Algebraic Multigrid

Presented to
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ATPESC Numerical Software Track

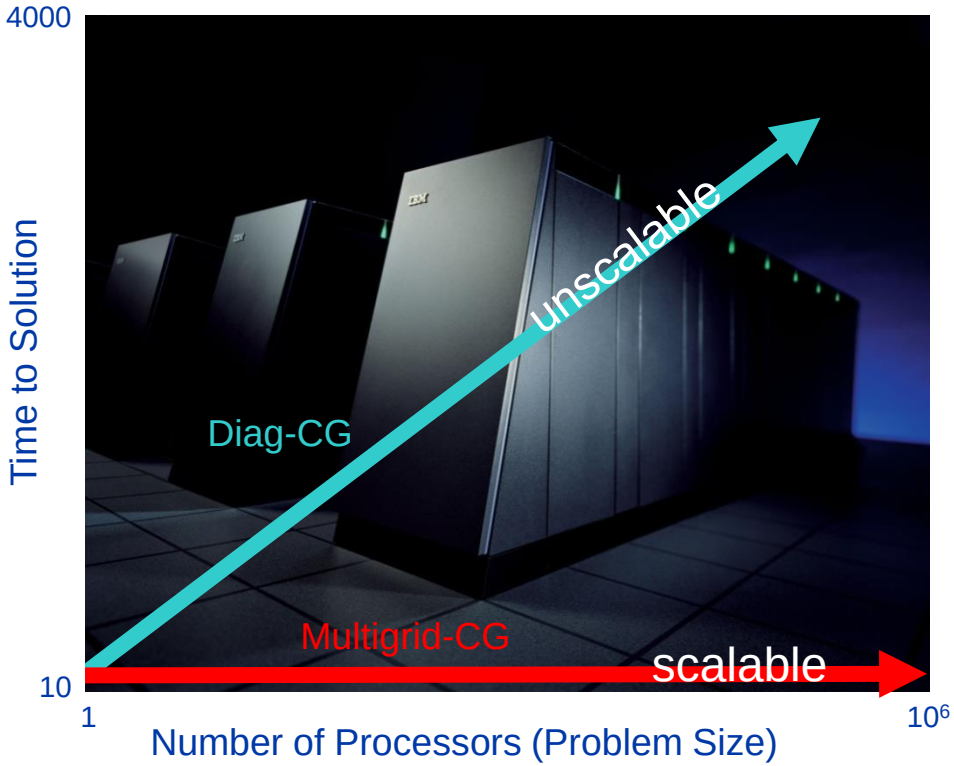
EXASCALE COMPUTING PROJECT

Argonne NATIONAL LABORATORY · BERKELEY LAB · Sandia National Laboratories · Rensselaer · SMU

Outline

- Why multigrid methods?
- Algebraic multigrid software
- How does multigrid work?
- Hypre software library – interfaces and solvers
  - Why different interfaces?
  - Solvers and data structures
- Effect of complexity on performance
- Hands-on exercises

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



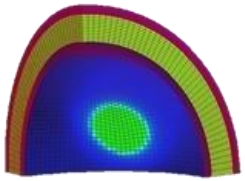
- Weak scaling – want constant solution time as problem size grows in proportion to the number of processors

Available multigrid software

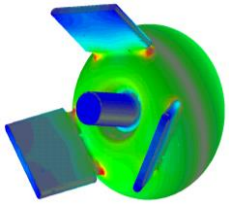
- ML, MueLu included in Trilinos
- GAMG in PETsc
- The *hypre* library provides various algebraic multigrid solvers, including multigrid solvers for special problems e.g. Maxwell equations, …
- All of these provide different flavors of multigrid and provide excellent performance for suitable problems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

The hypre software library provides structured and unstructured multigrid solvers

