Argonne Training Program on Extreme-Scale Computing

ATPESC 2020

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 and 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:

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

- 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)

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

  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
- Biconjugate Gradient Stabilized (BiCGSTAB)
  - 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

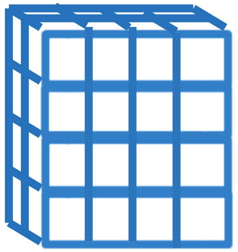
Hands-on Exercises: Krylov methods

- Go to https://xsdk-project.github.io/MathPackagesTraining2020/lessons/krylov_amg_hypre/

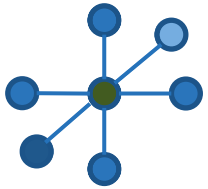
- Poisson equation: $-\Delta\varphi = \text{RHS}$

  with Dirichlet boundary conditions $\varphi = 0$

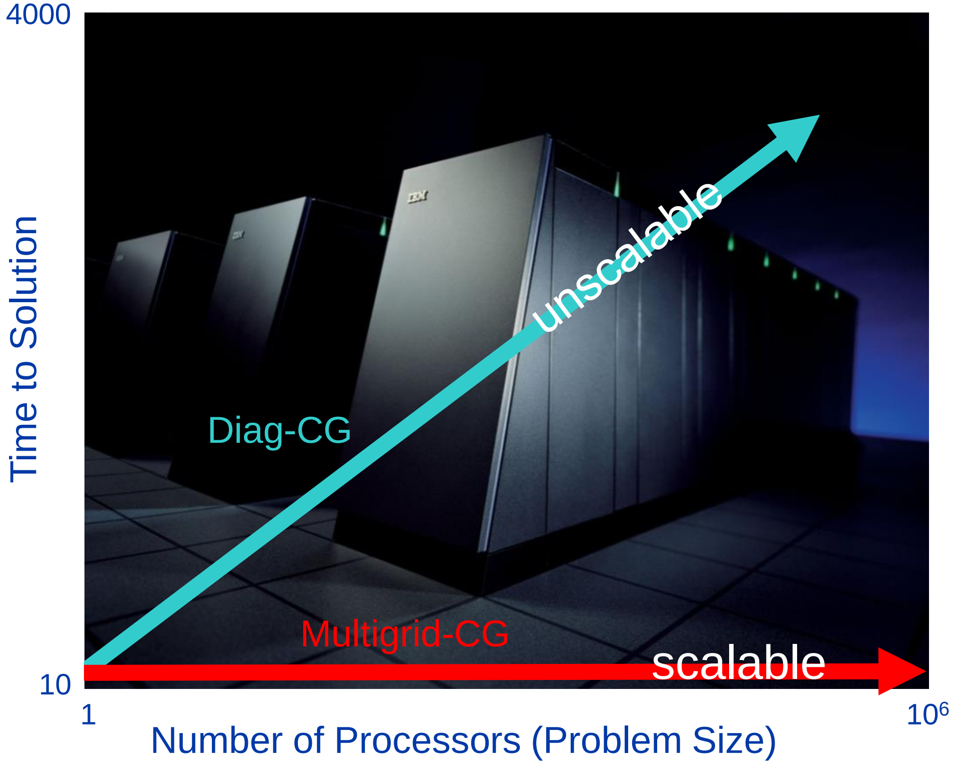
- Grid: cube



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



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

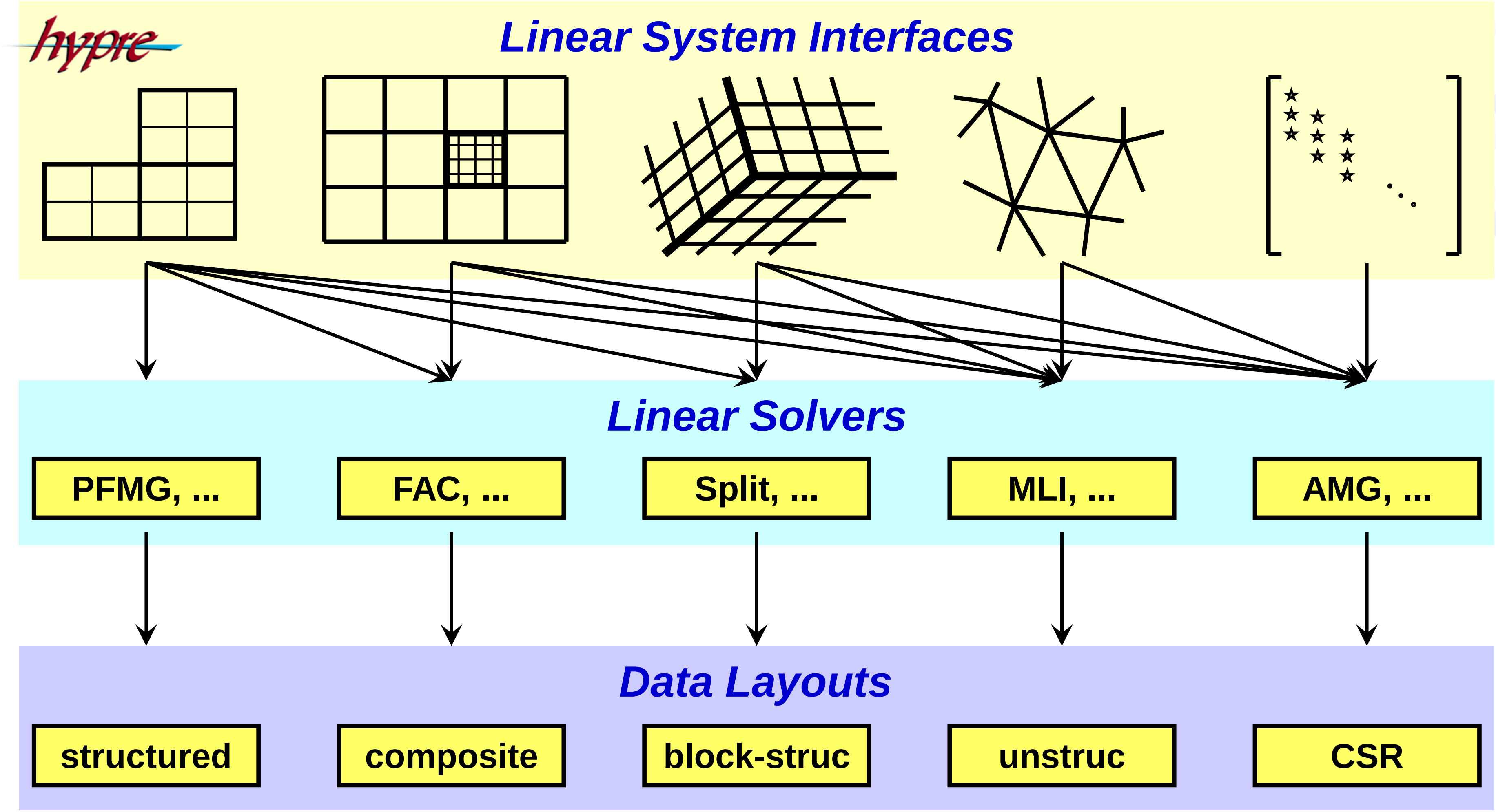


