Argonne Training Program on Extreme-Scale Computing

ATPESC 2024

Krylov Solvers and Algebraic Multigrid with *hypre*

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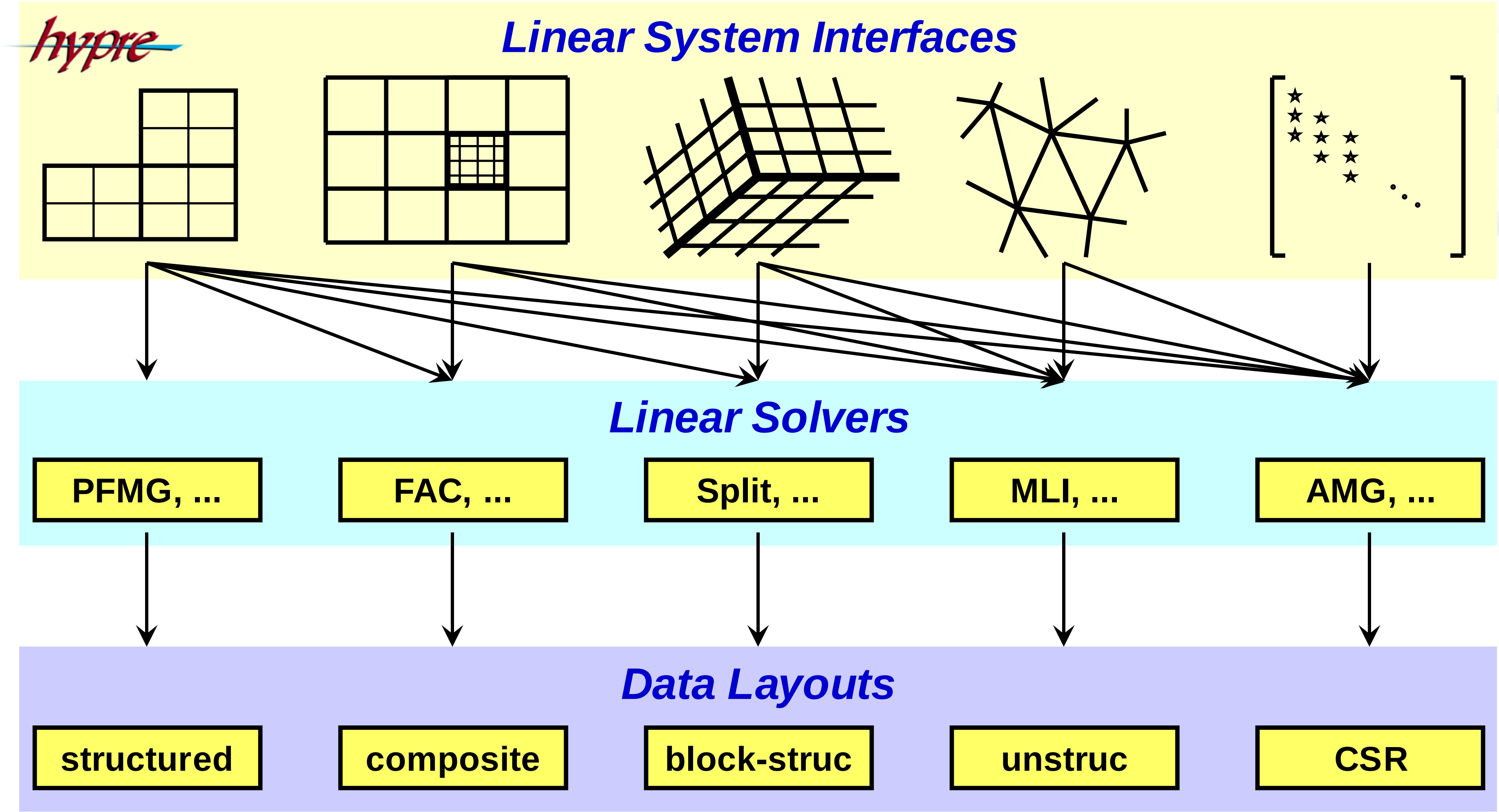
Outline

- Interfaces and Data Structures
  - IJ interface / ParCSR data structure
  - Structured interface / Struct data structure
- Iterative Solvers
  - Krylov Solvers
  - Multigrid solvers
- Some hands-on examples

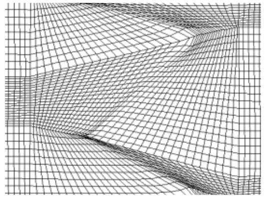
https://www.github.com/LLNL/hypre

	System Interfaces			
Solvers	**Struct**	**SStruct**	**FEI**	**IJ**
Jacobi	X	X		
SMG	X	X		
PFMG	X	X		
Split		X		
SysPFMG		X		
FAC		X		
Maxwell		X		
BoomerAMG		X	X	X
AMS		X	X	X
ADS		X	X	X
MLI		X	X	X
MGR				X
FSAI				X
ParaSails		X	X	X
ILU				X
Euclid		X	X	X
PILUT		X	X	X
PCG	X	X	X	X
GMRES	X	X	X	X
FlexGMRES	X	X	X	X
LGMRES	X	X		X
BiCGSTAB	X	X	X	X
Hybrid	X	X	X	X
LOBPCG	X	X		X

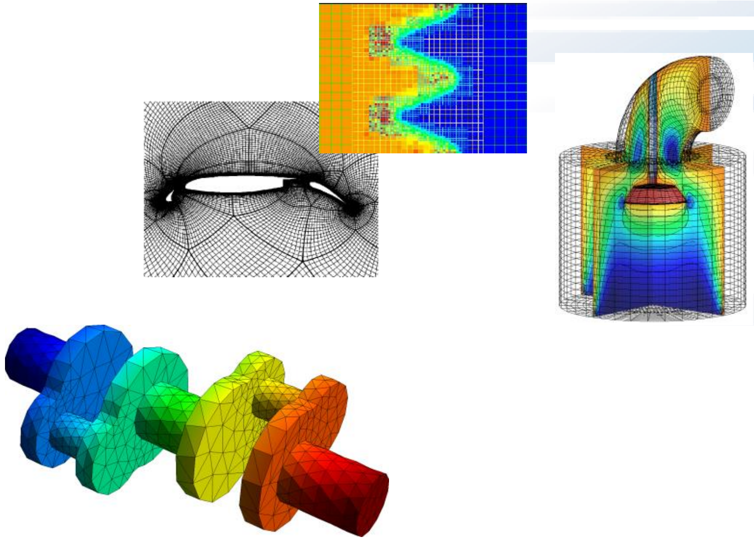
(Conceptual) linear system interfaces are necessary to provide "best" solvers and data layouts



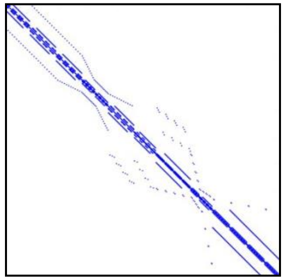
hypre supports these system interfaces



- 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*



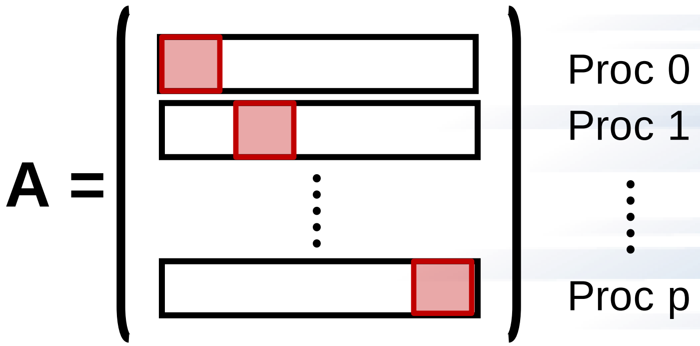
- Linear-Algebraic (`IJ`)
  - *general sparse linear systems*

