Exascale Co-design with Sandia's Structural Simulation Toolkit (SST)

Problem

- Exascale computing has been identified as a critical enabling technology for meeting numerous national challenges
- The nature of computing will change dramatically: billions of threads, faults, energy to solution, and time to solution are all critical issues
- Applications must be adapted before machines are available
 - Cost of adapting applications is high
- High cost of machines will require lower design margins
 - Provide what the application need but no more
 - Coarse measures such as bandwidth per FLOPS not sufficient

Solution

- The SST project is creating a multi-scale computer architecture simulator that will be used in the design and procurement of large-scale parallel machines as well as in the design of algorithms for these machines. Our goal is to become the preeminent simulator for performance prediction and analysis of applications running on large-scale machines
- Facilitate a consortium of industry, government, and academia to implement components and use them

Impact Measures

- ASC and ECDC applications team use SST to evaluate algorithms and programming models and act on results
- Leadership machine bids evaluated using SST
- Hardware vendors improve architecture in response to SST studies



Examples of SST usage and impact

SST Impact

Develop acceptance tests and estimate performance before machine is built.

Understand performance and issues for machines several years from deployment.

Allow co-design of advanced architectures and applications many years before deployment.

GREATER EFFORT AND IMPACT

SST Activity

Obtain traces for applications and compact applications. Use SST for parameter studies.

Write skeleton applications for extreme scale studies.

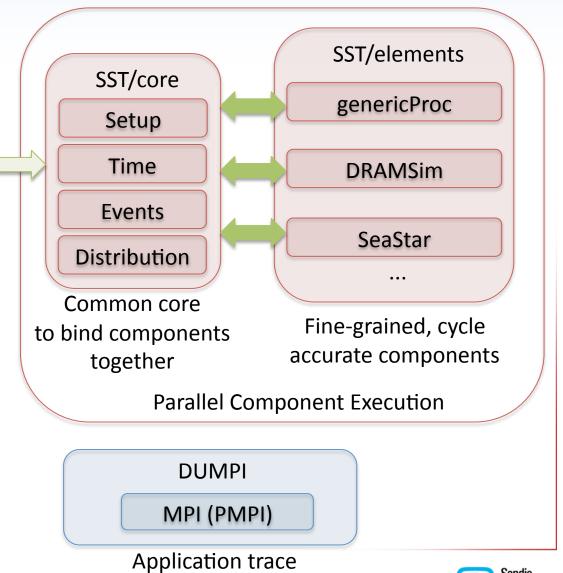
Simulate new architectural feature such as extended memory semantics and transactional memory.



SST System Architecture

SST/macro **Thread** Skeleton App. Trace Reader **Programming Model** MPI3 **Graph Scheduling Bandwidth Allocation Network Topology**

