ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

CSCS
Swiss National Supercomputing Centre

A Brief Compendium of GPU-enabled Numerical Libraries

Summer School 2014

Dr. William Sawyer, Dr. Karl Rupp, Dr. Michael Heroux, Dr. Dimitar Lukarski, Prof. Stan Tomov, Dr. Peter Messmer

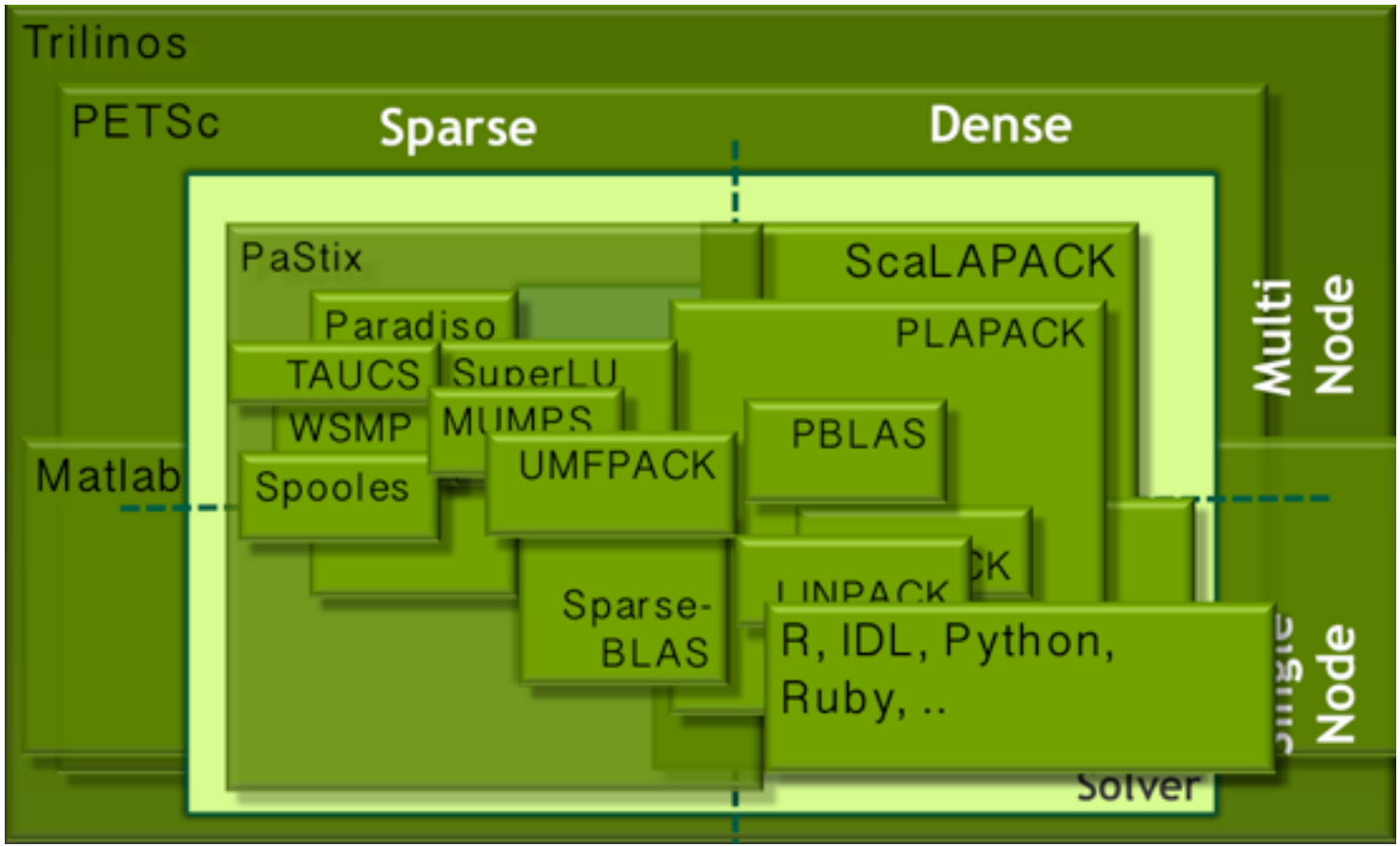
Tutorial Summary

- Introduction and library overview
  - Typical numerical and semi-numerical problems
  - Survey of some gpu-enabled libraries:
    - NVIDIA libraries: cuBLAS, cuFFT, cuRAND, cuSPARSE
    - MAGMA
    - Thrust / CuSP
    - ViennaCL
    - Paralution
    - PETSc
    - Trilinos
- More: https://github.com/fomics/GPU_Libraries_2013

Objectives of this tutorial

- Awareness of the available libraries
- Realization that it is not necessary for users to "recreate the wheel"
- *Subjective appraisal of the libraries to bet on*

Extensive CPU Library Ecosystem



Problems our users might like to solve

- Partial differential equations
- Dense linear algebra
- Sparse systems of linear equations
- Preconditioning of large systems
- Eigenvalue / singular value decompositions of sparse/dense matrices
- Partitioning large graphs
- Non-linear systems and optimization
- ...

For single node GPUs

Solid

Limited

Under development

NVIDIA's CUDA Libraries

- cuBLAS: simple linear algebra on vectors and matrices

  1: vectors: add, dot products, scaling, norms, rotations, ..

  2: matrix-vector: triangular/full/hermitian mat x vec, ...

  3: matrix-matrix: products, multiple rank updates, ...

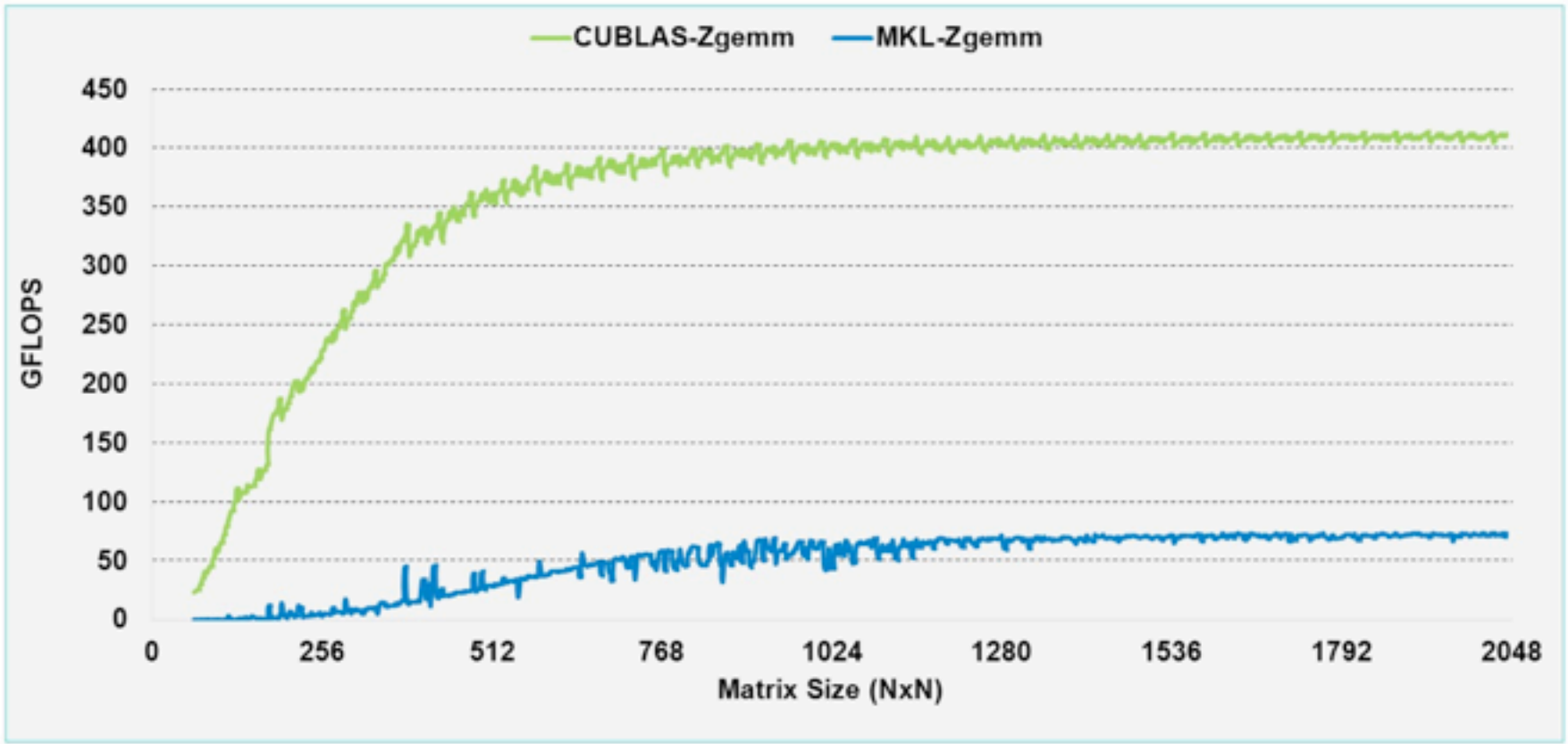
- cuSPARSE: Sparse linear algebra
  - ➡ matrix creation, various sparse matrix formats
  - ➡ indexed vector operations
  - ➡ sparse mat x vec, mat x mat operations
- cuFFT: fast Fourier transforms
- cuRAND: random number generators

➡ *offers single-GPU core support for user applications*

Example: simple SAXPY (vector add)

```
int N = 1 << 20;
cublasInit();
cublasAlloc(N, sizeof(float), (void**)&d_x);
cublasAlloc(N, sizeof(float), (void**)&d_y);

cublasSetVector(N, sizeof(x[0]), x, 1, d_x, 1); // CPU -> GPU
cublasSetVector(N, sizeof(y[0]), y, 1, d_y, 1); // CPU -> GPU

// Perform SAXPY: d_y[]=a*d_x[]+d_y[]

cublasSaxpy(N, 2.0, d_x, 1, d_y, 1)

cublasGetVector(N, sizeof(y[0]), d_y, 1, y, 1); // GPU -> CPU

cublasFree(d_x);
cublasFree(d_y);
cublasShutdown();
```

