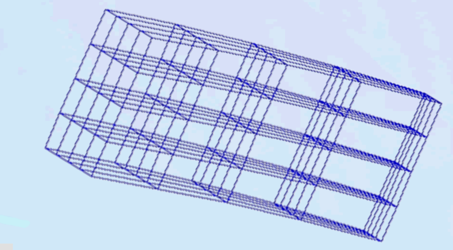
Leveraging Problem Structure within Multilevel Solvers to Improve Robustness & Performance on Advanced Architectures

SAND2018-1884D

P.I. R. Tuminaro, J. Hu, C. Siefert,
L. Berger-Vergiat, M. Mayr
Sandia National Labs, Albuquerque, NM & Livermore, CA



Abstract

Structured meshes will have enormous efficiency benefits on next generation platforms (NGPs). Consequently, we are designing solvers that fuse unstructured AMG ideas with structured multigrid ideas to tackle important classes of *partially* structured calculations. This fusion leads to computational math challenges that we address guided by applications in ice sheet modeling, magneto-hydrodynamics & hypersonic flow.

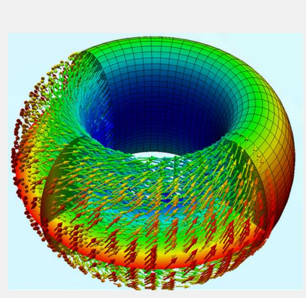
Motivation

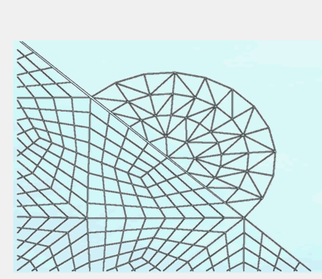
Structured mesh advantages for NGPs:
- ❖ lower memory bandwidth requirements
- ❖ less overall communication
- ❖ facilitates vectorization
- ❖ eases kernel development on special hardware (e.g., GPUs)
- ❖ less indirect addressing

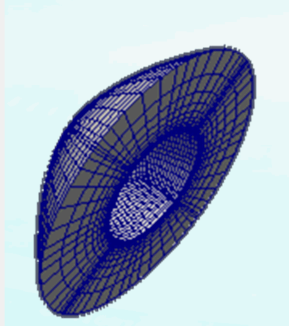
Attractive algorithmic features of structured solvers:
- ❖ low fill-in within hierarchical solvers & fewer MG coarser grid nonzeros
- ❖ specialized algorithms with superior robustness properties (e.g., black-box multigrid, line smoothing)
- ❖ relatively simplified preconditioner setup

Approach

We target scientists who traditionally focus on unstructured grids but are now reconsidering options for NGPs. New solvers must be numerically sound, fast and attractive to applied mathematicians & application scientists, who often have conflicting requirements. We leverage ASCR, ASC, and Sandia strengths in unstructured algebraic multigrid, structured multigrid, HPC algorithms/kernels, and unstructured discretization techniques. As complex applications are not fully structured, algorithm gaps must be addressed by fusing structured & unstructured MG ideas for meshes like:


extruded


uniformly refined within a set of sub-regions


block structured

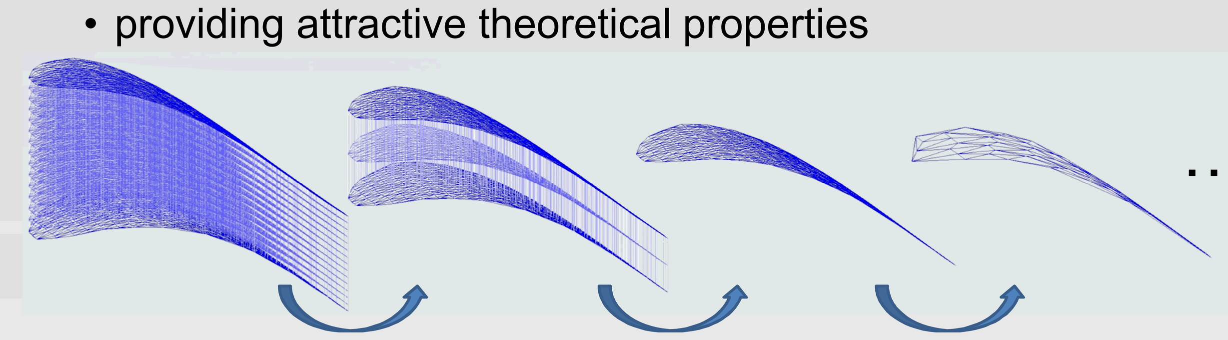
This fusion gives rise to math challenges:

