Lawrence Livermore National Laboratory

HYPRE: High Performance Preconditioners

August 7, 2015

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This work performed under the auspices of the U.S. Department of Energy by
Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

LLNL-PRES-231999

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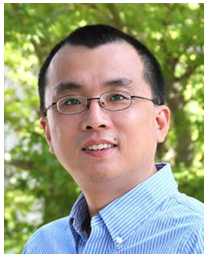
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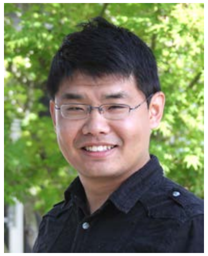
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hypre http://www.llnl.gov/casc/hypre/

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Outline

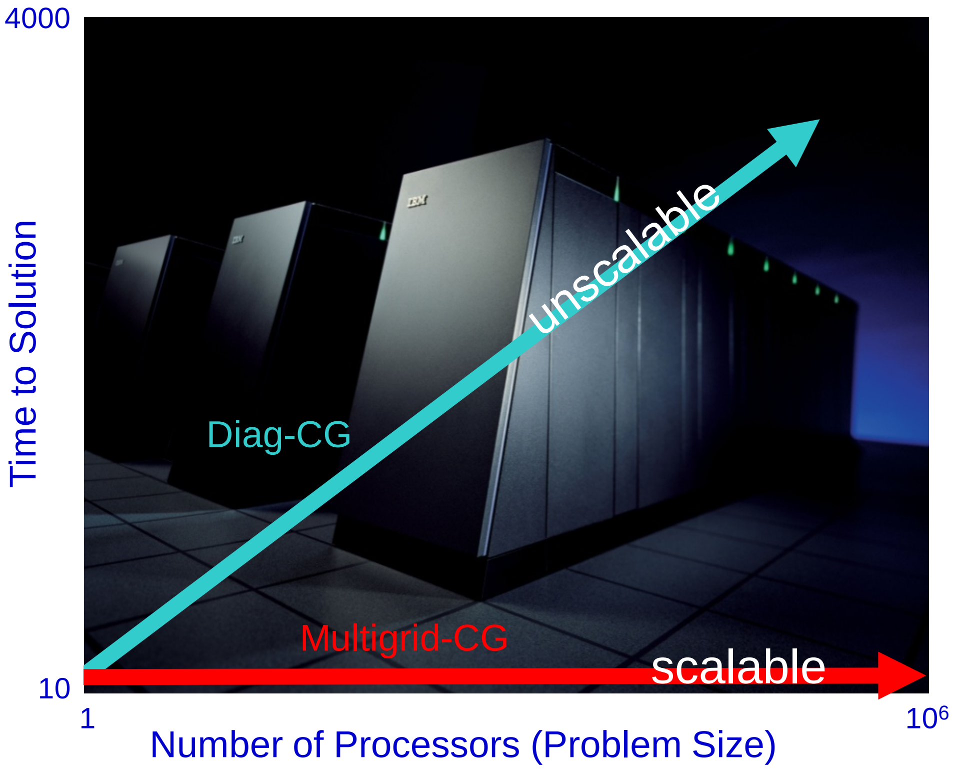
- Introduction / Motivation
- Getting Started / Linear System Interfaces

- Structured-Grid Interface (`Struct`)
- Semi-Structured-Grid Interface (`SStruct`)

- Solvers and Preconditioners
- Additional Information

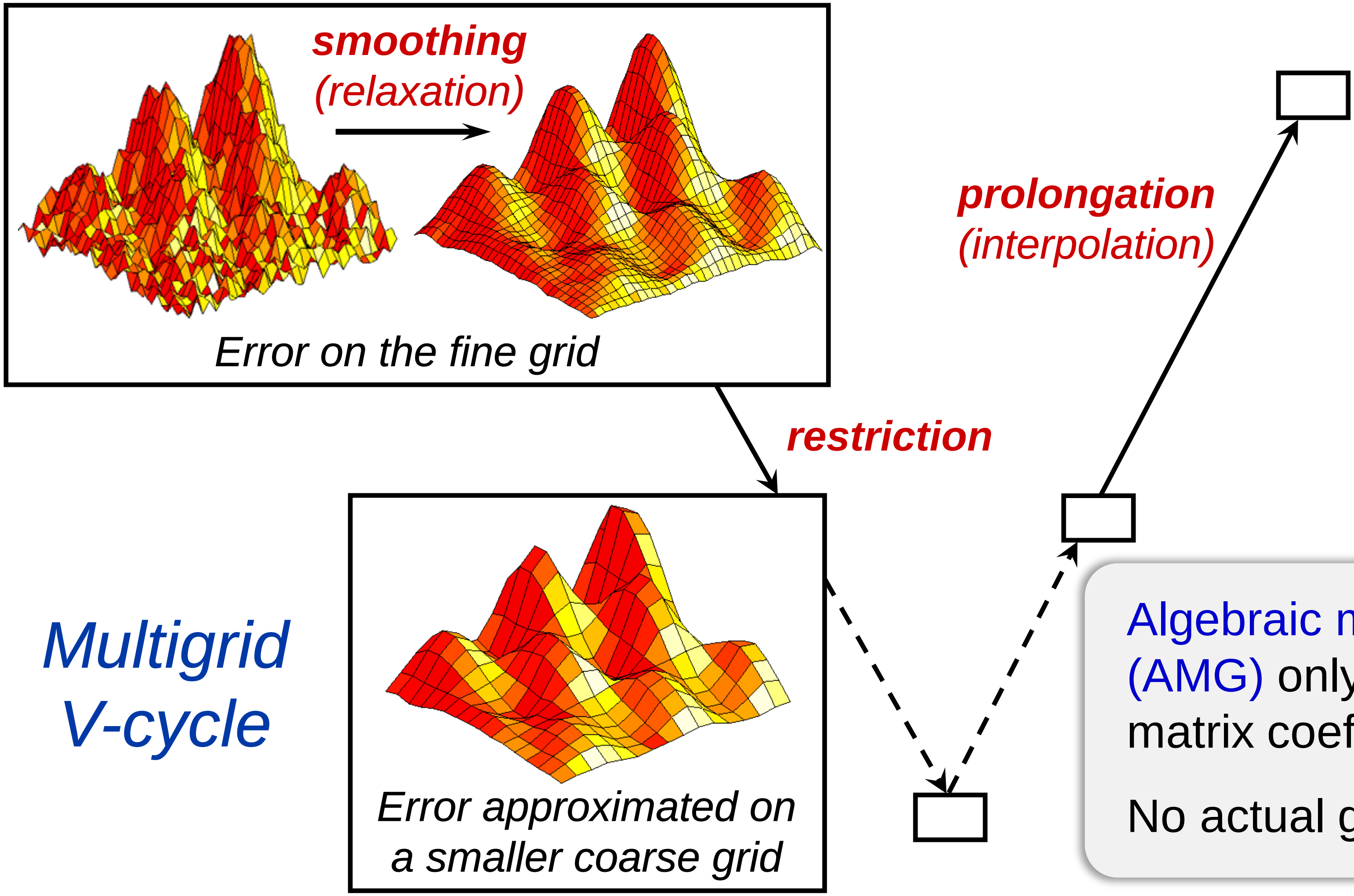
- Introduction to hands-on exercises

Multigrid solvers have $O(N)$ complexity, 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



smoothing

(relaxation)