CUBLAS ZGEMM Performance



- cuBLAS 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

•Performance may vary based on OS ver. and motherboard config.

cuSPARSE sparse linear algebra

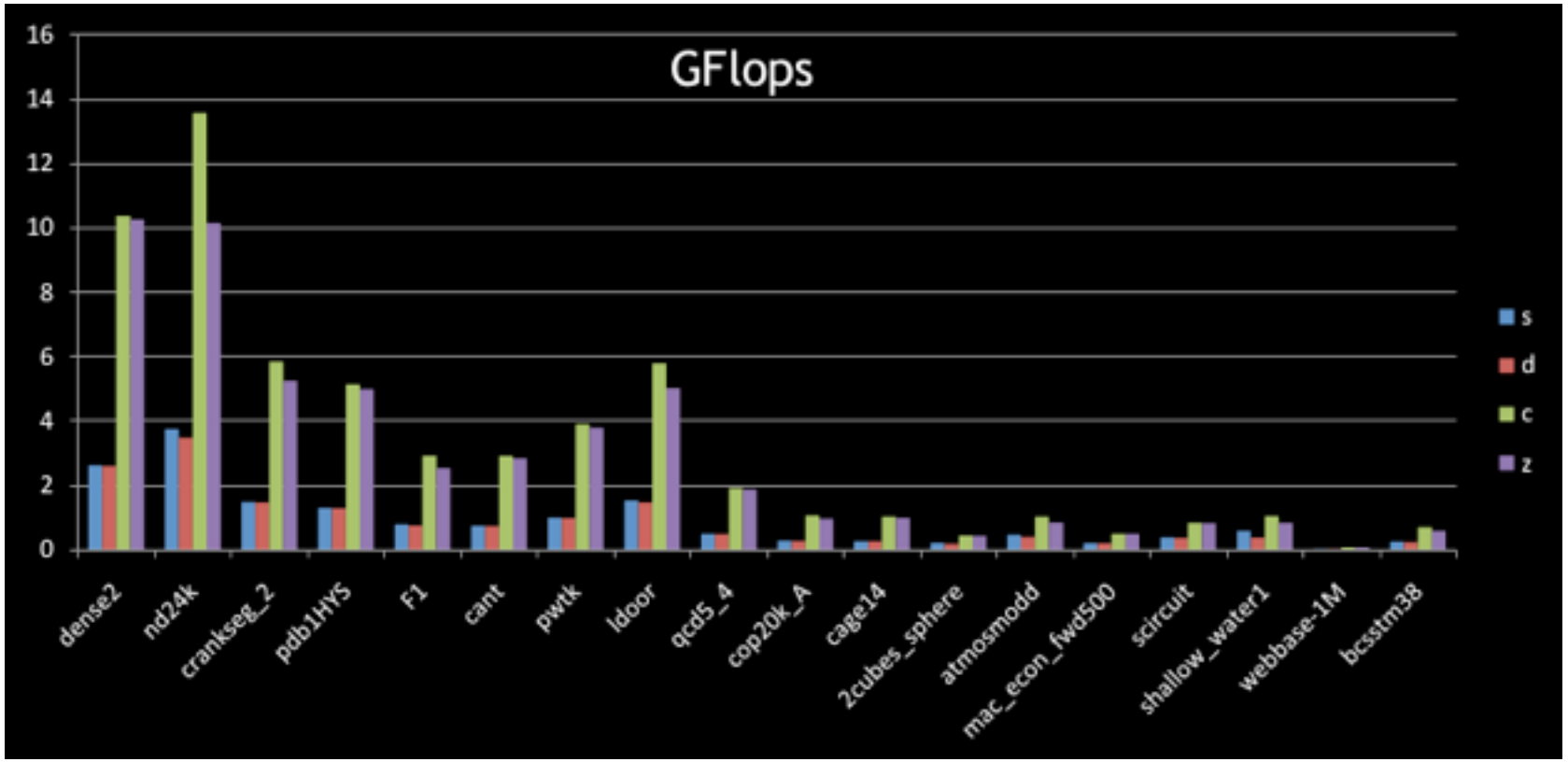
- Supports sparse (indexed) and dense formats for vectors, BLAS 1 operations for indexed vectors
- Various sparse formats for matrices (CSR, COO, ELL, hybrid ELL+COO, BSR, BSRx, ...)
- Matrix format conversions
- Sparse matrix-vector, matrix-matrix product
- Simplistic preconditioners

```
mkl_dcsrmv(transa, m, k,
alpha, descr, val, indx,
pntrb, pntre, x, beta, y);
```

```
err = cusparseDcsrmv(hdl,
transa, m, k, nnz, alpha,
desrc, val, indx, col,
x, beta, y);
```

cuSPARSE performance

CSR mat (transpose) x vec: C2050, ECC on,



https://developer.nvidia.com/cuSPARSE

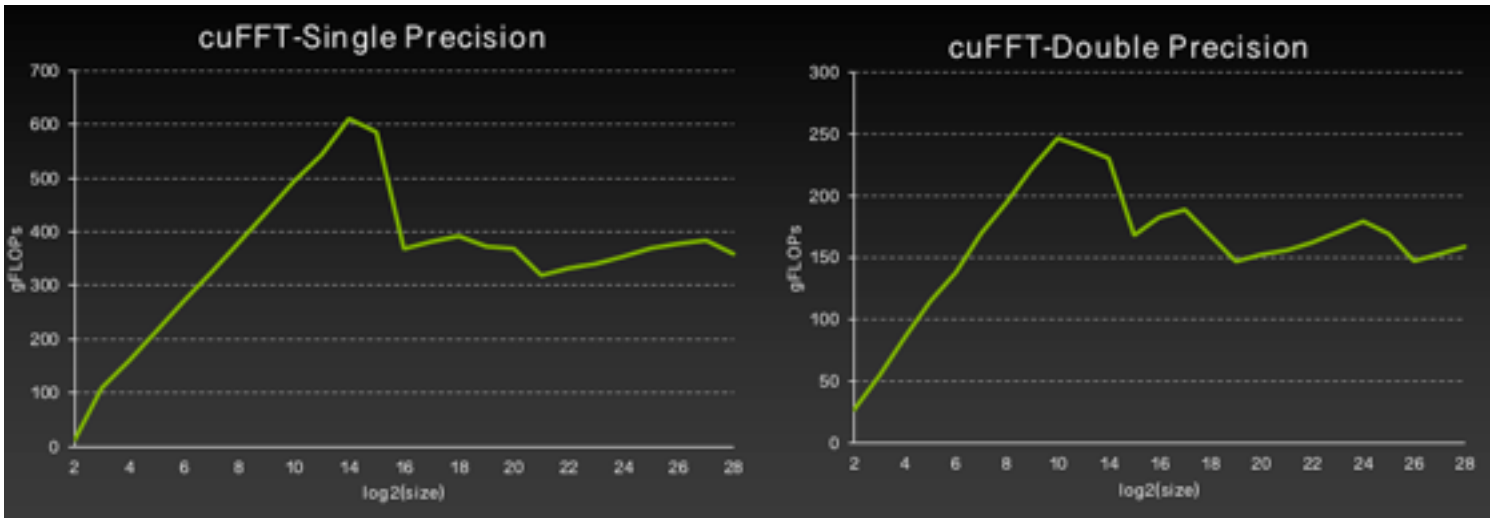
CUFFT Fast Fourier Transforms

Interface modeled after FFTW

```
fftw_plan PlanA;
fftw_plan_dft_2d(N, M, &PlanA,
data, data, FFT_FORWARD)
fftw_execute_dft(PlanA, data,
data);
```

```
cufftPlan2d PlanA;
cufftCreatePlan(N, M, &PlanA,
CUFFT_C2C);
cufftExecC2C(PlanA, d_data,
d_data, CUFFT_FORWARD);
```

1-D FFT perf. (NVIDIA)



cuRAND random numbers

- Large suite of high-quality random number generators
  - XORWOW, MRG323ka, MTGP32, scrambled Sobol
  - uniform, normal, log-normal
  - single and double precision
- Two APIs
  - Called from CPU: for large batches of random numbers

```
#include "curand.h"
curandCreateGenerator(&gen, CURAND_RNG_PSEUDO_DEFAULT);
curandGenerateUniform(gen, d_data, n);
```

  - Called from GPU: random numbers within kernels

```
#include "curand_kernel.h"
__global__ void generate_kernel(curandState *state) {
    int id = threadIdx.x + blockIdx.x * 64;
        x = curand(&state[id]);
}
```

MAGMA: Matrix Algebra on GPU and Multicore Architecture

- *MAGMA:* Matrix Algebra on GPU and Multicore Architectures http://icl.cs.utk.edu/magma
- Essentially LAPACK functionality on hybrid platforms
- CUDA + limited availability for Xeon Phi, OpenCL
- Developers/collaborators: UTK, UC Berkeley, UC Denver, INRIA, KAUST, others (including ETH)
- Distributed memory GPU platforms, coming soon??

