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Abstract: Multigrid methods play an important role in the numerical approximation of partial differential equations. As long as only a moderate number of processors is used, many alternatives can be used as solver for the coarsest grid. However, when the number of processors increases, then standard coarsening will stop while the problem is still large and the communication overhead for solving the corresponding coarsest grid problem may dominate. In this case, the coarsest grid must be agglomerated to only a subset of the processors. This article studies the use of sparse direct methods for solving the coarsest grid problem as it arises in a multigrid hierarchy. We use as test case a Stokes-type model and solve algebraic saddle point systems with up to $O(10^{11})$ degrees of freedom on a current peta-scale supercomputer. We compare the sparse direct solver with a preconditioned minimal residual iteration and show that the sparse direct method can exhibit better parallel efficiency.

Project TerraNeo:

High-Performance Computing

Numerics Geophysics

Multigrid framework : HHG

(Hierarchical Hybrid Grids)

The framework:

- Structured refinement of unstruct. tetrahedral meshes
- Matrix-free, stencil-based kernels
- Native PMINRES solver on the coarse grid

level 0 (no refinement) level 1 level 2

The MG: All-at-once Uzawa MG method
 ⚠ Potential convergence issue on the coarse grid
 Depending on the problem size/hardness

Scalability issue: agglomeration technique

For Direct solvers: Crumbling of the granularity in sub-systems:
Communication ≫ Computation

geometric multigrid
coarse solver
decreasing DOF
~50 DoFs per proc at coarsest

Sometimes less procs is better...
 ⇒ Master-Slave data agglomeration

Direct solver: MUMPS

(Multifrontal Massively Parallel Solver)

Parallel sparse direct solver for $Ax = b$ based on the multifrontal scheme.

Three phases

1. Analysis: ordering, scaling, symbolic factorization,
2. Factorization: $A=LU$,
3. Solve: $Ly=b$, then $Ux=y$

On the coarse grid

- Input in COO format: need a fully assembled matrix,
- ++ Analysis and Factorization (most of the cost) only required once in MG,
- ++ Robust (but too accurate)

MUMPS solver: <http://mumps-solver.org>

HPC JUWELS
Mantle Convection
TerraNeo
HHG Hierarchical Hybrid Grids
Agglomeration
MUMPS

Application: Stokes flow

(motivated by Mantle Convection)

Stokes problem on a spherical shell:

$$-\operatorname{div}\left(\frac{\nu}{2}(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)\right)+\nabla p=\mathbf{f}\quad\text{in}\Omega,$$

$$\operatorname{div}(\mathbf{u})=0\quad\text{in}\Omega,$$

$$\mathbf{u}=\mathbf{g}\quad\text{on}\partial\Omega$$

with \mathbf{u} : velocity, p : pressure, \mathbf{f} : forcing term

B.C → surface: Dirichlet from plate velocity data
 → core-mantle: free-slip (simplification)

⚠ viscosity $\nu(\mathbf{x}, T)$ impacts the coarse grid solver

Discretization:
 lowest equal-order FE method + PSPG stabilization
 Tetrahedral mesh hierarchy: uniform refinement
 → 2 levels for C.G., 6 for the MG scheme

Tets.	DoFs	DoFs coarse
1 920	5.37E+09	9.22E+04
15 360	4.29E+10	6.96E+05
43 200	1.21E+11	1.94E+06

Results on the application (JUWELS, JFZ)

Impact of viscosity

$\nu(\mathbf{x}, T)$ → iso-viscous
 → jump-410: marks asthenosphere frontier

Proc.	DoFs coarse	Visco.	PMINRES	MUMPS
			coarse(s)	coarse(s)
40	9.22E+04	iso	1.0	0.16
		jump	3.1	0.16
160	6.96E+05	iso	2.9	2.32
		jump	21.0	2.32
225	1.94E+06	iso	3.4	11.51
		jump	18.3	12.08

Comparison PMINRES-MUMPS

Run-time (s)

DOFs: 5.37 · 10⁹ 4.29 · 10¹⁰ 1.21 · 10¹¹

Proc.	PMINRES		MUMPS	
	Coarse(s)	Par. Eff.	Coarse(s)	Par. Eff.
1 920	3.1	1.00	0.16	1.00
15 360	21.0	0.73	2.32	0.87
43 200	28.3	0.66	12.08	0.76

Going further (HazelHen, HLRS):

Block Low Rank approximation

Controlled accuracy and mem/flops reduction

(a) Strong and weak interactions between clusters in the geometric domain.
 (b) Corresponding block-clusters in the matrix.

+ single precision arithmetic

Proc.	PMINRES		MUMPS-BLR-SP	
	fine(s)	Coarse(s)	fine(s)	Coarse(s)
1 920	75.5	3.56	75.8	0.18
15 360	84.0	21.44	82.1	1.79
43 200	88.7	33.61	85.26	5.9

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