An Abstract Node API for Heterogeneous and Multi-core Computing

Christopher G. Baker
Michael A. Heroux
Sandia National Laboratories

LACCS 2008

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

DMP vs. SMP

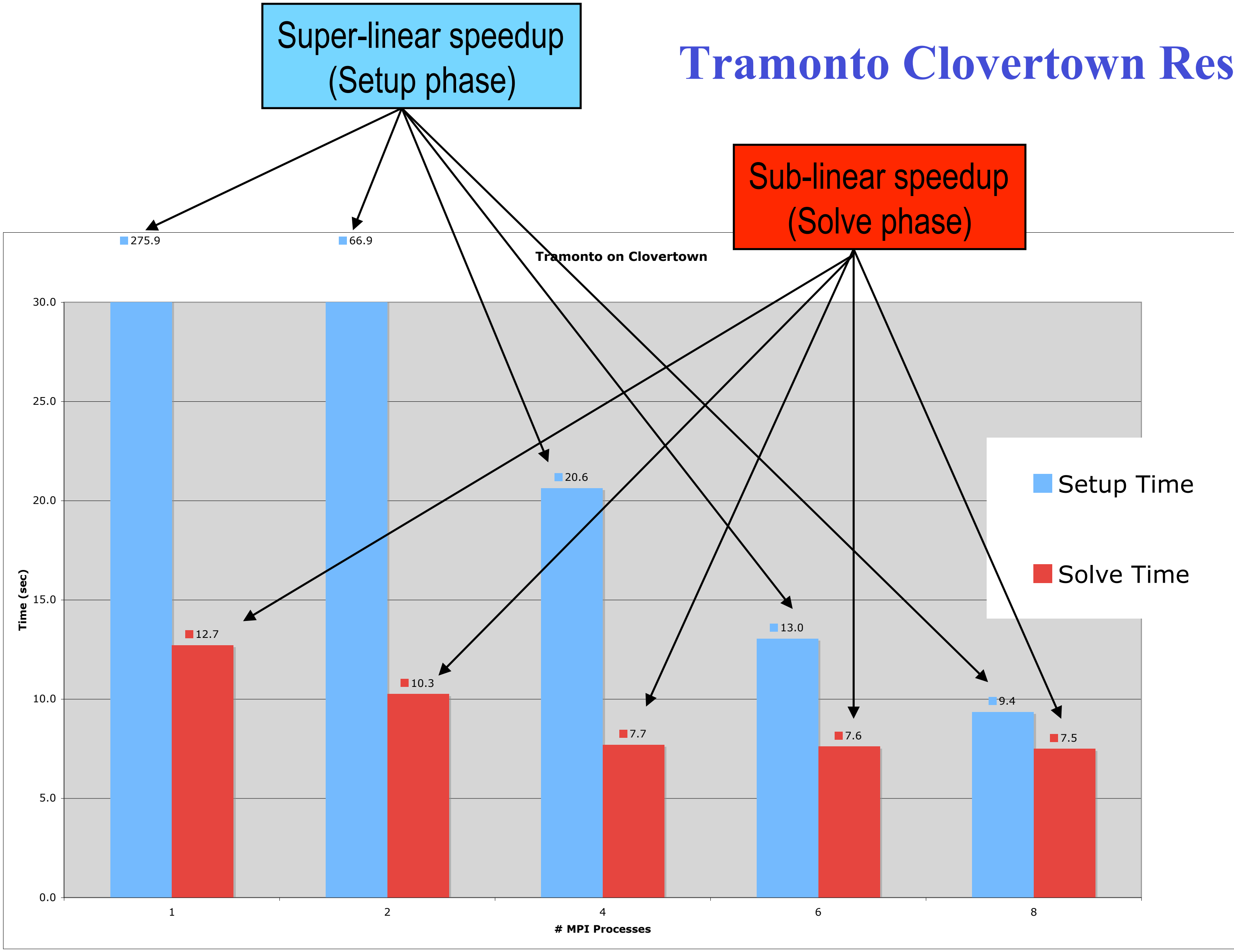
- Parallel computing has targeted two dominant architectures over the past decades.
- Highly scalable distributed systems:
  - programmed as a flat network of serial nodes
  - employs message passing interface, typically MPI
- Moderately scalable shared memory systems:
  - programmed indirectly using, e.g., OpenMP or directly via some threading API (e.g., Pthreads)
- The latter approach cannot be applied to systems of the former type.
- The former (MPI-based) approach **can** be used on systems of the latter type.

