SAND2011-8264P

A Tutorial on Anasazi and Belos

2011 Trilinos User Group Meeting
November 1st, 2011

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Outline

- Belos and Anasazi Framework
  - Background / Motivation
  - Framework overview
  - Available solver components
- Using Anasazi and Belos
  - Simple example
  - Through Stratimikos (Belos)
  - Through LOCA (Anasazi)
- Summary

Background / Motivation

- Several iterative linear solver / eigensolver libraries exist:
  - PETSc, SLAP, LINSOL, Aztec(OO), …
  - SLEPc, LOBPCG (hypre), ARPACK, …
- None of the linear solver libraries can efficiently deal with multiple right-hand sides or sequences of linear systems
- Stopping criteria are predetermined for most libraries
- The underlying linear algebra is static

AztecOO

- A C++ wrapper around Aztec library written in C
- Algorithms: GMRES, CG, CGS, BiCGSTAB, TFQMR
- Offers status testing capabilities
- Output verbosity level can be determined by user
- Interface requires Epetra objects
  - Double-precision arithmetic
- Interface to matrix-vector product is defined by the user through the EpetraOperator

ARnoldi PACKage
(ARPACK)

- Written in Fortran 77
- Algorithms: Implicitly Restarted Arnoldi/Lanczos
- Static convergence tests
- Output formatting, verbosity level is determined by user
- Uses LAPACK/BLAS to perform underlying vector space operations
- Offers abstract interface to matrix-vector products through reverse communication

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Scalable Library for Eigenvalue Problem Computations (SLEPc)

- Written in C (Hernández, Román, and Vidal, 2003).
- Provides some basic eigensolvers as well as wrappers around:
  - ARPACK (Lehoucq, Maschhoff, Sorensen, and Yang, 1998)
  - BLZPACK (Marques, 1995)
  - PLANSO (Wu and Simon 1997)
  - TRLAN (Wu and Simon, 2001)
- Native Algorithms: Power/Subspace Iteration, RQI, Arnoldi
- Wrapped Algorithms: IRAM/IRLM (ARPACK), Block Lanczos (BLZPACK), and Lanczos (PLANSO / TRLAN)
- Static convergence tests
- Uses PETSc to perform underlying vector space operations, matrix-vector products, and linear solves
- Allows the creation / registration of new matrix-vector products

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Anasazi and Belos

- Next generation linear solver (Belos) and eigensolver (Anasazi) libraries, written in templated C++.
  - Iterative methods for solving sparse, matrix-free systems
- Provide a generic interface to a collection of algorithms for solving linear problems and eigenproblems.
- Algorithms developed with generic programming techniques.
  - Algorithmic components:
    - Ease the implementation of complex algorithms
  - Operator/MultiVector interface *(and Teuchos::ScalarTraits)*:
    - Allow the user to leverage their existing software investment
    - Multi-precision solver capability
  - Design offers: Interoperability, extensibility, and reusability
- Includes block linear solvers and eigensolvers.

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Why are Block Solvers Useful?

- In general, block solvers enable the use of faster computational kernels.
- Block Eigensolvers ($Op(A)X = \Lambda X$):
  - Reliably determine multiple and/or clustered eigenvalues.
  - Example applications:
    - Stability analysis / Modal analysis
    - Bifurcation analysis (LOCA)
- Block Linear Solvers ($Op(A)X = B$):
  - Useful for when multiple solutions are required for the same system of equations.
  - Example applications:
    - Perturbation analysis
    - Optimization problems
    - Single right-hand sides where A has a handful of small eigenvalues
    - Inner-iteration of block eigensolvers

Belos Solver Categories

- Belos provides solvers for:
  - Single RHS: $Ax = b$
  - Multiple RHS (available simultaneously): $AX = B$
  - Multiple RHS (available sequentially): $Ax_i = b_i$, $i=1,\ldots,k$
  - Sequential Linear systems: $A_i x_i = b_i$, $i=1,\ldots,k$

- Leverage research advances of solver community:
  - Block methods: block GMRES [Vital], block CG/BICG [O'Leary]
  - "Seed" solvers: hybrid GMRES [Nachtigal, et al.]
  - "Recycling" solvers for sequences of linear systems [Parks, et al.]
  - Restarting, orthogonalization techiques

Belos Solvers

- Hermitian Systems ($A = A^H$)
  - Block CG
  - Pseudo-Block CG (Perform single-vector algorithm simultaneously)
  - RCG (Recycling Conjugate Gradients)
  - PCPG (Projected CG)
  - MINRES New!
- Non-Hermitian System ($A \neq A^H$)
  - Block GMRES
  - Pseudo-Block GMRES (Perform single-vector algorithm simultaneously)
  - Block FGMRES (Variable preconditioner)
  - Hybrid GMRES
  - TFQMR
  - GCRODR (Recycling GMRES)
  - Block GCRODR (Block variant of GCRODR) New!