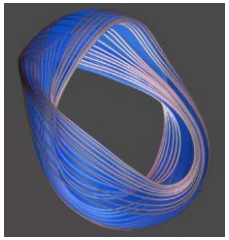
- Used in many applications



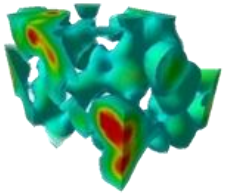
Elasticity/ Plasticity



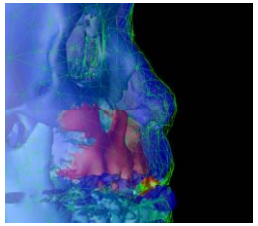
Electro-magnetics



Magneto-hydrodynamics

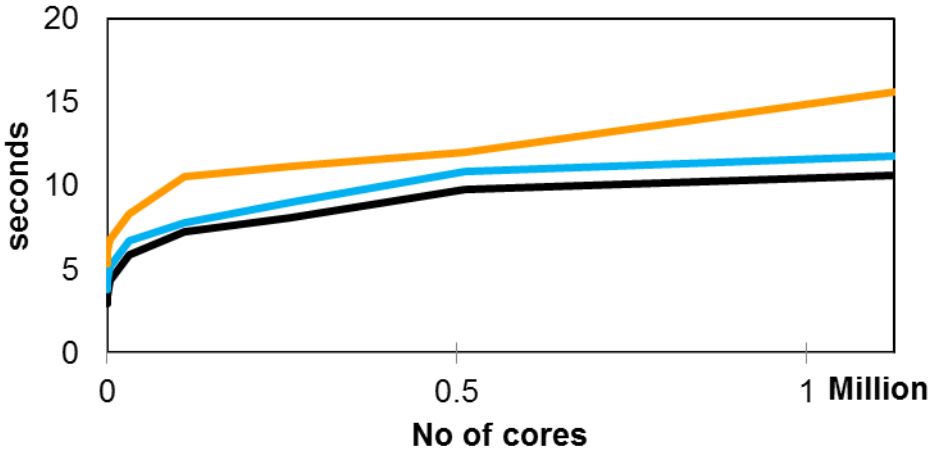


