European Research Council





DERDW Departement Erdwissenschaften

Numerical techniques for thermomechanical-fluid-flow modelling

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¹ETH Zürich.

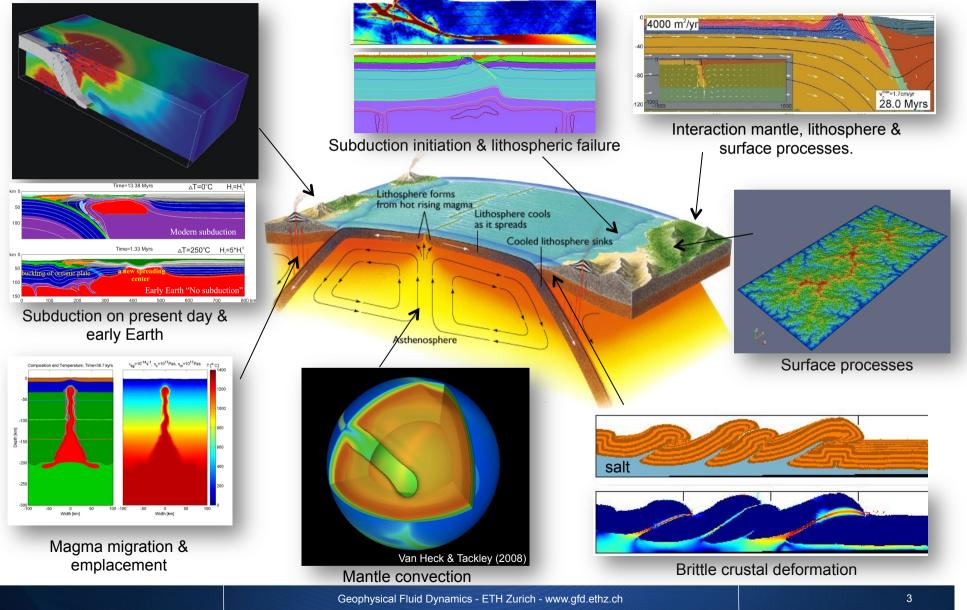
*Johannes-Gutenberg University Mainz (Germany) from next week onwards.

Outline

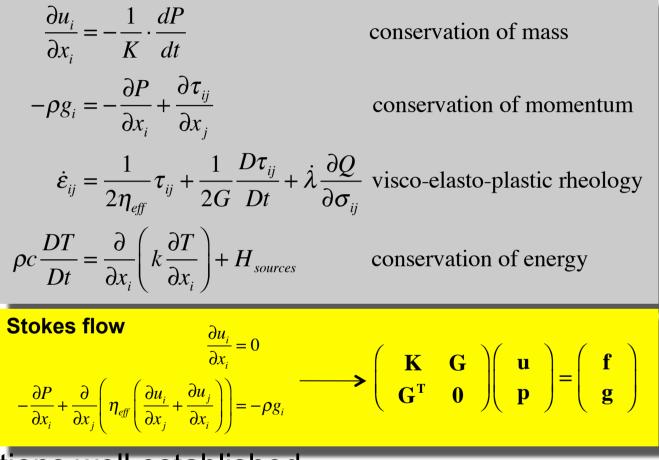
- Modelling of lithospheric deformation
 - Techniques
 - Progress
 - Challenges
- FEM or Finite Differences: what is better?
 - Accuracy, memory usage
 - Effect of element types
- Two-phase flow formulations coupled to lithospheric problems.



The Earth is a dynamical system



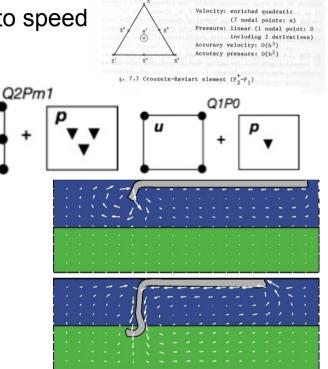
Equations for mantle & lithosphere deformation



- Equations well established
- Typically need to be solved numerically
- Often reduced to variable viscosity Stokes problem

2D Lithospheric deformation: FEM - MILAMIN_VEP

- Uses MILAMIN technology (Dabrowski et al. 2008) to speed up matrix assembly phase.
- Visco-elasto-plastic rheology.
- Unstructured OR structured finite elements.
- Q₁P₀, Q₂P₋₁, T₂P₋₁.
- Free surface.
- Thermo-mechanical coupling.
- Tracer-based or contour-based material properties
- Lagrangian with remeshing for large deformations
- Phase transitions.
- Set of MATLAB functions.
- Different setups have different needs -> easy to 'build' your own code using existing functions.
- Routinely being used by various people over the last few years.
- Disadvantages: 2D only, serial, uses direct solvers.



MILAMIN_VEP solver

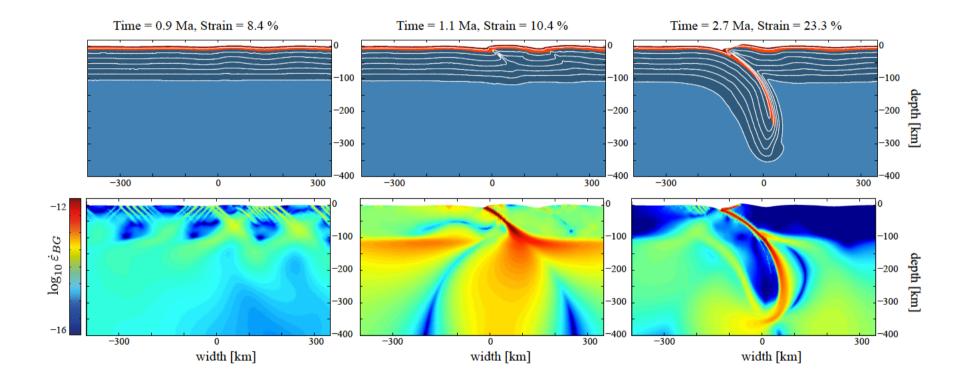
$$\begin{pmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{G}^{\mathrm{T}} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}$$
$$\begin{pmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{G}^{\mathrm{T}} & -\frac{1}{\kappa\Delta t} \mathbf{M}_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p}^{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} - \frac{1}{\kappa\Delta t} \mathbf{M}_{\mathbf{p}} \mathbf{p}^{n} \end{pmatrix}$$