Sandia National Laboratories

MPI-Only Programming Model

- Dominant approach: a collection of nodes communicate via message passing API such as MPI.
- In the presence of SMP nodes, possible approaches are:
  - MPI under MPI
  - employ hybrid MPI+threads approach
  - maintain the "flat" MPI-Only model
- Flat MPI: `k` cores each on `m` nodes → `O(k*m)` MPI processes
- "SMP-aware" MPI implementations allowed flat MPI approach to maintain dominance
  - shared memory copies for local communication
  - single copy of application per node reduces overhead
- Full performance benefit may not be fully realizable.

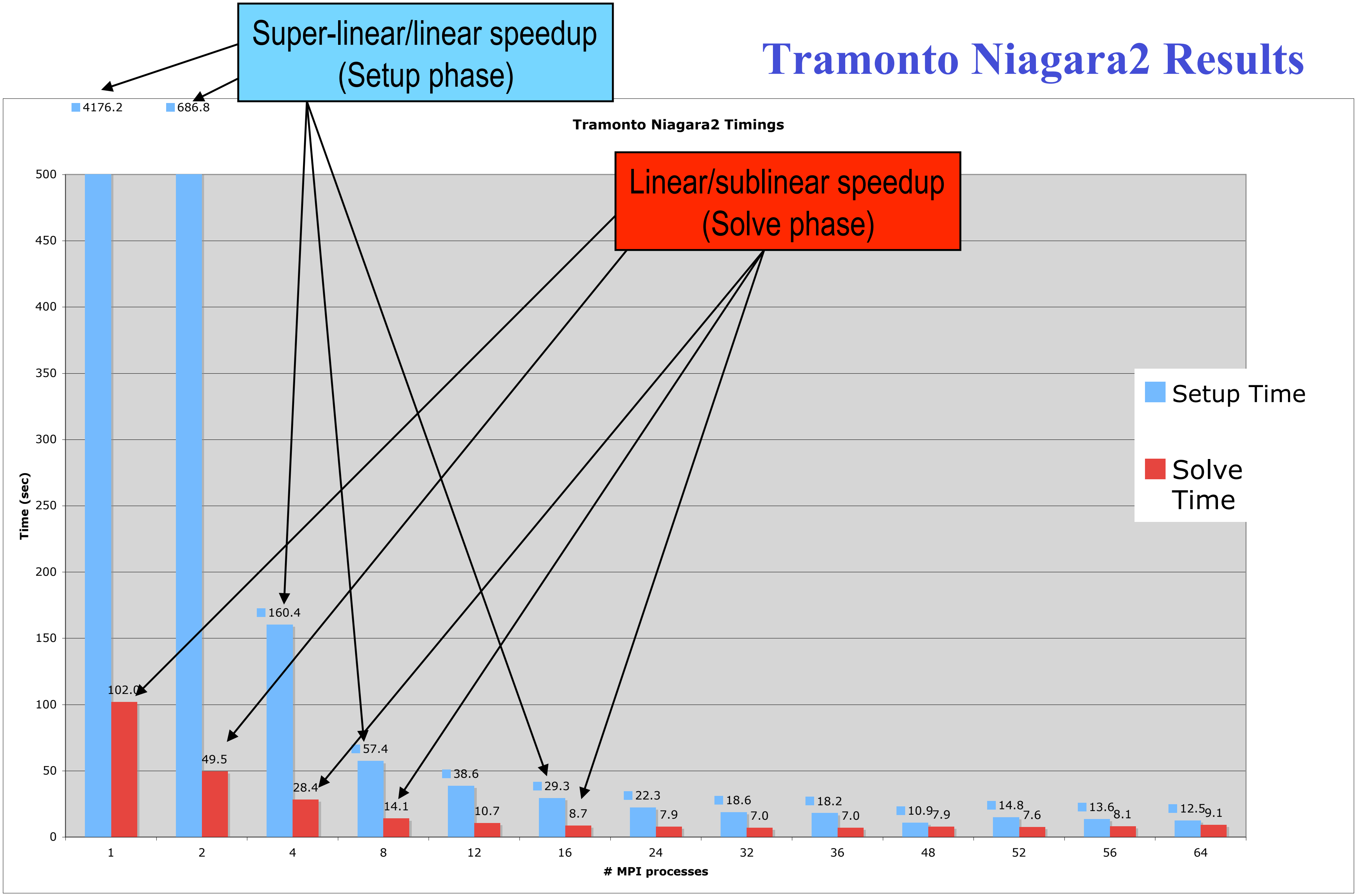
Tramonto Clovertown Results



- Setup (The application code itself): Excellent MPI-only.
- Solve (libraries): Much poorer. Inherent in algorithms.

Sandia National Laboratories

Tramonto Niagara2 Results



Addressing These and Other Issues

- Disappointing kernel performance is not due to poor implementation:
  - memory subsystem cannot fully exploit all cores on the node
  - solver algorithms may be handicapped by smaller domains
- General consensus is that the number of cores per node will continue to increase for a while.
  - These multicore architectures look like the SMP machines of yesterday.
  - However, now they are ubiquitous.
  - Furthermore, it seems necessary to exploit them due to slowing single-core performance gains.
  - Solution: Apply known SMP algorithms from the past decades of research.

Sandia National Laboratories

Other Items On Our Wishlist

- Support for multi-precision:
  - Double-precision is not always questioned in scientific computing.
  - Single-prec. floating point arithmetic can be significantly faster.
  - Smaller word size puts less strain on taxed memory hierarchy.
  - Multi-precision algorithms allow combination of fast arithmetic and need for higher accuracy.
- Support for newer architectures:
  - FPGA, GPU, CBE, ???
- Can achieve these via a general purpose programming environment with runtime support for desired platforms.
  - e.g., Sequoia, RapidMind
  - Too much trouble for me.
  - Instead, narrow scope to our libraries (i.e., those pesky solvers).

Sandia National Laboratories

Tpetra Abstract Interfaces

- We propose a set of abstract interfaces for achieving these goals in the Tpetra library of linear algebra primitives.
