HYPRE: High Performance Preconditioners

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

**Multigrid V-cycle**

- **Smoothing** (relaxation)
- **Restriction**
- **Prolongation** (interpolation)

Error on the fine grid

Error approximated on a smaller coarse grid

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)

- $m \times n$ 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**
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

\[
\begin{align*}
-\nabla^2 u &= f & \text{in the domain} \\
    u &= g & \text{on the boundary}
\end{align*}
\]
Structured-grid finite volume example:

Partition and distribute

Process 0

Process 1

Standard 5-point finite volume discretization

(-3,1)
Structured-grid finite volume example:
Setting up the grid on process 0

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

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 ilol[2] = {0,1};
int iupl[2] = {2,4};

HYPRE_StructGridSetExtents(grid, ilol, iupl);
```
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)

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

HYPRE_StructStencileCreate(ndim, size, &stencil);
```
Structured-grid finite volume example:
Setting up the stencil (all processes)

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

HYPRE_StructStencilSetElement(stencil, entry, offset);
```
Structured-grid finite volume example:
Setting up the stencil (all processes)

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

HYPRE_StructStencilSetElement(stencil, entry, offset);
```
Structured-grid finite volume example:
Setting up the stencil (all processes)

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

HYPRE_StructStencilSetElement(stencil, entry, offset);
```
Structured-grid finite volume example:
Setting up the stencil (all processes)

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

HYPRE_StructStencilsSetElement(stencil, entry, offset);
```
Structured-grid finite volume example:
Setting up the stencil (all processes)

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

HYPRE_StructStencilSetElement(stencil, entry, offset);
```
Structured-grid finite volume example:
Setting up the stencil (all processes)

That’s it!
There is no assemble routine
Structured-grid finite volume example:
Setting up the matrix on process 0

```
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 */
```

```c
S4
S1  S0  S2
S3
```

\[
\begin{pmatrix}
S4 \\
S1 & S0 & S2 \\
S3
\end{pmatrix} = 
\begin{pmatrix}
-1 \\
-1 & 4 & -1 \\
-1
\end{pmatrix}
\]
Structured-grid finite volume example:
Setting up the matrix bc’s on process 0

```c
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 */
...```

The diagram shows the coefficients for the matrix, including:

- `S4` with coefficients `-1` and `-1`.
- `S1` with coefficients `-1` and `4`.
- `S2` with coefficients `-1` and `0`.
- `S3` with coefficients `-1` and `4`.

The boundary conditions are set using the `HYPRE_StructMatrixSetBoxValues` function with the specified indices and values.
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);
```
Some solvers support symmetric storage.

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

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

For best efficiency, only set half of the coefficients:

\[
\begin{pmatrix}
0,1 \\
0,0 & 1,0
\end{pmatrix}
\leftrightarrow
\begin{pmatrix}
S2 \\
S0 & S1
\end{pmatrix}
\]

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
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 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**
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)

- We consider the interface calls made by process 3
Block-structured grid example:
Setting up the grid on process 3

```
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

```
int part = 3;
int ilower[2] = {1,1};
int iupper[2] = {4,4};

HYPRE_SStructGridSetExtents(grid, part, ilower, iupper);
```
Block-structured grid example:
Setting up the grid on process 3

```
int part, nvars = 3;
int vartypes[3] = {HYPRE_SSTRUCT_VARIABLE_CELL,
                   HYPRE_SSTRUCT_VARIABLE_XFACE,
                   HYPRE_SSTRUCT_VARIABLE_YFACE};

HYPRE_SStructGridSetVariables(grid, part, nvars, vartypes);
```
Block-structured grid example:
Setting up the grid on process 3

Set spatial relationship between parts 3 and 2

```c
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);
```
Block-structured grid example:
Setting up the grid on process 3

Set spatial relationship between parts 3 and 4

```
int part = 3, nbor_part = 4;
int ilower[2] = {0,1}, iupper[2] = {0,4};
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);
```
Block-structured grid example:
Setting up the grid on process 3

Assemble the grid

HYPRE_SStructGridAssemble(grid);
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).
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.
Block-structured grid example:
Setting up the graph on process 3

HYPRE_SStructGraph graph;

HYPRE_SStructGraphCreate(MPI_COMM_WORLD, grid, &graph);
Block-structured grid example:
Setting up the graph on process 3

Set the cell-centered stencil for each part

```c
int part;
int var = 0;
HYPRE_SStructStencil cell_stencil;

HYPRE_SStructGraphSetStencil(graph, part, var, cell_stencil);
```
Block-structured grid example:
Setting up the graph on process 3

Set the x-face stencil for each part

```c
int part;
int var = 1;
HYPRE_SStructStencil xStencil;

HYPRE_SStructGraphSetStencil(graph, part, var, xStencil);
```
Block-structured grid example:
Setting up the graph on process 3

