Scalability of Elliptic Solvers in Numerical Weather and Climate-Prediction

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NGWCP project

Next Generation Weather and Climate Prediction project

- Selection of numerical algorithms to simulate the atmosphere in weather and climate prediction which take advantage of massively parallel architectures.
- Develop new dynamical core for the Met Office Unified Model which scales up to $10^5 - 10^6$ cores
- Substantial increase in global model resolution
  \[ \sim 25\text{km} \rightarrow \sim \text{few km} \]
  \[ \Rightarrow \gtrsim 10^{10} \text{ degrees of freedom per atmospheric variable} \]
- Model runtime $\lesssim 1\text{hour}$ for 5 day forecast
- Solve elliptic PDE for pressure correction in $\ll 1\text{second}$
1 Background
   - Elliptic PDE in implicit time stepping
   - Model equation
   - Multigrid solvers

2 Scaling results
   - Massively parallel scaling on Hector

3 Tensor product geometric multigrid
   - Parallel scaling results
     - Weak scaling
     - Strong scaling
   - Implementation in DUNE-Grid

4 Summary and Outlook
Implicit timestepping

Large scale atmospheric flow: 
Navier Stokes equations

\[
\frac{D\mathbf{u}}{Dt} = -2\Omega \times \mathbf{u} - \frac{1}{\rho} \nabla p + \mathbf{g} + \mathbf{S}^u
\]

\[
\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{u}, \quad \ldots
\]

**Implicit** time stepping

- Unconditionally stable \(\Rightarrow\) Larger integration time step \(\Delta t\)
- Solve 3d **elliptic PDE** for pressure correction \(\pi'\) at every time step
  

\[
-(\alpha \Delta t)^2 c_s^2 \nabla \cdot (a \nabla \pi') + b \pi' = RHS
\]

- Significant proportion of model runtime
- Need **numerically efficient & scalable** solver
Does the solver scale?

Started by testing the following “black box” solvers:

**Distributed and Unified Numerics Environment (DUNE)**

ISTL Bastian et al. 2008, Blatt and Bastian 2007 & 2008

- CG preconditioned with aggregation AMG + ILU0 smoother

**Hypre** Developed at LLNL by U. Maier-Yang, R. Falgout and others

- CG preconditioned with BoomerAMG

⇒ “Matrix-free” geometric multigrid


- DUNE-based code with indirect horizontal-, direct vertical-addressing
Does the solver scale?

Comparison of **Multigrid solvers** for model equation

**Weak scaling** of # iter, total time +AMG setup time

all times in seconds

<table>
<thead>
<tr>
<th># proc</th>
<th># dof</th>
<th>AMG (DUNE)</th>
<th>BoomerAMG</th>
<th>geo MG</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>8.3 \cdot 10^6</td>
<td>11 6.92+4.13</td>
<td>12 8.72+2.59</td>
<td>6 1.99</td>
</tr>
<tr>
<td>64</td>
<td>3.4 \cdot 10^7</td>
<td>11 7.01+4.92</td>
<td>13 9.52+2.74</td>
<td>6 2.02</td>
</tr>
<tr>
<td>256</td>
<td>1.3 \cdot 10^8</td>
<td>11 7.18+4.88</td>
<td>12 8.98+2.82</td>
<td>6 2.04</td>
</tr>
<tr>
<td>1024</td>
<td>5.4 \cdot 10^8</td>
<td>11 7.32+5.89</td>
<td>12 9.04+3.18</td>
<td>6 2.06</td>
</tr>
<tr>
<td>4096</td>
<td>2.1 \cdot 10^9</td>
<td>13 8.64+6.32</td>
<td>12 8.99+3.56</td>
<td>6 2.06</td>
</tr>
<tr>
<td>16384</td>
<td>8.6 \cdot 10^9</td>
<td>12 8.16+8.06</td>
<td>11 9.43+5.75</td>
<td>6 2.10</td>
</tr>
<tr>
<td>65536</td>
<td>3.4 \cdot 10^{10}</td>
<td>11 7.49+10.92</td>
<td>9 20.20+7.09</td>
<td>6 2.24</td>
</tr>
</tbody>
</table>

+ matrix setup time for AMG solvers

Eike Mueller

Scalability of Elliptic Solvers in NWP
Model equation

Simplified model equation for \( u \equiv \pi' \) on spherical shell

\[
-\omega^2 \left[ \Delta_{(2d)} + \lambda^2 \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right] u + u = \text{RHS}
\]