Iterated penalty method / Powell Hesteness iterations

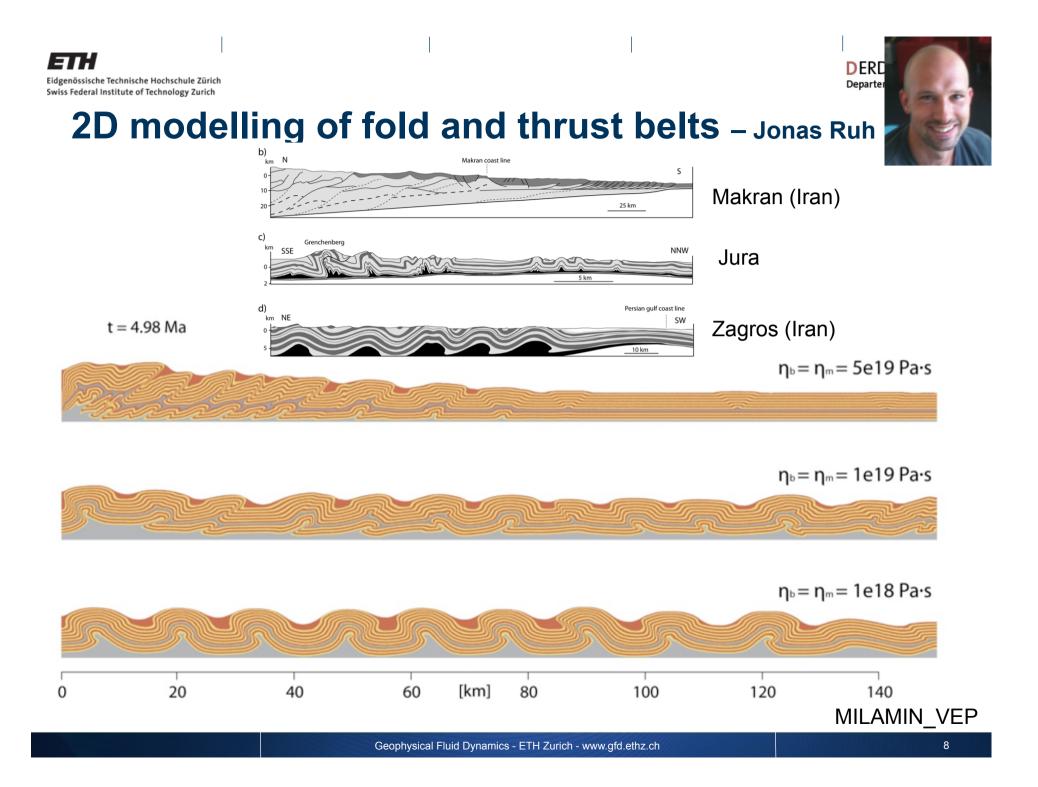
- Makes the system of equations slightly compressible
- Iterations are performed until $\mathbf{G}^{\mathrm{T}}\mathbf{u} < eps$
- Must be used in combination with a direct solver.
- Can deal with large viscosity contrasts O(10⁷).

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Subduction initiation – Marcel Thielmann



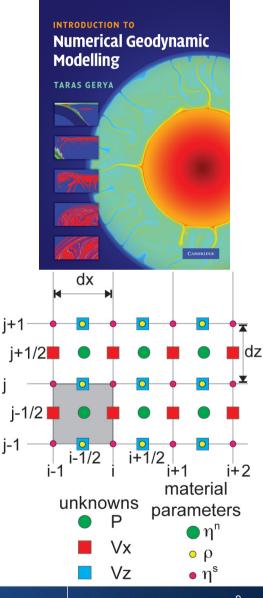
MILAMIN_VEP



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2D Lithospheric Deformation: Finite difference methods

- Easy for teaching.
- Various formulations:
 - Primitive variable staggered grid Velocity-Pressure formulation (Gerya, Tackley)
 - Streamfunction approach (Schmeling).
 - Rotated finite difference stencil.
- Which one is better?
- Doesn't really matter.
 - Interpolation of properties is more important (Deubelbeiss & Kaus, 2008)
 - Staggered grid is the easiest to implement.
- Optimal interpolation scheme:
 - Duretz, May, Gerya & Tackley (G³, 2011)
- Sticky air layer approximates free surface
 - Crameri et al. (submitted)

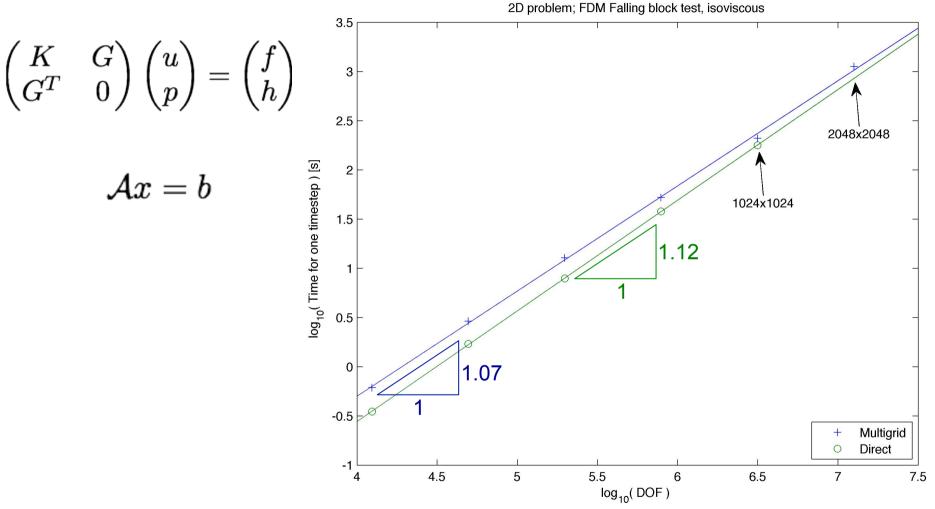




What are the challenges?

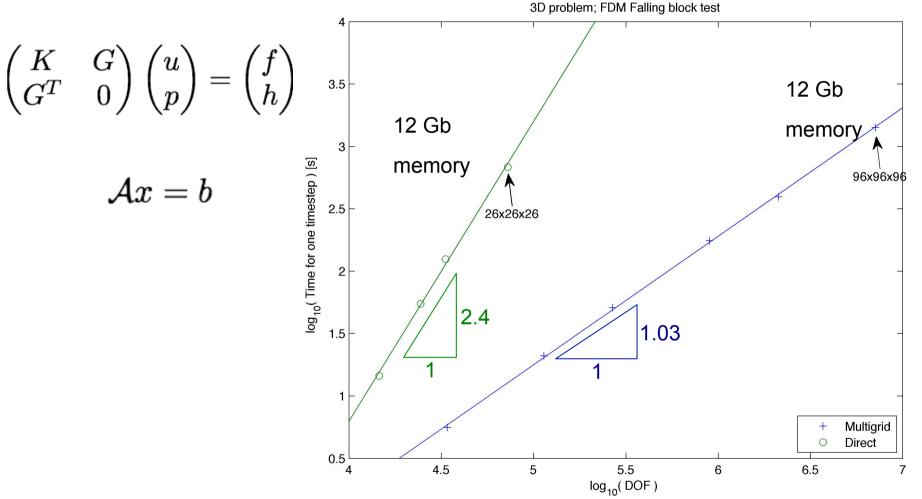
- Rheological/mechanical complexities (multiphase flow, melt migration etc.)
- 3D!!
 - Stokes solver should be:
 - Robust
 - Fast
 - Use little memory

Direct vs. iterative solvers – 2D



• 2D: direct solvers are quite fast and robust.