- Tpetra is a templated implementation of the Petra Object Model:
  - these classes provide data services for many other packages in the Trilinos project (*e.g., linear solvers, eigensolvers, non-linear solvers, preconditioners*)
  - successor to Trilinos's Epetra package
- Tpetra centered around the following interfaces:

• `Comm` for providing communication between nodes
• `Map` for describing layout of distributed objects.
• `DistObject` for redistributing distributed objects
• Linear algebra object interfaces (`Operator`, `Vector`)

Sandia National Laboratories

Satisfying Our Goals: Templates

- How do we support multiple data types?
  - C++ templating of the scalar type and ordinals.
  - Not new, not difficult.
  - Compiler support is good enough now.
- This provides generic programming capability, independent of data types.
- Templating implements compile time polymorphism.
- Pro: No runtime penalty.
- Con: Potentially large compile-time penalty.
  - This is okay. Compiling is a good use of multicore! :)
  - Techniques exist for alleviating this for common and user data types (explicit instantiation)

Sandia National Laboratories

Example

Standard method prototype for apply matrix-vector multiply:

```
template <typename OT, typename ST>
CrsMatrix::apply(const MultiVector<OT, ST> &x,
                       MultiVector<OT, ST> &y)
```

Mixed precision method prototype (DP vectors, SP matrix):

```
template <typename OT, typename ST>
CrsMatrix::apply(const MultiVector<OT,ScalarTraits<ST>::dp> &x,
                      MultiVector<OT,ScalarTraits<ST>::dp> &y)
```

Exploits traits class for scalar types:

```
typename ScalarTraits<ST>::dp;      // double precision w.r.t. ST
typename ScalarTraits<ST>::hp;      //   half precision w.r.t. ST
ST ScalarTraits<ST>::one();         // multiplicative identity
```

Sample usage in a mixed precision algorithm:

```
Tpetra::MultiVector<int, float> x, y;
Tpetra::CisMatrix<int, double> A;
A.apply(x, y);  // SP matrix applied to DP multivector
```

Sandia National Laboratories

C++ Templates

- Example was for `float/double` but works for:
  - `complex<float>` or `complex<double>`
  - Arbitrary precision (*e.g., GMP, ARPREC*)
  - The only requirement is a valid specialization of the traits class.