Quantum Chromodynamics

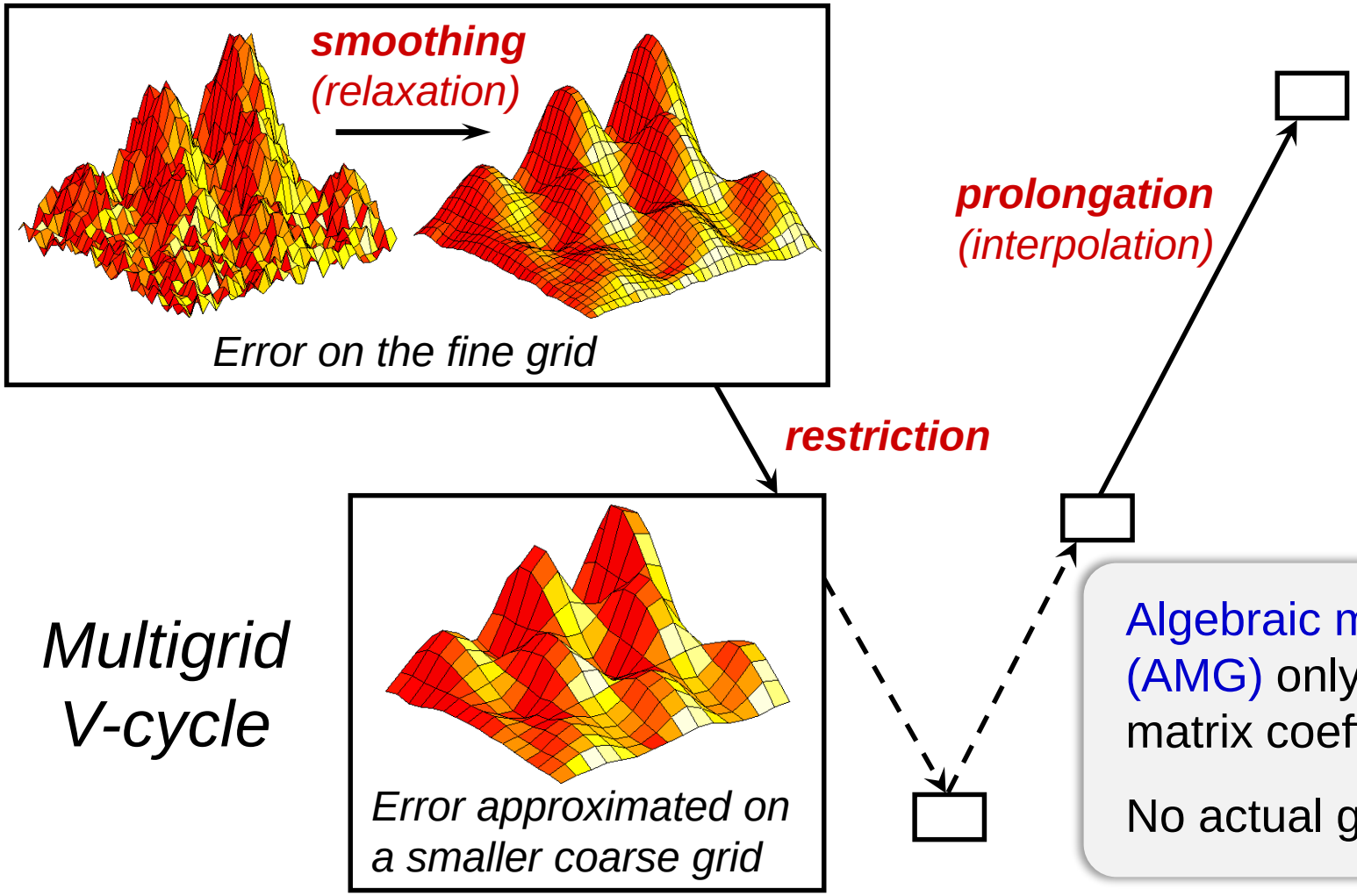


Facial surgery

- 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



Multigrid V-cycle

Algebraic multigrid (AMG) only uses matrix coefficients

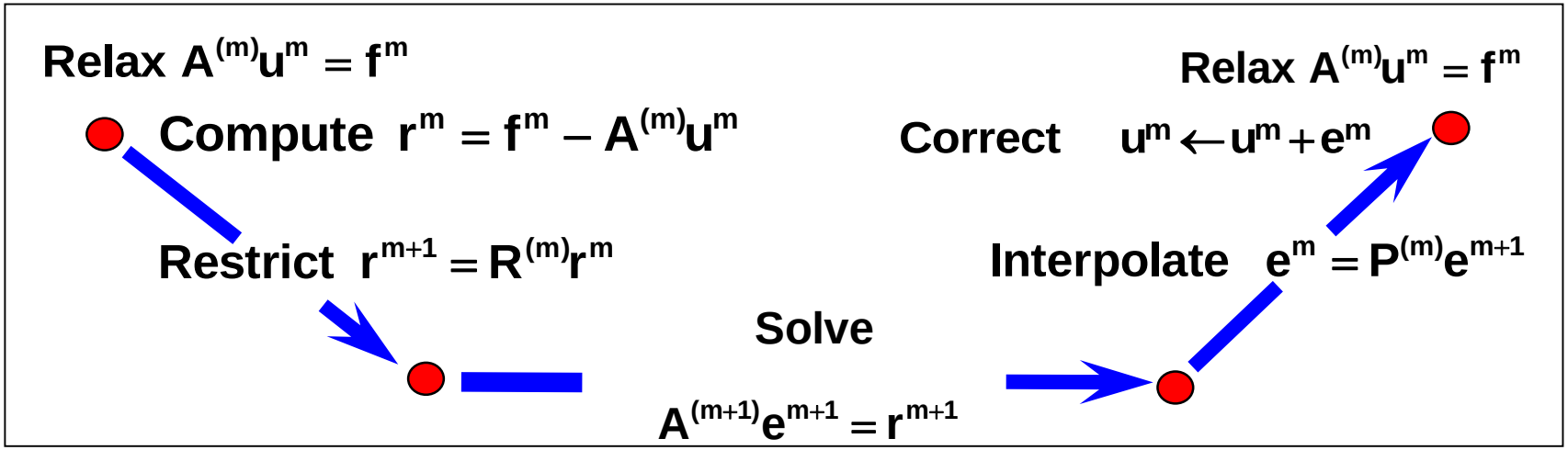
No actual grids!

