# 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

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

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

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

$$\dot{\mathcal{E}}_{ij}^{d} = \frac{1}{2} \left( \frac{\partial v_{i}}{\partial x_{j}} + \frac{\partial v_{j}}{\partial x_{i}} \right) - \frac{1}{3} \delta_{ij} \frac{\partial v_{k}}{\partial x_{k}} = \frac{1}{2G} \frac{D \tau_{ij}}{Dt} + \frac{1}{2\eta_{eff} (P, T, \tau_{II})} \tau_{ij}$$

#### Final effective viscosity

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

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

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

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

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

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

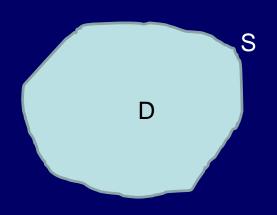
## Boundary conditions

#### General case

Boundary value problem: Lu=f,

were L 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:  $u(x,y \in S)=f1$ 

Neumann b. condition:  $\partial u / \partial \mathbf{n}$  (x,y $\in$ S)=f2– 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

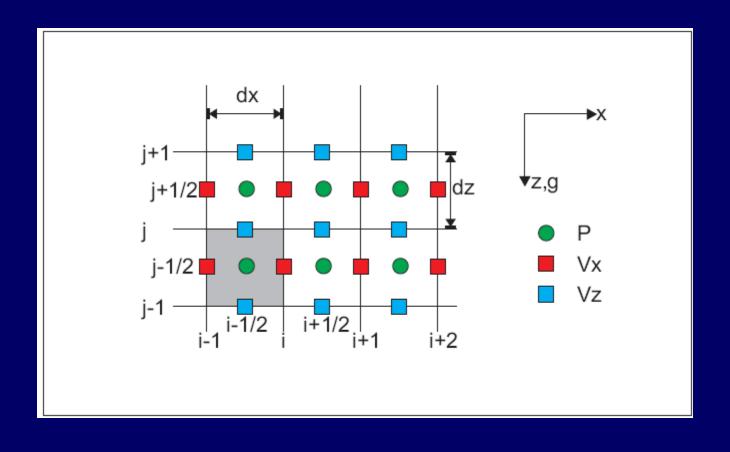
Finite Difference Method (FDM):

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

Finite Element Method (FEM):

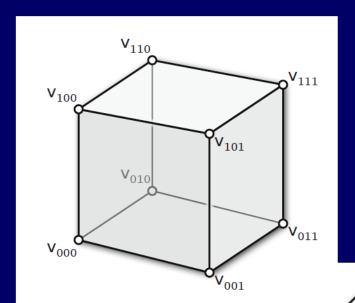
FEM uses exact operators but approximates the solution basis functions.