Error on the fine grid

restriction

Error approximated on a smaller coarse grid

prolongation

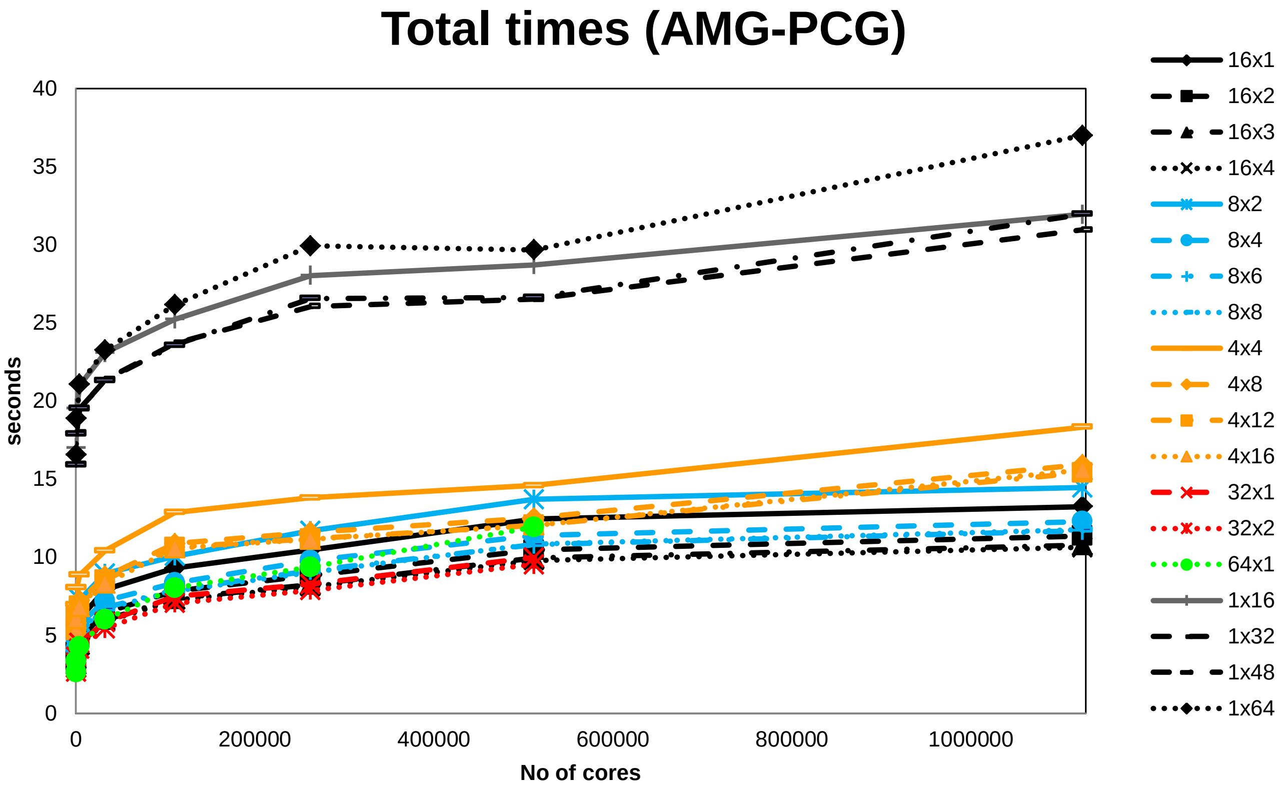
(interpolation)

Multigrid V-cycle

Algebraic multigrid (AMG) only uses matrix coefficients

No actual grids!

Parallel AMG in *hypre* now scales to 1.1M cores on Sequoia (IBM BG/Q)



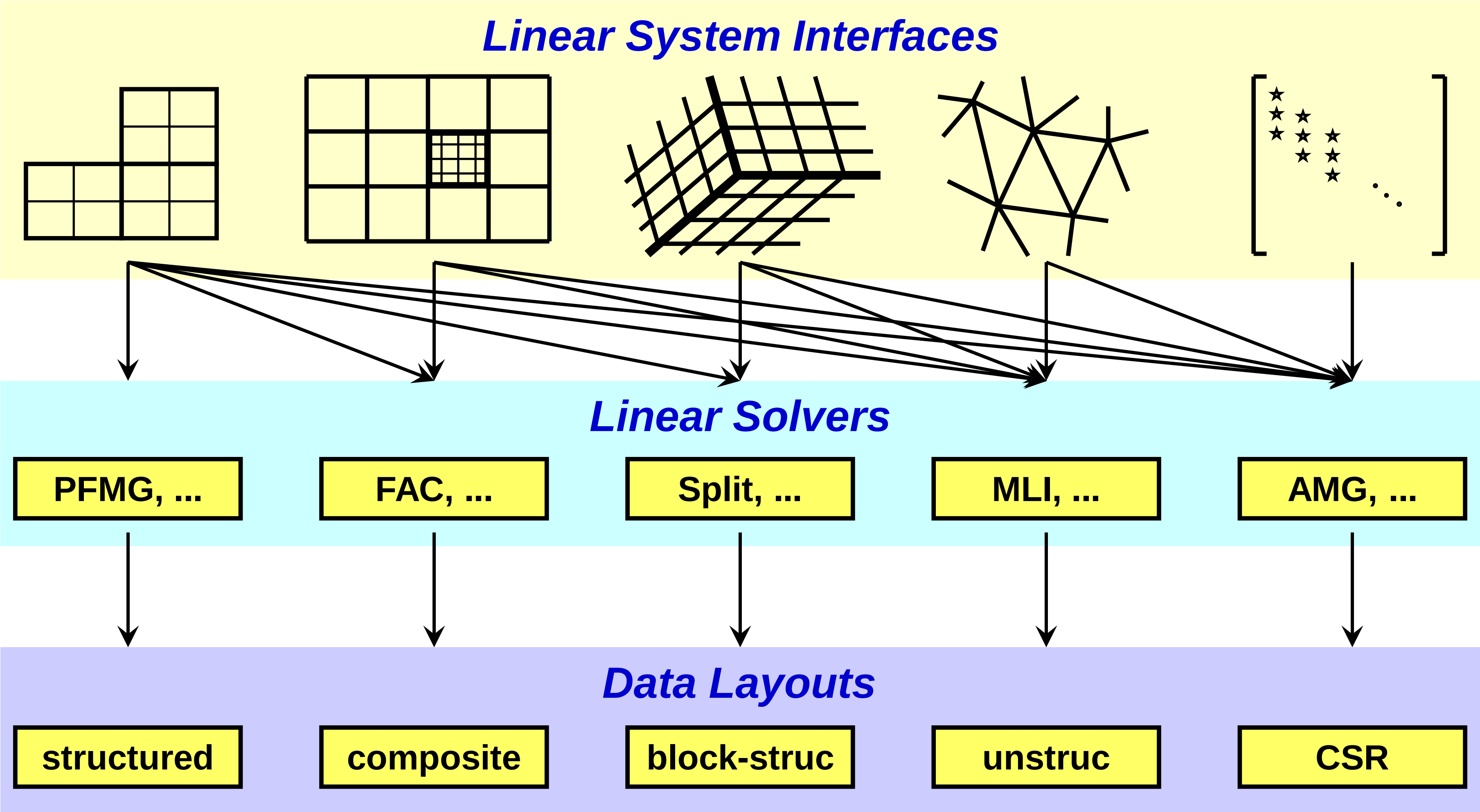
- *m* x *n* denotes *m* MPI tasks and *n* OpenMP threads per node
- Largest problem above: 72B unknowns on 1.1M cores

Getting Started

- Before writing your code:
  - choose a linear system interface
  - choose a solver / preconditioner
  - choose a matrix type that is compatible with your solver / preconditioner and system interface

- Now write your code:
  - build auxiliary structures (e.g., grids, stencils)
  - build matrix/vector through system interface
  - build solver/preconditioner
  - solve the system
  - get desired information from the solver

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



Linear System Interfaces

Linear Solvers

PFMG, ... | **FAC, ...** | **Split, ...** | **MLI, ...** | **AMG, ...**

Data Layouts

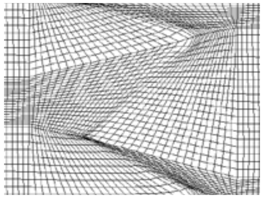
structured | **composite** | **block-struc** | **unstruc** | **CSR**

Why multiple interfaces? The key points

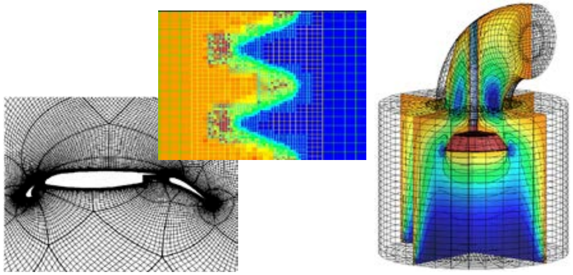
- Provides natural “views” of the linear system
- Eases some of the coding burden for users by eliminating the need to map to rows/columns
- Provides for more efficient (scalable) linear solvers
- Provides for more effective data storage schemes and more efficient computational kernels

Currently, *hypre* supports four system interfaces

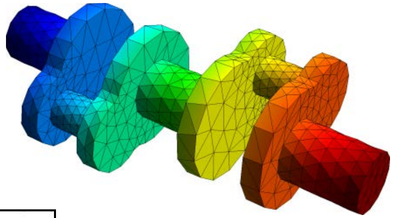
- Structured-Grid (`Struct`)
  - *logically rectangular grids*



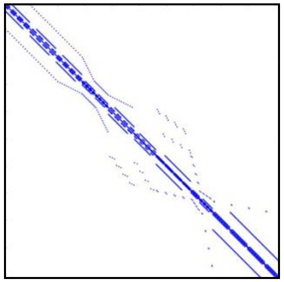
- Semi-Structured-Grid (`SStruct`)
  - *grids that are mostly structured*



