SAND2018-1883C

Leveraging Application Structure Within Next Generation Multigrid Solvers

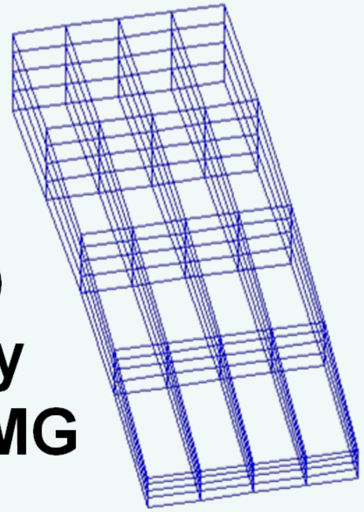
Ray Tuminaro @ Sandia

L. Berger-Vergiat, M. Mayr, J. Shadid, E. Cyr @ Sandia
M. Lupo Pasini @ Emory
P. Ohm @ Tufts

Mar., 2018

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, L.L.C., a wholly owned subsidiary of Honeywell International, Inc., for the U. S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline



Theme: adapting a Hierarchical Hybrid Grid (HHG) approach to a user community & code traditionally focused on fully unstructured finite elements & AMG

⇒ Math & Computer Science Challenges

- fully assembled matrices ⇒ regional oriented matrices
- supporting some unstructured regions
- interfacing with existing mature application codes

- leveraging an existing solver code framework
- data structures & performance

Trilinos

MueLu Multigrid Framework

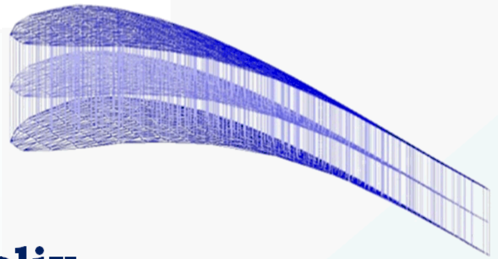
Motivation

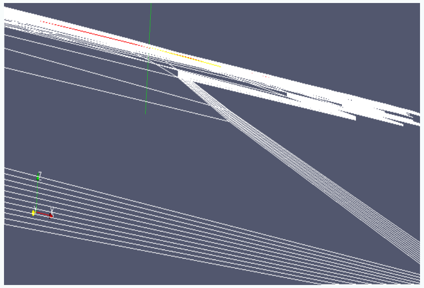
- **Architecture Advantages**
  - less memory bandwidth
  - less communication
  - facilitates vectorization
  - eases kernel development on special hardware (e.g., GPUs)
  - less indirect addressing

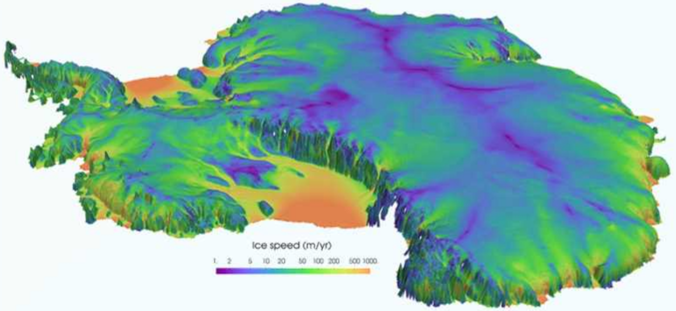
- **Solver Algorithm Advantages**
  - easier to reduce fill-in (e.g., coarse nnzs within multigrid)
  - algorithms applicable to structured grids have robustness advantages (e.g., black-box multigrid, line smoothing),
  - simplified preconditioner setup

Partially Structured Applications

- Ice sheets (extruded)