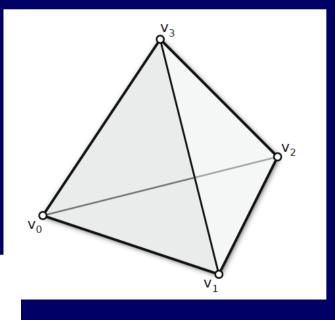
# FD Staggered grid



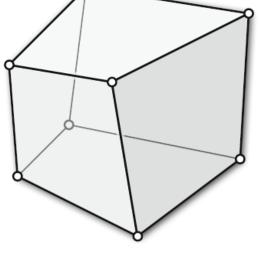
# Finite Elements

#### **Tetrahedron**

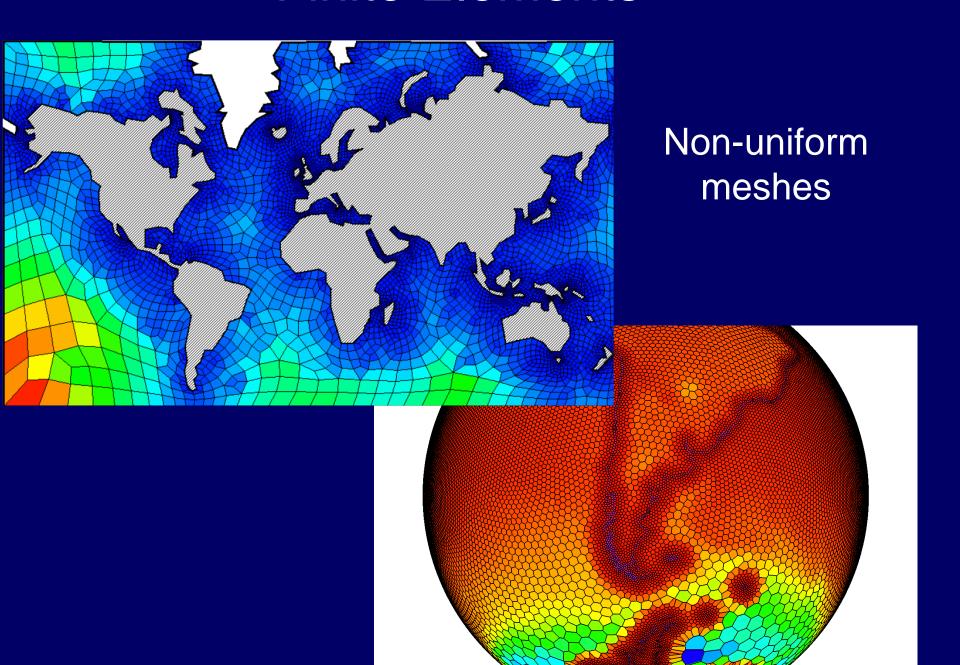




Hexahedron



# Finite Elements



# Interpolating Functions

nnod – number of degrees of freedom

Approximate solutions  $\ nnod$ 

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

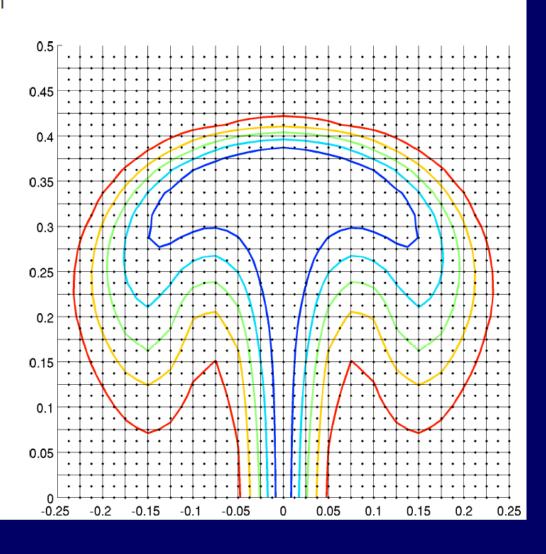
$$(\tilde{u}_y)x, y) = \sum_{i=1}^{nnod} N_i(x, y) u_y^i$$

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

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.

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

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

#### Should be:

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

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

## Explicit approximation:

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

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

## Explicit approximation:

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

#### Modified FLAC = LAPEX

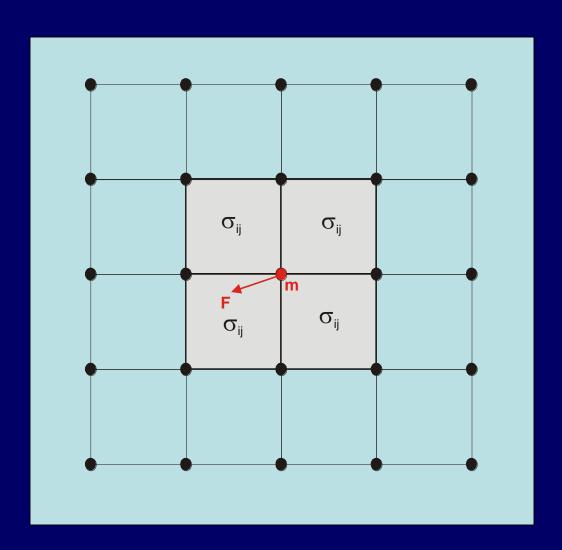
(Babeyko et al, EPSL2002)

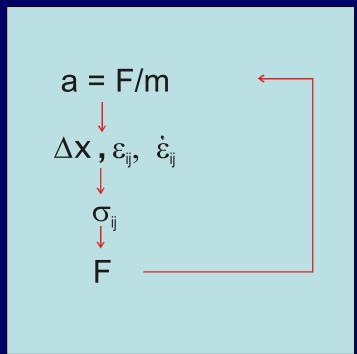
#### **Dynamic relaxation:**

$$-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i = \rho_{iner} \frac{D v_i}{D t},$$

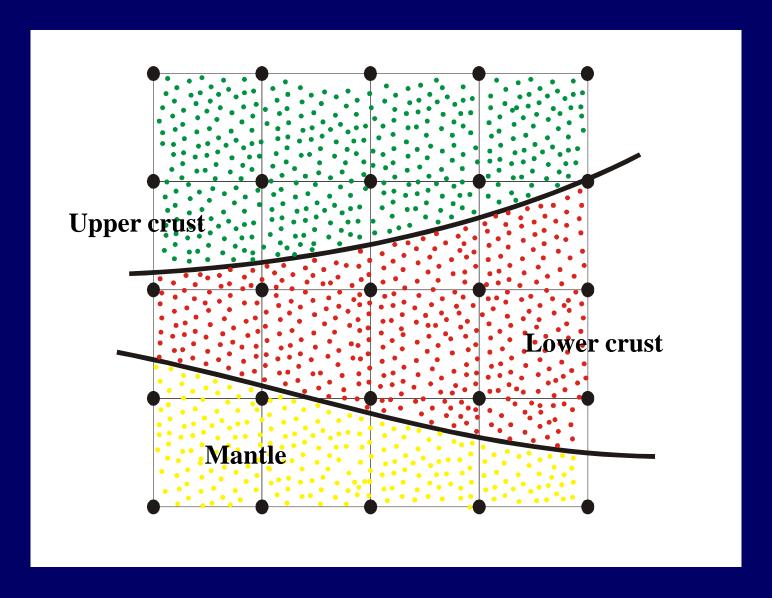
$$\left\| 
ho_{iner} \, rac{D v_i}{D t} 
ight\| << F_{tecto}$$

