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Production Implementations of Pipelined & Communication-Avoiding Iterative Linear Solvers

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DOE's ECP PEEKS

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- Pipelined & communication-avoiding Krylov solvers
  - Hide (overlap) or avoid (do less) communication (e.g., all-reduce)
  - May perform better, especially at large scales
- We want to make these solvers available in Trilinos
  - Goal: perform "well" for ECP applications on exascale computers
  - Also should be useful for non-exascale Trilinos users
- This talk
  - Is about resulting Trilinos software development challenges
  - Is NOT about algorithms or their performance

What is Trilinos?

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- Parallel math libraries for science & engineering applications
  - Parallel programming models
  - Sparse linear algebra
  - Linear & nonlinear solvers
  - Optimization algorithms
  - Space & time discretizations
- Mostly C++ with some C and Fortran
- Many users inside & outside Sandia
- Must work on many different platforms
  - CPUs: x86, KNL, POWER, ARM, …
  - GPUs: NVIDIA, later AMD
  - Future architectures (e.g., exascale)
- github.com/trilinos/Trilinos

Trilinos' linear solvers

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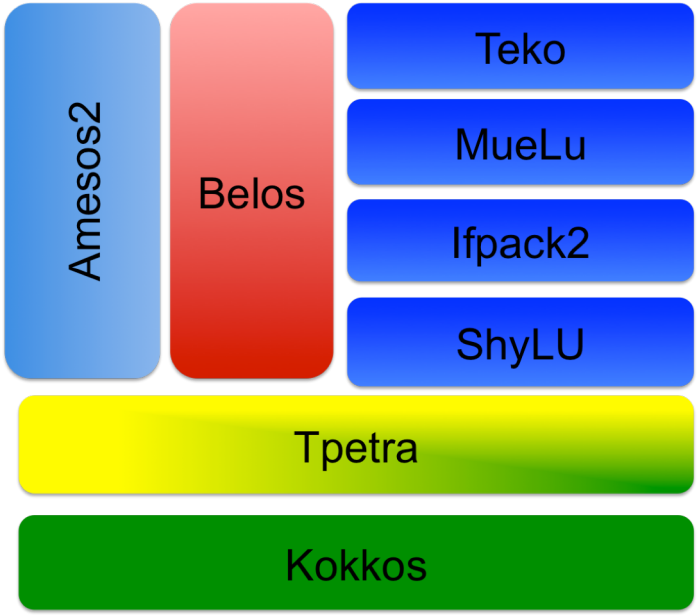
- Iterative (Krylov) solvers (Belos)
  - CG, GMRES, BiCGStab, TFQMR, recycling methods
- Linear algebra operations
  - Tpetra: Sparse graphs/matrices, dense vectors, parallel solve kernels, communication & redistribution
  - Teuchos: BLAS/LAPACK
- Sparse direct solvers (Amesos2)
- Direct+iterative solvers (ShyLU)
- Algebraic iterative solvers (Ifpack2)
  - Jacobi, SOR, polynomial, incomplete factorizations, additive Schwarz
- Algebraic multigrid (MueLu)
- Segregated block solvers (Teko)



Goal: “Productionize” solvers

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- Make pipelined & communication-avoiding iterative linear solvers available in Belos for Trilinos users
  - Must build & pass tests on all supported platforms
- Available to users via run-time choice (input deck)
  - Users don’t need to change their code
  - Plugging solvers through a custom solver “factory”
  - Not just dumping a class or function into the code repository

Software challenges

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1. Trilinos' iterative linear solvers package makes it hard to add new linear algebra operations

2. Trilinos must support many different build configurations
   - Older MPI versions may lack features needed for pipelined Krylov solvers
   - Default MPI implementation settings may not make progress on nonblocking collectives, thus taking away benefit of pipelined Krylov methods

Trilinos' Belos package

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- Trilinos' iterative linear solvers live in the Belos package
- Belos was written in the mid-2000's, to support Anasazi (iterative eigensolvers package)

- Belos works for any linear algebra (LA) implementation
  - Belos defines a fixed set of ops on Vectors & Linear Operators (matrices & preconditioners): e.g., dot, norm, axpy, apply(X,Y)
  - Fixed set of LA ops defined via (C++) traits classes

  - Belos' solvers are templated on Vector & Linear Operator & invoke LA ops by using traits classes
  - Belos provides specializations of traits for Trilinos' native LA types (e.g., Tpetra)

Belos solver interface

```
// Create a Belos::SolverManager for CG
// rcp / RCP are Trilinos' std::shared_ptr (Belos only needs C++98)
auto belosSolver = rcp (new Belos::PseudoBlockCGSolMgr<Scalar, Vec, LinOp>);

// Create and Set problem
typedef Belos::LinearProblem<Scalar, Vec, LinOp> linear_problem_type;
RCP<linear_problem_type > lp (new linear_problem_type (A, X, B));

belosSolver->setProblem (lp);
belosSolver->setParameters (params); // e.g., iteration count, convergence tolerance

// Solve the system
Belos::ReturnType belosResult = belosSolver->solve ();
```

- Same solver manager may be reused for multiple solves;
  e.g., for different b or A.
- A, b, x may be templated, e.g., with scalar, global/local ordinal, and node type

Belos solver implementation

```
typedef MultiVecTraits<Scalar, Vec> MVT;

RCP<Vec> P_;
RCP<Vec> AP_;

// Compute AP = A*P
lp_->applyOp( *P_, *AP_ );

// Compute P^T * A P
MVT::MvTransMv( one, *P_, *R_, alpha );
```

