Lecture 2. How to model: Numerical methods

Outline

- Brief overview and comparison of methods
- FEM LAPEX
- FEM SLIM3D
- Petrophysical modeling
- Supplementary: details for SLIM3D

Full set of equations

$$\frac{1}{K}\frac{DP}{Dt}-\alpha\frac{DT}{Dt}+\frac{\partial v_i}{\partial x_i}=0$$

mass

$$-\frac{\partial P}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}+\rho g_i=\rho\frac{Dv_i}{Dt}$$

momentum

$$\rho C_p\frac{DT}{Dt}=\frac{\partial}{\partial x_i}(\lambda\frac{\partial T}{\partial x_i})+\frac{1}{\eta_{eff}}\tau_{ij}\tau_{ij}+\rho A+\Delta H_{chem}$$

energy

$$\dot{\varepsilon}_{ij}^{d}=\frac{1}{2}(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i})-\frac{1}{3}\delta_{ij}\frac{\partial v_k}{\partial x_k}=\frac{1}{2G}\frac{D\tau_{ij}}{Dt}+\frac{1}{2\eta_{eff}(P,T,\tau_{II})}\tau_{ij}$$

Final effective viscosity

$$\frac{1}{2\eta_{eff}} = (\dot{\varepsilon}_L + \dot{\varepsilon}_N + \dot{\varepsilon}_P + \dot{\gamma}) / \tau_{II}$$

$$\dot{\varepsilon}_L = B_L\, \tau_{II} \exp\left(-\frac{H_L}{RT}\right)$$

$$\dot{\varepsilon}_N = B_N \left(\tau_{II}\right)^n \exp\left(-\frac{H_N}{RT}\right)$$

$$\dot{\varepsilon}_P = B_P \exp\left(-\frac{H_P}{RT}\left(1-\frac{\tau_{II}}{\tau_P}\right)\right)$$

$$\dot{\gamma} = 0 \quad \text{if} \quad \tau_{II} < c + \mu \cdot P$$

$$\dot{\gamma} \neq 0 \quad \text{if} \quad \tau_{II} = c + \mu \cdot P$$

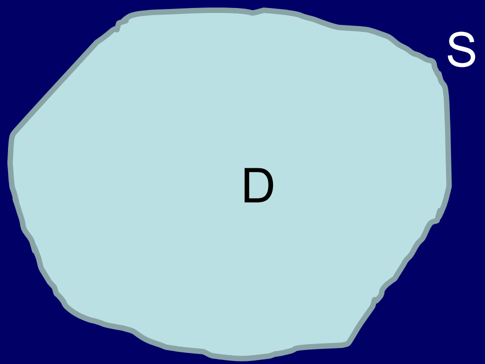
Boundary conditions

General case

Boundary value problem: $u=f$,

were is differential operator in space on unknown function u (like $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2$) and $f(x,y)$ is known function

Function $u(x,y)$ is defined in the domain D with the boundary S



Dirichlet b. condition $u(x,y\in S)=f_1$

Neumann b. condition $\partial u/\partial n\ (x,y\in S)=f_2$ – condition for flux

Boundary conditions

Kinematic boundary conditions

Dynamic boundary conditions:

Free surface

Free slip

Numerical methods

According to the type of parameterization in time:

Explicit, Implicit

According to the type of parameterization in space:

FDM, FEM, FVM, SM, BEM etc.

According to how mesh changes (if) within a deforming body:

Lagrangian, Eulerian, Arbitrary Lagrangian Eulerian (ALE)

Brief Comparison of Methods

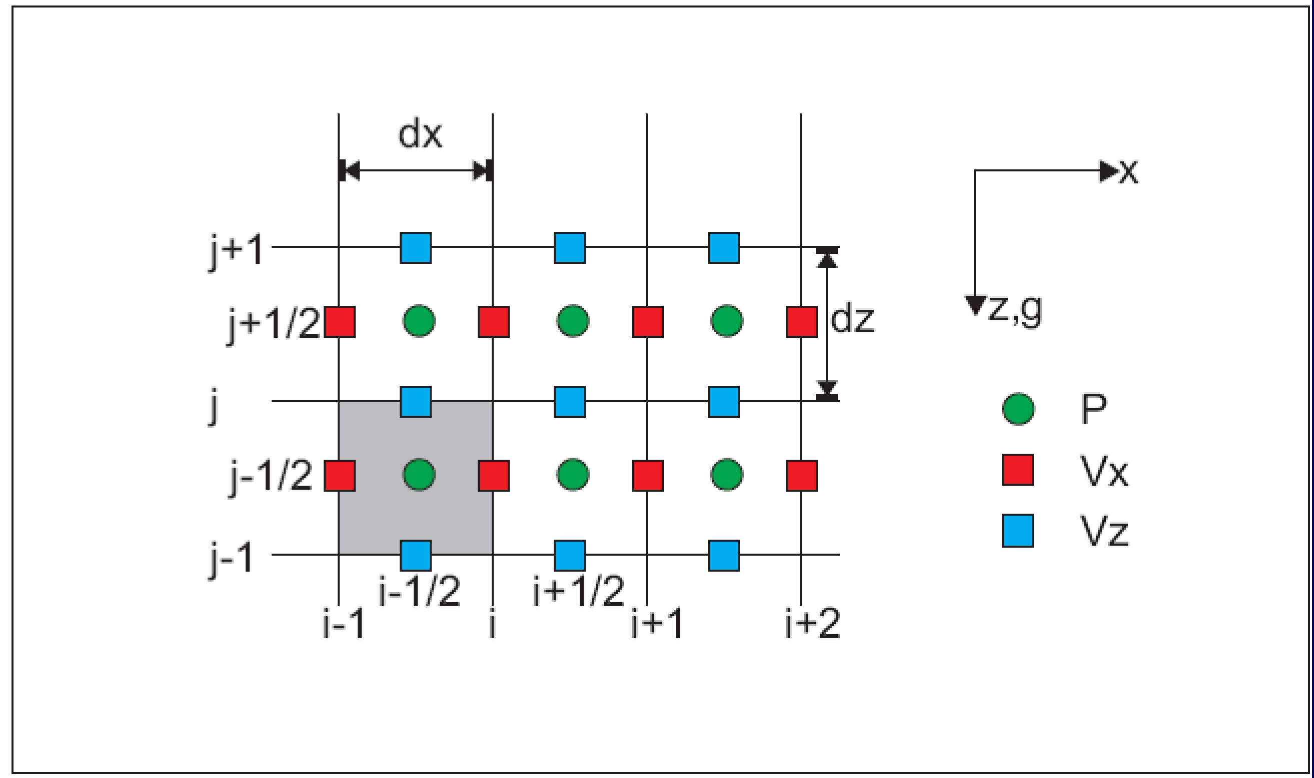
Finite Difference Method (FDM) :

FDM approximates an *operator* (e.g., the derivative)

Finite Element Method (FEM) :

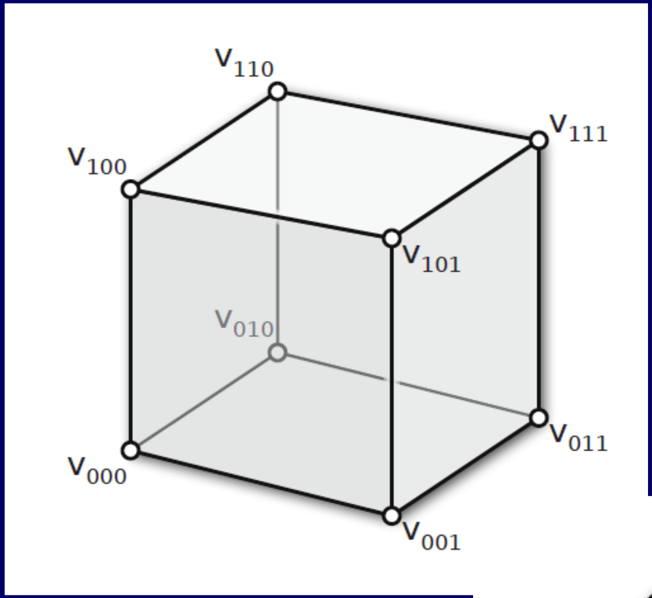
FEM uses exact operators but approximates the *solution basis functions.*