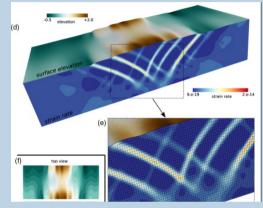
Direct vs. iterative solvers – 3D



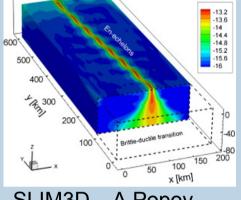
- 3D: multigrid is the only option for large resolutions.
- But: multigrid convergence deteriorates in presence of viscosity jumps.

Some 3D lithospheric deformation codes:

Finite Element Models



Fantom – C.Thieulot

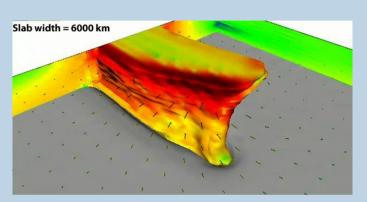


 $\log \dot{\epsilon}_{\parallel} [s^{-1}]$

SLIM3D – A.Popov

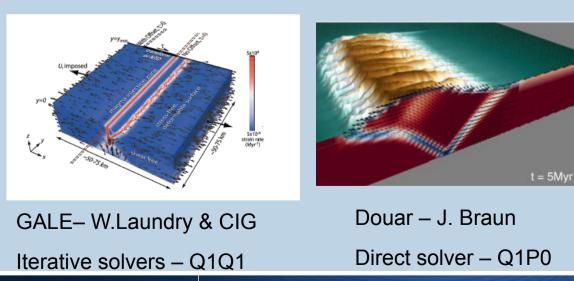
Geophysical Fluid Dynamics - ETH Zurich - www.gfd.ethz.ch

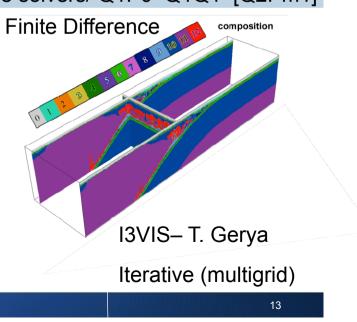
Direct solver, Q1P0 elements Direct solver – Q1P0



Underworld – L.Moresi & co

iterative solvers/ Q1P0–Q1Q1–[Q2Pm1]









FEM – LaMEM (Lithosphere and Mantle Evolution Model)

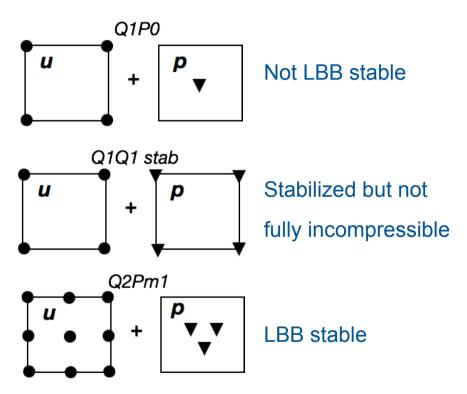
- 3D only, written in C, uses PETSc (fully MPI parallel).
- Main idea: we don't really know which iterative/multigrid solvers work well for 3D geodynamics problems.
- Use either a finite element OR a finite difference discretization.
- Particles to trace material properties.
- Most options (solvers etc.) configurable from commandline.
- Change element-type from the command-line.
 - ./LaMEM –vpt_element Q1P0/Q2Pm1_global/Q1Q1/FDSTAG

$$\left(\begin{array}{cc} \mathbf{K} & \mathbf{G} \\ \mathbf{G}^{\mathrm{T}} & \mathbf{0} \end{array}\right) \left(\begin{array}{c} \mathbf{u} \\ \mathbf{p} \end{array}\right) = \left(\begin{array}{c} \mathbf{f} \\ \mathbf{g} \end{array}\right)$$

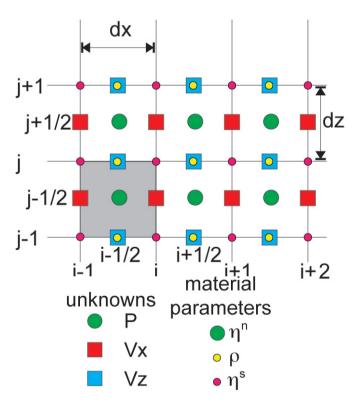
LaMEM – elements & discretization



Finite Element Method (FEM)



Finite Difference Method



- Only LBB stable ones are very reliable.
- Viscosity should be constant or smoothly varying within an element
- Staggered grid.
- Viscosity defined at two locations.

LaMEM – solver strategies

$$\left(\begin{array}{cc} K & G \\ G^T & 0 \end{array}\right) \left(\begin{array}{c} u \\ p \end{array}\right) = \left(\begin{array}{c} f \\ h \end{array}\right)$$

(1) Schur complement reduction

$$\begin{pmatrix} K & G \\ 0 & S \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ \hat{h} \end{pmatrix}$$
$$S = G^{T} K^{-1} G$$
$$\hat{h} = G^{T} K^{-1} f - h$$

1) solve for p: $Sp = \hat{h}$ 2) solve for u: Ku = f - Gp

y = Sx is computed as:

$$f^* = Gx$$
$$Ku^* = f^*$$
$$y = G^T u^*$$



(2) Fully coupled $\begin{pmatrix} K & G \\ G^T & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ h \end{pmatrix}$ is solved iteratively, with as preconditioner: $\begin{pmatrix} \hat{K} & G \\ 0 & -\hat{S} \end{pmatrix}$ where $\hat{S} = \frac{1}{\bar{\eta}^e} M_p$

(3) Powell-Hesteness iterations (penalty method)

$$\begin{pmatrix} K & G \\ G^T & -\frac{1}{\kappa\Delta t}M_p \end{pmatrix} \begin{pmatrix} u \\ p^n \end{pmatrix} \begin{pmatrix} f \\ -\frac{1}{\kappa\Delta t}M_pp^n \end{pmatrix}$$

Iterations are performed as the set of the set

LaMEM & multigrid – FC solver

1. Solve iteratively (e.g. using FGMRES) with as preconditioner:

$$\begin{pmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{p} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{0} & -\frac{1}{\overline{\eta}^{e}} \mathbf{M}_{p} \end{pmatrix}$$

 \mathbf{i}

u

p

g

2. Solve **Ku** iteratively (e.g. using FGMRES)

with as preconditioner:

$$\mathbf{K} \sim \begin{pmatrix} \mathbf{K}_{x,x} & \mathbf{K}_{x,y} & \mathbf{K}_{x,z} \\ \mathbf{K}_{y,x} & \mathbf{K}_{y,y} & \mathbf{K}_{y,z} \\ \mathbf{K}_{z,x} & \mathbf{K}_{z,y} & \mathbf{K}_{z,z} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{x} \\ \mathbf{u}_{y} \\ \mathbf{u}_{z} \end{pmatrix}$$
 'fieldsplit'
Solve with iterative method
(GMRES or CG) with an Algebraic $\sim \begin{pmatrix} \mathbf{K}_{x,x} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_{y,y} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{K}_{z,z} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{x} \\ \mathbf{u}_{y} \\ \mathbf{u}_{z} \end{pmatrix}$
or Geometric Multigrid method as $\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{z} \\ \mathbf{u}_{z} \\ \mathbf{u}_{z} \end{pmatrix}$
preconditioner.