Typical dense linear algebra algorithms

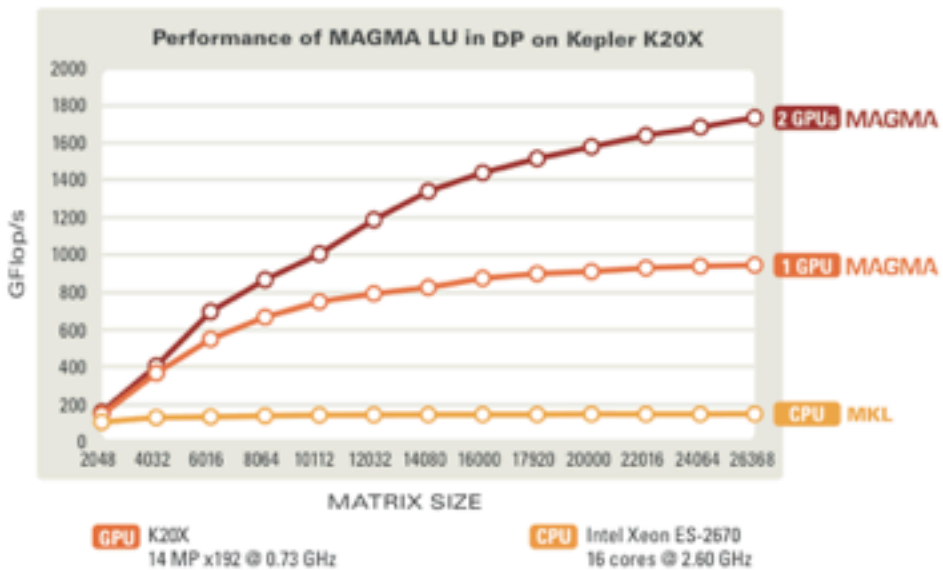
- Cholesky factorization: $A = A^T = LL^T \qquad i < j \Rightarrow L_{i,j} = 0$
- QR factorization: $A = QR \qquad Q^T Q = I \qquad i > j \Rightarrow R_{i,j} = 0$
- LU factorization: $A = P^T LU \qquad P^T P = I$
- Forward/back-substitution: $Ax = y \Rightarrow LUx = y \Rightarrow w = L^{-1}y \Rightarrow x = R^{-1}w$
- Eigenvalue decomposition: $Ax = \lambda x \Rightarrow A = QDQ^T$
- Generalized eigen-problem: $Ax = \lambda Bx$
- Singular value decomposition: $A = U\Sigma V^T \quad U^T U = I \quad V^T V = I$

MAGMA Overview (UTK)

HYBRID ALGORITHMS

MAGMA uses a hybridization methodology where algorithms of interest are split into tasks of varying granularity and their execution scheduled over the available hardware components. Scheduling can be static or dynamic. In either case, small non-parallelizable tasks, often on the critical path, are scheduled on the CPU, and larger more parallelizable ones, often Level 3 BLAS, are scheduled on the GPU.

PERFORMANCE

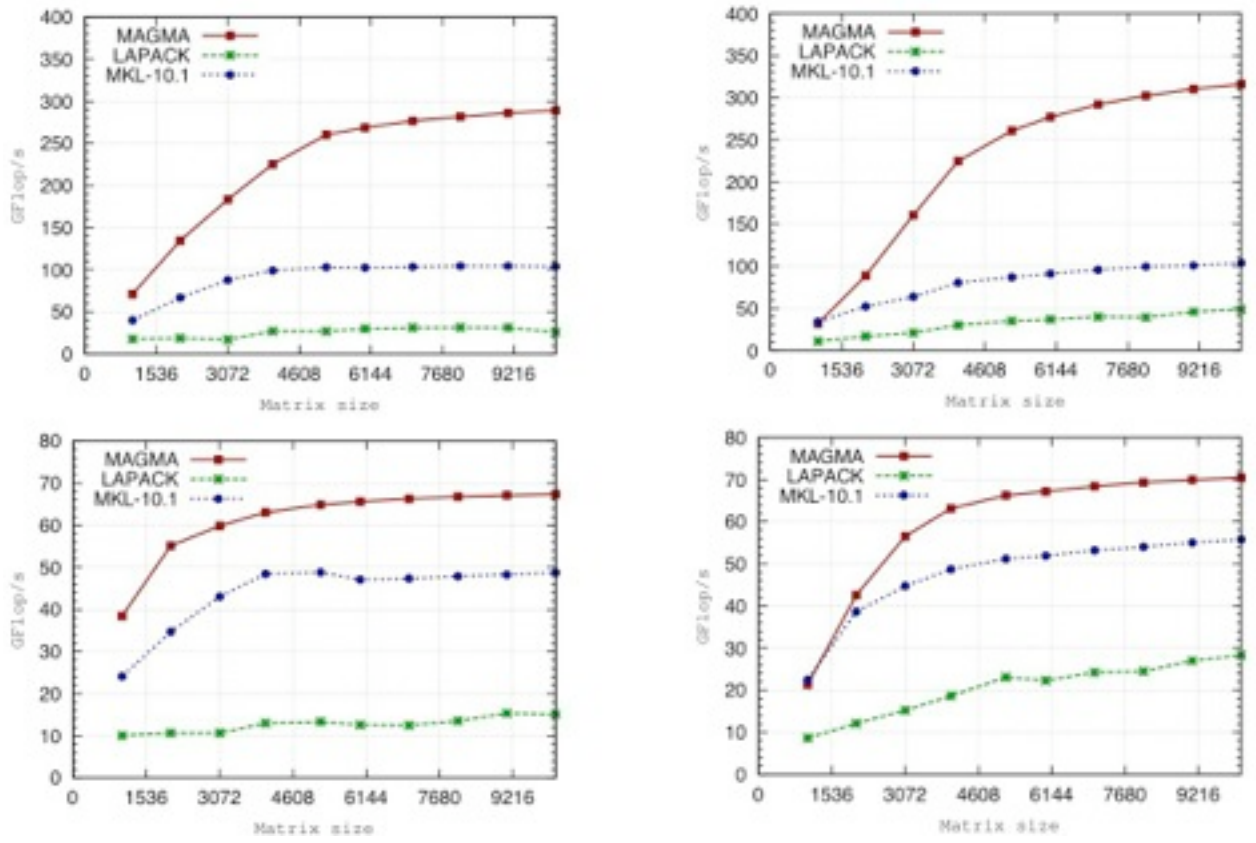


FEATURES AND SUPPORT

- MAGMA 1.3 FOR CUDA
- clMAGMA 1.0 FOR OpenCL
- MAGMA MIC 0.3 FOR Intel Xeon Phi

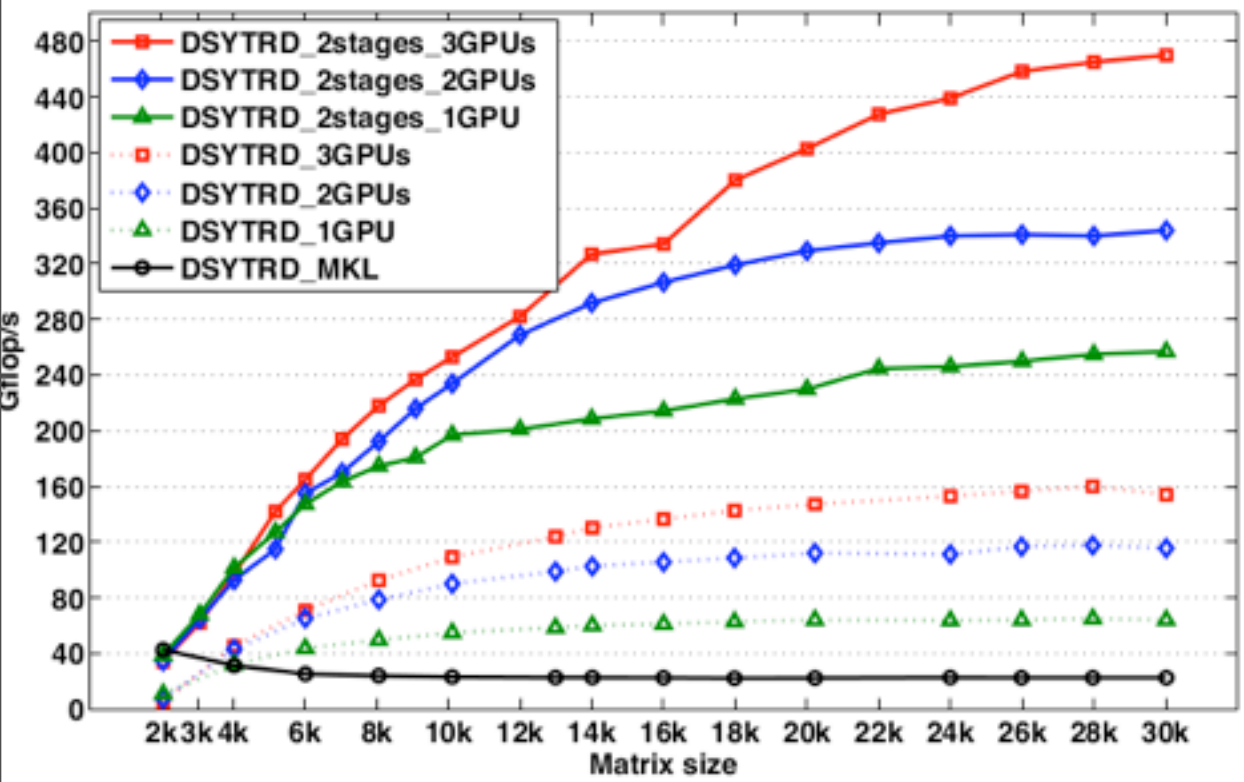
CUDA	OpenCL	Intel Xeon Phi	
●	●	●	Linear system solvers
●	●		Eigenvalue problem solvers
●			MAGMA BLAS
●			CPU Interface
●	●	●	GPU Interface
●	●	●	Multiple precision support
●			Non-GPU-resident factorizations
●			Multicore and multi-GPU support
●			Tile factorizations with StarPU dynamic scheduling
●	●	●	LAPACK testing
●	●	●	Linux
●			Windows
●			Mac OS

MAGMA Performance



MAGMA on GTX280 vs. Xeon quad core Left: QR decomp. SP/DP Right: LU decomp. SP/DP

MAGMA Gen EVP $Ax = \lambda Bx$



A. Haidar, S. Tomov, J. Dongarra, T. Schulthess, and R. Solca, *A novel hybrid CPU-GPU generalized eigensolver for electronic structure calculations based on fine grained memory aware tasks,* ICL Technical report, 03/2012.

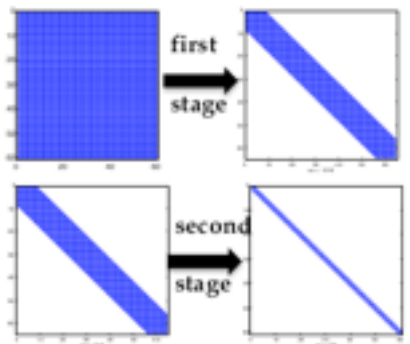
MKL Implementation

- Too many Blas-2 op,
- Relies on panel factorization,
- →Bulk sync phases,
- →Memory bound algorithm.

GPU 1-Stage

- Blas-2 GEMV moved to the GPU,
- Accelerate the algorithm by doing all BLAS-3
- →Bulk sync phases,
- →Memory bound algorithm.