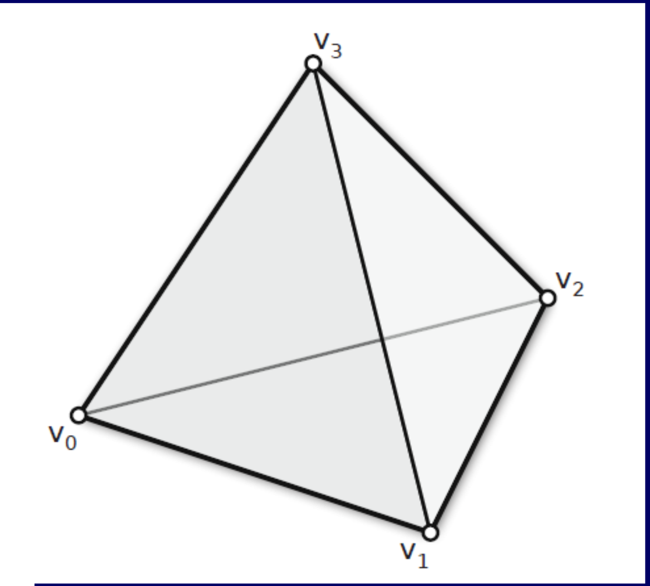
FD Staggered grid



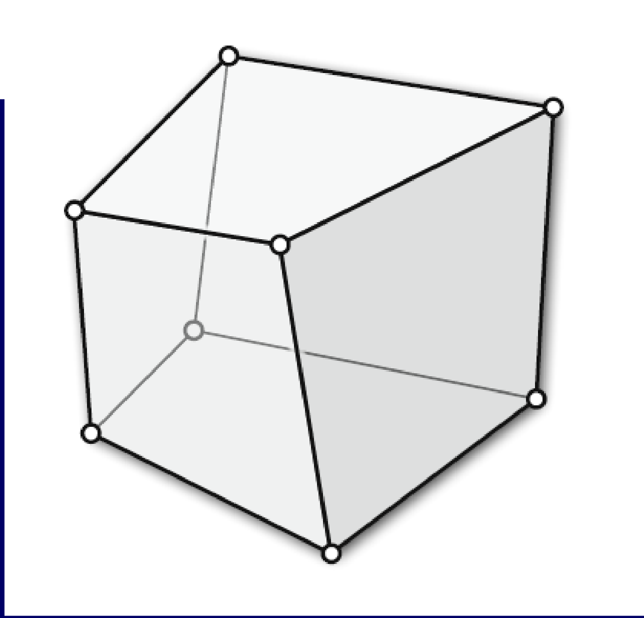
Finite Elements

Tetrahedron

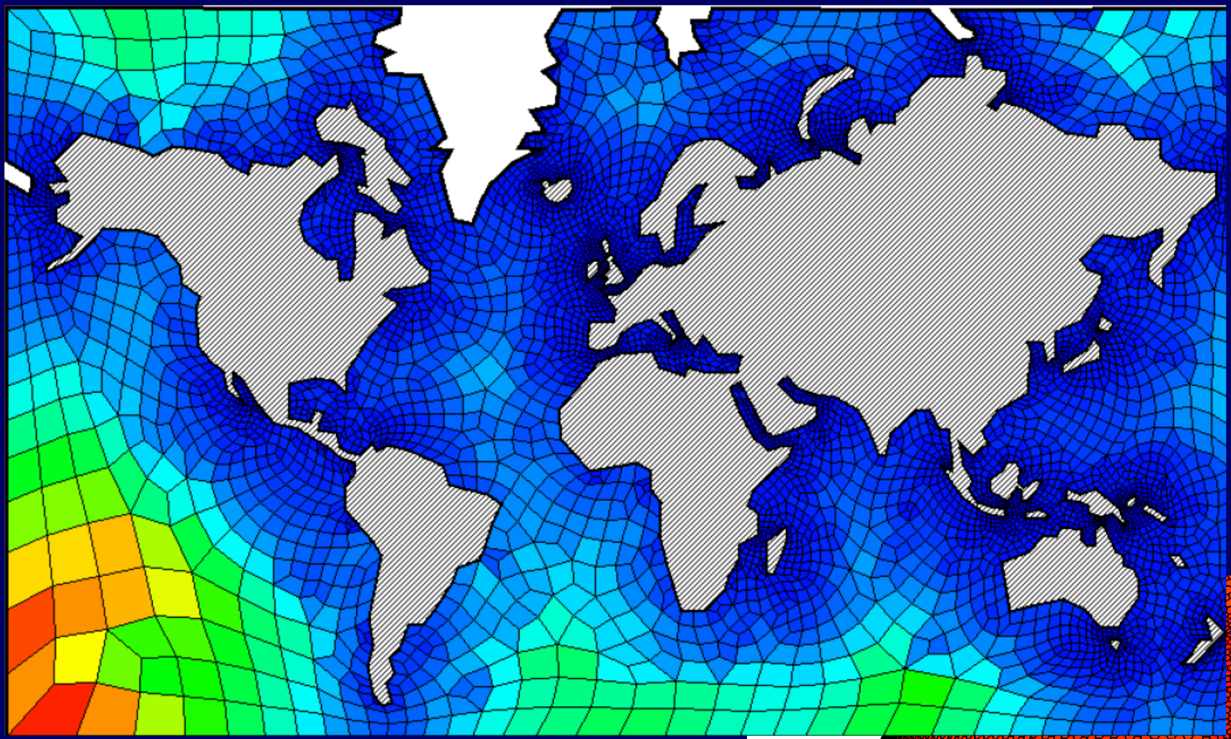


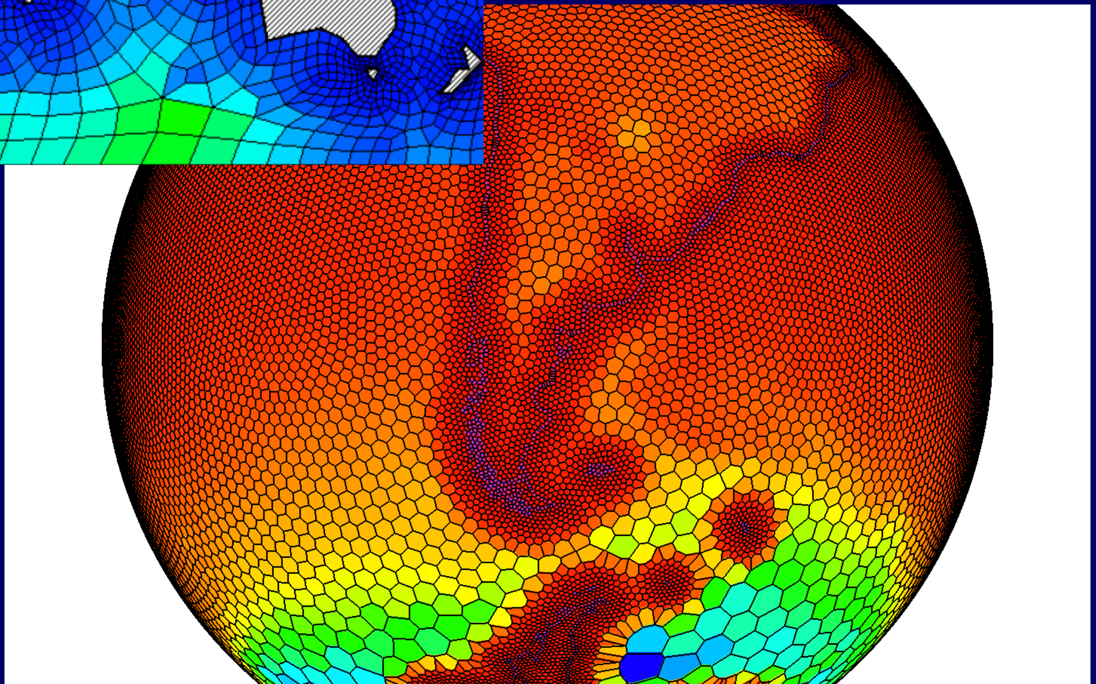


Hexahedron



Finite Elements





Non-uniform meshes

Interpolating Functions

nnod – number of degrees of freedom

Approximate solutions

$$\tilde{u}_x(x,y) = \sum_{i=1}^{nnod} N_i(x,y)\,u_x^i$$

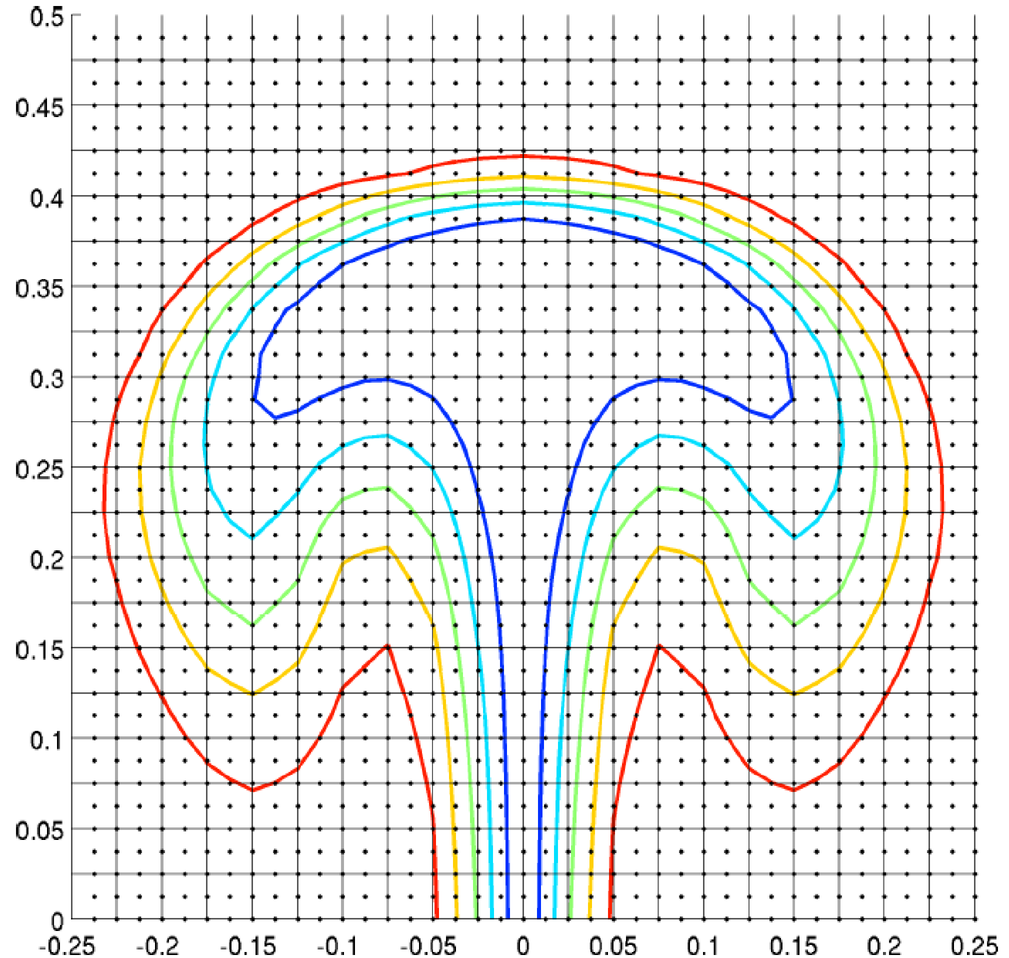
$$\tilde{u}_y(x,y) = \sum_{i=1}^{nnod} N_i(x,y)\,u_y^i$$

$$\tilde{p}(x,y) = \sum_{i=1}^{np} \Pi_i(x,y)\,p^i$$

Lagrangian Polynomials:

$$N_i(x) = \prod_{k \neq i} \frac{x - x_k}{x_i - x_k}$$

$$N_i(x_k) = \delta_{ik}$$



Brief Comparison of Methods

Spectral Methods (SM):

Spectral methods use global basis functions to approximate a solution across the entire domain.

Finite Element Methods (FEM):

FEM use compact basis functions to approximate a solution on individual elements.

Explicit vrs. Implicit

$$\frac{dX}{dt} = F(X, t)$$

Explicit vrs. Implicit

$$\frac{dX}{dt} = F(X, t)$$

Should be:

$$\frac{X(t+\Delta t) - X(t)}{\Delta t} = F(X(t+\Delta t/2), t+\Delta t/2)$$

Explicit vrs. Implicit

$$\frac{dX}{dt} = F(X,t)$$

Explicit approximation:

$$\frac{X(t+\Delta t) - X(t)}{\Delta t} = F(X(t),t))$$

Explicit vrs. Implicit

$$\frac{dX}{dt} = F(X,t)$$

Explicit approximation:

$$X(t+\Delta t) = X(t) + F(X(t),t)\Delta t$$

Modified FLAC = LAPEX

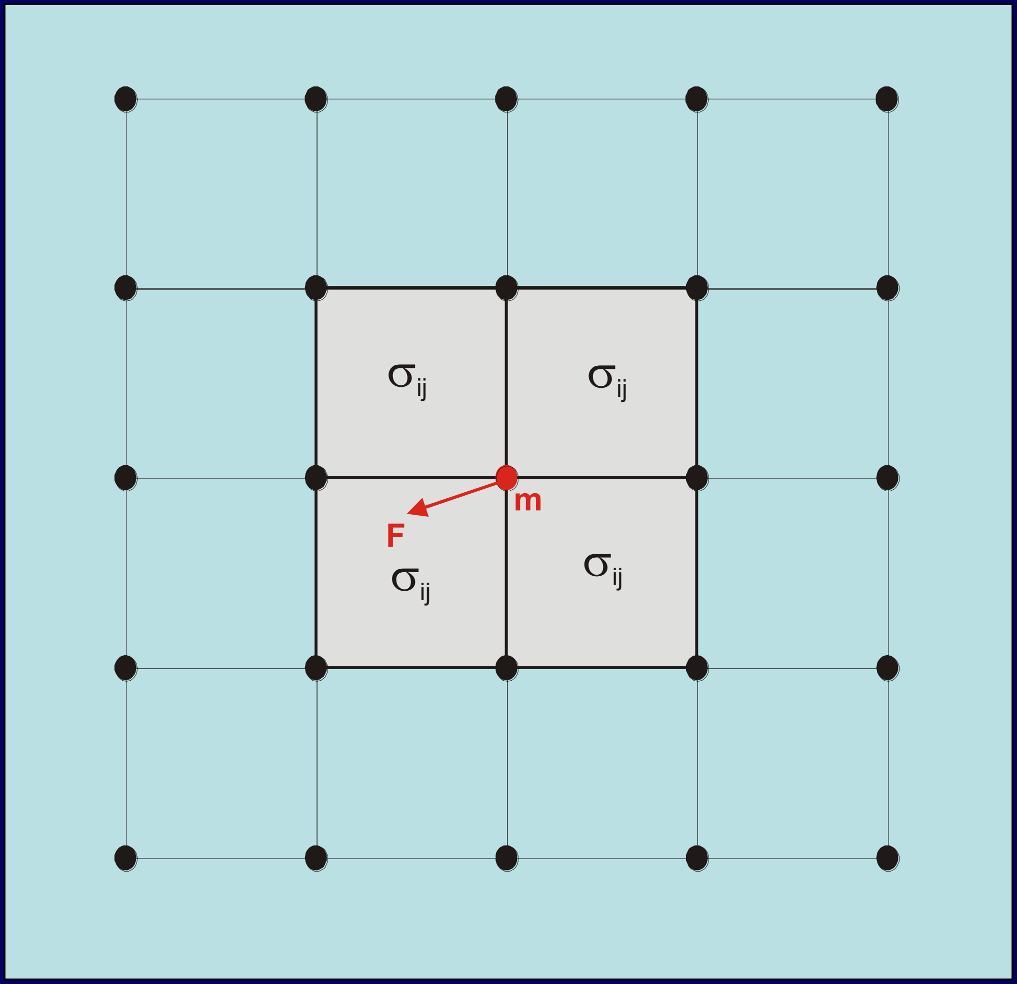
(Babeyko et al, EPSL2002)

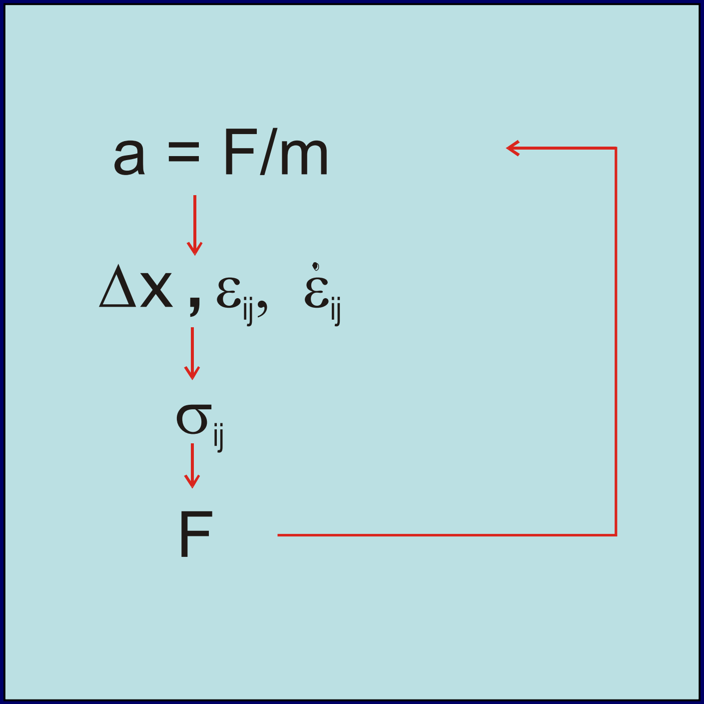
Dynamic relaxation:

$$-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i = \rho_{iner} \frac{Dv_i}{Dt},$$

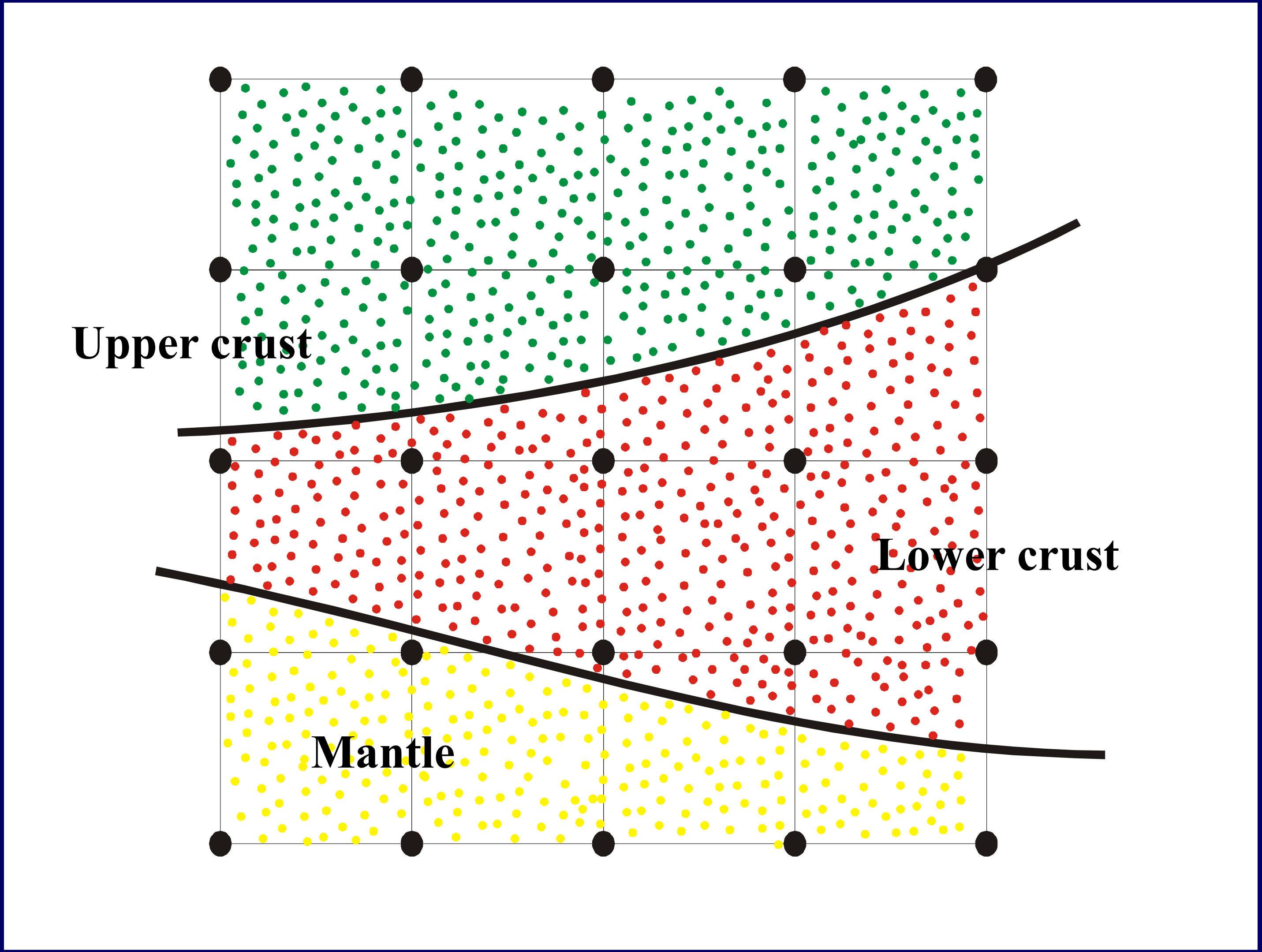
$$\left\| \rho_{iner} \frac{Dv_i}{Dt} \right\| << F_{tecto}$$