1

K

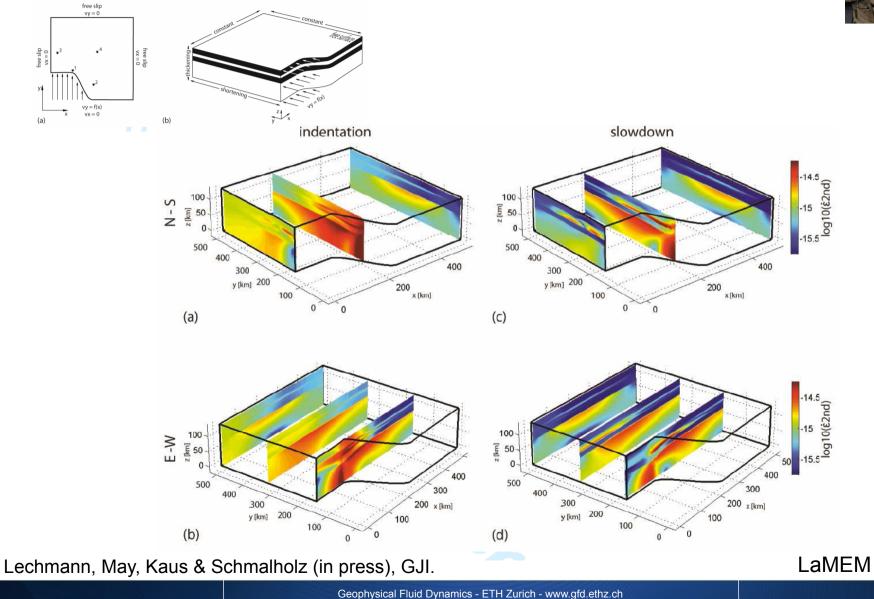
G^T







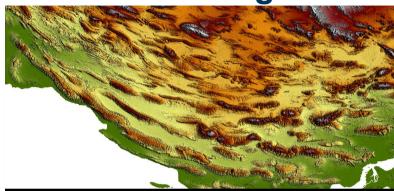
Thin sheet vs. 3D models – Sarah Lechmann



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3D modelling of detachment folding – Naiara Fernandez





velocity(cm/yr) Z

-0.01 **O** 0.01 0.02 0.03

0.03

-0.01

27x513x513 nodes

Using LaMEM & 1024 cores of Cray XT5 (Swiss Supercomputer center)

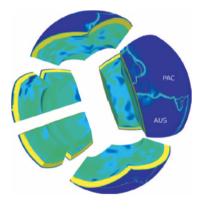
Geophysical Fluid Dynamics - ETH Zurich - www.gfd.ethz.ch

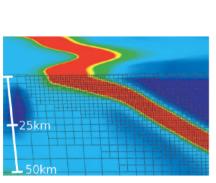
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FEM vs. FDM

The Dynamics of Plate Tectonics and Mantle Flow: From Local to Global Scales

Georg Stadler, ¹ Michael Gurnis, ² Carsten Burstedde, ¹ Lucas C. Wilcox, ¹ Laura Alisic, ² Omar Ghattas^{1,3,4}

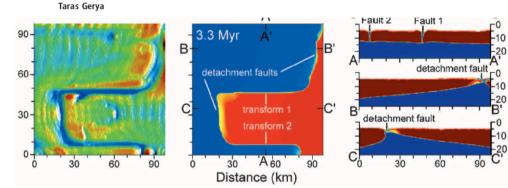




Dynamical Instability Produces Transform Faults at Mid-Ocean Ridges

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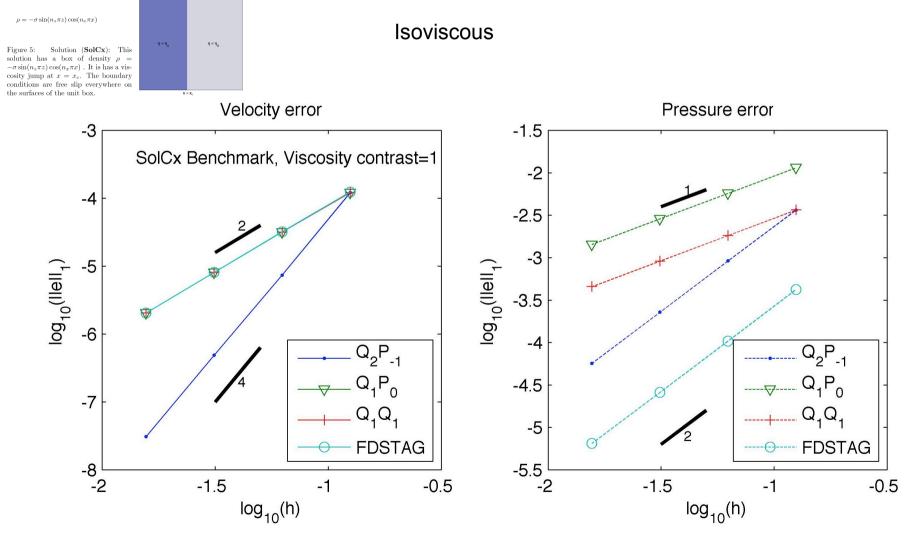
- RHEA
- FEM method, Q1Q1stab
- Adaptive Mesh Refinement (AMR)
- 1.2 billion DOF's on ~8000 processors
- ~150'000 DOF/processor
- 1 timestep: ~9 hours CPU time

- I3VIS
- Staggered grid FDM.
- Uniform mesh
- 197x197x96 nodes; ~15x10⁶ DOF's on 1 processor
- ~15 million DOF/processor
- 1 timestep:~5 hours CPU time (1th)
 - 2-3 minutes (subsequent)

FEM or Finite Difference?