GPU 2-Stage



tional intensity,
lly kernel,
ch,
equired, it has 1

MAGMA: conclusions

- Subset of LAPACK dense linear algebra functionality on hybrid multicore platforms (NVIDIA, Intel Xeon Phi, ...)
- *High quality, dependable implementation*
- Proven performance on single-node each with 1 or more GPUs
- *Clear need for distributed memory implementation*, some efforts are underway, e.g., `http://icl.cs.utk.edu/parsec` but no ScaLAPACK-like implementation in near future
- *Possible funding limitations...*

Thrust: Standard Template Library for GPUs

- A library of parallel algorithms resembling the C++ STL
- Allows easy access/manipulation of vectors on both host (CPU) and device (GPU); based on data *iterators*
- Defines straightforward vector data operators, e.g., :
  - ✳ initialize vectors
  - ✳ exchange existing values
  - ✳ copy one to another
  - ✳ transform with an operator
  - ✳ perform reductions (e.g., one-dimensional to scalar)
  - ✳ sorting and other operators

Thrust: typical operations

- Declare arrays on host or device

```
thrust::host_vector<int> H(4);
thrust::device_vector<int> D = H;
thrust::device_vector<int> Z(4, 1);  // All ones
```

- Initialize arrays, use iterators

```
thrust::sequence(H.begin(), H.end()); // H = (0,1,2,3)
thrust::fill(D.begin(), D.end(), 2);  // Fill with twos
```

- Transform arrays

```
thrust::transform(D.begin(), D.end(), Z.begin(), thrust::negate<int>());
thrust::replace(H.begin(), H.end(), 2, -2);
```

- Perform a reduction

```
int sum = thrust::reduce(D.begin(), D.end(), (int) 0, thrust::plus<int>());
```

- Sort array

```
thrust::sort(H, H + 4);
```

Thrust: simple manipulations

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>
#include <thrust/copy.h>
#include <thrust/fill.h>
#include <iostream>
int main(void)
{
  // initialize all ten integers of a device_vector to 1
  thrust::device_vector<int> D(10, 1);
  // initialize a host_vector with the first five elements of D
  thrust::host_vector<int> H(D.begin(), D.begin() + 5);
  // set the first seven elements of a vector to 9
  thrust::fill(D.begin(), D.begin() + 7, 9);
  // copy all of H back to the beginning of D
  thrust::copy(H.begin(), H.end(), D.begin());
  // print D
  for(int i = 0; i < D.size(); i++)
  {
    std::cout << "D[" << i << "] = " << D[i] << std::endl;
  }
  return 0;
}
```

Assignment: what values are printed?

Thrust: Exercise

- Compare host and device sorting of integer vectors
- Create device version from host version (given)
- `https://github.com/fomics/SummerSchool2014/wiki/Thrust-Exercise`
- Performance comparison

Thrust: conclusions

- Attempt to extend C++ STL functionality for host/device
- Based on CUDA, thus bound to NVIDIA GPUs
- Uses template meta-programming to find correct implementation at compile time
- Is an community, open-source project, *but appears to have long-term approval from NVIDIA* (bundled in SDK releases)
- *Development intended by NVIDIA to be demand-driven by community; in reality not really the case*

Linear solvers

Goal: Support the solution of linear systems,

$$Ax=b,$$

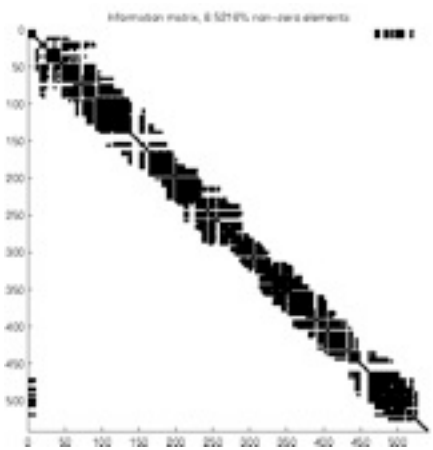
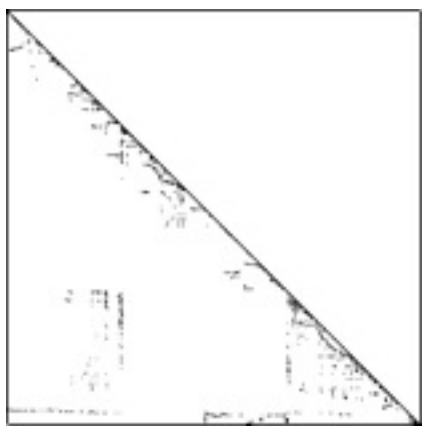
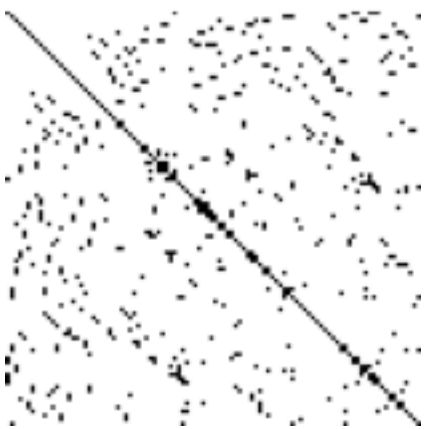
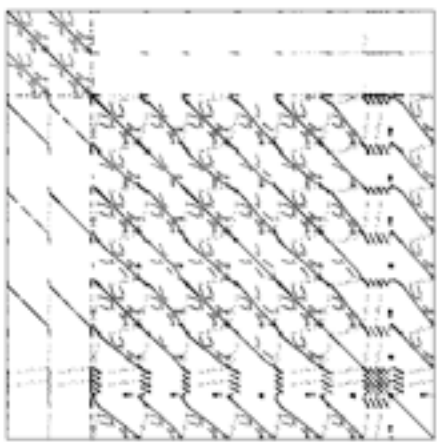
particularly for *sparse*, parallel problems, e.g., arising from PDE-based models.

User provides:

- *A (matrix or operator)*
- *b (right-hand side)*
- *u (initial guess)*

Libraries for Sparse Linear Algebra

- MAGMA limited to $m \times n$ matrices with $m,n = O(10^4)$
- Sparse matrices typically contain at least 90% zeros
- Number of non-zero (nz) elements, large: $nz = O(10^7)$
- Matrix market http://math.nist.gov/MatrixMarket/

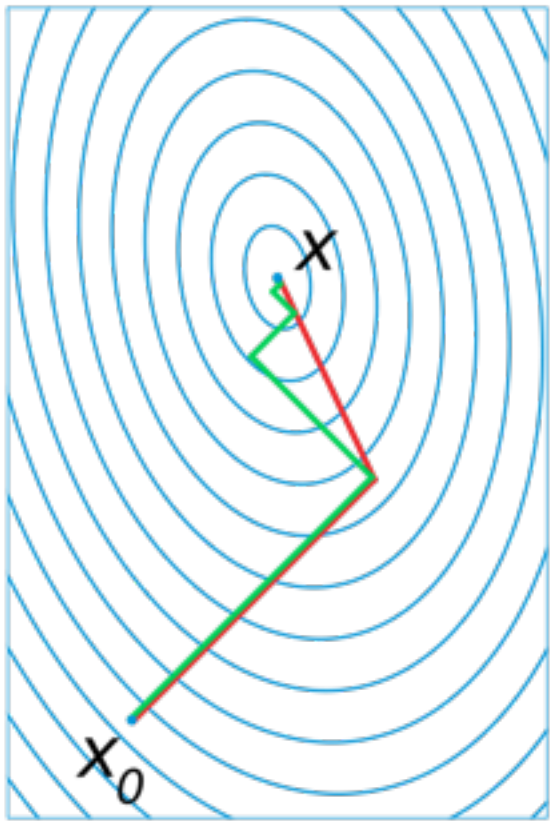





Linear System Solution: $Ax = b$

Two basic techniques:

- Direct methods, i.e. factorize matrix
  - good for multiple right hand sides
  - tend to be more robust
- Iterative methods
  - good if matrix known via operators
  - possibilities for approximate solutions

Hestenes/Stiefel, 1952: Conjugate Gradient



$$k = 0; \quad x_0 = 0; \quad r_0 = 0$$

$$while \quad r_k \neq 0 \quad \{$$

$$k = k + 1$$

$$if\,(k = 0) \Rightarrow p_1 = r_0$$

$$if\,(k > 0) \Rightarrow \beta_k = r_{k-1}^T r_{k-1} / r_{k-2}^T r_{k-2}; \quad p_k = r_{k-1} + \beta_k p_{k-1}$$

$$\alpha_k = r_{k-1}^T r_{k-1} / p_k^T A p_k$$

$$x_k = x_{k-1} + \alpha_k p_k$$

$$r_k = r_{k-1} - \alpha_k A p_k$$

$$\}$$

1980's: led to a wide class of iterative *Krylov subspace methods*

Preconditioners: KSM alone insufficient!

- CG method initially ignored due to slow convergence
  - Theoretical convergence after 2*n steps, but n is huge
  - Convergence rate related to ratio largest/smallest eigenvalue
- Easier problem: preconditioner $M \approx A$ $Ax = b \Rightarrow M^{-1}Ax = M^{-1}b$
  - Find an approximation for A where $M^{-1}x$ is 'easily' calculated
  - Possibilities:
    - Approximate inverse known through physical description
    - Incomplete LU decomposition
    - Sparse approximative inverse (assume inverse also sparse)
    - Multilevel (multigrid) preconditioners
    - More…

CUSP: Sparse Lin. Alg. for GPUs

- CUda SParse: a templated library for GPUs and CPUs, providing a high-level interface that hides GPU complexities (NVIDIA, Apache license)
- Built on top of Thrust (NVIDIA)

```
#include <cusp/hyb_matrix.h>
#include <cusp/io/matrix_market.h>
#include <cusp/krylov/cg.h>
int main(void)
{
    // create an empty sparse matrix structure (HYB format)
    cusp::hyb_matrix<int, float, cusp::device_memory> A;

    // load a matrix stored in MatrixMarket format
    cusp::io::read_matrix_market_file(A, "5pt_10x10.mtx");

