1.1_m15000_1_____1.1_1.1__1
```

2.2.5 Temperature box description

Arbitrary shapes of cubes are prescribed by setting the (x,y,z) coordinate of each of the 8 corners (Figure 1).

Parameter	Description
Type	Box type: 0 - simple box; 1&4 - age box; 5&6 - transitional
$[x_0, y_0, z_0]$	front upper left
$[x_1, y_1, z_1]$	front lower left with $x_1 = x_0$, $z_1 = z_0$
$[x_2, y_2, z_2]$	front upper right with $z_2 = z_0$
$[x_3, y_3, z_3]$	front lower right with $x_3 = x_2$, $z_3 = z_0$
$[x_4, y_4, z_4]$	back upper left with $x_4 = x_5$, $z_4 = z_7$
$[x_5, y_5, z_5]$	back lower left with $z_4 = z_7$
$[x_6, y_6, z_6]$	back upper right with $x_6 = x_7$, $z_6 = z_7$
$[x_7, y_7, z_7]$	back lower right
t_0	simple box: temperature P_0; age box: surface temperature
t_1	simple box: temperature P_1; age box: initial temperature
t_2	simple box: temperature P_2; age box: thermal diffusivity κ in P_0
t_3	simple box: temperature P_3; age box: thermal diffusivity κ in P_2
t_4	simple box: temperature P_4; age box: thermal diffusivity κ in P_4
t_5	simple box: temperature P_5; age box: thermal diffusivity κ in P_6
t_6	simple box: temperature P_6; age box: characteristic diffusion time
t_7	simple box: temperature P_7; age box: overprinted linear geotherm [$^\circ/m$]

Table 7: Temperature box parameters

Coordinates can be given either relative [0,1], or absolute [m0, mMAXSIZE], where MAXSIZE cannot be larger than the maximum domain size in this direction. With the leading 'm', the value is interpreted as an absolute value in meters.

Box type 0: simple box The given temperatures are set to the given coordinates and temperature is interpolated linearly within the box.

Box type 1&4: age box Within the given coordinates the temperature is given by conductive cooling in the following way:

$$T(y,t) = T_1 - (1 - erf(\frac{y}{2\sqrt{\kappa\tau}}))(T_1 - T_0), \tag{2.5}$$

where $\kappa = \dfrac{k}{\rho c_p}$ is the thermal diffusivity interpolated over the corner of the box and $\tau = \dfrac{l^2}{\kappa}$ is the characteristic diffusion time.

Box type 5&6: transitional box No new temperatures are set but existing temperatures at the coordinates of the box corners are read. Those are then interpolated linearly through out the box.

E.g. the continental crust and lithosphere is modelled in a simple box by a geothermal gradient of $\sim 17\,K/km$ spanning the whole width of the model and starting at $12\,km$ depth with a surface temperature of $273\,K$, going down to a depth of $90\,km$:

```
/T_BOXES_DESCRIPTION
/Typ__x0_________x2_______y0_________y1_______y2_______y3_______z0_______
_x5_______x7_______y4_______y5_______y6_______y7_______z7_______
t0___t1___t2___t3___t4___t5___t6___t7
/Oceanic_and_continental_geotherms
0      -0.000001  m350001   m12000      m90000     m12000      m90000  -0.000001
-0.000001  m350001   m12000      m90000   m12000      m90000   1.000001
273   1595  273   1595  273   1595  273   1595
```

2.3 mode.t3c

2.3.1 Timestepping description

The first/second line gives the filename and type of the initial file.

In the next very large block one timestep corresponds with one line and the data is only valid for one timestep. Seperate timestep parameters are given in table 8.