- Finite Element (`FEI`)
  - *unstructured grids with finite elements*



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

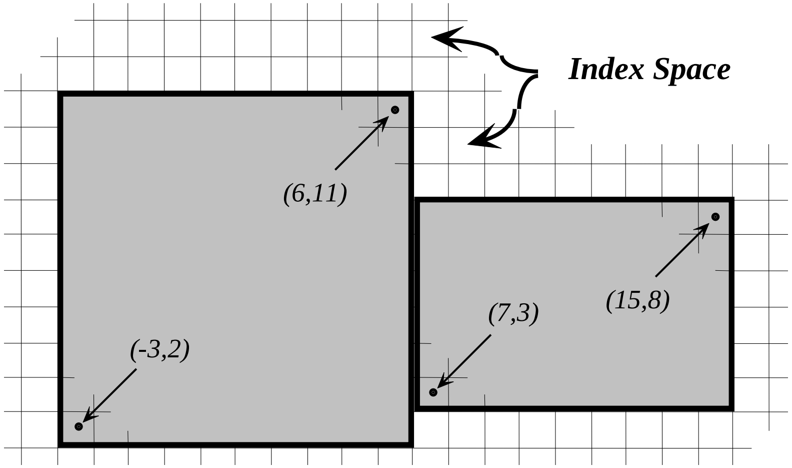


- More about the first two next…

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 scalar grid data is always associated with cell centers (unlike the more general SStruct interface)



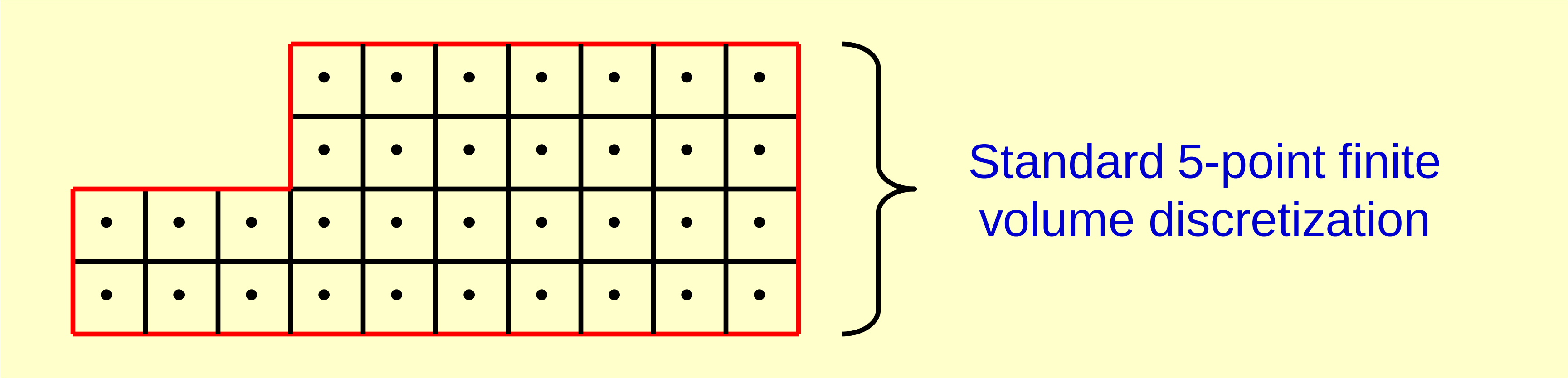
Structured-Grid System Interface (**`Struct`**)

- There are four basic steps involved:
  - set up the `Grid`
  - set up the `Stencil`
  - set up the `Matrix`
  - set up the right-hand-side `Vector`

- Consider the following 2D Laplacian problem

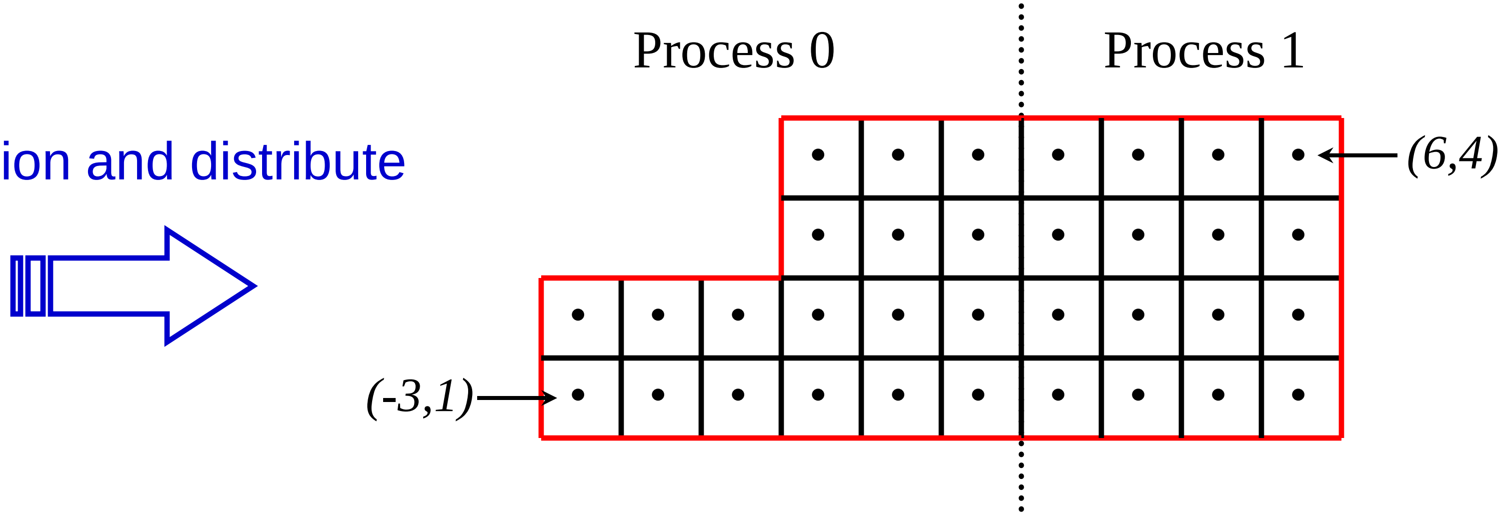
$$\begin{cases} -\nabla^2 u = f & \text{in the domain} \\ u = g & \text{on the boundary} \end{cases}$$

Structured-grid finite volume example:



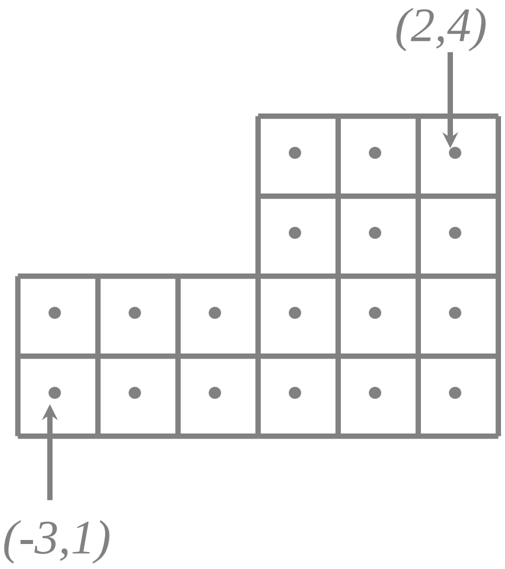
Standard 5-point finite volume discretization

Partition and distribute



Structured-grid finite volume example:

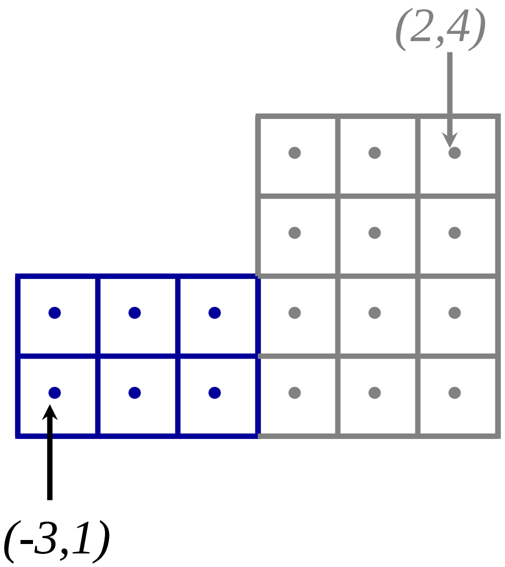
Setting up the grid on process 0



Create the grid object

```
HYPRE_StructGrid grid;
int ndim   = 2;

HYPRE_StructGridCreate(MPI_COMM_WORLD, ndim, &grid);
```

Structured-grid finite volume example:
Setting up the grid on process 0

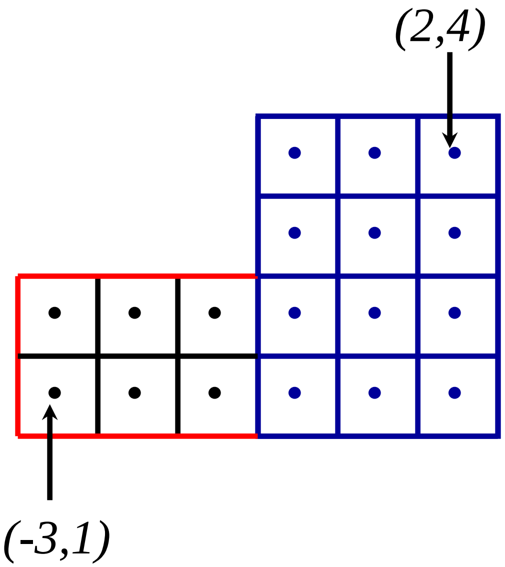


Set grid extents for first box

```
int ilo0[2] = {-3,1};
int iup0[2] = {-1,2};

HYPRE_StructGridSetExtents(grid, ilo0, iup0);
```

