



Argonne Training Program on Extreme-Scale Computing



ATPESC 2023

Krylov Solvers and Algebraic Multigrid with *hypre*

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Outline

- What are Krylov Solvers?
- Why are they used?
- Why multigrid methods?
- Algebraic multigrid software
- Hypre software library – interfaces
 - Why different interfaces?
- How does multigrid work?
- Unstructured vs structured multigrid solvers

Iterative Solvers

- Solve linear system $Ax = b$,
where A is a large sparse matrix of size n
- Direct solvers (e.g., Gaussian elimination) too expensive

- Iterative solvers

- Richardson iteration:

$$\begin{aligned}x^{n+1} &= x^n + (b - Ax^n) \\ e^{n+1} &= (I - A)e^n\end{aligned}$$

- Introduce a preconditioner B :

$$\begin{aligned}x^{n+1} &= x^n + B(b - Ax^n) \\ e^{n+1} &= (I - BA)e^n\end{aligned}$$

- Jacobi: $B = D^{-1}$; Richardson: $B = \lambda I$



Generalized Minimal Residual (GMRES)

- $x^{n+1} = x^n + B(b - Ax^n)$
- $\Rightarrow x^{n+1} = \sum_{i=0}^n \alpha_i (BA)^i Bb$
- $x^{n+1} \in K^n = \text{span}\{Bb, (BA)Bb, (BA)^2Bb, \dots, (BA)^n Bb\}$
Krylov space

- Now optimize by defining x^{n+1} through

$$\min_{x^{n+1} \in K^n} \|B(Ax^{n+1} - b)\|$$

- Construct a new basis for K^n through orthonormalization

$$\{q_0 = \frac{Bb}{\|Bb\|}, q_1, \dots, q_n\}$$

- Solve the minimization in the new basis
- q_i also called search directions

Some comments on GMRES

- GMRES consists of fairly simple operations:
 - Inner products and norms (global reductions)
 - Vector updates (embarrassingly parallel)
 - Matvecs (nearest neighbor updates)
 - Application of preconditioner (can be very complicated)
- Often used restarted as GMRES(k), i.e., after k iterations throw out q_i and start again using latest approximation
- Many variants to reduce and/or overlap communication (pipelined GMRES, etc)

Other Krylov solvers

- Conjugate Gradient (CG)
 - For symmetric positive definite matrices
 - Possesses like GMRES an orthogonality property
 - Uses a three-term concurrence
 - Requires only two inner products and a norm per iteration
- BiCGSTAB (Biconjugate Gradient Stabilized)
 - Like CG uses a three-term recurrence relation
 - No orthogonality property, can break down
 - Requires several inner products and a norm at each iteration (and two matvecs)
 - More erratic convergence than GMRES, but needs generally less memory

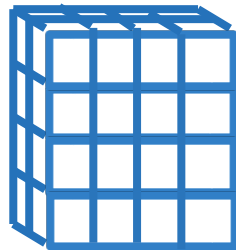
Hands-on Exercises: Krylov methods (First Set of Runs)

- Go to https://xsdk-project.github.io/MathPackagesTraining2023/lessons/krylov_amg_hypre/

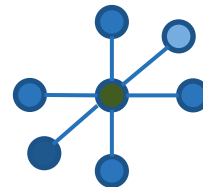
- Poisson equation: $-\Delta\varphi = \text{RHS}$

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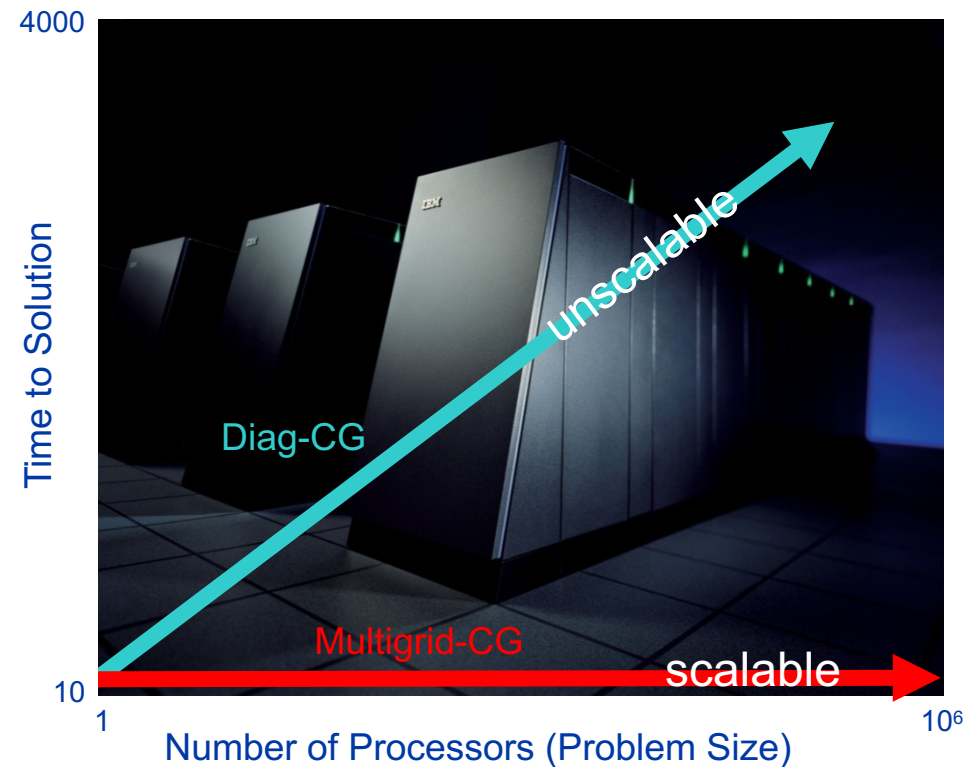
- Grid: cube



- Finite difference discretization:
 - Central differences for diffusion term
 - 7-point stencil

