Underworld – what have we learned?

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Auscope
Simulation, Analysis, Modelling Group
NeCTAR
eResearch Tools “Geology from Geodynamics”
Plate tectonics — a multi-scale problem
Integrated Earth modelling

- Evolution of basin structure
- Mantle instabilities
- Surface erosion and sediment transport
- Subduction zone thermal and mechanical evolution
- Simulation & data grid infrastructure
- 3D tomography and seismicity
- Reconstructed plate margins
- Seismic sections and interpretation
- Basin subsidence & stretching models
\[ \tau_{ij} = 2\eta D_{ij} = \eta (u_{i,j} + u_{j,i}) \]

\[ \tau_{ij,j} - p,i = f_i \]

\[ u_{i,i} = 0 \]

\[ f = g\rho_0 \alpha \Delta T \]

\[ T, t + u_k T,k = (\kappa T,k),k + Q \]

Stokes flow, incompressible
Elliptic problem - multigrid

Advection / diffusion

Ugly !!
This is a Rayleigh-Bénard convection model which evolves to a straightforward balance between thermal diffusion and thermal advection in narrow boundary layers.

At modest Rayleigh number, the structure which develops is steady despite strongly developed convective flow.

This system can be solved very efficiently on a fixed mesh.

Challenges: High strain accumulation during fluid-like deformation

\[
Ra = 10^7
\]
Challenges: Strain-dependence of lithospheric deformation

This is a simulation of continental crust being stretched in response to far field stresses imposed by plate motions.

At modest strain, the deformation will often localise onto faults which can be very long-lasting structures; very fine scale in width, but with large lateral dimension and relatively weak.

The history dependence of shear deformation is tractable if we use a Lagrangian reference frame.
In the **material point method** we can keep a mesh which is computationally efficient for diffusion-dominated problems (including Stokes flow) and material points — a.k.a. particles — for tracking history variables.

This is the technique implemented in Underworld and leads to a very natural approach to many “difficult” issues in geological thermal / mechanical models ([www.underworldproject.org](http://www.underworldproject.org))
Underworld for plate scale models with material history

- Underworld — finite element models with tracking of small-scale physics
- Highly parallel code for modern petascale machines
- Open source / based on open libraries (StGermain and PETSc)
- Checkpointed and so forth
Underworld — aims / successes

We wanted to build a code that would be widely used and useful.

- Easy to install
- Robust
- Easy to understand and use
- Highly parallel / efficient
- Very general
- Easy to maintain

More important than efficient

Better to build something effective

Community code

- No more heroes ?
- Vibrant community of users
- Everyone open source !
- Linked in to other workflows

Why knock the heroes ?

Work with everyone !
Robust solution is possible

The general approach is like this

\[ (G^T \tilde{K}^{-1} G)p = (G^T \tilde{K}^{-1}) F \]

solve for \( v \)

\[ Ku = F - Gp \]

mg configuration accuracy?

“outer” solve for \( p \)

which ksp / pc?

accuracy?

penalty?

“inner” mg solve for \( v^* \)

\[ \tilde{K} v_i^* = f_i^* \]

which ksp?

accuracy?

penalty?
**Multigrid “Inner solve”**

**Geometric multigrid**

- Multiple, nested grids sharing common nodes
- Solution is obtained by combining solutions on all grids
- Ideal for elliptic problems in which information propagation is not local and is instantaneous

![Diagram of multigrid](image)

- **Smoothing pc**
- **Approx solve (ksp)**
- **Final solve (ksp)**

**“V cycle” is MG preconditioner on final solver**
Robust and general preconditioners are hard to find

**Augmented Lagrangian Approach** — Takes advantage of the variational nature of the FE formulation. To add a constraint it is always possible to introduce via Lagrange multipliers. Because “exact” compliance with the incompressibility constraint produces a very stiff ill-conditioned system, we can instead use an approximate form and use it to improve iterative convergence

\[
Ku + \lambda G^T W^{-1} Gu + G\rho = F
\]

Minimization drives this term to \(O(1/\lambda)\)

Replaces the stiffness matrix in the Schur complement

\[
\tilde{K} = Ku + \lambda G^T W^{-1} Gu
\]

4  M. BENZI, M. A. OLSHANSKII AND Z. WANG

The equivalent augmented Lagrangian (AL) formulation [11] is given by

\[
\begin{pmatrix}
A + \gamma B^T W^{-1} B & B^T \\
B & 0
\end{pmatrix}
\begin{pmatrix}
u \\
p
\end{pmatrix} =
\begin{pmatrix}
f \\
g
\end{pmatrix},
\text{ or } \tilde{A} x = \tilde{b},
\]

where \(\tilde{f} := f + \gamma B^T W^{-1} g\), \(W\) is symmetric positive definite, and \(\gamma > 0\). A good choice of \(W\) is the pressure mass matrix, \(M_p\); in practice, we use the main diagonal of \(M_p\) instead, in order to maintain sparsity in \(A + \gamma B^T W^{-1} B\). The choice of \(\gamma\) is important and will be discussed below.

The use of the AL formulation (10) instead of the original one (9) can be justified in various ways; see for instance the discussion in [9, 10]. Here we justify this choice by the observation that preconditioning (10) allows us to circumvent the delicate issue of finding good approximations for the pressure Schur complement \(BA^{-1}B^T\) or its inverse, which is crucial when constructing preconditioners for the non-augmented system (9).
Augmented Lagrangian makes the condition number problem go away
But it’s a trade off between the inner and outer problems
Overview

Limit Summary

Instances
Used 1 of 80

VCPUs
Used 32 of 80

RAM
Used 128.0 GB of 320.0 GB

Security Groups
Used 2 of 10

Available Volumes
Used 2 of 5,000

Available Volume Storage
(includes volume snapshots)
Used 1.2TB of 4.9TB

Select a period of time to query its usage:

From: 2013-12-01 To: 2013-12-10 Submit
The date should be in YYYY-mm-dd format.

Active Instances: 1 Active RAM: 128GB This Period's VCPU-Hours: 21.46 This Period's GB-Hours: 20816.38

Usage Summary

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Displaying 1 item
ELLIPSIS modelling toolkit for UNDERWORLD

Lithospheric Modelling Recipe

- 2 cm/yr/wall extension.
- Strain-rate/temper dependent rheologies.
- 100 degree Iso-therms (from 293.15 K).

Time: 0.0000 Myr
Extension: 0.00%
Coupling with LECODE
Underworld and gPlates
Underworld — aims / successes

We wanted to build a code that would be widely used and useful.

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More important than efficient
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Community code

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