- Weak scaling – want constant solution time as problem size grows in proportion to the number of processors

Available 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

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

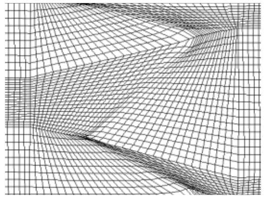


Why multiple interfaces? The key points

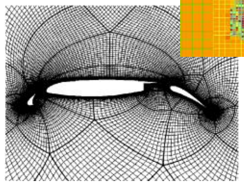
- Provides natural "views" of the linear system
- Eases some of the coding burden for users by eliminating the need to map to rows/columns
- Provides for more efficient (scalable) linear solvers
- Provides for more effective data storage schemes and more efficient computational kernels

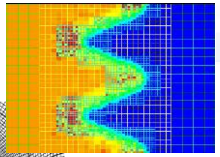
hypre supports these system interfaces

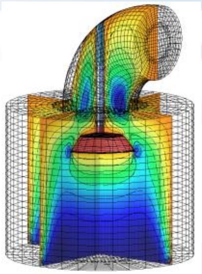
- Structured-Grid (`Struct`)
  - *logically rectangular grids*

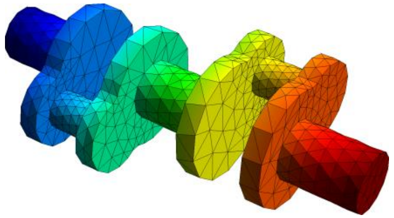


- Semi-Structured-Grid (`SStruct`)
  - *grids that are mostly structured*
  - *Examples: block-structured grids, structured adaptive mesh refinement grids, overset grids*
  - *Finite elements*