- If users want Belos to work for their own LA types, they must write their own specializations of traits classes

Challenge 1: New LA operation breaks build

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- What if we need new LA ops?
  - Pipelined Krylov: Nonblocking dot product
  - Communication-avoiding Krylov: Matrix powers kernel, TSQR
- Can't add new LA ops to Belos without breaking build!
  - OK for Trilinos' native LA
    - Belos just changes its traits class specializations
  - NOT OK for users' own LA
    - Users have their own Belos traits specializations
    - They would need to change their code to add new LA ops

Run-time vs. compile-time

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- **Mark**: “Not a C++ problem, but a design problem”
- Belos could have used run-time polymorphism (inheritance)
  - Adding new LA ops through “mix-in” classes without breaking backwards compatibility for libraries that lack them
- Belos chose compile-time polymorphism for historical reasons
  - Belos is in 1st generation of Trilinos packages using templates
  - Early C++ adopters for math codes worried about run-time overhead
  - C++ templates promised zero overhead
  - Trilinos developers have more experience w/ templates now
    - Tiny virtual method dispatch overhead vs. MPI communication
- Goal: no code changes for Belos users who want to use our new solvers

Traits classes too rigid here

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- One solver implementation for all LA ops, and one traits class contains all LA ops; but
  - Some solvers need specialized ops
  - Users or third-party libraries may have optimized entire solvers for specific LA; Belos users want to access them
- Solution: extend Belos to support LA-specific solvers
  - Belos::SolverFactory already takes solver name at run time & returns instance of the desired solver
  - NEW interface to inject a "**custom** solver factory" at run time
    - SolverFactory class templated on Vector & LinearOperator
      ➔ custom factory is specific to those types
    - custom solver needs to work for one LA
      ➔ they can code directly to that LA & use whatever ops they want
  - Solves a more general problem than pipelined & CA Krylov

Belos factory interface

```
// Create a Solver Manager
    Belos::SolverFactory<Scalar, Vect, LinOp> factory;
    RCP<solver_manager_type> solverManager = factory.create (args.solverName, params);

// Solve the system
    Belos::ReturnType belosResult = solverManager->solve ();
```

Behind the scenes:

```
// Create a Custom Solver Factory
    RCP<custom_factory_type> customFactory;
    customFactory = rcp (static_cast<custom_factory_type*> (new PeeksKrylovFactory<> ()));

// Add the Custom Factory
    factory.addFactory (customFactory);
```

Belos factory interface

```
// Create a Solver Manager
    Belos::SolverFactory<Scalar, Vect, LinOp> factory;
    RCP<solver_manager_type> solverManager = factory.create (args.solverName, params);

// Solve the system
    Belos::ReturnType belosResult = solverManager->solve ();
```

Behind the scenes:

```
void createSolver (const std::string& solverName)  {
   if (solverName == "PeeksCgPipeline") {
     this->solver_ = Teuchos::rcp( new CgPipeline<Scalar, LocalOrd, GlobalOrd, Node> () );
   } else if ( …
}
```

New Op for nonblocking all-reduce

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- Tpetra's interface to this new specialized op:
  - auto request = idot(&result, x, y); // ← MUST NOT BLOCK
  - /* … do other stuff ... Then */
  - request->wait();
- MPI-3 (2012) added support for nonblocking collectives
  - MPI_Iallreduce: nonblocking version of MPI_Allreduce
- What if Trilinos was built with MPI < 3?
  - Capture (&result, x, y) in a closure (C++11 lambda) that does blocking dot product; don't invoke closure yet
  - request->wait() just invokes the closure as std::function
- We write the solver once; & it works for all MPI versions

Challenge 2: nonblocking progress

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- "Nonblocking" ➔ return immediately after being called
- MPI could just defer all communication until MPI_Wait
  - MPI may only send/receive inside MPI functions
  - For asynchronous progress, must enable MPI_THREAD_MULTIPLE support & possibly also "progress thread" options at MPI build time
- Problems:
  - Users / sysadmins, not Trilinos, pick build MPI options
  - MPI_THREAD_MULTIPLE & progress thread incur overhead
  - Would we need to poll manually?
    - Paul Eller (UIUC): PETSc's implementation of pipelined Krylov needed manual MPI polling embedded inside the sparse matrix-vector multiply kernel in order for MPI_Iallreduce to be effective (!)

MPI progress: “work in progress”

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- Not sure what to do about this, yet
  - Manual polling? Impossible on GPUs, invasive in code
  - Programming model mismatch
    - Pipelined Krylov methods really want a dataflow model
    - MPI historically resisted “active messages” (that run a function asynchronously when I receive data from another process)
- MPI_THREAD_MULTIPLE overhead
  - Trilinos’ sparse matrix-vector multiply uses 2-sided
  - Cost: message queue locking for MPI 2-sided (send, recv)
  - Vendors recommended switching to MPI 1-sided (MPI_Win), since optimized implementations don’t use MPI message queues
  - Trilinos has plans to explore this, but not this year

Conclusions

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- We want to deploy pipelined & communication-avoiding Krylov methods in Trilinos
  - Implementations exist now
  - We will put them in Trilinos this year
- Software challenges, because we want it to work for production users, instead of just hacking it in there
- We addressed some Belos & MPI – related challenges
- We need a better approach to asynchronous progress for nonblocking MPI operations

Thank you!!

Thank you!!

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- ECP PEEKS: This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering and early testbed platforms, in support of the nations exascale computing imperative.