AMG Building Blocks

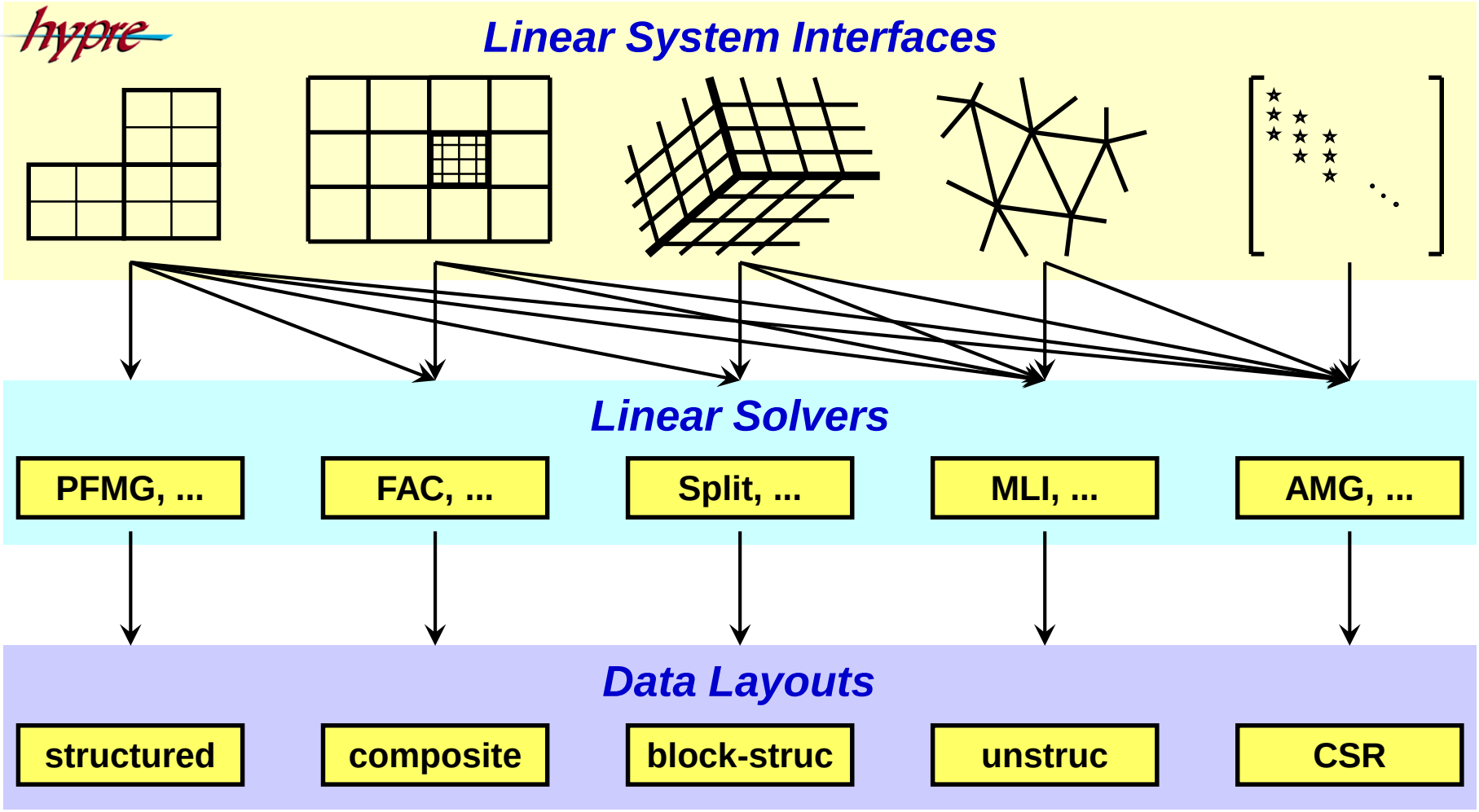
Setup Phase:

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

Solve Phase:



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

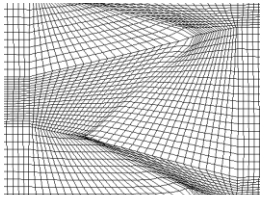


Why multiple interfaces? The key points

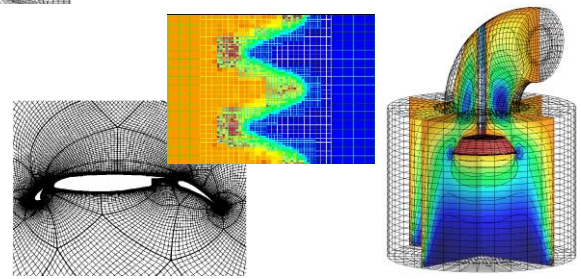
- Provides natural “views” of the linear system
- Eases some of the coding burden for users by eliminating the need to map to rows/columns
- Provides for more efficient (scalable) linear solvers
- Provides for more effective data storage schemes and more efficient computational kernels

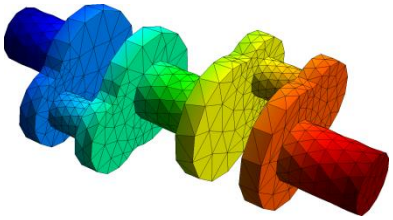
hypre supports these system interfaces

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

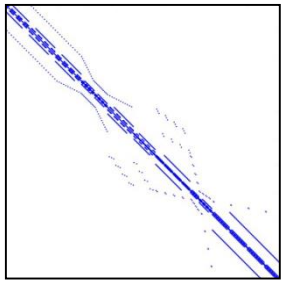


- Semi-Structured-Grid (`SStruct`)
  - *grids that are mostly structured*
  - *Examples: block-structured grids, structured adaptive mesh refinement grids, overset grids*
  - *Finite elements*