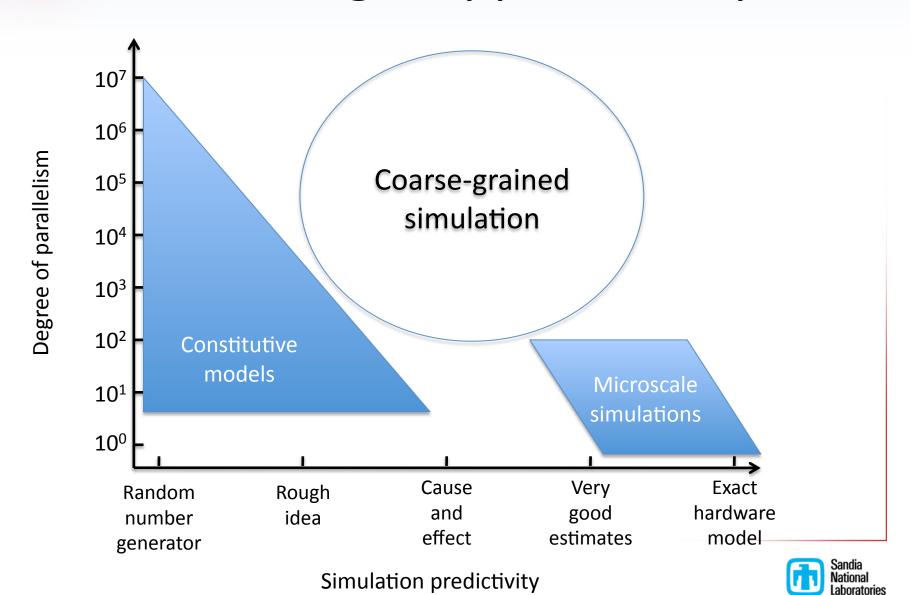
Coarse-grained Components



collection library



SST/macro target application space



SST/macro design goals

- Correctly identify causal relationships
 - Discrete inputs (network topology, node configuration, etc.)
 - Continuous inputs (noise/imbalance, bandwidth, latency, ...)
 - Emergent properties (resource contention, middleware behavior, ...)
- Play "what if" games
 - Interpolating and extrapolating runtime behavior
 - Implementation effects for communication routines
 - Multiple networks, perfect/"magic" operations
- Test changes to application, middleware, or resource management
 - Reordering code blocks, scheduling effects, etc.
- Test novel programming models
 - Fault-tolerant or fault-oblivious execution models
 - Alternatives to MPI, parallel runtime designs
 - Mixed programming models



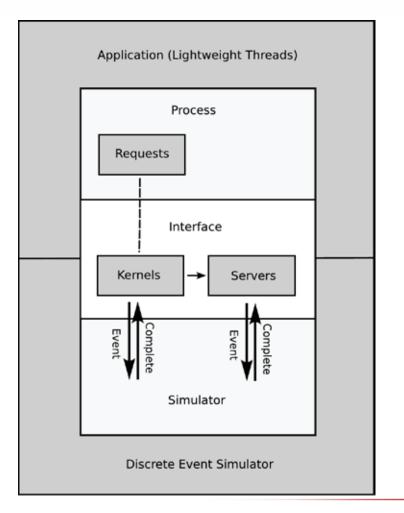
SST/macro approach

- To meet our design goals, we need:
 - A network model for resource contention
 - Very fast processor and memory models
 - Realistic middleware models (e.g. MPI)
 - Support for complex application models (no direct manipulation of state machines)
- We don't need the exact answer, but we need the correct macroscale behaviors
 - ... with a deterministic simulator
 - ... which must be reasonably fast
 - ... for a wide range of simulation system sizes (10¹-10⁶ nodes)
 - ... and realistic application workloads (10⁶-10⁹ MPI messages)



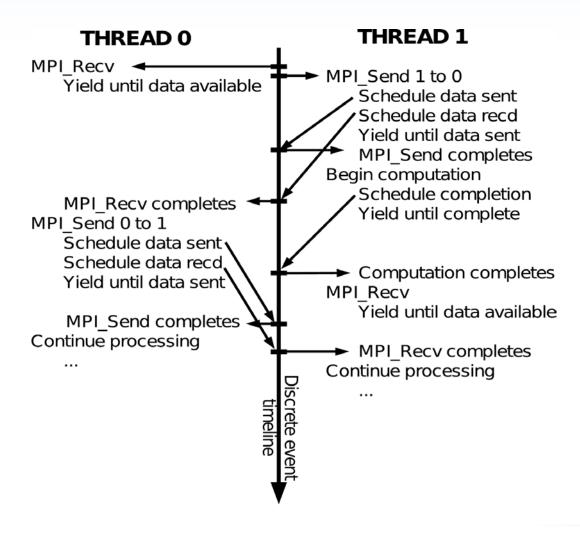
High-level simulator design

- "Process" holds application process state
 - User-space threads
 - Private stacks
- "Interface" bridges threads and DES
 - Context switching for blocking calls
 - Management of active/ blocked queues
- "Simulator" handles DES
 - Single-threaded (lock-free)