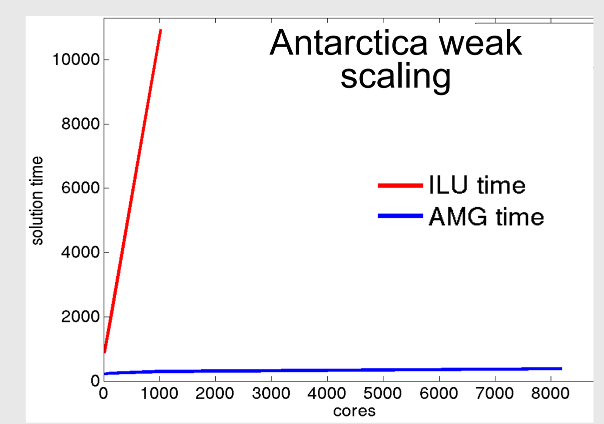
i) coarsening to maintain an extruded mesh structure throughout hierarchy,
ii) aligning grid transfers along interfaces between unstructured & structured sub-regions,
iii) non-conformal mesh issues when coarsening block structured meshes,
iv) avoiding a solver need for stiffness matrices, which are problematic for applications to supply.

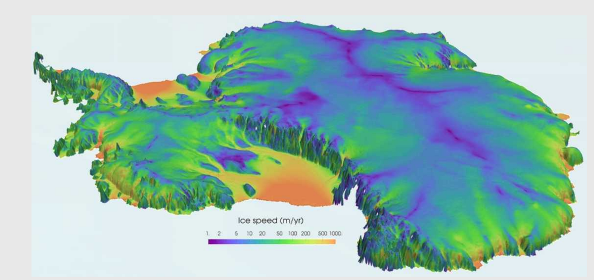
Results

Extruded Meshes

New **Trilinos** solver retains extruded features in MG hierarchy thereby overcoming convergence failures of traditional AMG due to anisotropic effects. Solver coarsens first in extruded direction followed by non-extruded coarsening. Highlights include
- generalizing box MG to meshes with only one structured direction
- aggressively coarsening to avoid HPC inefficiencies of deep hierarchies
- providing attractive theoretical properties



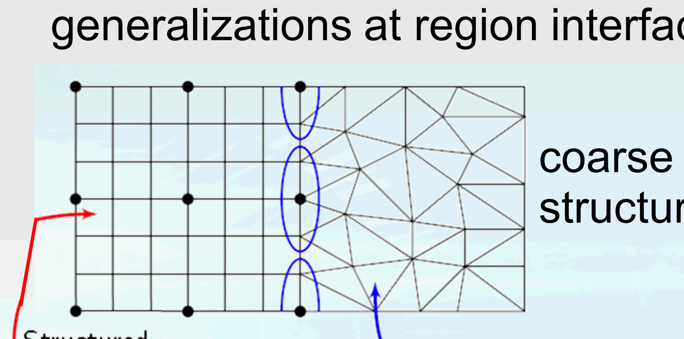




> *35x* run time gain over ILU while standard AMG does not converge
< 2x solution time increase (2.5 million dofs → 1.1 billion dofs)

Hybrid Structured/Unstructured Meshes

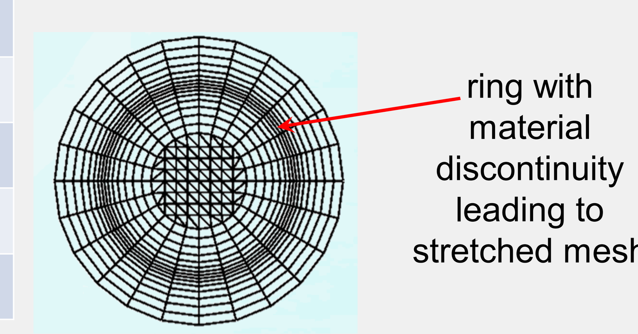
Hybrid solution strategy for grids with structured & unstructured sub-regions improves convergence over standard AMG on stretched meshes. AMG generalizations at region interfaces properly align inter-grid transfers.



coarse nodes & prolongator sparsity patterns from structured & unstructured MG agree on interface