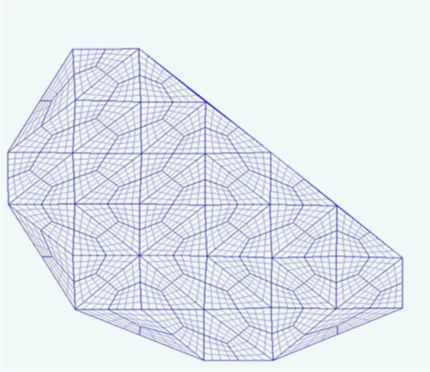


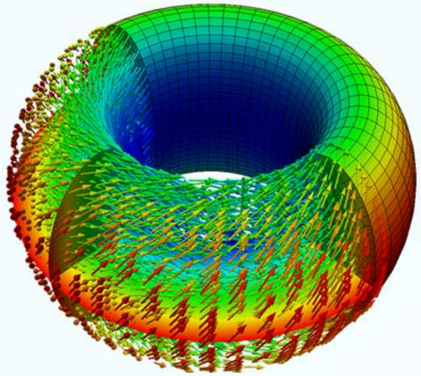




Albany/Felix

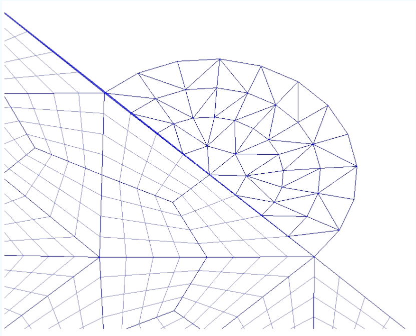
- MHD (regularly refined unstructured)

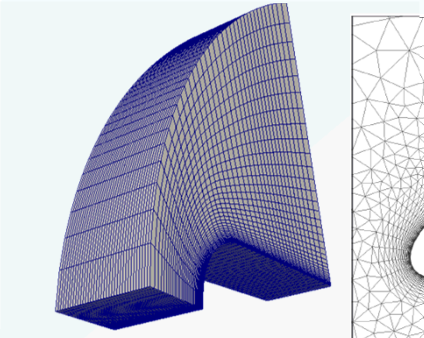


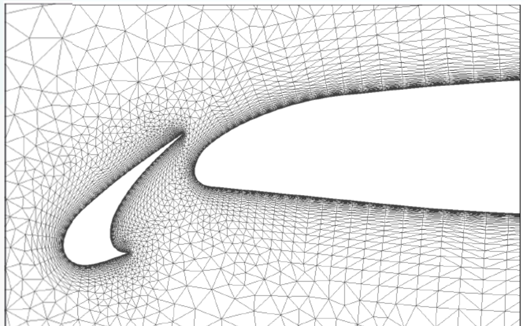


Drekar

- Hypersonic flow (block structured with some unstructured regions) **SPARC**







Hierarchical Hybrid Grids (HHG)

- Formed from regular refinement of coarse grid
  - Grid hierarchy containing regions of structured mesh
  - Each region corresponds to one element of original coarse mesh
- Sub-assemble stiffness matrices in each region
  - Implement multigrid in region-oriented fashion
  - Need to share information between neighboring regions

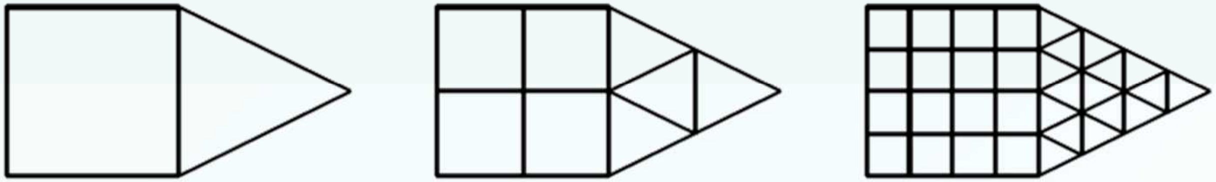
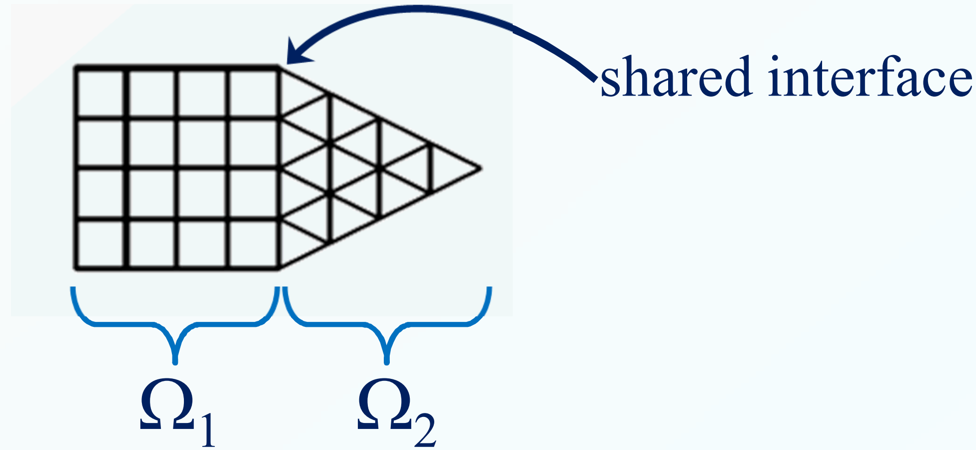


