Linear Solvers: Multilevel methods

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Emerging architectures are forcing the reevaluation of iterative solvers to ensure continued high performance. At the same time new algorithms need to be developed to solve increasingly complex problems. FASTMath linear solvers include various multilevel methods with excellent numerical scalability.

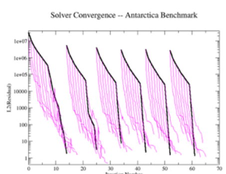
Solver Performance for BISICLES Ice Sheet Model with PETSc

Scientific Achievement

Improved linear solver robustness for Adaptive Mesh Refinement (AMR) composite-mesh solves.

Significance and Impact

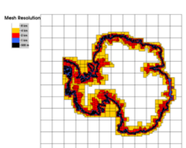
About 90% of run time in the BISICLES AMR Ice Sheet model is spent in the nonlinear momentum solve for the ice velocity field. Improving linear solver robustness directly improves BISICLES performance and robustness; coupling with PETSc AMG solvers enables solution of wider classes of problems which the native Chombo geometric multigrid solvers struggle to solve.



Solver convergence for full-continent ice velocity solves. Black lines are nonlinear residuals, blue are linear-solve residuals.

Research Details

- BISICLES spends 90% of run time in nonlinear ice velocity solves.
- FASTMath-developed Chombo-PETSc interface enables use of PETSc linear solvers for problems like ice sheets which feature sharp gradients in coefficients.
- Collaborative effort between FASTMath and ProSPecT BER SciDAC Partnership was able to significantly improve solver performance and robustness when solving realistic problems like Antarctica.
- Composite matrix construction for structured grid adaptive mesh refinement, Adams, Cornford, Martin, and McCorquodale, Conditionally accepted to Computer Physics Communications.



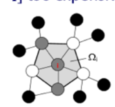
AMR resolution distribution for Antarctic simulations

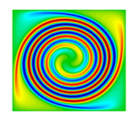
Contact: Mark Adams, LBNL

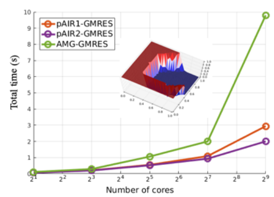
Parallel Approximate Ideal Restriction (pAIR)

AMG solver for nonsymmetric advection-dominated problems, occurring e.g. in transport, which conventional AMG methods are unable to solve or only solve poorly;

- Uses a different restriction than P^T
- Consider $A = \begin{bmatrix} A_{FF} & A_{FC} \\ A_{CF} & A_{CC} \end{bmatrix}$ ordered based on F- and C-points
- Ideal restriction: $R^* = [-A_{CF}A_{FF}^{-1} \quad I]$ too expensive
- Use localized ideal R^* constructed from principal submatrices

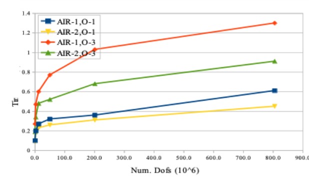






Weak scalability for a nonsymmetric problem (solution pictured) comparing pAIR and AMG

Time-dependent advection equation discretized by DG (order 1 and 3) using MFEM



Weak scalability (up to 16384 cores) of pAIR. Standard AMG combined with GMRES only solves the 2 smallest problems, but much (~4x,~8x) slower

Contact: Ruipeng Li, LLNL

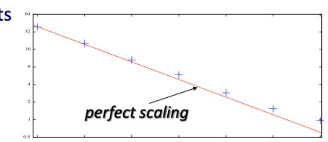
A Low-Communication Method to Solve Poisson's Equation on Locally-Structured Grids

- Poisson's equation arises in astrophysics, plasma physics, electrostatics, and fluid dynamics. Solve it with infinite-domain boundary conditions
- Method of Local Corrections (MLC)
  - Represent potential f as linear superposition of local discrete convolutions, with global coupling represented in a non-iterative form of geometric multigrid
  - Communication cost like that of a single iteration of multigrid
  - Computational kernels are multidimensional FFTs on small domains
- Comparison with geometric multigrid (GMG) with 10 V-cycles for 27-point Laplacian

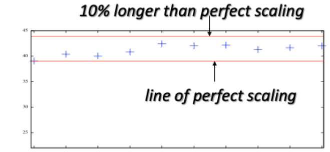
Algorithm	Flops per gridpoint	Loads (bytes) / gridpoint	Stores (bytes)/ gridpoint	Messages/ phase
GMG	1210	3840	1920	20
MLC	4637+398=5035	344	351	2

step 1 / everything else

- Scaling Tests



64 – 4K cores, strong scaling efficiency > 60%



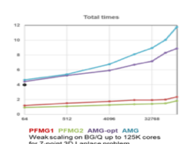
92% weak scaling efficiency

Contact: Peter McCorquodale, LBNL

Development of a new semi-structured AMG in hypre

Motivation:

- Current computer architecture trends favor regular compute patterns for high performance.
- Structured PFMG much faster than unstructured AMG
- But PFMG restricted to problems on structured grids and cannot be used on semi-structured grids!
- Solution: develop new semi-structured AMG based on PFMG



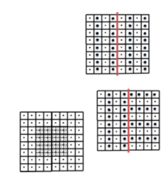
Contact: Ulrike Yang, LLNL

Algorithm:

- SStructMatrix is split into structured and unstructured couplings: A = S +U, where U is a very small portion of the matrix
- Generate interpolation and restriction for structured parts only: P_S, $R_S = P_S^T$
  Adjust weights at part boundaries as needed
- Generate coarse grid operator: $A_C = R_SAP_S = R_SSP_S + R_SUP_S = S_C + U_C$
- mostly structured ops with good potential for efficient performance
- Using 2-point interpolation, U_C restricted to part boundaries, no growth into interior
- Apply weighted Jacobi smoother to $S_C + U_C$

Convergence Tests:

- Tested for $u_{xx} + cu_{yy} + u_{zz} = b$ with $c = 1, 0.01$
- Mixed anisotropy problem (an. 0.001)
- AMR problem
- Compared to PFMG-CG, AMG-CG,(P: 2 nnz/row)
- Number of Iterations:



	PFMG			AMG			SSAMG		
n	32	64	128	32	64	128	32	64	128
C=1; 2D	8	8	9	11	12	14	9	12	15
C=0.01; 2D	6	6	7	6	7	8	13	15	18
Mix; 2D	55	98	145	11	13	16	16	22	31
AMR; 2D	-	-	-	11	13	15	13	16	18
C=1; 3D	9	9	9	12	17	26	9	10	11
C=0.01; 3D	8	8	8	8	9	11	9	11	13
Mix; 3D	36	68	107	11	13	17	12	14	20
AMR; 3D	-	-	-	13	17	22	16	18	20

Conclusions/Future Work:

- SSAMG-CG converges
- achieves better scalability in 3D than 2D
- Future research will investigate inclusion of unstructured portion into interpolation: $P_S + P_U$

More Information: http://www.fastmath-scidac.org or contact Ulrike Yang, LLNL, yang11@llnl.gov, 925-422-2850

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