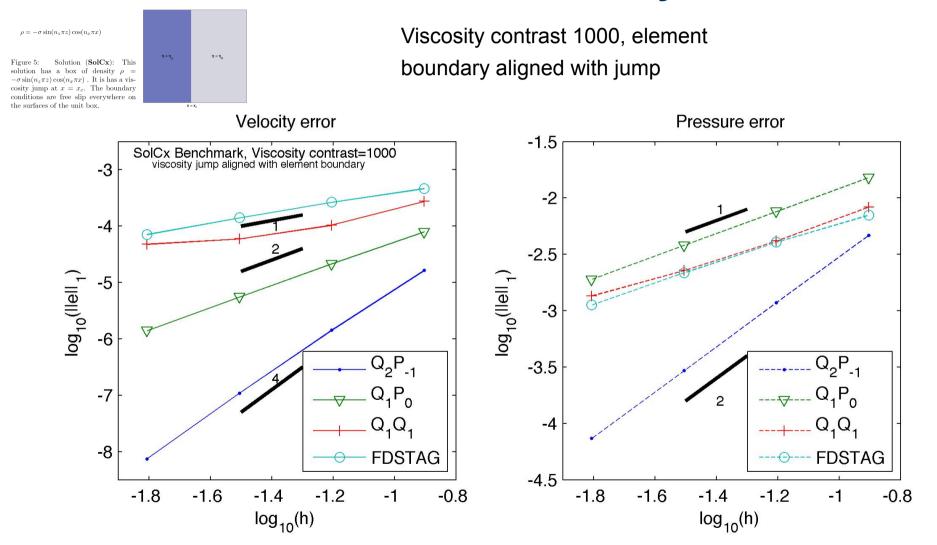
- (1) Accuracy
- (2) Memory usage
- (3) Speed
- (4) How well do they work with iterative solvers?

FEM vs. Finite difference - accuracy benchmark



High-order element wins for velocity

FEM vs. Finite difference - accuracy benchmark



High-order element wins.

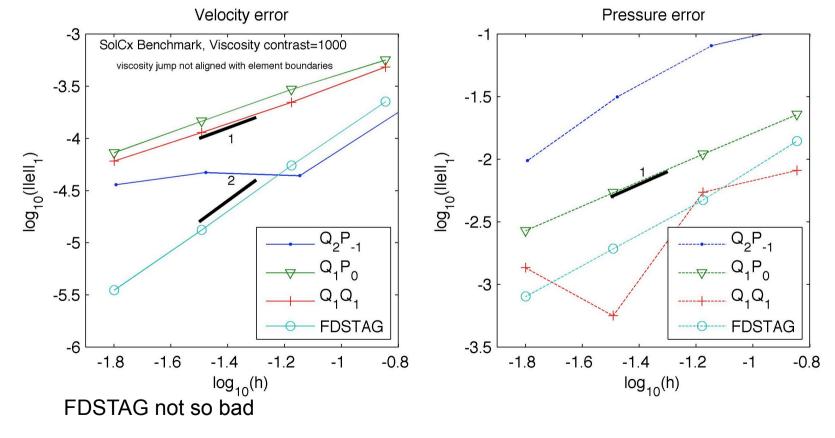
FEM vs. Finite difference - accuracy benchmark

 $\rho = -\sigma \sin(n_z \pi z) \cos(n_x \pi x)$

Figure 5: Solution (SolCx): This solution has a box of density $\rho = -\sigma \sin(n_{\pi} x_2) \cos(n_{\pi} x_{\pi} x)$. It is has a viscosity jump at $x = x_c$. The boundary conditions are free slip everywhere on the surfaces of the unit box.

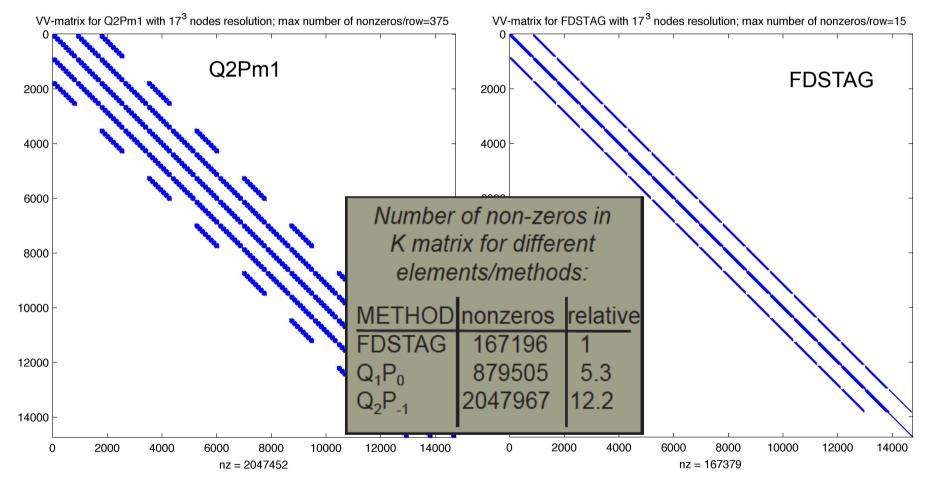


Viscosity contrast 1000, element boundary NOT aligned with jump



High-order element sucks.

FEM vs. FDSTAG – memory usage

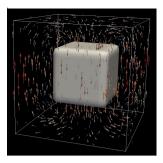


FDSTAG requires significantly less memory!

Matrix-vector multiplications much faster!



FEM vs. FDSTAG – iterative performance



SCR method, Falling block test with viscosity contrast 10³

# nodes	Q ₂ P ₋₁	Q ₁ P ₀	Q_1Q_1	FDSTAG
173	8/33.0 (46.1s)	24/24.0 (36.4s)	9/25.4 (44.7s)	13/53.4 (29.1s)
33 ³	8/33.5 (408s)	31/24.8 (297.0s)	9/26.6 (337.1s)	12/67.5 (162.0s)
65 ³	8/47.9 (4630.7s)	44/23.8 (2787.8s)	10/24.5 (2817.1s)	11/78.2(1233.8s)

Reported numbers: # of Schur iterations/ Average number of inner iterations (time in s). In all simulations, 2-3 ML solves are used.

/LaMEM restart 0 -levels 1 -mumax 1e3 -UzawaSolver 1 -SolverType 2 -schur_ksp_type figmres -schur_ksp_tenson-schur_ksp_monitor -schur_ksp_tol 1e-5 -mat_schur_ksp_type figmres -mat_schur_ksp_tol 1.0e-6 -mat_schur_pc_type fieldspit

-mat_schur_fieldspilt_pc_type mi-mat_schur_ksp_converged_reason-mat_schur_pc_fieldspilt_type ADDITIVE -mat_schur_pc_fieldspilt_block_size 3-vpt_element Q1P0 -nnode_x 17 -nnode_y 17 -nnode_y z

FC method, Falling block test with viscosity contrast 10³

	LBB stable	Not LBB stable	Stabilized	
# nodes	Q ₂ P ₋₁	Q_1P_0	Q_1Q_1	FDSTAG
173	13/8.5 (17.7s)	38/8.8 (22.0s)	13/9.7 (19.7s)	22/10.2 (20.0s)
33 ³	14/10.3 (154.7s)	47/7.4 (123.9s)	15/8.8 (139.9s)	22/10.0 (48.3s)
65 ³	14/10.9 (1367.6s)	58/5.7 (793.8s)	16/9.1 (1284.2s)	23/11.7 (318.8s)

Reported numbers: # of FC iterations/ Average number of inner iterations (time in s).

