Scalability of Elliptic Solvers in Numerical Weather and Climate- Prediction

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NGWCP project

Next **G**eneration **W**eather and **C**limate **P**rediction 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**

$$\sim 25\text{km} \quad \rightarrow \quad \sim \text{few km}$$

$$\Rightarrow \gtrsim 10^{10} \text{ degrees of freedom per atmospheric variable}$$

- Model runtime $\lesssim$ 1hour for 5 day forecast
- Solve **elliptic PDE** for pressure correction in $\ll$ 1second

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

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

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\boldsymbol{u}, \qquad \ldots$$

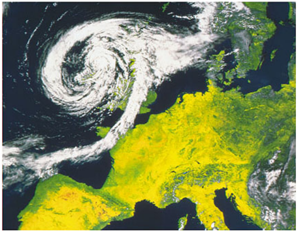


image source: NASA

Implicit time stepping

- Unconditionally stable ⇒ Larger integration time step Δt
- Solve 3d **elliptic PDE** for pressure correction π' at every time step [Davies et al. Q J Royal Met Soc, 131 (608):1759-1782, 2005, . . .]

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

- 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 (+ AMG) setup costs?

$\Rightarrow$ **"Matrix-free" geometric multigrid**

- Hand-written Fortran code based on tensor-product multigrid idea Börm, Hiptmair 2001. Numerical Algorithms. 26: 219234
- 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

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

+ matrix setup time for AMG solvers

Model equation

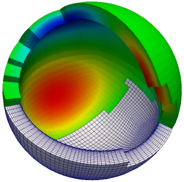
Simplified model equation for $u \equiv \pi'$ on spherical shell

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

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

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

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



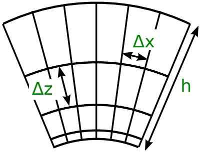
Model equation

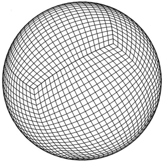
Properties

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

$$-\omega^2 D^{(2)} u + u = RHS$$

- 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

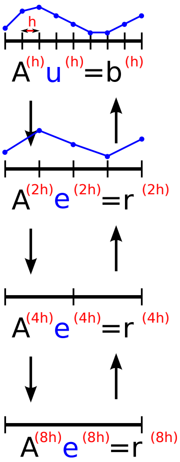
$$A^{(H)} e^{(H)} = r^{(H)}$$

$\Rightarrow$ **Work on coarse grids is cheap!**

- Algorithmically optimal

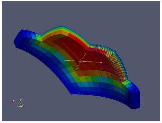
$$Cost(MG) = \mathcal{O}(n)$$

- 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

$$n_x \mapsto 2n_x, \qquad n_y \mapsto 2n_y, \qquad n_z = 128, \qquad p \mapsto 4p$$

- Keep Courant number $\nu = c_g \Delta t / \Delta x \sim 10$ fixed†
  (i.e. Δt decreases)

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

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

*OpenMP in vertical direction?

†NB explicit scheme requires $\nu \lesssim 1$

Weak Scaling

"Black box" AMG solvers: # iterations & time per iteration

Residual reduction: $||r||/||r_0|| \leq 10^{-5}$ all times in seconds

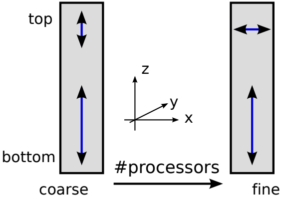
		AMG (DUNE)†			BoomerAMG†		
# proc	# dof	# iter	t_{iter}	eff.	# iter	t_{iter}	eff.
16	$8.3 \cdot 10^6$	11	0.63		12	0.73	
64	$3.4 \cdot 10^7$	11	0.64	[98%]	13	0.73	[100%]
256	$1.3 \cdot 10^8$	11	0.65	[97%]	12	0.75	[97%]
1024	$5.4 \cdot 10^8$	11	0.67	[94%]	12	0.75	[97%]
4096	$2.1 \cdot 10^9$	13	0.66	[95%]	12	0.75	[97%]
16384	$8.6 \cdot 10^9$	12	0.68	[92%]	11	0.86	[84%]
65536	$3.4 \cdot 10^{10}$	11	0.68	[92%]	9	2.24	[32%]

† 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**

Börm, Hiptmair 2001. Numerical Algorithms. 26: 219234

Tensor-product multigrid

Tensor product operator

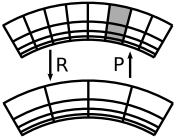
$$A \quad = \quad A^{(r)} \otimes M_h^{(horiz)} + M^{(r)} \otimes A_h^{(horiz)} \qquad \text{[for operator } \; -\nabla(\alpha\nabla\cdot) \text{]}$$

Vertical “eigenmodes”

$$A^{(r)} e_j^{(r)} = \omega_t M^{(r)} e_j^{(r)} \qquad u(r, \boldsymbol{x}) = \sum_{j=1}^{n_z} u_j(\boldsymbol{x}) e_j^{(r)}(r)$$

Börm, Hiptmair 2001. Numerical Algorithms. 26: 219234

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



$\Rightarrow$ 2d multigrid convergence rate

$$\rho^{(2d)} \quad \leftarrow \quad \max_j \left\{ \rho^{(horiz)} [e_j^{(r)}] \right\}$$

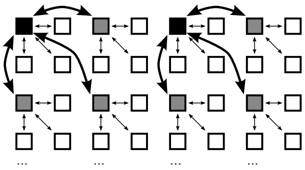
Meteorological application on 3d lat-lon grid:

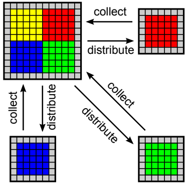
Buckeridge, Cullen, Scheichl and Wlasak 2011. Q J Royal Met Soc 137 (657):1083-1094.

