New Advances in *hypre* 3.0 for Mixed Precision and Semi-Structured Problems

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CASC
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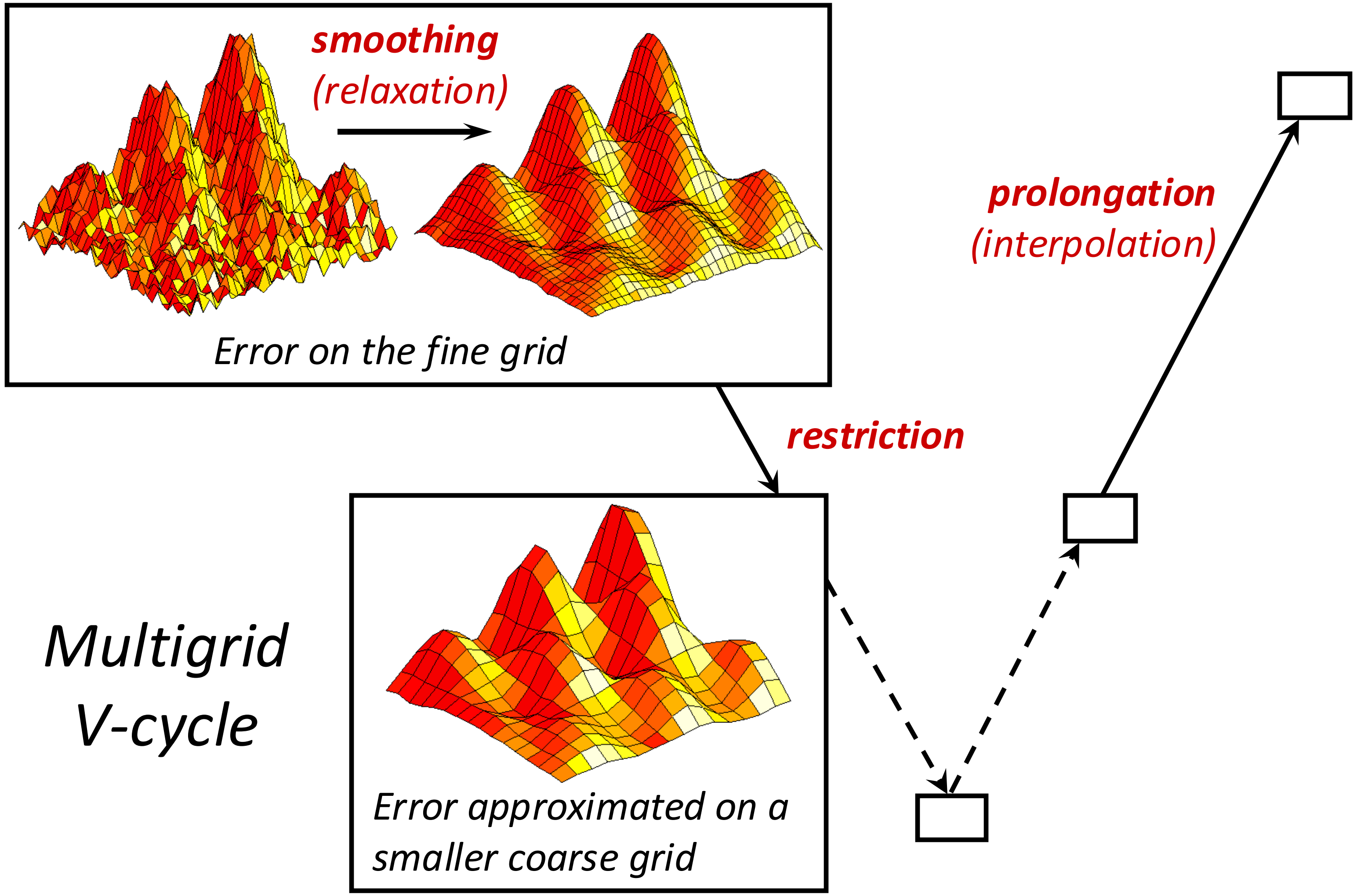
Multigrid (MG) is among the fastest and most scalable linear solvers
– uses a sequence of coarse grids to accelerate the fine grid solution

Multigrid V-cycle

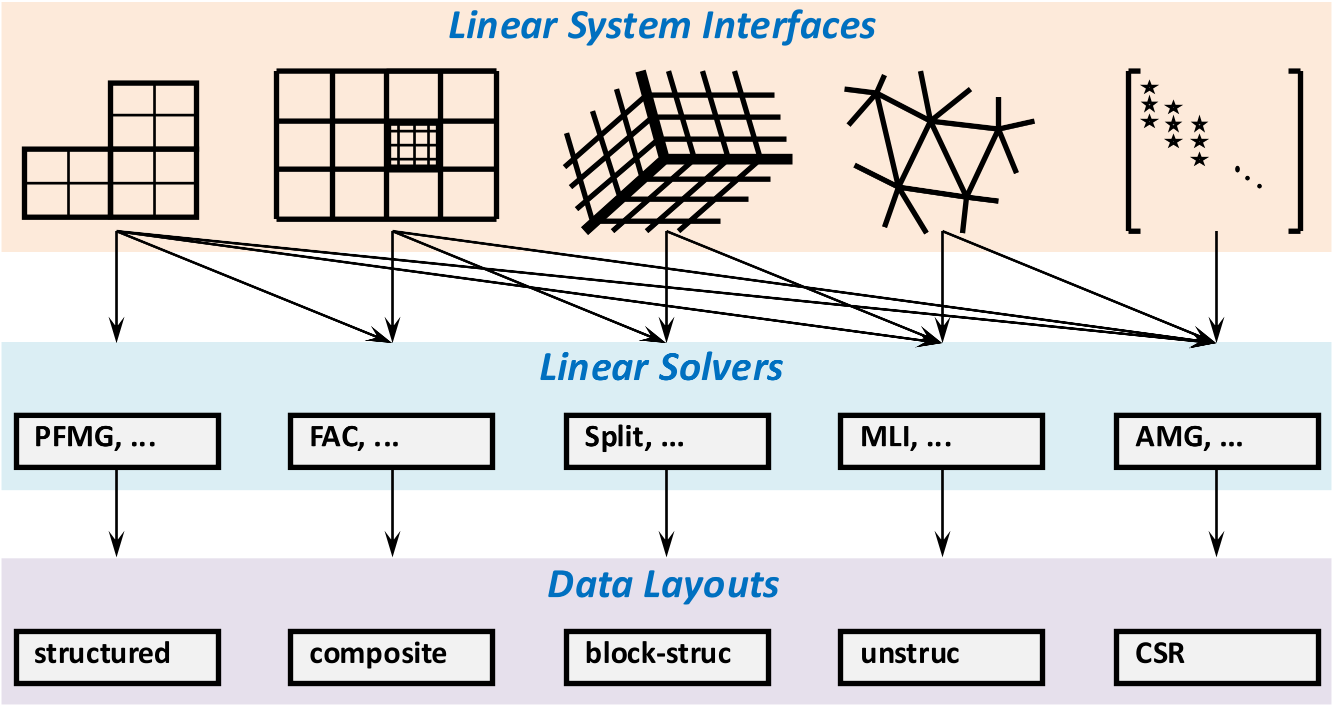


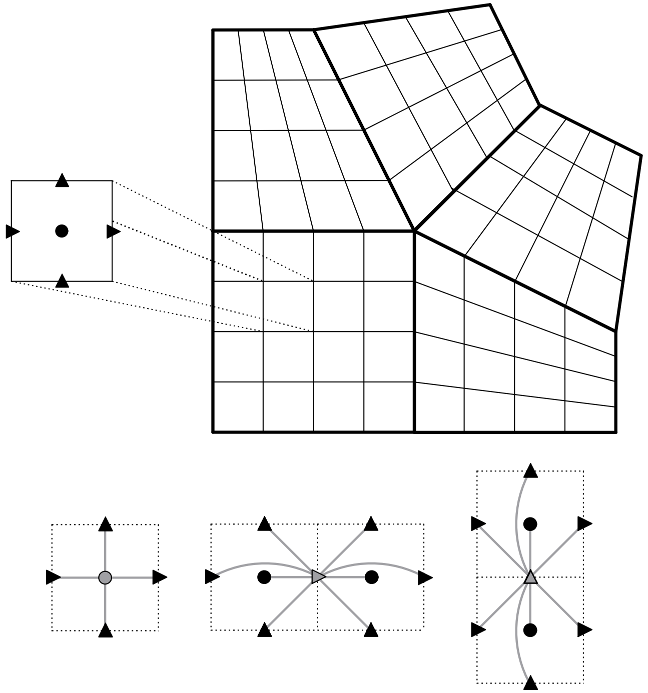
hypre

Widely used at LLNL, the DOE, and around the world

- Scalable, $O(N)$
- Many algorithms
- Geometric / algebraic
- Linear / nonlinear
- Math & CS research