Structured-grid finite volume example:

Setting up the grid on process 0

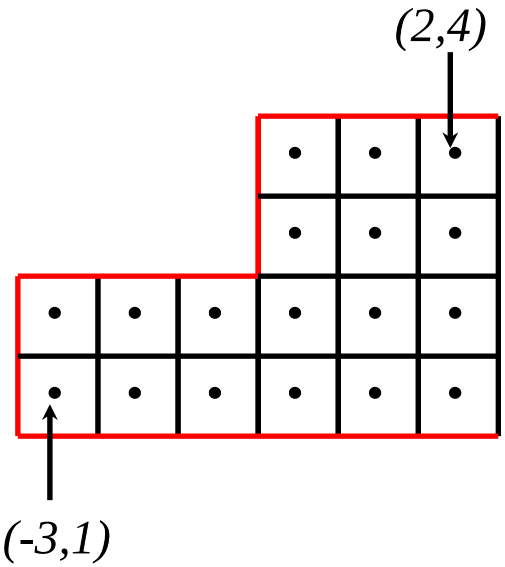


Set grid extents for second box

```
int ilo1[2] = {0,1};
int iup1[2] = {2,4};

HYPRE_StructGridSetExtents(grid, ilo1, iup1);
```

Structured-grid finite volume example:

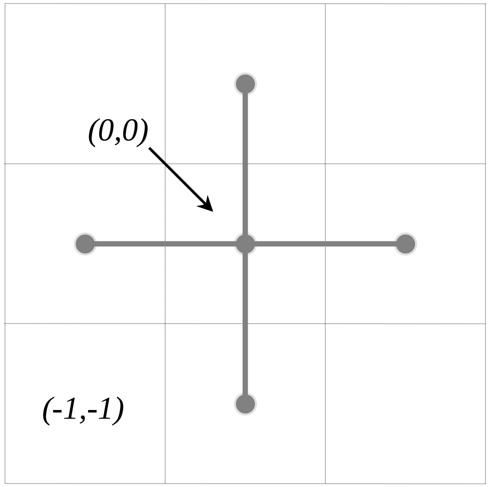
Setting up the grid on process 0



Assemble the grid

```
HYPRE_StructGridAssemble(grid);
```

Structured-grid finite volume example:
Setting up the stencil (all processes)



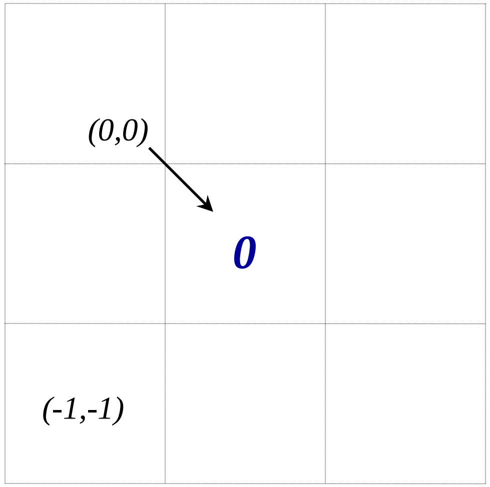
stencil entries		geometries
0	⟷	(0, 0)
1	⟷	(-1, 0)
2	⟷	(1, 0)
3	⟷	(0,-1)
4	⟷	(0, 1)

Create the stencil object

```
HYPRE_StructStencil stencil;
int ndim = 2;
int size = 5;

HYPRE_StructStencilCreate(ndim, size, &stencil);
```

Structured-grid finite volume example:

Setting up the stencil (all processes)

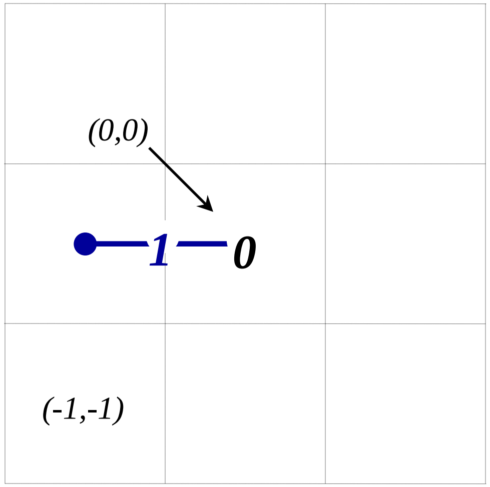


stencil entries		geometries
0	⟷	(0, 0)
1	⟷	(-1, 0)
2	⟷	(1, 0)
3	⟷	(0,-1)
4	⟷	(0, 1)

Set stencil entries

```
int entry = 0;
int offset[2] = {0,0};

HYPRE_StructStencilSetElement(stencil, entry, offset);
```

Structured-grid finite volume example:
Setting up the stencil (all processes)



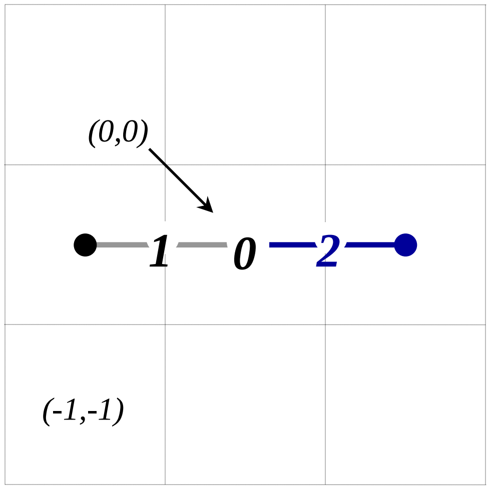
stencil entries	geometries
0	(0, 0)
1	(-1, 0)
2	(1, 0)
3	(0,-1)
4	(0, 1)

Set stencil entries

```
int entry = 1;
int offset[2] = {-1,0};

HYPRE_StructStencilSetElement(stencil, entry, offset);
```

Structured-grid finite volume example:

Setting up the stencil (all processes)



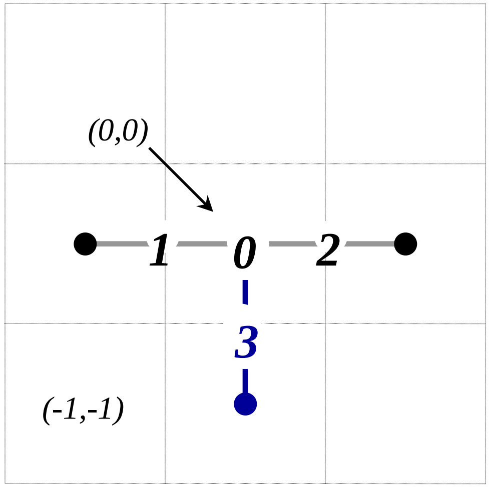
stencil entries		geometries
0	⟷	(0, 0)
1	⟷	(-1, 0)
2	⟷	(1, 0)
3	⟷	(0,-1)
4	⟷	(0, 1)

Set stencil entries

```
int entry = 2;
int offset[2] = {1,0};

HYPRE_StructStencilSetElement(stencil, entry, offset);
```

Structured-grid finite volume example:

Setting up the stencil (all processes)

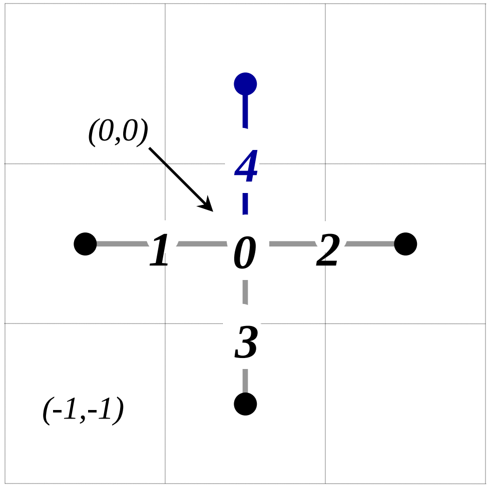


stencil entries		geometries
0	⟷	*(0, 0)*
1	⟷	*(-1, 0)*
2	⟷	*(1, 0)*
3	⟷	*(0,-1)*
4	⟷	*(0, 1)*

Set stencil entries

```
int entry = 3;
int offset[2] = {0,-1};

HYPRE_StructStencilSetElement(stencil, entry, offset);
```

Structured-grid finite volume example:
Setting up the stencil (all processes)