./LaMEM -restart 0 -mumax 1e3 -SolverType 2 -A11_ksp_type fgmres -A11_ksp_type fieldsplit_A11_fieldsplit_pc_type ml -A11_fieldsplit_ksp_trlo1 1e-2 -A11_pc_fieldsplit_type ADDITIVE -levels 1 -A11_ksp_converged_reason -A11_pc_fieldsplit_block_size 3

-A11_fieldsplit_ksp_type preonly -fc_ksp_atol 1.0e-13 -fc_ksp_rtol 1.0e-5 -use_stokes_relative_norm -use_stokes_norm_L2 -vpt_element FDSTAG -nnode_x 65 -nnode_y 65 -nnode_z 65

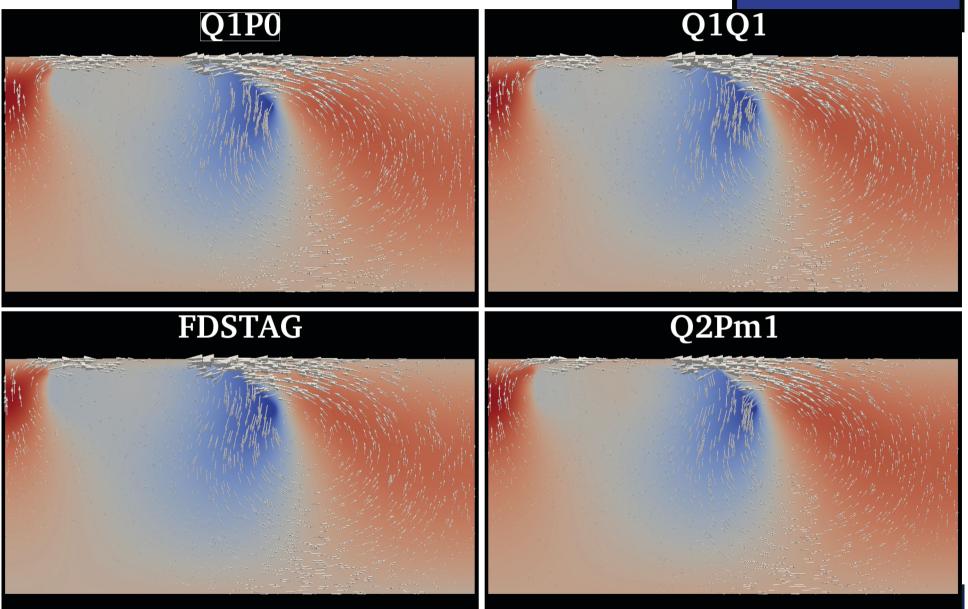
Non-stable elements are bad for iterative solvers

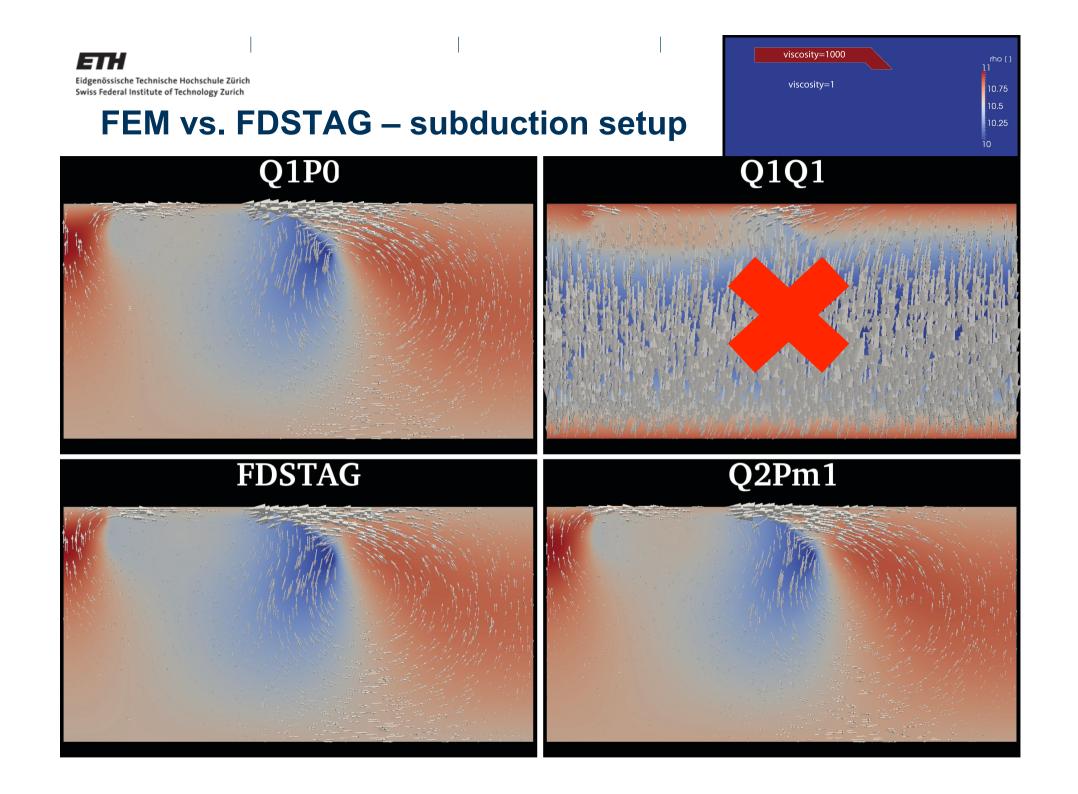
FDSTAG behaves like a **stable** element.



FEM vs. FDSTAG – subduction setup



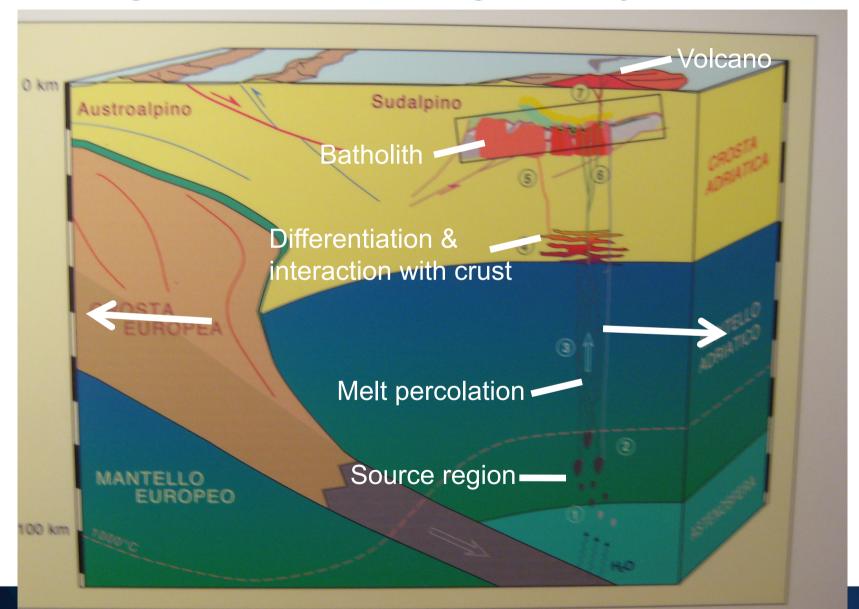




Summary part 1

- Modelling high-resolution 3D lithospheric deformation is challenging.
- Need to use iterative solvers.
- Better use a stable element.
- The staggered grid finite difference method behaves like an ideal (small) stable finite element
 - Small
 - Cheap
 - Equally accurate as other linear elements