    // allocate storage for solution (x) and right hand side (b)
    cusp::array1d<float, cusp::device_memory> x(A.num_rows, 0);
    cusp::array1d<float, cusp::device_memory> b(A.num_rows, 1);

    // solve the linear system A * x = b with the Conjugate Gradient
method
    cusp::krylov::cg(A, x, b);
    return 0;
}
```

CUSP: some extensions

- CUSP implementation of sparse approximate inverse preconditioner at CSCS/USI
- Requires least-squares minimization (QR factorization)
- GMRES solver (like CG for non-symmetric matrices)

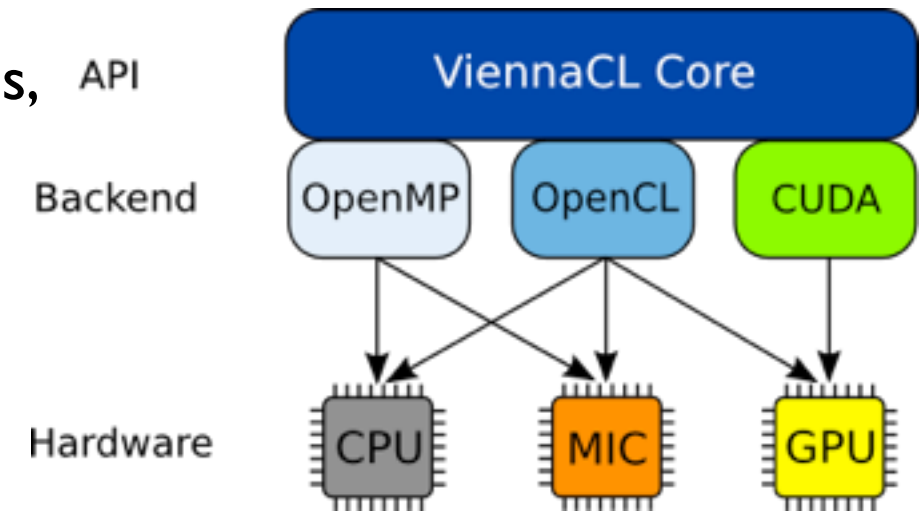
```
        std::cout << "\nSolving with SPAI preconditioner" << std::endl;
// allocate storage for solution (x) and right hand side (b)
        cusp::array1d<ValueType, MemorySpace> x(A.num_rows, 0);
        cusp::array1d<ValueType, MemorySpace> b(A.num_rows, 1);
              // set stopping criteria (iteration_limit = 1000, relative_tolerance = 1e-6)
        cusp::default_monitor<ValueType> monitor(b, 1000, 1e-6)

// setup preconditioner
        cusp::precond::spai<ValueType, MemorySpace> M(A, A);

// solve
        cusp::krylov::gmres(A, x, b, monitor, M);
```

CUSP: Some conclusions

- Template metaprogramming: conceptually easy to specify one template for different data types, e.g., single/double precision
- Only supports single node execution (*multi-node implementation should be at a higher level, anyway*)
- Has only CUDA backends: only for NVIDIA GPUs
- *Not supported by NVIDIA! Future: uncertain*
- Community effort, driven by user demand
- Location: `https://github.com/cusplibrary`

ViennaCL: Sparse Lin. Algebra on multiple platforms

- Linear algebra library for many core architectures (GPUs, CPUs, Intel Xeon Phi)
- Supports BLAS 1-3
- Iterative solvers
- Sparse row matrix-vector multiplication, solvers
- Goals:
  - ➡ Simplicity, minimal dependencies
  - ➡ Compatible with Boost.uBLAS, Eigen,...
  - ➡ Open source, header-only library



Boost: Solve linear system

```
using namespace boost::numeric::ublas;
matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);

/* Fill A, x, rhs here */

// Some operations
rhs += 2.0 * x;
double val = inner_prod(x, rhs);
matrix += val * outer_prod(x, rhs);

x = solve(A, rhs, upper_tag()); // Upper triangular solver

std::cout << " 2-norm: " << norm_2(x) << std::endl;
std::cout << "sup-norm: " << norm_inf(x) << std::endl;
```

ViennaCL: Solve linear system

```
using namespace viennacl;
using namespace viennacl::linalg;

matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);

/* Fill A, x, rhs here */

// Some operations
rhs += 2.0 * x;
double val = inner_prod(x, rhs);
matrix += val * outer_prod(x, rhs);

x = solve(A, rhs, upper_tag()); // Upper triangular solver

std::cout << " 2-norm: " << norm_2(x) << std::endl;
std::cout << "sup-norm: " << norm_inf(x) << std::endl;
```

ViennaCL: Memory Model

Memory buffers need to be managed differently for each of the compute backends (OpenMP, CUDA, OpenCL)

- Memory domain abstraction in class `viennacl::backend::mem_handle`
- Raw handles from `cuda_handle()`, `opencl_handle()` and `ram_handle()`
- backend is required to support:
  - ➡ `memory_create()`: Create a memory buffer
  - ➡ `memory_copy()`: Copy the (partial) contents of one buffer to another
  - ➡ `memory_write()`: Write from a memory location in CPU RAM to the buffer
  - ➡ `memory_read()`: Read from the buffer to a memory location in CPU RAM

ViennaCL: Interoperability

Standard C++ vectors and Boost uBLAS vectors can be passed to/from ViennaCL vectors:

```
std::vector<double> std_x(100)
ublas::vector<double> ublas_x(100);
viennacl::vector<double> vcl_x1, vcl_x2;

/* setup of std_x and ublas_x omitted */
viennacl::copy(std_x.begin(), std_x.end(), vcl_x1.begin());
viennacl::copy(ublas_x.begin(), ublas_x.end(), vcl_x2.begin());
```

ViennaCL: Solve sparse system

```
using namespace viennacl;
using namespace viennacl::linalg;
compressed_matrix<double> A(1000, 1000);  // sparse matrix format
vector<double> x(1000), rhs(1000);
/* Fill A, x, rhs here */
x = solve(A, rhs, cg_tag()); // Conjugate Gradient solver
x = solve(A, rhs, bicgstab_tag()); // BiCGStab solve
x = solve(A, rhs, gmres_tag()); // GMRES solver
```

uBLAS has no iterative solvers, but thanks to compatibility

```
using namespace boost::numeric::ublas;
using namespace viennacl::linalg;
compressed_matrix<double> A(1000, 1000);
vector<double> x(1000), rhs(1000);
/* Fill A, x, rhs here */
x = solve(A, rhs, cg_tag()); // Conjugate Gradient solver
x = solve(A, rhs, bicgstab_tag()); // BiCGStab solver
x = solve(A, rhs, gmres_tag()); // GMRES solver
```

ViennaCL: temporaries

Consider the expression

```
vec1 = vec2 + alpha * vec3 - beta * vec4;
```

With naive C++ this could be equivalent to

