#### **Lawrence Livermore National Laboratory**

### **HYPRE: High Performance Preconditioners**

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Center for Applied Scientific Computing

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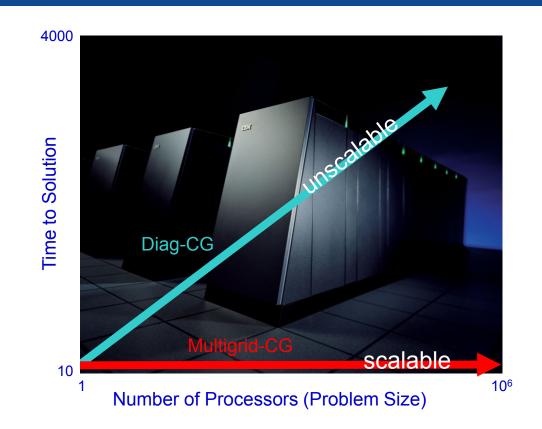


### Outline

- Introduction / Motivation
- Getting Started / Linear System Interfaces
- Structured-Grid Interface (Struct)
- Semi-Structured-Grid Interface (SStruct)
- Finite Element Interface (FEI)
- Linear-Algebraic Interface (IJ)
- Solvers and Preconditioners
- Additional Information

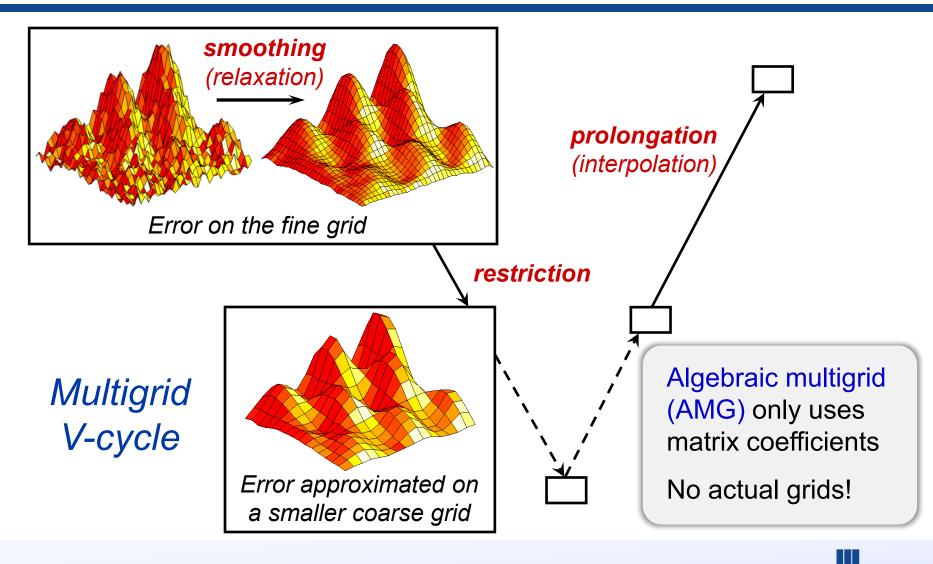


# Multigrid solvers have O(N) complexity, and hence have good scaling potential

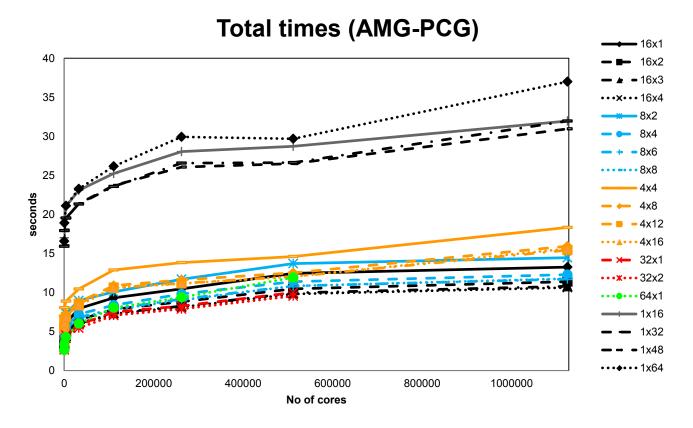


 Weak scaling – want constant solution time as problem size grows in proportion to the number of processors

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



# 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

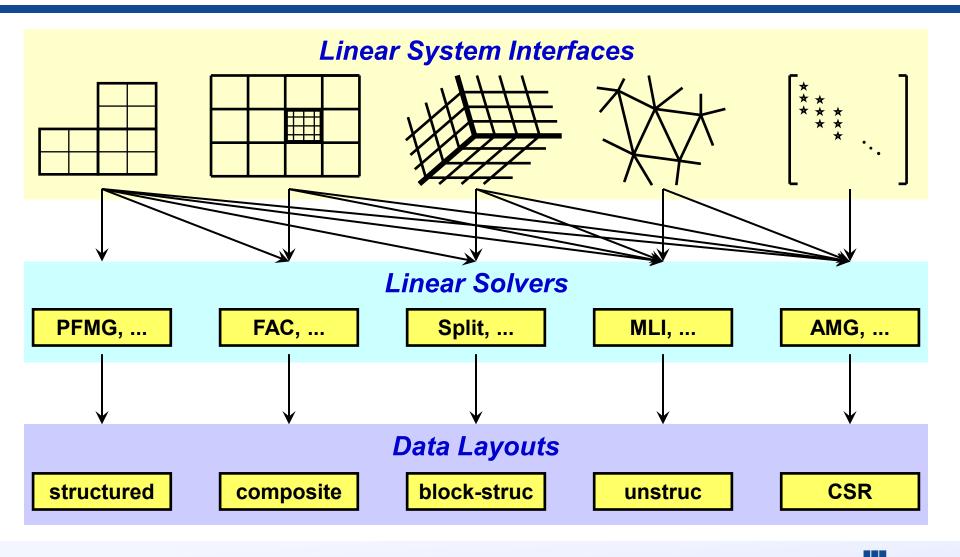


### **Getting Started**

- 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

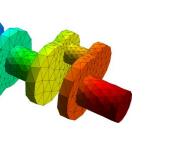


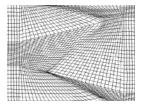
### Why multiple interfaces? The key points

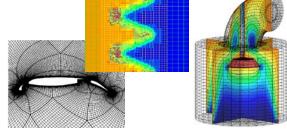
- Provides natural "views" of the linear system
- Eases some of the coding burden for users by eliminating the need to map to rows/columns
- Provides for more efficient (scalable) linear solvers
- Provides for more effective data storage schemes and more efficient computational kernels