Explicit finite element method



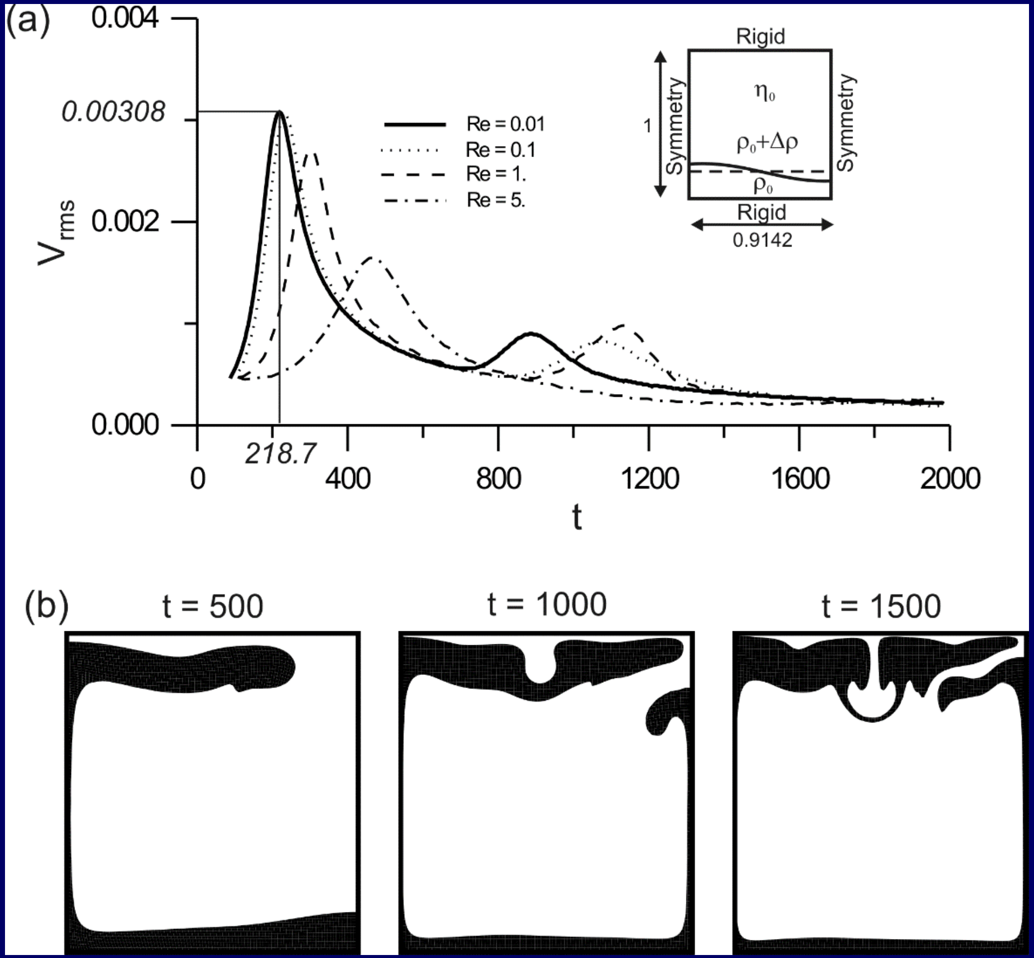


Markers track material and history properties

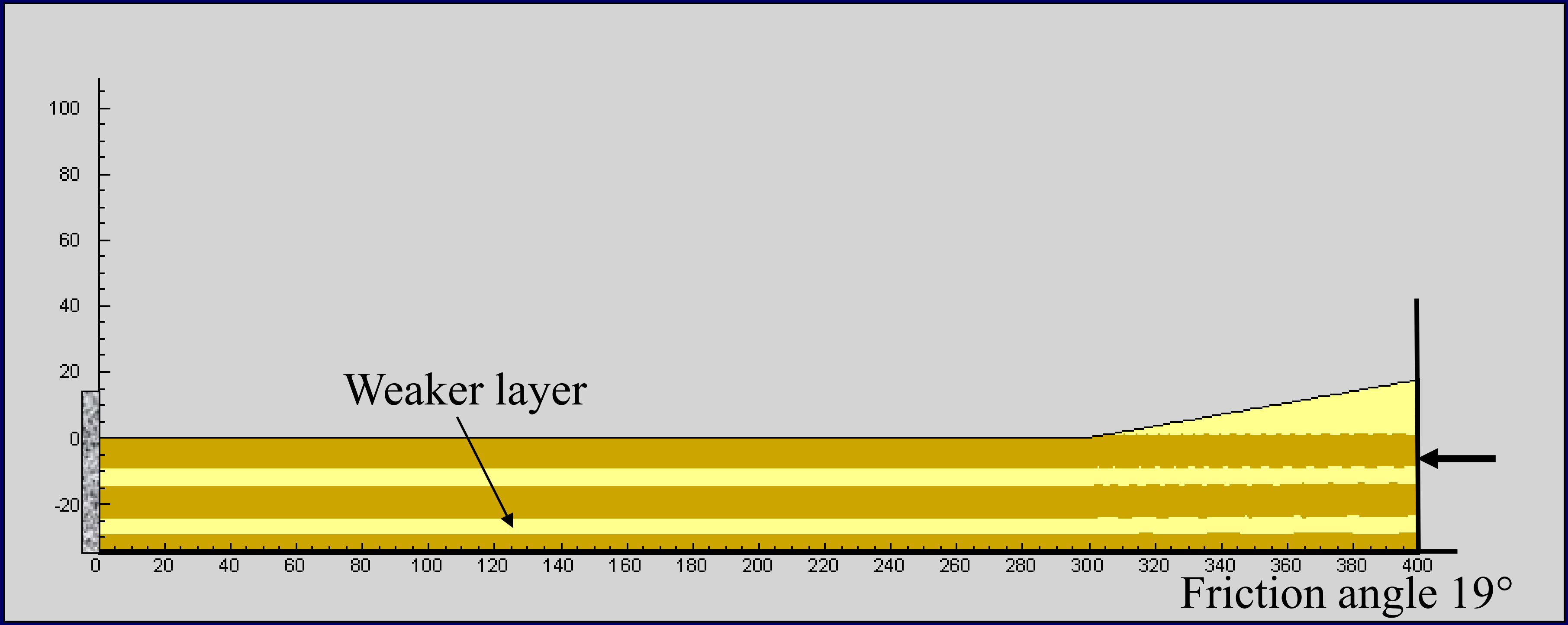


Benchmark: Rayleigh-Taylor instability

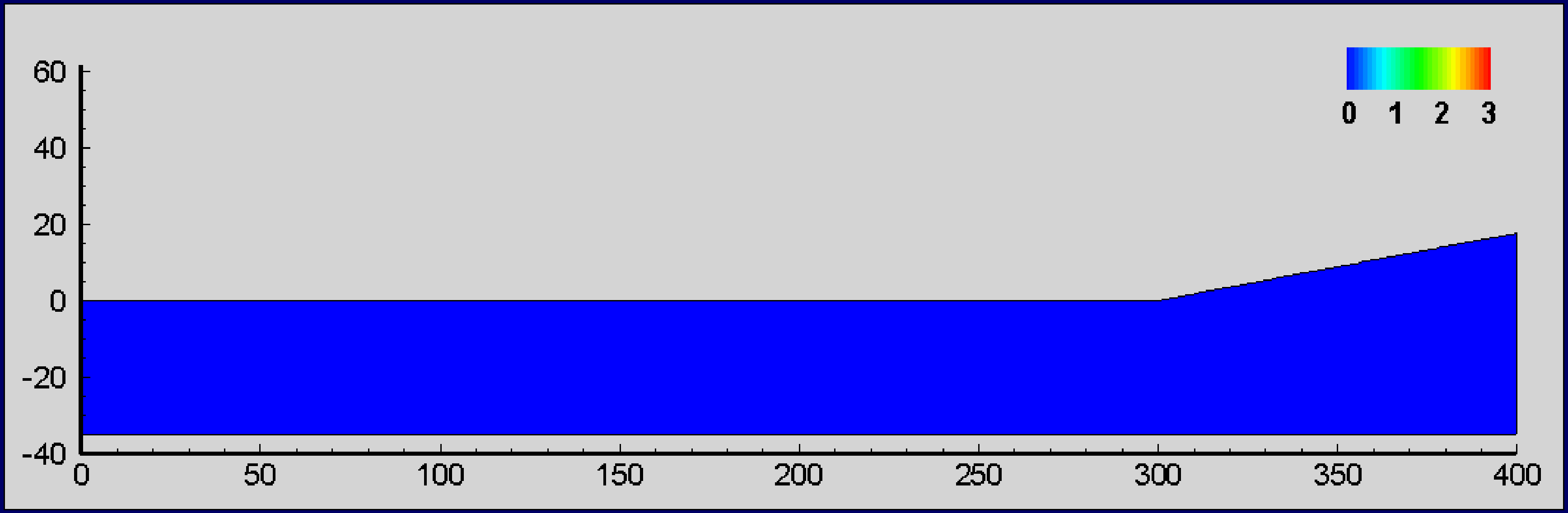
van Keken et al. (1997)

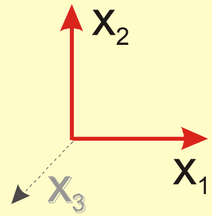
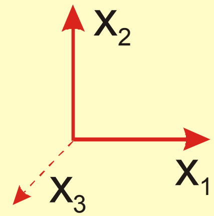
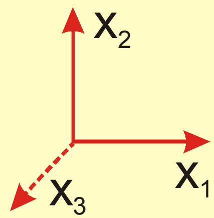
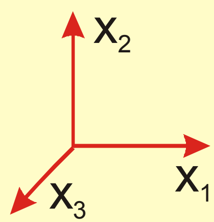


Sand-box benchmark movie



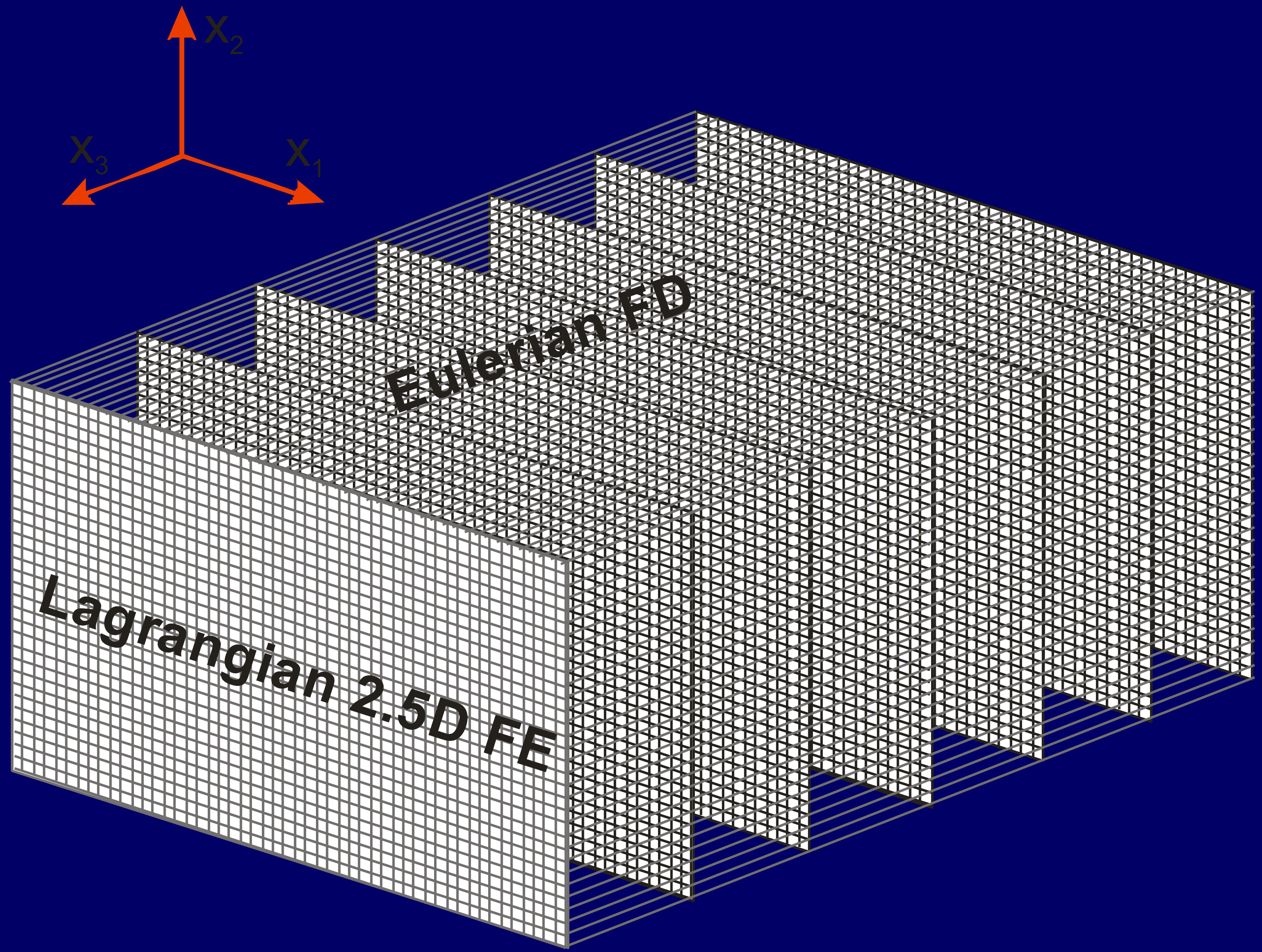
Sand-box benchmark movie



2D models		$v_3 = 0$, $\partial/\partial x_3 = 0$, $\sigma_{13} = \sigma_{23} = 0$
2.5D models		$v_3 \neq 0$, $\partial/\partial x_3 = 0$, $\sigma_{ij} \neq 0$
3D- models		$\partial/\partial x_3 \neq 0$, $\lvert\partial/\partial x_3\rvert << \lvert\partial/\partial x_{1,2}\rvert$
Fully 3D models		no restrictions

v_i – velocity vector component, σ_{ij} - stress tensor component

Simplified 3D concept.