#### Explicit finite element method



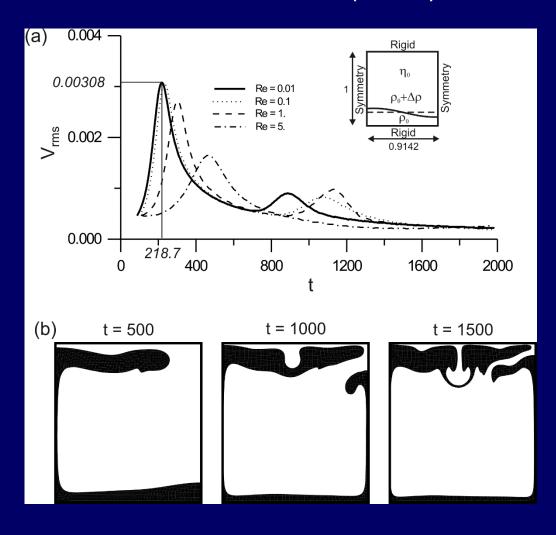


#### Markers track material and history properties

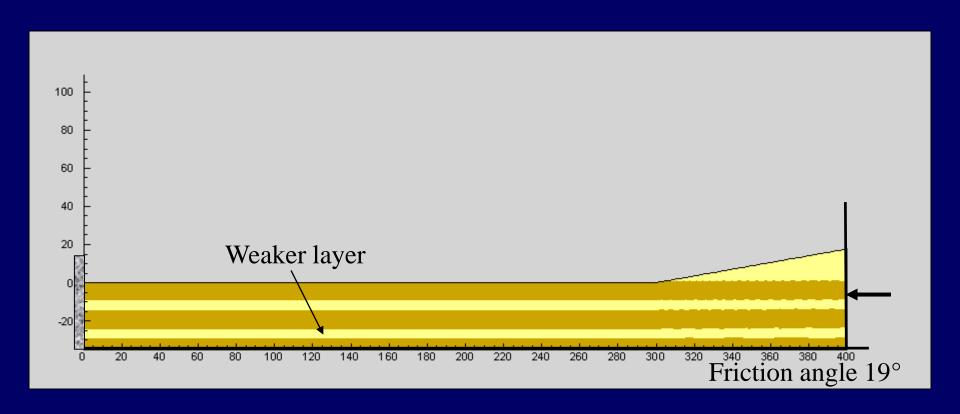


## Benchmark: Rayleigh-Taylor instability

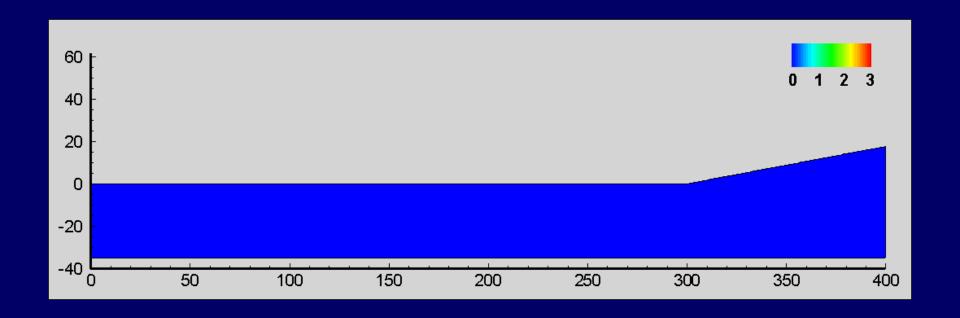
van Keken et al. (1997)