Dimensional analysis: \( r \in [1, 1 + h] \) with \( h = H/R_{\text{earth}} = 10^{-2} \):

\[
\omega^2 \sim \left( \frac{c_s \alpha \Delta t}{R_{\text{earth}}} \right)^2 \quad \lambda^2 \sim \frac{1}{1 + (\alpha \Delta t)^2 (N^*0)^2}
\]

- Acoustic waves: \( c_s \approx 550 \text{ms}^{-1} \)
- Buoyancy frequency \( N^*0 = 0.018 \text{s}^{-1} \)
- Off-centering parameter \( \alpha = \frac{1}{2} \)
  (fully implicit: \( \alpha = 1 \), fully explicit: \( \alpha = 0 \))
Model equation

Properties

- \( h = \frac{H}{R_{\text{earth}}} \approx 1/100 \Rightarrow \frac{\lambda^2}{h^2} \gg 1 \)
- Strong **vertical anisotropy** \( \left( \frac{\lambda}{h} \cdot \frac{\Delta x}{\Delta z} \right)^2 \)
- **Constant term** improves condition number (on coarser MG levels)

\[- \omega^2 D^{(2)} u + u = \text{RHS} \]

- Horizontal grid e.g. cubed sphere, icosahedral, . . .
- **no pole singularity** as in lat/lon grid
Multigrid solvers

Multigrid idea:
Eliminate error on all scales

- Hierachy of grids $h, 2h, 4h, \ldots$
- Apply smoother (e.g. SOR) on all levels, restrict/prolongate between levels
- Residual equation on coarser grids

\[ A^{(H)} e^{(H)} = r^{(H)} \]

⇒ Work on coarse grids is cheap!
- Algorithmically optimal

\[ \text{Cost}(MG) = O(n) \]
- Robust & parallelisable
Setup

Weak scaling

- 1/6 of cubed sphere grid
  (have also run on entire sphere)
- Horizontal partitioning only* (atmos. physics)
- # processors $\propto$ problem size

\[ n_x \mapsto 2n_x, \quad n_y \mapsto 2n_y, \quad n_z = 128, \quad p \mapsto 4p \]

- Keep Courant number $\nu = c_g \Delta t / \Delta x \sim 10$ fixed\(^{\dagger}\)
  (i.e. $\Delta t$ decreases)

\[ \omega \propto \Delta t \propto \Delta x, \quad \lambda^2 = \frac{1}{1 + (\alpha \Delta t)^2 (N^*0)^2} \]

- All runs carried out on Hector Cray XE6 supercomputer
  2816 nodes of 2 x AMD Opteron 16-core Interlagos 2.3GHz = 90,122 cores

*OpenMP in vertical direction?
\(^{\dagger}\)NB explicit scheme requires $\nu \lesssim 1$
Weak Scaling

“Black box” AMG solvers: # iterations & time per iteration

Residual reduction: \( \|r\|/\|r_0\| \leq 10^{-5} \)

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<th>BoomerAMG†</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td># iter</td>
<td>( t_{iter} )</td>
</tr>
<tr>
<td>16</td>
<td>8.3 ( \cdot ) 10^6</td>
<td>11</td>
<td>0.63</td>
</tr>
<tr>
<td>64</td>
<td>3.4 ( \cdot ) 10^7</td>
<td>11</td>
<td>0.64</td>
</tr>
<tr>
<td>256</td>
<td>1.3 ( \cdot ) 10^8</td>
<td>11</td>
<td>0.65</td>
</tr>
<tr>
<td>1024</td>
<td>5.4 ( \cdot ) 10^8</td>
<td>11</td>
<td>0.67</td>
</tr>
<tr>
<td>4096</td>
<td>2.1 ( \cdot ) 10^9</td>
<td>13</td>
<td>0.66</td>
</tr>
<tr>
<td>16384</td>
<td>8.6 ( \cdot ) 10^9</td>
<td>12</td>
<td>0.68</td>
</tr>
<tr>
<td>65536</td>
<td>3.4 ( \cdot ) 10^{10}</td>
<td>11</td>
<td>0.68</td>
</tr>
</tbody>
</table>

† as preconditioner for CG
Setup costs + Anisotropy

AMG has **coarse level** & **matrix** setup costs

**Rotating anisotropy** due to vertical grading

- Grid-aligned anisotropy
- Operator “well-behaved” in horizontal direction

⇒ **Tensor-product matrix-free geometric multigrid**

Tensor-product multigrid

Tensor product operator

\[ A = A^{(r)} \otimes M^{(\text{horiz})}_h + M^{(r)} \otimes A^{(\text{horiz})}_h \]

[for operator \( -\nabla (\alpha \nabla \cdot) \)]