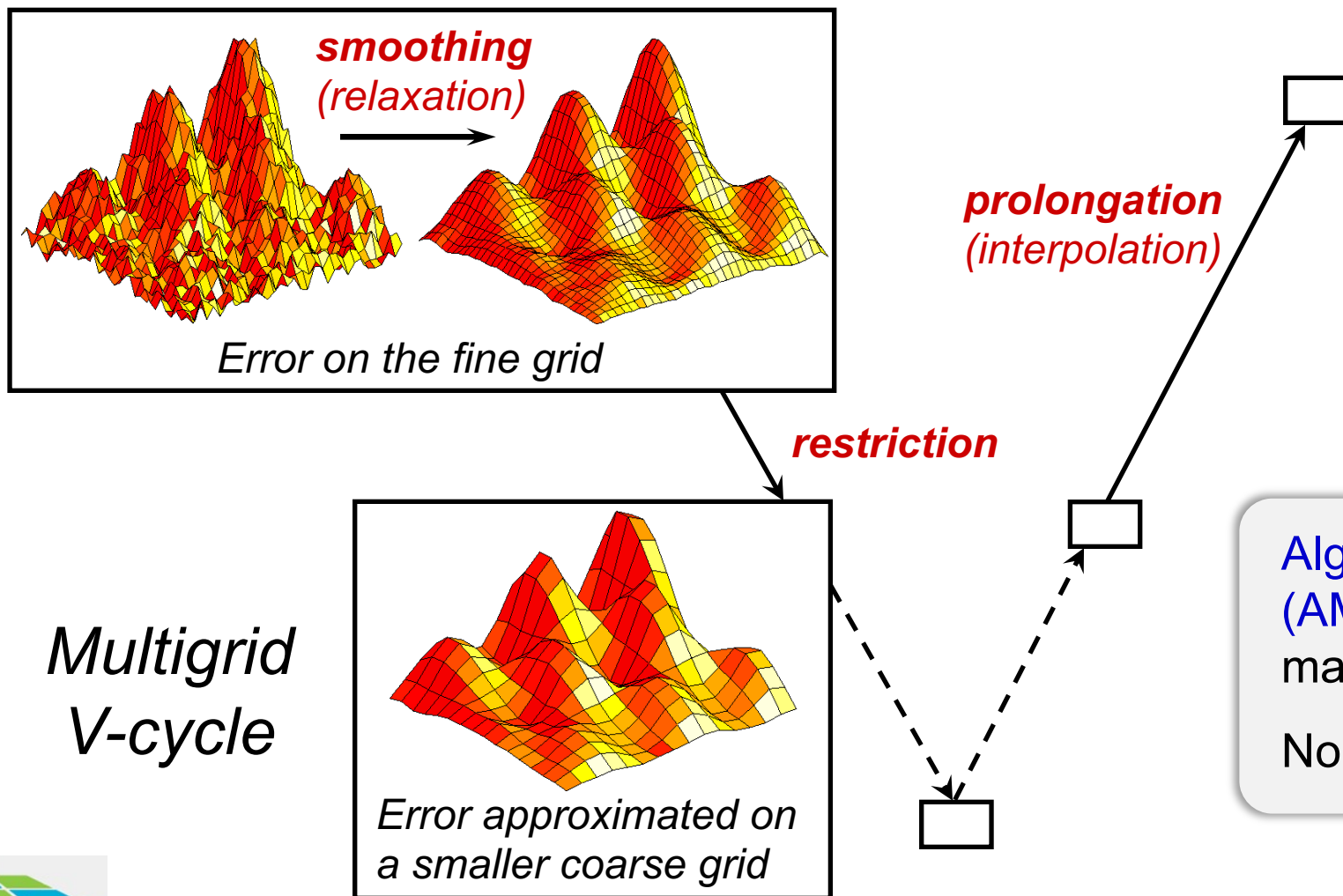


Multigrid linear solvers are optimal ($O(N)$ operations), and hence have good scaling potential



- Weak scaling – want constant solution time as problem size grows in proportion to the number of processors

Multigrid (MG) uses a sequence of coarse grids to accelerate the fine grid solution



Multigrid V-cycle

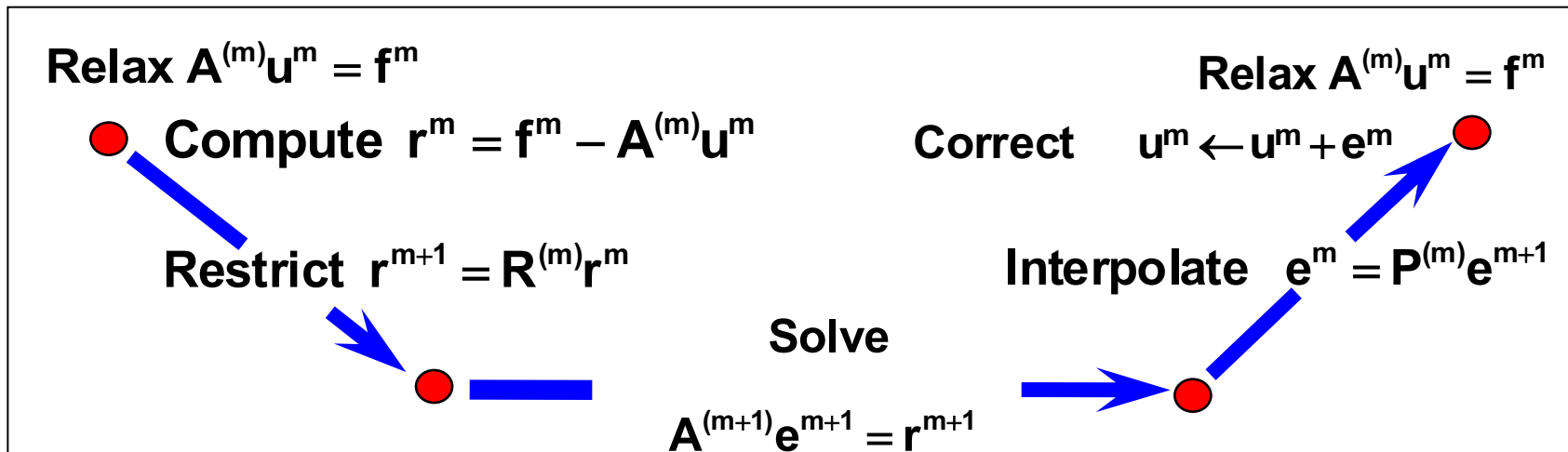
Algebraic multigrid (AMG) only uses matrix coefficients
No actual grids!

AMG Building Blocks



Setup Phase:

- Select coarse “grids”
- Define interpolation: $\mathbf{P}^{(m)}$, $m = 1, 2, \dots$
- Define restriction: $\mathbf{R}^{(m)}$, $m = 1, 2, \dots$, often $\mathbf{R}^{(m)} = (\mathbf{P}^{(m)})^T$
- Define coarse-grid operators: $\mathbf{A}^{(m+1)} = \mathbf{R}^{(m)} \mathbf{A}^{(m)} \mathbf{P}^{(m)}$
Galerkin product

Solve Phase:

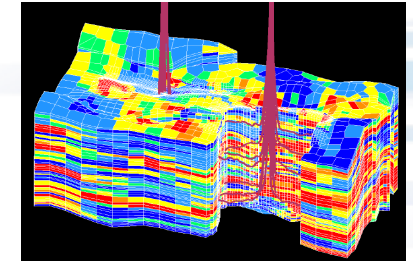
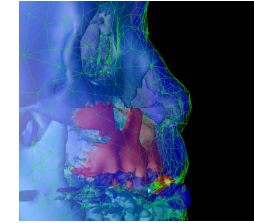
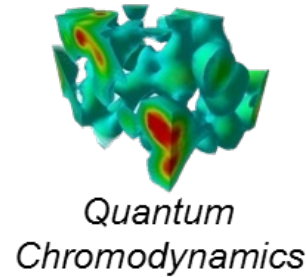
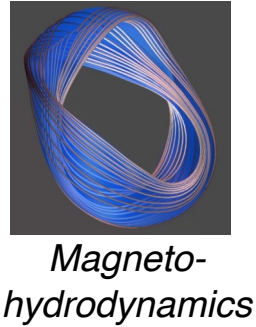
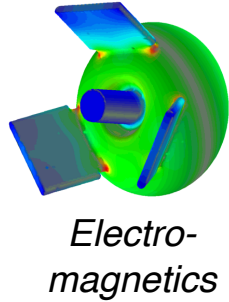
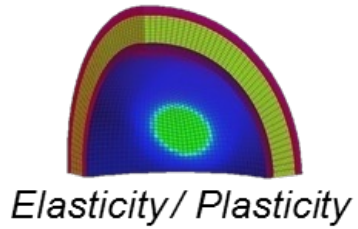


Multigrid software

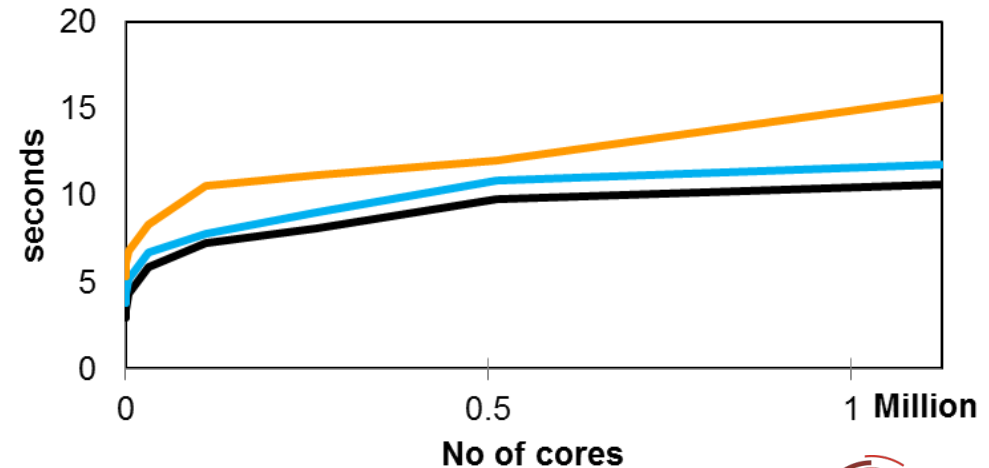
- ML, MueLu included in 
- GAMG in  PETSc
- The *hypra* library provides various algebraic multigrid solvers, including multigrid solvers for special problems e.g., Maxwell equations, ...
- ...
- All of these provide different flavors of multigrid and provide excellent performance for suitable problems
- Focus here on *hypra*

The *hypr* software library provides structured and unstructured multigrid solvers