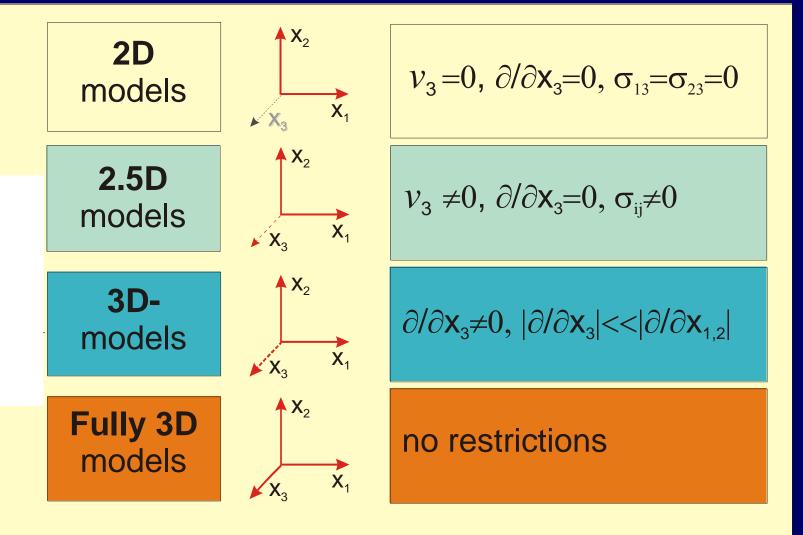


#### Sand-box benchmark movie



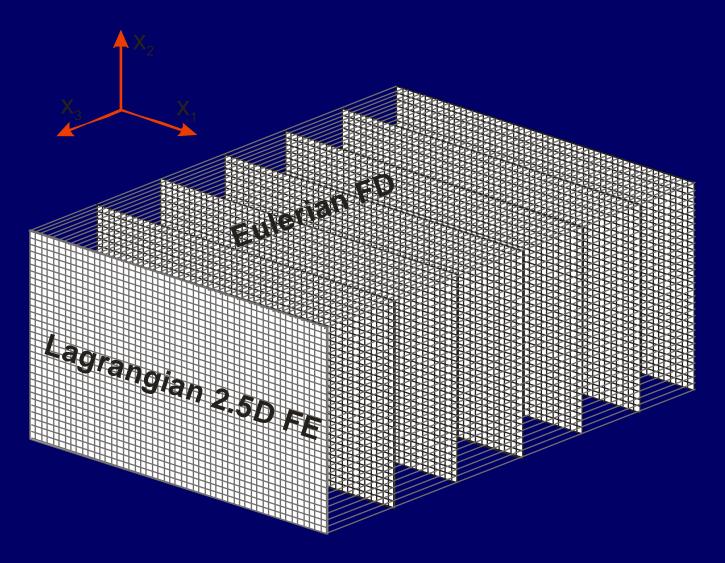
#### Sand-box benchmark movie





 $\mathcal{V}_{i}$  - velocity vector component,  $\sigma_{ij}$  - 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

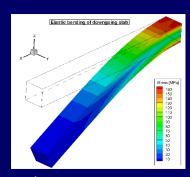
(Popov and Sobolev, 2008)

#### Physical background

#### Balance equations

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

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



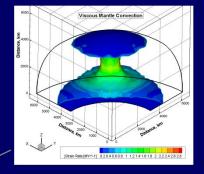
#### **Deformation mechanisms**

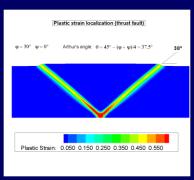
$$\dot{\mathcal{E}}_{ij} = \dot{\mathcal{E}}^{el}_{ij} + \dot{\mathcal{E}}^{vs}_{ij} + \dot{\mathcal{E}}^{pl}_{ij}$$

Elastic strain:  $\dot{\varepsilon}_{ij}^{el} = \frac{1}{2G} \hat{\tau}_{ij}$ 

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

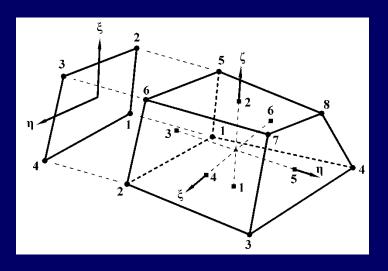
Plastic strain:  $\dot{\varepsilon}_{ij}^{pl} = \dot{\gamma} \frac{\partial Q}{\partial \tau_{ij}}$  
Mohr-Coulomb





#### Numerical background

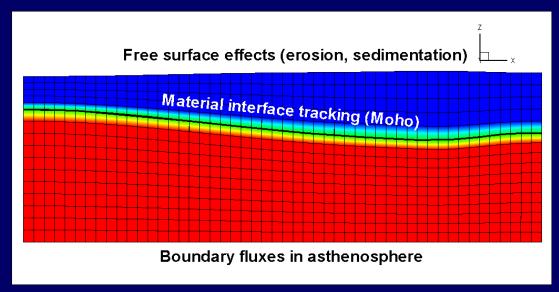
Discretization by Finite Element Method



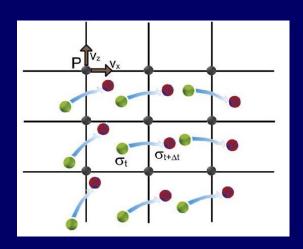
Fast implicit time stepping + Newton-Raphson solver

$$\mathbf{u}_{k+1} = \mathbf{u}_k - \mathbf{K}_k^{-1} \mathbf{r}_k$$
 $\mathbf{r} - \mathbf{Residual Vector}$ 
 $\mathbf{K} = \frac{\partial \mathbf{r}}{\partial \Delta \mathbf{u}} - \mathbf{Tangent Matrix}$ 