Figure: Example of regular refinement of a mesh

matrix dis-assembly



$$A = A^{\Omega_1} + A^{\Omega_2}$$

user supplied

region matrices

- convenient for region-oriented MG code
- HPC advantages

  Note: $RAP = R^{\Omega_1} A^{\Omega_1} P^{\Omega_1} + R^{\Omega_1} A^{\Omega_2} P^{\Omega_1}$
- useful for some algorithms, e.g. black-box MG

[redacted]

- want regional MG to *resemble* MG applied to A
- applications don't want to supply A^{Ω_k}'s
- mathematically, no $(A^{\Omega_k})_{ij}$ edge $\not\in$ interior(Ω_ℓ) for $k \neq \ell$

A^{Ω_k} should be "good" for black box MG

convergence & dis-assembly

The operator splitting is not unique

$$\overline{A}_{h,k}(i,j) = \begin{cases} A_h(i,j) & \text{if node } i \text{ and/or } j \text{ are interior points of } \mathcal{Q}_{h,k} \\ 0 & \text{if node } i \text{ or } j \text{ do not belong to } \mathcal{Q}_{h,k} \\ ? & \text{if node } i \text{ and } j \text{ are points of } \Gamma \end{cases}$$

A decision must be made to split $A_h(i,j)$ when both nodes i and j lie on internal boundary Γ

$A_{h,k} = R_k \overline{A}_{h,k} P_k$ is used to construct $R^{h_2}_{h_1,k}$ and $P^{h_1}_{h_2,k}$ via BoxMG
$\Rightarrow$ The splitting affects the region grid transfer operators

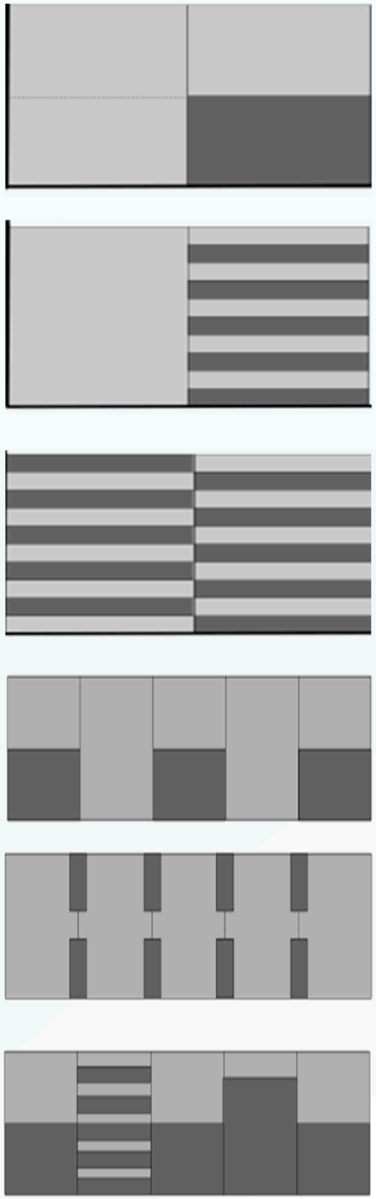
	Regional	Composite	Basic splitting
Test case 1	13	13	13
Test case 2	15	14	14
Test case 3	16	14	14
Test case 4	25	22	22
Test case 5	24	24	24
Test case 6	19	15	15
Test case 7	15	15	15
Test case 8	31	24	24

CG iterations for different splittings across test cases (material jumps & mesh stretching)

$$-\nabla \cdot (a(\mathbf{x})\nabla u) = 1 \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \Gamma_D$$
$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_N$$