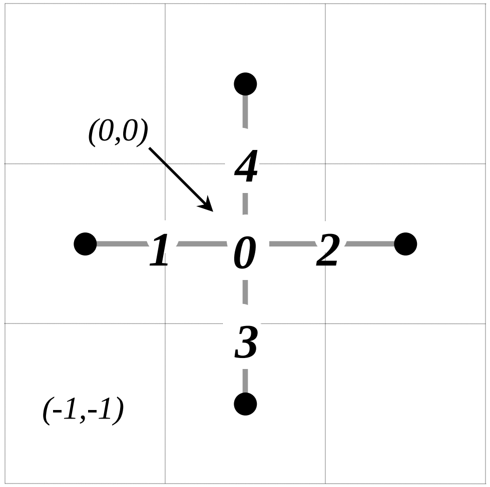
stencil entries		geometries
0	⟷	(0, 0)
1	⟷	(-1, 0)
2	⟷	(1, 0)
3	⟷	(0,-1)
4	⟷	(0, 1)

Set stencil entries

```
int entry = 4;
int offset[2] = {0,1};

HYPRE_StructStencilSetElement(stencil, entry, offset);
```

Structured-grid finite volume example:

Setting up the stencil (all processes)

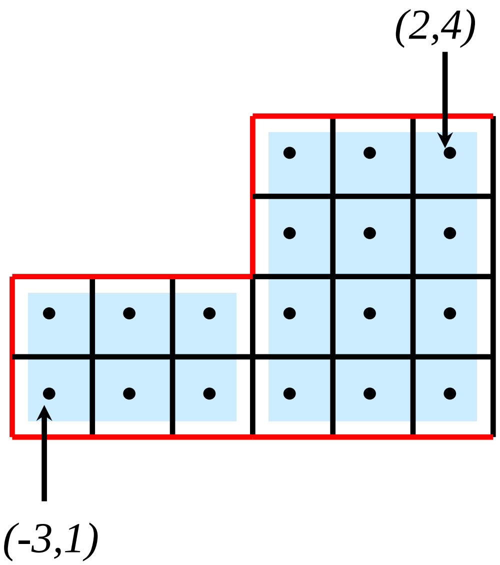


stencil entries		geometries
0	⟷	(0, 0)
1	⟷	(-1, 0)
2	⟷	(1, 0)
3	⟷	(0,-1)
4	⟷	(0, 1)

That's it!

There is no assemble routine

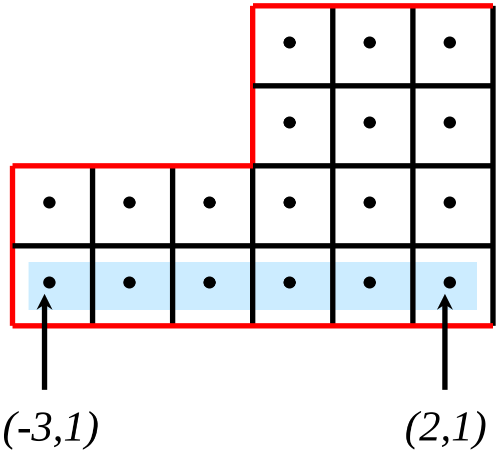
Structured-grid finite volume example :
Setting up the matrix on process 0



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

```
HYPRE_StructMatrix  A;
double  vals[24] = {4, -1, 4, -1, …};
int  nentries = 2;
int  entries[2] = {0,3};

HYPRE_StructMatrixCreate(MPI_COMM_WORLD,
   grid, stencil, &A);
HYPRE_StructMatrixInitialize(A);

HYPRE_StructMatrixSetBoxValues(A,
   ilo0, iup0, nentries, entries, vals);
HYPRE_StructMatrixSetBoxValues(A,
   ilo1, iup1, nentries, entries, vals);

/* set boundary conditions */
…
HYPRE_StructMatrixAssemble(A);
```

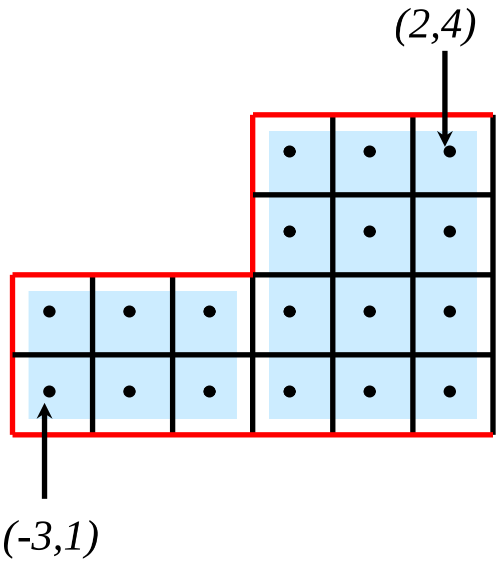
Structured-grid finite volume example :
Setting up the matrix bc's on process 0



$$\begin{bmatrix} & S4 & \\ S1 & S0 & S2 \\ & S3 & \end{bmatrix} = \begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & 0 & \end{bmatrix}$$

```
int  ilo[2] = {-3, 1};
int  iup[2] = { 2, 1};
double  vals[6] = {0, 0, …};
int nentries = 1;

/* set interior coefficients */
…

/* implement boundary conditions */
…

i = 3;
HYPRE_StructMatrixSetBoxValues(A,
   ilo, iup, nentries, &i, vals);

/* complete implementation of bc’s */
…
```

A structured-grid finite volume example :
Setting up the right-hand-side vector on process 0



```
HYPRE_StructVector  b;
double  vals[12] = {0, 0, …};

HYPRE_StructVectorCreate(MPI_COMM_WORLD,
   grid, &b);
HYPRE_StructVectorInitialize(b);

HYPRE_StructVectorSetBoxValues(b,
   ilo0, iup0, vals);
HYPRE_StructVectorSetBoxValues(b,
   ilo1, iup1, vals);

HYPRE_StructVectorAssemble(b);
```

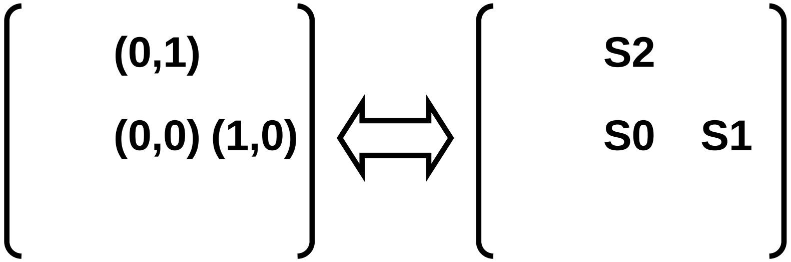
Symmetric Matrices

- Some solvers support symmetric storage

- Between `Create()` and `Initialize()`, call:

```
HYPRE_StructMatrixSetSymmetric(A, 1);
```

- For best efficiency, only set half of the coefficients



(0,1)

(0,0) (1,0)

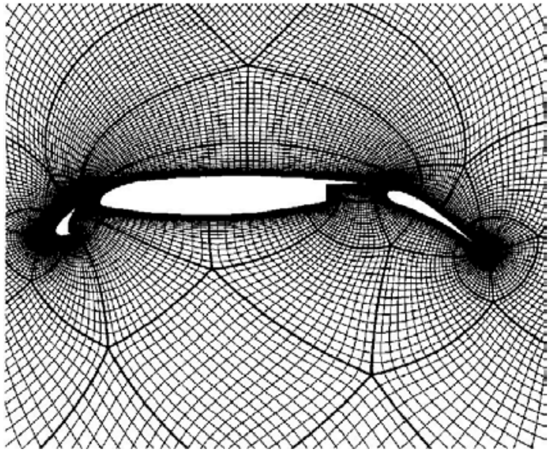
S2

S0 S1

- This is enough info to recover the full 5-pt stencil

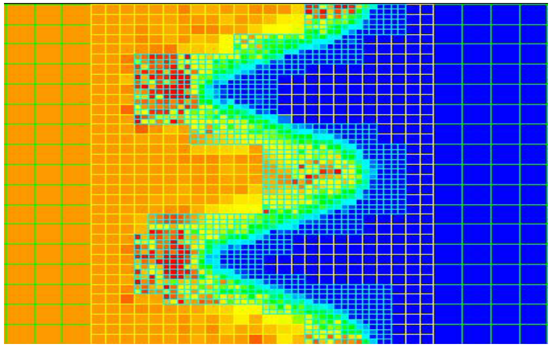
Semi-Structured-Grid System Interface (`SStruct`)

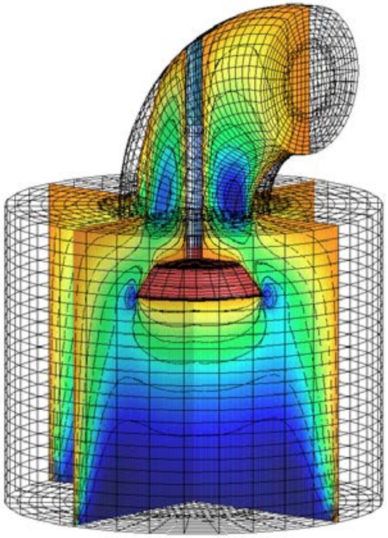
- Allows more general grids:
  - Grids that are mostly (but not entirely) structured
  - Examples: *block-structured grids, structured adaptive mesh refinement grids, overset grids*