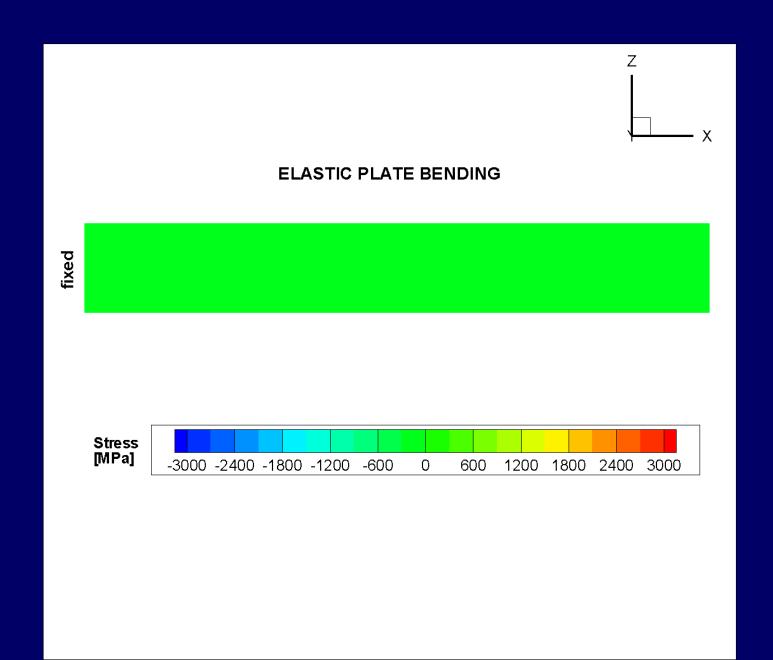
Arbitrary Lagrangian-Eulerian kinematical formulation