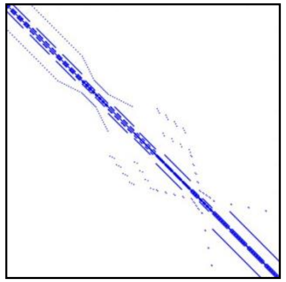






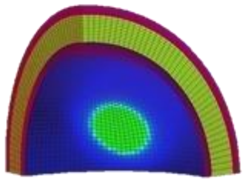


- Linear-Algebraic (`IJ`)
  - *general sparse linear systems*

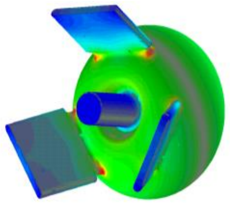


The *hypre* software library provides structured and unstructured multigrid solvers

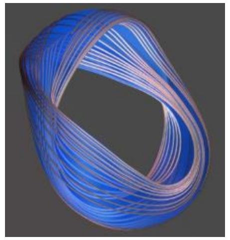
- Used in many applications



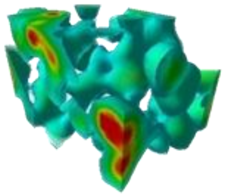
Elasticity/ Plasticity



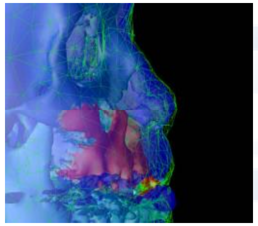
Electro-magnetics



Magneto-hydrodynamics

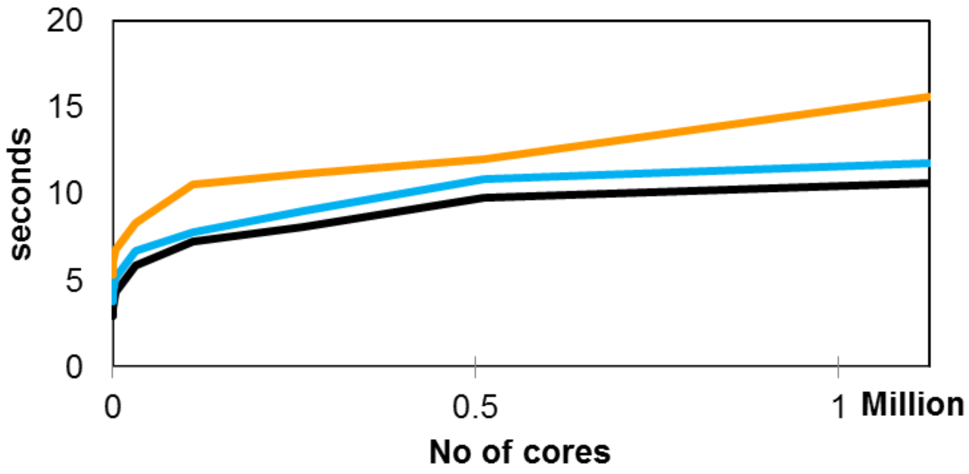


Quantum Chromodynamics

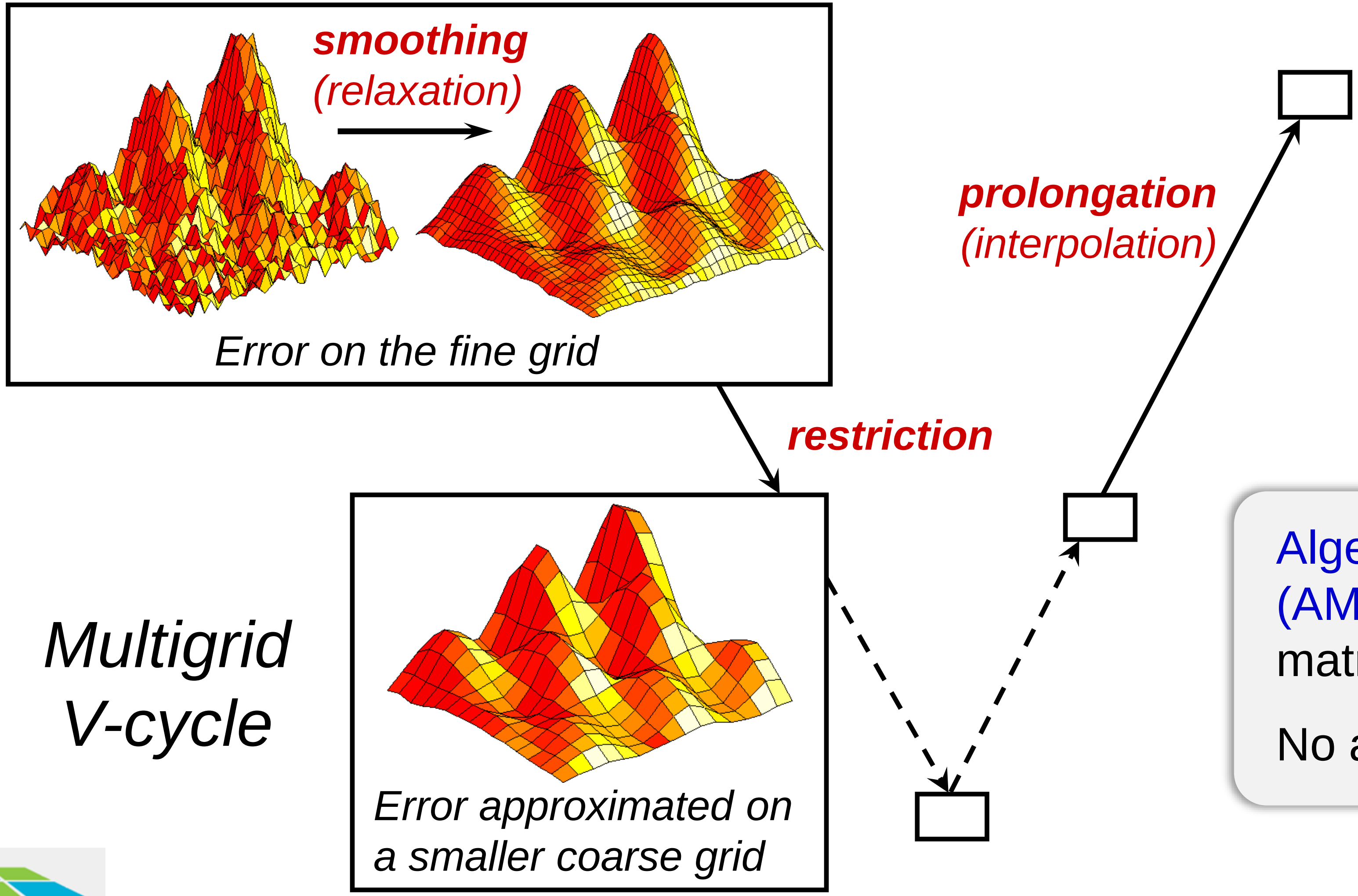


Facial surgery