Set the y-face stencil for each part

```c
int part;
int var = 2;
HYPRE_SStructStencils y_stencil;

HYPRE_SStructGraphSetStencils(graph, part, var, y_stencil);
```
Block-structured grid example:
Setting up the graph on process 3

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 \texttt{Struct} interface

- Matrix coefficients are set with the routines
  - \texttt{HYPRE_SStructMatrixSetValues()}
  - \texttt{HYPRE_SStructMatrixAddToValues()}

- Vector values are set with similar routines
  - \texttt{HYPRE_SStructVectorSetValues()}
  - \texttt{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

\[
\begin{align*}
\n-\nabla^2 u &= 1 \quad \text{in } \Omega \\
u &= 0 \quad \text{on } \Gamma
\end{align*}
\]

- FEM stiffness matrix

\[
\begin{pmatrix}
0 & 1 & 2 & 3 \\
0 & 4-k & -1 & -2+k & -1 \\
1 & -1 & 4+k & -1 & -2-k \\
2 & -2+k & -1 & 4-k & -1 \\
3 & -1 & -2-k & -1 & 4+k
\end{pmatrix} \alpha
\]

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

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).
- We consider the interface calls made by process 0.
FEM example: Setting up the grid on process 0

Create the grid object

HYPRE_SStructGrid grid;
int ndim   = 2;
int nparts = 6;

HYPRE_SStructGridCreate(MPI_COMM_WORLD, ndim, nparts, &grid);
FEM example: Setting up the grid on process 0

```
int part = 0;
int ilower[2] = {1,1};
int iupper[2] = {9,9};

HYPRE_SStructGridSetExtents(grid, part, ilower, iupper);
```
**FEM example:** Setting up the grid on process 0

```
int part;
int nvars = 1;
int vartypes[3] = {HYPRE_SSTRUCT_VARIABLE_NODE};

HYPRE_SStructGridSetVariables(grid, part, nvars, vartypes);
```

Set grid variables for each part
**FEM example: Setting up the grid on process 0**

Set FEM ordering of variables on part 0

```c
int part = 0;
int ordering[12] = { 0, -1, -1,
                     0, +1, -1,
                     0, +1, +1,
                    0, -1, +1 };

HYPRE_SStructGridSetFEMOrdering(grid, part, ordering);
```
**FEM example:** Setting up the grid on process 0

```c
int part = 0, spart = 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);
```
**FEM example:** Setting up the grid on process 0

```c
int part = 0, spart = 5;
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);
```
FEM example: Setting up the grid on process 0

```c
int part = 0, spart = 2;
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);
```
**FEM example:** Setting up the grid on process 0

```c
int part = 0, spart = 3;
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);
```
FEM example: Setting up the grid on process 0

Set shared variables for parts 0 and 4

```
int part = 0, spart = 4;
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);
```
**FEM example:** Setting up the grid on process 0

HYPRE_SStructGridAssemble(grid);

Assemble the grid
FEM example: Setting up the graph on process 0

Create the graph object

HYPRE_SStructGraph graph;

HYPRE_SStructGraphCreate(MPI_COMM_WORLD, grid, &graph);
FEM example: Setting up the graph on process 0

Set FEM instead of stencils for each part
(Set nonzero pattern of local stiffness matrix)

```c
int part;

HYPRE_SStructGraphSetFEM(graph, part);

/* Optional: HYPRE_SStructGraphSetFEMSparsity() */
```
FEM example: Setting up the graph on process 0

Assemble the graph

/* 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

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

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

- For vectors, pass in local variable values

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

- After `Assemble()`, call:
  ```c
  HYPRE_SStructMatrixGetObject(A, &parcsr_A);
  ```

- Now, use the ParCSR matrix with compatible solvers such as BoomerAMG (algebraic multigrid)
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Setup and use of solvers is largely the same (see Reference Manual for details)

- Create the solver
  
  ```c
  HYPRE_SolverCreate(MPI_COMM_WORLD, &solver);
  ```

- Set parameters
  
  ```c
  HYPRE_SolverSetTol(solver, 1.0e-06);
  ```

- Prepare to solve the system
  
  ```c
  HYPRE_SolverSetup(solver, A, b, x);
  ```

- Solve the system
  
  ```c
  HYPRE_SolverSolve(solver, A, b, x);
  ```

- Get solution info out via system interface
  
  ```c
  HYPRE_StructVectorGetValues(struct_x, index, values);
  ```

- Destroy the solver
  
  ```c
  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:** \texttt{SStruct}, \texttt{FEI}, \texttt{IJ}
- **Matrix Class:** \texttt{ParCSR}
- Solves definite problems:
  \[ \nabla \times \alpha \nabla \times E + \beta E = f, \quad \alpha > 0, \beta \geq 0 \]
- 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 $M$
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.llnl.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 *hype* from Fortran

- **C code:**

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

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

- **Corresponding Fortran code:**

```fortran
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!

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