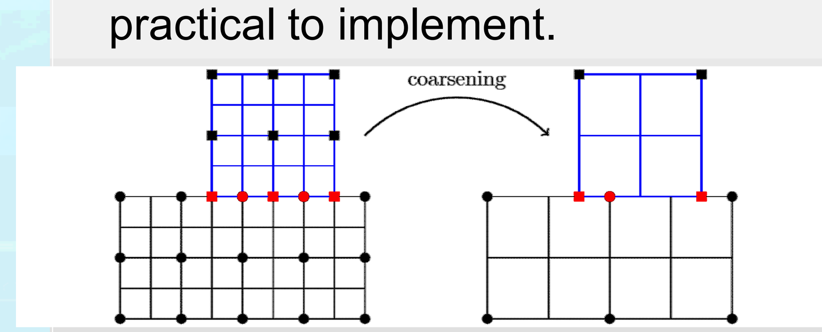
# dofs	max mesh aspect ratio	CG iters	
		AMG	Hybrid AMG
285	132.7	31	12
2417	124.4	89	14
21501	121.6	nc	19
192773	120.6	nc	26

Line smoothing within structured outer ring improves robustness

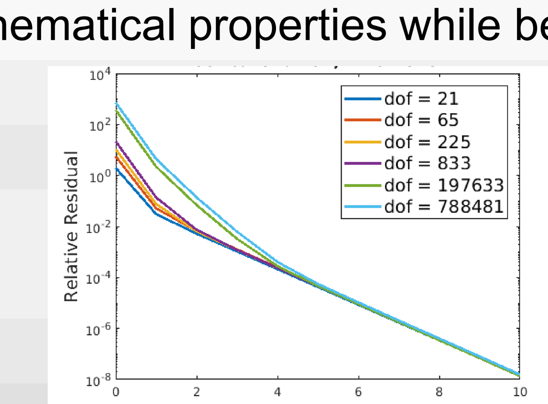


Blocked Structured Meshes

Maintaining structure on block structured grids requires algorithm adaptations for non-conformal coarse meshes. We have devised structured coarsening algorithms that preserve desirable mathematical properties while being practical to implement.



Structured coarsening illustration leading to non-conformal coarse nodes



mesh independent convergence with new algorithm that addresses non-conformity

Conclusions and Future Work

Solver algorithms that exploit partial mesh structure will play a major role in efficiently utilizing NGPs. Our new solvers leverage structure & demonstrate:
- ability to retain structure throughout MG hierarchy without burdensome application requirements
- convergence benefits of structured solvers over their unstructured counter-parts in important situations
- scalability on large systems for extruded mesh solver

We continue to extend, develop, optimize algorithms for partially structured meshes to leverage NGPs.

1 yr DOE impact extruded capability essential for PISCEES ice sheet modeling scalability. Expect to leverage for weapons project.

5 yr DOE impact will significantly boost scalability for incompressible magneto-hydrodynamics & hypersonic flow modeling.

10 yr impact we believe that leveraging partial structure will be key toward maximizing NGP performance for a wide range of DOE applications.

Areas in which we can help

We partner with application teams (2 ASCR & 1 ASC funded) who anticipate significant performance benefits within their codes on NGPs. The partially structured paradigm leads to new math/computer science questions (e.g., alternative solver algorithms, communication avoiding, software design, kernel optimization) that spur new research.

Areas in which we need help

We partner with SciDAC (PISCEES, FASTMATH), the Exascale Computing Project, an ASCR base math program, and ASC projects on NGP kernels & specific applications. The switch to partially structured algorithms is a major shift requiring significant effort within the DOE labs. Further partnering will be needed to tackle the transformation toward partially structured meshes.

References

R. Tuminaro, M. Perego, I. Tezaur, A. Salinger, S. Price, M.Perego, S. Price, "A Matrix Dependent/Algebraic Multigrid Approach for Extruded Meshes with Applications to Ice Sheet Modeling", SIAM J. Sci. Comput.,38(5), pp. C5041-C532, 2016.

P.B. Ohm and R.S. Tuminaro, Hybrid Multigrid Methods for Nearly Structured Meshes, in Center for Computing Research Summer Proceedings 2016, J.B. Carleton and M.L. Parks, eds., Technical Report SAND2017-1294R, Sandia National Laboratories, 2016, pp. 53--62, https://cfwebprod.sandia.gov/cfdocs/CompResearch/docs/proceedings/ccr16.pdf .

This project funded related structure leveraging ideas leading to

Prokopenko A, Tuminaro RS. An algebraic multigrid method for Q2-Q1 mixed discretizations of the Navier-Stokes equations. Numer. Linear Algebra Appl. 2017;e2109. https://doi.org/10.1002/nla.2109