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

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,



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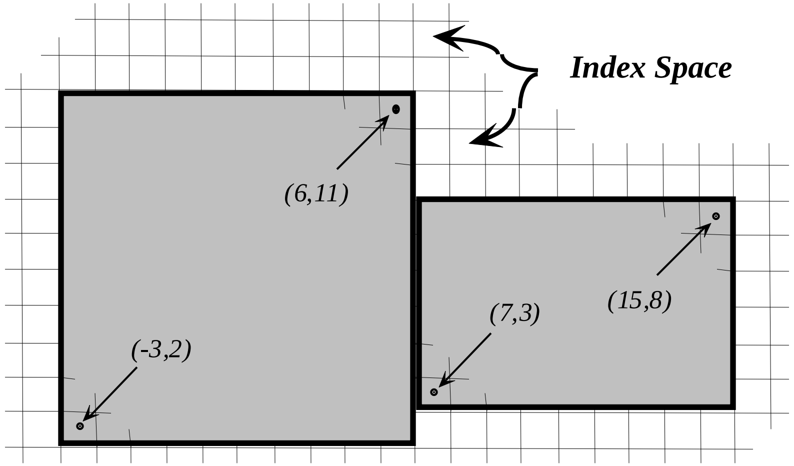
Structured-Grid System Interface (`Struct`)

- 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



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

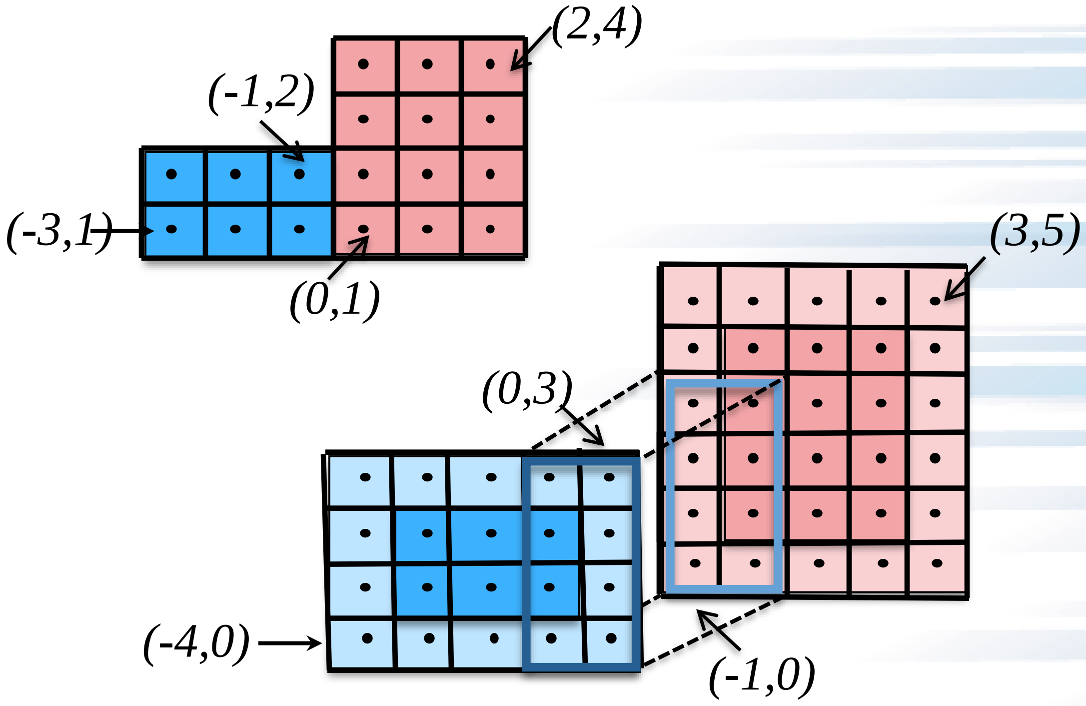
StructMatrix data structure

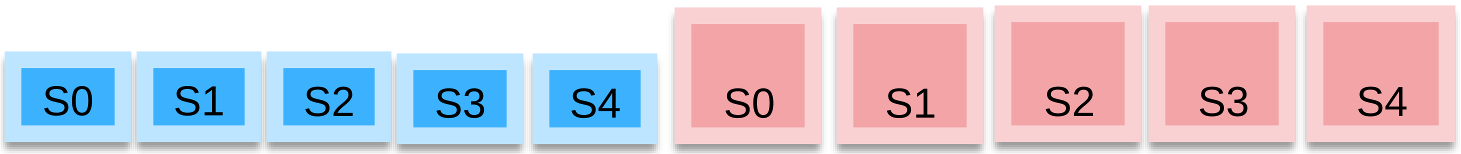
- Stencil $\begin{bmatrix} & S4 & \\ S1 & S0 & S2 \\ & S3 & \end{bmatrix} = \begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix}$

- 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)**

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:

$$x^{n+1} = x^n + (b - Ax^n)$$
$$e^{n+1} = (I - A)e^n$$

- Introduce a preconditioner B:

$$x^{n+1} = x^n + B(b - Ax^n)$$
$$e^{n+1} = (I - BA)e^n$$

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

Generalized Minimal Residual (GMRES)

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

  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

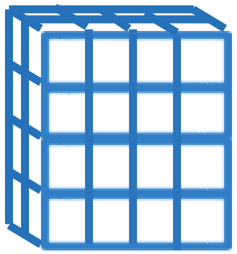
Hands-on Exercises: Krylov methods (First Set of Runs)

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

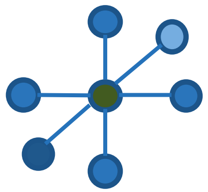
- Poisson equation: $-\Delta\varphi$ = RHS