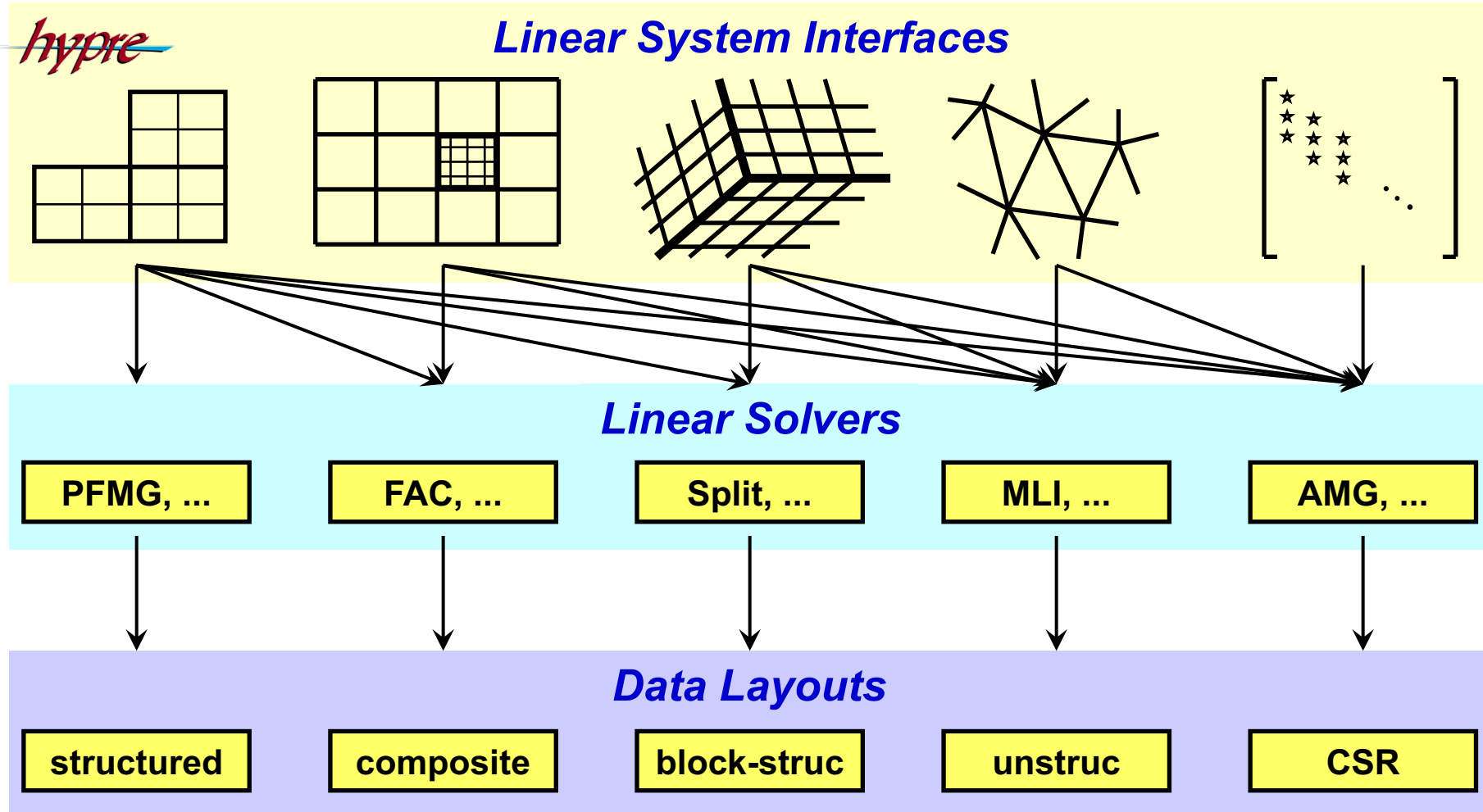
- Used in many applications



- Displays **excellent weak scaling** and **parallelization properties** on BG/Q type architectures



(Conceptual) linear system interfaces are necessary to provide “best” solvers and data layouts

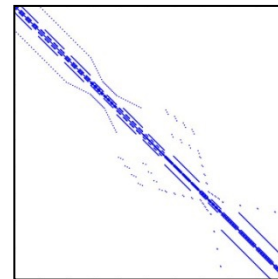
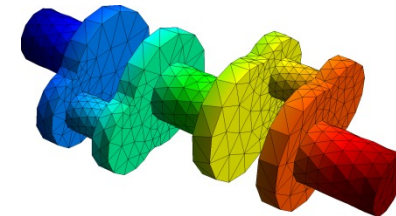
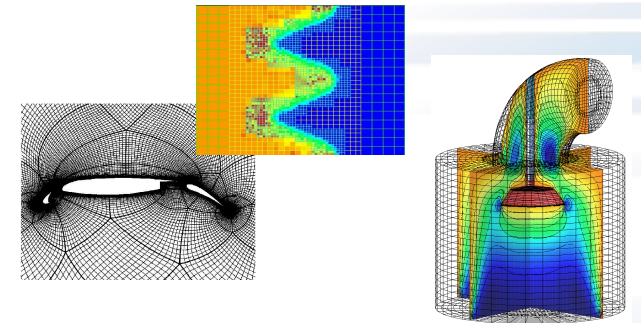
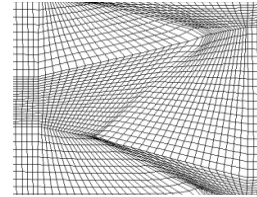


Why multiple interfaces? The key points

- Provides natural “views” of the linear system
- Eases some of the coding burden for users by eliminating the need to map to rows/columns
- Provides for more efficient (scalable) linear solvers
- Provides for more effective data storage schemes and more efficient computational kernels

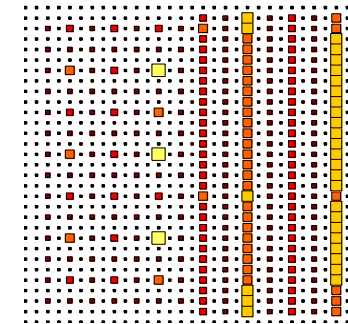
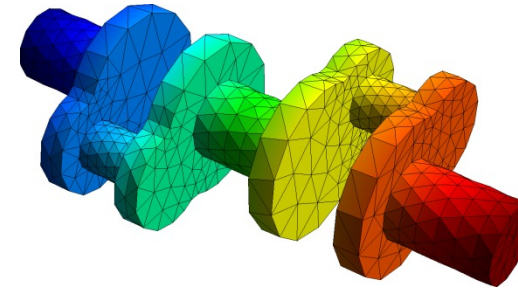
hydre supports these system interfaces

- Structured-Grid (`Struct`)
 - *logically rectangular grids*
- Semi-Structured-Grid (`SStruct`)
 - *grids that are mostly structured*
 - *Examples: block-structured grids, structured adaptive mesh refinement grids, overset grids*
 - *Finite elements*
- Linear-Algebraic (`IJ`)
 - *general sparse linear systems*