Unique software interfaces in *hypre* enable more efficient solvers, kernels, and storage



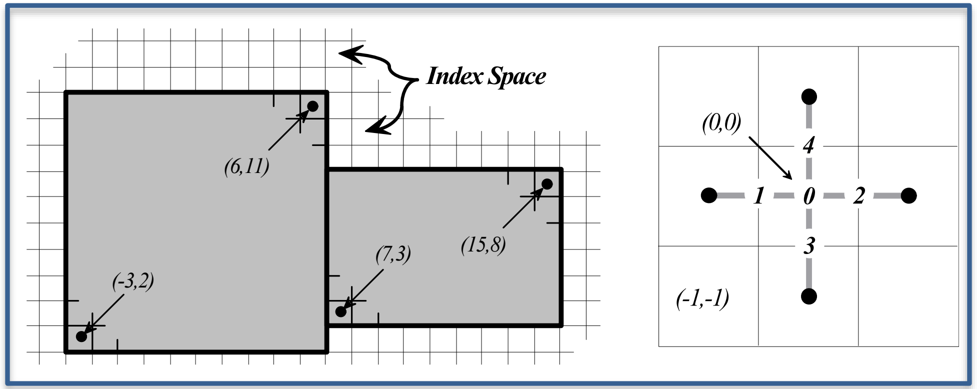


Block-structured grid with 3 variable types and 3 discretization stencils

- Example: *hypre*'s interface for semi-structured grids
  - Based on "grids" and either "stencils" or "finite elements"
  - Allows for specialized solvers for semi-structured problems
  - Also provides for more general solvers like AMG

There are three matrix object types (data structures) in *hypre*

- Struct matrix
  - Grid (list of boxes)
  - Stencil
  - Data array
  - Optimizations for constant coefficients and symmetric



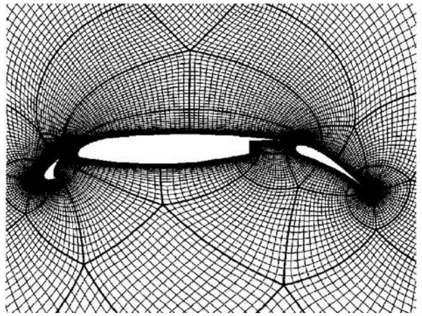
- ParCSR matrix
  - Two CSR matrices (diag, offd)
  - Mapping for off-proc connections

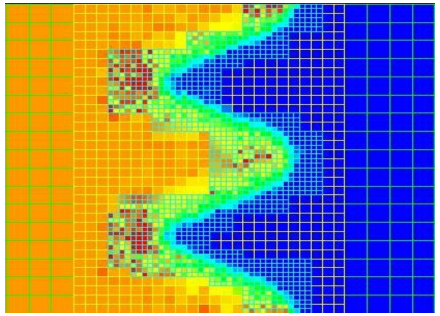
Row Pointer: $[i_0, i_1, i_2, \ldots, i_{Nrows}]$

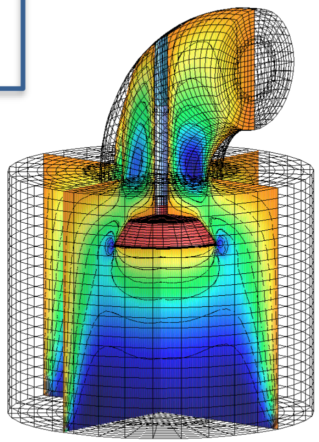
Column Indices: $[j_0, j_1, j_2, \ldots, j_{NNZ}]$

Data: $[a_0, a_1, a_2, \ldots, a_{NNZ}]$

- SStruct (semi-struct) matrix
  - Struct matrices for each part
  - ParCSR matrix for part connections

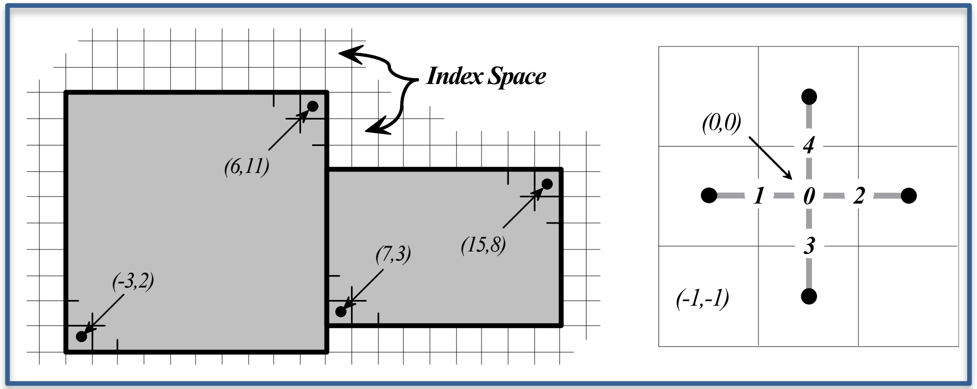




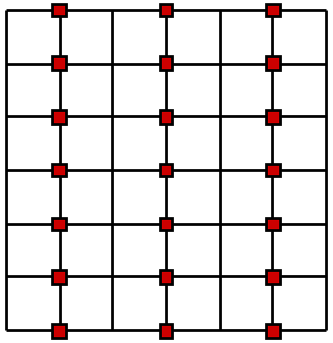


(S)Struct multigrid solver development in *hypre* has been hampered by limited matrix-vector tools

- (S)Struct matrices must be square
  - Struct matrix uses a stencil applied to a single grid
  - SStruct matrix depends on Struct: $A = A_s + A_u$
  - Matrix-vector multiply (Matvec) is only for square matrices
  - Matrix-matrix multiply (Matmat) is not available



- Struct solvers
  - SMG: semi-coarsening with plane/line smoothing
  - PFMG: semi-coarsening with point smoothing
  - Interpolation and coarse-grid operators are hard-coded for specific stencil cases



- SStruct (semi-structured) solvers
  - Split SMG/PFMG: approximate block Jacobi with SMG/PFMG on each part
  - True multigrid solvers are difficult to implement!

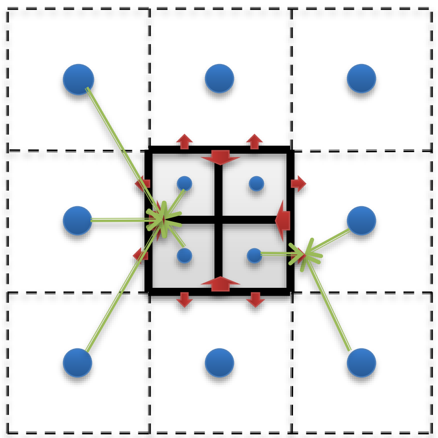
Overhaul of (S)Struct code in hypre-3.0 enhances matrix-vector tools and provides new SStruct solver SSAMG

- Matmat and Matvec are key kernels, but they often involve rectangular matrices
  - E.g., Interpolation/restriction, RAP in multigrid, RAP in AMR interface

- Matrix-vector class has been extended beyond square matrices (also added Matmat)
  - Implementation supports both variable and constant-coefficients (and combinations)
  - Struct matrix still based on stencils, but with domain/range grids
  - Simplifies implementation of multigrid algorithms and AMR interface
  - Centralizes code optimization to a few core routines (but optimization is trickier)
  - Allows for faster solvers – implemented semi-structured AMG (SSAMG) algorithm

- (S)Struct re-design began in about 2014
  - hypre-3.0 release was in September 2025
  - It's been a long process

- Longer term work
  - Additional solver updates (SMG, PFMG extensions, etc.)
  - Finish implementing an AMR interface