Parameter	Description
SAVEFILE	name of the file (if this name is non-unique, the file will be overwritten without warning)
TYPE	file type: b = binary (no other supported)
cyc0max	number of repetitions done for each timestep
maxxystep	maximum step size in dimension
maxtkstep	maximum step size in temperature
maxtmstep	maximum step size in time
nubeg	global lower viscosity cut-off
nuend	global upper viscosity cut-off
p0koef	Pressure penalty factor, Relaxation parameter in Continuity equation
p1koef	Pressure update interpolation from coarser multigrid levels
p2koef	Pressure penalty factor in inertia term, $p2koef = 0$: no inertia, $p2koef \approx -\frac{2}{3} * p0koef$
p0koef0	Alternative for p0koef after switch multinum2
p1koef1	Alternative for p1koef after switch multinum2
p2koef2	Alternative for p2koef after switch multinum2
multinum	number of multigrid levels
stp1	number of iterations/cycles with *multinum*, after stp1 cycles switch to *multinum2*, *p0koef1*, *p1koef1*, *p2koef1*
multinum2	number of multigrid levels 2, switched to after stp1 cycles

Table 8: Timestep parameters

2.3.2 General parameters

The following parameters are mainly used to control the general behaviour of the program.

Parameter	Description	Default
loadmod	load from data file (1) or set initial conditions (0)	1
printmod	print information on the monitor, Yes (1)/ No (2)	1
crustmod	print information on crustthickness in files for each nth timestep; 0 = disable	-
dynamod	do dynamo calculations for each nth timestep; 0 = disabled	-
fl0num	number of otput file Names	-
movemod	do velocity-pressure iterations, solve continuity and Stokes equation	1
tempmod	do temperature iterations, solve heat transfer equation	1
markmod	move markers Y(1-simple,2-Runge-Kutta4)/N(0)	2
gridmod	recalculate density and viscosity	1
outgrid	marker move out of grid Y(0)/N(1) Orthogonal Only (2)	2
densimod	mode of density calculation: 0-constant, 1-PT-dependent, 2-TDbase 3-PT-dependent+WaterTDbase	3
stp100	maximum total distance for immobile markers without getting reseted	9000
CTreset	composition/temperature reset for water/air at 100 km above surface Y(1)/N(0)	1
smeltextract	extract melt when moving markers Y(1)/N(0)	1
sthdatabase	Use of Mars thermodynamic database Y(1) or standard database N(0)	1
p2vmod	convert each nth prn to vtr /N(0)	10
filestop	number of timesteps to execute before exiting	50

Table 9: General parameters

2.3.3 Erosion and Sedimentation parameters

Parameter	Description	Initial value
eroslev	Erosion level: markers above this depth which are neither sticky air nor water get converted to sticky air	8000
sedilev	Sedimentation level: sticky air or water below this depth gets converted to sediments	20000
waterlev	Water level: sticky air markers below water level are converted to water and water markers above water level are converted to sticky air	12000

Table 10: Erosion and Sedimentation parameters

2.3.4 Velocity- and Pressure-iterations parameters

The following parameters are mainly needed to solve the Continuity and Stokes equation with multigrid. Some these parameters already appeared in table 8 and their global value given here will be overwritten with the new value for each timestep.

Parameter	Description	Initial value
cyc1max	unused	3000
DIVVMIN	Continuity equation lower error bound	$3e{-}03$
STOKSMIN	Stokes equation lower error bound	$5e{+}01$
DIVVMAX	Continuity equation upper error bound	$0e{-}03$
STOKSMAX	Stokes equation upper error bound	$3e{-}03$
multinum	number of multigrid levels; overwritten by separate timestep value	4
multicyc	Number of whole multigrid V-cycle iterations	1
multinnn	V-cycle structure: number of GS-iterations for each multigrid level in upcycle and downcycle.	4 16 16 32 0; 4 16 16 32 64
p0koef	Global pressure penalty factor 1, Relaxation parameter in Continuity equation; overwritten by separate timestep value	$3.0e{-}01$
p1koef	Global pressure update interpolation from coarser multigrid level; overwritten by separate timestep value	$1.0e{-}00$
p2koef	Global pressure penalty factor 2, Relaxation parameter in Continuity equation; overwritten by separate timestep value	$0.0e{-}00$
v0koef	Velocity penalty facto. Relaxation parameter in vx-,vy-,vz-Stokes equation	$1.0e{-}00$
v1koef	MG velocity relaxation parameter. Velocity field prolongation	$1.0e{-}00$
nubeg	global lower viscosity cut-off; overwritten by separate timestep value	$1e{+}18$
nuend	global upper viscosity cut-off; overwritten by separate timestep value	$1e{+}25$
nukoef	Average ν for pressure optimisation	0.0
viscmod	Effective viscosity mode. 0 = lin. interp; 1 = exp. interp; 2 = inverse interp;	0
viscoutermod	viscosity in space/air/water; 1-gradual increase in space, 2-gradual increase in water/air	2
spheryn	Spherical gravity. 0 = off; 1 = on;	0

Table 11: V and P iterations parameters

viscmod: Effective viscosity interpolation Type of interpolation done to obtain effective viscosity. viscmod = 0 uses linear interpolation (eq. 2.6a), viscmod = 1 uses exponential interpolation (eq. 2.6b) and viscmod = 2 uses inverse interpolation (eq. 2.6c).