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



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



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: $R^{(m)}, \quad m = 1,2,\ldots, \quad \text{often } R^{(m)} = (P^{(m)})^T$
- 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 $A^{(m+1)} e^{m+1} = r^{m+1}$

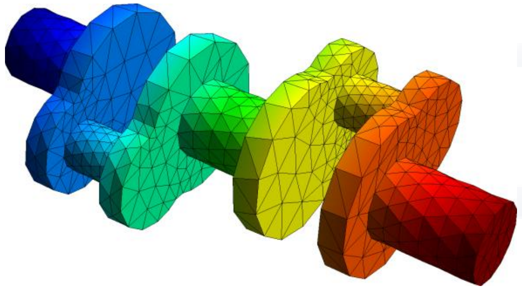
Interpolate $e^m = P^{(m)} e^{m+1}$

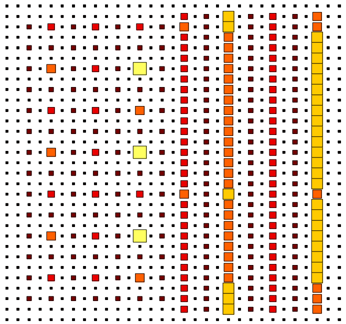
Correct $u^m \leftarrow u^m + e^m$

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

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 (limited options)