Vertical “eigenmodes”

\[ A^{(r)} e^{(r)}_j = \omega_t M^{(r)} e^{(r)}_j \]

\[ u(r, x) = \sum_{j=1}^{n_z} u_j(x) e^{(r)}_j(r) \]


- Vertical line relaxation (e.g. RB Gauss-Seidel)
- Semi-coarsening in horizontal direction only

\[ \Rightarrow 2d \text{ multigrid convergence rate} \]

\[ \rho^{(2d)} \leftarrow \max_j \left\{ \rho^{(\text{horiz})}_j [e^{(r)}_j] \right\} \]

Meteorological application on 3d lat-lon grid:
**Geometric multigrid**

**Implementation**

- RB Line Gauss-Seidel (1× pre-/post-smoothing)
- Halo exchange after each smoothing step & prolongation
  ⇒ Overlap calculation/communication
- collect/distribute coarse grid data when # procs > # columns
Geometric multigrid

**Parallel Multigrid**: volume/interface ratio decreases on coarser levels Hülsemann et al., Lect. Notes in Comp. Science and Engineering (2005)

**BUT**

Well conditioned on coarser levels \((-\omega^2 D^{(2)} u + u = \text{RHS})\)

Horizontal coupling vs. constant term:

\[
4 \frac{\omega^2}{\Delta x^2_\ell} = 4 \frac{\omega^2}{\Delta x^2_0} \times 2^{-2\ell} \leq 2^{8-2\ell}
\]

⇒ Reduce number of levels

- Coarsen to 1 column (standard MG)
- Coarsen to 1 column/processor (7 levels, shallow MG)
- 4 levels (very shallow MG)
- 1-level method to check robustness
Weak scaling results

Different number of multigrid levels

| # proc | # dof  | standard MG | | iter | # lev = 7 | | iter | # lev = 4 | | iter |
|--------|--------|-------------|--------|--------|-------------|--------|-------------|--------|--------|
| 16     | $8.3 \cdot 10^6$ | 6 | 0.332 | 6 | 0.332 | 6 | 0.333 |
| 64     | $3.4 \cdot 10^7$ | 6 | 0.337 [99%] | 6 | 0.335 [99%] | 6 | 0.335 [99%] |
| 256    | $1.3 \cdot 10^8$ | 6 | 0.340 [98%] | 6 | 0.338 [98%] | 6 | 0.337 [99%] |
| 1024   | $5.4 \cdot 10^8$ | 6 | 0.343 [97%] | 6 | 0.342 [97%] | 5 | 0.340 [98%] |
| 4096   | $2.1 \cdot 10^9$ | 6 | 0.343 [98%] | 6 | 0.340 [98%] | 5 | 0.342 [97%] |
| 16384  | $8.6 \cdot 10^9$ | 6 | 0.350 [95%] | 6 | 0.342 [97%] | 5 | 0.342 [97%] |
| 65536  | $3.4 \cdot 10^{10}$ | 6 | 0.373 [89%] | 6 | 0.351 [95%] | 5 | 0.342 [97%] |

all times in seconds
Strong scaling results

Standard **geometric multigrid**

Problem size: $n \times n \times 256$

\[
\text{efficiency} = \frac{p_0 \cdot T(p_0)}{p \cdot T(p)} \times 100\%
\]
Multigrid on arbitrary spherical grids

Grid structure

Tensor product grid structure

- 2-sphere
- 1-column

Size of vertical column $O(100)$

- "Hide" indirect addressing in horizontal direction by work in vertical direction
- MacDonald et al., Int J of HPC Appl (2011)
- Naturally maps to DUNE data model: Attach vector of size $n_z$ to each cell of the 2d host grid
- Multigrid hierarchy only on host grid
Comparison to DUNE geometric MG code

**Time per iteration** [Intel(R) Core(TM)2 Duo CPU E8400 3.00GHz]

\[ t_{\text{iter}} = A(\text{grid}) + B \cdot n_z \]

Implemented together with Andreas Dedner (Warwick)
Summary

- Multigrid solvers for elliptic PDE in NWP implicit time stepping
- Verified weak & strong scaling to 65536 cores (HECToR)
- Access to bigger machines?
- Geometric multigrid code avoids AMG- and matrix setup costs
- **Anisotropy**: Tensor product multigrid
  - semi-coarsening + vertical line relaxation
- Problem well-conditioned on coarser grids
  - ⇒ use small number of multigrid levels
- Geometric multigrid robust

Outlook

- Hybrid MPI+OpenMP parallelisation
- More realistic problems (ENDGame?): non-symmetry, non-smoothness,…
- GPGPUs