  with Dirichlet boundary conditions $\varphi = 0$

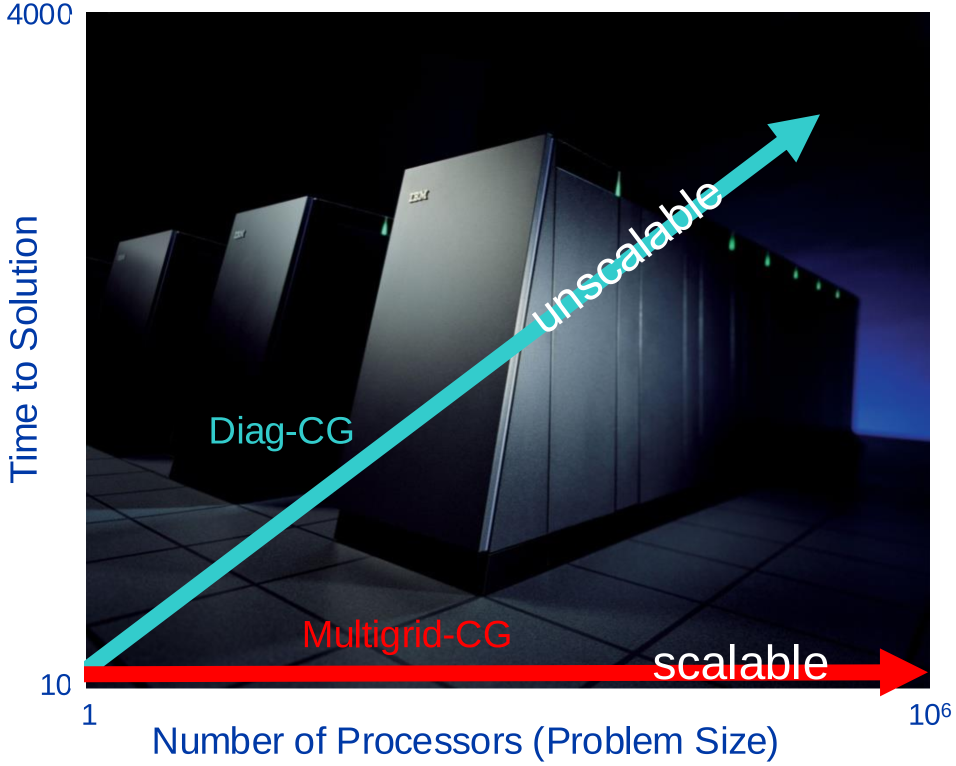
- Grid: cube



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

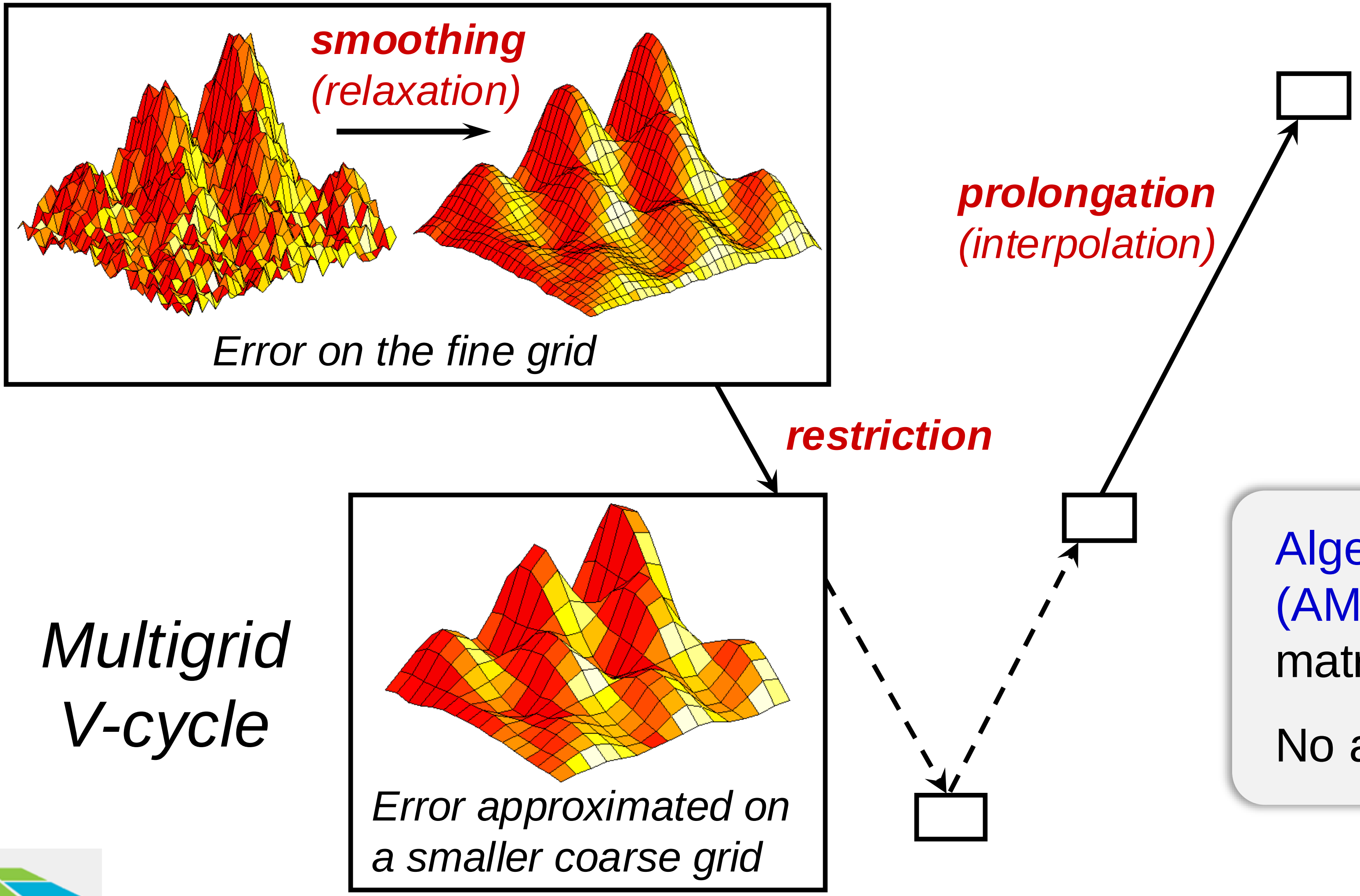


Multigrid linear solvers are optimal ($O(N)$ operations), and hence have good scaling potential



- 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: $P^{(m)}, \quad m = 1,2,\ldots$
- Define restriction: $R^{(m)}, \quad m = 1,2,\ldots, \quad$ often $R^{(m)} = (P^{(m)})^T$
- Define coarse-grid operators: $A^{(m+1)} = R^{(m)} A^{(m)} P^{(m)}$

  Galerkin product

Solve Phase:

Relax $A^{(m)} u^m = f^m$

Compute $r^m = f^m - A^{(m)} u^m$

Restrict $r^{m+1} = R^{(m)} r^m$

Solve $A^{(m+1)} e^{m+1} = r^{m+1}$

Interpolate $e^m = P^{(m)} e^{m+1}$

Correct $u^m \leftarrow u^m + e^m$

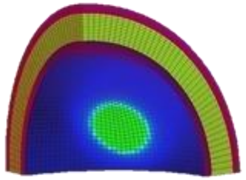
Relax $A^{(m)} u^m = f^m$

Multigrid software

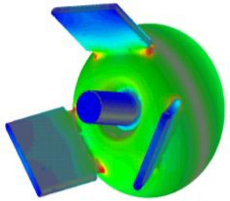
- ML, MueLu included in TRILINOS
- GAMG in PETSc
- The hypre library provides various algebraic multigrid solvers, including multigrid solvers for special problems e.g., Maxwell equations, …
- …
- All of these provide different flavors of multigrid and provide excellent performance for suitable problems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