$$\eta_{eff} = \frac{1}{8}\sum_i \eta_i \tag{2.6a}$$

$$\eta_{eff} = exp\left(\frac{1}{8}\sum_i \left(log\left(\eta_i\right)\right)\right) \tag{2.6b}$$

$$\eta_{eff} = \frac{1}{\frac{1}{8}\sum_i \frac{1}{\eta_i}} \tag{2.6c}$$

2.3.5 Temperature-iterations parameters

The following parameters are mainly needed to solve the temperature equation with multigrid.

Parameter	Description	Initial value
cyc2max	unused	2500
HEATMIN	Temperature equation lower error bound	$1e{-}4$
multinumt	Number of multigrid levels	0
multicyct	Number of whole multigrid V-cycle iterations	1
multittt	V-cycle structure: number of GS-iterations for each multigrid level in upcycle and downcycle	1; 0
t0koef	Temperature penalty factor. Relaxation parameter in Continuity equation	$1.0e{-}00$
t1koef	MG temperature relaxation parameter. Temperature field prolongation	$1.0e{-}00$
heatdif	Numerical heat diffusion coefficient in subgrid diffusion	1.0
frictyn	Switch viscous friction heat	1
adiabyn	Switch adiabatic heat calculation	1

Table 12: T iterations parameters

2.3.6 Hydration and melting parameters

Parameter	Description	Initial value
tkpor	Maximum temperature for porosity	97300000.0
zmpor	Maximum depth for porosity	75000
vyfluid	Initial fluid velocity	$-3e{-}09$
vymelt	Initial melt velocity	$-3e{-}09$
dmwamin	Minimum water release difference	$1e{-}1$
tdeep	Bottom temperature reset	1880.0
dtdeep	Tolerance for bottom temperature	100.0
drdeep	Bottom density change	000.0
zdeep	Depth for temperature reset	660000.0
vdeep	Depth for viscosity reset	670000.0
nudeep	Bottom viscosity reset	$1e{+}21$
dxwater	Fluid extension in x	$2e{+}3$
dywater	Fluid extension in y	$2e{+}3$
dzwater	Fluid extension in z	$2e{+}3$
maxwater	Maximum water content in peridotite melt	$5e{-}1$
minmelt	Minimum remaining melt	$1e{-}2$
maxmelt	Maximum melt, start melt extraction	$1e{-}2$
maxpmelt	Maximum pressure for dry mantle melting	

Table 13: Hydration and melting parameters

2.3.7 Collision velocity parameters

Linearly change collision velocity. Use initial constant velocity set from boundary conditions. Between *timebeg* and *timeend* linearly change the collision velocity to the final velocity *velocitykf*.