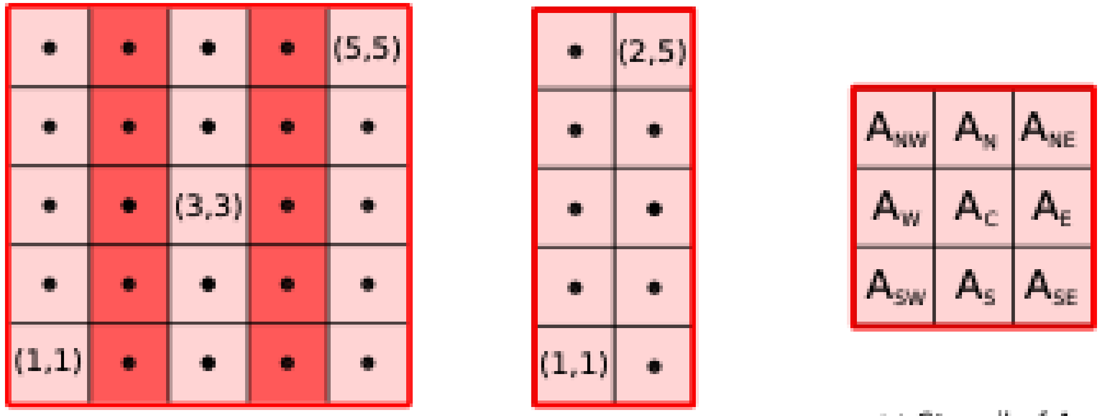
- hypre-3.0 was the first major release since hypre-2.0 in December of 2006!

Struct rectangular matrices are also based on stencils and grids but extend the current implementation

- Matrices have a domain and range grid where each coarsens a common base grid
- Matrix stencils act on an index space that is the same or finer than either grid
  - The stencil grid need not be the same as the base grid (currently they are the same)
  - Either the matrix or its transpose must be representable by a single “range stencil”
- Example: Interpolation in PFMG (semi-coarsened coarse grid in x)

$$
\begin{aligned}
P &\sim [P_W \quad 1 \quad P_E]_c \\
&= [P_W \quad * \quad P_E]_c^{r_\mathrm{f}} \oplus [* \quad 1 \quad *]_c^{r_\mathrm{c}}
\end{aligned}
$$

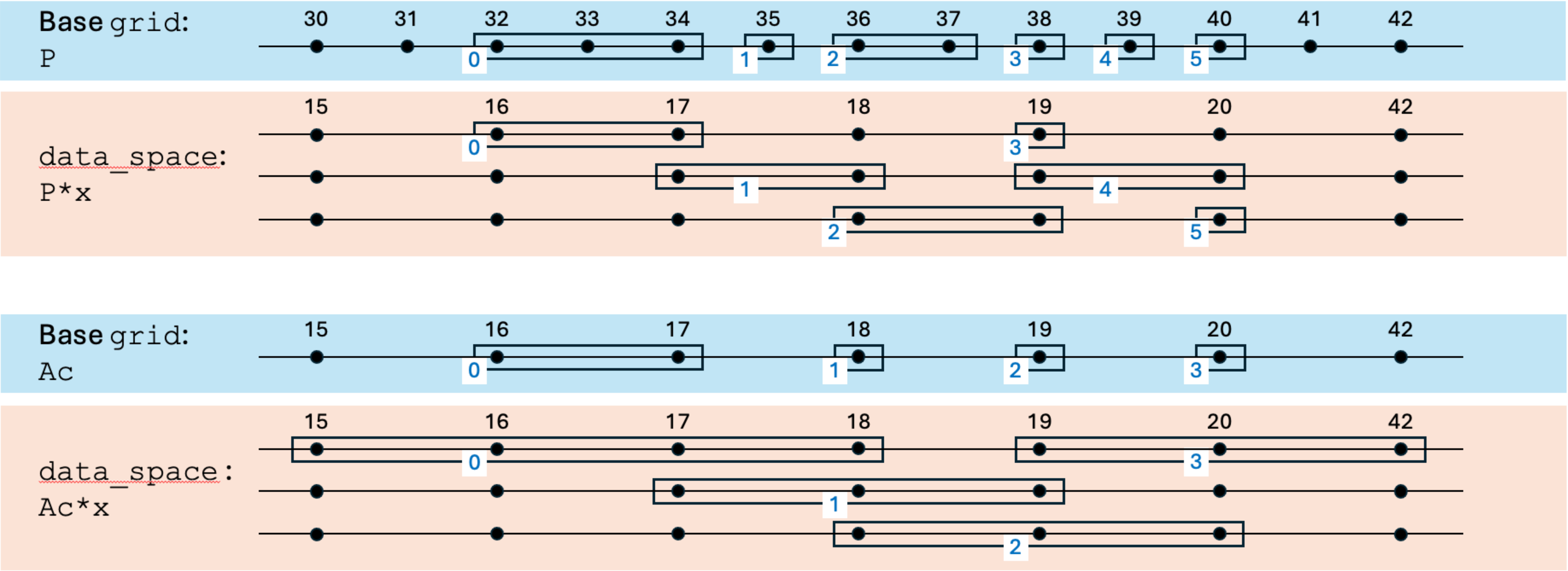
$$
\begin{aligned}
(P\boldsymbol{u})_{i,j} &= P_W u_{i-1,j} + P_E u_{i+1,j}\,, & (i,j) \in r_\mathrm{f} \\
(P\boldsymbol{u})_{i,j} &= u_{i,j}\,, & (i,j) \in r_\mathrm{c}
\end{aligned}
$$



(a) Fine grid (b) Coarse grid (c) Stencil of A centered at (3,3)

Struct Matvec uses ghost zones for communication – these are now determined automatically

- Ghost zone size for a vector $\boldsymbol{x}$ depends on how it's used – hard for users to specify
  - Example: Matvec with two different matrices P and A_c in multigrid



Struct Matmat also produces a stencil-based matrix with constant/variable coefficients

- Stencil algebra determines the product stencil and equations for computing its entries
  - Use the fact that $stencil(AB) = B^T stencil(A)$

$$ABC = \begin{bmatrix} X_{i,j}^{-1,1} & X_{i,j}^{0,1} & X_{i,j}^{1,1} \\ X_{i,j}^{-1,0} & X_{i,j}^{0,0} & X_{i,j}^{1,0} \\ X_{i,j}^{-1,-1} & X_{i,j}^{0,-1} & X_{i,j}^{1,-1} \end{bmatrix}, \qquad X_*^* = \sum a_*^* \, b_*^* \, c_*^*$$

- Assume 2 “data spaces”, compute necessary ghost zones, aggregate communication, use mask if needed for constant coefficient stencil entries, unroll kernel loops
- Kernel – write $abc = \alpha \, v_1 v_2 v_3$ where
  - the constant α is 1x the product of the constant coefficient entries in $\{a, b, c\}$ (if any)
  - the v_i associated with each constant coefficient entry is set to a $mask = \{0, 1\}$
  - each v_i is associated with one of possibly two ”data spaces” → 3 cases to implement in 3D
- Symmetric matrices – store and compute only “half” of the entries

Struct Matmat currently has two kernel implementations

- Loop unrolling works well on CPUs – matches current hardcoded $P^T A\ P$ code

$$X_i \mathrel{+}= \sum \alpha v_1 v_2 v_3$$

- Loop fusion is better for GPUs – fewer kernel launches

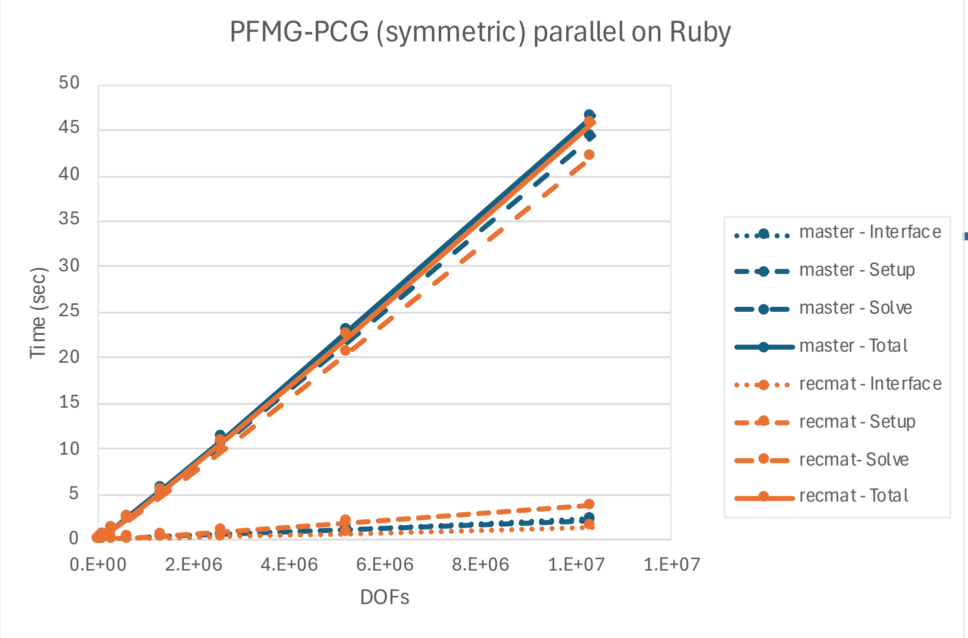
$$X_1 \mathrel{+}= \alpha v_1 v_2 v_3$$
$$X_2 \mathrel{+}= \alpha v_1 v_2 v_3$$
$$\ldots$$