### 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

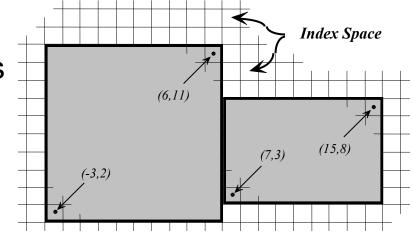








- Appropriate for scalar applications on structured grids with a fixed stencil pattern
- Grids are described via a global *d*-dimensional *index* space (singles in 1D, tuples in 2D, and triples in 3D)
- A box is a collection of cell-centered indices, described by its "lower" and "upper" corners
- The scalar grid data is always associated with cell centers (unlike the more general SStruct interface)

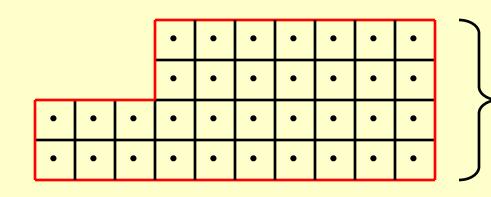


- There are four basic steps involved:
  - set up the Grid
  - set up the Stencil
  - set up the Matrix
  - set up the right-hand-side Vector
- Consider the following 2D Laplacian problem

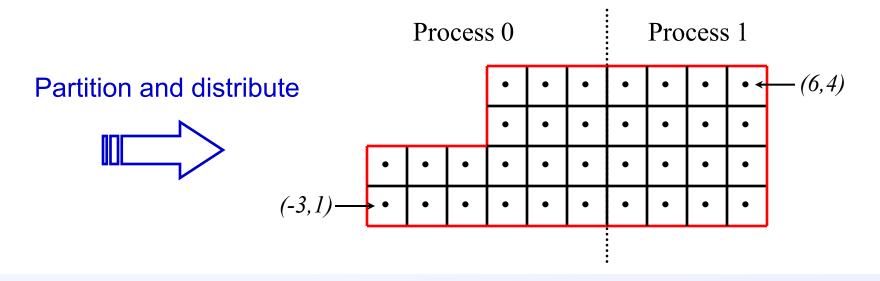
$$\left\{ \begin{array}{ll} -\nabla^2 u = f & \text{in the domain} \\ u = g & \text{on the boundary} \end{array} \right.$$

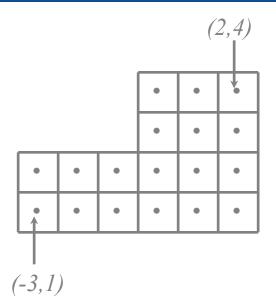


#### **Structured-grid finite volume example:**



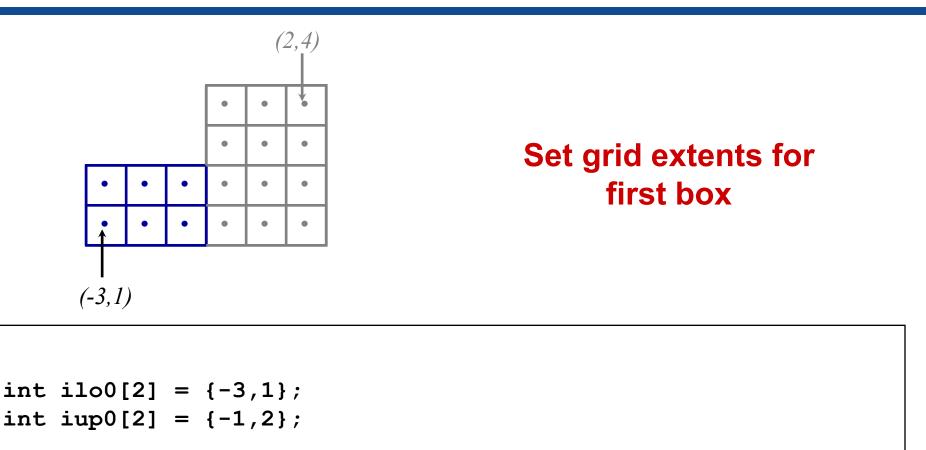
### Standard 5-point finite volume discretization





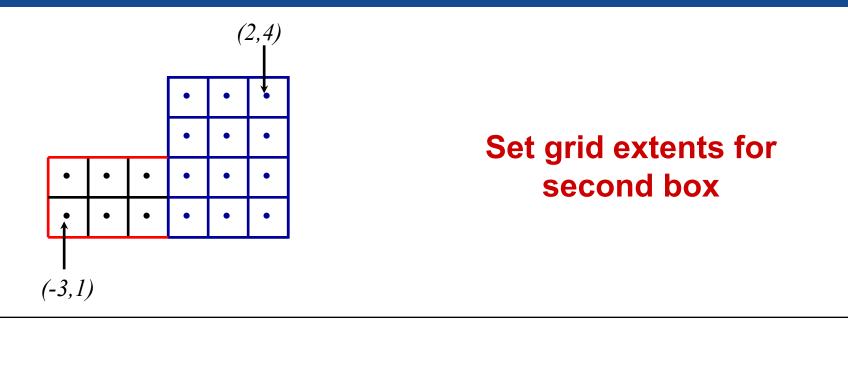
#### **Create the grid object**





```
HYPRE StructGridSetExtents(grid, ilo0, iup0);
```

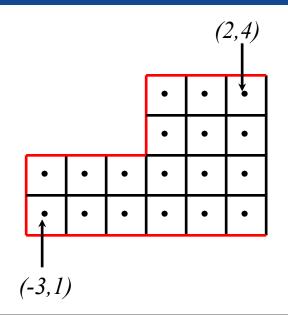




```
int ilo1[2] = {0,1};
int iup1[2] = {2,4};
```