Parameter	Description	Initial value
timebeg	Begin velocity change	$20e{+}6$
timeend	End velocity change	$25e{+}6$
velocitykf	Final collision velocity	0

Table 14: Collision velocity parameters

3 Raw output files: .prn

Valid for subduction/collision setup

3.1 Part I: General Information

Parameter	Description	Initial value	Unit
xnumx	Number of nodes in x	$16N + 5$ (4 multi-grid levels)	-
ynumy	Number of nodes in y	$16N + 5$ (4 multi-grid levels)	-
znumz	Number of nodes in z	$16N + 5$ (4 multi-grid levels)	-
mnumx	Number markers per cell in x	-	-
mnumy	Number markers per cell in y	-	-
mnumz	Number markers per cell in z	-	-
xsize	Dimension of model in x	-	$[m]$
ysize	Dimension of model in y	-	$[m]$
zsize	Dimension of model in z	-	$[m]$
pxinit	x-coordinate of initial pressure cell	$(xnumx - 1)/2$	-
pyinit	y-coordinate of initial pressure cell	$(ynumy - 1)/2$	-
pzinit	z-coordinate of initial pressure cell	-	-
pinit	Initial pressure in initial pressure cell	-	$[Pa]$
GXKOEFF	Gravitational acceleration in x	-	$[m/s^2]$
GYKOEFF	Gravitational acceleration in y	-	$[m/s^2]$
GZKOEFF	Gravitational acceleration in z	-	$[m/s^2]$
rocknum			
bondnum			
marknum			
n1			
timesum	Starting time	-	$[years]$
ival1			
gridcur			
gridtot			

Table 15: prn-file general information block

3.2 Part II: Rock type information

Parameter	Description	Unit
markn0	Individual lower viscosity limit	$[Pa * s]$
markn1	Individual upper viscosity limit	$[Pa * s]$
marks0	Maximum pore water content	[%]
marks1	Individual upper stress limit (= maximum brittle-ductile transition)	$[Pa]$
marknu	Newtonian viscosity	$[Pa^{MM} * s]$
markdh	Activation energy	$[J]$
markdv	Activation volume	$[J/bar]$
markss	Dislocation/diffusion creep stress threshold	$[Pa]$
markmm	Stress exponent	$(Power)$
markll	Pore fluid pressure factor	$(koef)$
marka0	Cohesion	$[Pa]$
marka1	Cohesion 2	$[Pa]$
markb0	Sine of dry friction angle	$[-]$
markb1	Sine of dry friction angle 2	$[-]$
marke0	Lower strain threshold for brittle/ductile transition	$[-]$
marke1	Upper strain threshold for brittle/ductile transition	$[-]$
markro	Density	$[kg/M^3]$
markbb	Density koef b	$[1/K]$
markaa	Density koef a	$[1/kbar]$
markcp	Heat capacity	$[J/kg]$
markkt	Thermal conductivity	$[W/(m * K)]$
markkf	Temperature dependency koef in conductivity	$[W/(m)]$
markkp	Pressure dependency koef in conductivity	$[Pa^{-1}]$
markht	heat generation	$[W/kg]$

Table 16: prn-file Rock type information block, see also tbl 3.

3.3 Part III: Nodes information

For each node the following parameters are given. The order is the following, where n is the number of nodes *nodenum*:

$$pr_0, vx_0, ...ht_0, pr_1, .., ht_1, .., pr_n, .., ht_n$$

Parameter	Description	Unit
pr	Pressure	$[Pa]$
vx	Velocity in x	$[m/s]$
vy	Velocity in y	$[m/s]$
vz	Velocity in z	$[m/s]$
ro	Density	$[kg/m^3]$
nu	Viscosity	$[Pa * s]$
tk	Temperature	$[K]$
cp	Heat capacity	$[J/kg]$
et	Thermal expansivity	$[1/K]$
kt	Thermal conductivity	$[Wt/m/K]$
ht	Heat sources	$[Wt/kg]$

Table 17: prn-file Node information block

3.4 Part IV: Gridline positions

Position of gridlines in x direction $xnumx$ numbers are given

Position of gridlines in y direction $ynumy$ numbers are given

Position of gridlines in z direction $znumz$ numbers are given

3.5 Part V: Boundary Condition Equations

For each boundary condition there are 5 values needed. The total number of boundary conditions is *bondnum*. The boundary conditions are all of the following general form:

$$CURPAR = CONST + KOEF1 * PAR1$$

Parameter	Description
m2	Index in Indexmatrix bondm
m3	Index in BC-matrices, saved in bondm
bondv1[m3][0]	$CONST$ value in BC equ.
bondv1[m3][1]	$KOEF1$ value in BC equ.
bondn1[m3]	$PAR1+1$ value in BC equ., $PAR1 = 0$ means no boundary

Table 18: prn-file boundary condition information block

3.6 Part VI: Markers

The total number of markers is *marknum*. For each marker the following parameters is given:

Parameter	Description	Unit
markx	Marker position in x	$[m]$
marky	Marker position in y	$[m]$
markz	Marker position in z	$[m]$
markk	Temperature	$[K]$
markw	Water percentage	[%]
markd	Density	$[kg/m^3]$
markex	Accumulated meltfraction	[%]
marktm	Creation time	$[s]$
markc1	Melt composition: Granitic part	[%]
markc2	Melt composition: Dacite part	[%]
markt	Rock type	$[nr.]$

Table 19: prn-file Marker information block

4 Numerical problems and solutions

- *Program stops because pressure gets too high.*

  Solution: This might indicate an awkward or inappropriate model setup. Try to lower the two pressure penalty factors from table 8 to $[0.5, 0.3, 0.1, 0.001]$. If that doesn't help, try another model setup.