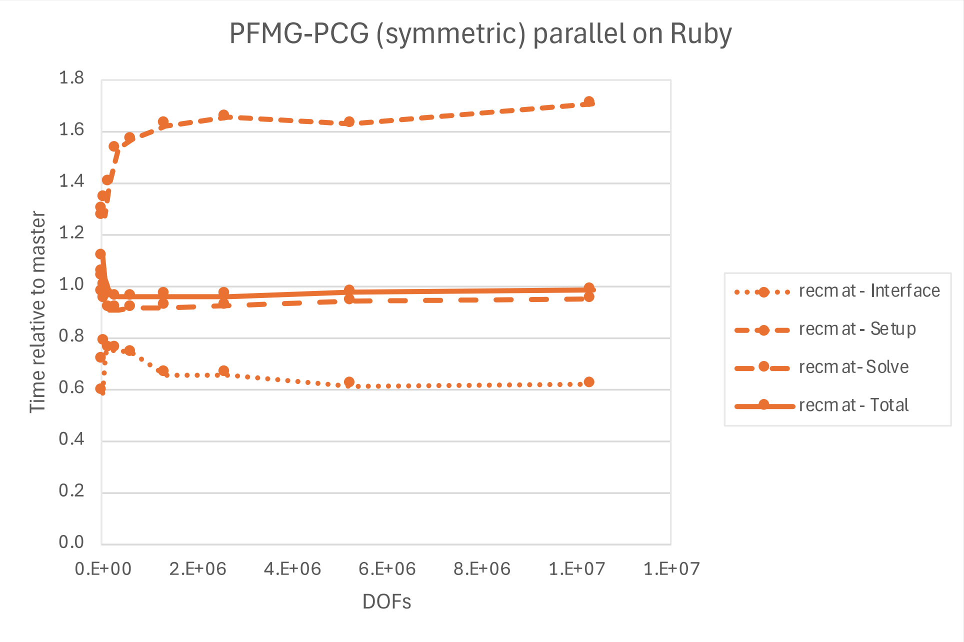
Performance optimizations in Struct

- Optimizations to bring performance in line with main branch
  - Matvec and Matmat loop unrolling
  - Smarter handling of ghost zone resizing
  - Support for symmetric matrices in mat-mat

- PFMG optimizations Jan-Apr 2025
  - Improved setup by 3.8x
  - Improved solve by 1.8x
  - Total times are now slightly faster than master

- Ruby at LLNL
  - Intel Supermicro Zeon
  - 85,568 cores = 1512 nodes * 56 cores/node
  - #310 on June Top 500, 3.7 PFlops/s LINPACK



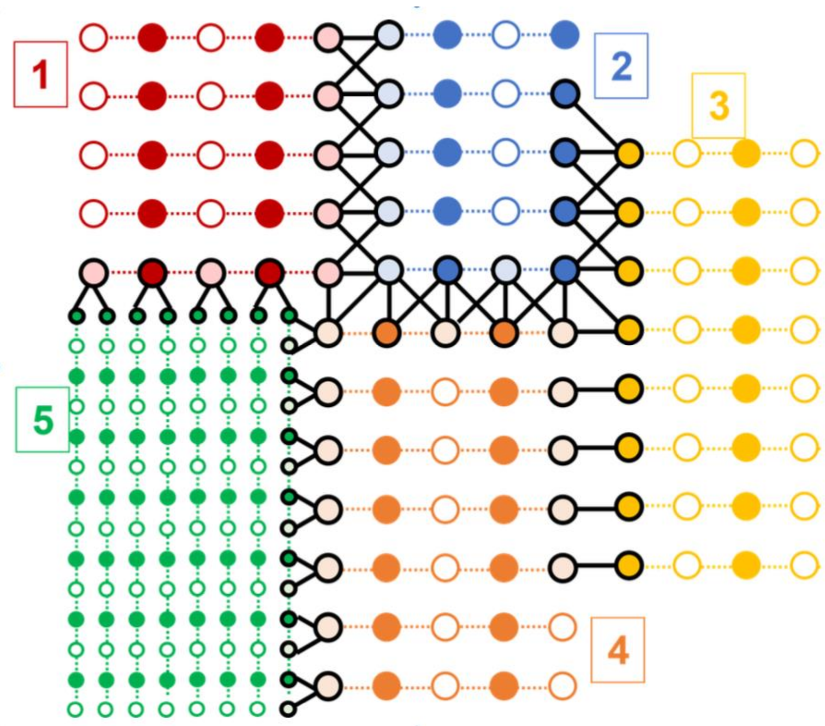


Semi-structured algebraic multigrid (SSAMG) combines the structured PFMG solver with BoomerAMG

- Structured behavior within parts (PFMG)
  - Semi-coarsening
  - Operator-based, two-point structured interpolation
- Unstructured behavior at part boundaries
  - One-sided structured interpolation: $P = P_s$
  - Full interpolation (WIP) can greatly improve convergence (e.g., 7 iterations instead of 20): $P = P_s + P_u$
- Galerkin coarse-grid operator

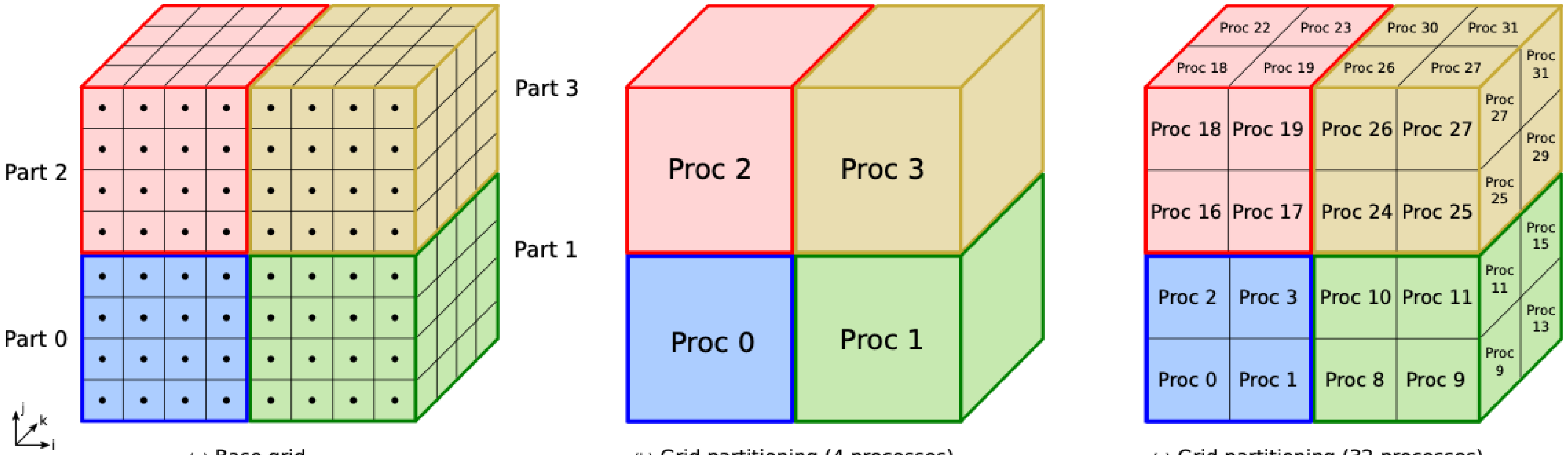
$$P^T A P = (P_s + P_u)^T (A_s + A_u)(P_s + P_u)$$