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

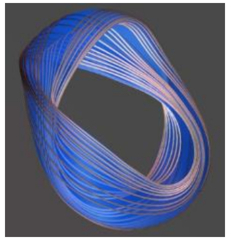
- Used in many applications



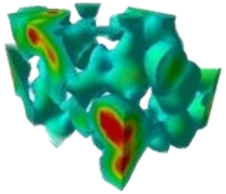
Elasticity/ Plasticity



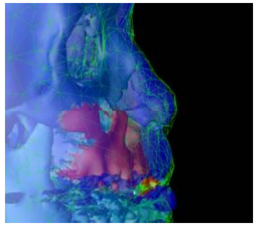
Electro-magnetics



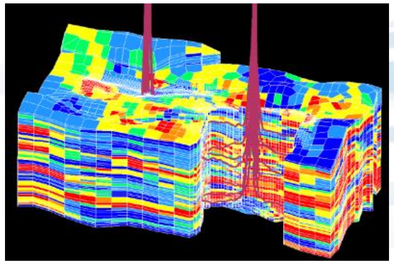
Magneto-hydrodynamics



Quantum Chromodynamics

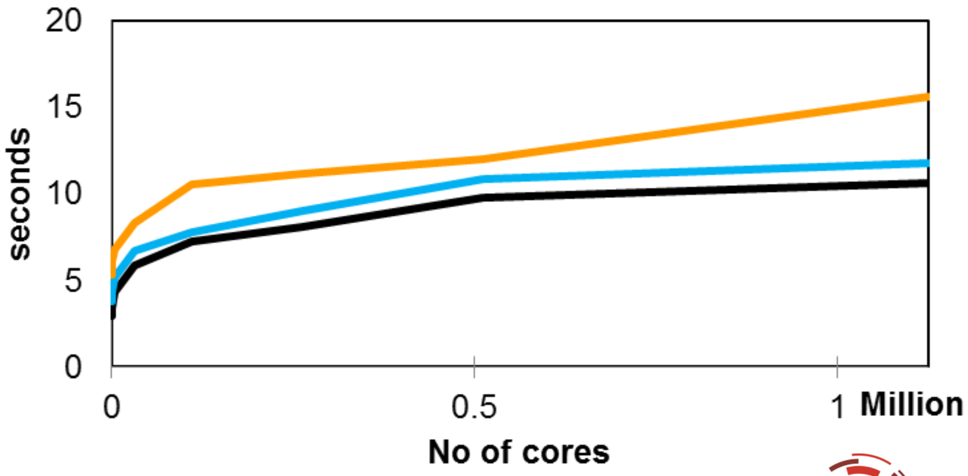


Facial surgery



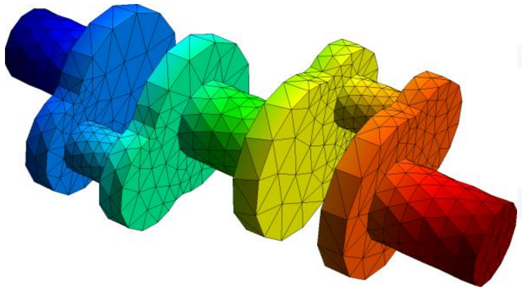
Subsurface simulations

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

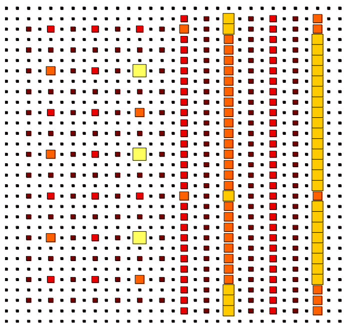


BoomerAMG is an algebraic multigrid method for unstructured grids

- Interface: `SStruct, IJ`
- Matrix Class: `ParCSR`

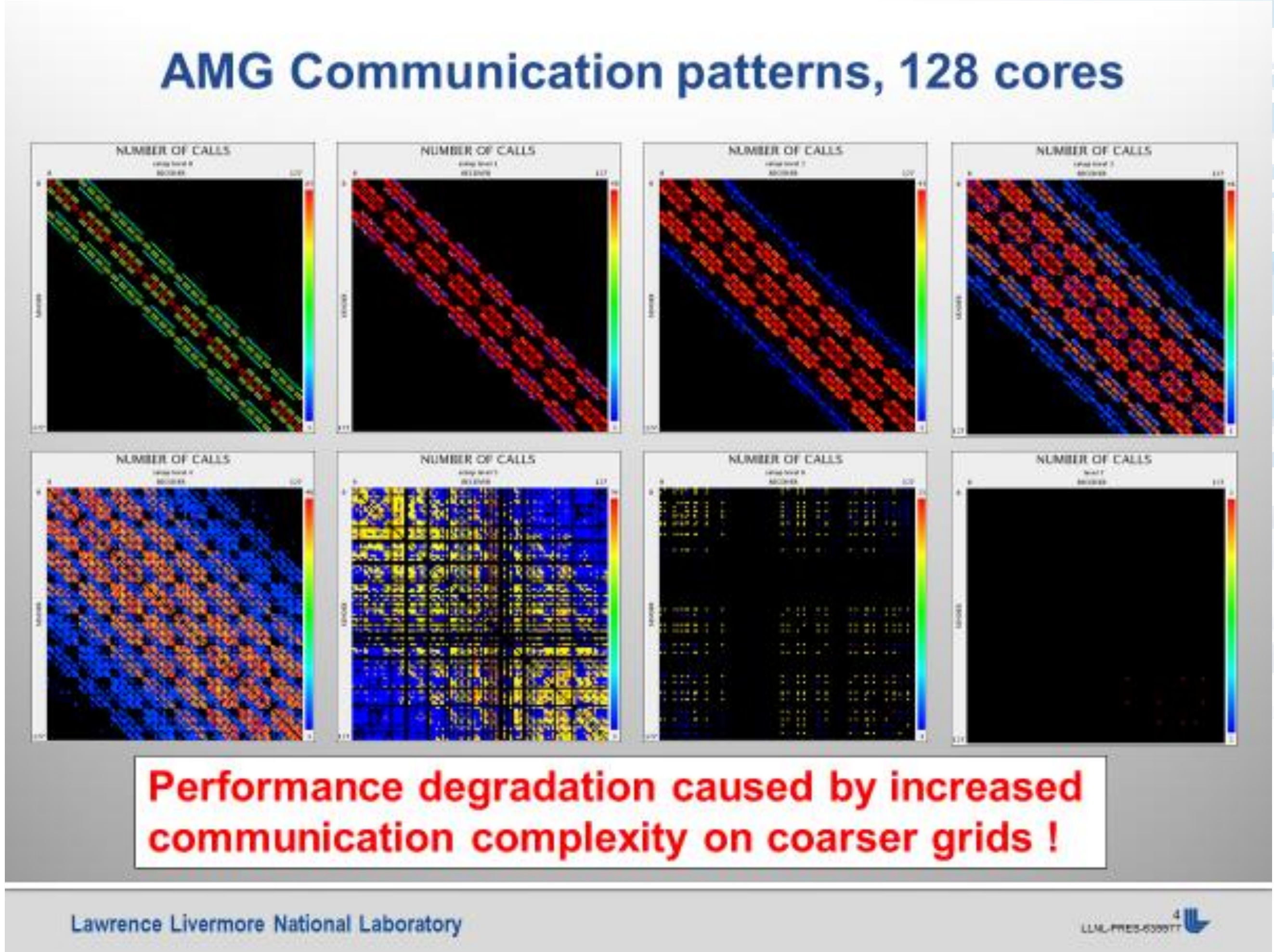


- Originally developed as a general matrix method (i.e., assumes given only A, x, and b)
- Various coarsening, interpolation and relaxation schemes
- Automatically coarsens “grids”
- Can solve systems of PDEs if additional information is provided
- Can also be used through PETSc and Trilinos
- Can be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