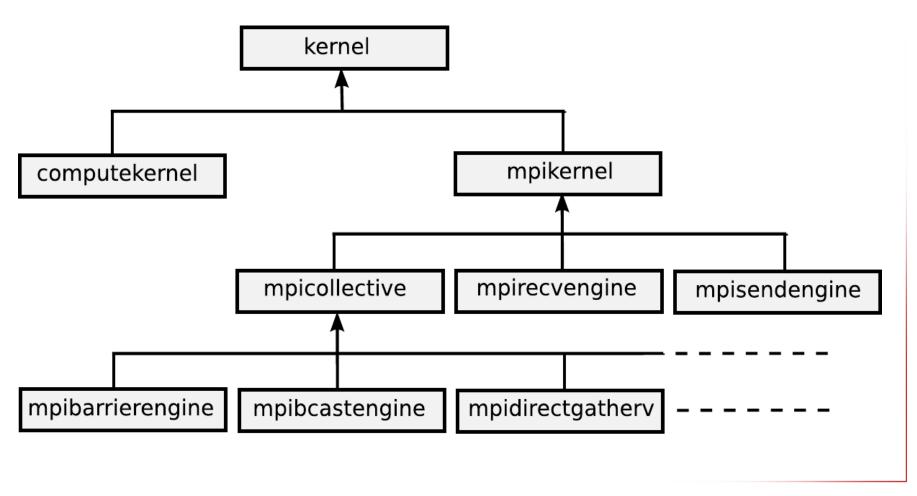
Example process control flow



Two simulated processes exchanging data via MPI send/recv pairs

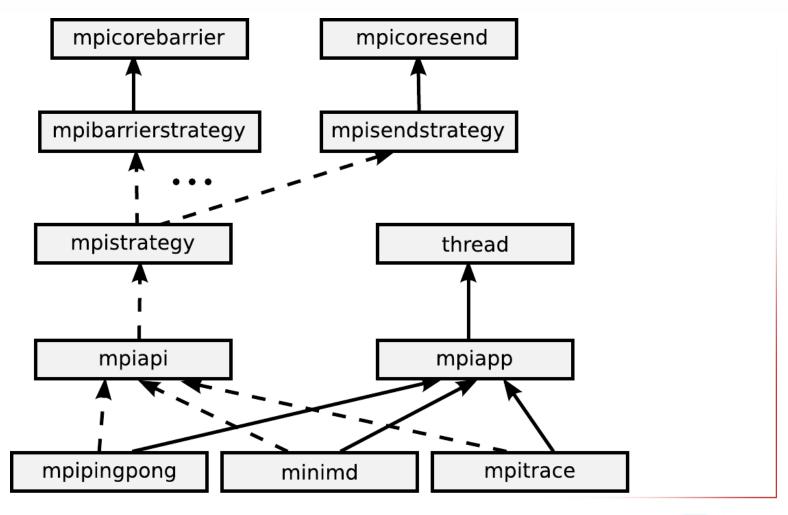


Example inheritance diagram





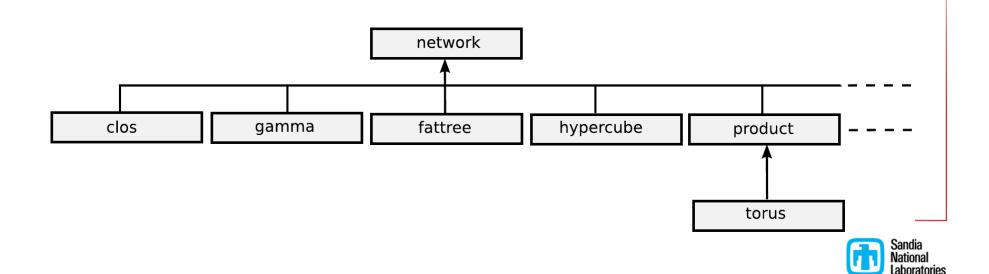
Partial collaboration diagram for MPI



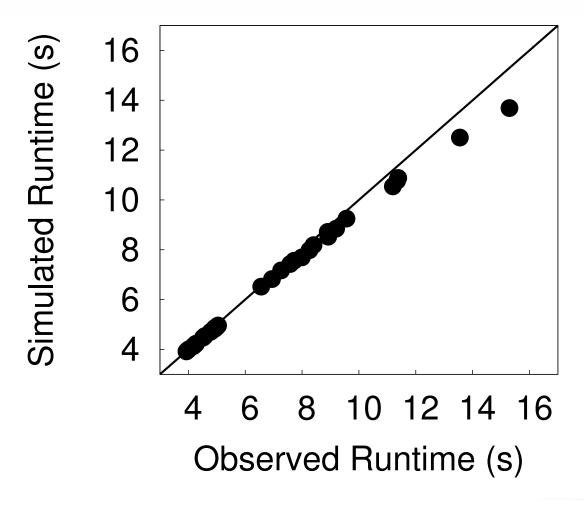


Networks

- Currently supports simplified network routing/ sharing
 - 1. Contention-free
 - 2. Circuit with fair sharing for concurrent flows
- Multiple topologies supported