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

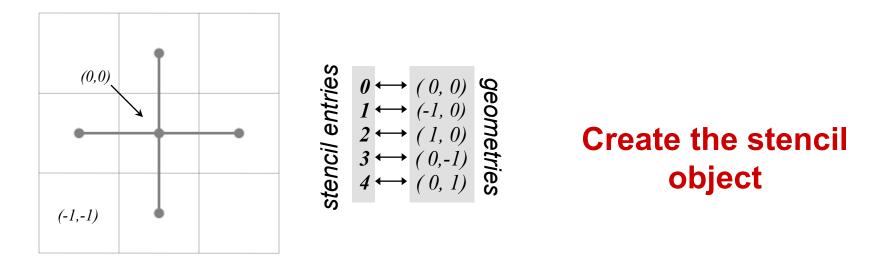




#### Assemble the grid

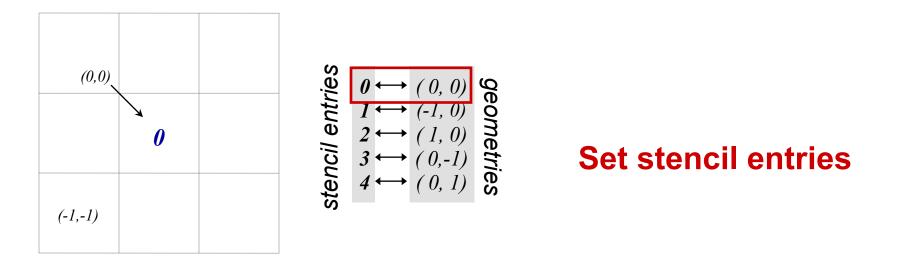
HYPRE StructGridAssemble(grid);





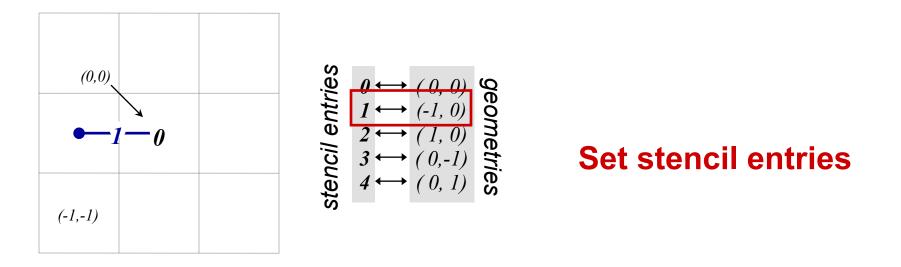
```
HYPRE_StructStencil stencil;
int ndim = 2;
int size = 5;
HYPRE_StructStencilCreate(ndim, size, &stencil);
```





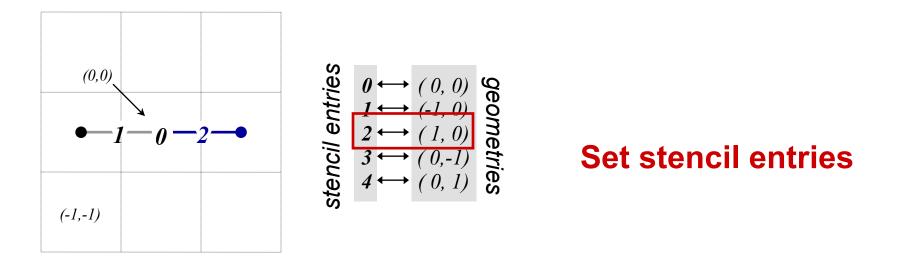






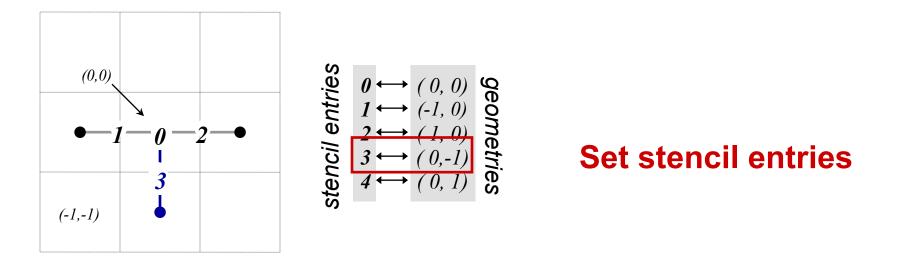
int entry = 1; int offset[2] = {-1,0}; HYPRE\_StructStencilSetElement(stencil, entry, offset);





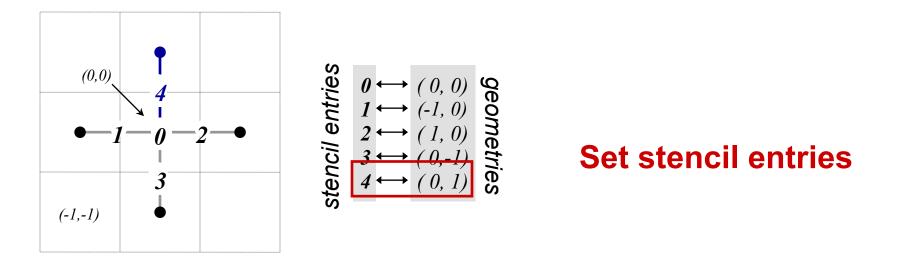
int entry = 2; int offset[2] = {1,0}; HYPRE\_StructStencilSetElement(stencil, entry, offset);



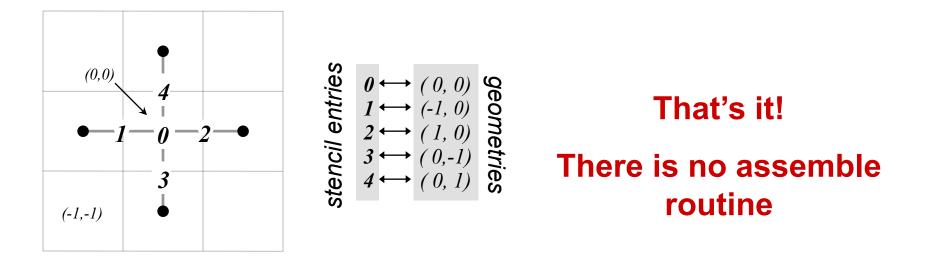


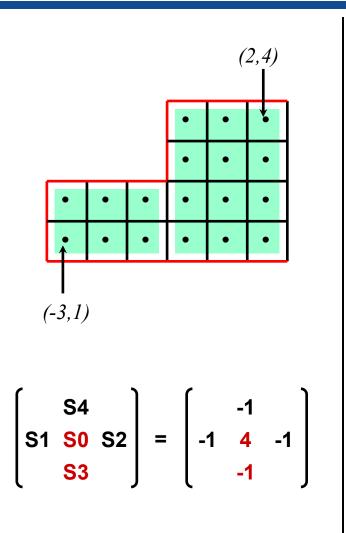
int entry = 3; int offset[2] = {0,-1}; HYPRE\_StructStencilSetElement(stencil, entry, offset);





int entry = 4; int offset[2] = {0,1}; HYPRE\_StructStencilSetElement(stencil, entry, offset);