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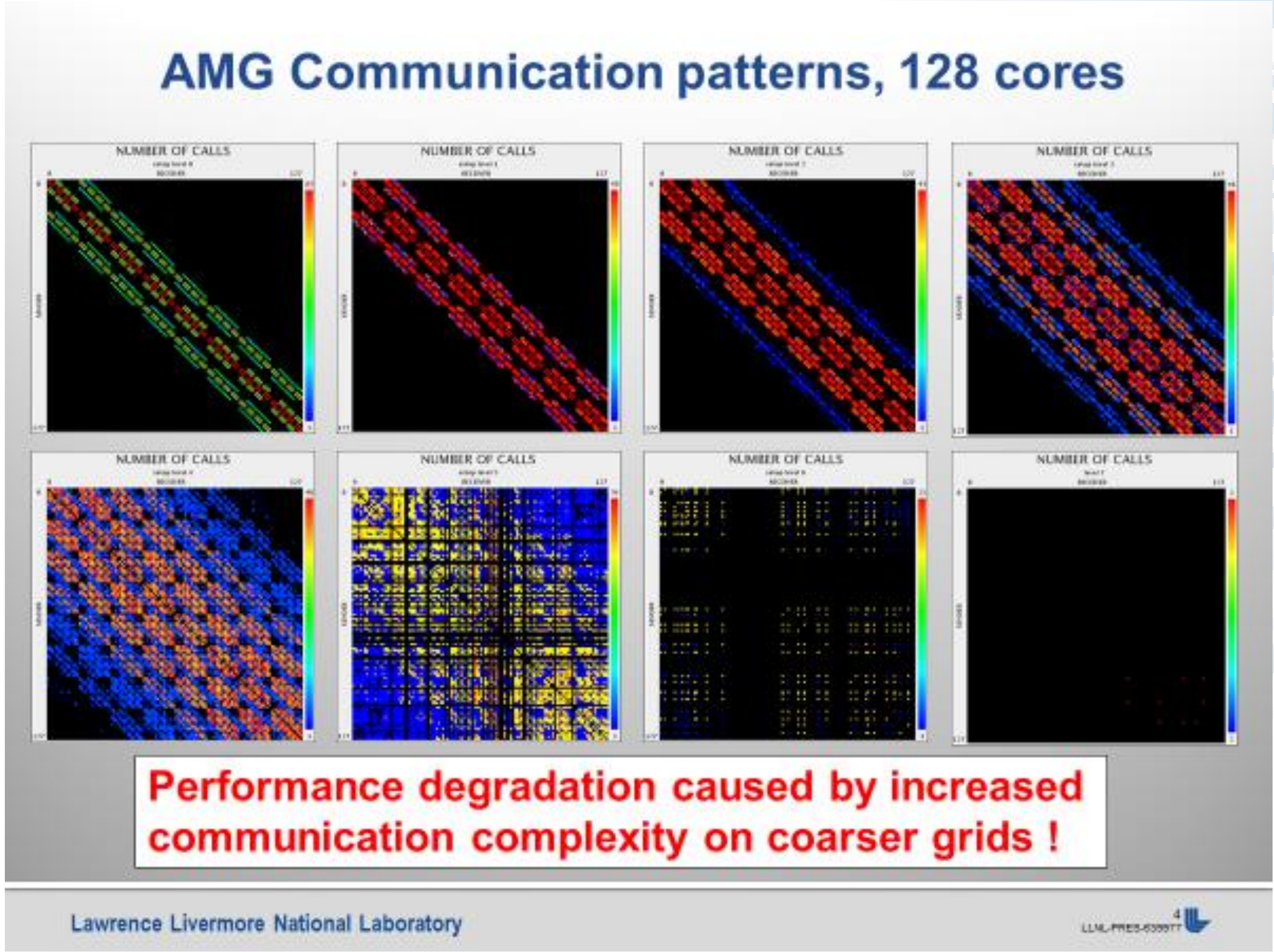
Complexity issues

- Coarse-grid selection in AMG can produce unwanted side effects
- Operator (RAP) “stencil growth” reduces efficiency
- For BoomerAMG we will therefore 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