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Anasazi Solvers

- Hermitian Eigenproblems
  - Block Davidson
  - Locally-Optimal Block Preconditioned Conjugate Gradient (LOBPCG)
  - Implicit Riemannian Trust-Region (IRTR)
- Non-Hermitian Eigenproblems
  - Block Krylov-Schur (BKS)

Anasazi and Belos

(Algorithmic components)

$x^{(0)}$ is an initial guess
for $j = 1, 2, ...$
  Solve r from $Mr = b - Ax^{(0)}$
  $v^{(1)} = r/\|r\|_2$
  $s := \|r\|_2 e_1$
  for $i = 1, 2, ..., m$
    Solve w from $Mw = Av^{(i)}$
    for $k = 1, ..., i$
      $h_{k,i} = (w, v^{(k)})$
      $w = w - h_{k,i}v^{(k)}$
    end
    $h_{i+1,i} = \|w\|_2$
    $v^{(i+1)} = w/h_{i+1,i}$
    apply $J_1, ..., J_{i-1}$ on $(h_{1,i}, ..., h_{i+1,i})$
    construct J_i, acting on ith and $(i+1)$st component
    of $h_{.,i}$, such that $(i+1)$st component of $J_i h_{.,i}$ is 0
    $s := J_i s$
    if $s(i+1)$ is small enough then (UPDATE$(\tilde{x}, i)$ and quit)
  end
  UPDATE$(\tilde{x}, m)$
end

GMRES Example

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Anasazi and Belos

(Algorithmic components)

SolverManager Class

$x^{(0)}$ is an initial guess
for $j = 1, 2, ...$
  Solve r from $Mr = b - Ax^{(0)}$
  $v^{(1)} = r/\|r\|_2$
  $s := \|r\|_2 e_1$
  for $i = 1, 2, ..., m$
    Solve w from $Mw = Av^{(i)}$
    for $k = 1, ..., i$
      $h_{k,i} = (w, v^{(k)})$
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end

GMRES Example

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Anasazi and Belos

(Algorithmic components)

SolverManager Class

Iteration Class

$x^{(0)}$ is an initial guess
for $j = 1, 2, \ldots$
  Solve r from $Mr = b - Ax^{(0)}$
  $v^{(1)} = r/\|r\|_2$
  $s := \|r\|_2 e_1$
  for $i = 1, 2, \ldots, m$
    Solve w from $Mw = Av^{(i)}$
    for $k = 1, \ldots, i$
      $h_{k,i} = (w, v^{(k)})$
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GMRES Example

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Anasazi and Belos

(Algorithmic components)

SolverManager Class

Problem Classes / Operator Classes

Iteration Class

$x^{(0)}$ is an initial guess
for $j = 1, 2, \ldots$
  Solve r from $Mr = b - Ax^{(0)}$
  $v^{(1)} = r/\|r\|_2$
  $s := \|r\|_2 e_1$
  for $i = 1, 2, \ldots, m$
    Solve w from $Mw = Av^{(i)}$
    for $k = 1, \ldots, i$
      $h_{k,i} = (w, v^{(k)})$
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  end
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end

GMRES Example

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(Algorithmic components)

SolverManager Class

Problem Classes / Operator Classes

Iteration Class

MultiVector Classes

$x^{(0)}$ is an initial guess
for $j = 1, 2, \ldots$
  Solve r from $Mr = b - Ax^{(0)}$
  $v^{(1)} = r/\|r\|_2$
  $s := \|r\|_2 e_1$
  for $i = 1, 2, \ldots, m$
    Solve w from $Mw = Av^{(i)}$
    for $k = 1, \ldots, i$
      $h_{k,i} = (w, v^{(k)})$
      $w = w - h_{k,i} v^{(k)}$
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GMRES Example

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Anasazi and Belos

(Algorithmic components)

SolverManager Class

Problem Classes / Operator Classes

Iteration Class

MultiVector Classes

OrthoManager Class

(ICGS, IMGS, DGKS, TSQR)

$x^{(0)}$ is an initial guess
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GMRES Example

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Anasazi and Belos

(Algorithmic components)

SolverManager Class

Problem Classes / Operator Classes

Iteration Class

MultiVector Classes

OrthoManager Class

(ICGS, IMGS, DGKS, TSQR)

StatusTest Class

$x^{(0)}$ is an initial guess
for $j = 1, 2, \ldots$
  Solve r from $Mr = b - Ax^{(0)}$
  $v^{(1)} = r/\|r\|_2$
  $s := \|r\|_2 e_1$
  for $i = 1, 2, \ldots, m$
    Solve w from $Mw = Av^{(i)}$
    for $k = 1, \ldots, i$
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GMRES Example

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(Algorithmic components)

SolverManager Class

Problem Classes / Operator Classes

Iteration Class

MultiVector Classes

OrthoManager Class

(ICGS, IMGS, DGKS, TSQR)

StatusTest Class

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    $s := J_i s$
    if $s(i+1)$ is small enough then (UPDATE($\tilde{x}, i$) and quit)
  end
  UPDATE($\tilde{x}, m$)
end