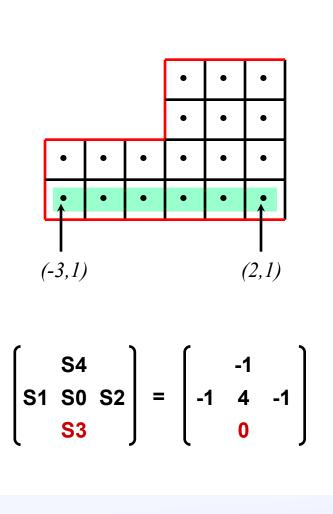


```
HYPRE_StructMatrix A;
double vals[24] = {4, -1, 4, -1, ...};
int nentries = 2;
int entries[2] = {0,3};
```

```
HYPRE_StructMatrixCreate(MPI_COMM_WORLD,
    grid, stencil, &A);
HYPRE StructMatrixInitialize(A);
```

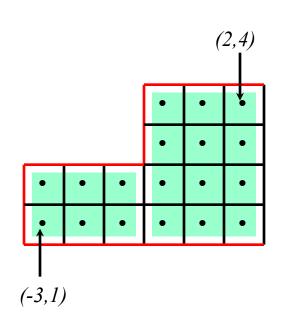
/\* set boundary conditions \*/

HYPRE\_StructMatrixAssemble(A);



```
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\_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

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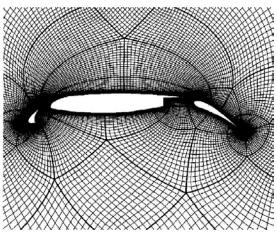
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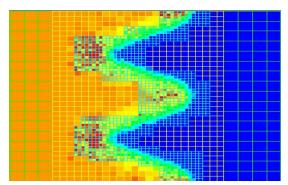
This is enough info to recover the full 5-pt stencil

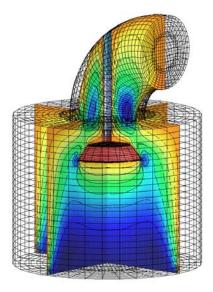
- Allows more general grids:
  - Grids that are mostly (but not entirely) structured
  - Examples: block-structured grids, structured adaptive mesh refinement grids, overset grids



Block-Structured

Adaptive Mesh Refinement

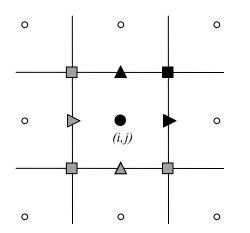




Overset



- 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

- The SStruct grid is composed out of structured grid parts
- The interface uses a graph to allow nearly arbitrary relationships between part data
- The graph is constructed from stencils or finite element stiffness matrices (new) plus additional data-coupling information set either
  - directly with GraphAddEntries(), or
  - by relating parts with GridSetNeighborPart() and GridSetSharedPart() (new)
- We will consider two examples:
  - block-structured grid using stencils
  - star-shaped grid with finite elements (new)

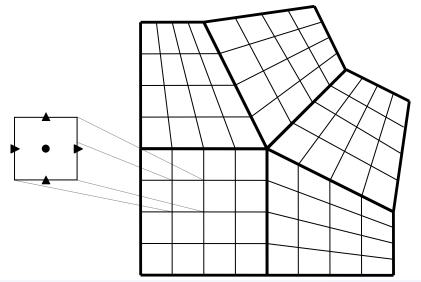
- There are five basic steps involved:
  - set up the Grid
  - set up the Stencils
  - set up the Graph
  - set up the Matrix
  - set up the right-hand-side Vector

#### Block-structured grid example (SStruct)

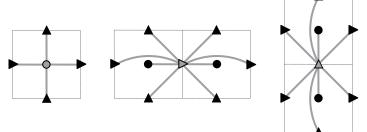
 Consider the following block-structured grid discretization of the diffusion equation

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



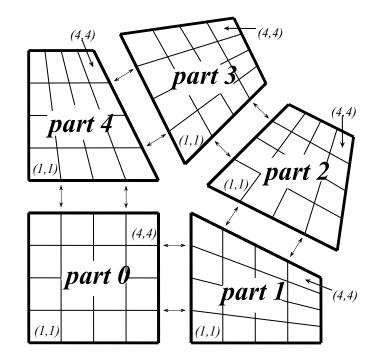


The 3 discretization stencils

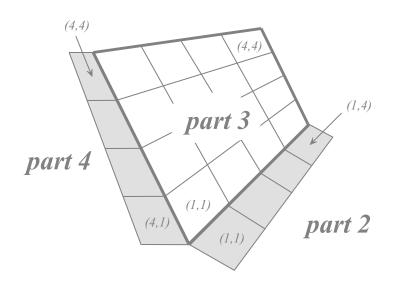


#### Block-structured grid example (SStruct)

- The Grid is described via 5 logically-rectangular parts
- We assume 5 processes such that process p owns part p (user defines the distribution)
- We consider the interface calls made by process 3



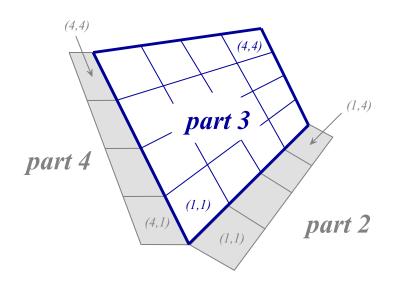
#### **Block-structured grid example:** Setting up the grid on process 3



#### **Create the grid object**

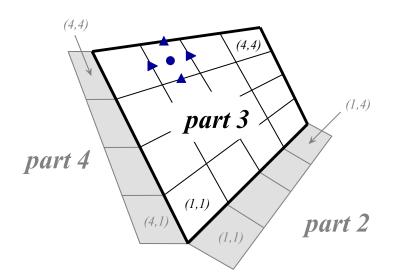
HYPRE\_SStructGrid grid; int ndim = 2; int nparts = 5; HYPRE\_SStructGridCreate(MPI\_COMM\_WORLD, ndim, nparts, &grid);

#### **Block-structured grid example:** Setting up the grid on process 3

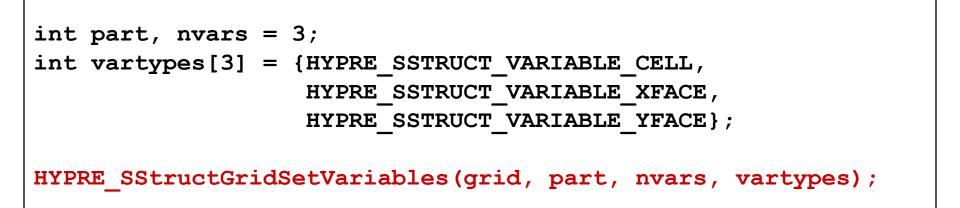


### Set grid extents for part 3

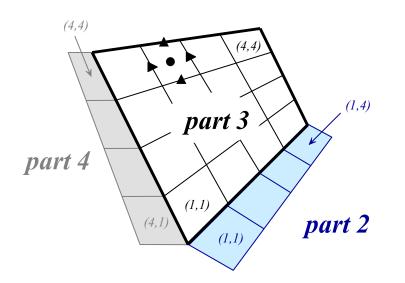
int part = 3; int ilower[2] = {1,1}; int iupper[2] = {4,4}; HYPRE\_SStructGridSetExtents(grid, part, ilower, iupper);



#### Set grid variables for each part

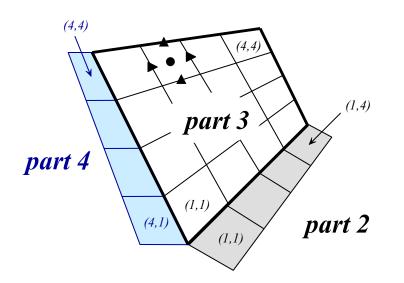






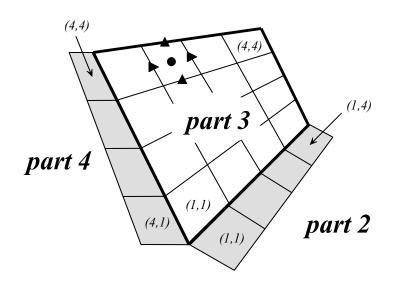
## Set spatial relationship between parts 3 and 2