  - Rectangular structured mat-mats
  - Need to multiply Struct and ParCSR matrices
- BoomerAMG as coarsest-grid solver
  - Workhorse multigrid solver (uses ParCSR)
  - Variation of classical AMG



Numerical results show qualitatively similar results to earlier work but with improved performance

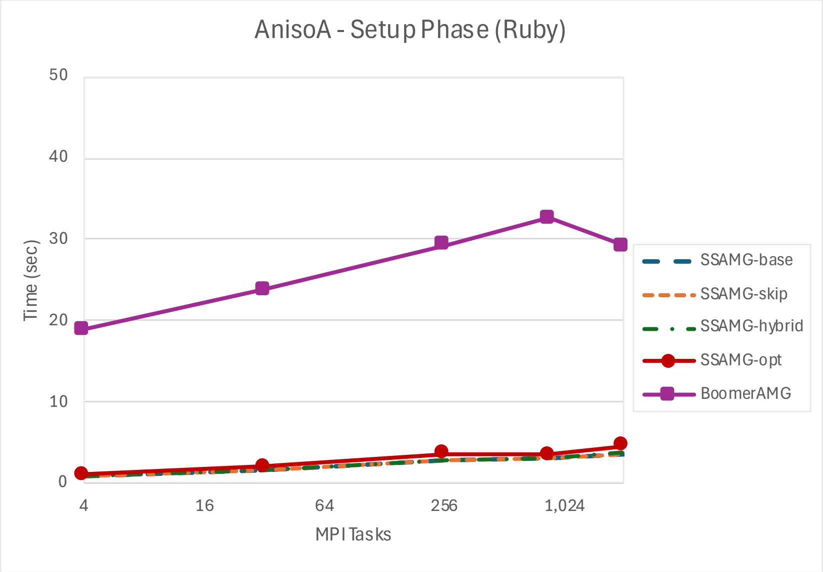
- 3D cubic grid with four parts, 128 x 128 x 128 grid per MPI task
- Three scenarios (A, B, C) of anisotropies in each part
- Discretization stencil: $A \sim [-\gamma] \begin{bmatrix} & -\beta & \\ -\alpha & 2(\alpha+\beta+\gamma) & -\alpha \\ & -\beta & \end{bmatrix} [-\gamma]$

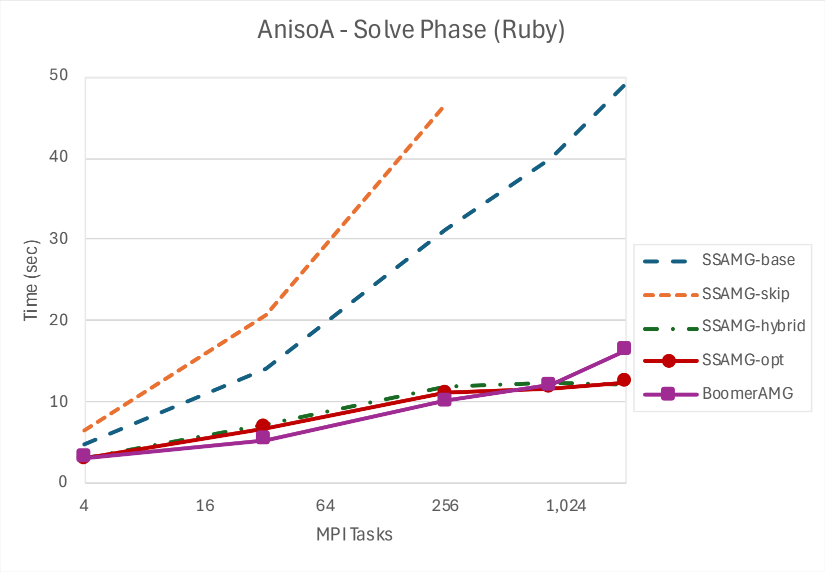


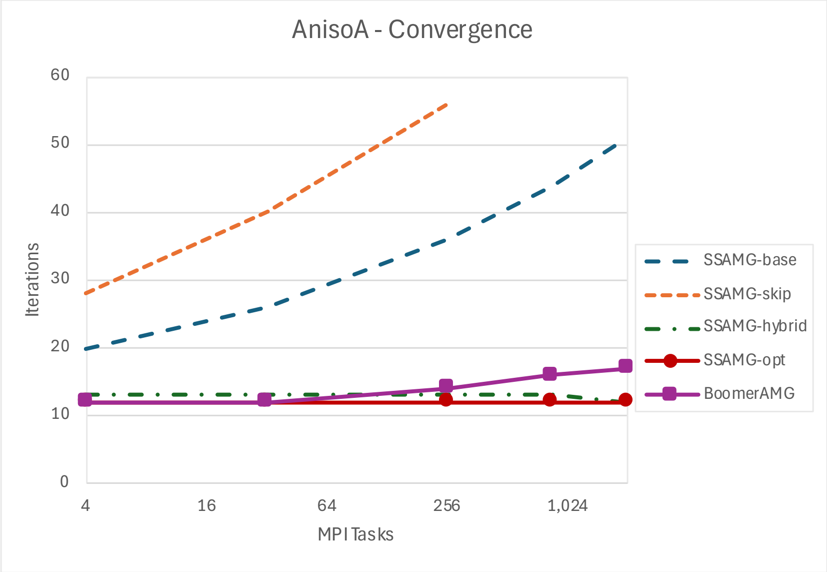
(a) Base grid (b) Grid partitioning (4 processes) (c) Grid partitioning (32 processes)

1. Magri, Falgout, Yang, "A new semi-structured algebraic multigrid method", *SIAM J. Sci. Comput.* (2023)

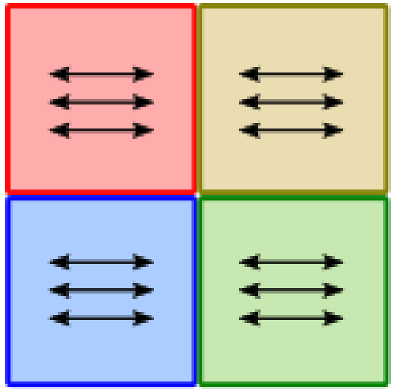
Results (A) – SSAMG Setup is more than 7x faster than AMG