Explicit method vs. implicit

- Advantages
  - Easy to implement, small computational efforts per time step.
  - No global matrices. Low memory requirements.
  - Even highly nonlinear constitutive laws are always followed in a valid physical way and without additional iterations.
  - Straightforward way to add new effects (melting, shear heating, ...)
  - Easy to parallelize.
- Disadvantages
  - Small technical time-step (order of a year)

Implicit ALE FEM SLIM3D

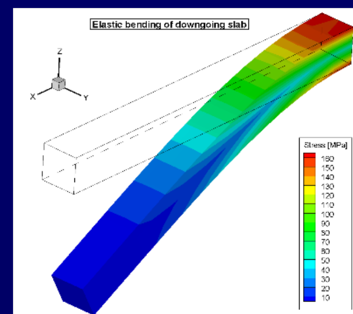
(Popov and Sobolev, 2008)

Physical background

Balance equations

Momentum: $$\frac{\partial \sigma_{ij}}{\partial x_j} + \Delta\rho g\, z_i = 0$$

Energy: $$\frac{DU}{Dt} = -\frac{\partial q_i}{\partial x_i} + r$$



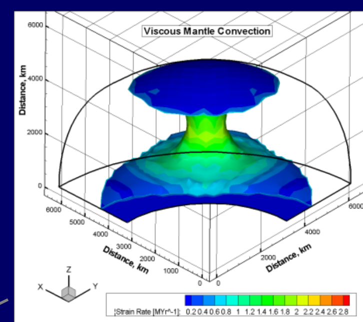
Deformation mechanisms

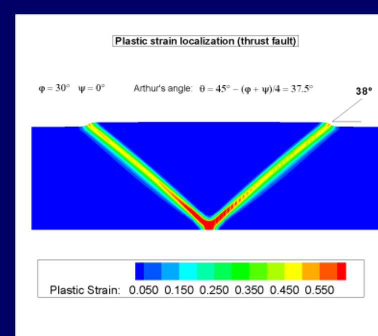
$\dot{\varepsilon}_{ij}$ $\dot{\varepsilon}_{ij}$ $\dot{\varepsilon}_{ij}$ $\dot{\varepsilon}_{ij}$

Elastic strain: $\dot{\varepsilon}_{ij}$ $\frac{1}{2G}$ $_{ij}$

Viscous strain: $\dot{\varepsilon}_{ij}$ $\frac{1}{2\eta_{eff}}\tau_{ij}$

Plastic strain: $\dot{\varepsilon}_{ij}$ $\dot{\lambda}\frac{\partial Q}{\partial \tau_{ij}}$
Mohr-Coulomb

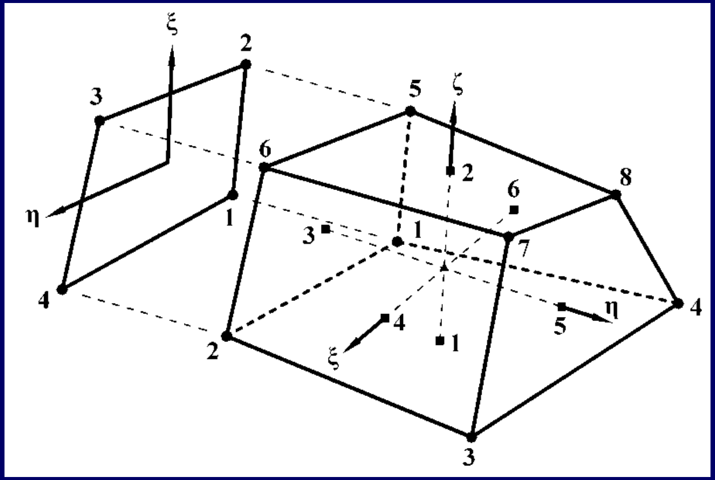




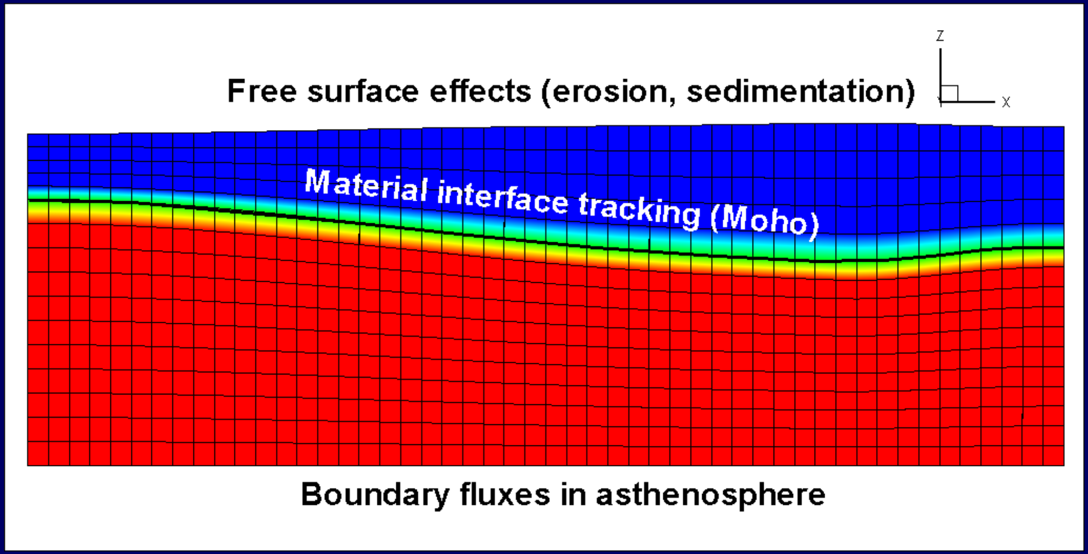
Popov and Sobolev (2008)

Numerical background

Discretization by Finite Element Method



Arbitrary Lagrangian-Eulerian kinematical formulation



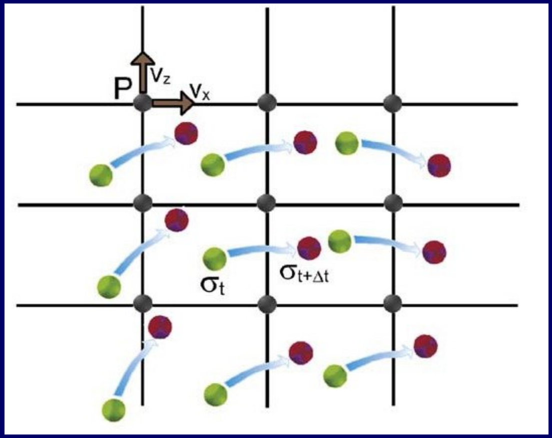
Fast implicit time stepping + Newton-Raphson solver

$$\mathbf{u}_{k+1} = \mathbf{u}_k - \mathbf{K}_k^{-1}\mathbf{r}_k$$

$\mathbf{r}$ – **Residual Vector**

$\mathbf{K} = \dfrac{\partial \mathbf{r}}{\partial \Delta \mathbf{u}}$ – **Tangent Matrix**

Remapping of entire fields by Particle-In-Cell technique



Popov and Sobolev (2008)

Finite element discretization

Interpolation and shape functions

$$(\bullet) = N^A (\bullet)^A, \quad N^A(\xi,\eta,\zeta) = \frac{1}{8}\left(1+\underline{\xi}^A\xi\right)\left(1+\underline{\eta}^A\eta\right)\left(1+\underline{\zeta}^A\zeta\right)$$

Discrete equilibrium equation

$$\int_{\Omega^e} \boldsymbol{\sigma}\cdot\mathbf{b}^A \; d\Omega^e = \int_{\Omega^e} N^A \rho\mathbf{g}\, d\Omega^e + \int_{\Gamma^e} N^A \,\bar{\mathbf{t}}\, d\Gamma^e, \quad \mathbf{b}^A = \mathrm{grad}[N^A]$$

Uniform gradient vectors + stabilization

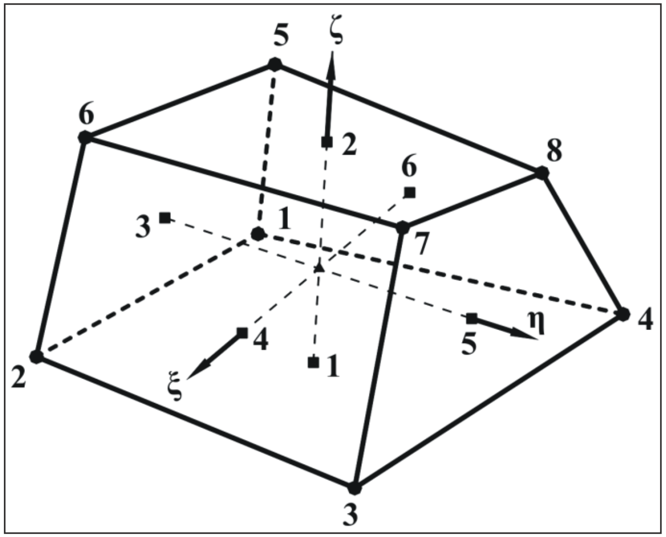
$$\tilde{\mathbf{b}}^A = \frac{1}{\Omega^e}\int_{\Omega^e} \mathbf{b}^A \; d\Omega^e, \quad \mathbf{b}^A \approx \tilde{\mathbf{b}}^A + \xi\,\partial_\xi \tilde{\mathbf{b}}^A + \eta\,\partial_\eta \tilde{\mathbf{b}}^A + \zeta\,\partial_\zeta \tilde{\mathbf{b}}^A$$

Internal force vector (reduced integration)

$$\mathbf{f}^{\mathrm{int}} = \mathop{\mathbf{A}}_{e=1}^{N_E}\left\{\frac{1}{4}\Omega^e \boldsymbol{s}\cdot\sum_{Q=1}^{4}\mathbf{b}^A\left(\xi_Q,\eta_Q,\zeta_Q\right) + \Omega^e\bar{\sigma}\,\tilde{\mathbf{b}}^A\right\}$$

External force vector (gravity and Winkler)

$$\mathbf{f}^{\mathrm{ext}} = \mathop{\mathbf{A}}_{e=1}^{N_E}\left\{\frac{1}{8}\Omega^e\rho\,\mathbf{g} + \int_{-1}^{+1}\int_{-1}^{+1} p\,N^A\,\partial_\xi\mathbf{x}\times\partial_\eta\mathbf{x}\,d\xi\,d\eta\right\}$$



Time discretization and nonlinear solution

Time discretization

$$[0, \mathrm{T}] = \bigcup_{n=1}^{\mathrm{N_S}} [t_n, t_{n+1}], \quad \Delta t = t_{n+1} - t_n$$

Displacement increment (major solution variable)

$$\Delta \mathbf{u} = \mathbf{x}_{n+1} - \mathbf{x}_n$$

Incremental stress update (strain driven problem)

$$\boldsymbol{\sigma}_{n+1} \leftarrow \wp(\boldsymbol{\sigma}_n, \ \Delta\mathbf{u}, \Delta t \ldots)$$

Nonlinear residual equation

$$\mathbf{r}_{n+1}(\Delta\mathbf{u}, t_{n+1}) = \mathbf{f}_{n+1}^{\mathrm{int}}(\Delta\mathbf{u}, t_{n+1}) - \mathbf{f}_{n+1}^{\mathrm{ext}}(\Delta\mathbf{u}, t_{n+1}) = \mathbf{0}$$

Taylor series expansion of the residual equation

$$\mathbf{r} + \mathbf{K}\,\boldsymbol{\delta}\mathbf{u} + O(\boldsymbol{\delta}\mathbf{u}^2) = \mathbf{0}, \qquad \mathbf{K} = \partial_{\boldsymbol{\delta}\mathbf{u}}\mathbf{r} - \text{tangent matrix}$$

Newton-Raphson iterative solution with line search

$$\boldsymbol{\delta}\mathbf{u}^{\{i+1\}} = -\left[\mathbf{K}^{\{i\}}(\Delta\mathbf{u}^{\{i\}})\right]^{-1}\mathbf{r}^{\{i\}}(\Delta\mathbf{u}^{\{i\}}), \qquad \Delta\mathbf{u}^{\{i+1\}} = \Delta\mathbf{u}^{\{i\}} + \alpha^{\{i+1\}}\boldsymbol{\delta}\mathbf{u}^{\{i+1\}}$$

Objective stress integration

Trial pseudo-elastic stress

$$\boldsymbol{s}^{\mathrm{tr,e}}_{n+1} = 2G\,\mathrm{dev}[\Delta\boldsymbol{\varepsilon}] + \Delta\boldsymbol{R}\,\boldsymbol{s}_n\,\Delta\boldsymbol{R}^T, \quad \bar{\sigma}^{\mathrm{tr,e}}_{n+1} = K\,\mathrm{tr}[\Delta\boldsymbol{\varepsilon}] + \bar{\sigma}_n$$

Strain increment: $\boldsymbol{h}_{n+1/2} = \Delta\mathbf{u}^A \otimes \tilde{\mathbf{b}}^A_{n+1/2}, \quad \Delta\boldsymbol{\varepsilon} = \frac{1}{2}\left(\boldsymbol{h}_{n+1/2} + \boldsymbol{h}^T_{n+1/2}\right)$

Rotation: $\Delta\boldsymbol{\omega} = \frac{1}{2}\left(\boldsymbol{h}_{n+1/2} - \boldsymbol{h}^T_{n+1/2}\right), \quad \Delta\boldsymbol{R} = \boldsymbol{1} + \left(\boldsymbol{1} - \frac{1}{2}\Delta\boldsymbol{\omega}\right)^{-1}\Delta\boldsymbol{\omega}$

Viscous stress update

$$\boldsymbol{s}^{\mathrm{tr,\,v}}_{n+1} = \beta_{\mathrm{v}}\boldsymbol{s}^{\mathrm{tr,\,e}}_{n+1}$$

$$\beta_{\mathrm{v}} \leftarrow f(\beta_{\mathrm{v}}) = (1-\beta_{\mathrm{v}})\left\|\boldsymbol{s}^{\mathrm{tr,\,e}}_{n+1}\right\| - 2G\,\Delta t\,\dot{\gamma}^{\mathrm{v}}_{n+1}\left(\beta_{\mathrm{v}}, \left\|\boldsymbol{s}^{\mathrm{tr,\,e}}_{n+1}\right\|\right) = 0$$