```
int part = 3, nbor_part = 2;
int ilower[2] = {1,0}, iupper[2] = {4,0};
int nbor_ilower[2] = {1,1}, nbor_iupper[2] = {1,4};
int index_map[2] = {1,0}, index_dir[2] = {1,-1};
HYPRE_SStructGridSetNeighborPart(grid, part, ilower, iupper,
nbor_part, nbor_ilower, nbor_iupper, index_map, index_dir);
```



## Set spatial relationship between parts 3 and 4

```
int part = 3, nbor_part = 4;
int ilower[2] = {0,1}, iupper[2] = {0,4};
int nbor_ilower[2] = {4,1}, nbor_iupper[2] = {4,4};
int index_map[2] = {0,1}, index_dir[2] = {1,1};
HYPRE_SStructGridSetNeighborPart(grid, part, ilower, iupper,
nbor_part, nbor_ilower, nbor_iupper, index_map, index_dir);
```

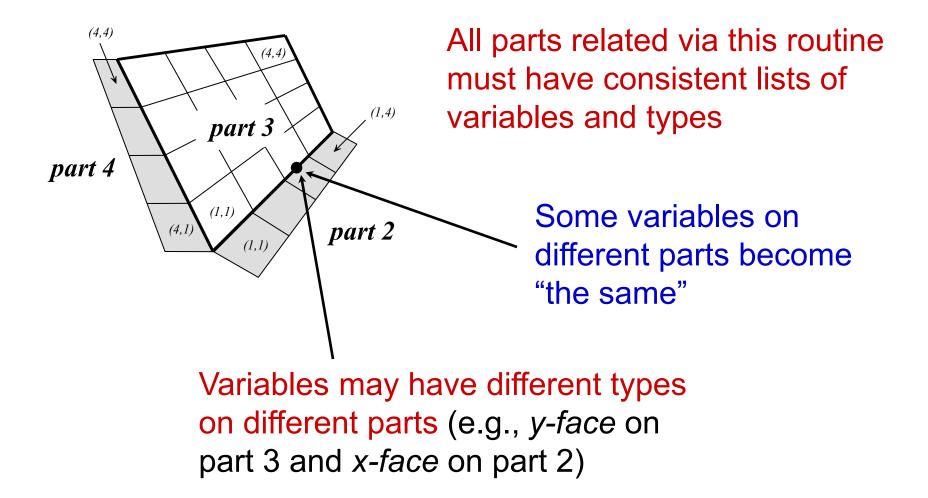


**Assemble the grid** 

HYPRE SStructGridAssemble(grid);

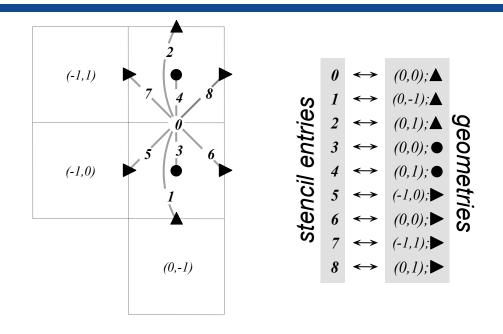


# Block-structured grid example: some comments on SetNeighborPart()





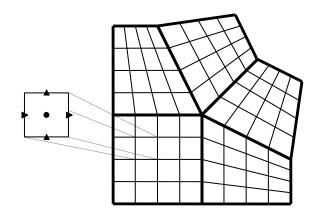
#### **Block-structured grid example:** Setting up the three stencils (all processes)



#### 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*



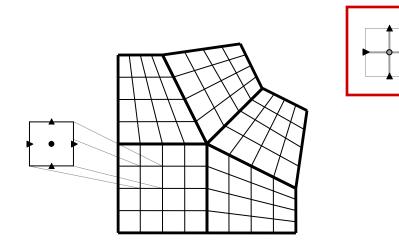


## Create the graph object

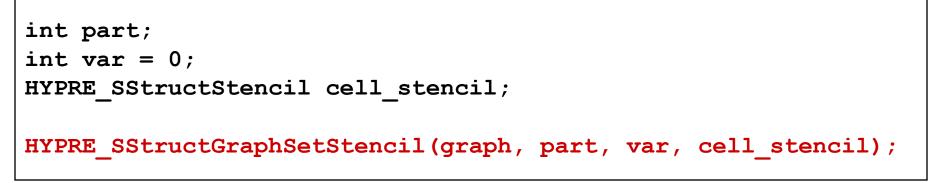
HYPRE SStructGraph graph;

HYPRE SStructGraphCreate(MPI COMM WORLD, grid, &graph);

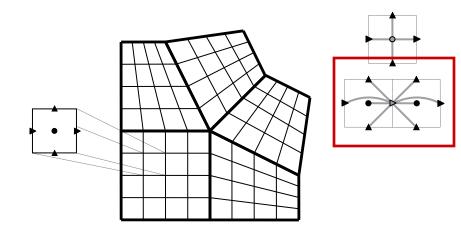




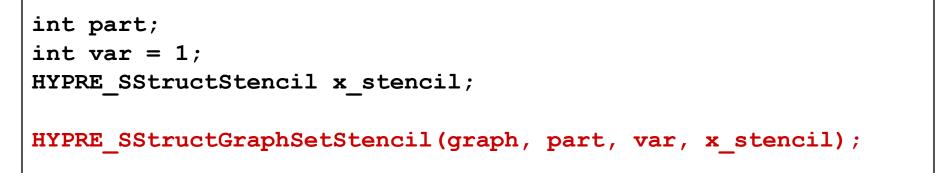
## Set the cell-centered stencil for each part





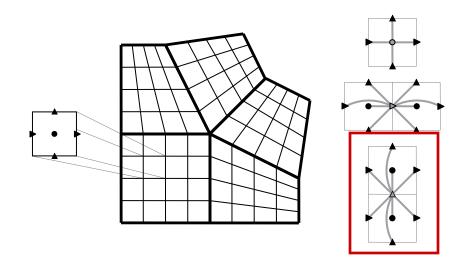


## Set the x-face stencil for each part

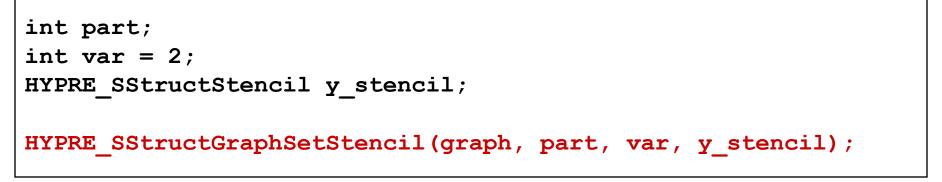




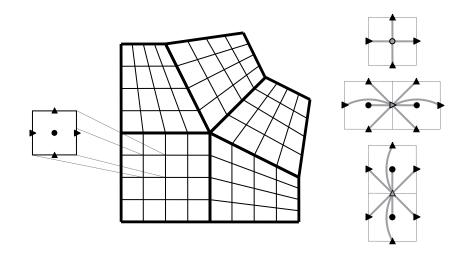




## Set the y-face stencil for each part







#### Assemble the graph

/\* No need to add non-stencil entries
 \* with HYPRE\_SStructGraphAddEntries() \*/

HYPRE\_SStructGraphAssemble(graph);