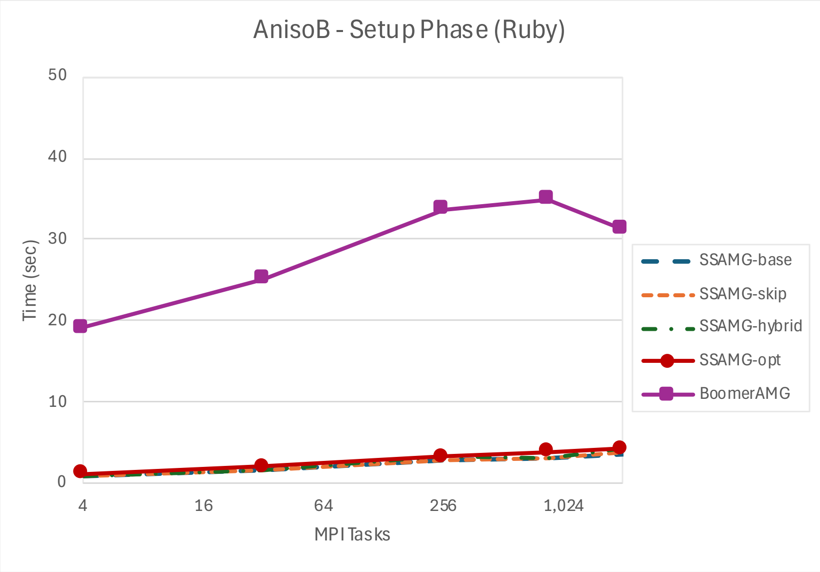


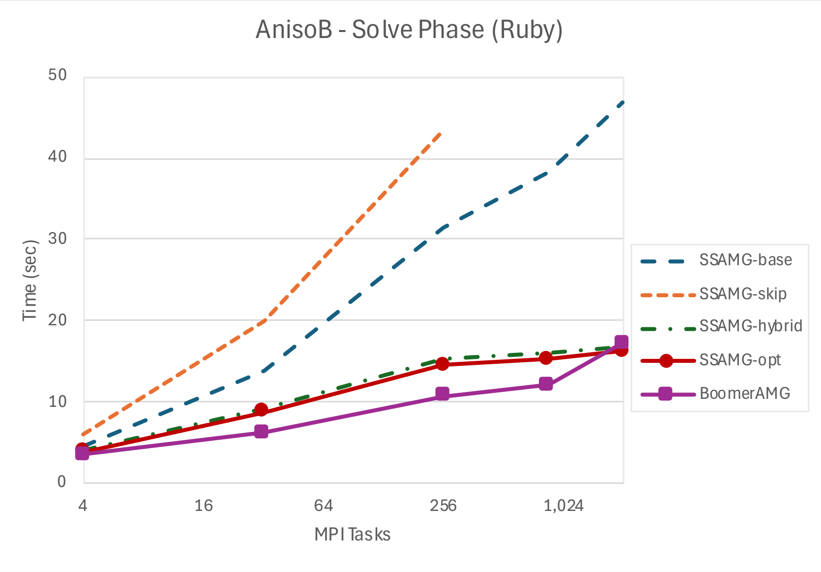
- Solvers:
  - SSAMG-base – L1 Jacobi smoother, $\omega = 3/2$
  - SSAMG-skip – SSAMG-base with skip-relaxation option
  - SSAMG-hybrid – switch to BoomerAMG on level 10
  - SSAMG-opt – switch to BoomerAMG on level 7
  - BoomerAMG – one level aggressive coarsening, L1 GS, $\theta = 0.25$, ext+i interpolation

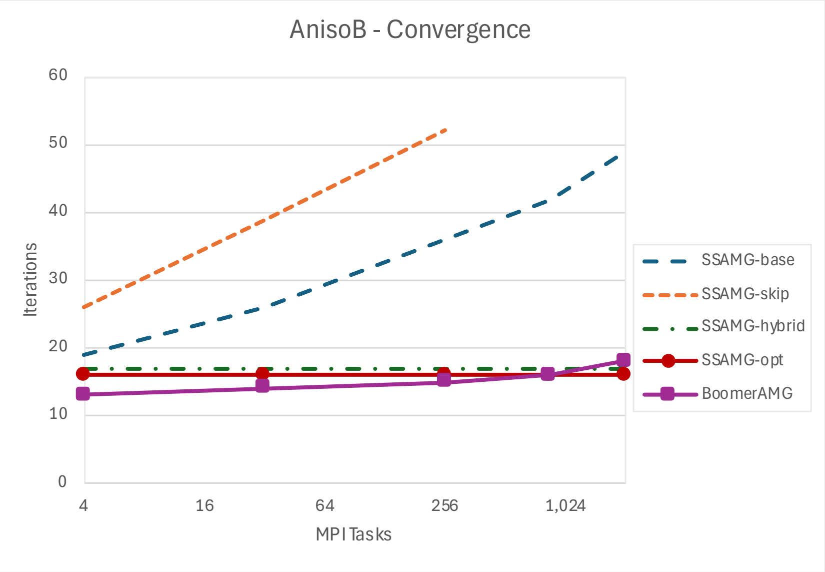


1. Magri, Falgout, Yang, "A new semi-structured algebraic multigrid method", *SIAM J. Sci. Comput.* (2023)

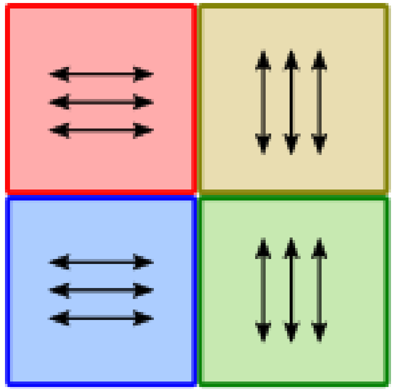
Results (B) – SSAMG Setup is more than 7x faster than AMG





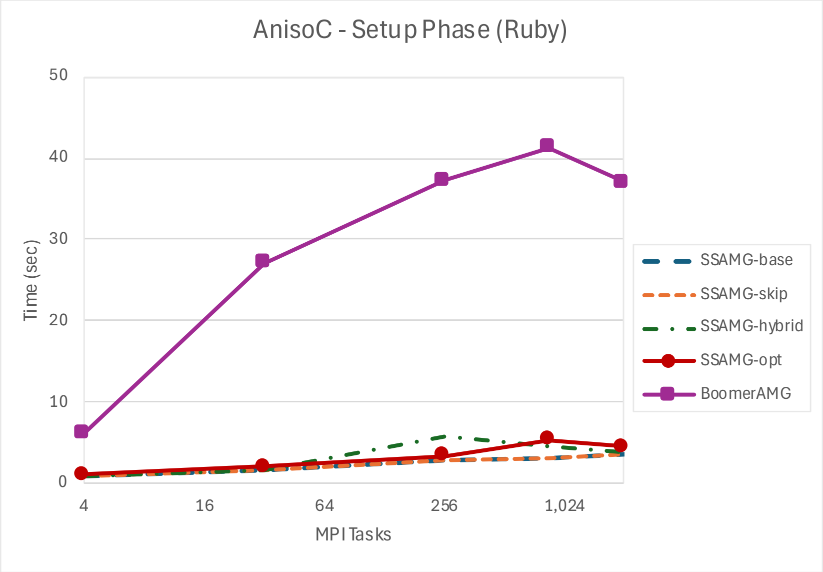


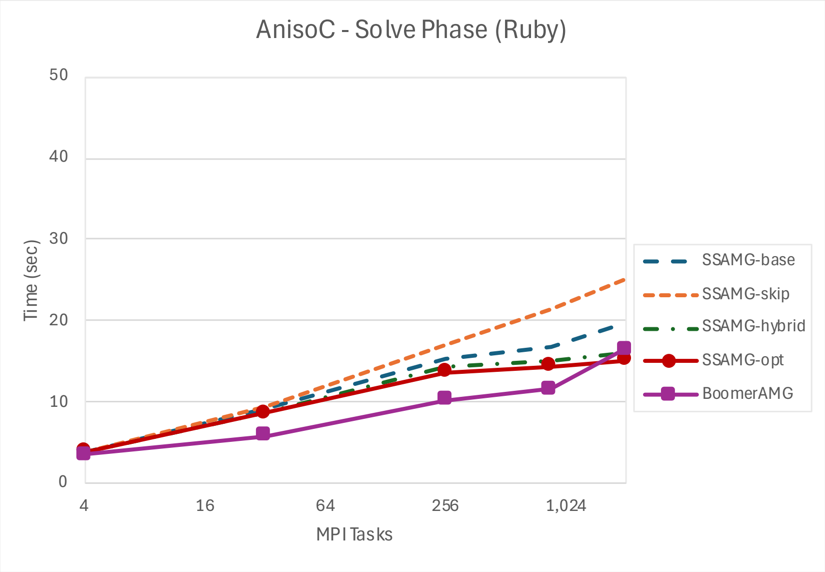
- Solvers:
  - SSAMG-base – L1 Jacobi smoother, $\omega = 3/2$
  - SSAMG-skip – SSAMG-base with skip-relaxation option
  - SSAMG-hybrid – switch to BoomerAMG on level 10
  - SSAMG-opt – switch to BoomerAMG on level 7
  - BoomerAMG – one level aggressive coarsening, L1 GS, $\theta = 0.25$, ext+i interpolation