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

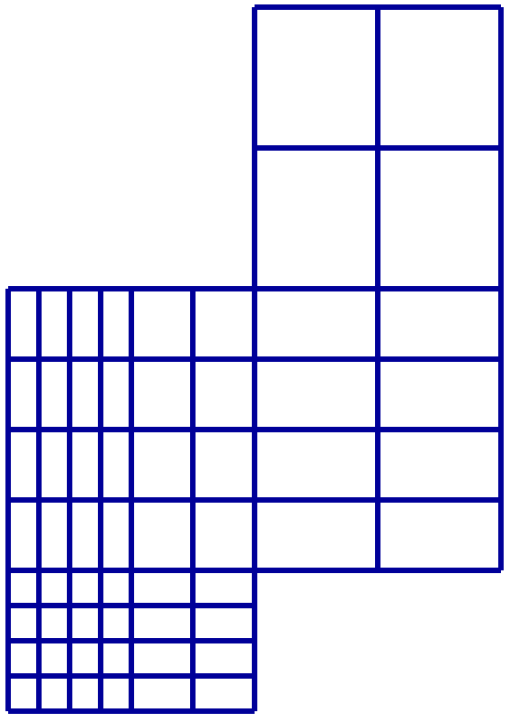


SMG and PFMG are semicoarsening multigrid methods for structured grids

- 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

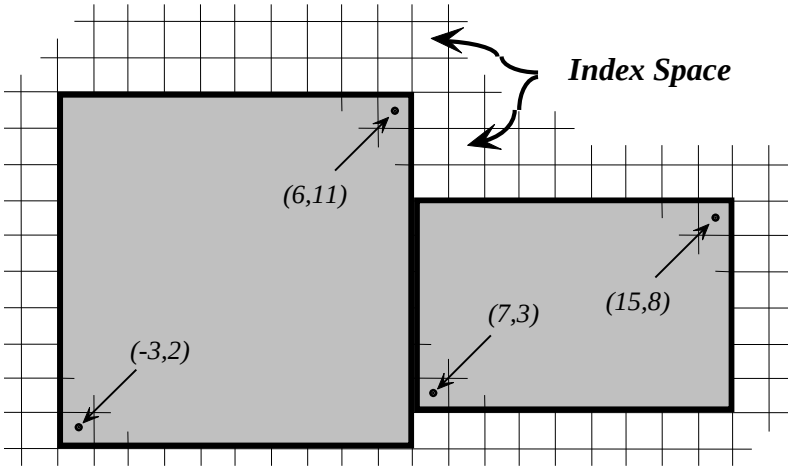
- Constant-coefficient versions!



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

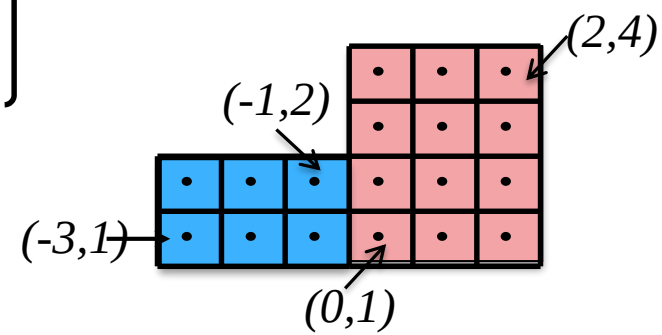
$$\begin{pmatrix} & S4 & \\ S1 & S0 & S2 \\ & S3 & \end{pmatrix} = \begin{pmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{pmatrix}$$



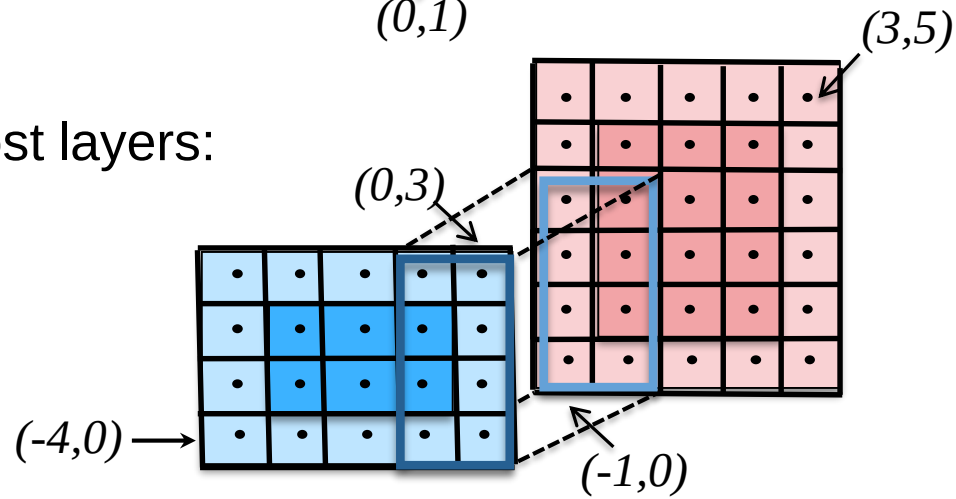
StructMatrix data structure

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

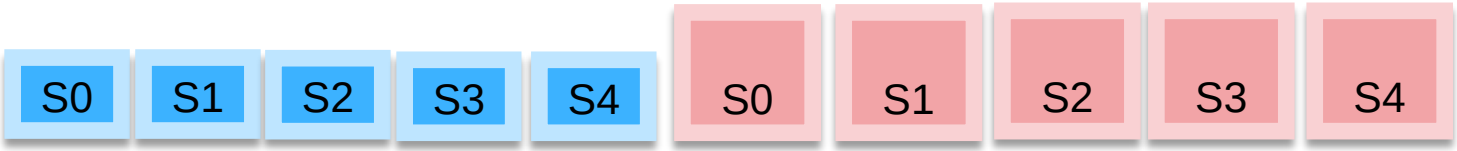
- Grid boxes: [(-3,1), (-1,2)]
  [(0,1), (2,4)]