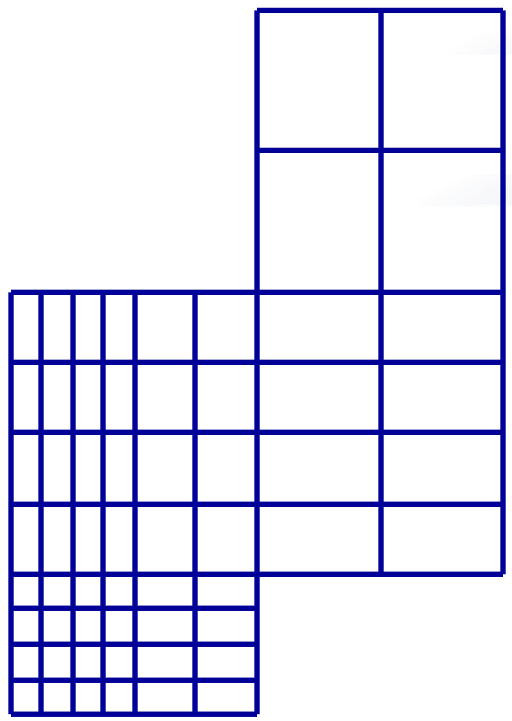
Complexity issues

- 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



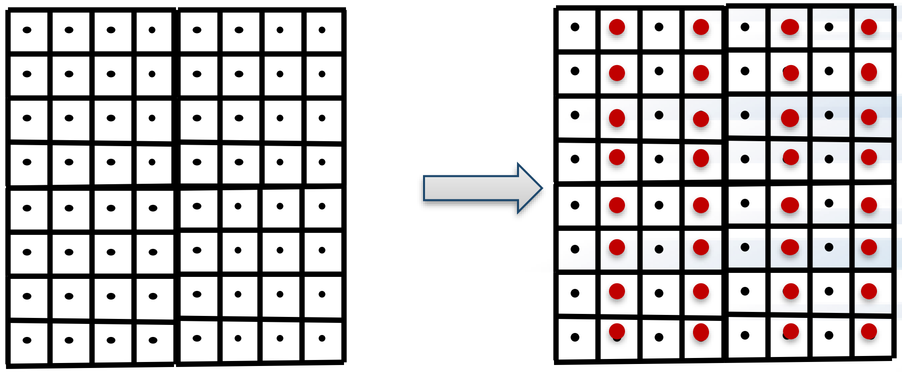
SMG and PFMG are semicoarsening multigrid methods for structured grids

- 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, SYCL, RAJA, Kokkos)



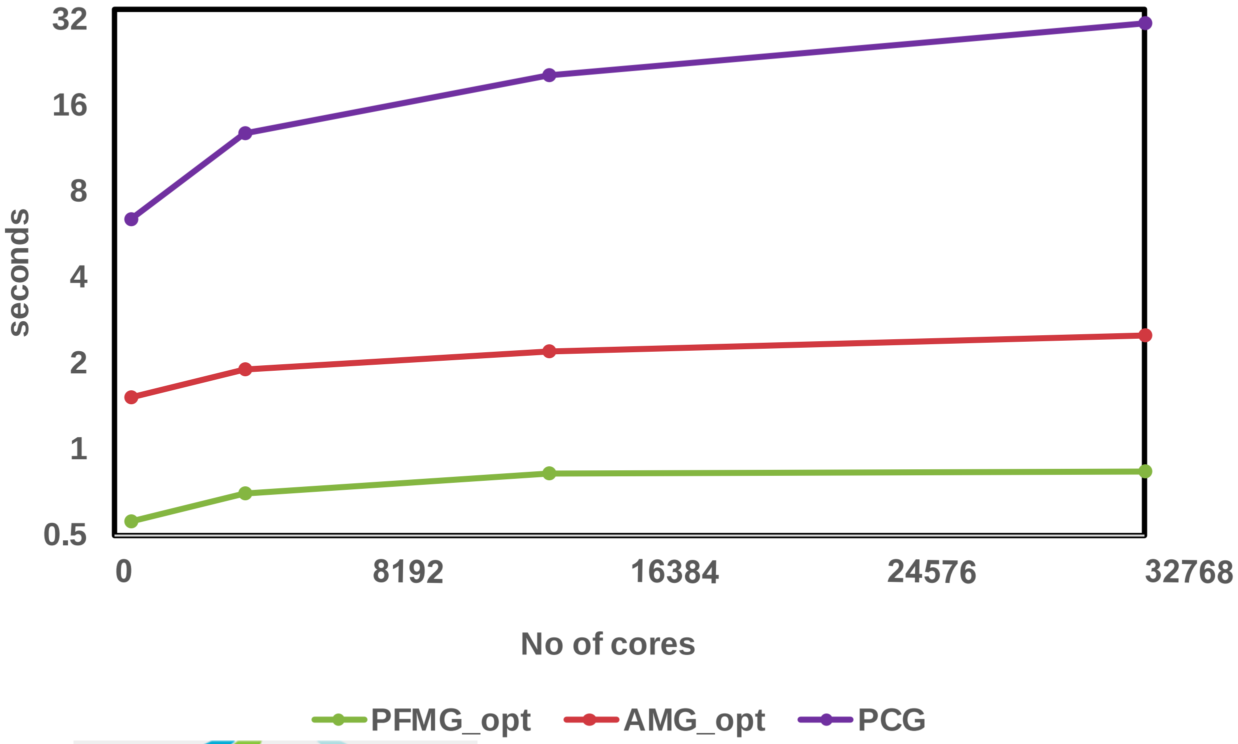
PFMG is an algebraic multigrid method for structured grids

- 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



Algebraic multigrid as preconditioner

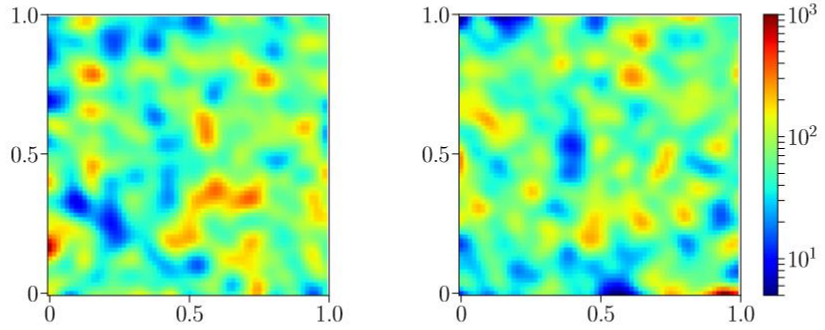
- Generally algebraic multigrid methods are used as preconditioners to Krylov methods, such as conjugate gradient (CG) or GMRES
- This often leads to additional performance improvements



Classic porous media diffusion problem:

$$-\nabla \cdot \kappa \nabla \mathrm{u} = \mathrm{f}$$

with κ having jumps of 2-3 orders of magnitude



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

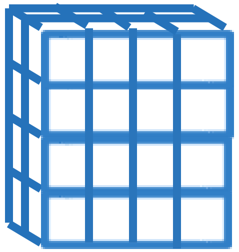
Hands-on Exercises: Algebraic multigrid (Second Set of Runs)

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

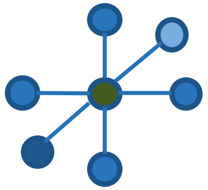
- Poisson equation: $-\Delta\varphi$ = RHS