Plastic stress update

$$\boldsymbol{s}_{n+1} = \boldsymbol{s}^{\mathrm{tr,\,v}}_{n+1} - 2G\Delta\gamma\,\boldsymbol{n}, \quad \bar{\sigma}_{n+1} = \bar{\sigma}^{\mathrm{tr,e}}_{n+1} - K\Delta\gamma\,\kappa_{\psi}$$

$$\Delta\gamma \leftarrow f(\boldsymbol{\sigma}_{n+1}) = 0$$

Linearization and tangent operator

Global tangent matrix

$$\mathbf{K} = \mathbf{K}^{\text{int}} - \mathbf{K}^{\text{ext}} = \partial_{\boldsymbol{\delta}\mathbf{u}} \mathbf{f}^{\text{int}}_{n+1} - \partial_{\boldsymbol{\delta}\mathbf{u}} \mathbf{f}^{\text{ext}}_{n+1}$$

$$\mathbf{K}^{\text{int}} = \mathop{\mathsf{A}}_{e=1}^{N_E} \int_{\Omega^e_{n+1}} \underbrace{\left(\partial_{\Delta\boldsymbol{\varepsilon}} \boldsymbol{\sigma}_{n+1}\right) : \left(\mathbf{b}^A_{n+1} \otimes \mathbf{b}^B_{n+1}\right)}_{\text{material stiffness}} + \underbrace{\left(\mathbf{b}^A_{n+1} \cdot \boldsymbol{\sigma}_{n+1} \cdot \mathbf{b}^B_{n+1}\right) \boldsymbol{I}}_{\text{geometric stiffness}} \, \mathrm{d}\Omega^e_{n+1}$$

$$\mathbf{K}^{\text{ext}} = \mathop{\mathsf{A}}_{e=1}^{N_E} \int_{-1}^{+1}\int_{-1}^{+1} N^A N^B \, \partial_{\boldsymbol{\delta}\mathbf{u}} p_{n+1} \otimes \left(\partial_\xi \mathbf{x}_{n+1} \times \partial_\eta \mathbf{x}_{n+1}\right) \mathrm{d}\xi \, \mathrm{d}\eta$$

Consistent tangent operator

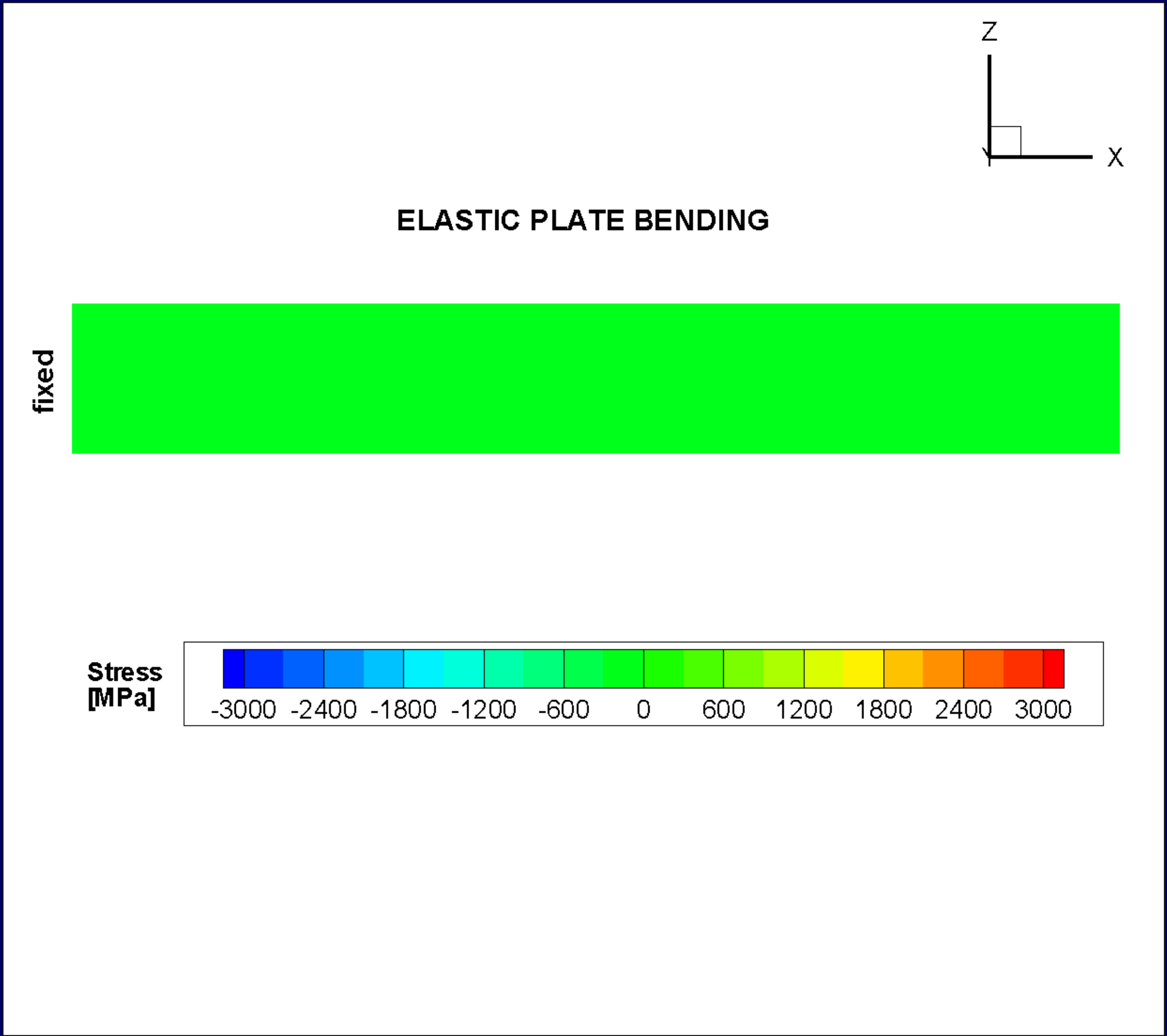
$$C^{\text{tg}} = \partial_{\Delta\boldsymbol{\varepsilon}} \boldsymbol{\sigma}_{n+1}$$

Example (Drucker-Prager model)

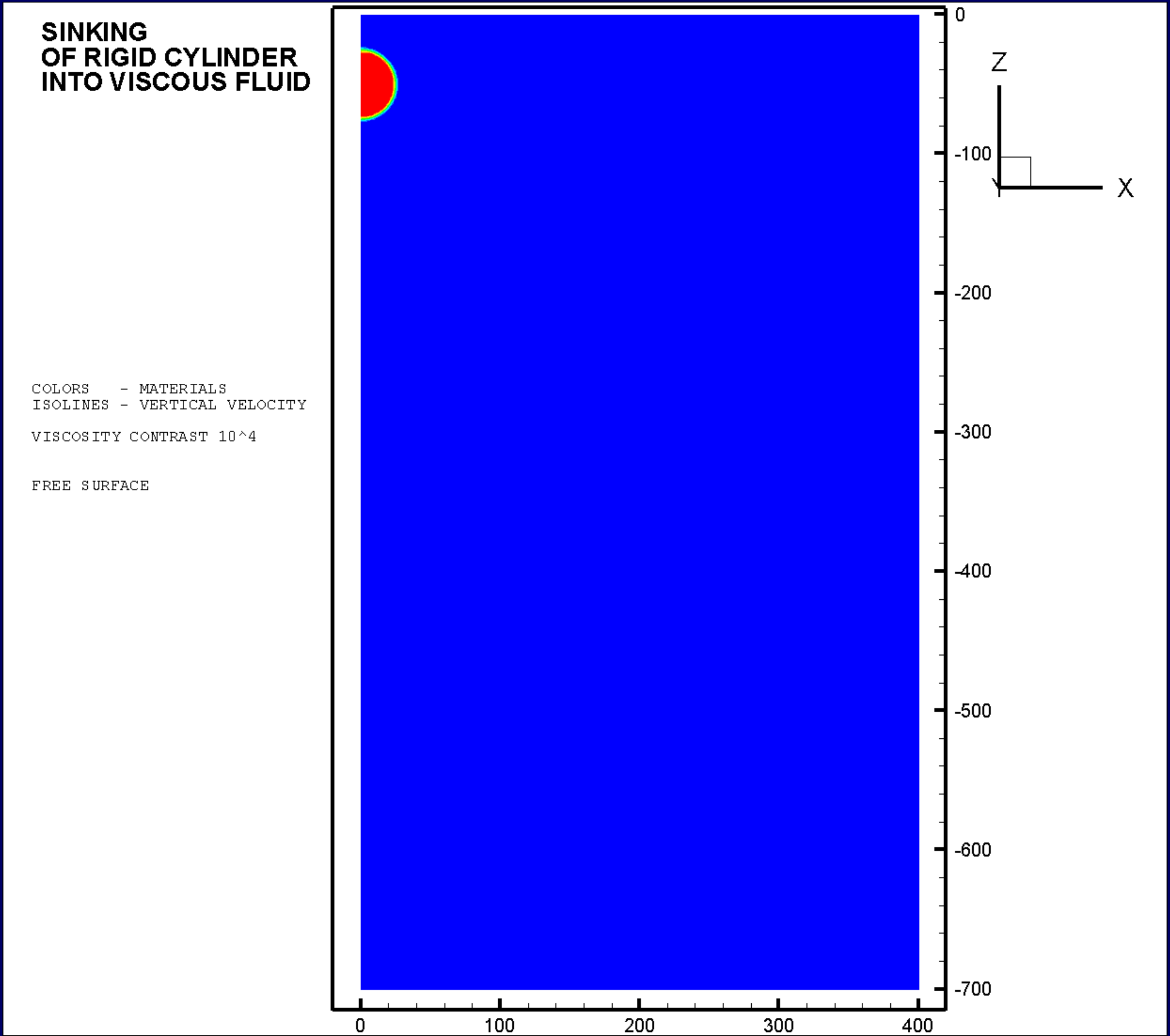
$$C^{\text{tg}} = \left(K - \kappa_\varphi \kappa_\psi \frac{K^2}{2G^*}\right) \boldsymbol{1} \otimes \boldsymbol{1} + 2G\left(1 - \frac{2G\Delta\gamma}{\left\| \boldsymbol{s}^{\text{tr, v}}_{n+1} \right\|}\right) \boldsymbol{I}^D - 2G\left(\frac{G}{G^*} - \frac{2G\Delta\gamma}{\left\| \boldsymbol{s}^{\text{tr, v}}_{n+1} \right\|}\right) \boldsymbol{n} \otimes \boldsymbol{n}$$

$$-\frac{\kappa_\varphi KG}{G^*} \boldsymbol{n} \otimes \boldsymbol{1} - \frac{\kappa_\psi KG}{G^*} \boldsymbol{1} \otimes \boldsymbol{n}, \quad \boldsymbol{I}^D = \frac{1}{2}\left(\boldsymbol{1} \,\overline{\otimes}\, \boldsymbol{1} + \boldsymbol{1} \,\underline{\otimes}\, \boldsymbol{1}\right) - \frac{1}{3} \boldsymbol{1} \otimes \boldsymbol{1}, \quad G^* = G + \frac{1}{2} \kappa_\varphi \kappa_\psi K$$