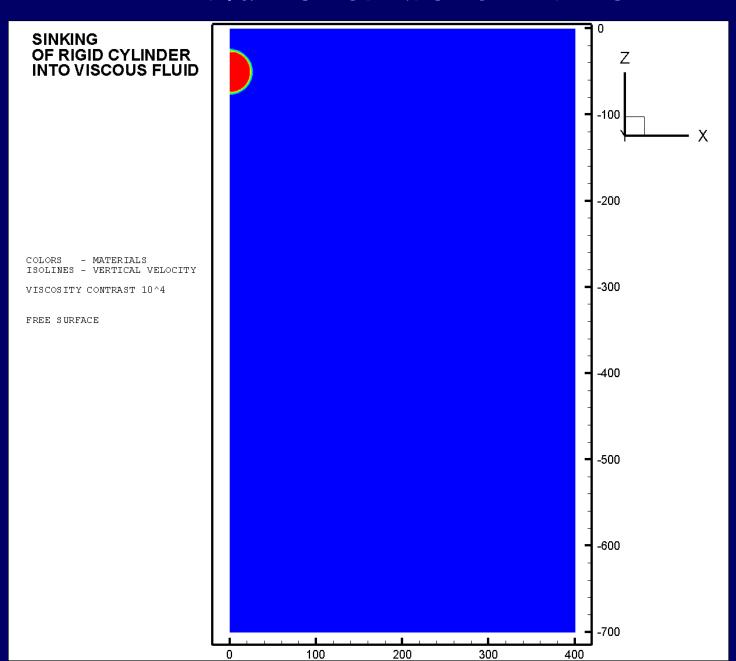


Remapping of entire fields by Particle-In-Cell technique

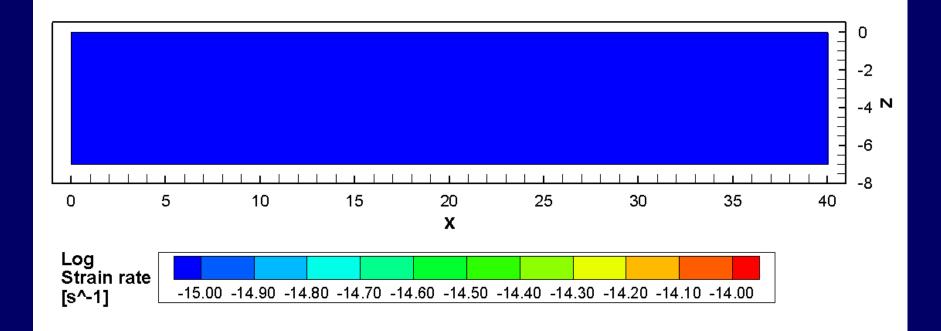


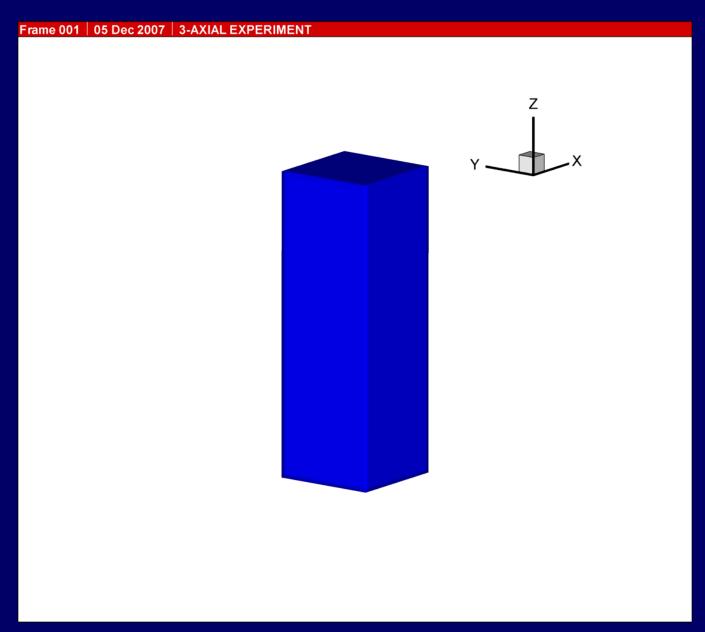
Popov and Sobolev (2008)