  with Dirichlet boundary conditions $\varphi = 0$

- Grid: cube



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

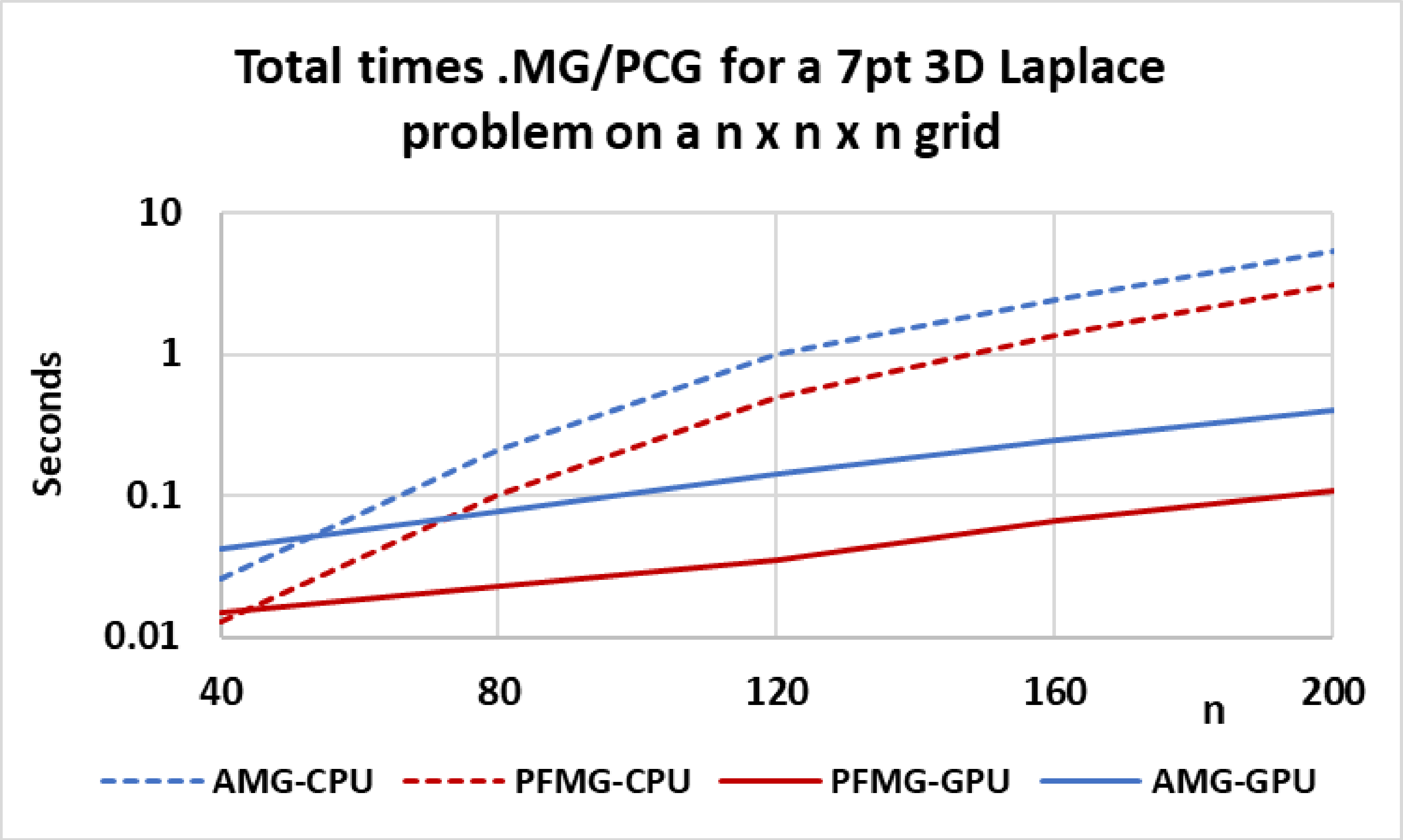


Porting to GPUs required inclusion of new programming models and different strategies for structured/unstructured interfaces

- 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 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



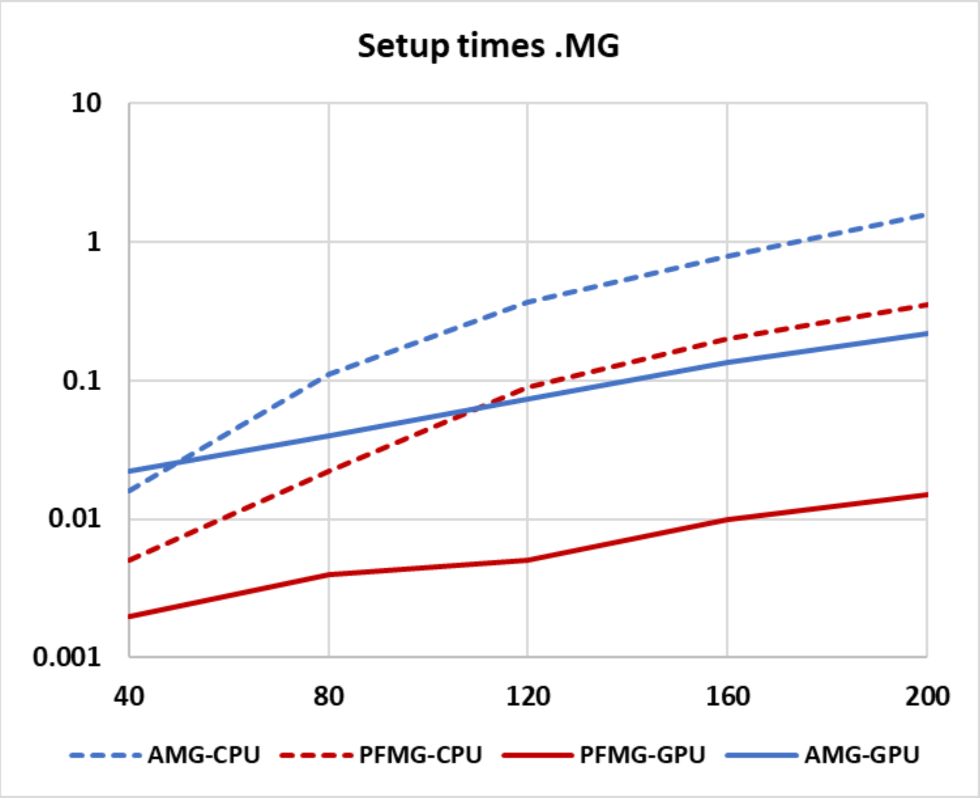
ThetaGPU
GPU: 1 Nvidia A100
CPU: 16 MPI tasks

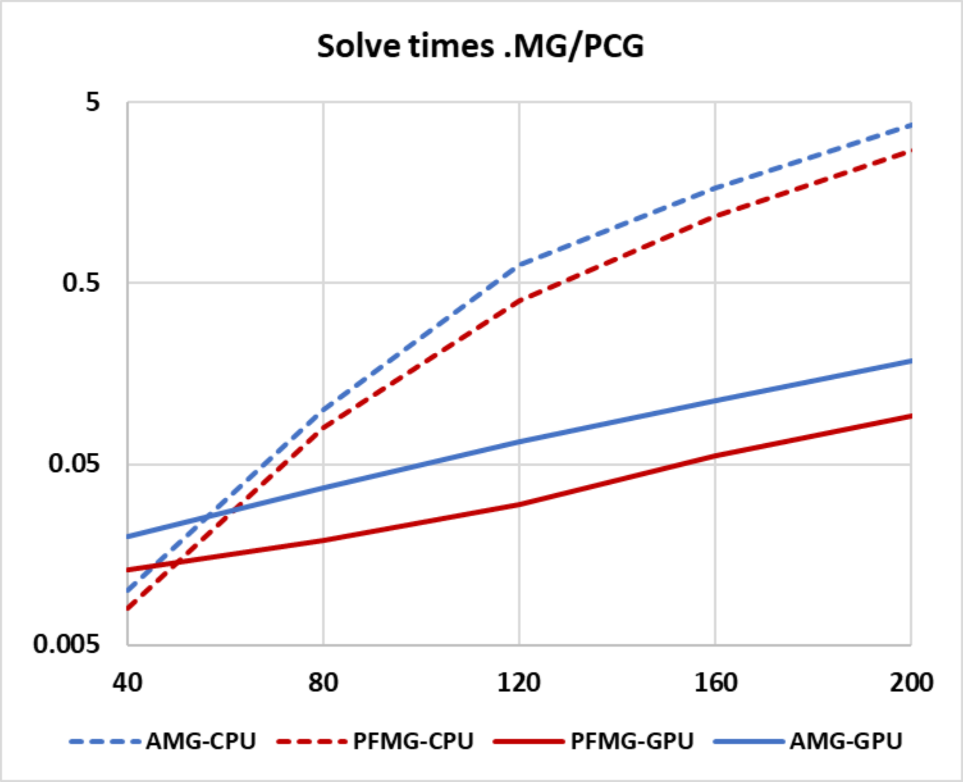
Used optimal settings for AMG, which are different for CPU and GPU!