OutputManager Class

SortManager Class

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Example (Step #1 – Initialize System)

```
int main(int argc, char *argv[]) {
  MPI_Init(&argc,&argv);
  Epetra_MpiComm Comm(MPI_COMM_WORLD);
  int MyPID = Comm.MyPID();

  typedef double                              ST;
  typedef Teuchos::ScalarTraits<ST>          SCT;
  typedef SCT::magnitudeType                  MT;
  typedef Epetra_MultiVector                  MV;
  typedef Epetra_Operator                     OP;
  typedef Belos::MultiVecTraits<ST,MV>       MVT;
  typedef Belos::OperatorTraits<ST,MV,OP>    OPT;

  using Teuchos::ParameterList;
  using Teuchos::RCP;
  using Teuchos::rcp;

  // Get the problem
  std::string filename("orsirr1.hb");
  RCP<Epetra_Map> Map;
  RCP<Epetra_CrsMatrix> A;
  RCP<Epetra_MultiVector> B, X;
  RCP<Epetra_Vector> vecB, vecX;
  EpetraExt::readEpetraLinearSystem(filename, Comm, &A, &Map, &vecX, &vecB);
  X = Teuchos::rcp_implicit_cast<Epetra_MultiVector>(vecX);
  B = Teuchos::rcp_implicit_cast<Epetra_MultiVector>(vecB);
```

Parameters for Templates

Get linear system from disk

Trilinos/packages/belos/epetra/example/BlockGmres/BlockGmresEpetraExFile.cpp

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Example (Step #2 – Solver Params)

```
bool verbose = false, debug = false, proc_verbose = false;
int frequency = -1;          // frequency of status test output.
int blocksize = 1;           // blocksize
int numrhs = 1;              // number of right-hand sides to solve for
int maxiters = 100;          // maximum number of iterations allowed
int maxsubspace = 50;        // maximum number of blocks
int maxrestarts = 15;        // number of restarts allowed
MT tol = 1.0e-5;             // relative residual tolerance

const int NumGlobalElements = B->GlobalLength();

ParameterList belosList;
belosList.set( "Num Blocks", maxsubspace);            // Maximum number of blocks in Krylov
  factorization
belosList.set( "Block Size", blocksize );             // Blocksize to be used by iterative solver
belosList.set( "Maximum Iterations", maxiters );      // Maximum number of iterations allowed
belosList.set( "Maximum Restarts", maxrestarts );     // Maximum number of restarts allowed
belosList.set( "Convergence Tolerance", tol );        // Relative convergence tolerance requested
int verbosity = Belos::Errors + Belos::Warnings;
if (verbose) {
  verbosity += Belos::TimingDetails + Belos::StatusTestDetails;
  if (frequency > 0)
    belosList.set( "Output Frequency", frequency );
}
if (debug) {
  verbosity += Belos::Debug;
}
belosList.set( "Verbosity", verbosity );
```

Solver Parameters

ParameterList for SolverManager

Trilinos/packages/belos/epetra/example/BlockGmres/BlockGmresEpetraExFile.cpp

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Example (Step #3 – Solve)

```
// Construct linear problem instance.
Belos::LinearProblem<double,MV,OP> problem( A, X, B );
bool set = problem.setProblem();
if (set == false) {
  std::cout << std::endl << "ERROR:  Belos::LinearProblem failed to
  set up correctly!" << std::endl;
  return -1;
}
```

LinearProblem Object

Template Parameters

SolverManager Object

```
// Start block GMRES iteration
Belos::OutputManager<double> My_OM();
// Create solver manager.
RCP< Belos::SolverManager<double,MV,OP> > newSolver =
  rcp( new Belos::BlockGmresSolMgr<double,MV,OP>(rcp(&problem,false), rcp(&belosList,false)));
// Solve
Belos::ReturnType ret = newSolver->solve();
if (ret!=Belos::Converged) {
  std::cout << std::endl << "ERROR:  Belos did not converge!" << std::endl;
  return -1;
}
std::cout << std::endl << "SUCCESS:  Belos converged!" << std::endl;
return 0;
```

Trilinos/packages/belos/epetra/example/BlockGmres/BlockGmresEpetraExFile.cpp

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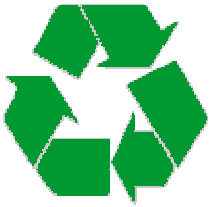
Spotlight on Recycling