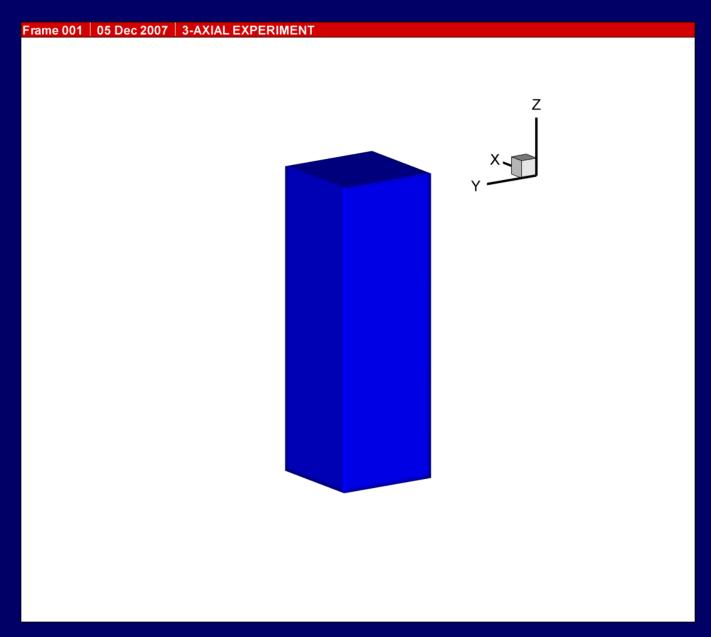


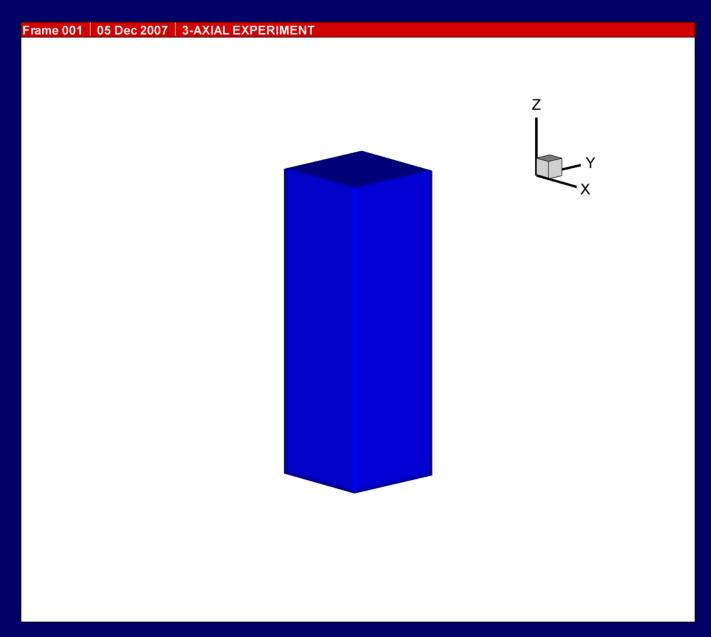


#### COMPRESSION

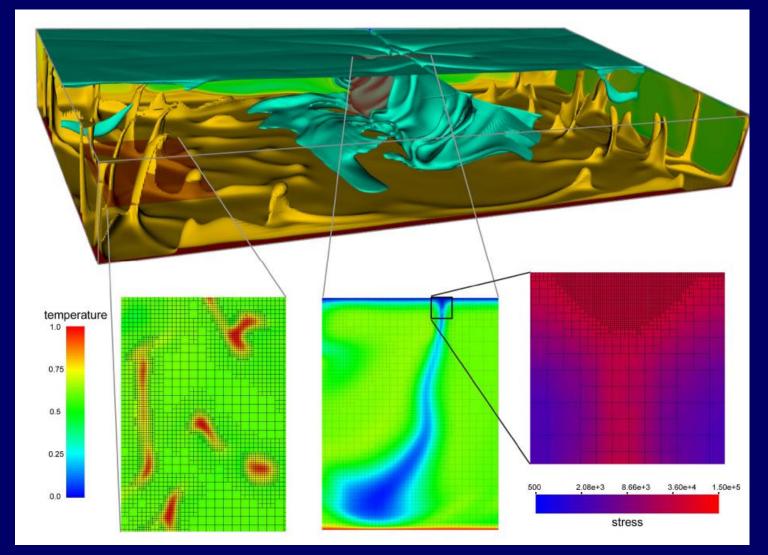






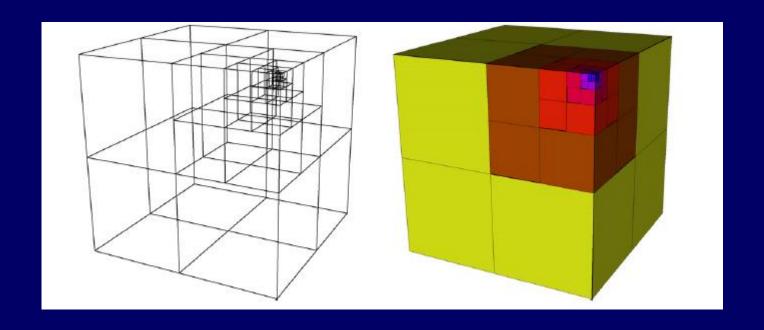


# Solving Stokes equations with code Rhea (adaptive mesh refinement similar to ASPECT)

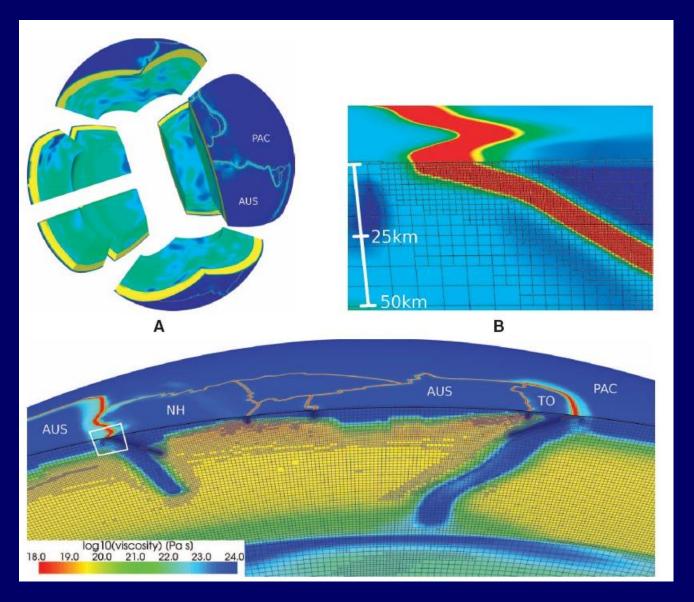


Burstedde et al.,2008-2010

## Mesh refinement: octree discretization



### Solving Stokes equations with code Rhea



# Open codes

#### Available from CIG (<a href="http://geodynamics.org">http://geodynamics.org</a>)

**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 small-strain lithospheric modeling problems.

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

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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

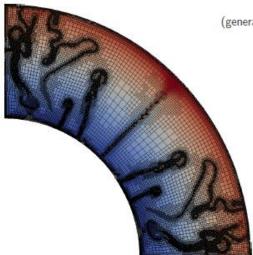
COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)

# 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, <u>Juliane Dannberg</u>, William Durkin, <u>René Gaßmöller</u>. Thomas Geenen, Anne Glerum, Ryan Grove, Eric Heien, Martin Kronbichler, <u>Elvira Mulyukova</u>, Jonathan Perry-Houts, Ian Rose, Cedric Thieulot, Iris van Zelst, Siqi Zhang

geodynamics.org

## Full set of equations

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

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

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

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

# 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<sub>2</sub>O<sub>3</sub>

MgO + (P,T)

CaO

FeO

Na<sub>2</sub>O

 $K_2O$ 



Density and elastic properties optionally with cracks and anisotropy

given chemical composition and PT-conditions

### 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  $\mu_i$  are the number of moles and chemical potential of substance i (end-member of solid solution or mineral of constant composition). The chemical potential  $\mu_i$  is defined by

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

where  $\mu_i^0$  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  $\alpha_i$ ,  $\beta_i$  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,  $\gamma_i$  is its activity coefficient. For plagioclase we accept an ideal contribution according to the Alavoidance model by Kerrick and Darken (1975).