Sandia National Laboratories

The Rest: C++ Virtual Functions

- How do we address our desire to support multiple implementations for these objects?
  - C++ virtual functions and inheritance.
- This provides runtime polymorphism.
- Use abstract base classes to encapsulate data and behavior.
- Specific concrete implementations of these interfaces provide adapters to target architectures.
- We will "abstract away" communication, data allocation /placement and computation.

Tpetra Communication Interface

- `Teuchos::Comm` is a pure virtual class:
  - Has no executable code, interfaces only.
  - Encapsulates behavior and attributes of the parallel machine.
  - Defines interfaces for basic comm. services between "nodes", e..g.:
    - collective communications
    - gather/scatter capabilities
  - Allows multiple parallel machine implementations.
  - Generalizes `Epetra_Comm`.
- Implementation details of parallel machine confined to `Comm` subclasses.
- In particular, Tpetra (and rest of Trilinos) has no dependence on any particular API (*e.g., MPI*).

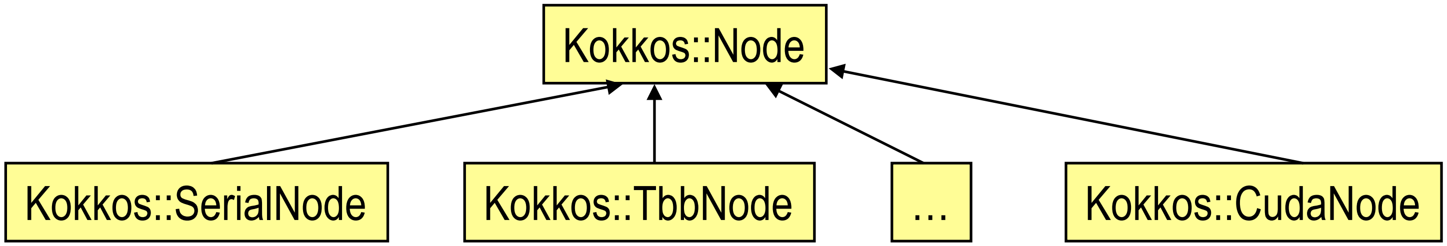
Comm Methods

```
getRank()
getSize()
barrier()
broadcast<Packet>(Packet *MyVals, int count, int Root)
gatherAll<Packet>(Packet *MyVals, Packet *AllVals, int count)
reduceAll<Packet>(ReductionOp op,
                  int count, const Packet *local, Packet *global)
scan<Packet>(ReductionOp op,
             int count, const Packet *send, Packet *scans)
```

Comm Implementations

- `SerialComm` simultaneous supports of serial and parallel coding.
- `MpiComm` is a thin wrapper around MPI communication routines.
- `MpiSmpComm` allows use of shared-memory nodes.

Abstract Node Class



- Trilinos/Kokkos: Trilinos compute node package.
- Abstraction definition in progress.
  - Node currently envisioned as an abstract factory class for computational objects.

Example:

```
Kokkos::LocalCrsMatrix<int,double> lclA;
lclA = myNode.createCrsMatrix(…);
lclA.submitEntries(…); // fill the matrix
Kokkos::LocalMultiVector<int,double> lclX = myNode.createMV(…),
                                     lclY = myNode.createMV(…);
lclA.apply(lclX,lclY); // apply the matrix operator
```

Abstract Node Class (2)

- Node handles platform-specific details, such as:
  - how to allocate memory for the necessary data structures?
    - significant in the case of attached accelerators with distinct memory space.
  - How to perform the necessary computations?
    - Tpetra is responsible only for invoking global communication, via the abstract Comm class.
    - In addition to supporting multiple architectures, Tpetra/Kokkos becomes a test bench for research into primitives.
- These abstractions *(hopefully)* provide us with flexibility to tackle a number of platforms.
- Cons:
  - `m` kernels, `p` platforms → `m*p` implementations
  - Heros can't improve code they don't have access to.