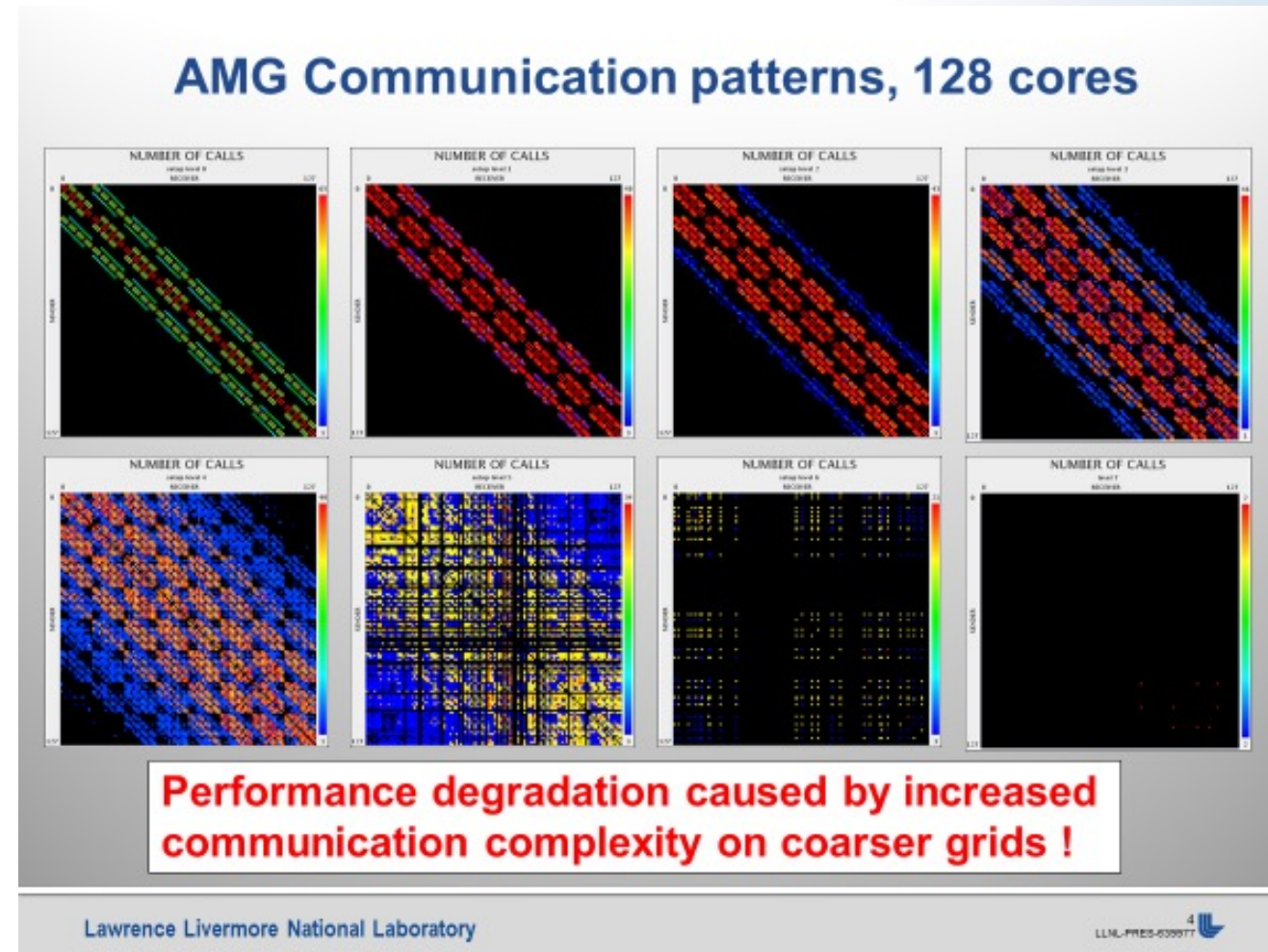
BoomerAMG is an algebraic multigrid method for unstructured grids

- Interface: `SStruct`, `IJ`
- Matrix Class: `ParCSR`
- Originally developed as a general matrix method (i.e., assumes given only A , x , and b)
- Various coarsening, interpolation and relaxation schemes
- Automatically coarsens “grids”
- Can solve systems of PDEs if additional information is provided
- Can also be used through PETSc and Trilinos
- Can now also be used on GPUs (CUDA, HIP)



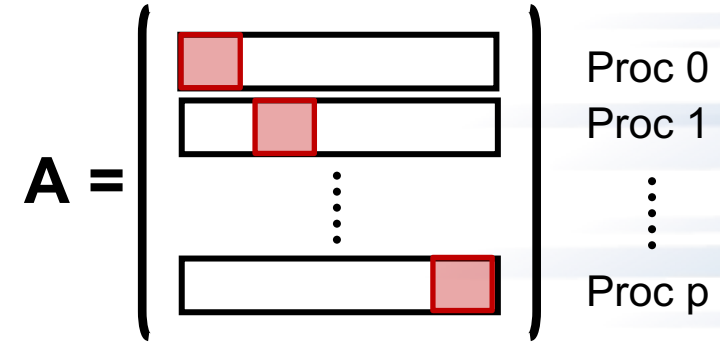
Complexity issues

- Coarse-grid selection in AMG can produce unwanted side effects
- Operator (RAP) “stencil growth” reduces efficiency
- For BoomerAMG, we will also consider complexities:
 - Operator complexity:
$$C_{op} = (\sum_{i=0}^L nnz(A_i)) / nnz(A_0)$$
 - Affects flops and memory
 - Generally, would like $C_{op} < 2$, close to 1
- Can control complexities in various ways
 - varying strength threshold
 - more aggressive coarsening
 - Operator sparsification (interpolation truncation, non-Galerkin approach)
- Needs to be done carefully to avoid excessive convergence deterioration



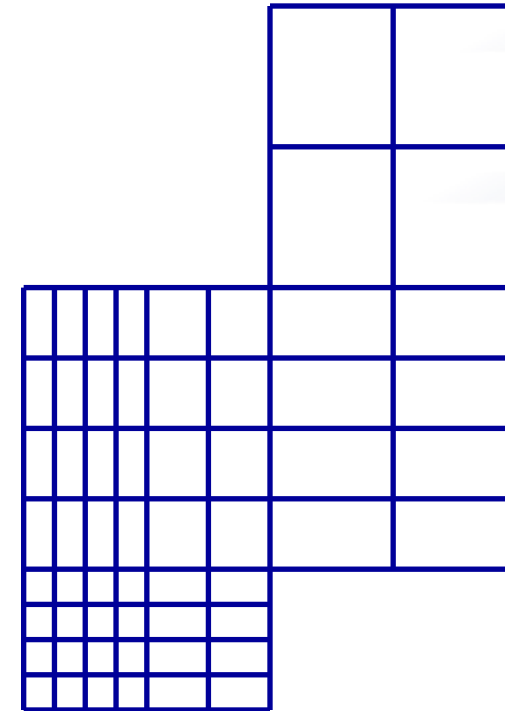
ParCSRMatrix data structure

- Based on compressed sparse row (CSR) data structure
- Consists of two CSR matrices:
 - One containing **local coefficients** connecting to local column indices
 - The other (Offd) containing coefficients with column indices pointing to off processor rows
- Also contains a mapping between local and global column indices for Offd
- Requires much indirect addressing, integer computations, and computations of relationships between processes etc,



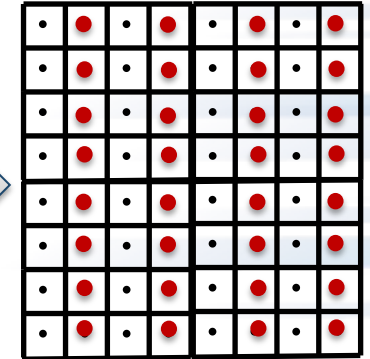
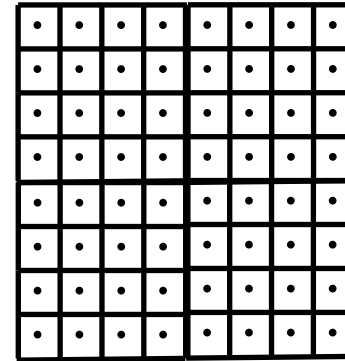
SMG and PFMG are semicoarsening multigrid methods for structured grids

- Interface: `Struct`
- Matrix Class: `Struct`
- SMG uses plane smoothing in 3D, where each plane “solve” is affected by one 2D V-cycle
- SMG is very robust
- PFMG uses simple pointwise smoothing, and is less robust
- Note that stencil growth is limited for SMG and PFMG (to at most 27 points per stencil in 3D)
- Constant-coefficient versions
- Can be used on GPUs (CUDA, HIP, RAJA, Kokkos)



PFMG is an algebraic multigrid method for structured grids

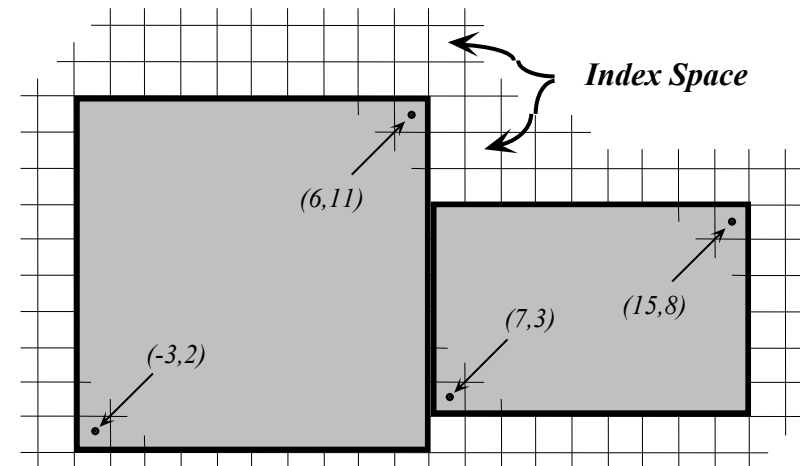
- Matrix defined in terms of grids and stencils
- Uses semicoarsening
- Simple 2-point interpolation
→ limits stencil growth to at most 9pt (2D), 27pt (3D)
- Optional non-Galerkin approach (Ashby, Falgout), uses geometric knowledge, **preserves stencil size**
- Pointwise smoothing
- Highly efficient for suitable problems