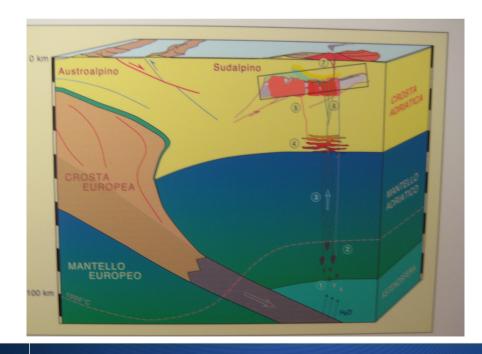
Geological cartoon of magmatic systems



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Challenges:

- Two phase flow formulation required.
- Dikes, melt channels or diapirs?
 - Requires elasto-plastic formulation.
- Magmatic evolution and emplacement of batholiths
- Take (2D) lithospheric deformation into account.







Modeling of two-phase flow – Tobias Keller

- Overcoming limitations
 - Possible to treat regions of magma accumulation as Stokes flow at lower cutoff viscosity?
 - Lithosphere deforms as visco-elasto-plastic medium,
 -> use full visco-elasto-plastic compaction rheology
- Overcoming challenges
 - Use implementation style of standard Stokes codes
 - Use primitive variables without flow decomposition
 - Code in progress: FEM2PHAST (Finite Element Model of 2-PHase and STokes flow)



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V_s

Two-phase flow equations

Bulk momentum conservation

$$\nabla \cdot \left[(1 - \phi) \cdot \boldsymbol{\sigma}_{s}^{d} \right] - \nabla P_{e} - \nabla P_{f} - \rho_{b} g \hat{\mathbf{z}} = 0$$

Solid mass conservation

$$\nabla \cdot \mathbf{v}_{s} + \frac{1}{\eta_{s,vep}^{v}} P_{e} - \frac{\chi^{v}}{\eta_{s,vep}^{v}} P_{e}^{old} - \dot{\lambda} \sin \psi = 0 \qquad P_{e}$$

Bulk mass conservation

$$\nabla \cdot \mathbf{v}_{s} - \nabla \cdot \left[\frac{k_{\phi}}{\eta_{f}} \cdot \nabla P_{f} + \rho_{f} g \hat{\mathbf{z}}\right] - \dot{M} \cdot \frac{\Delta \rho}{\rho_{s} \rho_{f}} = 0 \qquad \qquad P_{f}$$

Porosity conservation

$$\frac{D_s\phi}{Dt} + (1-\phi)\nabla \cdot \mathbf{v}_s - \frac{\dot{M}}{\rho_s} = 0$$

Energy Conservation

 $\phi \rho_f C_f \frac{D_f T}{Dt} + (1 - \phi) \rho_s C_s \frac{D_s T}{Dt} = -\nabla \cdot [k_b \nabla T] + H_r + L \cdot \dot{M} + (1 - \phi) \cdot \left(\boldsymbol{\sigma}_s^d \dot{\boldsymbol{\varepsilon}}_{s,vp}^d + \boldsymbol{\eta}_{s,vp}^v [\nabla \cdot \mathbf{v}_s]_{vp}^2\right) + \frac{\eta_f}{k_{\phi}} \mathbf{q}_D^2 \qquad \mathbf{T}$



Compaction rheology

Effective mean stress / volumetric strain rate

$$\sigma_s^* = P_e = P_b - P_f \qquad \dot{\varepsilon}_s^v = -\frac{1}{3} (\nabla \cdot \mathbf{v}_s)$$

Maxwell visco-elasto-plastic rheology (sum strain rates)

$$\dot{\varepsilon}_{s,tot}^{v} = \dot{\varepsilon}_{s,vis}^{v} + \dot{\varepsilon}_{s,ela}^{v} + \dot{\varepsilon}_{s,pla}^{v} = \frac{1}{3\eta_{s}^{v}}\sigma_{s}^{*} + \frac{1}{3K_{\phi}}\frac{D_{s}\sigma_{s}^{*}}{Dt} + \frac{\dot{\lambda}}{3}tr\left(\frac{\partial Q^{t}}{\partial\sigma_{s}^{*}}\right)$$

Visco-elasto-plasticity (effective viscosity approach)



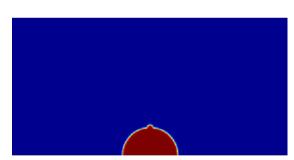
First results in progress

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- Simple setup to test rheological regimes
 - Kinematic boundaries: extension 2.e-15 s-1
 - 10% melt region in 0.1% background material
 - Inhomogeneity at tip of melt region
 - Hydrostatic fluid pressure lower boundary
 - Porosity-weakening of viscosities

$$\eta_s^d = \eta_s^{ref} \cdot \exp(-25 \cdot \phi) \qquad \eta_s^v = \frac{\eta_s^{ref}}{\phi}$$

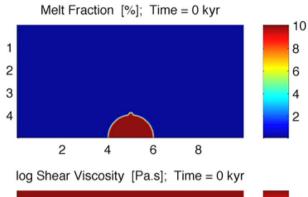
 Gradually increase background viscosity from 1.e19 to 1.e24 Pa.s

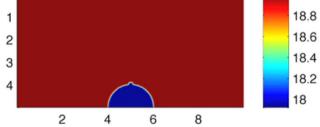




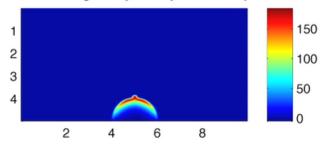


eta_ref = 1.*e*19 *Pa.s*





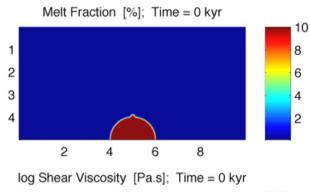
Matrix Divergence [1e-15/s]; Time = 0 kyr

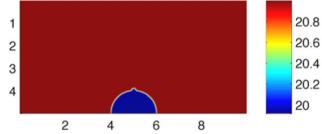


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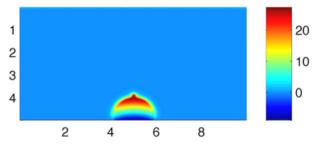








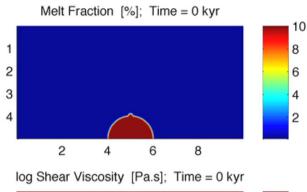
Matrix Divergence [1e-15/s]; Time = 0 kyr

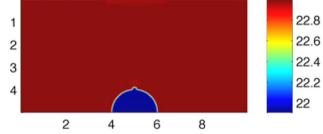


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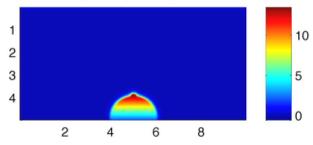