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Sequences of Linear Systems

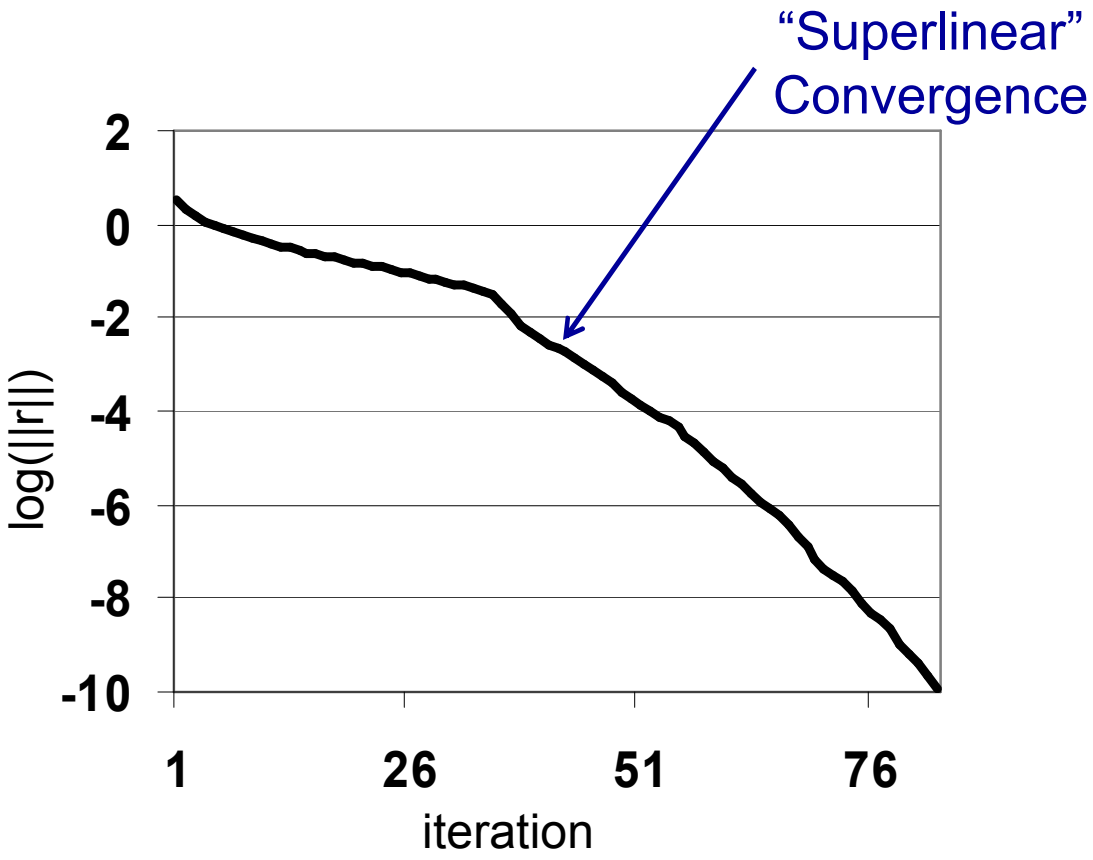
- Consider sequence of linear systems

$$\mathbf{A}^{(i)}\mathbf{x}^{(i)} = \mathbf{b}^{(i)} \qquad i=1,2,3,\ldots$$

- Applications:
  - Newton/Broyden method for nonlinear equations
  - Materials science and computational physics
  - Transient circuit simulation
  - Crack propagation
  - Optical tomography
  - Topology optimization
  - Large-scale fracture in disordered materials
  - Electronic structure calculations
  - Stochastic finite element methods
- Iterative (Krylov) methods build search space and select optimal solution from that space
- **Building search space is dominant cost**
- For sequences of systems, get fast convergence rate and good initial guess immediately by **recycling** selected search spaces from previous systems

Why Recycle?

- Typically, dominant subspace exists such that almost any Krylov space (from any starting vector) has large components in that space (why restarting is bad)



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Why Recycle?

- Typically, dominant subspace exists such that almost any Krylov space (from any starting vector) has large components in that space (why restarting is bad)
- Optimality derives from orthogonal projection
  - new search directions should be far from this dominant subspace for fast convergence
- If such a dominant subspace persists (approximately) from one system to the next, it can be recycled
  - Typically true when changes to problem are small and/or highly localized

Matrix	Off-the-shelf solver	Recycling Solver	Release
General	GMRES	GCRODR	Trilinos 8
SPD	CG	Recycling CG (RCG)	Trilinos 10
Symmetric Indefinite	MINRES	Recycling MINRES (RMINRES)	N/A

Deflation

- Invariant subspace associated with small eigenvalues delays convergence
- Corresponds to smooth modes that change little for small localized changes in the problem

- Remove them to improve convergence!
  - Recycle space = approximate eigenspace

$$\min_{z \in K^m(A, r_0)} \|r_0 - Az\|_2 = \min_{P_m(0)=1} \|p_m(A) r_0\|_2$$
$$\leq \kappa(V) \|r_0\|_2 \min_{P_m(0)=1} \max_{\lambda \in \Lambda(A)} |p_m(\lambda)|$$

- If $\kappa(V)$ is not large (normality assumption) we can improve bound by removing select eigenvalues