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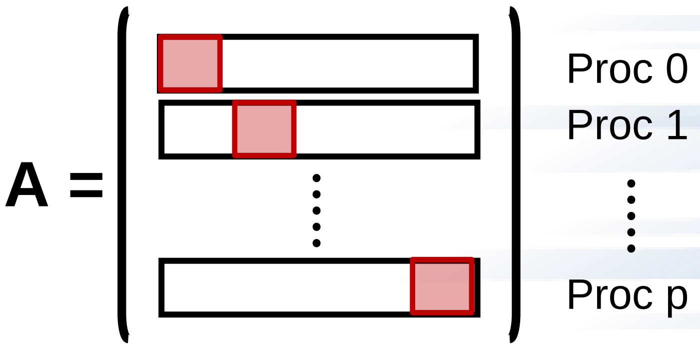
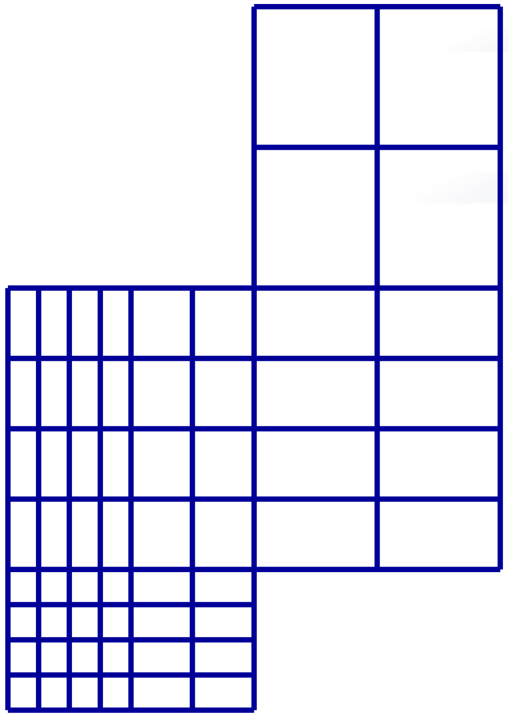
ParCSRMatrix data structure



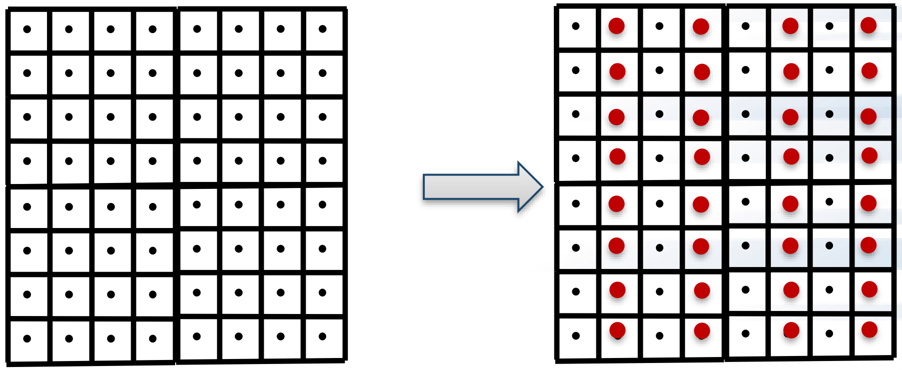
- Based on compressed sparse row (CSR) data structure
- Consists of two CSR matrices:
  - One containing local coefficients connecting to local column indices
  - The other (Offd) containing coefficients with column indices pointing to off processor rows
- Also contains a mapping between local and global 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, SStruct`
- Matrix Class: `Struct`
- SMG uses plane smoothing in 3D, where each plane “solve”
  is effected 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, RAJA, Kokkos)



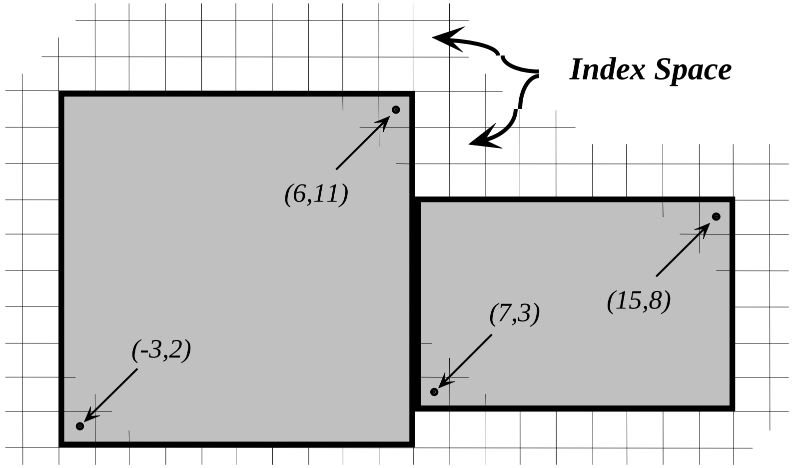
PFMG is an algebraic multigrid method for structured grids