```
tmp1 <- alpha * vec3
tmp2 <- beta * vec4;
tmp3 <- tmp1 - tmp2;
tmp4 <- vec2 + tmp3;
vec1 <- tmp4;
```

Temporaries are costly on CPUs, even more so on GPUs

➡ *Expression templates* reduce usage of temporaries

ViennaCL: Exercises

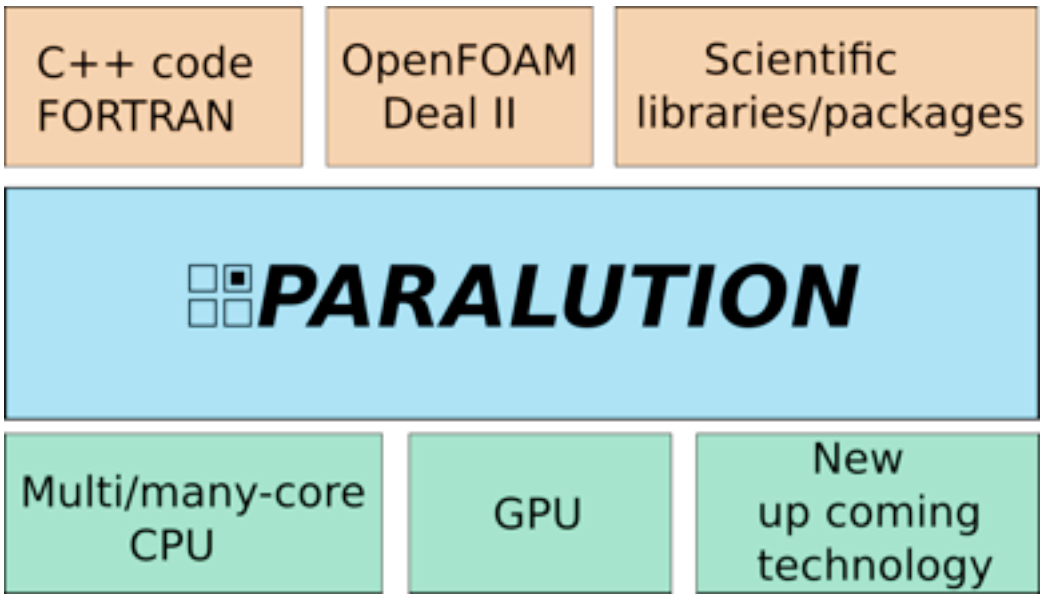
- Compile and run uBLAS version of sparse matrix-vector multiply version on CPU
- Create device version from host version (given)
- https://github.com/fomics/SummerSchool2014/wiki/ViennaCL-Exercise
- Performance comparison

ViennaCL Conclusions

- A logical extension of Boost uBLAS template library
- Backends for OpenMP, OpenCL and CUDA
- Runs on CPUs, Intel Xeon Phi, NVIDIA + AMD GPUs
- Actively supported by ViennaCL team
- Krylov-subspace solvers, minimal spectrum of preconditioners
- *Performance results are evolving*
- Interoperates with other libraries:
  - Eigen
  - PETSc
  - others...

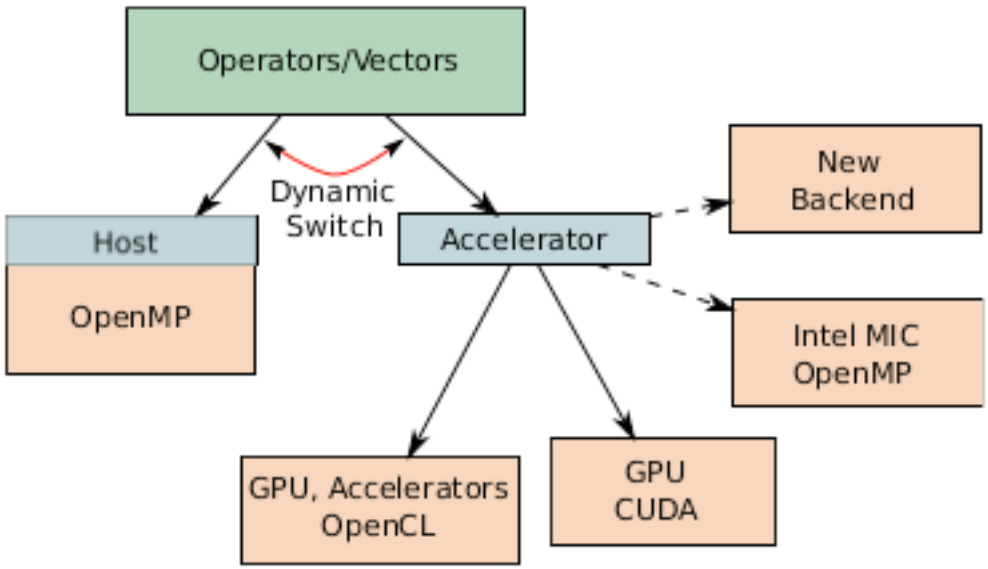
➡ *Promising library supporting high-level linear algebra*

PARALUTION: Sparse Linear Algebra on multiple platforms



- *Sparse Iterative solvers & preconditioners*
- *Targeted: CPUs + accelerators*
- *Hardware abstraction*
- *OpenMP/CUDA/OpenMP opaque to user*
- *Code portable*
- *GPL v3*
- *http://www.paralution.com*

Dynamic switch to accelerator



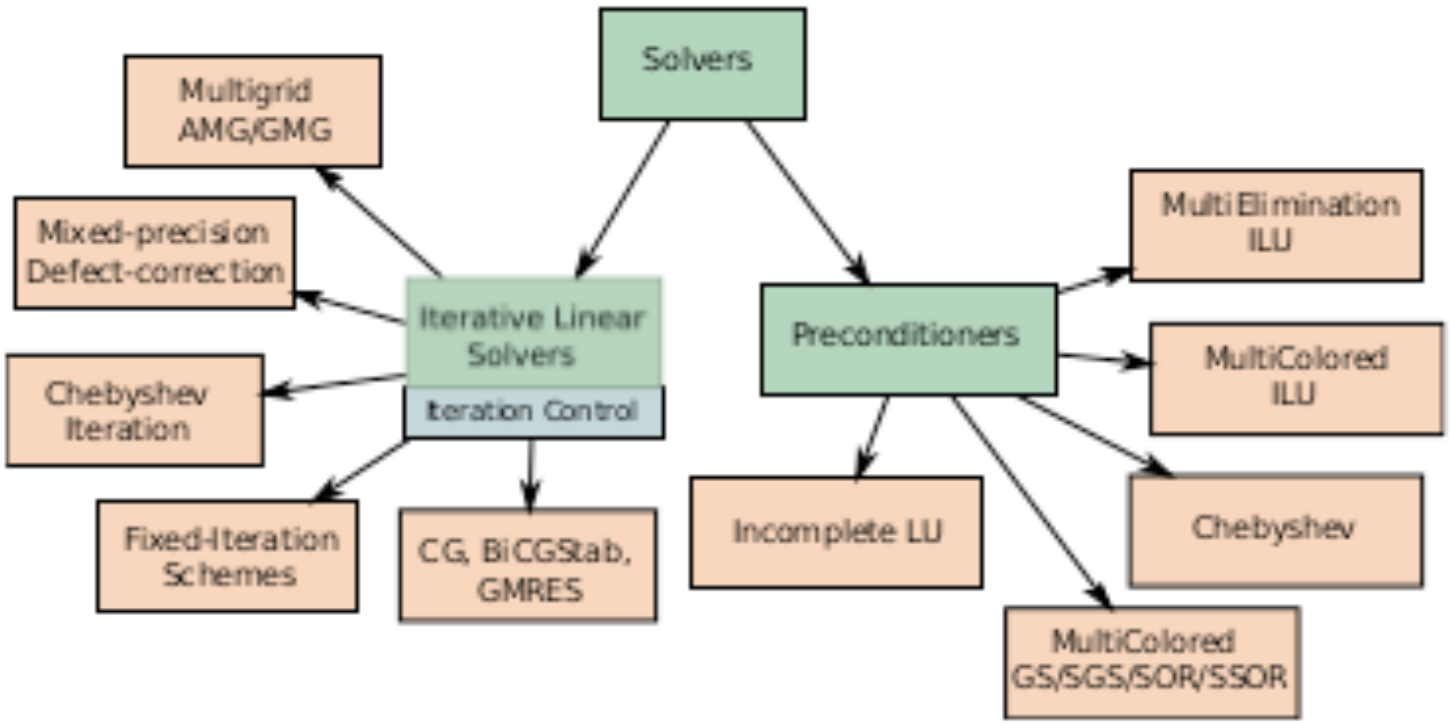
Accelerated execution takes place on accelerator, if one found at run time

Paralution: matrix-vector product

```
LocalMatrix<ValueType> A;
LocalVector<ValueType> x, y ;
A.ReadFileMTX("my_matrix.mtx");
x.Allocate("vector1", mat.get_nrow());
y.Allocate("vector2", mat.get_ncol());
// y = A x
A.Apply(x, &y);
// Print the product of x and y
std::cout << x.Dot(y) << std::endl;
```


```
A.MoveToAccelerator();
x.MoveToAccelerator();
y.MoveToAccelerator();
A.Apply(x, &y);
std::cout << x.Dot(y) << std::endl;
```

Paralution: solvers, preconditioners



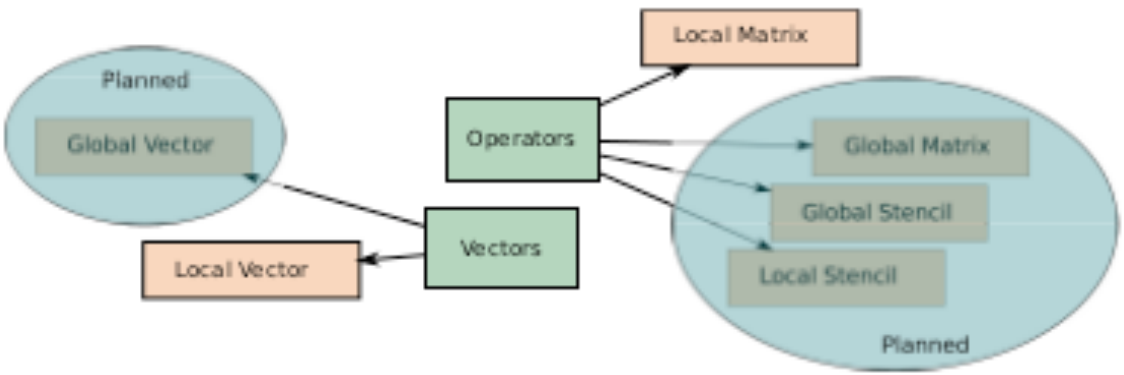
Paralution: solver example

```
CG<LocalMatrix<ValueType>, LocalVector<ValueType>, ValueType > ls;
MultiColoredILU<LocalMatrix<ValueType>, LocalVector<ValueType>, ValueType > p;

ls.SetOperator(mat);
ls.SetPreconditioner(p);
ls.Build();

ls.MoveToAccelerator();
mat.MoveToAccelerator();
rhs.MoveToAccelerator();
x.MoveToAccelerator();