Block-Structured

Adaptive Mesh Refinement

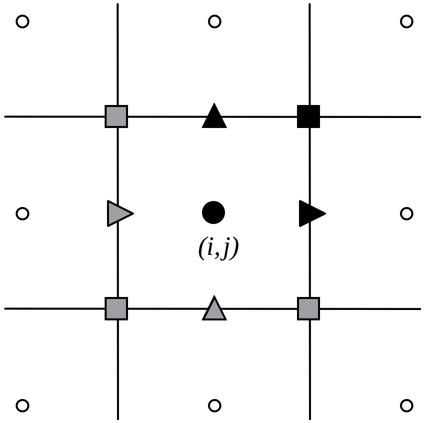




Overset

Semi-Structured-Grid System Interface (**`SStruct`**)

- Allows more general PDE’s
  - Multiple variables (system PDE’s)
  - Multiple variable types (cell centered, face centered, vertex centered, …)



Variables are referenced by the abstract cell-centered index to the left and down

Semi-Structured-Grid System Interface (**`SStruct`**)

- The interface calls are very similar to `Struct`

- The `SStruct` grid is composed out of structured grid *parts*

- A *graph* enables nearly arbitrary relationships between parts
- The graph is constructed from stencils or finite elements plus additional data-coupling information set either
  - directly with `GraphAddEntries()`, or
  - by relating parts with `GridSetNeighborPart()` and `GridSetSharedPart()`

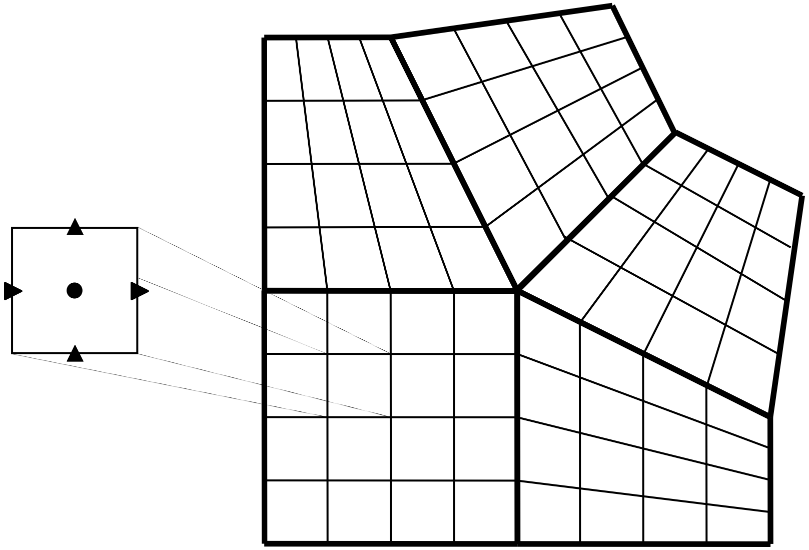
- We will briefly consider two examples:
  - block-structured grid using stencils
  - star-shaped grid with finite elements

Block-structured grid example (**`SStruct`**)

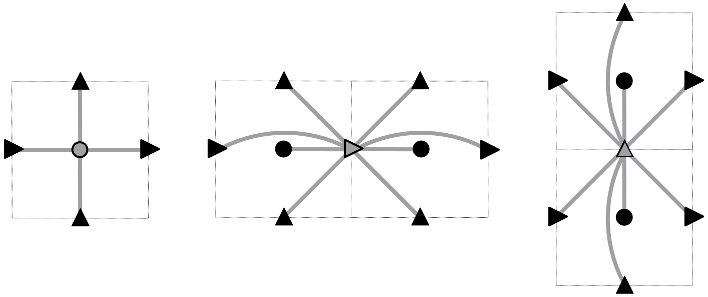
- Consider the following block-structured grid discretization of the diffusion equation

$$-\nabla \cdot \mathbf{K}\nabla u + \sigma u = f$$

A block-structured grid with 3 variable types



The 3 discretization stencils

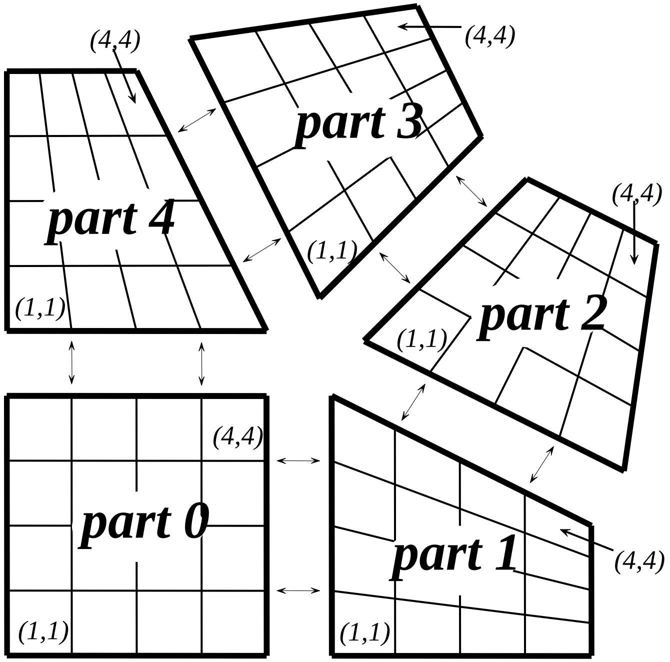


Block-structured grid example (`SStruct`)

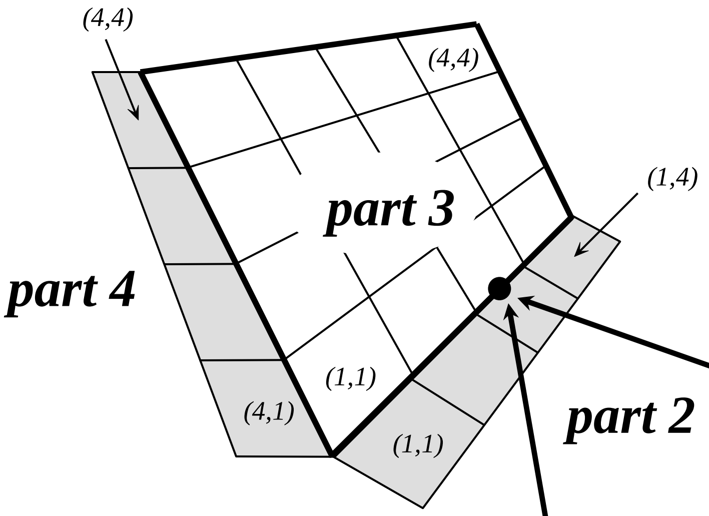
- The `Grid` is described via 5 logically-rectangular parts

- We assume 5 processes such that process *p* owns part *p* (user defines the distribution)

- Consider the interface calls made by process 3
  - Part 3 is set up similarly to `Struct`, then `GridSetNeighborPart()` is used to connect it to parts 2 and 4



Block-structured grid example: some comments on **`SetNeighborPart()`**

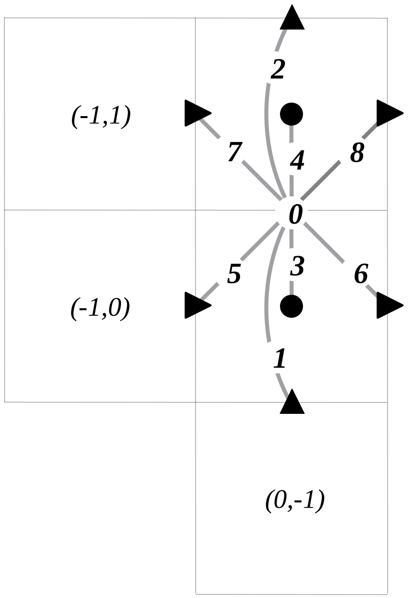


All parts related via this routine must have consistent lists of variables and types

Some variables on different parts become “the same”

Variables may have different types on different parts (e.g., *y-face* on part 3 and *x-face* on part 2)

Block-structured grid example:
Setting up the three stencils (all processes)



stencil entries		geometries
0	↔	(0,0);▲
1	↔	(0,-1);▲
2	↔	(0,1);▲
3	↔	(0,0);●
4	↔	(0,1);●
5	↔	(-1,0);▶
6	↔	(0,0);▶
7	↔	(-1,1);▶
8	↔	(0,1);▶

The y-face stencil

- Setting up a stencil is similar to the `Struct` interface, requiring only one additional *variable* argument
  - Example: Above *y-face* stencil is coupled to variables of types *x-face*, *y-face*, and *cell-centered*