- Matrix defined in terms of grids and stencils
- Uses semicoarsening
- Simple 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



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

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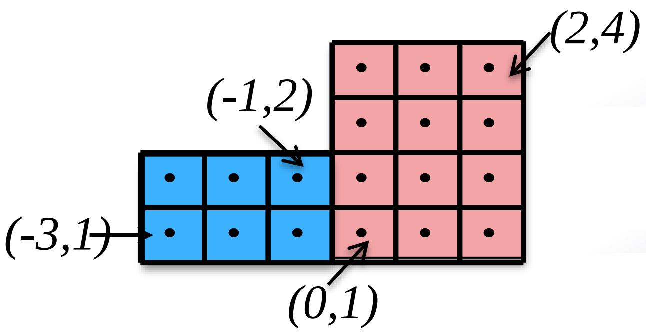
ECP EXASCALE COMPUTING PROJECT

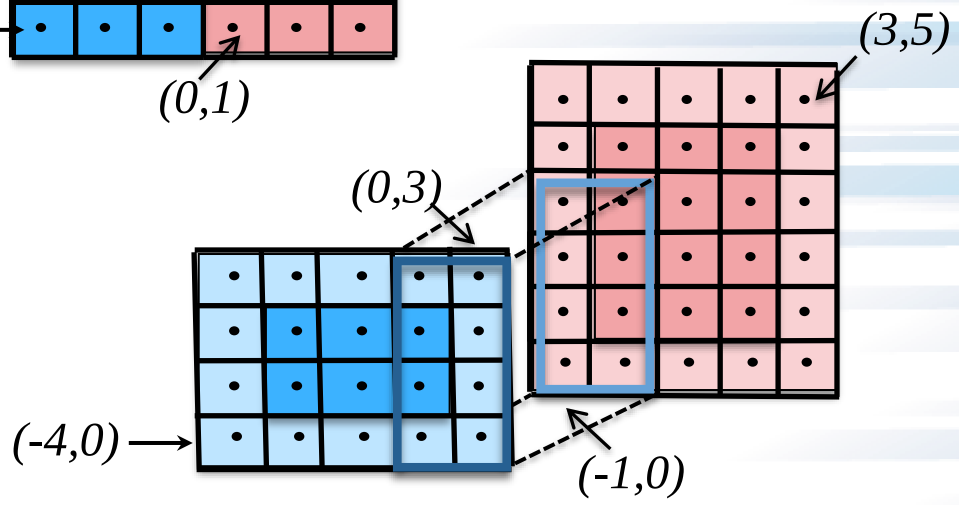
StructMatrix data structure

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

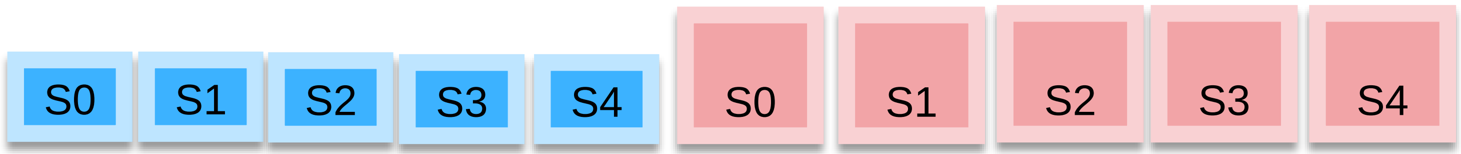
- Grid boxes: [(-3,1), (-1,2)] [(0,1), (2,4)]



- Data Space: grid boxes + ghost layers: [(-4,0), (0,3)] , [(-1,0), (3,5)]



