Argonne Training Program on Extreme-Scale Computing

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Krylov Solvers and Algebraic Multigrid with *hypre*

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Outline

• What are Krylov Solvers?
• Why are they used?
• Why multigrid methods?
• Algebraic multigrid software
• Hypre software library – interfaces
  – Why different interfaces?
• How does multigrid work?
• Unstructured and structured multigrid solvers
Iterative Solvers

• Solve linear system $Ax = b$, where $A$ is a large sparse matrix of size $n$

• Direct solvers (e.g. Gaussian elimination) too expensive

• Iterative solvers
  
  • Richardson iteration:
    
    $x^{n+1} = x^n + (b - Ax^n)$
    
    $e^{n+1} = (I - A)e^n$

  • Introduce a preconditioner $B$:
    
    $x^{n+1} = x^n + B(b - Ax^n)$
    
    $e^{n+1} = (I - BA)e^n$

• Jacobi: $B = D^{-1}$; Richardson: $B = \lambda I$
Generalized Minimal Residual (GMRES)

- \( x^{n+1} = x^n + B(b - Ax^n) \)
- \( \Rightarrow x^{n+1} = \sum_{i=0}^{\infty} \alpha_i (BA)^i Bb \)
- \( x^{n+1} \in K^n = \text{span}\{Bb, (BA)Bb, (BA)^2Bb, ..., (BA)^nBb\} \)

Krylov space

- Now optimize by defining \( x^{n+1} \) through
  \[ \min_{x^{n+1} \in K^n} \|B(Ax^{n+1} - b)\| \]
- Construct a new basis for \( K^n \) through orthonormalization
  \[ Bb \]
  \[ \{q_0 = \frac{Bb}{\|Bb\|}, q_1, ..., q_n\} \]
- Solve the minimization in the new basis
- \( q_i \) also called search directions
Some comments on GMRES

• GMRES consists of fairly simple operations:
  – Inner products and norms (global reductions)
  – Vector updates (embarrassingly parallel)
  – Matvecs (nearest neighbor updates)
  – Application of preconditioner (can be very complicated)

• Often used restarted as GMRES(k), i.e. after k iterations throw out $q_i$ and start again using latest approximation

• Many variants to reduce and/or overlap communication (pipelined GMRES, etc)
Other Krylov solvers

• Conjugate Gradient (CG)
  – For symmetric positive definite matrices
  – Possesses like GMRES an orthogonality property
  – Uses a three-term concurrence
  – Requires only two inner products and a norm per iteration

• Biconjugate Gradient Stabilized (BiCGSTAB)
  – Like CG uses a three-term recurrence relation
  – No orthogonality property, can break down
  – Requires several inner products and a norm at each iteration (and two matvecs)
  – More erratic convergence than GMRES, but needs generally less memory
Hands-on Exercises: Krylov methods

• Go to https://xsdk-project.github.io/MathPackagesTraining2020/lessons/krylov_amg_hypre/

• Poisson equation: \(-\Delta \varphi = \text{RHS}\)
  
  with Dirichlet boundary conditions \(\varphi = 0\)

• Grid: cube

• Finite difference discretization:
  – Central differences for diffusion term
  – 7-point stencil
Multigrid linear solvers are optimal ($O(N)$ operations), and hence have good scaling potential.

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

• ML, MueLu included in TRILINOS

• GAMG in PETSc

• The hypre library provides various algebraic multigrid solvers, including multigrid solvers for special problems e.g. Maxwell equations, ...