Sample Code Comparison: MV::dot()

MPI-only:

```
double dot(int len,
           double *x,
           double *y)
{
  double lcl = 0.0, gbl;
  for (int i=0; i<len; ++i)
    lcl += x[i]*y[i];
  MPI_ALLREDUCE(lcl,gbl,…);
  return gbl;
}
```

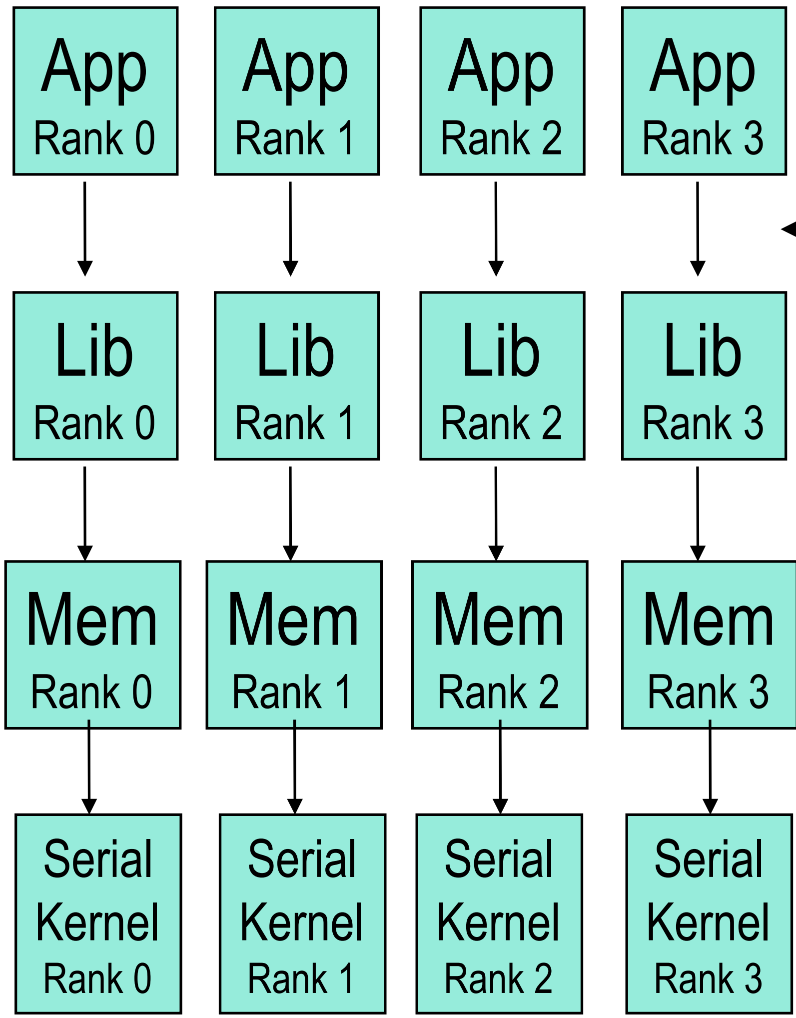
Tpetra/Kokkos:

```
template <typename ST>
ST Tpetra::MultiVector<ST>::dot(
       Comm comm,
       Kokkos::LocalVector<ST> x,
       Kokkos::LocalVector<ST> y)
{
  Scalar lcl, gbl;
  lcl = x.dot(y);
  reduceAll<ST>(comm,SUM,lcl,gbl);
  return gbl;
}
```

- For appropriate choices of Node and Comm, both implementations are equivalent.
- Right hand example is limited only by the available implementations of these classes:
  - can determine whether library was compiled with support for GPU, MPI, etc.
  - can compose different nodes for heterogeneous