- *Timestep doesn't converge within the time-limit of the Brutus queue.*

  Solution: Use a longer queue, e.g. 24h-queue instead of the 8h-queue. If the problem still persists try one of the following:

  a) Increase continuity equation error limit DIVMIN in tbl. 11 to $3e{-}3$

  b) Decrease multinum1 and multinum2 in tbl. 8 to 3.

  c) Increase both pressure penalty factors in tbl. 8. Choose something along $[0.05, 0.11, 0.31, 0.41]$.

  d) Decrease continuity equation error limit DIVMIN in tbl. 11 to $1e{-}3$.

  e) Try the following configurations for the pressure penalty factors [p0koef,p1koef,p2koef,p3koef] = $[0.31, 1.00, 0, 0]$, $[0.41, 1.00, 0, 0]$, $[0.11, 0.50, 0, 0]$

  f) Make 4 v-cycles series. In tbl. 11 set multicyc = 4.

- *Unstable model, model goes into very fast convection*

  Solution: Try one of the following:

  a) Decrease maximum timestep *maxtkstep* from 500 to 100.

b) Decrease maximum timestep *maxtmstep* from $5e3$ to $1e3$.

c) Increase lower viscosity limit from 10^{18} to 10^{19}.

- *Program stops because of NaN velocities.*

Solution: Try one of the following:

a) In case you are using a low resolution, with few nodes in any direction (< 181), check the amount of cores your job is using on Euler. If this is larger than 2, you are probably getting NaN velocities because of a bug in the solver where parallellisation fails (processors start to compete on coarsest mutligrid levels). Taras says it's in theory fixable, but for now it doesn't work. Try running the job on 2 cores.

b) Reconsider the volume balancing.
To conserve mass, material coming in needs to be balanced by material going out of the box (air and non-air):

$$V_{in} = \sum A_{app} * \bar{v} \tag{4.1}$$

where A_{app} is the area where the (average) velocity $\bar{v}$ is applied. Sticky air surplus or deficits (the net in- or outflow of air) must be compensated by assigning a flux at the upper boundary (deficit divided by area of model box). Likewise, net non-air fluxes must be balanced by in- or outgoing fluxes at the lower boundary, usually with asthenosphere. Especially important in this aspect is if you are using a permeable lower boundary, signified by a $Koef$ of 0.99 in the /Lower_bondary part of the initfile. In that case, do the following to calculate the flux at the lower boundary:

i. Add a virtual 99 nodes to the nodes in the y direction, e.g. 101 -> 200. Your new ysize will be 400 instead of 200 km if you're using a 2 km resolution.

ii. Calculate the net inflow of non-air material follwing equation 4.1

iii. Divide the net inflow of non-air material by the horizontal surface area (xsize * ysize). This value is the flux at the bottom of the 99 "extra nodes" below the lower boundary

iv. Divide this answer by 100 to get the outflow at the actual lower boundary

c) If you changed the model resolution with respect to your previous setup, check if the external grid uses the new resolution, and don't forget to modify the step100 parameter in *mode.t3c*, which needs to be 4.5 times the x-resolution.

5 Usage of paraview

5.1 Conversion from raw output to Paraview files

prn2vtr

5.2 Visualisation with Paraview

5.2.1 Visualize composition

Use the following pipeline:

- Threshold filter:
  set upper and lower threshold to the same composition number. Don't set the 'All Scalars' option.
- Contour filter:
  Contour by composition. Choose x.001 as value for the isosurface.
- GenerateSurfaceNormals filter:
  This generates a polygonal mesh, which has a smoothing effect.

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