#### **Block-structured grid example:** Setting up the matrix and vector

- The matrix and vector objects are constructed in a manner similar to the Struct interface
- Matrix coefficients are set with the routines
  - HYPRE\_SStructMatrixSetValues()
  - HYPRE\_SStructMatrixAddToValues()
- Vector values are set with similar routines
  - HYPRE\_SStructVectorSetValues()
  - HYPRE\_SStructVectorAddToValues()

# New 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

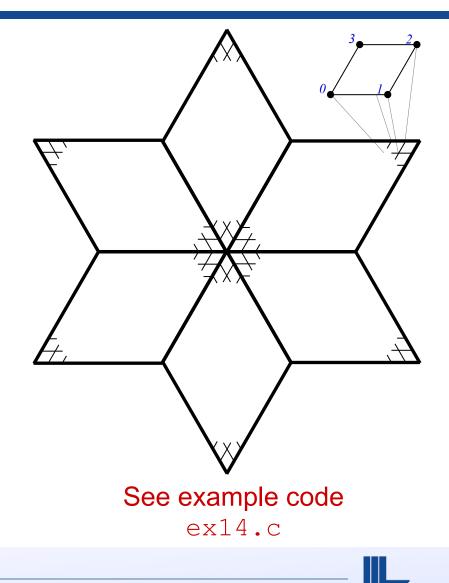


### Finite Element (FEM) example (SStruct)

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

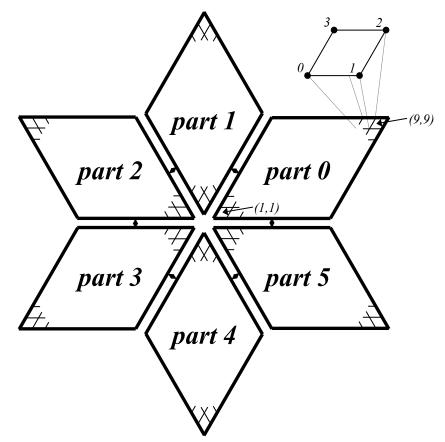
$$\begin{cases} -\nabla^2 u = 1 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma \end{cases}$$

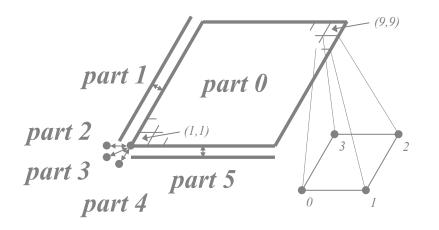
FEM stiffness matrix



### FEM example (SStruct)

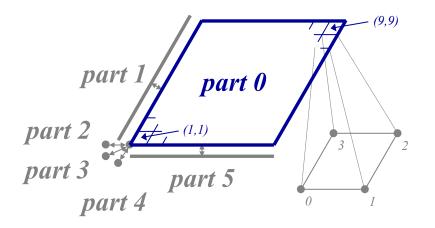
- The Grid is described via 6 logically-rectangular parts
- We assume 6 processes, where process p owns part p
- The Matrix is assembled from stiffness matrices (no stencils)
- We consider the interface calls made by process 0





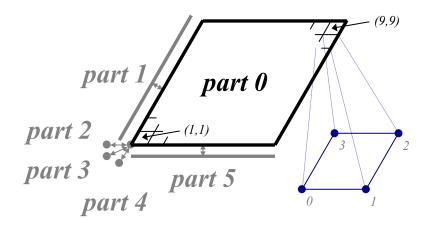
#### **Create the grid object**

HYPRE\_SStructGrid grid; int ndim = 2; int nparts = 6; HYPRE\_SStructGridCreate(MPI\_COMM\_WORLD, ndim, nparts, &grid);

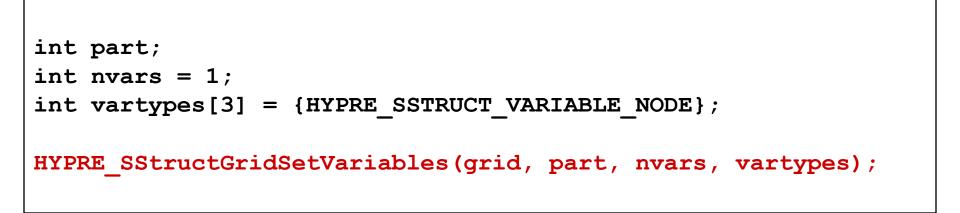


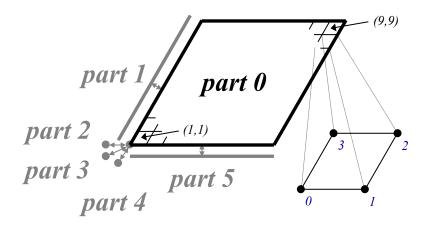
## Set grid extents for part 0

int part = 0; int ilower[2] = {1,1}; int iupper[2] = {9,9}; HYPRE\_SStructGridSetExtents(grid, part, ilower, iupper);



#### Set grid variables for each part

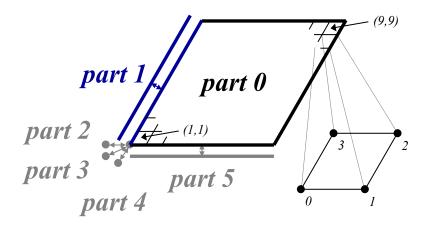




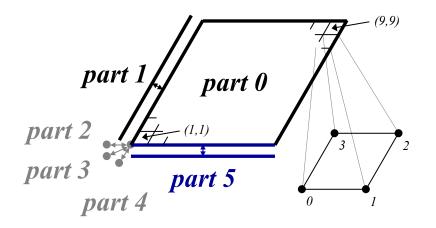
## Set FEM ordering of variables on part 0

HYPRE\_SStructGridSetFEMOrdering(grid, part, ordering);



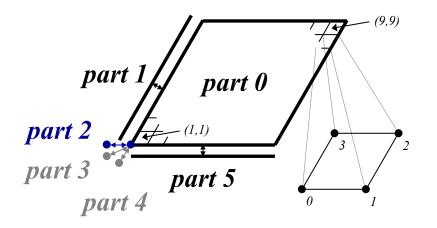