Structured-Grid System Interface (Struct)

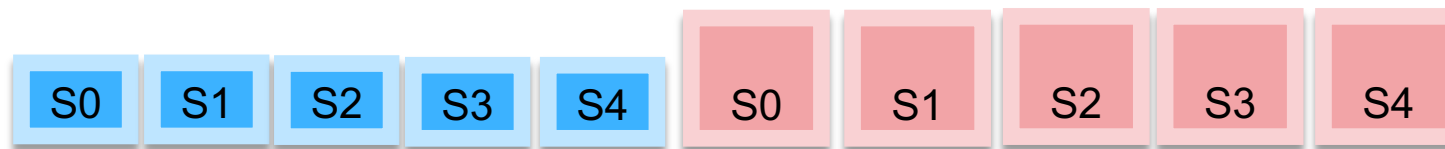
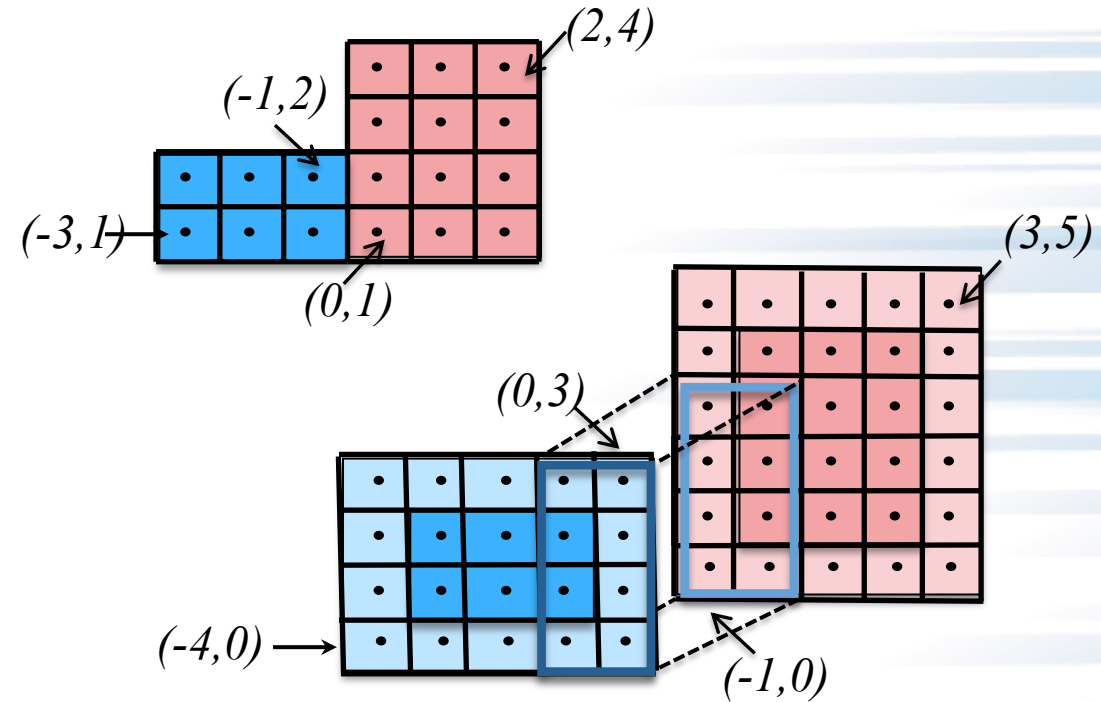
- Appropriate for scalar applications on structured grids with a fixed stencil pattern
- Grids are described via a global d -dimensional *index space* (singles in 1D, tuples in 2D, and triples in 3D)
- A *box* is a collection of cell-centered indices, described by its “lower” and “upper” corners
- The grid is a collection of boxes
- Matrix coefficients are defined via stencils

$$\begin{pmatrix} & \mathbf{S4} & & \\ \mathbf{S1} & \mathbf{S0} & \mathbf{S2} & \\ & \mathbf{S3} & & \end{pmatrix} = \begin{pmatrix} & & & -1 \\ -1 & 4 & & -1 \\ & & & -1 \end{pmatrix}$$



StructMatrix data structure

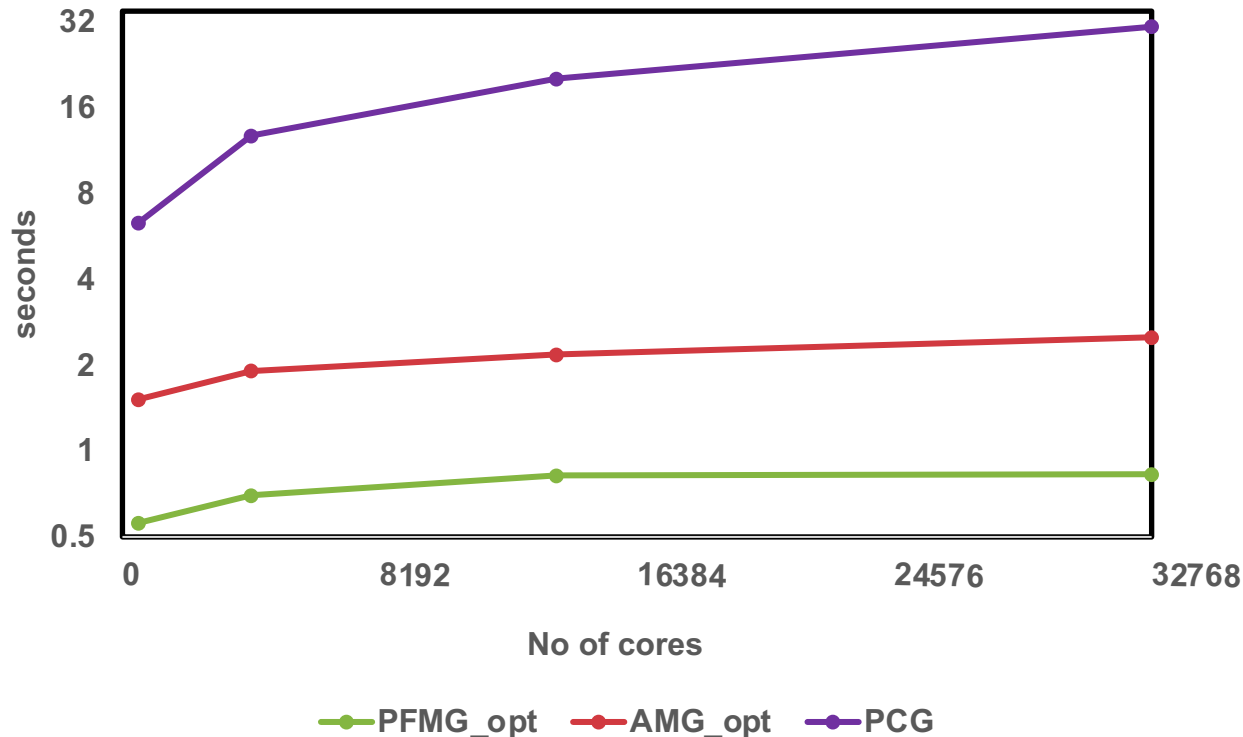
- Stencil $\begin{bmatrix} & S4 & & & \\ S1 & S0 & S2 & & \\ & S3 & & & \end{bmatrix} = \begin{bmatrix} & -1 & & & \\ -1 & 4 & -1 & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}$
- Grid boxes: $[(-3,1), (-1,2)] [(0,1), (2,4)]$
- Data Space: grid boxes + ghost layers: $[(-4,0), (0,3)] , [(-1,0), (3,5)]$
- Data stored



- **Operations applied to stencil entries per box (corresponds to matrix (off) diagonals from a matrix point of view)**