Finite element (FEM) style interface for SStruct as an alternative to stencils

- Beginning with *hypre* version 2.6.0b

- `GridSetSharedPart()` is similar to `SetNeighborPart`, but allows one to specify shared cells, faces, edges, or vertices
- `GridSetFEMOrdering()` sets the ordering of the unknowns in an element (always a cell)
- `GraphSetFEM()` indicates that an FEM approach will be used to set values instead of a stencil approach
- `GraphSetFEMSparsity()` sets the nonzero pattern for the stiffness matrix
- `MatrixAddFEMValues()` and `VectorAddFEMValues()`

- See examples: `ex13.c`, `ex14.c`, and `ex15.c`

Finite Element (FEM) example (`SStruct`)

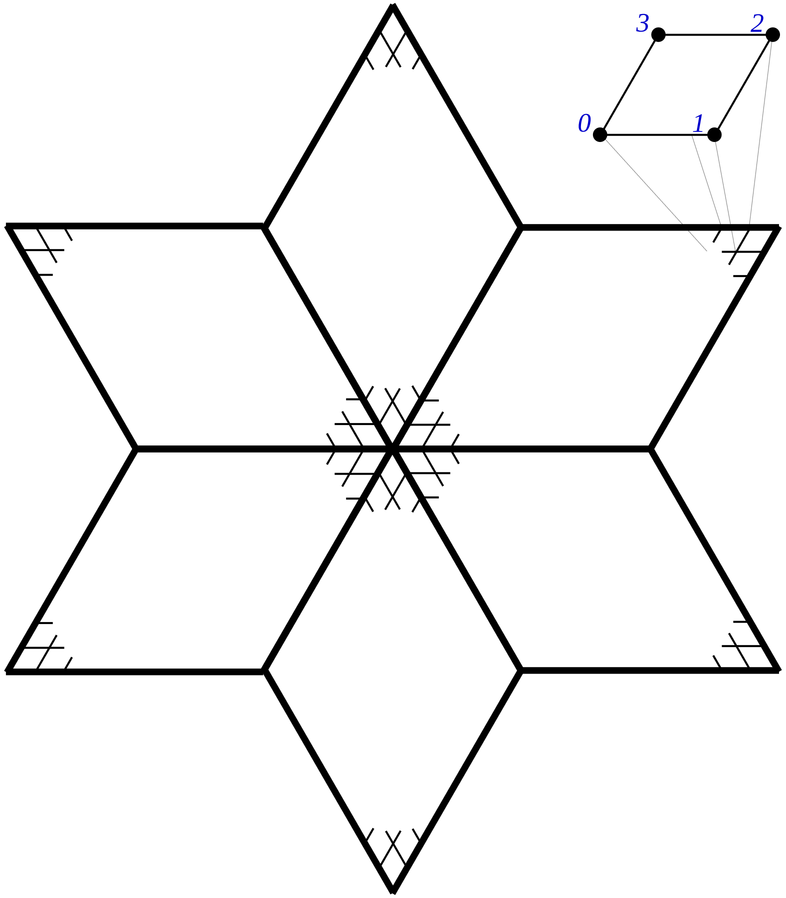
- FEM nodal discretization of the Laplace equation on a star-shaped domain

$$\begin{cases} -\nabla^2 u = 1 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma \end{cases}$$

- FEM stiffness matrix

$$\begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{cccc} \quad 0 \quad & \quad 1 \quad & \quad 2 \quad & \quad 3 \quad \end{array} \\ \begin{pmatrix} 4-k & -1 & -2+k & -1 \\ -1 & 4+k & -1 & -2-k \\ -2+k & -1 & 4-k & -1 \\ -1 & -2-k & -1 & 4+k \end{pmatrix} \alpha \end{array}$$

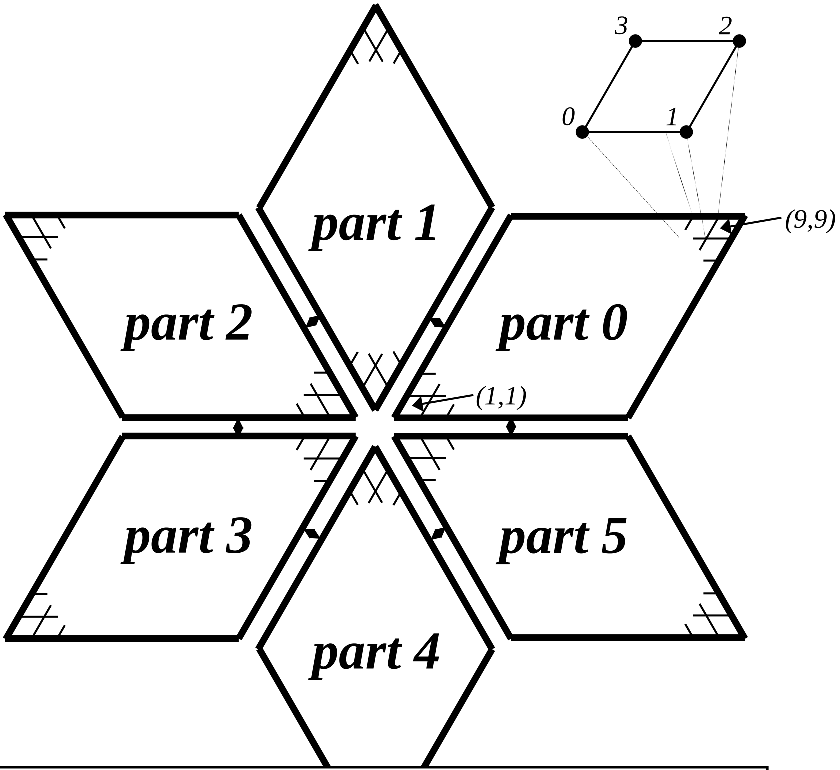
$$\alpha = (6\sin(\gamma))^{-1}, \quad k = 3\cos(\gamma), \quad \gamma = \pi/3$$



See example code `ex14.c`

FEM example (**`SStruct`**)

- The `Grid` is described via 6 logically-rectangular parts
- We assume 6 processes, where process *p* owns part *p*
- The `Matrix` is assembled from stiffness matrices (no stencils)



```
int part = 0, index[2] = {i,j};
double values[16] = {…};

HYPRE_SStructMatrixAddFEMValues(A, part, index, values);
```

Building different matrix/vector storage formats with the `SStruct` interface

- Efficient preconditioners often require specific matrix/vector storage schemes

- Between `Create()` and `Initialize`(), call:

```
HYPRE_SStructMatrixSetObjectType(A, HYPRE_PARCSR);
```

- After `Assemble()`, call:

```
HYPRE_SStructMatrixGetObject(A, &parcsr_A);
```

- Now, use the `ParCSR` matrix with compatible solvers such as BoomerAMG (algebraic multigrid)

Current solver / preconditioner availability via *hypre*'s linear system interfaces

Data Layouts	Solvers	System Interfaces			
		Struct	SStruct	FEI	IJ
Structured	Jacobi	✓	✓		
	SMG	✓	✓		
	PFMG	✓	✓		
Semi-structured	Split		✓		
	SysPFMG		✓		
	FAC		✓		
	Maxwell		✓		
Sparse matrix	AMS, ADS		✓	✓	✓
	BoomerAMG		✓	✓	✓
	MLI		✓	✓	✓
	ParaSails		✓	✓	✓
	Euclid		✓	✓	✓
	PILUT		✓	✓	✓
Matrix free	PCG	✓	✓	✓	✓
	GMRES	✓	✓	✓	✓
	BiCGSTAB	✓	✓	✓	✓
	Hybrid	✓	✓	✓	✓

Setup and use of solvers is largely the same (*see Reference Manual for details*)

- Create the solver

```
HYPRE_SolverCreate(MPI_COMM_WORLD, &solver);
```

- Set parameters

```
HYPRE_SolverSetTol(solver, 1.0e-06);
```

- Prepare to solve the system

```
HYPRE_SolverSetup(solver, A, b, x);
```

- Solve the system

```
HYPRE_SolverSolve(solver, A, b, x);
```

- Get solution info out via system interface

```
HYPRE_StructVectorGetValues(struct_x, index, values);
```