• All of these provide different flavors of multigrid and provide excellent performance for suitable problems

• Focus here on hypre
(Conceptual) linear system interfaces are necessary to provide “best” solvers and data layouts.
Why multiple interfaces? The key points

• Provides natural “views” of the linear system

• Eases some of the coding burden for users by eliminating the need to map to rows/columns

• Provides for more efficient (scalable) linear solvers

• Provides for more effective data storage schemes and more efficient computational kernels
hypre supports these system interfaces

- Structured-Grid (Struct)
  - logically rectangular grids

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

- Linear-Algebraic (IJ)
  - general sparse linear systems
The *hypre* software library provides structured and unstructured multigrid solvers

- Used in many applications

- Displays excellent weak scaling and parallelization properties on BG/Q type architectures

![Diagram showing weak scaling and parallelization properties](image)
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!
AMG Building Blocks

Setup Phase:

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

Solve Phase:

\[
\text{Relax } A^{(m)} u^m = f^m \\
\text{Compute } r^m = f^m - A^{(m)} u^m \\
\text{Restrict } r^{m+1} = R^{(m)} r^m \\
\text{Solve } A^{(m+1)} e^{m+1} = r^{m+1} \\
\text{Correct } u^m \leftarrow u^m + e^m \\
\text{Interpolate } e^m = P^{(m)} e^{m+1}
\]
BoomerAMG is an algebraic multigrid method for unstructured grids

- **Interface:** SStruct, IJ
- **Matrix Class:** ParCSR
- Originally developed as a general matrix method (i.e., assumes given only $A$, $x$, and $b$)
- Various coarsening, interpolation and relaxation schemes
- Automatically coarsens “grids”
- Can solve systems of PDEs if additional information is provided
- Can also be used through PETSc and Trilinos
- Can now also be used on GPUs (limited options)
Complexity issues

- Coarse-grid selection in AMG can produce unwanted side effects
- Operator (RAP) “stencil growth” reduces efficiency
- For BoomerAMG we will therefore also consider complexities:
  - Operator complexity: 
    \[ C_{op} = \frac{\sum_{i=0}^{L} nnz(A_i))}{nnz(A_0)} \]
    - Affects flops and memory
    - Generally would like \( C_{op} < 2 \), close to 1
- Can control complexities in various ways
  - varying strength threshold
  - more aggressive coarsening
  - Operator sparsification (interpolation truncation, non-Galerkin approach)
- Needs to be done carefully to avoid excessive convergence deterioration
ParCSRMatrix data structure

- Based on compressed sparse row (CSR) data structure

- Consists of two CSR matrices:
  - One containing local coefficients connecting to local column indices
  - The other (Offd) containing coefficients with column indices pointing to off processor rows

- Also contains a mapping between local and global column indices for Offd

- Requires much indirect addressing, integer computations, and computations of relationships between processes etc,
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
- Note that stencil growth is limited for SMG and PFMG (to at most 27 points per stencil in 3D)
- **Constant-coefficient versions**
- Can be used on GPUs (CUDA, RAJA, Kokkos)
PFMG is an algebraic multigrid method for structured grids

• Matrix defined in terms of grids and stencils

• Uses semicoarsening

• Simple interpolation
  \(\rightarrow\) limits stencil growth to at most 9pt (2D), 27pt (3D)

• Optional non-Galerkin approach (Ashby, Falgout), uses geometric knowledge, preserves stencil size

• Pointwise smoothing

• Highly efficient for suitable problems
Structured-Grid System Interface (Struct)

• Appropriate for scalar applications on structured grids with a fixed stencil pattern
• Grids are described via a global $d$-dimensional index space (singles in 1D, tuples in 2D, and triples in 3D)
• A box is a collection of cell-centered indices, described by its “lower” and “upper” corners
• The grid is a collection of boxes
• Matrix coefficients are defined via stencils

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

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

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

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

- Data stored

- Operations applied to stencil entries per box (corresponds to matrix (off) diagonals from a matrix point of view)
Algebraic multigrid as preconditioner

- Generally algebraic multigrid methods are used as preconditioners to Krylov methods, such as conjugate gradient (CG) or GMRES
- This often leads to additional performance improvements

Classic porous media diffusion problem:
\[-\nabla \cdot (\kappa \nabla u) = f\]
with \(\kappa\) having jumps of 2-3 orders of magnitude

Weak scaling: 32x32x32 grid points per core, BG/Q
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Thank you!
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