Geometric multigrid

Implementation

- RB Line Gauss-Seidel ($1\times$ pre-/post-smoothing)
- Halo exchange after each smoothing step & prolongation
  $\Rightarrow$ 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 ($-\omega^2 D^{(2)} u + u = RHS$)
Horizontal coupling vs. constant term:

$$4\frac{\omega^2}{\Delta x_\ell^2} \quad = \quad 4\frac{\omega^2}{\Delta x_0^2} \times 2^{-2\ell} \lesssim 2^{8-2\ell}$$

$\Rightarrow$ 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

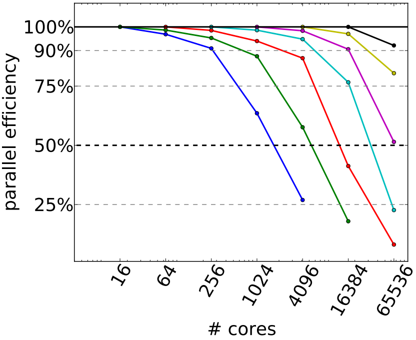
Different number of multigrid levels

all times in seconds

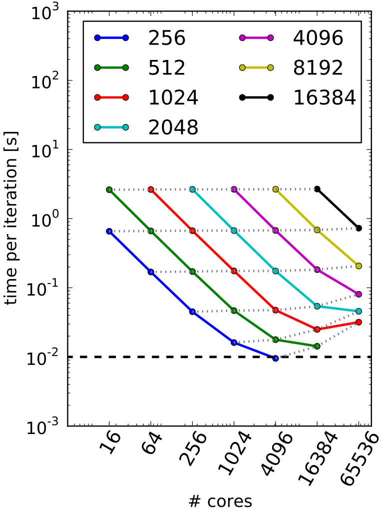
		standard MG		$n_{lev} = 7$		$n_{lev} = 4$	
# proc	# dof	#	t_{iter}	#	t_{iter}	#	t_{iter}
16	$8.3 \cdot 10^6$	6	0.332	6	0.332	6	0.333
64	$3.4 \cdot 10^7$	6	0.337 [99%]	6	0.335 [99%]	6	0.335 [99%]
256	$1.3 \cdot 10^8$	6	0.340 [98%]	6	0.338 [98%]	6	0.337 [99%]
1024	$5.4 \cdot 10^8$	6	0.343 [97%]	6	0.342 [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%]**

Strong scaling results

Standard **geometric multigrid**
Problem size: $n \times n \times 256$

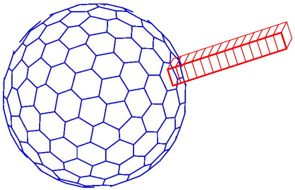


$$efficiency = \frac{p_0 \cdot T(p_0)}{p \cdot T(p)} \times 100\%$$



Multigrid on arbitrary spherical grids

Grid structure



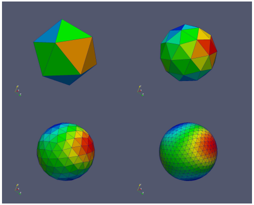
Tensor product grid structure

2-sphere ⊗ 1-column

host grid — directly addressed

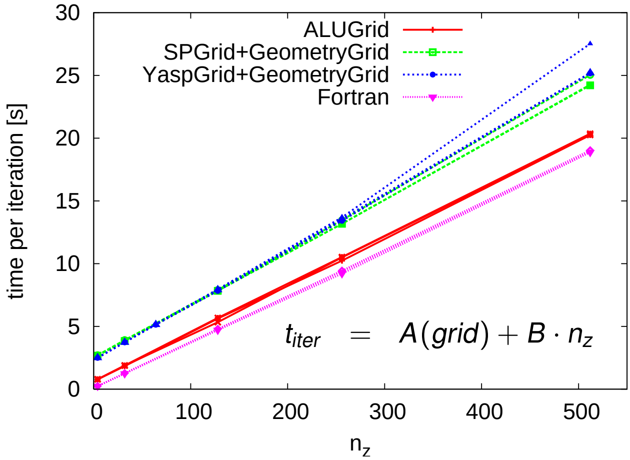
Size of vertical column $\mathcal{O}(100)$

- "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]



Implemented together with Andreas Dedner (Warwick)

Summary and outlook

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**
  $\Rightarrow$ use small number of multigrid levels
- Geometric multigrid robust

Outlook

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