```
int part = 0, spart = 1;
int ilo[2] = {1,1}, iup[2] = {1,9}, offset[2] = {-1,0};
int silo[2] = {1,1}, siup[2] = {9,1}, soffset[2] = {0,-1};
int index_map[2] = {1,0}, index_dir[2] = {-1,1};
HYPRE_SStructGridSetSharedPart(grid, part, ilo, iup, offset,
spart, silo, siup, soffset, index_map, dir_map);
```



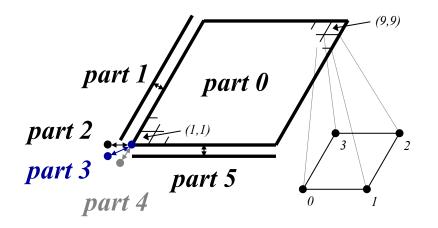
```
int part = 0, spart = 5;
int ilo[2] = {1,1}, iup[2] = {9,1}, offset[2] = {0,-1};
int silo[2] = {1,1}, siup[2] = {1,9}, soffset[2] = {-1,0};
int index_map[2] = {1,0}, index_dir[2] = {1,-1};
HYPRE_SStructGridSetSharedPart(grid, part, ilo, iup, offset,
spart, silo, siup, soffset, index_map, dir_map);
```





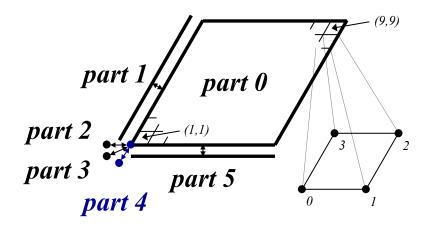
```
int part = 0, spart = 2;
int ilo[2] = {1,1}, iup[2] = {1,1}, offset[2] = {-1,-1};
int silo[2] = {1,1}, siup[2] = {1,1}, soffset[2] = {-1,-1};
int index_map[2] = {0,1}, index_dir[2] = {-1,-1};
HYPRE_SStructGridSetSharedPart(grid, part, ilo, iup, offset,
spart, silo, siup, soffset, index_map, dir_map);
```





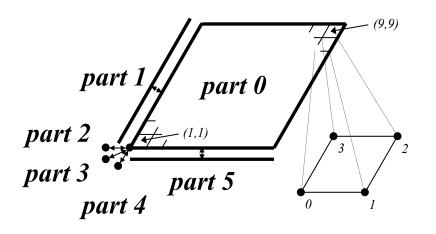
```
int part = 0, spart = 3;
int ilo[2] = {1,1}, iup[2] = {1,1}, offset[2] = {-1,-1};
int silo[2] = {1,1}, siup[2] = {1,1}, soffset[2] = {-1,-1};
int index_map[2] = {0,1}, index_dir[2] = {-1,-1};
HYPRE_SStructGridSetSharedPart(grid, part, ilo, iup, offset,
spart, silo, siup, soffset, index_map, dir_map);
```





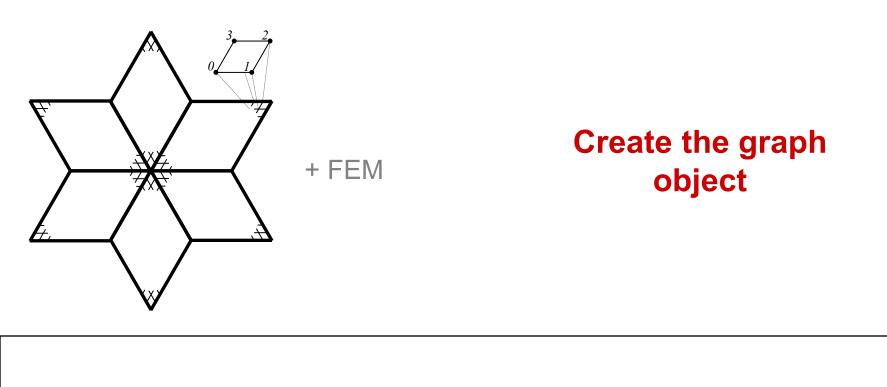
```
int part = 0, spart = 4;
int ilo[2] = {1,1}, iup[2] = {1,1}, offset[2] = {-1,-1};
int silo[2] = {1,1}, siup[2] = {1,1}, soffset[2] = {-1,-1};
int index_map[2] = {0,1}, index_dir[2] = {-1,-1};
HYPRE_SStructGridSetSharedPart(grid, part, ilo, iup, offset,
spart, silo, siup, soffset, index_map, dir_map);
```





#### Assemble the grid

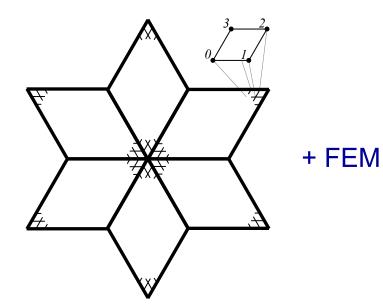
HYPRE SStructGridAssemble(grid);



HYPRE SStructGraph graph;

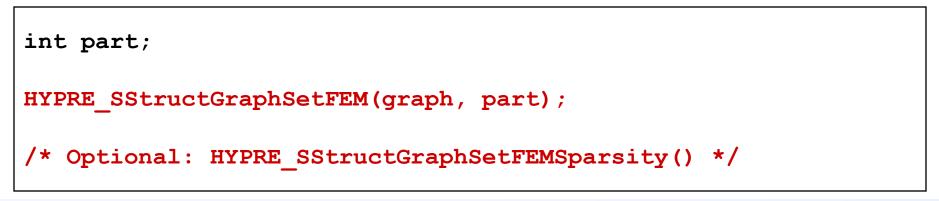
HYPRE\_SStructGraphCreate(MPI\_COMM\_WORLD, grid, &graph);



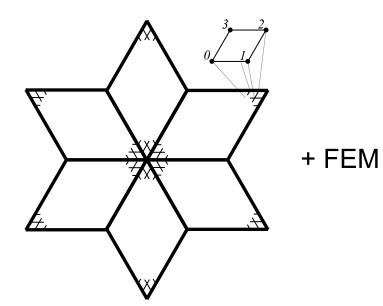


## Set FEM instead of stencils for each part

(Set nonzero pattern of local stiffness matrix)









/\* No need to add non-stencil entries
 \* with HYPRE SStructGraphAddEntries() \*/

HYPRE\_SStructGraphAssemble(graph);



### FEM example: Setting up the matrix and vector

- Matrix and vector values are set one element at a time
- For matrices, pass in local stiffness matrix values

