Scaling Finite Element Multigrid Solvers to Ten Trillion ($10^{13}$) Unknowns

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joint work with B. Gmeiner, D. Thoennes, U. Rüde (FAU)
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Solver for Earth Mantle Convection

• Why simulations?
  • Driving force for plate tectonics
  • Cause of earthquakes and mountain formation

• Coupled multiphysics problem

• Problem dimensions
  • $10^9$ years time scale
  • 6400 km Earth radius
  • 3000 km Earth mantle thickness

$\Rightarrow 10^{12}$ degrees of freedom (1 km resolution)
Simplified model

\[-\nabla \cdot (2\mu(\vartheta, \mathbf{x})\varepsilon(\mathbf{u})) + \nabla p = \rho(\vartheta, \mathbf{x}) g\]
\[\nabla \cdot \mathbf{u} = 0\]
\[\partial_t \vartheta + \mathbf{u} \cdot \nabla \vartheta - \nabla \cdot (\kappa \nabla \vartheta) = \gamma\]

Stokes equation: \[-\text{div}(\nabla \mathbf{u} - p \mathbf{I}) = \mathbf{f},\]
\[\text{div} \mathbf{u} = 0\]

\[\begin{array}{l}
\mathbf{u} & \text{velocity} \\
\mu & \text{viscosity} \\
\varepsilon = \frac{1}{2} \left( \nabla \mathbf{u} + \nabla \mathbf{u}^\top \right) & \text{strain rate tensor} \\
\rho & \text{dynamic pressure} \\
\vartheta & \text{temperature} \\
\rho & \text{density} \\
g & \text{gravity} \\
\kappa & \text{thermal conductivity} \\
\gamma & \text{heat sources}
\end{array}\]

FEM Discretization: [1]
\[a(u_l, v_l) + b(v_l, p_l) = L(v_l) \quad \forall v_l \in V_l, \]
\[b(u_l, q_l) - c(p_l, q_l) = 0 \quad \forall q_l \in Q_l,\]
with: \[a(u, v) := \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v} \, dx, \quad b(u, q) := -\int_\Omega \text{div} \mathbf{u} \cdot q \, dx\]

Schur-complement formulation:
\[
\begin{bmatrix}
A_l & B_l^\top \\
0 & C_l + B_l A_l^{-1} B_l^\top
\end{bmatrix}
\begin{bmatrix}
\mathbf{u}_l \\
\mathbf{p}_l
\end{bmatrix}
= \begin{bmatrix}
\mathbf{f}_l \\
B_l A_l^{-1} \mathbf{f}_l
\end{bmatrix}
\]

Hierarchical Hybrid Grids (HHG)

• Parallelize multigrid for tetrahedral finite elements
  • partition domain
  • parallelize all operations on all grids
  • use clever data structures
  • matrix free implementation

• Elliptic problems always require global communication
  ➞ Coarser grids for the global data transport
Tetrahedral discretization
HHG Concepts

• Structured refinement of unstructured base mesh
• Geometrical hierarchy: Volume, face, edge, vertex
• Parallel grid traversal:

for each vertex do
  apply operation to vertex
  update vertex primary dependencies
for each edge do
  copy from vertex interior
  apply operation to edge
  copy to vertex halo
update edge primary dependencies
for each element do
  copy from edge/vertex interiors
  apply operation to element
  copy to edge/vertex halos
update secondary dependencies
Coupled flow and transport (const. viscosity)

- Iso-surfaces of temperature distribution \(^{[1]}\)

\[
-\nabla u + \nabla \rho = -Ra \nabla \Theta \hat{r} \\
\nabla \cdot u = 0 \\
\partial_t \Theta + u \cdot \nabla \Theta = Pe^{-1} \Delta \Theta
\]

- Finite Elements with \(6.5 \cdot 10^9\) DoF, 10 000 time steps
- Run-time 7 days on mid-size cluster (LSS): 288 cores (9 nodes)

Rheology in asthenospheric channel

- Viscosity model $^{[1]}$ (asthenosphere thickness 410 km)

$$\mu(\varphi, r) = \left( e^{4.61 \frac{1-r}{1-r_{\text{inner}}}} - 2.99 \varphi \right) \begin{cases} 10^{-3} d_a^3 & \text{for } r > 1 - d_a \\ \frac{1}{10} & \text{else} \end{cases}$$

- Temperature distribution $^{[2,3]}$ recovered from seismic data

$\begin{align*}
d_a & \quad \text{relative asthenosphere thickness} \\
r_{\text{inner}} & \quad \text{relative core radius}
\end{align*}$


Temperature distribution
Velocity boundary conditions


Stationary velocity
Towards exa-scale computing

• Strong scaling is examined for two problems
  • Laplace problem with full multigrid
  • Stokes problem with pressure correction scheme [1]

• Weak scaling of Stokes problem is investigated
  with an all-at-once (Uzawa) multigrid [2]


Strong scaling results

Poisson problem

Stokes problem

Reduction scalability of Stokes problem results from saddle point problem and growing coarsest grid cost
Weak scaling results

- Optimized for minimal memory consumption
  - $10^{13}$ unknowns correspond to 80 TByte for solution vector
  - JUQUEEN has 450 TByte memory
  - Matrix-free implementation essential

<table>
<thead>
<tr>
<th>nodes</th>
<th>threads</th>
<th>DoFs</th>
<th>multigrid iterations</th>
<th>time to solution</th>
<th>parallel efficiency</th>
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</thead>
<tbody>
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<td>5</td>
<td>80</td>
<td>$2.7 \cdot 10^9$</td>
<td>10</td>
<td>685 s</td>
<td>100 %</td>
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<td>776 s</td>
<td>88 %</td>
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➡ Excellent weak scalability up to $10^{13}$ degrees of freedom (DoF) for Stokes problem
Conclusion

- $10^{13}$ degrees of freedom for FE are possible
- Multigrid scales to Peta (and beyond)
- Excellent time to solution
- HHG - lean matrix-free implementation

- Next: Re-design for higher-order finite elements