ls.Solve(rhs, &x);
```

Paralution Conclusions

- Accelerator support more hidden, determined at run-time
- Multiple backends for OpenMP, OpenCL and CUDA
- Actively supported by Paralution team
- Krylov-subspace solvers, minimal spectrum of preconditioners
- Performance results are evolving

➡ Plans for multi-node implementation, stencil operators



Beyond single node linear algebra

So perhaps single-node sparse/dense linear algebra is covered

- What about distributed memory parallelism?
- What about problems beyond linear algebra?
- Fact: there are solid MPI-GPU development efforts ongoing:
  - ➡ D-MAGMA (e.g. ParSEC, related efforst)
  - ➡ PETSc (next slides)
  - ➡ Trilinos (next slides)
- *Current multi-node GPU support for non-linear problems, optimizations, eigenvalue problems and others is provisional at best!*

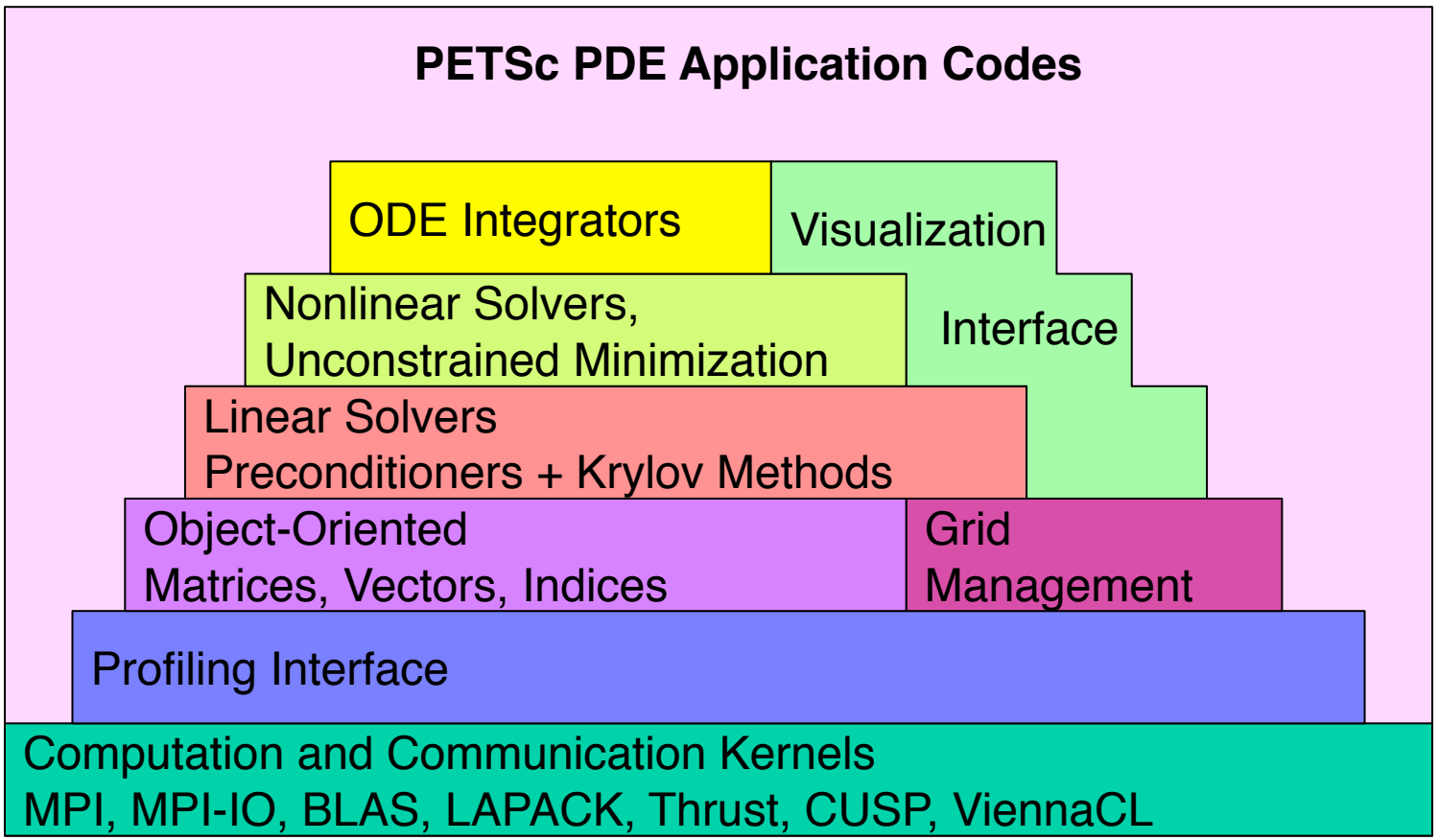
What is PETSc ?

- Supports non-linear PDE problems
- A freely available (and supported!) research code
  - Available via http://www.mcs.anl.gov/petsc
  - Free for everyone, including industrial users
  - Hyperlinked documentation and manual pages for all routines
  - Many tutorial-style examples
  - Support via email: petsc-maint@mcs.anl.gov
  - Current version: 3.3 (released Jun. 5, 2012)
- Portable to any parallel system supporting MPI
  - Tightly coupled systems, e.g., Cray XK6, XE6

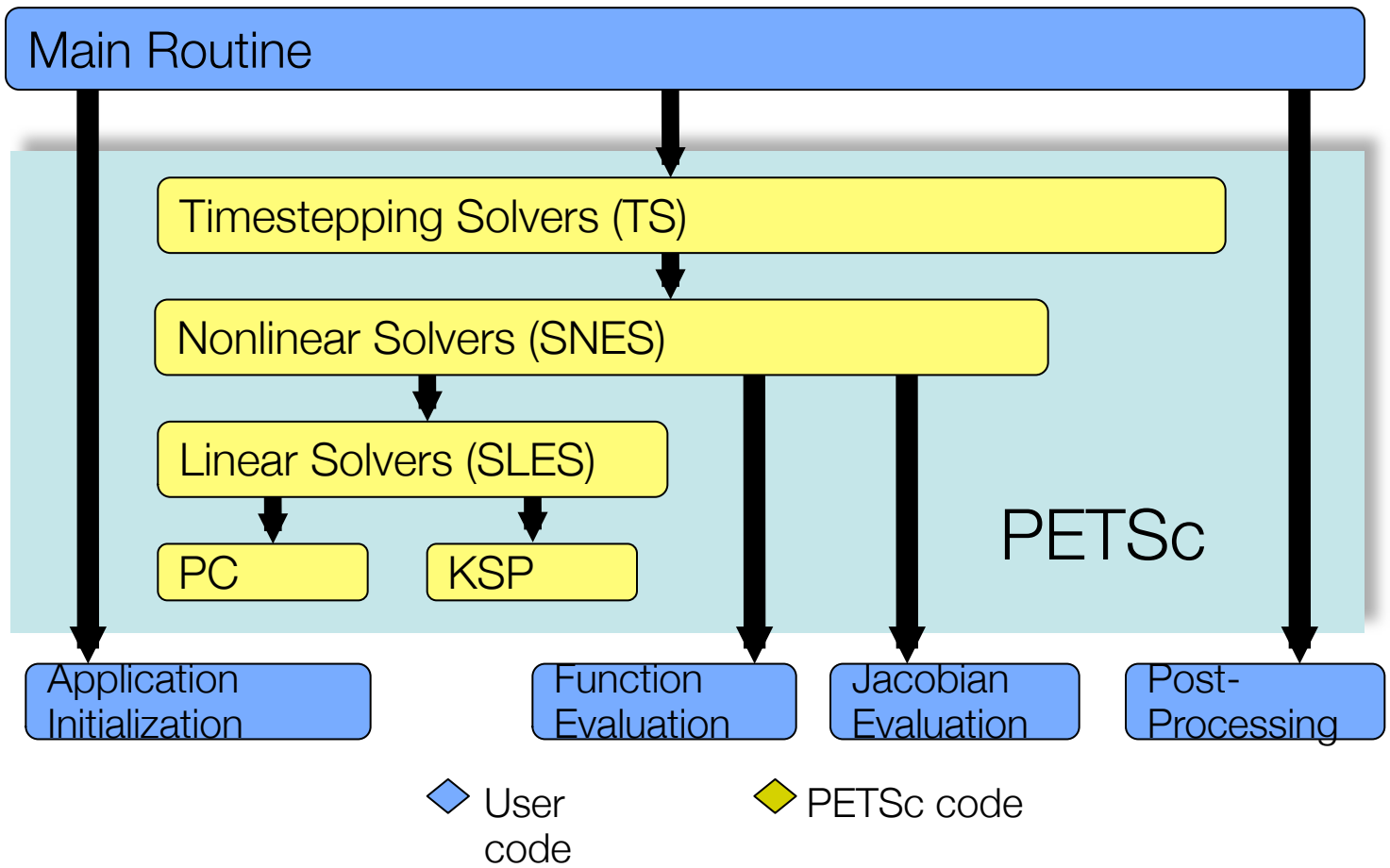
PETSc Concepts

- To specify the mathematics of the problem:
  - Programmer manipulates mathematical objects (sparse matrices, nonlinear equations), algorithmic objects (solvers) and discrete geometry (meshes)
- To solve the problem:
  - Solvers: linear, nonlinear, and time stepping (ODE)
- Parallel computing considerations:
  - Parallel data layout, e.g., structured and unstructured meshes

Structure of PETSc



Flow control for PDE solution



PETSc Programming Model

- **Goals**
  - Portable, runs everywhere, including heterogeneous multi-core
  - Performance
  - Scalable parallelism
- **Approach**
  - Distributed memory, “shared-nothing”
    - Access to data on remote machines or nodes through MPI
  - Can still exploit node parallelism on each node (e.g., SMP), with limitations (see PETSc home page)
  - Hide within parallel objects the details of the communication
  - User orchestrates communication at a higher abstract level than message passing
  - Additional classes added for GPU support

PETSc Data Objects

- Vectors (Vec)
  - focus: field data arising in nonlinear PDEs
- Matrices (Mat)
  - focus: linear operators arising in nonlinear PDEs (i.e., Jacobians)

beginner	• Object creation
beginner	• Object assembly
intermediate	• Setting options
intermediate	• Viewing
advanced	• User-defined customizations

Parallel Vector and Matrix Assembly

- Processors may generate any entries in vectors and matrices
- Entries need not be generated on the processor on which they ultimately will be stored
- PETSc automatically moves data during the assembly process if necessary

PETSc Communication

- MPI communicators (MPI_Comm) specify collectivity (processors involved in a computation)
- All PETSc creation routines for solver and data objects are collective with respect to a communicator, e.g.,

– `VecCreate(MPI_Comm comm, int m, int M, Vec *x)`

- Some operations are collective, while others are not, e.g.,

– collective: `VecNorm()`

– not collective: `VecGetLocalSize()`

- If a sequence of collective routines is used, they **must** be called in the same order on each processor

PETSc Linear Solvers (subset)

Krylov Methods (KSP)

- Conjugate Gradient
- GMRES
- CG-Squared
- Bi-CG-stab
- Transpose-free QMR
- etc.

Preconditioners (PC)

- Block Jacobi
- Overlapping Additive Schwarz
- ICC, ILU via BlockSolve95
- ILU(k), LU (sequential only)
- etc.

PETSc: evolving GPU support

PETSc GPU Model

- Each MPI process has access to a single GPU, which has its own memory
- Backends for CUSP, CUSparse and ViennaCL available
- New implementations of **Vec** and **Mat (type at run-time)**
  - ➡ Vectors with types `VECSEQCUSP`, `VECMPICUSP`, or `VECCUSP`
  - ➡ Matrices with types `MATSEQAIJCUSP`, `MATMPIAIJCUSP`, or `MATAIJCUSP`
  - ➡ Matrices with types `MATSEQAIJCUSPARSE`, `MATMPIAIJCUSPARSE`, or `MATAIJCUSPARSE`

PETSc: GPU support

Objects support both CPU and GPU copy of data, and carry flags indicated the validity of the data

PETSC_CUDA_UNALLOCATED	Memory not allocated on GPU
PETSC_CUDA_GPU	Values on GPU are current
PETSC_CUDA_CPU	Values on CPU are current
PETSC_CUDA_BOTH	Values on both devices current

Implementations for GPU-CPU data movement

- `VecCUDACopyToGPU`
- `VecCUDACopyFromGPU`
- `...`

these are generally used internally in solvers

PETSc: GPU support

How it works, at least conceptually

- User needs to specify types of vectors and matrices at run time
- Functionality invoked from backend (CUSP, CUSparse, ViennaCL, if available)
- Implementation should be transparent to user
- Alternatively, user can program in CUDA and access device objects directly, directly call thrust:: and cusp:: operators, etc.

PETSc Summary

- PETSc library of PDE/ODE solvers
- *Extensive selection of solvers, high quality, good support, free*
- *However: much more effective for new code*
- *Saddled by design choices, e.g., not thread-safe*
- Monolithic: one package tries to solve all, though there are adaptors to other libraries
- *MPI-GPU support in development version, in principle can be invoked at run-time. Interfaces to CUSP, CUSparse, ViennaCL*

Trilinos: a 'pearl necklace' of packages

Object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems

- http://trilinos.sandia.gov
- http://code.google.com/p/trilinos/wiki/TrilinosHandsOnTutorial

Trilinos: parallel packages (with GPU support)

- Basic linear algebra: *Epetra/EpetraExt (C++), Tpetra (C++ templates)*
- Preconditioners: *AztecOO, Ifpack2, ML, Meros*
- Iterative linear solvers: *AztecOO, Belos*
- Direct linear solvers: *Amesos (SuperLU, UMFPACK, MUMPS, ScaLAPACK, …)*
- Non-linear / optimization solvers: *NOX, MOOCHO*
- Eigensolvers: *Anasazi*
- Mesh generation / adaptivity: *Mesquite, PAMGEN*
- Domain decomposition: *Claps*
- Partitioning / load balance: *Isorropia, Zoltan2*

Trilinos: *Kokkos* Compute Model

- How to make shared-memory programming generic:
  - ➡Parallel reduction is the intersection of dot() and norm1()
  - ➡Parallel for loop is the intersection of axpy() and mat-vec
  - ➡We need a way of fusing kernels with these basic constructs.
- *Template meta-programming* is the answer
  - ➡This is the same approach that Intel TBB and Thrust take
  - ➡Has the effect of requiring that Tpetra objects be templated on Node type.

Trilinos: Generic Parallel Constructs

Node provides generic parallel constructs, user fills in the rest

Parallel FOR:

```
template <class WDP> void Node::parallel_for(int beg, int end, WDP workdata);
```

Work-Data Pair (WDP) struct provides:

- loop body via `WDP::execute(i)`

Parallel REDUCE:

```
template <class WDP> WDP::ReductionType
Node::parallel_reduce(int beg, int end, WDP workdata);
```

Work-Data Pair (WDP) struct provides:

- Reduction type `WDP::ReductionType`
- Element generation via `WDP::generate(i)`
- Reduction via `WDP::reduce(x,y)`

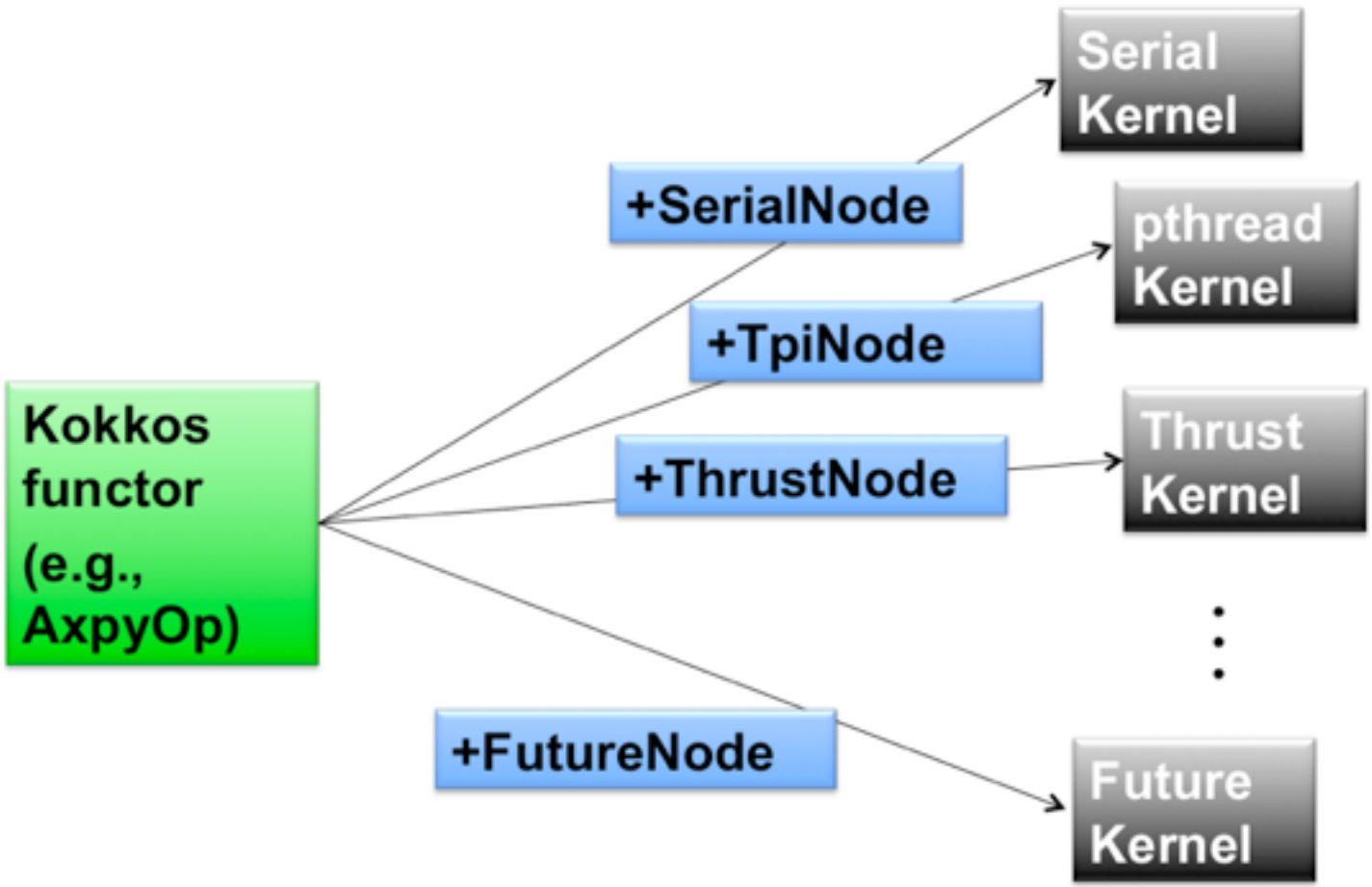
Kokkos: axpy implementation

```
template <class WDP> void
Node::parallel_for(int beg, int end, WDP workdata);

template <class T> struct AxpyOp
{const T* x;
  T* y;
  T alpha, beta;
  void execute(int i) { y[i] = alpha*x[i] + beta*y[i]; }
};

AxpyOp<double> op;
op.x = ...; op.alpha = ...;  op.y = ...;  op.beta = ...;
node.parallel_for< AxpyOp<double> > (0, length, op);
```

Kokkos: dot product

```
template <class WDP> WDP::ReductionType
Node::parallel_reduce(int beg, int end, WDP workdata);

template <class T> struct DotOp
{typedef T ReductionType;
  const T* x, y;
  T identity() { return (T)0;}T alpha, beta;
  T generate(int i) { return x[i]*y[i]; }
  T reduce(T x, T y) { return x + y; }
};

DotOp <float> op;
op.x = ...; op.y = ...;
float dot;
dot = node.parallel_reduce < DotOp<float> > (0, length, op);
```

Kokkos: compile-time kernel specialization



Anasazi: Eigenvalues/vectors of large, sparse matrices

- Techniques based on Lanczos iteration (symm. A)

$$r_0 = q_1; \quad \beta_0 = 1; \quad q_0 = 0; \quad j = 0$$

$$while \quad \beta_j \neq 0 \quad \{$$

$$q_{j+1} = r_j / \beta_j; \quad j = j + 1; \quad \alpha_j = q_j^T A q_j$$

$$r_j = (A - \alpha_j I) q_j - \beta_{j-1} q_{j-1}; \quad \beta_j = \left\| r_j \right\|_2$$

$$\}$$

- Lanczos vectors: q_j
- Form tridiagonal matrix T: diagonal α_j subdiagonal β_j
- Diagonalization of T is stable iterative procedure

Anasazi: classes for $Ax = \lambda Bx$

- `Anasazi::Eigenproblem`
  - Contains components of eigen-problem
  - setOperator, SetA, SetB, setPrec, setInitVec
- `Anasazi::Eigensolution`
  - Manages the solution of the eigen-problem
- `Anasazi::Eigensolver`
  - Defines interface which must be met by any solver
  - Currently implemented solvers: BlockDavidson, BlockKrylovSchur, LOBPCG
- `Anasazi::SolverManager`
  - 'Turn-key' class to use existing eigen-solvers

NOX: non-linear equations

- Solve $F(x) = 0$ with $F(x) = \begin{pmatrix} f_1(x_1, \cdots, x_n) \\ \vdots \\ f_n(x_1, \cdots, x_n) \end{pmatrix}$ and $J_{i,j} = \frac{\partial F_i}{\partial x_j}(x)$
- User supplies:
  - Function F(x) evaluation
  - Optional: Jacobian evaluation, preconditioner
- With good guess, convergence quadratic
- Heuristics used to improve first guess
- PETSc interface available
- http://trilinos.sandia.gov/packages/nox/

Trilinos Summary

- Non-monolithic set of packages, some interoperating tightly, some loosely, some not at all
- Large development team, free software, technically advanced, latest solvers, following emerging technologies (e.g. GPUs)
- Solvers are opaque, hard to see internals, bugs can be hard to deal with
- GPU implementation through Kokkos abstraction, only *NOX, Tpetra,Belos, Anasazi, Ifpack2, Zoltan2*

GPU-enabled Libraries Summary

- The take home message is:

  Don't recreate the wheel

- A limited number of GPU-libraries available, e.g. CUxxxx (vendor), Thrust, ViennaCL, ...
- Parallel distributed memory libraries in development, e.g., D-MAGMA, PETSc, Trilinos, within overarching message-passing framework
- *BUT: current GPU library support is sobering*

Acknowledgments

- The PETSc team
- Trilinos team
- UT, Knoxville: Innovative Computing Laboratory
- NVIDIA