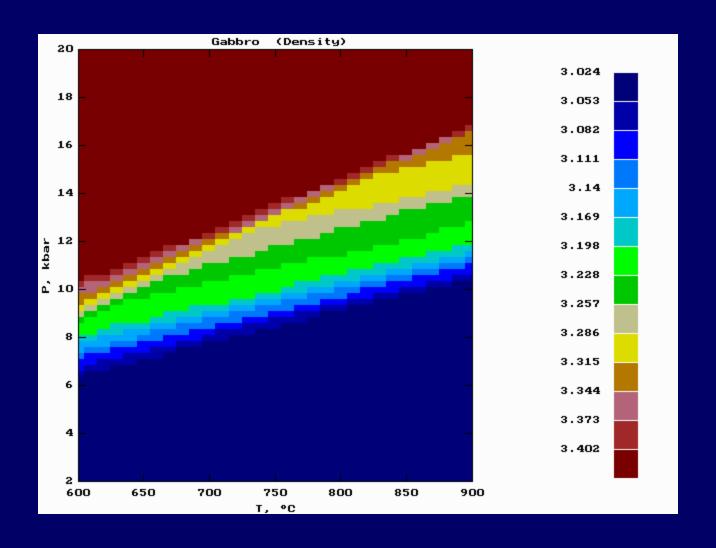
Non-ideal contributions to the activity can be expressed through binary interactions according to Bertrand *et al.* (1983):

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

where

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

## Density P-T diagram for average gabbro composition



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

# Finite element discretization (SLIM3D)

#### 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

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

### **Uniform gradient vectors + stabilization**

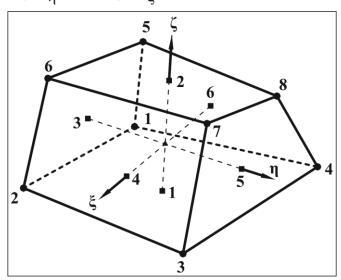
$$\tilde{\mathbf{b}}^{A} = \frac{1}{\mathbf{O}^{e}} \int_{\Omega^{e}} \mathbf{b}^{A} d\Omega^{e}, \quad \mathbf{b}^{A} \approx \tilde{\mathbf{b}}^{A} + \xi \partial_{\xi} \tilde{\mathbf{b}}^{A} + \eta \partial_{\eta} \tilde{\mathbf{b}}^{A} + \zeta \partial_{\zeta} \tilde{\mathbf{b}}^{A}$$

### Internal force vector (reduced integration)

$$\mathbf{f}^{\text{int}} = \mathbf{A}_{e=1}^{N_E} \left\{ \frac{1}{4} \Omega^e \mathbf{s} \cdot \sum_{Q=1}^{4} \mathbf{b}^A \left( \boldsymbol{\xi}_Q, \boldsymbol{\eta}_Q, \boldsymbol{\zeta}_Q \right) + \Omega^e \boldsymbol{\bar{\sigma}} \, \tilde{\mathbf{b}}^A \right\}$$

### External force vector (gravity and Winkler)

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



# Time discretization and nonlinear solution (SLIM3D)

#### Time discretization

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

Displacement increment (major solution variable)

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

Incremental stress update (strain driven problem)

Nonlinear residual equation

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

Taylor series expansion of the residual equation

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

Newton-Raphson iterative solution with line search

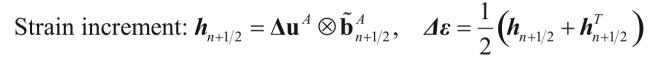
$$\delta \mathbf{u}^{\{i+1\}} = - \left[ \mathbf{K}^{\{i\}} \left( \Delta \mathbf{u}^{\{i\}} \right) \right]^{-1} \mathbf{r}^{\{i\}} \left( \Delta \mathbf{u}^{\{i\}} \right), \qquad \Delta \mathbf{u}^{\{i+1\}} = \Delta \mathbf{u}^{\{i\}} + \alpha^{\{i+1\}} \delta \mathbf{u}^{\{i+1\}}$$

$$\Delta \mathbf{u}^{\{i+1\}} = \Delta \mathbf{u}^{\{i\}} + \alpha^{\{i+1\}} \delta \mathbf{u}^{\{i+1\}}$$

# Objective stress integration (SLIM3D)

#### **Trial pseudo-elastic stress**

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



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



#### Viscous stress update

$$oldsymbol{s}_{n+1}^{ ext{tr, v}} = eta_{ ext{v}} oldsymbol{s}_{n+1}^{ ext{tr, e}}$$

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



#### Plastic stress update

$$\mathbf{s}_{n+1} = \mathbf{s}_{n+1}^{\text{tr, v}} - 2G\Delta\gamma \, \mathbf{n}, \quad \overline{\sigma}_{n+1} = \overline{\sigma}_{n+1}^{\text{tr, e}} - K\Delta\gamma \, \kappa_{\psi}$$
$$\Delta\gamma \leftarrow f\left(\boldsymbol{\sigma}_{n+1}\right) = 0$$





# Linearization and tangent operator (SLIM3D)

### **Global tangent matrix**

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

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

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

### Consistent tangent operator

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

### **Example (Drucker-Prager model)**

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

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