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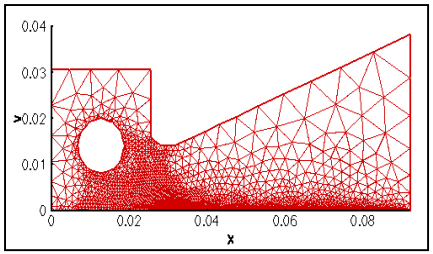
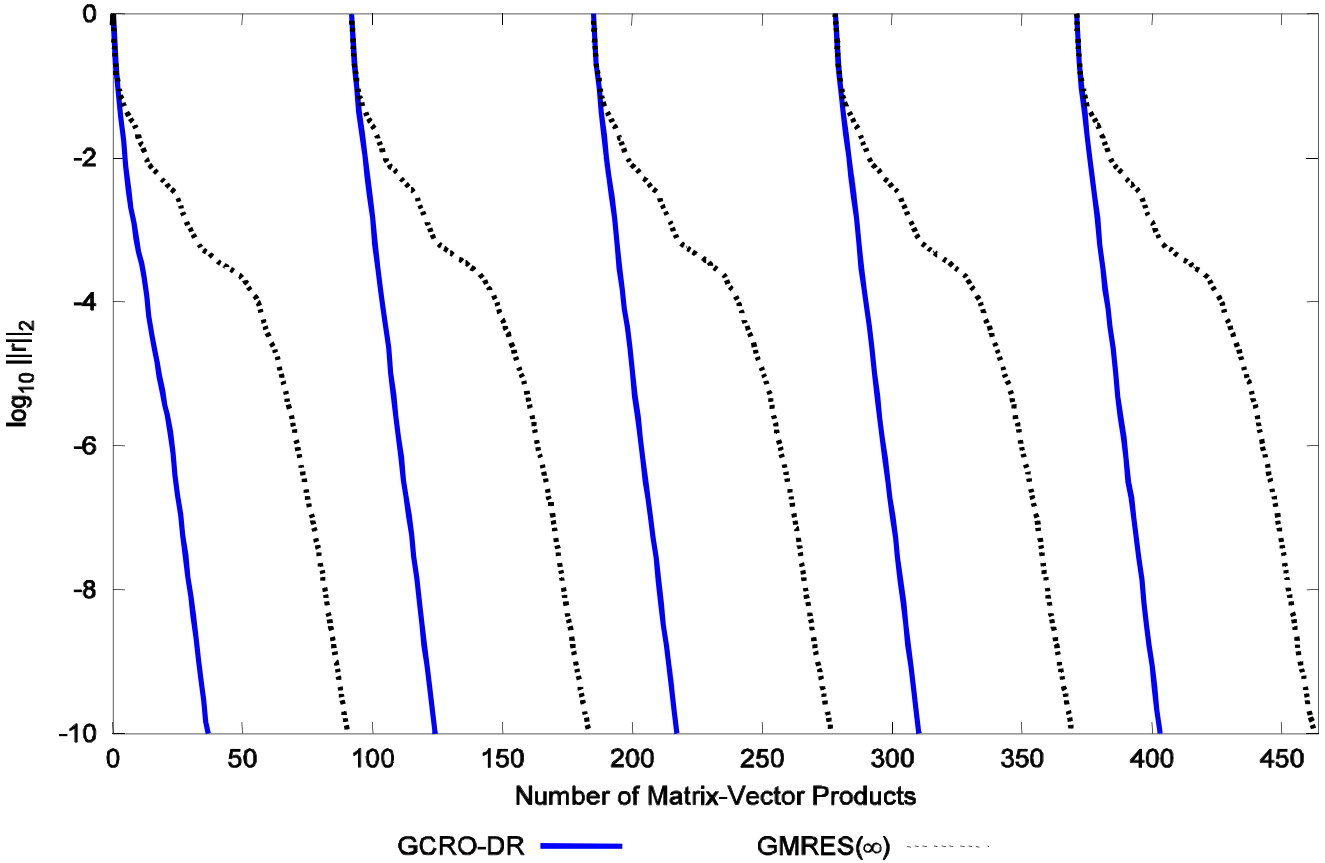
Typical Convergence with Recycling

- IC(0) preconditioner
- GMRES – full recurrence
- All Others – Max subspace size 40





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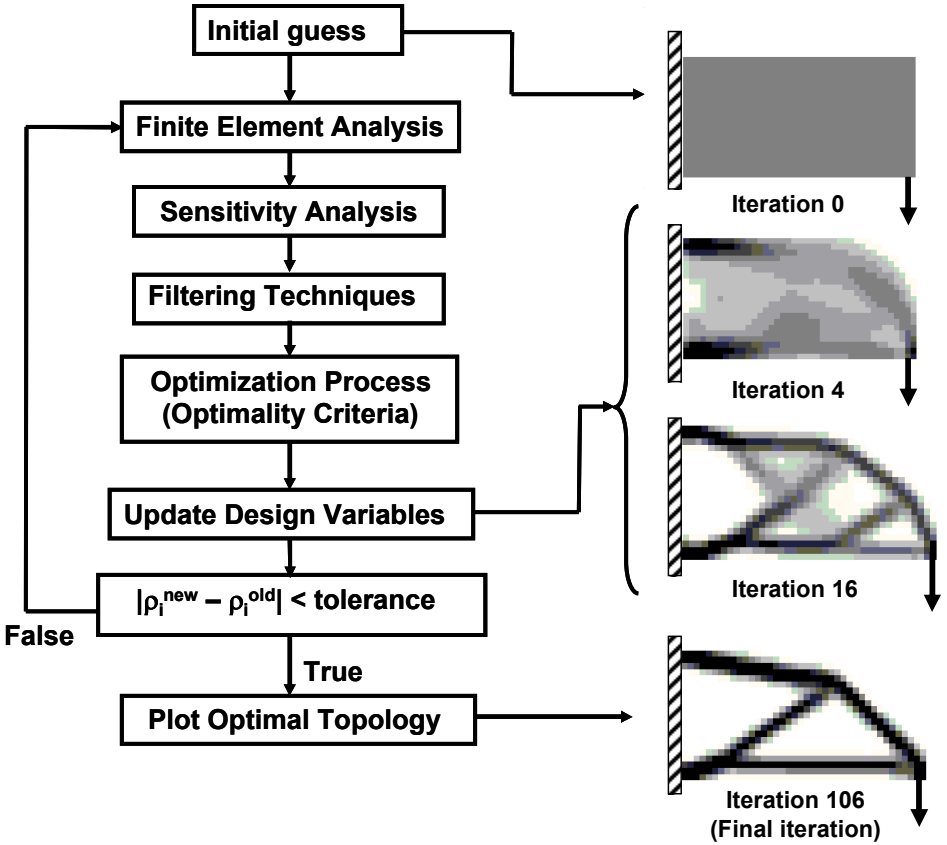
Example #1 Topology Optimization*