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

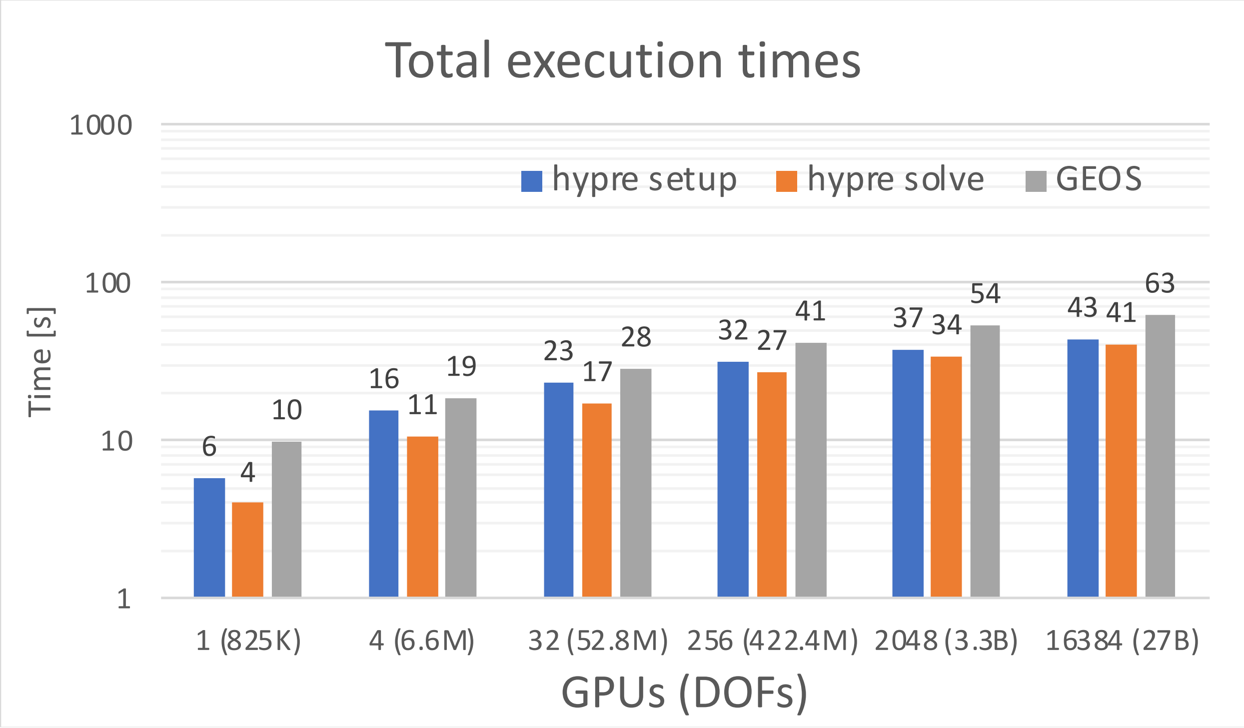


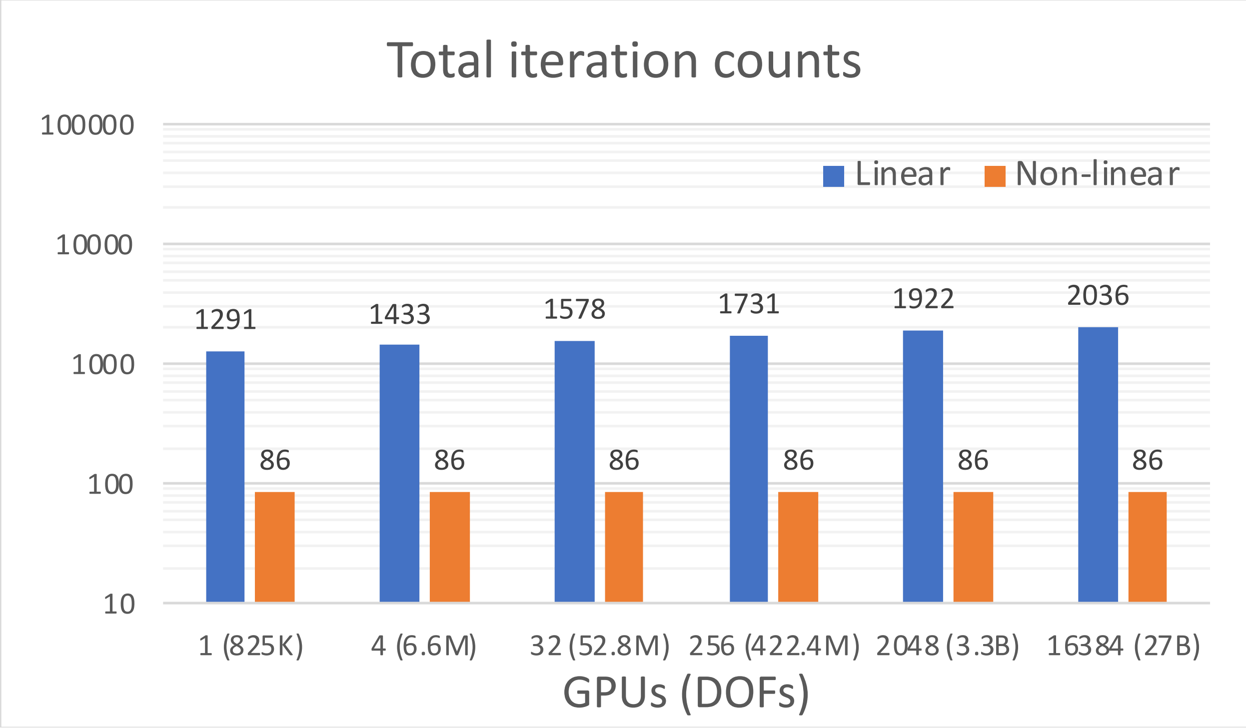


Setup		Solve	
Speedup GPU/CPU (AMG)	7.2	Speedup GPU/CPU (AMG)	20.1
Speedup GPU/CPU (PFMG)	23.3	Speedup GPU/CPU (PFMG)	29.3
CPU Speedup PFMG/AMG	4.5	CPU Speedup PFMG/AMG	1.4
GPU Speedup PFMG/AMG	14.5	GPU Speedup PFMG/AMG	2.0

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 ~ O(log(N)); Iteration counts ~ O(1).