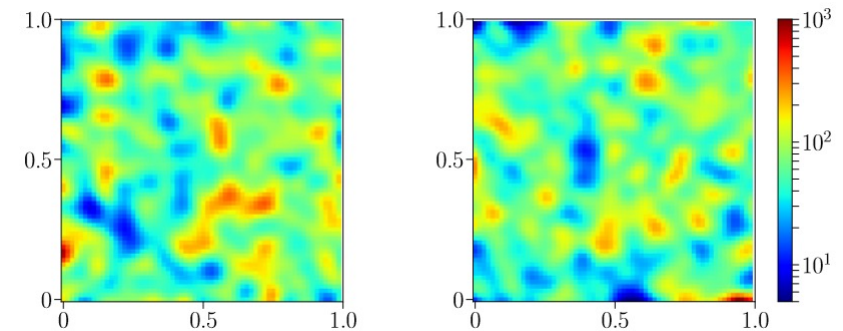
Algebraic multigrid as preconditioner

- Generally algebraic multigrid methods are used as preconditioners to Krylov methods, such as conjugate gradient (CG) or GMRES
- This often leads to additional performance improvements



Classic porous media diffusion problem:
$$-\nabla \cdot \kappa \nabla u = f$$

with κ having jumps of 2-3 orders of magnitude



Weak scaling: 32x32x32 grid points per core,
BG/Q

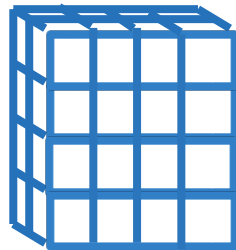
Hands-on Exercises: Algebraic multigrid (Second Set of Runs)

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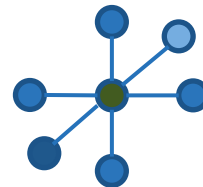
- Poisson equation: $-\Delta\varphi = \text{RHS}$

with Dirichlet boundary conditions $\varphi = 0$

- Grid: cube



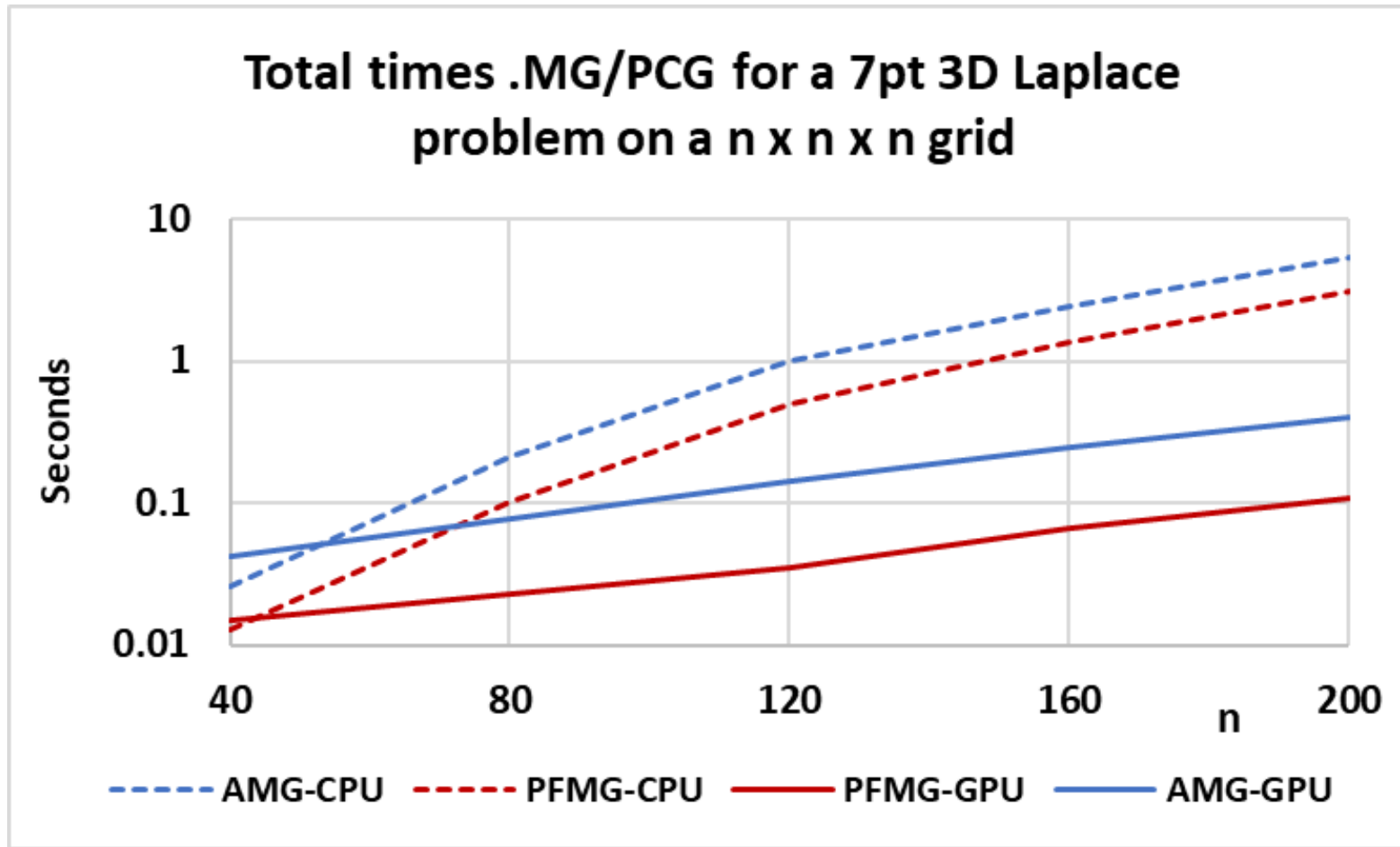
- Finite difference discretization:
 - Central differences for diffusion term
 - 7-point stencil



Porting to GPUs required inclusion of new programming models and different strategies for structured/unstructured interfaces

- Strategy for structured interface and solvers
 - Include new programming models (CUDA, HIP, RAJA, Kokkos, OMP, and SYCL) in `hypre_BoxLoops` (macros that operate on data in loops).
- Strategy for unstructured interface and solvers
 - CSR-based matrix data structures
 - Modularize into smaller chunks/kernels to be ported to CUDA for Nvidia GPUs initially
 - Convert CUDA kernels to HIP for AMD GPUs and SYCL for Intel GPUs
 - Develop new algorithms for portions not suitable for GPUs (interpolation operators, smoothers)
 - different defaults for CPU and GPU use
 - Various special solvers (e.g., Maxwell solver AMS, ADS, AME, pAIR, MGR) built on BoomerAMG benefit from this strategy

Structured multigrid methods perform significantly better than unstructured ones on CPUs and - even more - on GPUs