- Optimize material distribution, ρ, in design domain
- Minimize compliance $u^T K(\rho)u$, where $K(\rho)u=f$



*S. Wang, E. de Sturler, and G. H. Paulino, *Large-scale topology optimization using preconditioned Krylov subspace methods with recycling*, International Journal for Numerical Methods in Engineering, Vol. 69, Issue 12, pp. 2441—2468, 2007.

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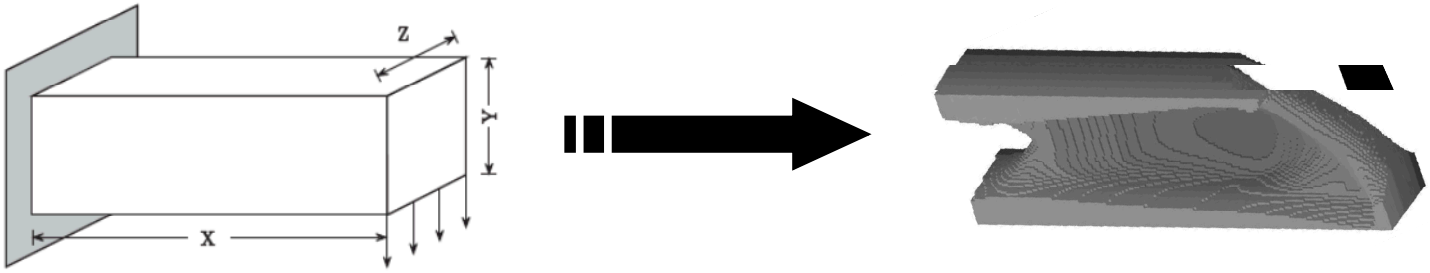
Example #1: Topology Optimization



Size	Num. DOFs	Direct Solve Time	Recycling Solve Time
Small	**9,360**	**0.96**	**1.68**
Medium	**107,184**	**179.30**	**50.41**
Large	**1,010,160**	**26154.00**	**1196.30**

Recycling Solve = RMINRES + IC(0) PC

Direct Solve = multifrontal, supernodal Cholesky factorization from TAUCS

[*]S. Wang, E. de Sturler, and G. H. Paulino, *Large-scale topology optimization using preconditioned Krylov subspace methods with recycling*, International Journal for Numerical Methods in Engineering, Vol. 69, Issue 12, pp. 2441—2468, 2007.

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Example #2 Stochastic PDEs*

- Stochastic elliptic equation

$$-\nabla \cdot \big(\mathbf{a}(\mathbf{x},\omega)\big)\nabla \mathbf{u}(\mathbf{x},\omega) = \mathbf{f}(\mathbf{x}) \qquad \mathbf{x} \in \mathbf{D}, \omega \in \Omega$$
$$\mathbf{u}(\mathbf{x},\omega) = \mathbf{0} \qquad \mathbf{x} \in \partial\mathbf{D}, \omega \in \Omega$$

- KL expansion + double orthogonal basis + discretization
  - Separate deterministic and stochastic components
  - Yield sequence of uncoupled equations

$$\mathbf{A}^{(i)}\mathbf{x}^{(i)} = \mathbf{b}^{(i)} \qquad \mathbf{i=1,2,3,\ldots}$$

- Preprocess for recycling Krylov solver
  - Use reordering scheme to minimize change in spectra of linear system

*C. Jin, X-C. Cai, and C. Li, *Parallel Domain Decomposition Methods for Stochastic Elliptic Equations,* SIAM Journal on Scientific Computing, Vol. 29, Issue 5, pp. 2069—2114, 2007.

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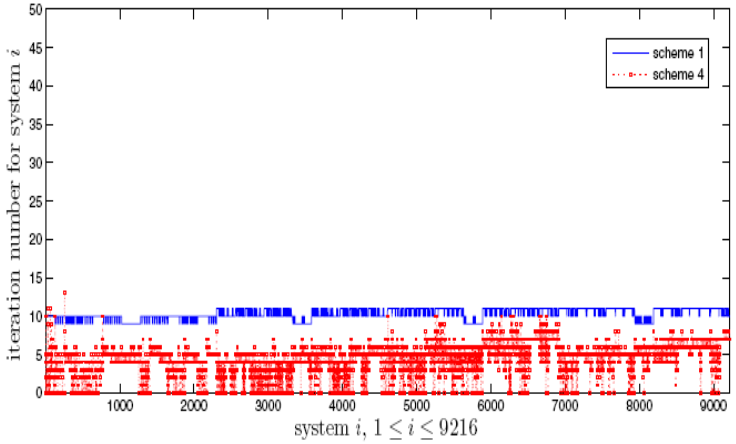
Example #2 Stochastic PDEs*

- Scheme #1: No Krylov recycling
- Scheme #4: Recycle Krylov spaces using reordering
- Many systems require zero iterations!