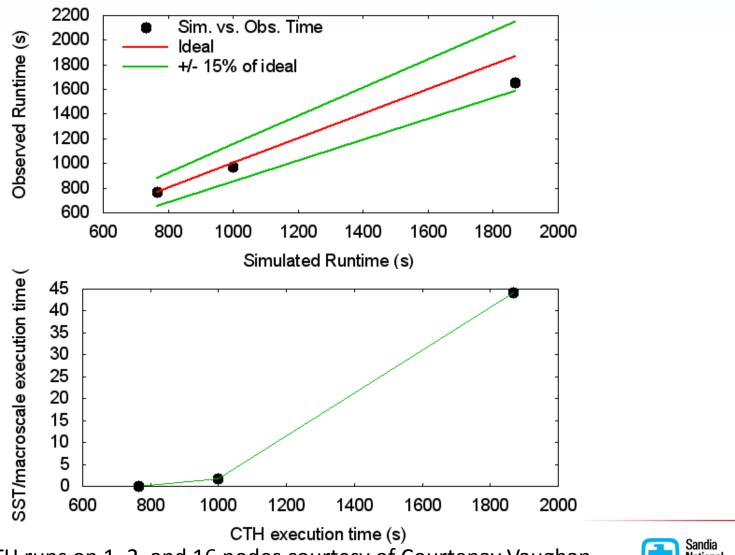
MPI trace example: AMG2006



AMG2006 on a variety of node counts and decompositions.



MPI trace example: CTH





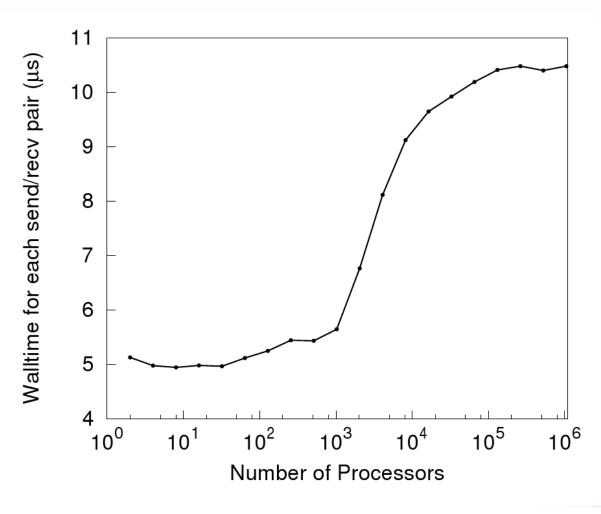


Skeleton applications

```
void mpipingpong::run() {
  this->mpi_->init();
  mpicomm world = this->mpi_->comm_world();
  mpitype type = mpitype::mpi_double;
  int rank = world.rank().id;
  int size = world.size().id;
  if(! ((size \% 2) \&\& (rank+1 >= size))) {
    // With an odd number of nodes, rank (size-1) sits out
    mpiid peer(rank ^ 1); // partner nodes 0<=>1, 2<=>3, etc.
    mpiapi::const_mpistatus_t stat;
    for(int half_cycle = 0; half_cycle < 2*niter; ++half_cycle) {</pre>
       if((half_cycle + rank) & 1)
         mpi_->send(count_, type, peer, mpitag(0), world);
       else
         mpi_->recv(count_, type, peer, mpitag(0), world, stat);
  mpi_->finalize();
```



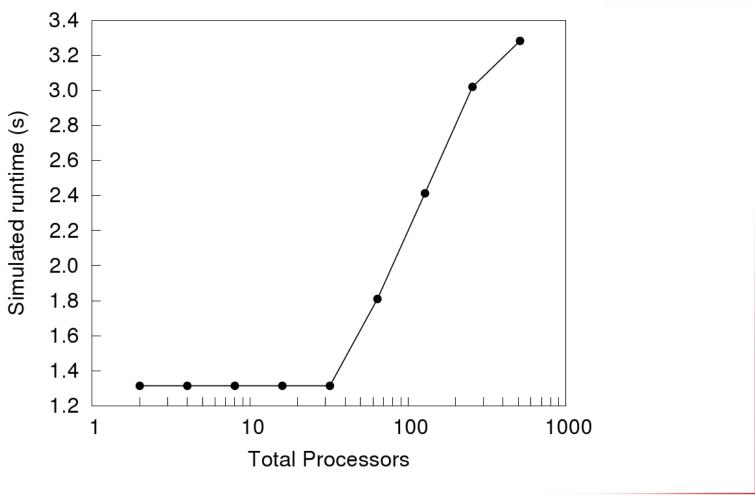
Simulator performance



MPI ping-pong on a contention-free network. Total of 4M messages.