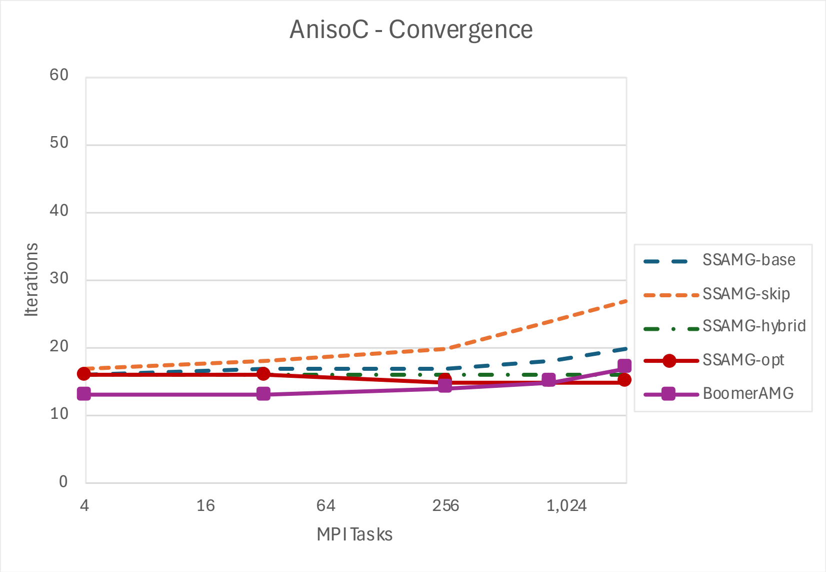


1. Magri, Falgout, Yang, "A new semi-structured algebraic multigrid method", *SIAM J. Sci. Comput.* (2023)

Results (C) – SSAMG Setup is more than 6x faster than AMG

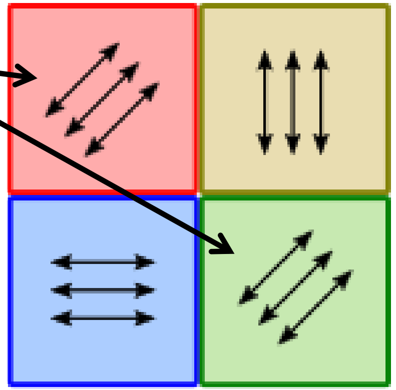






- Solvers:
  - SSAMG-base – L1 Jacobi smoother, $\omega = 3/2$
  - SSAMG-skip – SSAMG-base with skip-relaxation option
  - SSAMG-hybrid – switch to BoomerAMG on level 10
  - SSAMG-opt – switch to BoomerAMG on level 7
  - BoomerAMG – one level aggressive coarsening, L1 GS, $\theta = 0.25$, ext+i interpolation

Anisotropic in z



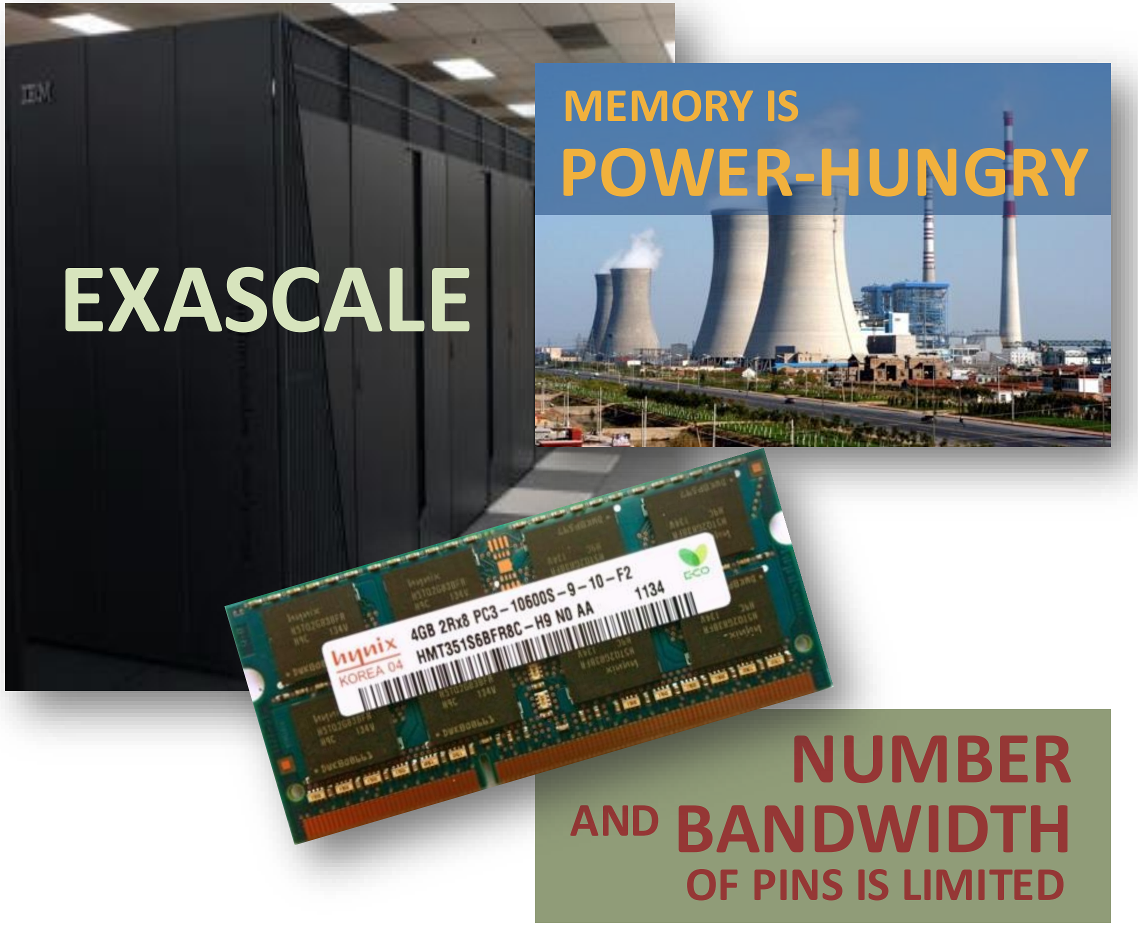
1. Magri, Falgout, Yang, "A new semi-structured algebraic multigrid method", *SIAM J. Sci. Comput.* (2023)

Mixed Precision

Mixed precision solver development is driven by several factors

- HPC support for low precision arithmetic
  - Single (or lower) precision can be more than 2x faster
  - Tensor core hardware on NVIDIA GPUs

- Data motion and memory capacity are becoming limiting factors in HPC
  - Better bandwidth utilization



Mixed precision in hypre-3.0 has several goals and features

- Terminology
  - multiprecision – a solver, function, or feature that uses one precision at a time
  - mixed precision – a solver, function, or feature that uses different precisions simultaneously
- Mixed precision is primarily intended to
  - provide multiple precisions at runtime
  - provide faster and more memory efficient mixed-precision solvers
- Features include
  - User code runs as before without requiring modification
  - All compile-time precisions are available at runtime
  - Precision can be set globally at runtime and requires minimal changes to user code
  - [Future] Precision of objects (e.g., matrices) determines the precision of related methods (e.g., `Matvec`)
  - Mixed precision solvers are available

HYPRE provides runtime multiprecision and mixed precision capabilities with minimal impact on users

- Multiprecision has been available for many years

```
--enable-single        (autotools)
-DHYPRE_SINGLE=ON      (CMake)
```

- With hypre-3.0: multiprecision and mixed precision are available at runtime

```
--enable-mixed-precision.          (autotools)
-DHYPRE_ENABLE_MIXED_PRECISION=ON  (CMake)
```

- Users can turn on mixed precision without changing code
  - Code will compile and run as before
- Several levels of support for using runtime precision
  - Code changes required

Runtime precision is available in several ways

- Every function `Foo` in hypre (e.g., `HYPRE_PCGSolve`) is available in fixed precision

`Foo_flt`	(precision in C = `float`)
`Foo_dbl`	(precision in C = `double`)
`Foo_long_dbl`	(precision in C = `long double`)

- Prototypes are the same as before except for real types
  – `HYPRE_Real` maps to specific C types (e.g., `float` for function `Foo_flt`)

- Every user-API function `Foo` has precision determined (globally) by
  – `HYPRE_Int HYPRE_SetGlobalPrecision(HYPRE_Precision precision)`
  – where `precision` has value `HYPRE_REAL_DOUBLE` for example (default value is set at configuration time by the user)

- Prototypes for `Foo` are different because they need to support all precisions
  – Scalar `HYPRE_Real` becomes `long double`, while array `HYPRE_Real*` becomes `void*`
  – No casting is necessary, but care is needed to manage arrays

- Function `Foo_pre(precision, …)` is useful for writing mixed precision code

Test driver `sstruct` illustrates use of runtime multiprecision (example drivers are to come)

- Additional `-precision` argument switches the global runtime precision

```
> sstruct -in TEST_sstruct/sstruct.in.cube -precision 0
...
Iterations = 4
Final Relative Residual Norm = 2.187087e-07
```