One-Level ASM



Two-Level ASM

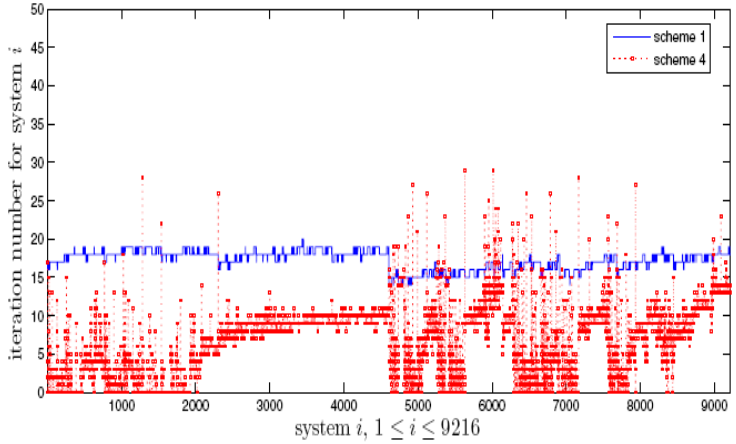


TABLE 4.1
Running time for different schemes and preconditioning (seconds).

Preconditioner	Scheme			
	1	2	3	4
One-level ASM	12030	7693	4205	3882
Two-level ASM	20980	14130	10740	8476

*C. Jin, X-C. Cai, and C. Li, *Parallel Domain Decomposition Methods for Stochastic Elliptic Equations,* SIAM Journal on Scientific Computing, Vol. 29, Issue 5, pp. 2069—2114, 2007.

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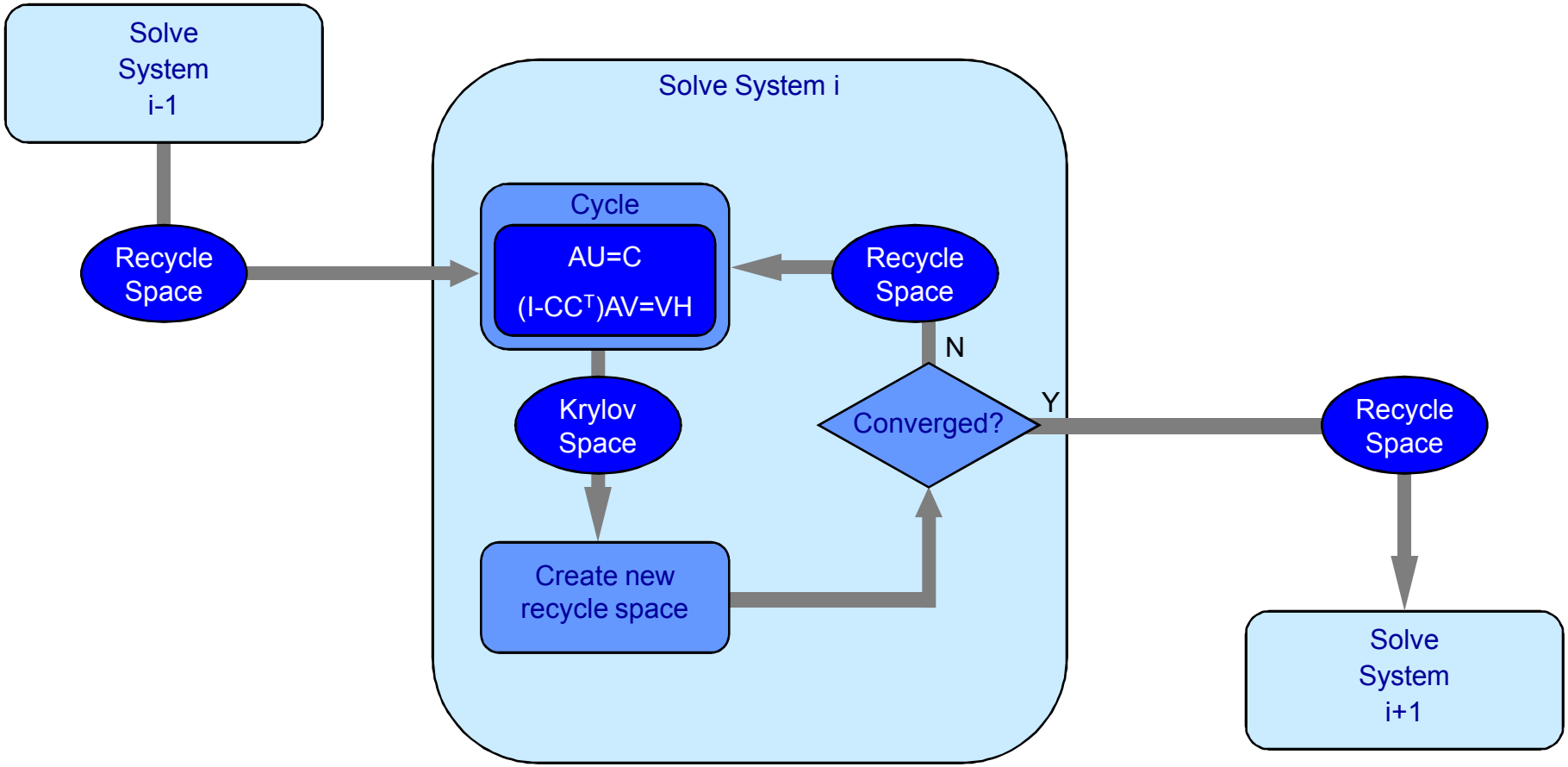
Structure of Recycling Solver