Sandia National Laboratories

Example: MPI-Only $Ax=b$



App passes matrix and vector values to library data classes

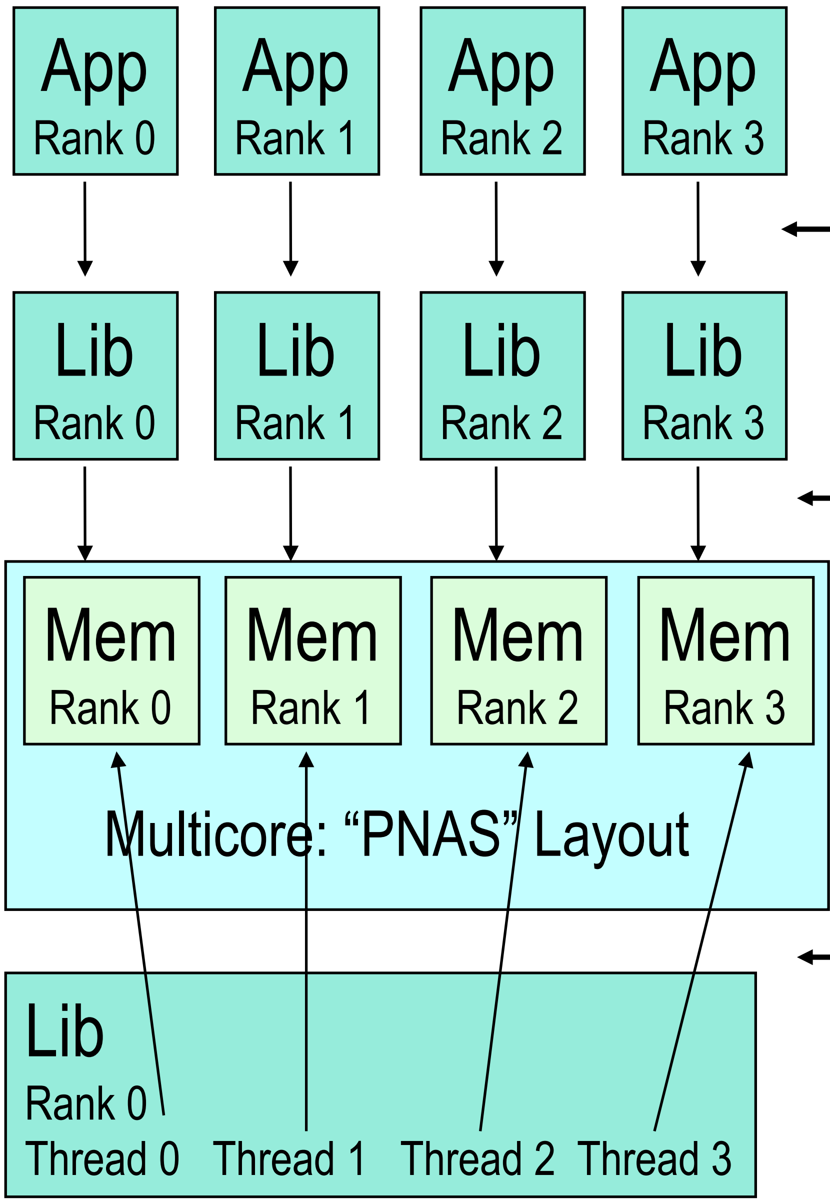
All ranks store *A, x, b* data in locally-visible address space