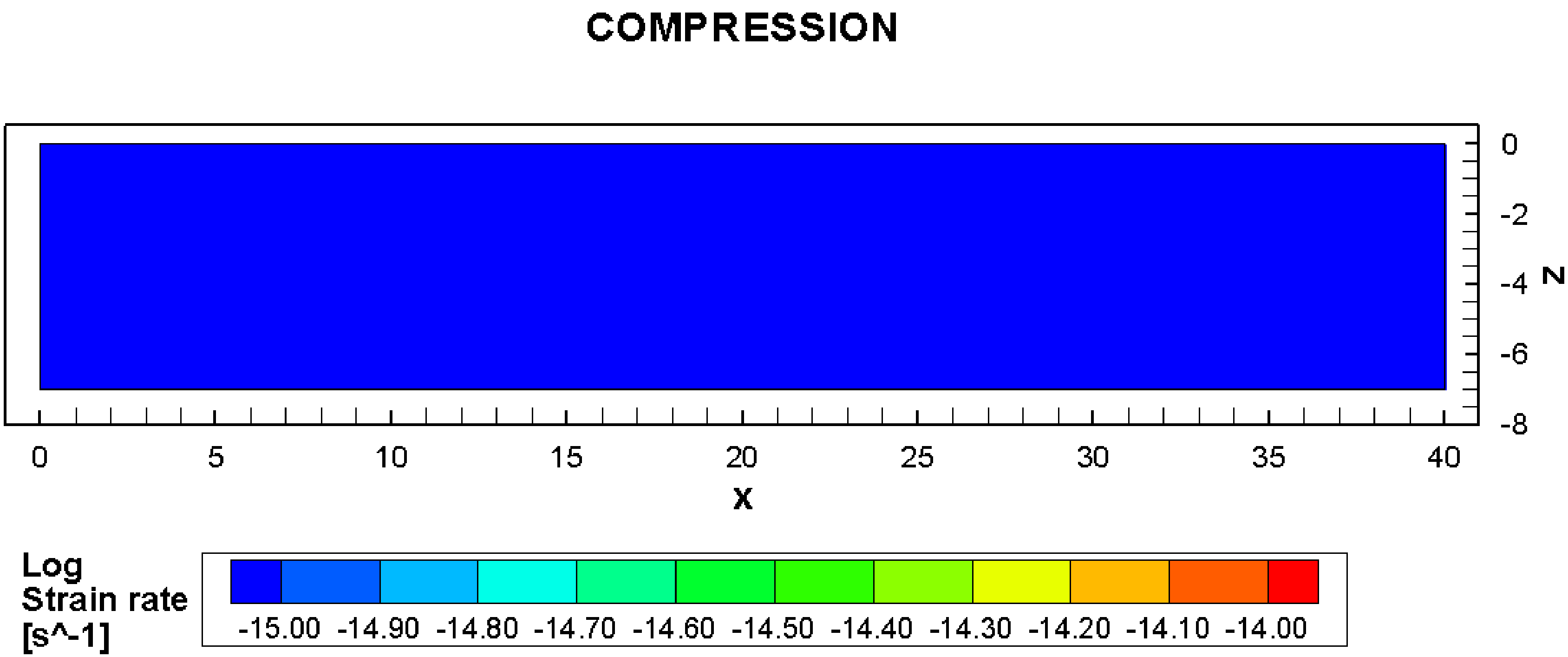
Numerical benchmarks



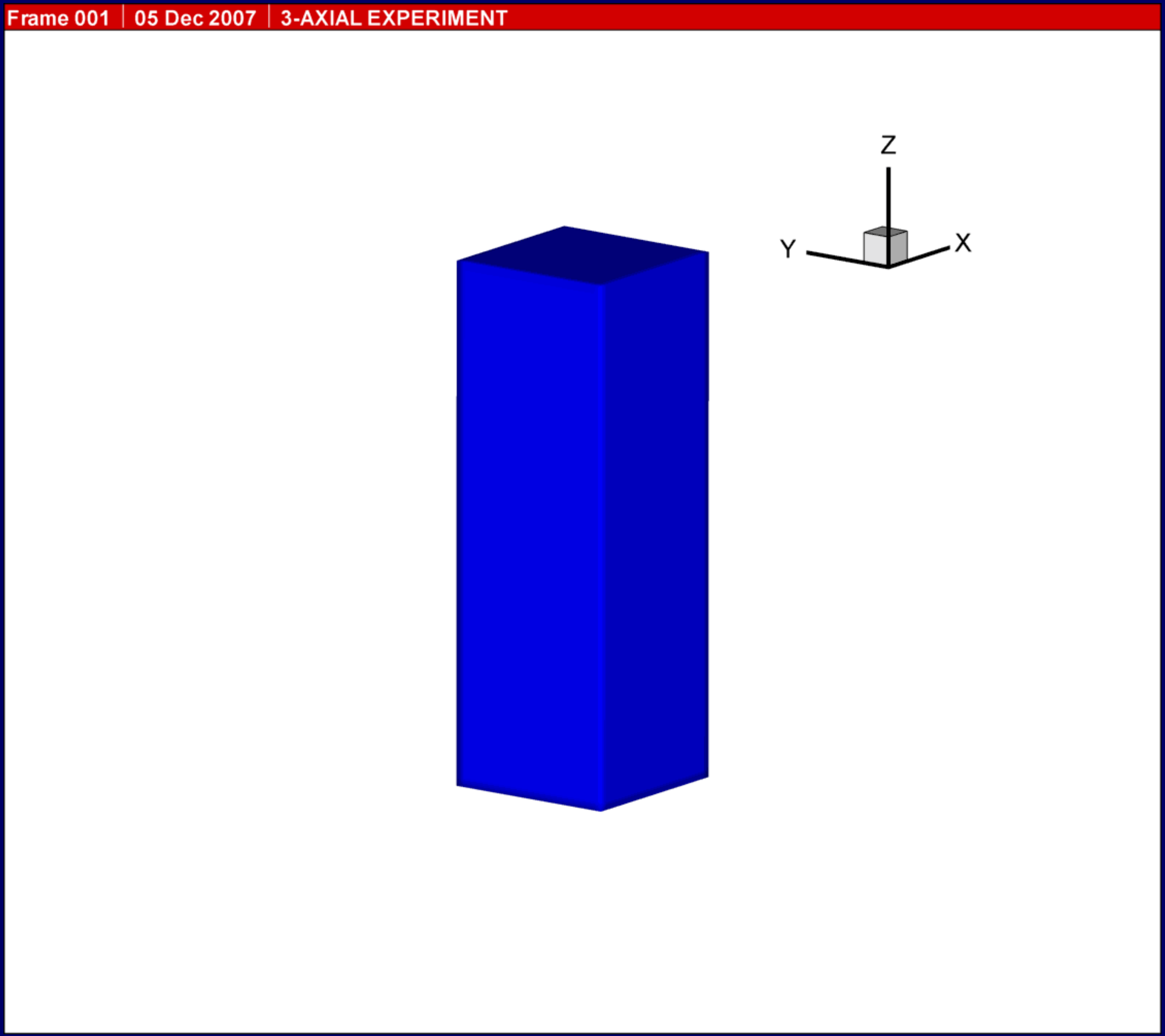
Numerical benchmarks



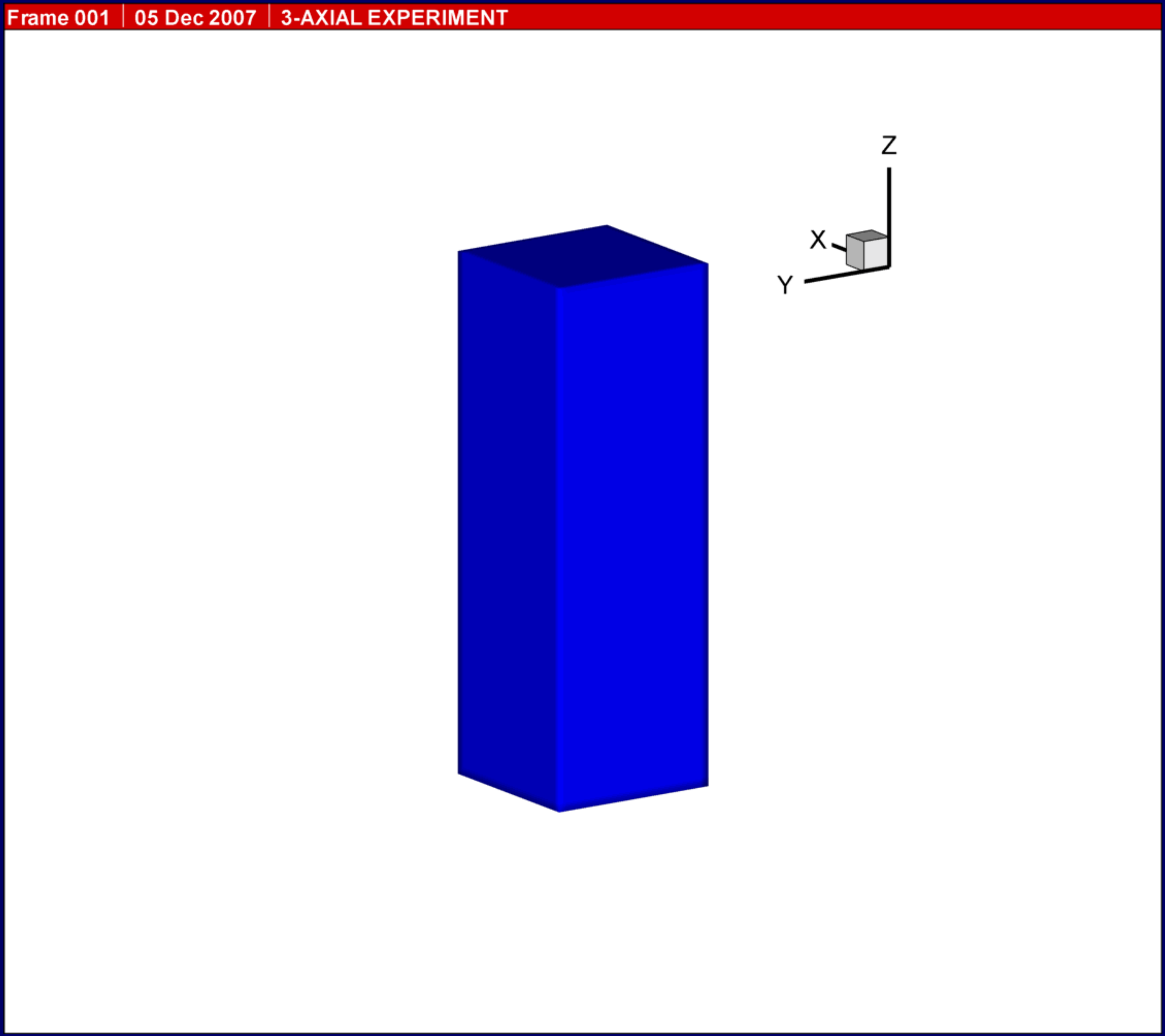
Numerical benchmarks



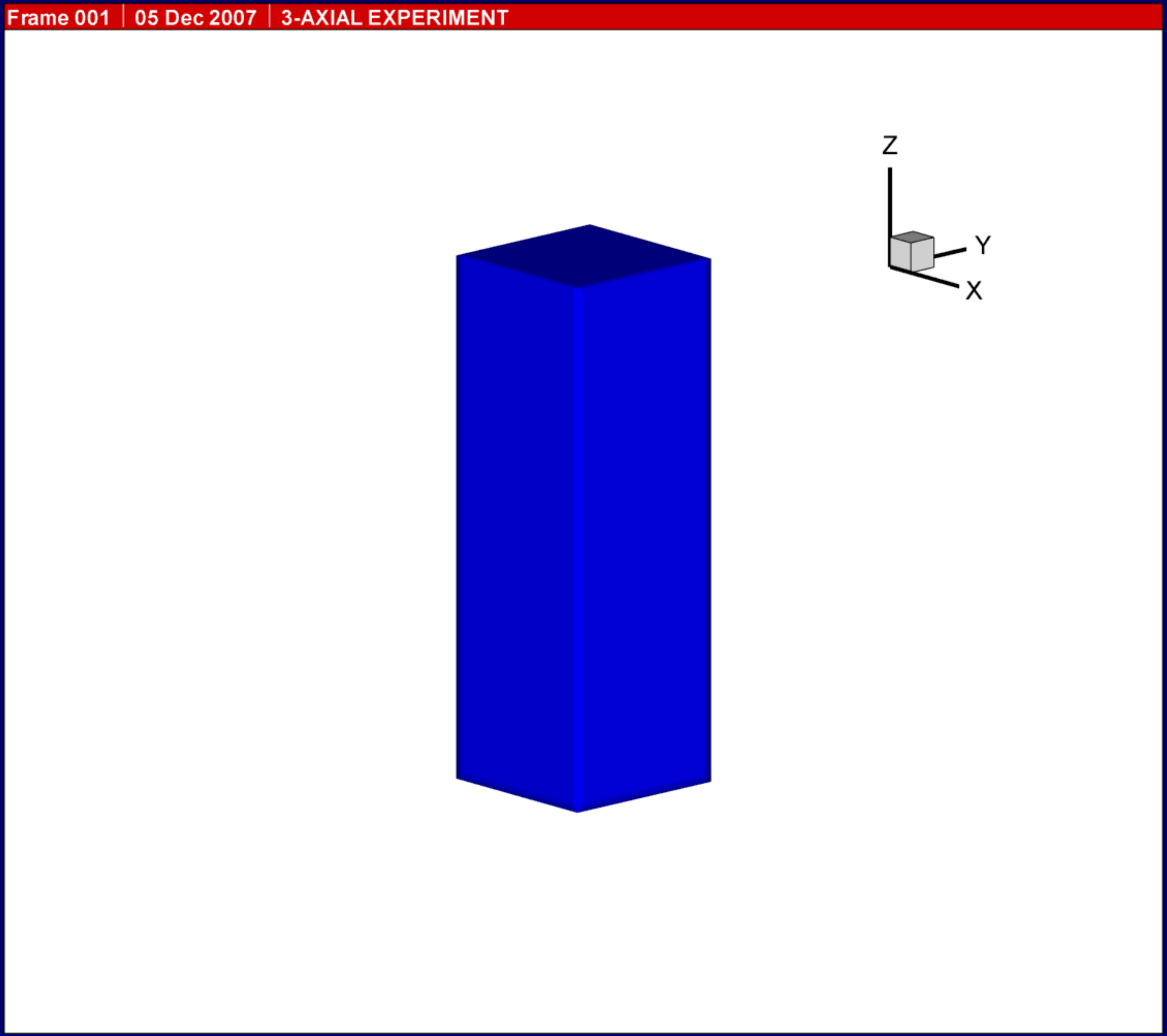
Numerical benchmarks



Numerical benchmarks

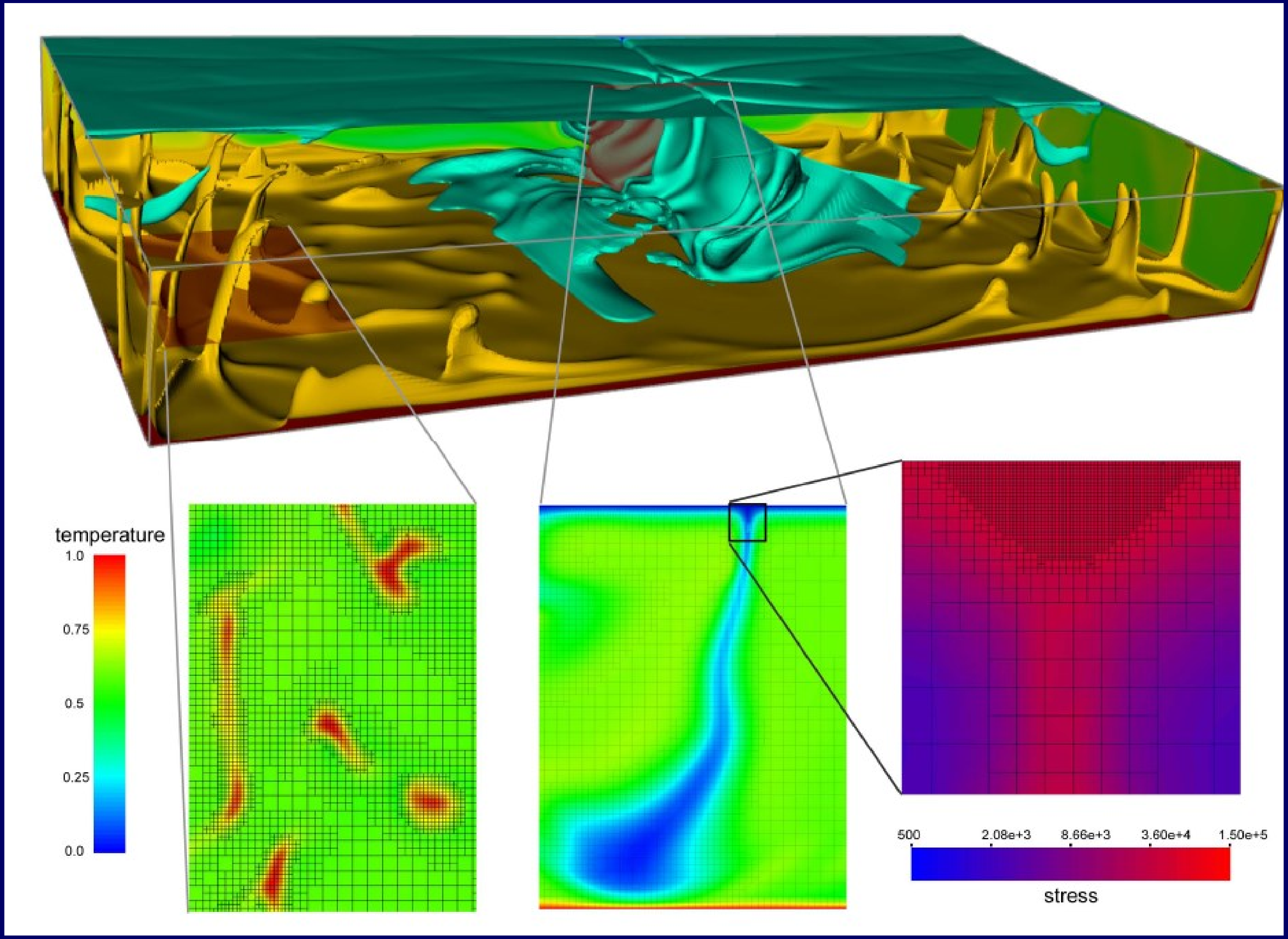


Numerical benchmarks



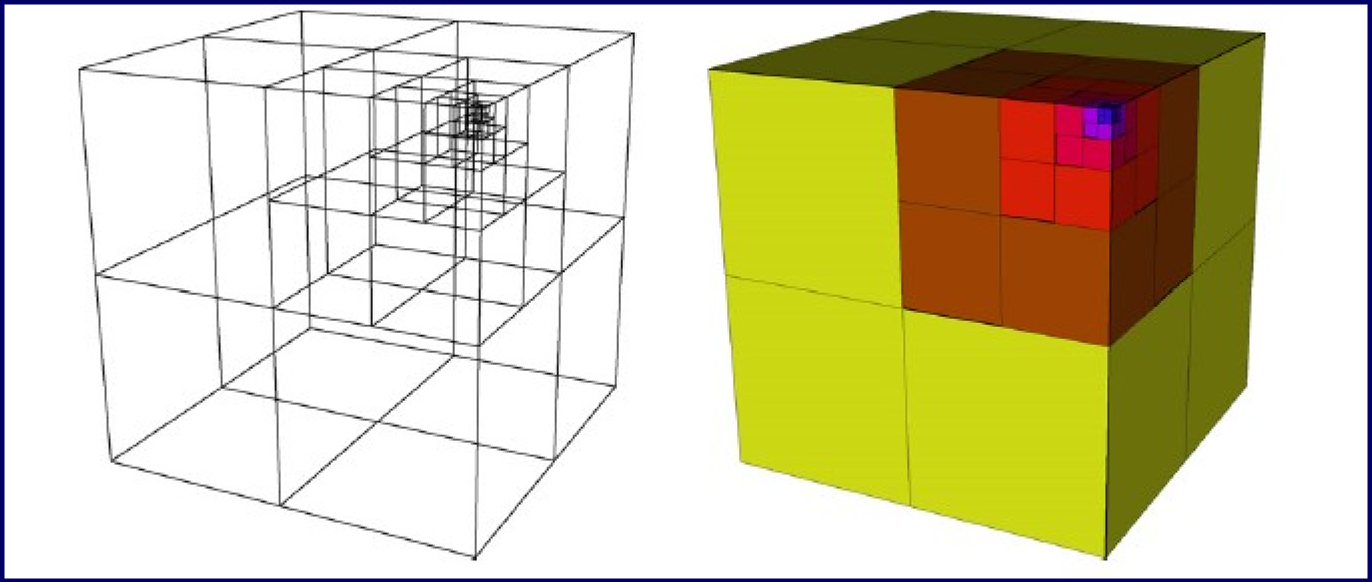
Solving Stokes equations with code Rhea and ASPECT

(adaptive mesh refinement)

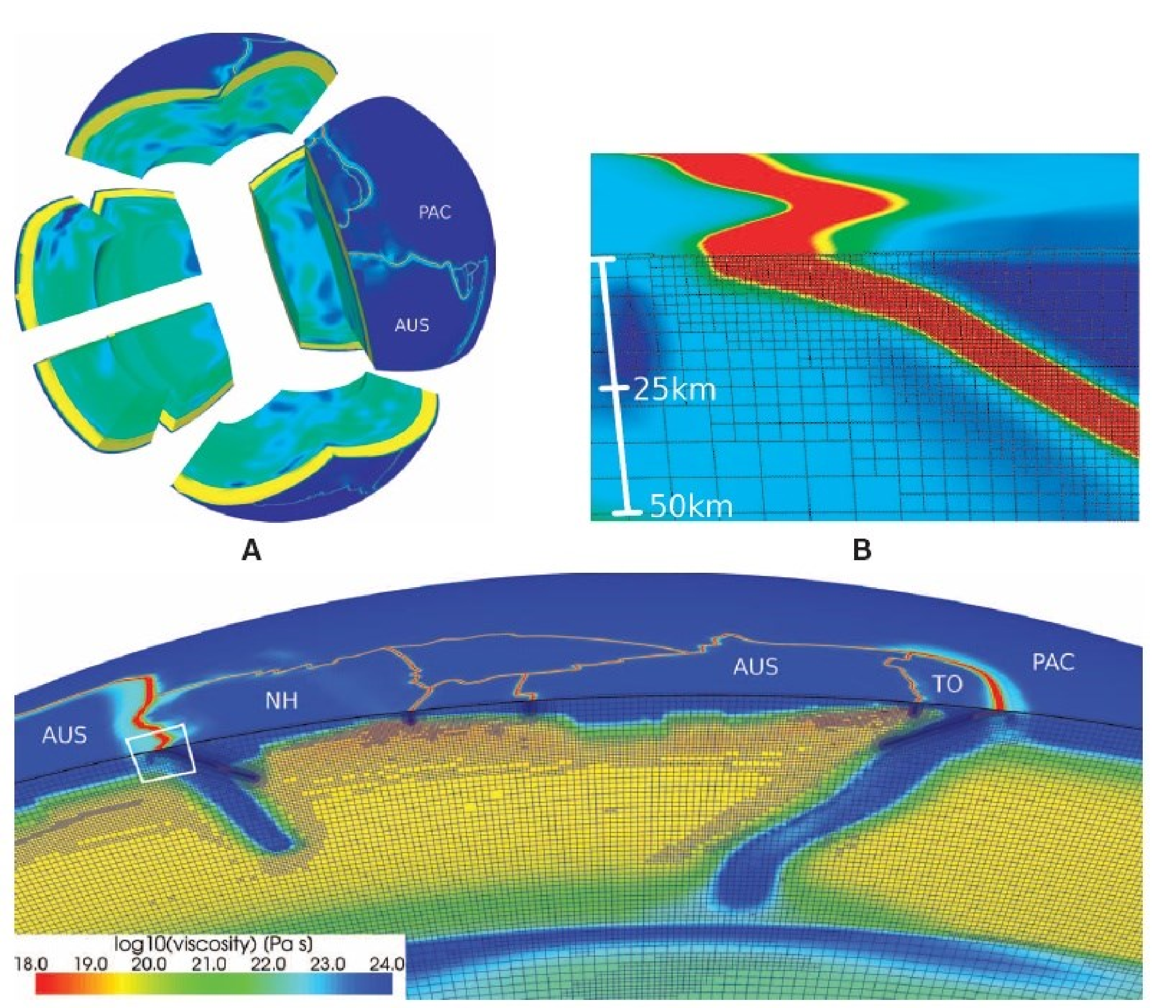


Burstedde et al.,2008-2010

Mesh refinement: octree discretization



Solving Stokes equations with codes Rhea and ASPECT



Stadler et al., 2010

Open codes

Available from CIG (http://geodynamics.org)

CitComCU. A finite element E parallel code capable of modelling thermo-chemical convection in a 3-D domain appropriate for convection within the Earth's mantle. Developed from CitCom (Moresi and Solomatov, 1995; Moresi *et al*., 1996).

CitComS.A finite element E code designed to solve thermal convection problems relevant to Earth's mantle in 3-D spherical geometry, developed from CitCom by Zhong *et al*.(2000).

Ellipsis3D. A 3-D particle-in-cell E finite element solid modelling code for viscoelastoplastic materials, as described in O'Neill *et al*. (2006).

Gale. An Arbitrary Lagrangian Eulerian (ALE) code that solves problems related to orogenesis, rifting, and subduction with coupling to surface erosion models. This is an application of the Underworld platform listed below.

PyLith . A finite element code for the solution of viscoelastic/ plastic deformation that was designed for lithospheric modeling problems.

SNAC is a L explicit finite difference code for modelling a finitely deforming elasto-visco-plastic solid in 3D.

Available from http://milamin.org/.

MILAMIN. A finite element method implementation in MATLAB that is capable of modelling viscous flow with large number of degrees of freedom on a normal computer Dabrowski *et al*. (2008).

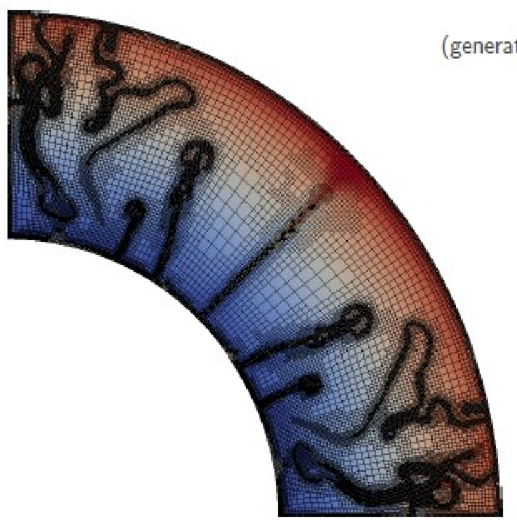
Open code Aspect

COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)

ASPECT

Advanced Solver for Problems in Earth's ConvecTion

User Manual
Version 1.2
(generated January 23, 2015)



Wolfgang Bangerth
Timo Heister
with contributions by:
Jacky Austermann, Markus Bürg, Juliane Dannberg, William Durkin, René Gaßmöller, Thomas Geenen, Anne Glerum, Ryan Grove, Eric Heien, Martin Kronbichler, Elvira Mulyukova, Jonathan Perry-Houts, Ian Rose, Cedric Thieulot, Iris van Zelst, Siqi Zhang

geodynamics.org

Full set of equations

$$\frac{1}{K}\frac{DP}{Dt}-\alpha\frac{DT}{Dt}+\frac{\partial v_i}{\partial x_i}=0$$ mass