```
int part = 0;
int index[2] = {i,j};
double values[16] = {...};
HYPRE_SStructMatrixAddFEMValues(A, part, index, values);
```

For vectors, pass in local variable values

```
double values[4] = {...};
HYPRE_SStructVectorAddFEMValues(v, 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		System Interfaces			
	Solvers	Struct	SStruct	FEI	IJ
Structured {	Jacobi	$\checkmark$	$\checkmark$		
	SMG	$\checkmark$	$\checkmark$		
	PFMG	$\checkmark$	$\checkmark$		
Semi-structured	Split		$\checkmark$		
	SysPFMG		$\checkmark$		
	FAC		$\checkmark$		
	Maxwell		$\checkmark$		
Sparse matrix	AMS, ADS		$\checkmark$	$\checkmark$	$\checkmark$
	BoomerAMG		$\checkmark$	$\checkmark$	$\checkmark$
	MLI		$\checkmark$	$\checkmark$	$\checkmark$
	ParaSails		$\checkmark$	$\checkmark$	$\checkmark$
	Euclid		$\checkmark$	$\checkmark$	$\checkmark$
	PILUT		$\checkmark$	$\checkmark$	$\checkmark$
Matrix free {	PCG	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
	GMRES	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
	BICGSTAB	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
	Hybrid	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$

# **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);
```

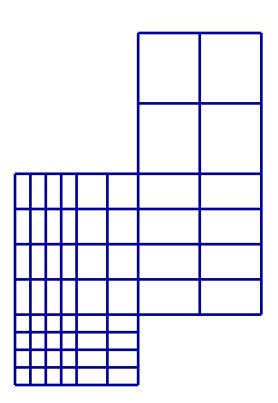
```
/* set preconditioner */
HYPRE_StructPCGSetPrecond(solver,
    HYPRE_StructSMGSolve, HYPRE_StructSMGSetup, precond);
```

```
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

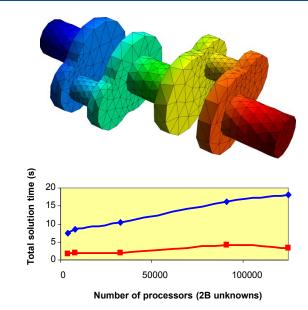


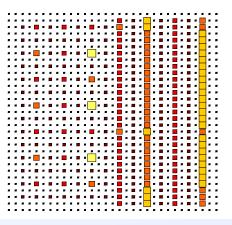
Constant-coefficient versions!



# 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





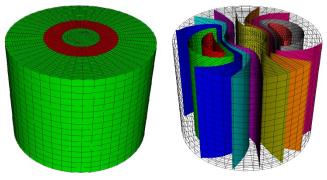


# AMS is an auxiliary space Maxwell solver for unstructured grids

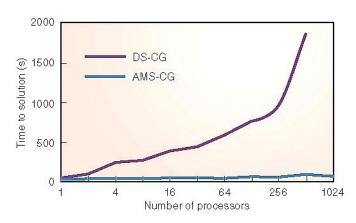
- Interface: SStruct, FEI, IJ
- Matrix Class: ParCSR
- Solves definite problems:

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

- 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<sup>6</sup>



#### 25x faster on 80M unknowns

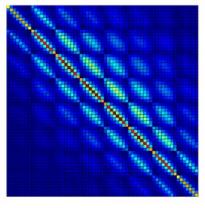


# ParaSAILS is an approximate inverse method for sparse linear systems

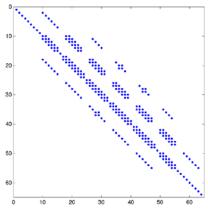
- Interface: SStruct, FEI, IJ
- Matrix Class: ParCSR

- 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**

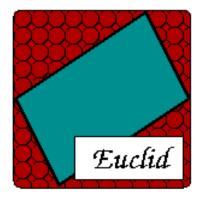


Approx inverse



# 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



## **Getting the code**

To get the code, go to

#### http://www.IInl.gov/CASC/hypre/

- User's / Reference Manuals can be downloaded directly
- A short form must be filled out (just for our own records)



## **Building the library**

- Usually, hypre can be built by typing configure followed by 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

Release includes example programs!

## 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, general usage questions

Send email to:

hypre-support@llnl.gov

 We use a tool called Roundup to automatically tag and track issues

## 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.