- Destroy the solver

```
HYPRE_SolverDestroy(solver);
```

Solver example: SMG-PCG

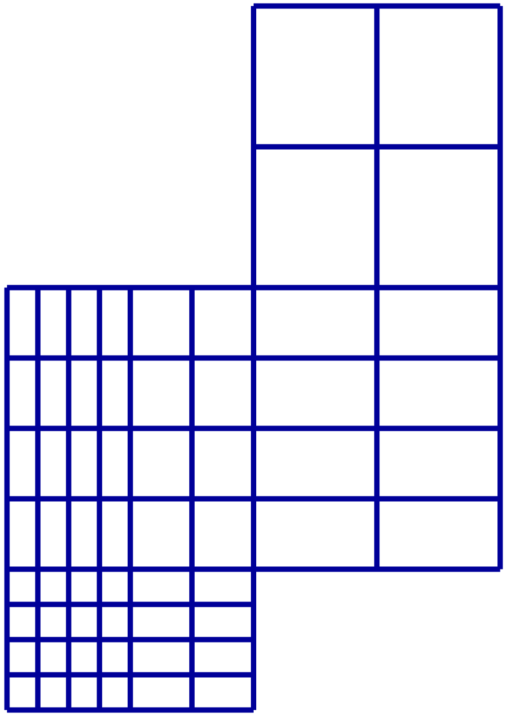
```
/* define preconditioner (one symmetric V(1,1)-cycle) */
HYPRE_StructSMGCreate(MPI_COMM_WORLD, &precond);
HYPRE_StructSMGSetMaxIter(precond, 1);
HYPRE_StructSMGSetTol(precond, 0.0);
HYPRE_StructSMGSetZeroGuess(precond);
HYPRE_StructSMGSetNumPreRelax(precond, 1);
HYPRE_StructSMGSetNumPostRelax(precond, 1);

HYPRE_StructPCGCreate(MPI_COMM_WORLD, &solver);
HYPRE_StructPCGSetTol(solver, 1.0e-06);

/* set preconditioner */
HYPRE_StructPCGSetPrecond(solver,
   HYPRE_StructSMGSolve, HYPRE_StructSMGSetup, precond);

HYPRE_StructPCGSetup(solver, A, b, x);
HYPRE_StructPCGSolve(solver, A, b, x);
```

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

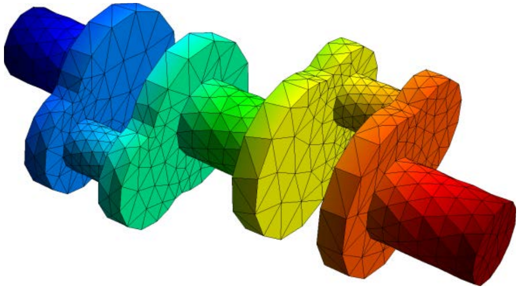
- Constant-coefficient versions!

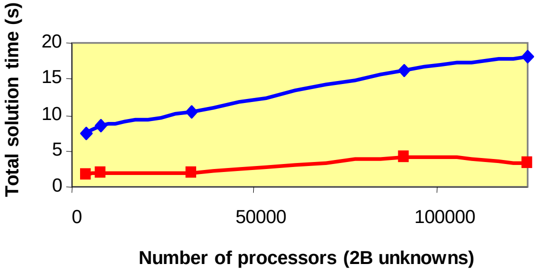


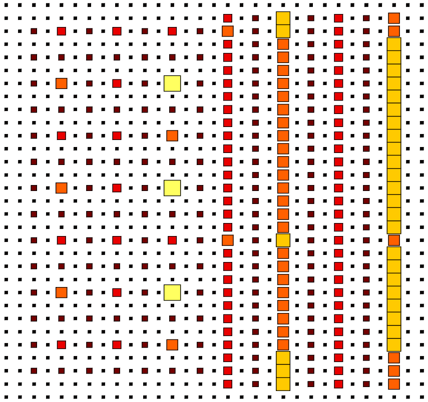
BoomerAMG is an algebraic multigrid method for unstructured grids

- Interface: `SStruct, FEI, 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





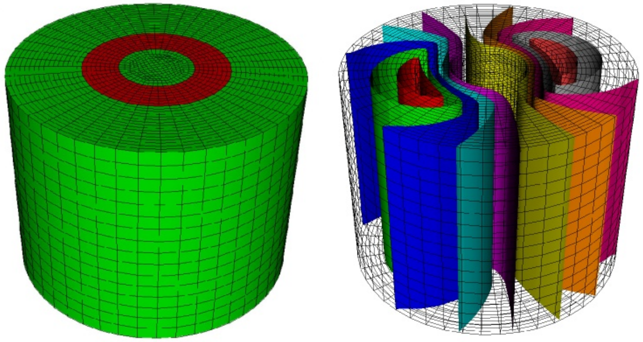


AMS is an auxiliary space Maxwell solver for unstructured grids

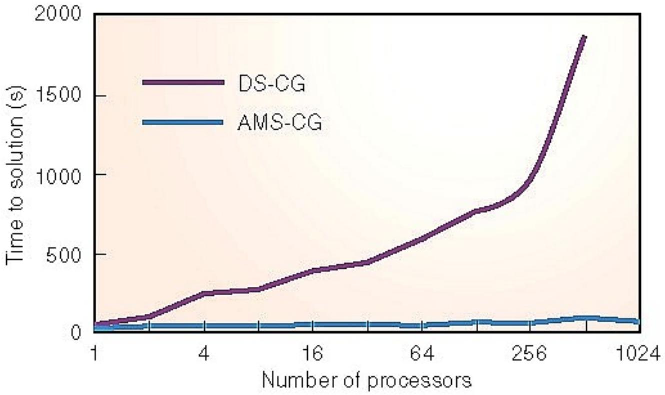
- Interface: `SStruct`, `FEI`, `IJ`
- Matrix Class: `ParCSR`
- Solves definite problems:

$$\nabla \times \alpha \nabla \times E + \beta E = f, \;\; \alpha > 0, \beta \geq 0$$

- Requires additional gradient matrix and mesh coordinates
- Variational form of Hiptmair-Xu
- Employs BoomerAMG
- Only for FE discretizations
- ADS is a related solver for FE grad-div problems.



Copper wire in air, conductivity jump of 10^6



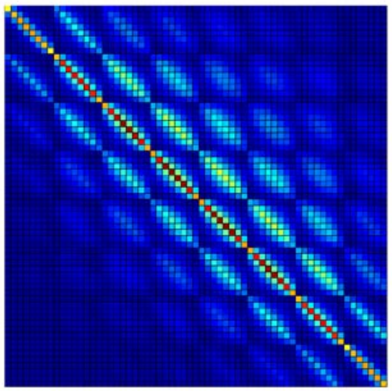
25x faster on 80M unknowns

ParaSAILS is an approximate inverse method for sparse linear systems

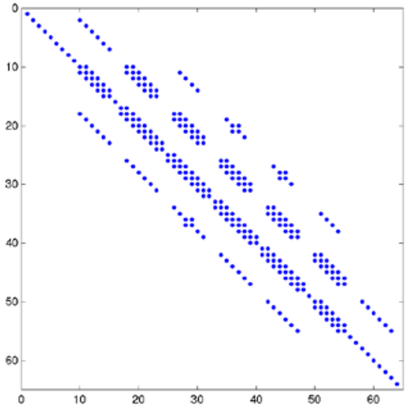
- Interface: `SStruct`, `FEI`, `IJ`
- Matrix Class: `ParCSR`

- Approximates the inverse of A by a sparse matrix M by minimizing the Frobenius norm of $I - AM$
- Uses graph theory to predict good sparsity patterns for M

Exact inverse

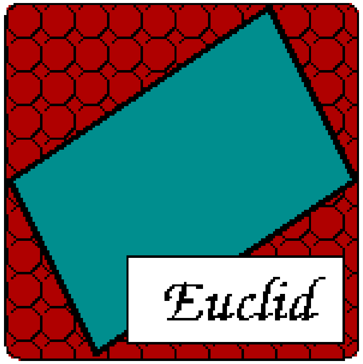


Approx inverse



Euclid is a family of Incomplete LU methods for sparse linear systems

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



- Obtains scalable parallelism via local and global reorderings
- Good for unstructured problems

http://www.cs.odu.edu/~pothen/Software/Euclid

Solver parameters can greatly impact performance!

- Defaults are usually chosen to perform well across some (possibly small) set of problems
  - They may be poor choices for other problems
- All parameters have pros and cons
- BoomerAMG example:
  - HMIS coarsening, long-range interpolation, and truncation reduce communication but degrade convergence
  - For Diffusion, this is an overall win in time-to-solution
- Don’t hesitate to contact hypre-support for guidance

Getting the code

- To get the code, go to

http://www.llnl.gov/CASC/hypre/

- User’s / Reference Manuals can be downloaded directly

- Release includes example programs!

Building the library

- Usually, *hypre* can be built by typing `configure` then `make`
- Configure supports several options (for usage information, type '`configure --help`'):

  '`configure --enable-debug`' - turn on debugging
  '`configure --with-openmp`' - use openmp
  '`configure --disable-fortran`' - disable Fortran tests
  '`configure --with-CFLAGS=…`' - set compiler flags

- CMake is also supported
  - Ideal for Windows environment

- See `INSTALL` file for more details

Calling *hypre* from Fortran

- C code:

```
HYPRE_IJVector vec;
int            nvalues, *indices;
double        *values;

HYPRE_IJVectorSetValues(vec, nvalues, indices, values);
```

- Corresponding Fortran code:

```
integer*8        vec
integer          nvalues, indices(NVALUES)
double precision values(NVALUES)

call HYPRE_IJVectorSetValues(vec, nvalues, indices, values, ierr)
```

Reporting bugs, requesting features, usage questions

- Send email to the following address:

hypre-support@llnl.gov

- We use an email-centered tool called Roundup to automatically tag and track issues

Introduction to hypre hands-on exercises

- Open `hypre/README.html`

Thank You!

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.