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



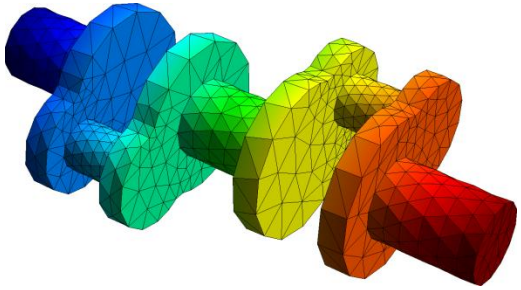
- Data stored



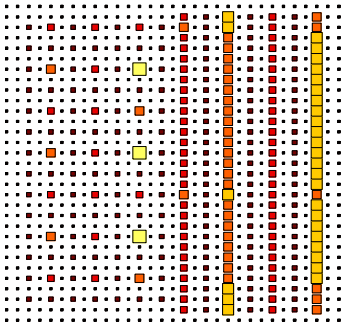
- **Operations applied to stencil entries per box (corresponds to matrix (off) diagonals from a matrix point of view)**

BoomerAMG is an algebraic multigrid method for unstructured grids

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

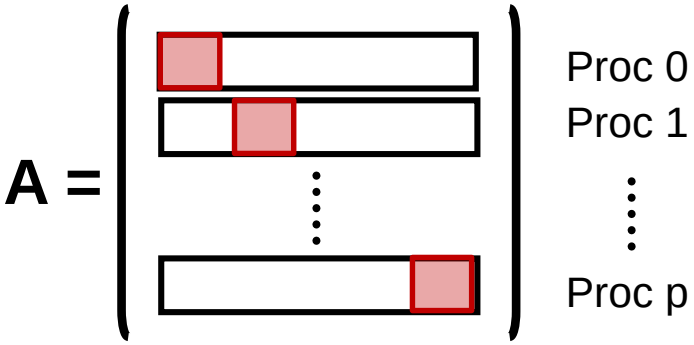


- Originally developed as a general matrix method (i.e., assumes given only A, x, and b)
- Various coarsening, interpolation and relaxation schemes
- Automatically coarsens “grids”
- Can solve systems of PDEs if additional information is provided
- Can also be used through PETSc and Trilinos