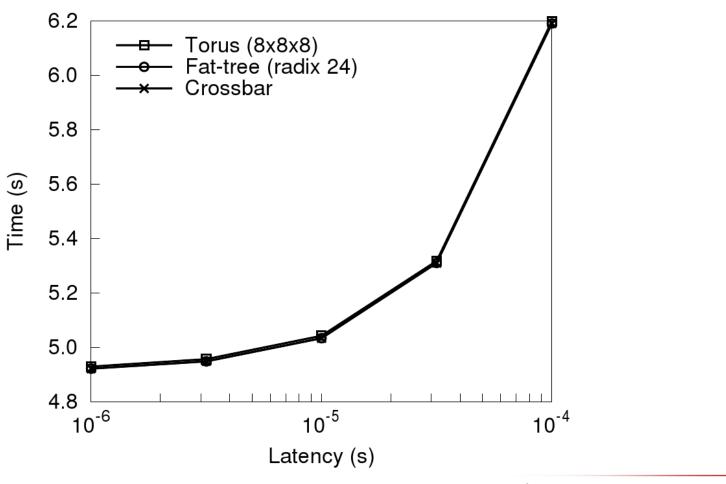
Simulated traffic congestion







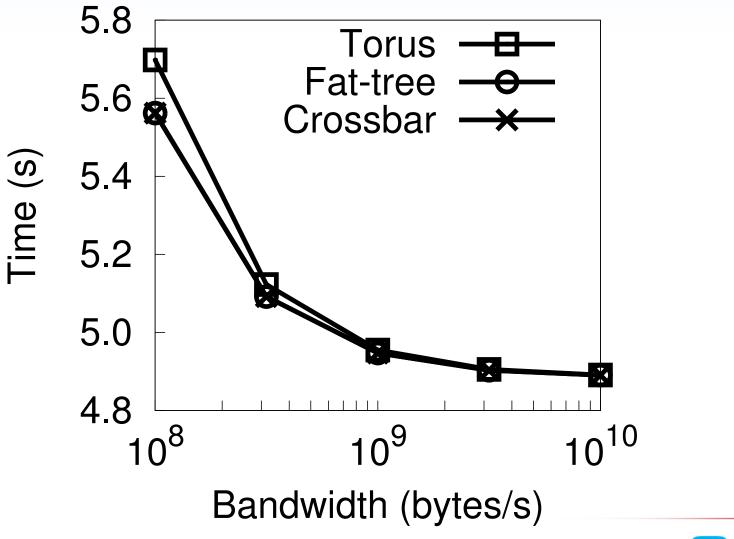
Example parameter sweep: Latency







Example parameter sweep: Bandwidth



AMG2006 on 128 nodes. Latency constant at 3 μ s.



DUMPI: The MPI tracer

- PMPI link-time library for trace file generation
- Full fingerprints for all MPI-2 functions
- Writes a (reasonably compact) binary trace file
- Negligible runtime overhead
- Reasonably portable C code

libdumpi

PMPI bindings
Type mapping
Call tree tracing (gcc/icc)

common

MPI type identifiers
MPI function identifiers
Trace file IO
Timers
Performance counters

libundumpi

Parsing of trace files



Example of data output by DUMPI

(converted using dumpi2ascii)

```
MPI_Allgatherv entering at walltime 1274314439.744512000,  
cputime 0.201756000 seconds in thread 0.
int commsize=16
int sendcount=1024
MPI_Datatype sendtype=14 (MPI_DOUBLE)
int recvcounts[16]=[1024, 1024, 1024, 1024, 1024, 1024, 1024, 1024, 1024, 1024, 1024, 1024, 1024, 1024]
int displs[16]=[0, 1024, 2048, 3072, 4096, 5120, 6144, 7168,  
8192, 9216, 10240, 11264, 12288, 13312, 14336, 15360]
MPI_Datatype recvtype=14 (MPI_DOUBLE)
MPI_Comm comm=2 (MPI_COMM_WORLD)
MPI_Allgatherv returning at walltime 1274314439.749554000,  
cputime 0.202159000 seconds in thread 0.
```



Callback-driven parsing of DUMPI files

Each MPI call is assigned a callback function

 The full set of arguments to the MPI function is passed to the callback in a struct

```
typedef struct dumpi_allgatherv {
    /** Not an MPI argument. Added to index relevant data in the struct.

*/

int commsize;
    /** Argument value before PMPI call */
    int sendcount;
    /** Argument value before PMPI call */
    dumpi_datatype sendtype;
    /** Argument value before PMPI call. Array of length [commsize] */
    int * recvcounts;
    /** Argument value before PMPI call. Array of length [commsize] */
    int * displs;
    /** Argument value before PMPI call */
    dumpi_datatype recvtype;
    /** Argument value before PMPI call */
    dumpi_comm comm;
} dumpi allaathery:
```



SST/macro Team Members

Contributors

Curtis Janssen (PI)
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Scott Cranford (I/O modeling)
Damian Dechev (Skeleton app. generation)
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Jackson Mayo (Interested observer)
Ali Pinar (Network models)