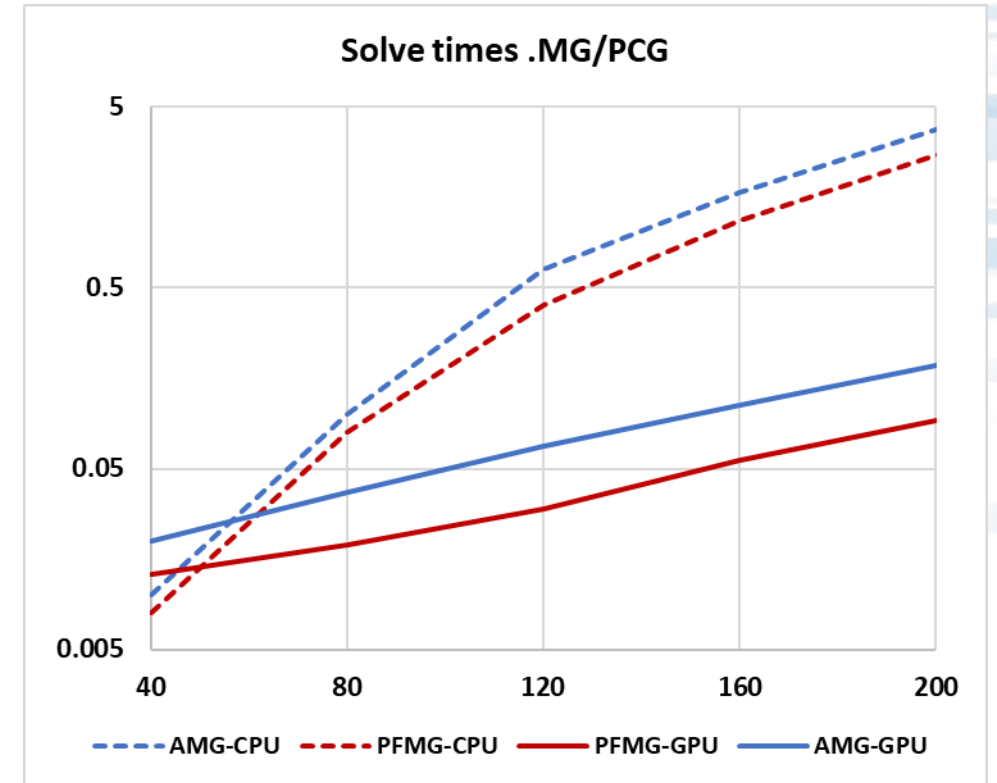
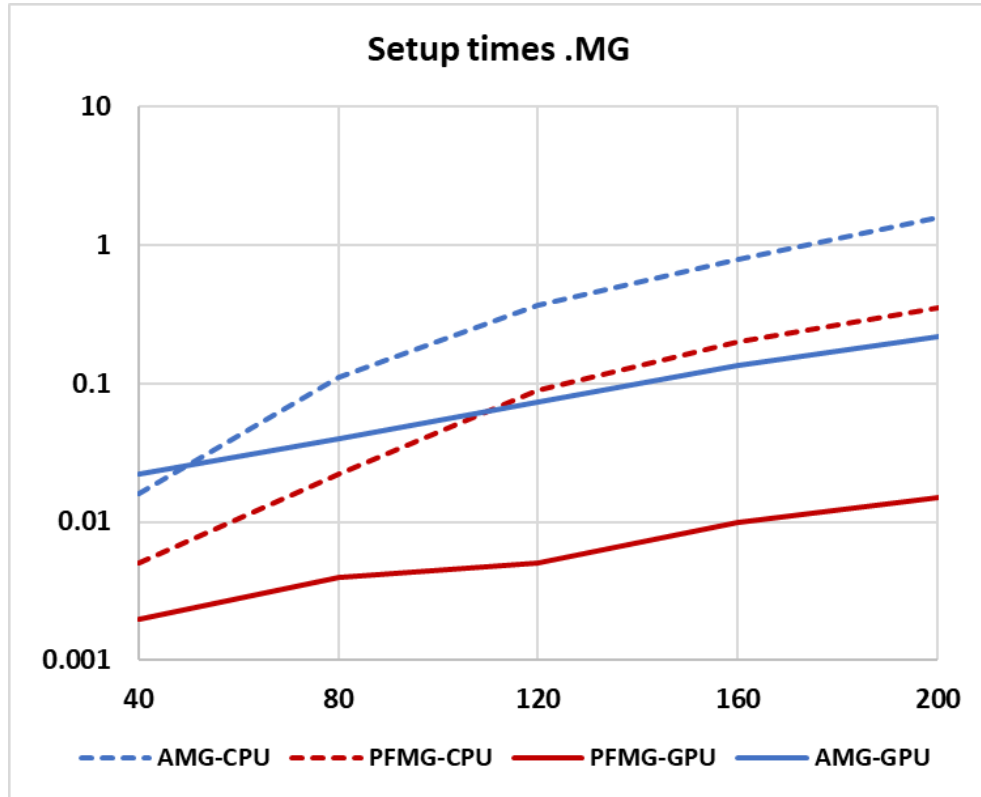
ThetaGPU
GPU: 1 Nvidia A100
CPU: 16 MPI tasks

Used optimal settings for AMG, which are different for CPU and GPU!

Speedups at $n=200$

Speedup GPU/CPU 13.2	CPU Speedup PFMG/AMG 1.7
Speedup GPU/CPU 28.5	GPU Speedup PFMG/AMG 3.8

Most gains of PFMG over AMG in setup phase

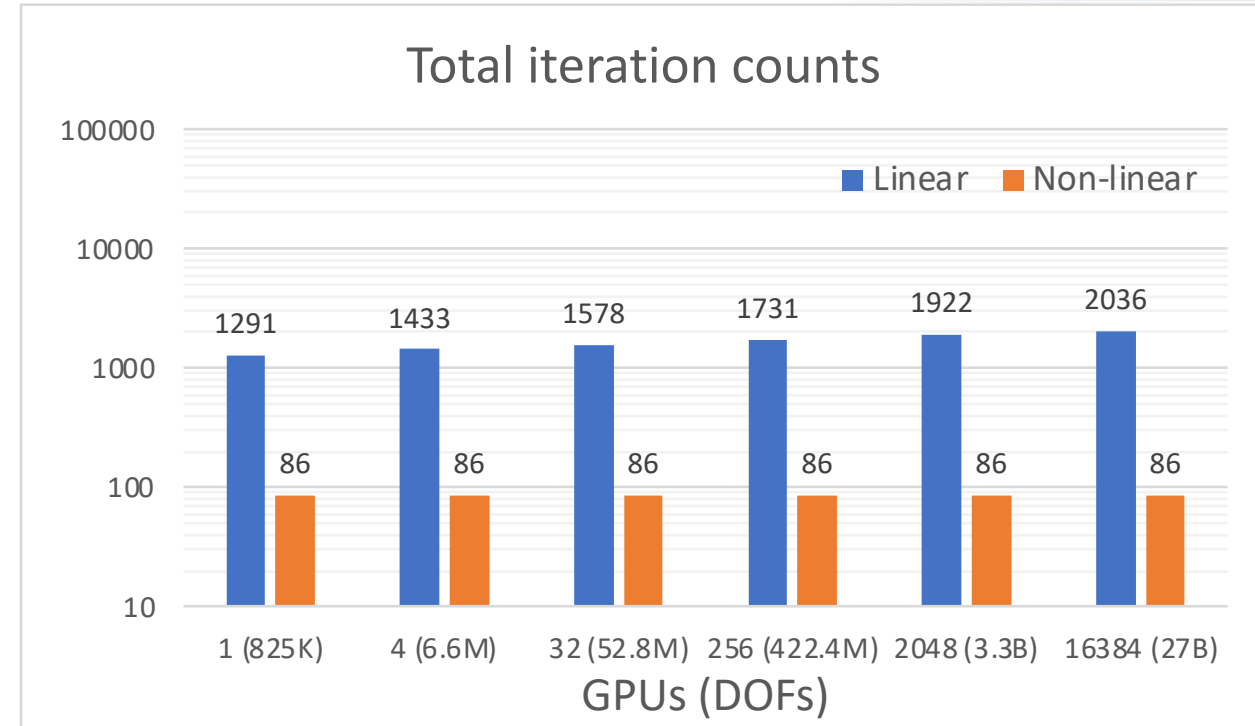
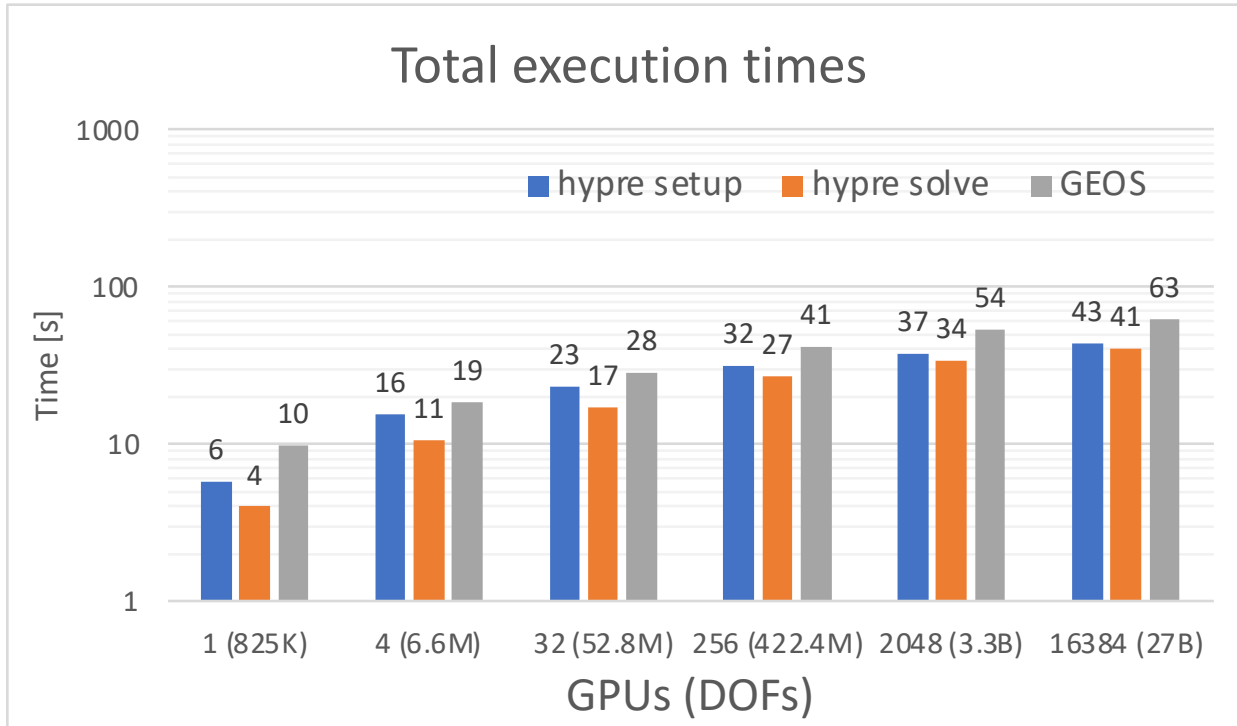