Library solves *Ax=b* using distributed memory algorithm, communicating via MPI

Using: SerialNode, MpiComm

Sandia National Laboratories

Example: MPI+Threads $Ax = b$



App passes matrix and vector values to library data classes

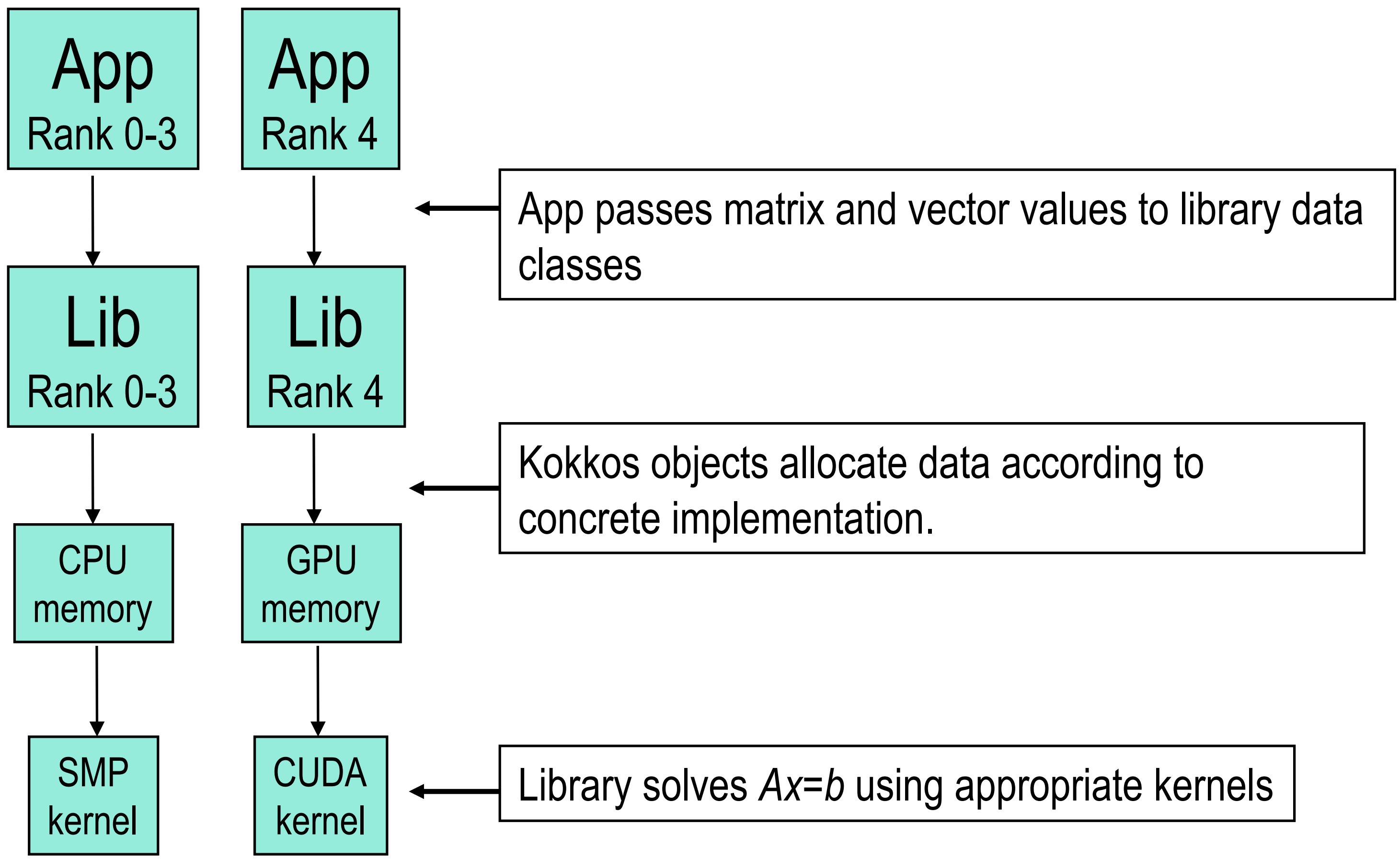
All ranks store *A, x, b* data in memory visible to rank 0

Library solves *Ax*=*b* using shared memory algorithms on the node

Using: SmpNode, SerialComm

Sandia National Laboratories

Example: Multicore + GPU $Ax=b$



Using: SmpNode, CudaNode, SerialComm, CudaComm

Sandia National Laboratories

Conclusion

- I wish I had some results.
- C++ polymorphism:
  - allows library user to run apps on a wide variety of platforms
  - allows/**requires** library developer to isolate implementation from interface
  - gives hacker/hero a hook for experimentation/salvation
- Abstract Comm has been in use in Epetra for years; some use of abstract interfaces to hide implementation have already seen experimental use.
- Development of this API for Tpetra is currently in progress; expect limited release in March ‘09, general release in Sept ‘09.