$$-\frac{\partial P}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}+\boxed{\rho(P,T)}g_i=\rho\frac{Dv_i}{Dt}$$ momentum

$$\rho C_p\frac{DT}{Dt}=\frac{\partial}{\partial x_i}(\lambda\frac{\partial T}{\partial x_i})+\tau_{II}\dot{\varepsilon}_{II}+\rho A$$ energy

$$\dot{\varepsilon}_{ij}=\frac{1}{2}(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i})=\frac{1}{2G}\frac{D\tau_{ij}}{Dt}+\frac{1}{2\eta_{eff}}\tau_{ij}$$

Petrophysical modeling

Goals of the petrophysical modeling

To establish link between rock composition and its physical properties.

Direct problems:

prediction of the density and seismic structure (also anisotropic)

incorporation in the thermomechanical modeling

Inverse problem:

interpretation of seismic velocities in terms of composition

Petrophysical modeling

Internally-consistent dataset of thermodynamic properties of minerals and solid solutions
(Holland and Powell '90, Sobolev and Babeyko '94)

Gibbs free energy minimization algorithm
After de Capitani and Brown '88

SiO_2
Al_2O_3
Fe_2O_3
MgO + (P,T)
CaO
FeO
Na_2O
K_2O

Equilibrium mineralogical composition of a rock
given chemical composition and PT-conditions

Density and elastic properties
optionally with cracks and anisotropy

Gibbs energy

The Gibbs free energy of a multicomponent system is given by

$$G = \sum_i n_i \cdot \mu_i,$$

where n_i and μ_i are the number of moles and chemical potential of substance i (end-member of solid solution or mineral of constant composition). The chemical potential μ_i is defined by

$$\mu_i = \mu_i^0(P,T) + RT \ln a_i,$$

where μ_i^0 is the standard chemical potential, R is the gas constant and a_i is the activity (for minerals of constant composition $a_i = 1$). In solid systems the following simplified relations for standard potentials can be used (Wood (1987)):

$$\mu_i^0(P,T) = H_i^f(1000) + c_{p,i}(1000) \cdot (T - 1000) - T \cdot (S_i(1000)$$
$$+c_{p,i} \cdot \ln(T/1000)) + V_i(1,298) \cdot (1 + \alpha_i \cdot (T - 298) + \beta_i \cdot P/2) \cdot P,$$

where $H_i^f(1000)$, $S_i(1000)$ and $c_{p,i}$ (1000) are the standard enthalpy, entropy and heat capacity at T = 1000 K and P = 1 bar, V_i(1,298) is the molar volume at T = 298 K and P = 1 bar and α_i, β_i are the thermal expansion coefficient and compressibility, respectively.

Solid solutions model

$$RT \ln a_i = RT \ln x_i + RT \ln \gamma_i.$$

Here x_i is the molar fraction of end-member i in solid solution, γ_i is its activity coefficient. For plagioclase we accept an ideal contribution according to the Al-avoidance model by Kerrick and Darken (1975).