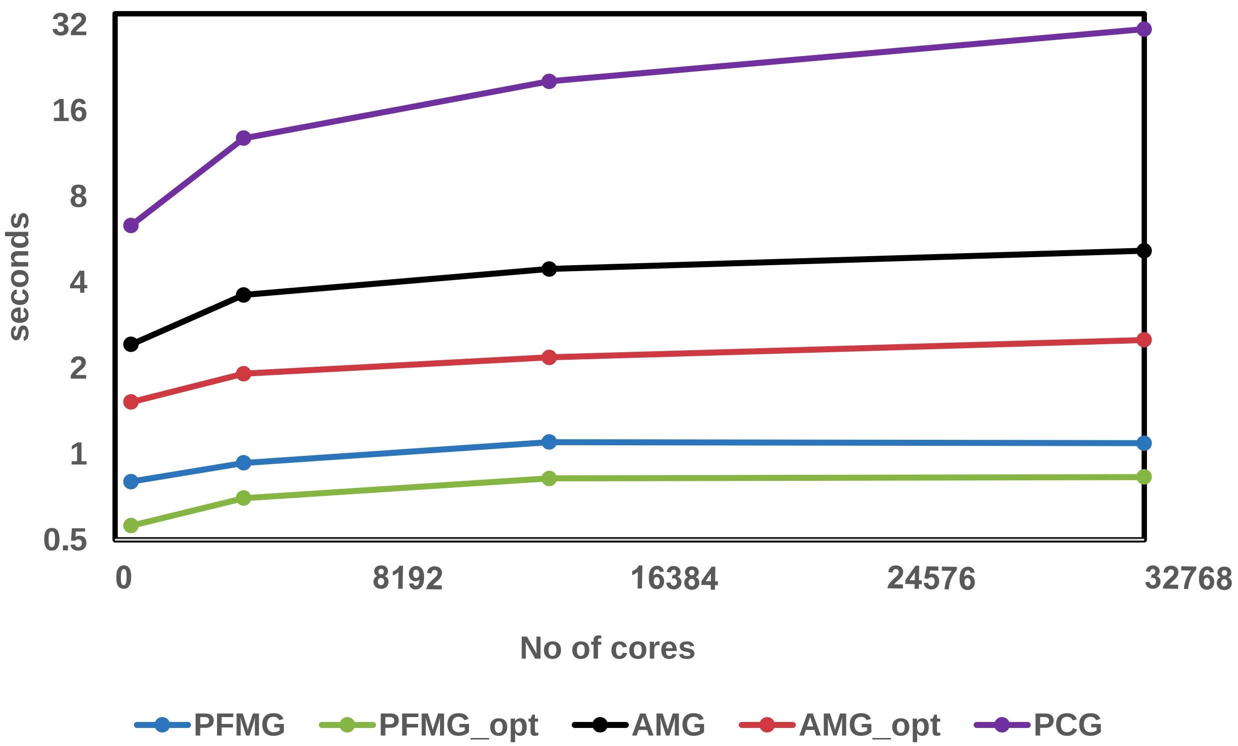
- Data stored



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

Algebraic multigrid as preconditioner

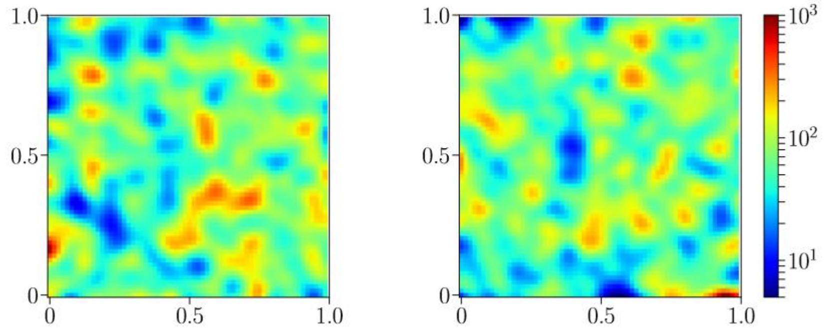
- Generally algebraic multigrid methods are used as preconditioners to Krylov methods, such as conjugate gradient (CG) or GMRES
- This often leads to additional performance improvements



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

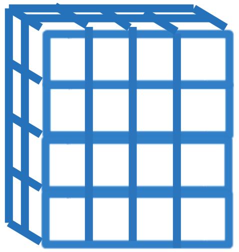
Hands-on Exercises: Algebraic multigrid methods

- Go to https://xsdk-project.github.io/MathPackagesTraining2020/lessons/krylov_amg_hypre/

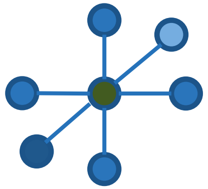
- Poisson equation: $-\Delta\varphi = \text{RHS}$

  with Dirichlet boundary conditions $\varphi = 0$

- Grid: cube



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



Thank you!

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