$$\Omega = [0,2] \times [0,1]$$

Γ_D : left/right
Γ_N : top/bottom
2 regions with interface @ x=1



Different a()'s

software & dis-assembly

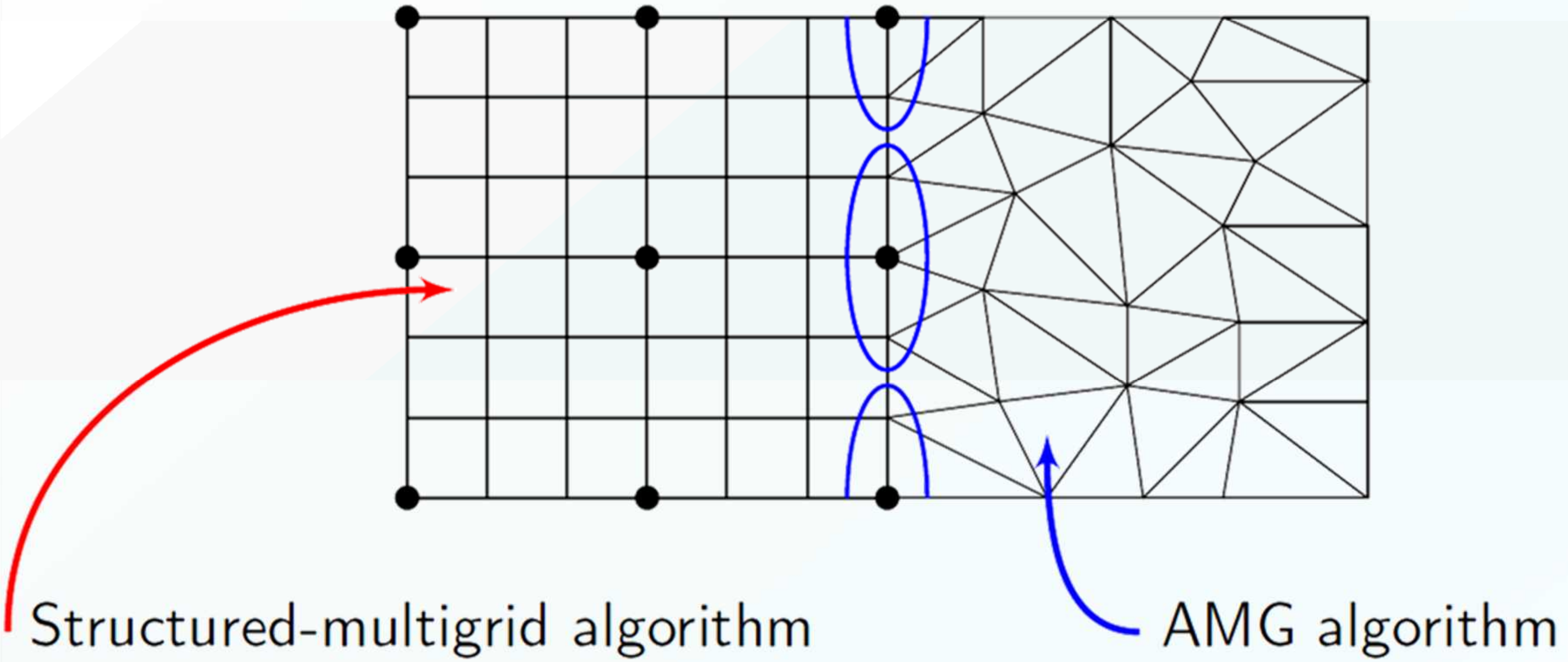
– Use Trilinos overlapping Schwarz-like capabilities + splitting of "overlapped" rows to create region matrices
  - leverage Trilinos import/export
  - lots of care required
  - some complex configurations not allowed

    e.g., processors that only own a "piece" of a region cannot own multiple regions or multiple region pieces
  - region operators explicitly defined within hierarchy while composite residual can be implicitly computed

– Users supply
  - list of region ids for all region pieces that a processor owns
  - a list of region ids that share each composite dof
  - function region(compID,region) that defines local region id of each composite id

HHG with an unstructured region

Modify the HHG scheme to allow for unstructured regions



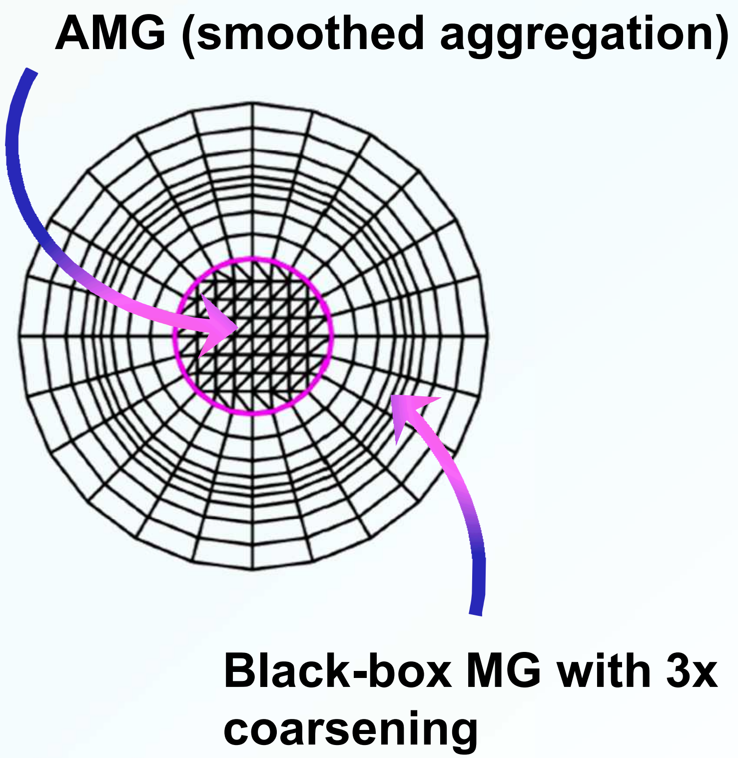
- Need coarse points on interface to agree between regions
- Want interpolation at non-coarse interface points to depend only on coarse points on the interface
- Want sparsity pattern of operators to agree on the interface