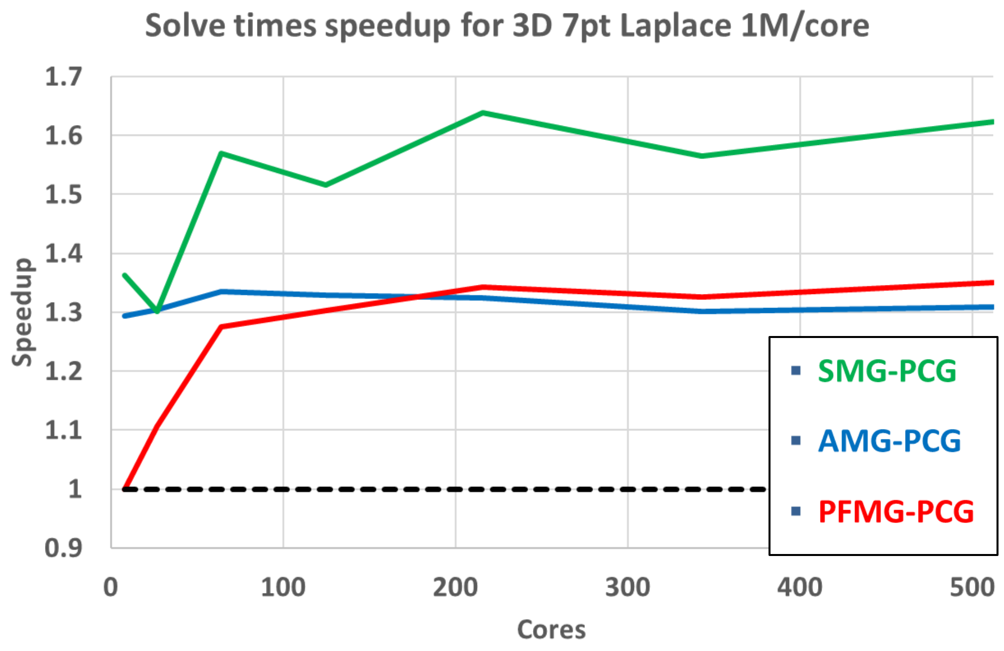
```
> sstruct -in TEST_sstruct/sstruct.in.cube -precision 1
...
Iterations = 4
Final Relative Residual Norm = 5.459331e-16
```

- Code changes needed
  - Add call to `HYPRE_SetGlobalPrecision()`
  - Manage real arrays with various utility routines (to keep things clean) such as
    `hypre_MuPDataCopyToMP(h_values, values, values_size);`

Mixed precision solver availability is limited to lower-precision preconditioned Krylov methods – more capability coming soon

- Using lower-precision preconditioners requires minimal code changes:
  - Add `SetPrecondMatrix()` call
  - Utilities available for creating lower-precision matrix
- Results for single-precision preconditioners
  - Need flexible CG for convergence at lower tolerances
  - Solve phase speedups for AMG and PFMG are comparable, with larger speedups for SMG
  - Structured solvers have higher per-iteration speedups
- Within a month or two:
  - GPU support for mixed precision (draft PR in progress)
  - Mixed precision BoomerAMG (results on next slide)

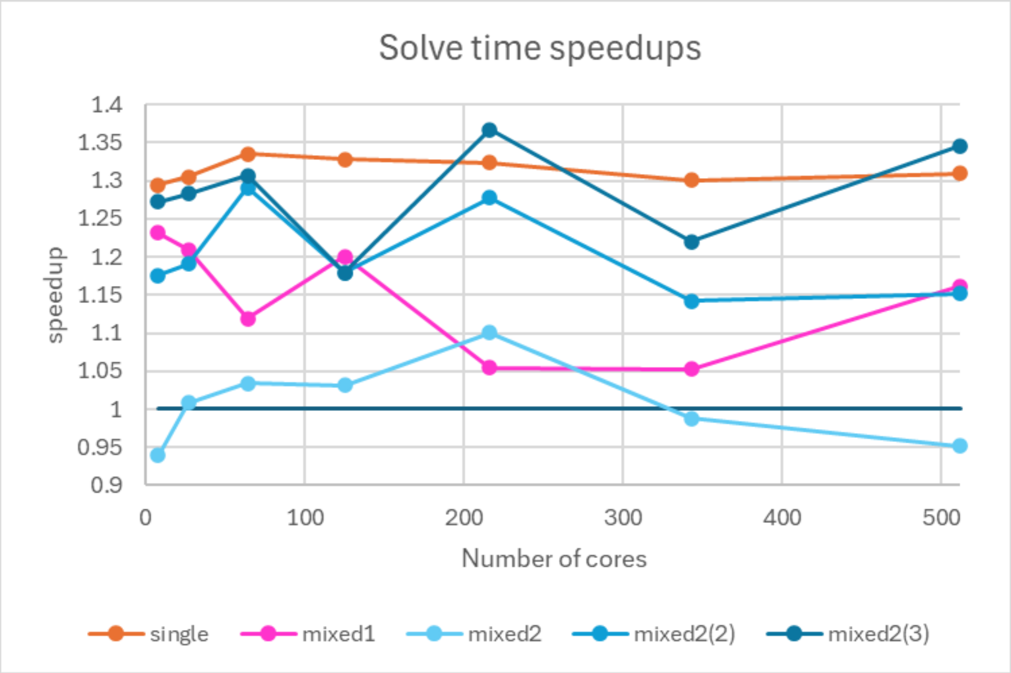
Speedups for single-precision preconditioners (double-precision PCG solve) on LLNL RZHound (Intel Sapphire Rapids) with 100x100x100 = 1M/core for 7pt Laplace problem. Results for AMG, PFMG, and SMG.



Mixed precision AMG uses different precisions on each grid level

- Setup phase
  - Additional creation of a lower precision matrix
- Solve phase
  - Additional precision conversions of the residual and error during restriction and prolongation
- Different API
  - `HYPRE_BoomerAMGSolve_mp()` (for example)
- Major challenge – size of AMG data structure
- Results:
  - Defaults: HMIS coarsening, ext+i(4), L1-GS
  - Setup: no real benefit
  - Solve: using single precision on lower levels is best

Results for mixed-precision AMG-PCG with different precision variations on each grid level. 7pt 3D Laplace problem with 100x100x100 = 1M/core on RZHound (Intel Sapphire Rapids).



Automation is used as much as possible to implement and maintain the mixed precision support in hypre-3.0

- Developers use scripts (awk, sed) to auto-generate multiprecision wrapper code
  - Keep lists of library symbols in special files (e.g., `mup.functions`)
  - Run `mup_check` to check library symbols – update lists as needed
  - Run `mup_code` to generate wrapper code
  - Commit everything to the repo

- HYPRE build is more involved:
  - Compiles 3 times to generate fixed-precision symbols
  - Compiles extra auto-generated code

Build Type / Function List	mup.fixed	mup.functions	mup.methods
MP_BUILD_SINGLE	Foo_flt	Foo_flt	Foo_flt
MP_BUILD_DOUBLE	Foo_dbl	Foo_dbl	Foo_dbl
MP_BUILD_LONGDOUBLE	Foo_long_dbl	Foo_long_dbl	Foo_long_dbl
No MP (standard compile)	Foo	Foo, Foo_pre	Foo, Foo_pre

```
HYPRE_Int
HYPRE_BiCGSTABSetTol_pre( HYPRE_Precision precision, HYPRE_Solver solver, hypre_long_double tol )
{
   switch (precision)
   {
      case HYPRE_REAL_SINGLE:
         return HYPRE_BiCGSTABSetTol_flt( solver, (hypre_float)tol );
      case HYPRE_REAL_DOUBLE:
         return HYPRE_BiCGSTABSetTol_dbl( solver, (hypre_double)tol );
      case HYPRE_REAL_LONGDOUBLE:
         return HYPRE_BiCGSTABSetTol_long_dbl( solver, (hypre_long_double)tol );
      default:
```

Summary / Conclusions

- (S)Struct rectangular matrix-vector tools
  - Implemented and optimized for CPUs and GPUs
  - SSAMG can outperform BoomerAMG on semi-structured problems – more optimizations to come
  - New tools will simplify solver development and enable solver improvements

- Mixed precision algorithms
  - Multi-precision code is available at runtime
  - Mixed-precision solvers have potential for GPUs (coming soon)

- We look forward to getting feedback on these new features!

Our Multigrid / Parallel-in-Time Research Team and Alumni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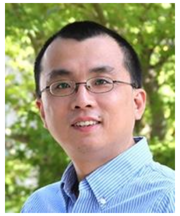
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- University collaborators and former interns
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- Software, publications, and other information

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

XBRAID http://llnl.gov/casc/xbraid

Hyperbolic PinT


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Thank You!

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