Non-ideal contributions to the activity can be expressed through binary interactions according to Bertrand *et al.* (1983):

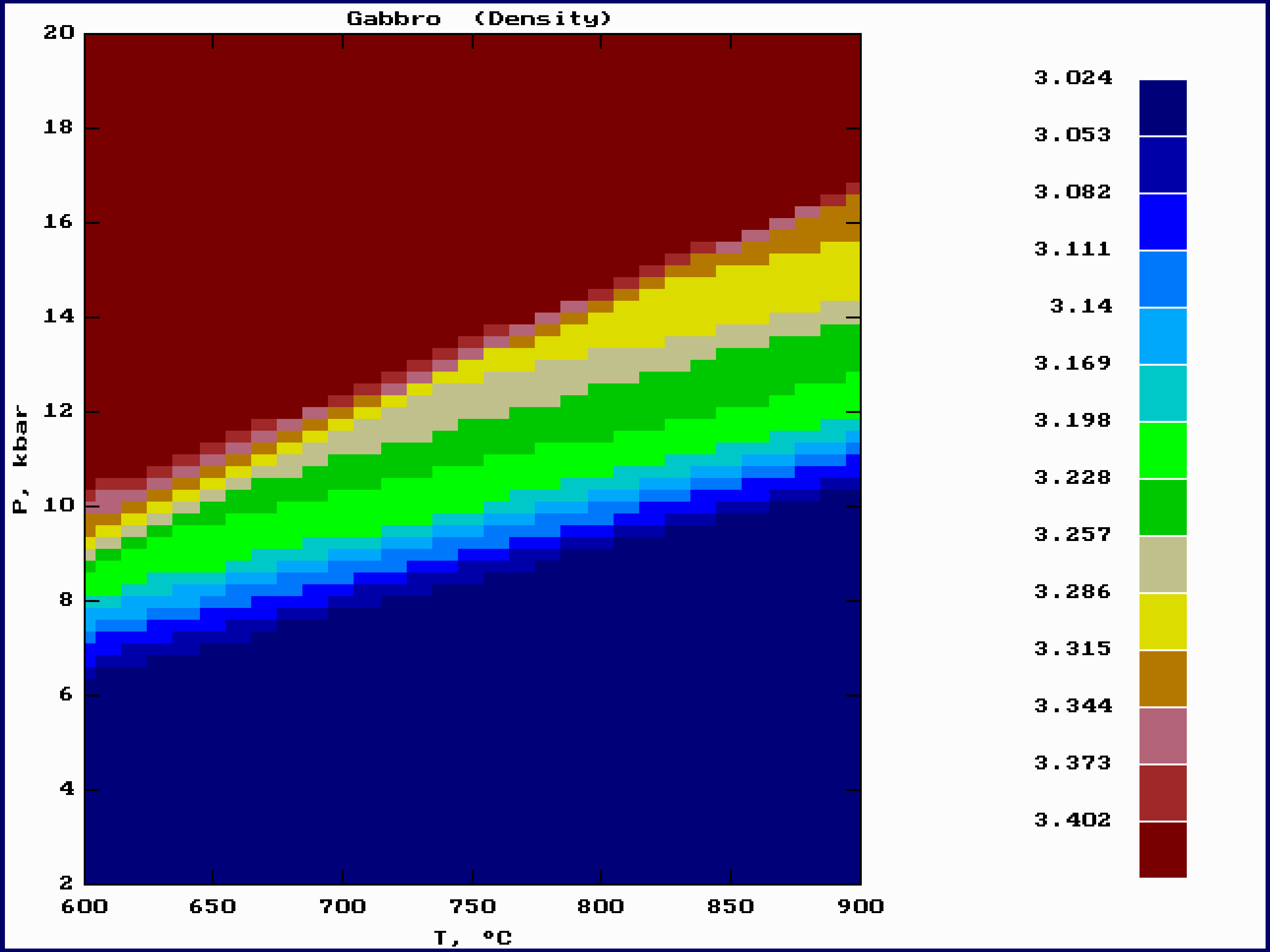
$$RT \ln \gamma_i = \sum_{j \neq i} (x_i + x_j) \cdot (RT \ln \gamma_i^{ij} + (1 - x_i - x_j) \cdot \Delta G_{ij}^{\text{ex}})$$

$$- \sum_j \sum_{k>j} (x_j + x_k) \cdot \Delta G_{jk}^{\text{ex}},$$

where

$$\Delta G_{ij}^{\text{ex}} = x_i^{ij} \cdot RT \ln \gamma_i^{ij} + x_j^{ij} \cdot RT \ln \gamma_j^{ij},$$

Density P-T diagram for average gabbro composition



Supplement: details for FEM SLIM3D (Popov and Sobolev, PEPI, 2008)

Finite element discretization

Interpolation and shape functions

$$(\bullet) = N^A (\bullet)^A, \quad N^A(\xi,\eta,\zeta) = \frac{1}{8}\left(1+\underline{\xi}^A\xi\right)\left(1+\underline{\eta}^A\eta\right)\left(1+\underline{\zeta}^A\zeta\right)$$

Discrete equilibrium equation

$$\int_{\Omega^e} \boldsymbol{\sigma}\cdot\mathbf{b}^A \, \mathrm{d}\Omega^e = \int_{\Omega^e} N^A \rho\,\mathbf{g}\, \mathrm{d}\Omega^e + \int_{\Gamma^e} N^A \,\bar{\mathbf{t}}\, \mathrm{d}\Gamma^e, \quad \mathbf{b}^A = \mathrm{grad}[N^A]$$

Uniform gradient vectors + stabilization

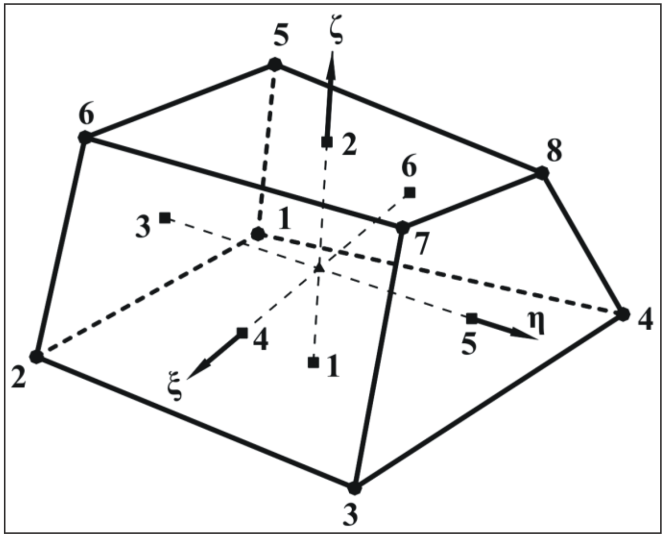
$$\tilde{\mathbf{b}}^A = \frac{1}{\Omega^e}\int_{\Omega^e}\mathbf{b}^A \,\mathrm{d}\Omega^e, \quad \mathbf{b}^A \approx \tilde{\mathbf{b}}^A + \xi\,\partial_\xi \tilde{\mathbf{b}}^A + \eta\,\partial_\eta\tilde{\mathbf{b}}^A + \zeta\,\partial_\zeta\tilde{\mathbf{b}}^A$$

Internal force vector (reduced integration)

$$\mathbf{f}^{\mathrm{int}} = \mathop{\mathbf{A}}_{e=1}^{N_E}\left\{\frac{1}{4}\Omega^e \boldsymbol{s}\cdot\sum_{Q=1}^{4}\mathbf{b}^A\left(\xi_Q,\eta_Q,\zeta_Q\right) + \Omega^e\bar{\sigma}\,\tilde{\mathbf{b}}^A\right\}$$

External force vector (gravity and Winkler)

$$\mathbf{f}^{\mathrm{ext}} = \mathop{\mathbf{A}}_{e=1}^{N_E}\left\{\frac{1}{8}\Omega^e\rho\,\mathbf{g} + \int_{-1}^{+1}\int_{-1}^{+1} p\,N^A\,\partial_\xi\mathbf{x}\times\partial_\eta\mathbf{x}\,\mathrm{d}\xi\,\mathrm{d}\eta\right\}$$



Time discretization and nonlinear solution

Time discretization

$$[0, \mathrm{T}] = \bigcup_{n=1}^{\mathrm{N_S}} [t_n, t_{n+1}], \quad \Delta t = t_{n+1} - t_n$$

Displacement increment (major solution variable)

$$\boldsymbol{\Delta}\mathbf{u} = \mathbf{x}_{n+1} - \mathbf{x}_n$$

Incremental stress update (strain driven problem)

$$\boldsymbol{\sigma}_{n+1} \leftarrow \wp\left(\boldsymbol{\sigma}_n,\ \boldsymbol{\Delta}\mathbf{u}, \Delta t \ldots\right)$$

Nonlinear residual equation

$$\mathbf{r}_{n+1}\left(\boldsymbol{\Delta}\mathbf{u}, t_{n+1}\right) = \mathbf{f}_{n+1}^{\mathrm{int}}\left(\boldsymbol{\Delta}\mathbf{u}, t_{n+1}\right) - \mathbf{f}_{n+1}^{\mathrm{ext}}\left(\boldsymbol{\Delta}\mathbf{u}, t_{n+1}\right) = \mathbf{0}$$

Taylor series expansion of the residual equation

$$\mathbf{r} + \mathbf{K}\,\boldsymbol{\delta}\mathbf{u} + O\left(\boldsymbol{\delta}\mathbf{u}^2\right) = \mathbf{0}, \qquad \mathbf{K} = \partial_{\boldsymbol{\delta}\mathbf{u}}\mathbf{r} - \text{tangent matrix}$$

Newton-Raphson iterative solution with line search

$$\boldsymbol{\delta}\mathbf{u}^{\{i+1\}} = -\left[\mathbf{K}^{\{i\}}\left(\boldsymbol{\Delta}\mathbf{u}^{\{i\}}\right)\right]^{-1}\mathbf{r}^{\{i\}}\left(\boldsymbol{\Delta}\mathbf{u}^{\{i\}}\right), \qquad \boldsymbol{\Delta}\mathbf{u}^{\{i+1\}} = \boldsymbol{\Delta}\mathbf{u}^{\{i\}} + \alpha^{\{i+1\}}\boldsymbol{\delta}\mathbf{u}^{\{i+1\}}$$

Objective stress integration

Trial pseudo-elastic stress

$$\boldsymbol{s}_{n+1}^{\mathrm{tr,e}} = 2G\,\mathrm{dev}[\Delta\boldsymbol{\varepsilon}] + \Delta\boldsymbol{R}\,\boldsymbol{s}_n\,\Delta\boldsymbol{R}^T, \quad \bar{\sigma}_{n+1}^{\mathrm{tr,e}} = K\,\mathrm{tr}[\Delta\boldsymbol{\varepsilon}] + \bar{\sigma}_n$$

Strain increment: $\boldsymbol{h}_{n+1/2} = \Delta\mathbf{u}^A \otimes \tilde{\mathbf{b}}_{n+1/2}^A, \quad \Delta\boldsymbol{\varepsilon} = \frac{1}{2}\left(\boldsymbol{h}_{n+1/2} + \boldsymbol{h}_{n+1/2}^T\right)$

Rotation: $\Delta\boldsymbol{\omega} = \frac{1}{2}\left(\boldsymbol{h}_{n+1/2} - \boldsymbol{h}_{n+1/2}^T\right), \quad \Delta\boldsymbol{R} = \boldsymbol{1} + \left(\boldsymbol{1} - \frac{1}{2}\Delta\boldsymbol{\omega}\right)^{-1}\Delta\boldsymbol{\omega}$

Viscous stress update

$$\boldsymbol{s}_{n+1}^{\mathrm{tr,\,v}} = \beta_{\mathrm{v}}\boldsymbol{s}_{n+1}^{\mathrm{tr,\,e}}$$

$$\beta_{\mathrm{v}} \leftarrow f\left(\beta_{\mathrm{v}}\right) = \left(1 - \beta_{\mathrm{v}}\right)\left\|\boldsymbol{s}_{n+1}^{\mathrm{tr,\,e}}\right\| - 2G\,\Delta t\,\dot{\gamma}_{n+1}^{\mathrm{v}}\left(\beta_{\mathrm{v}}, \left\|\boldsymbol{s}_{n+1}^{\mathrm{tr,\,e}}\right\|\right) = 0$$

Plastic stress update

$$\boldsymbol{s}_{n+1} = \boldsymbol{s}_{n+1}^{\mathrm{tr,\,v}} - 2G\Delta\gamma\,\boldsymbol{n}, \quad \bar{\sigma}_{n+1} = \bar{\sigma}_{n+1}^{\mathrm{tr,e}} - K\Delta\gamma\,\kappa_{\psi}$$

$$\Delta\gamma \leftarrow f\left(\boldsymbol{\sigma}_{n+1}\right) = 0$$

Linearization and tangent operator

Global tangent matrix

$$\mathbf{K} = \mathbf{K}^{\text{int}} - \mathbf{K}^{\text{ext}} = \partial_{\boldsymbol{\delta}\mathbf{u}} \mathbf{f}_{n+1}^{\text{int}} - \partial_{\boldsymbol{\delta}\mathbf{u}} \mathbf{f}_{n+1}^{\text{ext}}$$

$$\mathbf{K}^{\text{int}} = \mathop{\mathsf{A}}_{e=1}^{N_E} \int_{\Omega_{n+1}^e} \underbrace{\left(\partial_{\Delta\boldsymbol{\varepsilon}} \boldsymbol{\sigma}_{n+1}\right) : \left(\mathbf{b}_{n+1}^A \otimes \mathbf{b}_{n+1}^B\right)}_{\text{material stiffness}} + \underbrace{\left(\mathbf{b}_{n+1}^A \cdot \boldsymbol{\sigma}_{n+1} \cdot \mathbf{b}_{n+1}^B\right) \boldsymbol{1}}_{\text{geometric stiffness}} \, \mathrm{d}\Omega_{n+1}^e$$

$$\mathbf{K}^{\text{ext}} = \mathop{\mathsf{A}}_{e=1}^{N_E} \int_{-1}^{+1}\int_{-1}^{+1} N^A N^B \, \partial_{\boldsymbol{\delta}\mathbf{u}} p_{n+1} \otimes \left(\partial_\xi \mathbf{x}_{n+1} \times \partial_\eta \mathbf{x}_{n+1}\right) \mathrm{d}\xi \, \mathrm{d}\eta$$

Consistent tangent operator

$$C^{\text{tg}} = \partial_{\Delta\boldsymbol{\varepsilon}} \boldsymbol{\sigma}_{n+1}$$

Example (Drucker-Prager model)

$$C^{\text{tg}} = \left(K - \kappa_\varphi \kappa_\psi \frac{K^2}{2G^*}\right) \boldsymbol{1} \otimes \boldsymbol{1} + 2G\left(1 - \frac{2G\Delta\gamma}{\left\| \boldsymbol{s}_{n+1}^{\text{tr, v}} \right\|}\right) \boldsymbol{I}^D - 2G\left(\frac{G}{G^*} - \frac{2G\Delta\gamma}{\left\| \boldsymbol{s}_{n+1}^{\text{tr, v}} \right\|}\right) \boldsymbol{n} \otimes \boldsymbol{n}$$

$$-\frac{\kappa_\varphi KG}{G^*} \boldsymbol{n} \otimes \boldsymbol{1} - \frac{\kappa_\psi KG}{G^*} \boldsymbol{1} \otimes \boldsymbol{n}, \quad \boldsymbol{I}^D = \frac{1}{2}\left(\boldsymbol{1} \,\overline{\otimes}\, \boldsymbol{1} + \boldsymbol{1} \,\underline{\otimes}\, \boldsymbol{1}\right) - \frac{1}{3} \boldsymbol{1} \otimes \boldsymbol{1}, \quad G^* = G + \frac{1}{2} \kappa_\varphi \kappa_\psi K$$