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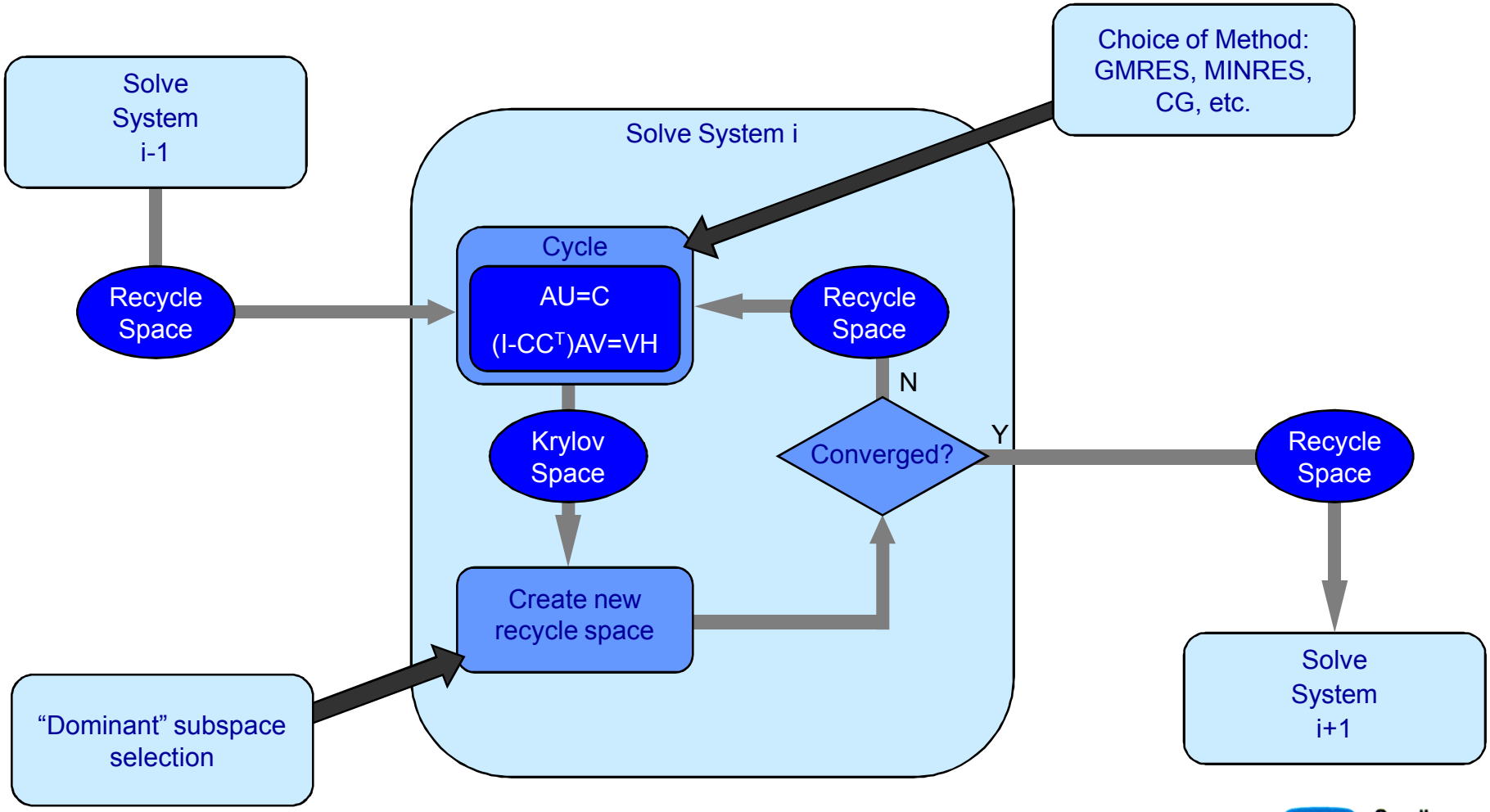
Structure of Recycling Solver



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Summary

- Belos and Anasazi are **next-generation** linear and eigensolver libraries
  - Designed for interoperability, extensibility, and reusability
- Belos and Anasazi are readily available:
  - Can be used as standalone linear and eigensolvers
  - Belos available through Stratimikos
  - Anasazi available through LOCA
- Check out the Trilinos Tutorial
  `http://trilinos.sandia.gov/Trilinos10.8Tutorial.pdf`
- See website for more:
  `http://trilinos.sandia.gov/packages/belos`
  `http://trilinos.sandia.gov/packages/anasazi`

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