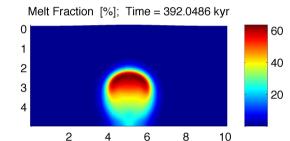
Matrix Divergence [1e-15/s]; Time = 0 kyr



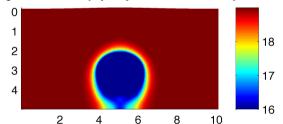
Three (preliminary) regimes

diapirs

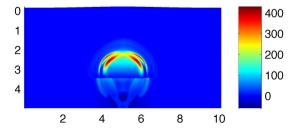
porosity weakening



log Shear Viscosity [Pa.s]; Time = 392.0486 kyr

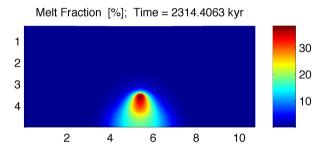


Matrix Divergence [1e-15/s]; Time = 392.0486 kyr

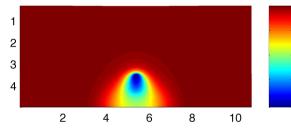


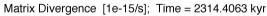
channels

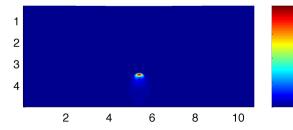
decompaction weakening



log Shear Viscosity [Pa.s]; Time = 2314.4063 kyr

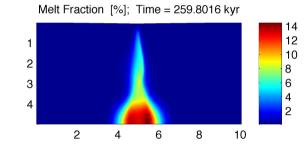






dikes

mode-1 plasticity



log Shear Viscosity [Pa.s]; Time = 259.8016 kyr

20

19

18

17

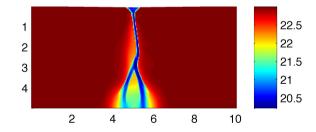
40C

300

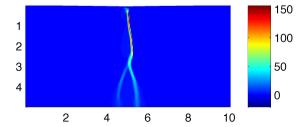
200

100

Ω



Matrix Divergence [1e-15/s]; Time = 259.8016 kyr







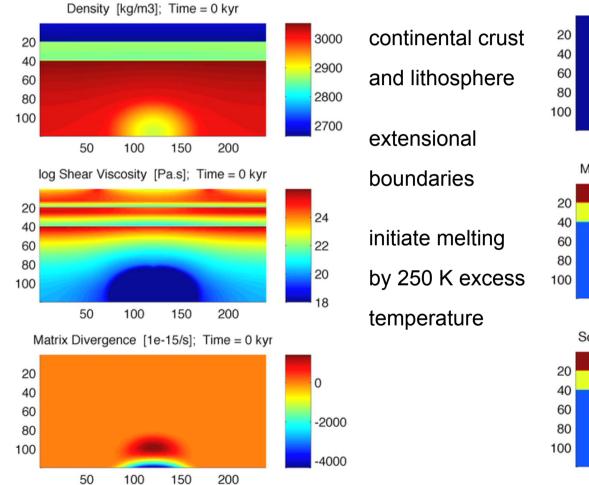
Magmatic evolution model

- Melting model
 - Katz (2003) plus some additions
 - Melt fraction depends on P, T, H2O and composition
- Magmatic evolution of melt and solid
 - Melt evolution index: 0% (primordial) to 100% (evolved)
 - Solid evolution index: 0% (ultramafic) to 100% (felsic)
 - > compute melting rate / solve energy equation during each iteration of non-linear solver

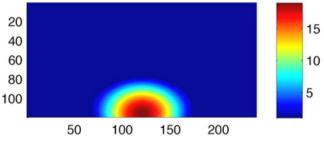


First results...

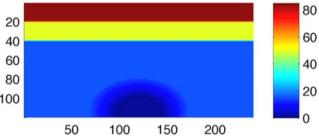




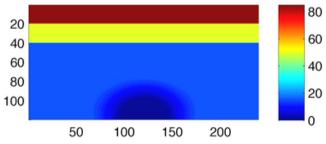
Melt Fraction [%]; Time = 0 kyr



Melt Evolution Index [%]; Time = 0 kyr



Solid Evolution Index [%]; Time = 0 kyr





Conclusions

- Code development was/is and remains important in geodynamics.
- 3D is challenging particularly for lithospheric dynamics.
- The staggered finite difference method is (surprisingly) competitive.
- Magmatic systems require including two-phase flow formulations within lithospheric codes.
- Preliminary results produce diapirs, dikes and channelized flow.



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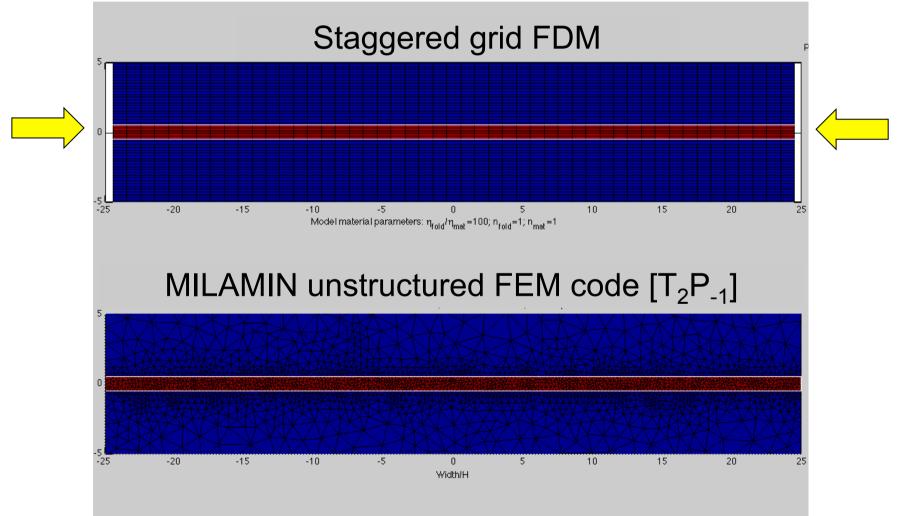


DERDW Departement Erdwissenschaften

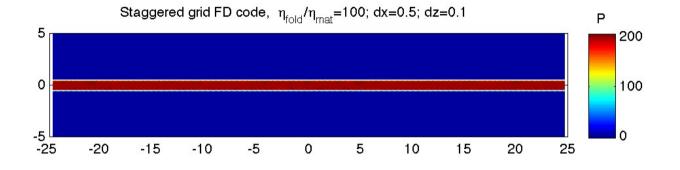
Additional slides

FEM vs. Finite Differences – Model setup

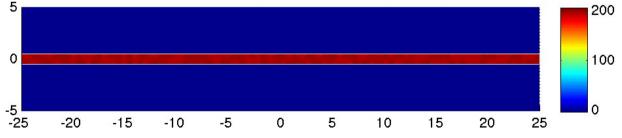
Folding setup, viscosity contrast 100.



FEM vs. Finite Differences







FDSTAG is doing pretty well.