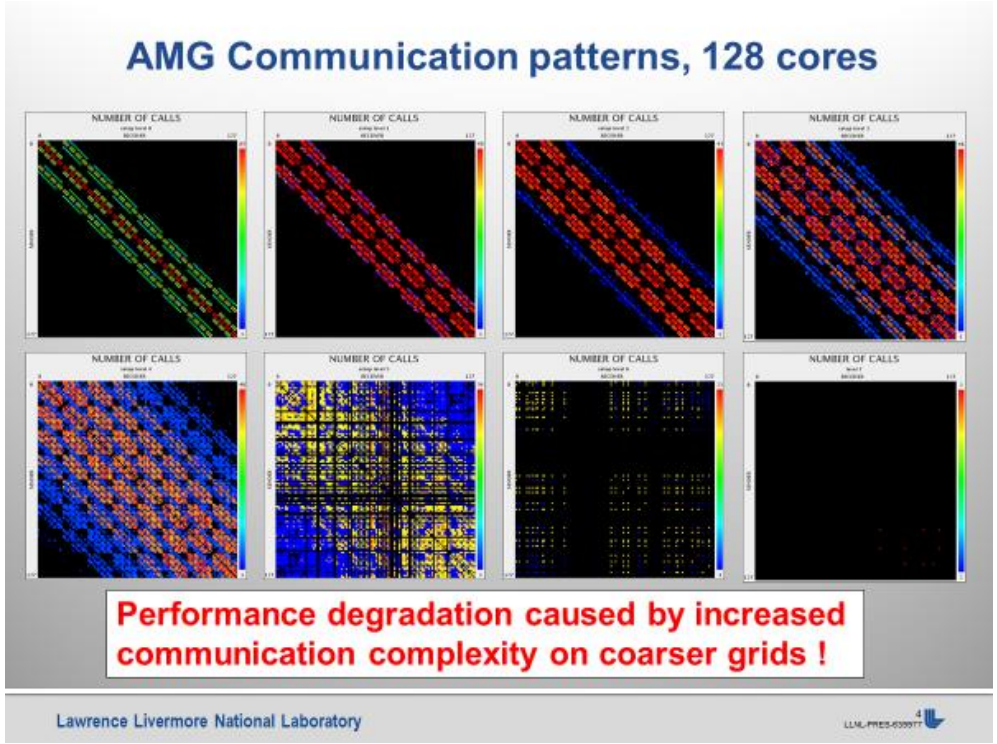
ParCSRMatrix data structure

- 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,



Complexity issues

- Coarse-grid selection in AMG can produce unwanted side effects
- Operator (RAP) “stencil growth” reduces efficiency
- Not so much an issue for SMG and PFMG, for which stencil growth is limited (to at most 27 points per stencil in 3D)



- For BoomerAMG we will therefore also consider complexities:
  - Operator complexity: $C_{op} = (\sum_{i=0}^{L} nnz\,(A_i))/nnz(A_0)$
  - Generally would like this to be less than 2, close to 1
  - Affects flops and memory
- Can ameliorate with more aggressive coarsening

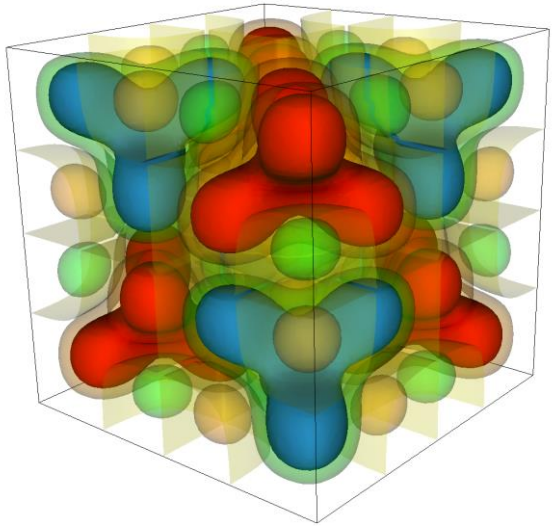
Algebraic multigrid as preconditioner

- 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

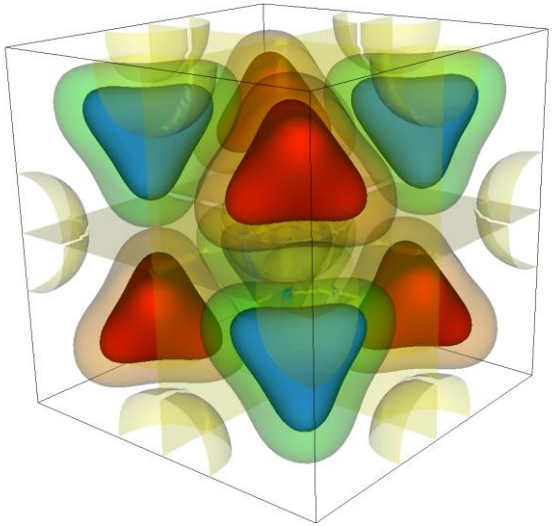
Hands-on Exercises

- Equation: $\varphi - \Delta \cdot \beta \nabla \varphi$ = RHS , Dirichlet boundary conditions
- Grid: 128 x 128 x 128, block structured, consisting of (at least) 8 subgrids

RHS:



solution:



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