Speedup GPU/CPU 7.2	Speedup GPU/CPU 23.3	CPU Speedup PFMG/AMG 4.5	GPU Speedup PFMG/AMG 14.5
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Speedup GPU/CPU 20.1	Speedup GPU/CPU 29.3	CPU Speedup PFMG/AMG 1.4	GPU Speedup PFMG/AMG 2.0
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Successfully used hypre on Frontier (AMD GPUs) for solving complex multiphysics simulations

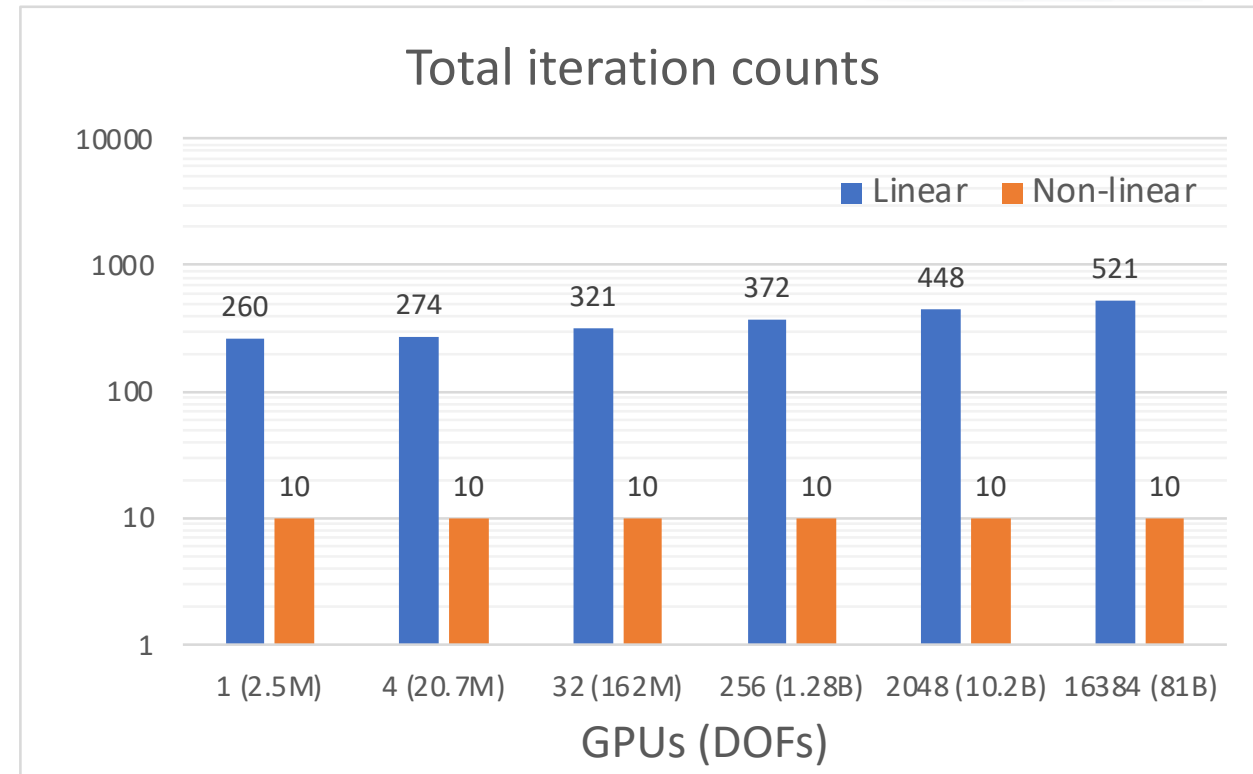
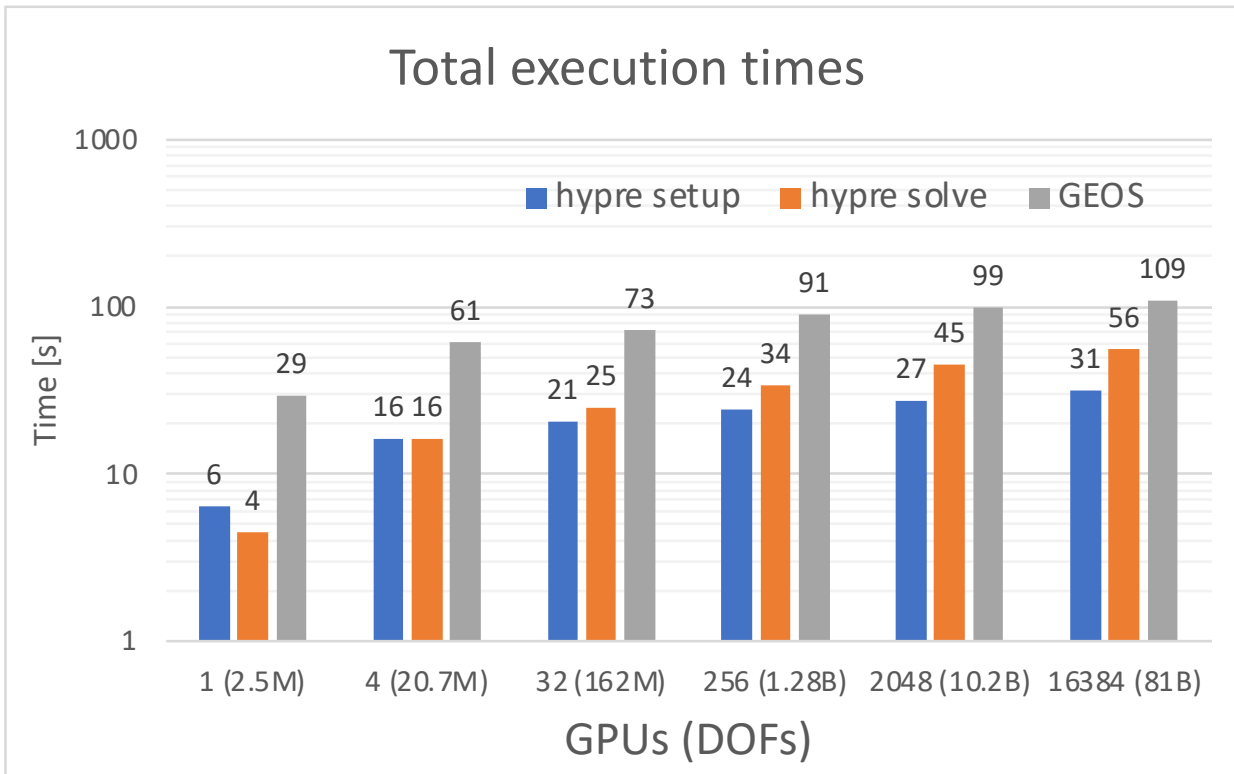
Single-phase flow (Poisson-like problem)



- Weak scaling with BoomerAMG/GMRES(50)
- Time complexity $\sim O(\log(N))$; Iteration counts $\sim O(1)$.

Frontier (AMD GPUs) results - Solved system with 80B DOFs using less than 25% of the machine

Mechanics (linear elasticity problem)



- Weak scaling with BoomerAMG/GMRES(40)

Hands-on Exercises: Comparing GPU to CPU Performance

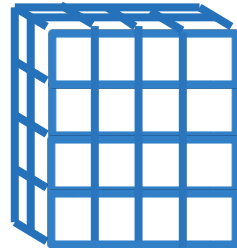
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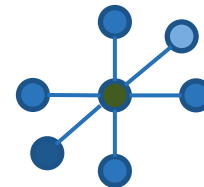
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Thank you!



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