Sandia National Laboratories

Structured/Unstructured MG combination

Algorithm: Line Smoothing with interface communication

1. **angular line smoother in outer ring**
2. **overwrite shared values**
3. **Jacobi smoother in disk center**
4. **overwrite shared values**
5. **radial line smoother in outer ring**
6. **overwrite shared values**
7. **Jacobi smoother in disk center**
8. **overwrite shared values**



Numerical Illustration
anisotropic mesh

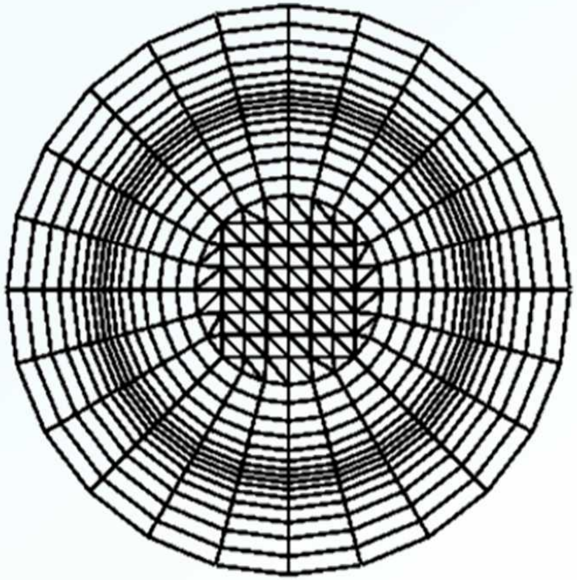
Poisson-like PDE

$$(\rho(x,y)u_x)_x + (\rho(x,y)u_y)_y = f$$

on the domain $x^2 + y^2 \leq 9$, with $u(x,y) = 0$ for $x^2 + y^2 = 9$, and

$$f(x,y) = \begin{cases} 1 & \text{for } ((x-1)^2 + (y-1)^2) \leq (1.25)^2 \\ 0 & \text{otherwise} \end{cases}$$

$$\rho(x,y) = \begin{cases} 100 & \text{for } (1.9)^2 \leq (x^2 + y^2) \leq (2.1)^2 \\ 1 & \text{otherwise} \end{cases}$$



Sandia National Laboratories

Multigrid
Numerical Results

Total Unknowns	Max Aspect Ratio	pcg iterations		
			hybrid methods	
		AMG	Jacobi	Line Smooth
285	4.8	21	20	11
2417	4.8	31	27	13
21501	4.7	49	30	18
192773	4.7	62	32	27
717	14.2	45	47	12
6305	14.2	94	81	14
56493	14.2	-	90	18

Total Unknowns	Max Aspect Ratio	pcg iterations		
			hybrid methods	
		AMG	Jacobi	Line Smooth
285	132.7	31	29	12
2417	124.4	89	72	14
21501	121.6	-	-	19
192773	120.6	-	-	26
717	372.4	60	64	13
6305	364.7	99	-	14
56493	361.9	-	-	18

Sandia National Laboratories

Concluding Remarks

HHG for pre-existing unstructured finite elements software

- Algorithms & Software on-going
  - interface with existing solvers & apps
  - allow for some unstructured regions
  - allow for some block structured meshes
  - matrix dis-assembly requires some care
  - minimize application re-factoring

Structured algorithms advantages: line smoothers on anisotropic cases

Lots to do …

- Still working on general Trilinos implementation
- Performance & data structures
- Thinking about conforming issues & block structured grids

…