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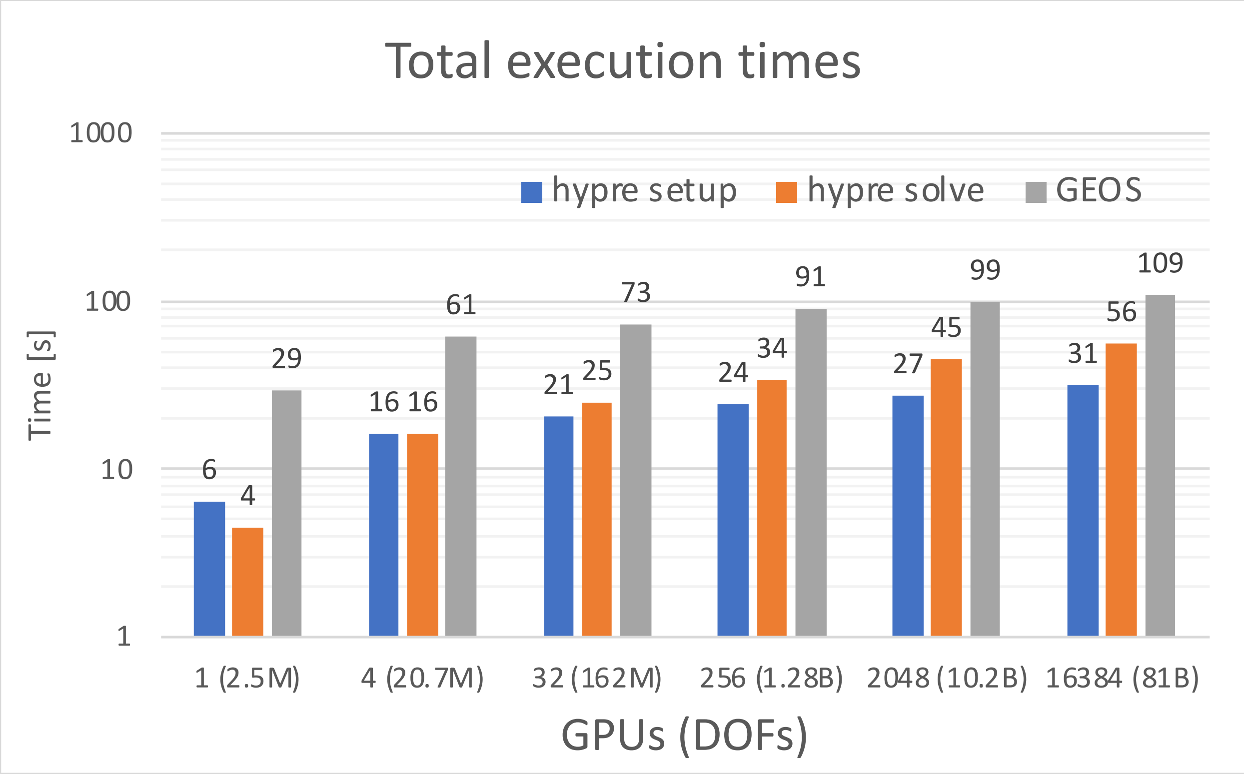
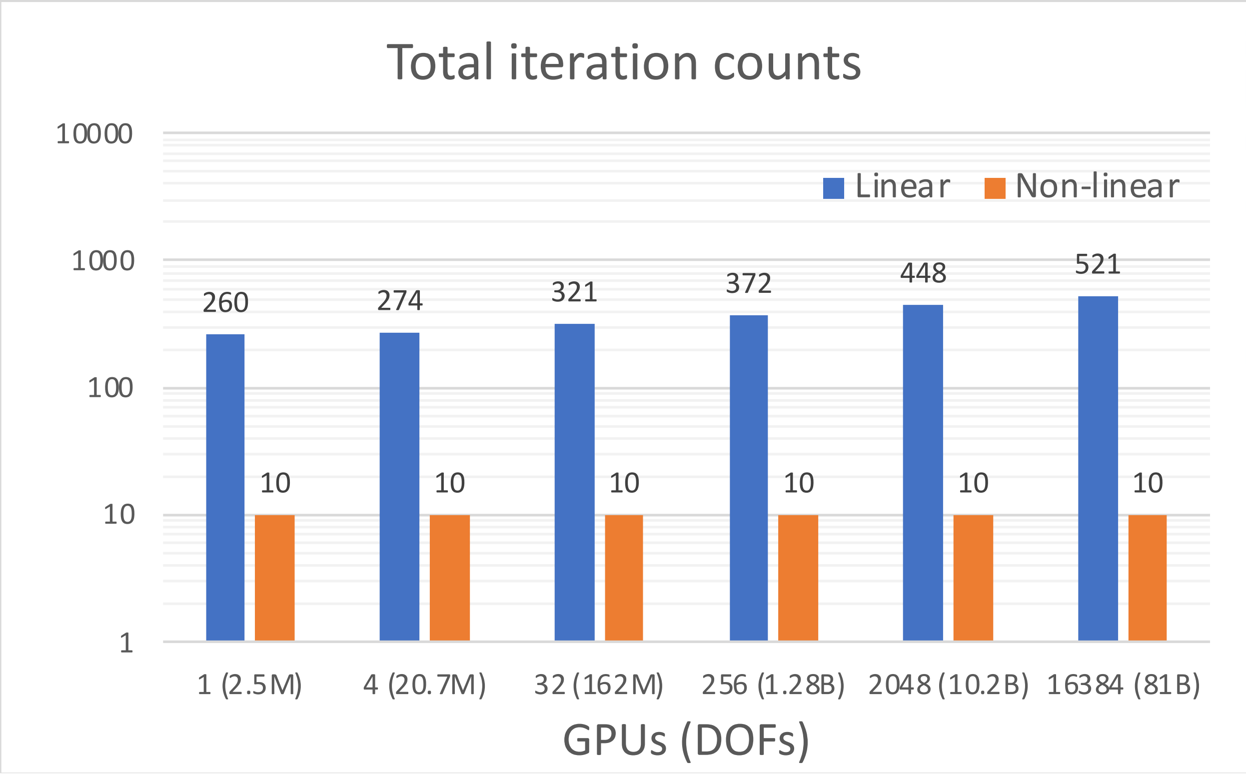
Frontier (AMD GPUs) results - Solved system with 80B DOFs using less than 25% of the machine

Mechanics (linear elasticity problem)





- Weak scaling with BoomerAMG/GMRES(40)

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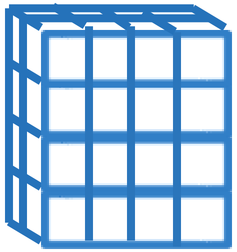
Hands-on Exercises: Comparing GPU to CPU Performance Algebraic Multigrid methods (Third Set of Runs)

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

- Poisson equation: $-\Delta\varphi$ = RHS

  with Dirichlet boundary conditions $\varphi = 0$

- Grid: cube



- Finite difference discretization:
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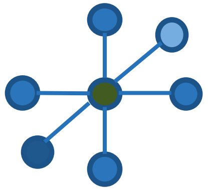
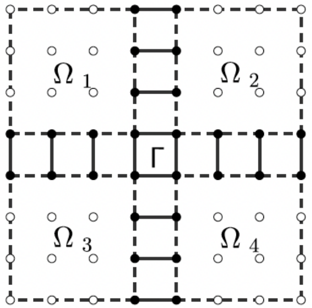
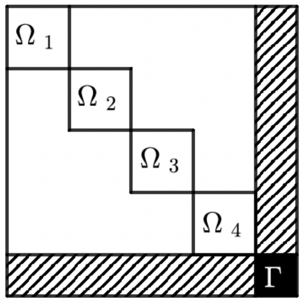
  - 7-point stencil



Some special general purpose solvers in hypre

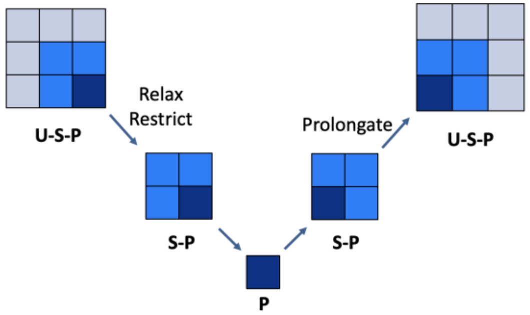
- Incomplete LU factorization
  - Based on a domain decomposition framework
    - Local ILU solve with global Schur complement solve
    - Various combinations of local ILU and global Schur solvers
  - GPU support available (for certain options)





- Multigrid reduction for PDE systems and Multiphysics applications
  - Reduction-based solver in a multigrid framework
  - Utilizes BoomerAMG as coarse solver
  - Effective Multiphysics preconditioner
  - GPU support available

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix}$$



FASTMATH

EXASCALE COMPUTING PROJECT

Thank you!

CASC

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