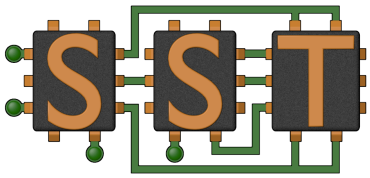
SST/macro 6.0: User's Manual

Sandia National Labs
Livermore, CA

July 14, 2016



Contents

Chapter 1

Introduction

1.1 Overview

The SST/macro software package provides a simulator for large-scale parallel computer architectures. It permits the coarse-grained study of distributed-memory applications. The simulator is driven from either a trace file or skeleton application. The simulator architecture is modular, allowing it to easily be extended with additional network models, trace file formats, software services, and processor models.

Simulation can be broadly categorized as either off-line or on-line. Off-line simulators typically first run a full parallel application on a real machine, recording certain communication and computation events to a simulation trace. This event trace can then be replayed post-mortem in the simulator. Most common are MPI traces which record all MPI events, and SST/macro provides the DUMPI utility (3.8) for collecting and replaying MPI traces. Trace extrapolation can extend the usefulness of off-line simulation by estimating large or untraceable system scales without having to collect a trace, it is typically only limited to strictly weak scaling.

We turn to on-line simulation when the hardware or applications parameters need to change. On-line simulators instead run real application code, allowing native C/C++/Fortran to be compiled directly into the simulator. SST/macro intercepts certain function calls, estimating how much time passes rather than actually executing the function. In MPI programs, for example, calls to MPI_Send are linked to the simulator instead of passing to the real MPI library. If desired, SST/macro can actually be a full MPI *emulator*, delivering messages between ranks and replicating the behavior of a full MPI implementation.

Although SST/macro supports both on-line and off-line modes, on-line simulation is encouraged because event traces are much less flexible, containing a fixed sequence of events. Application inputs and number of nodes cannot be changed. Without a flexible control flow, it also cannot simulate dynamic behavior like load balancing or faults. On-line simulation can explore a much broader problem space since they evolve directly in the simulator.

For large, system-level experiments with thousands of network endpoints, high-accuracy cycle-accurate simulation is not possible, or at least not convenient. Simulation requires coarse-grained approximations to be practical. SST/macro is therefore designed for specific cost/accuracy tradeoffs. It should still capture complex cause/effect behavior in applications and hardware, but be efficient enough to simulate at the

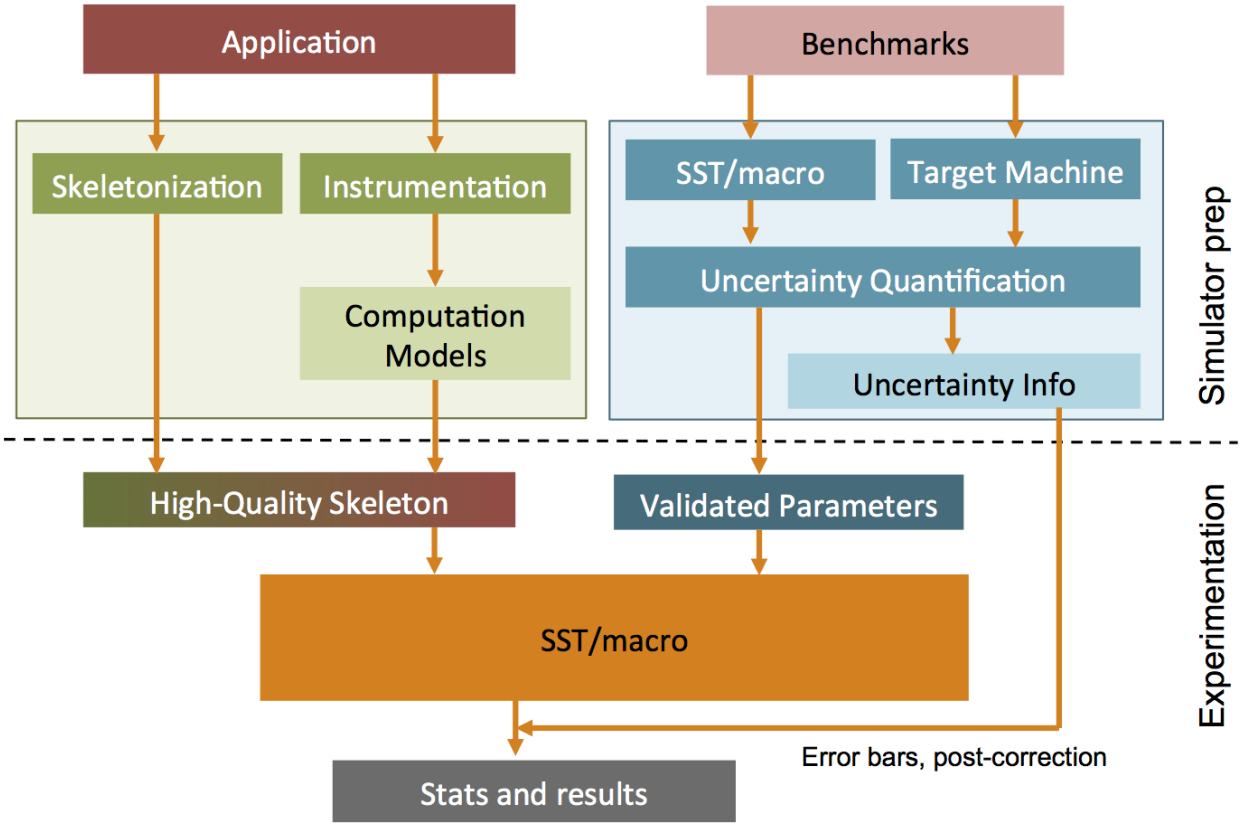


Figure 1.1: SST/macro workflow.

system-level. For speeding up simulator execution, we encourage *skeletonization*, discussed further in Chapter 5. A high-quality skeleton is an application model that reproduces certain characteristics with only limited computation. We also encourage uncertainty quantification (UQ) for validating simulator results, to be detailed in a pending SAND report. Skeletonization and UQ are the two main elements in the "canonical" SST/macro workflow (Figure 1.1).

1.2 Currently Supported

1.2.1 Programming APIs

Because of its popularity, MPI is one of our main priorities in providing programming model support. We currently test against the MPICH test suite. All tests compile, so you should never see compilation errors. However, since many of the functions are not typically used in the community, we only test commonly-used functions. See Section 1.3.2 for functions that are not supported. Functions that are not implemented will throw a `unimplemented_error`, reporting the function name.

1.2.2 Analysis Tools and Statistics

The following analysis tools are currently available in SST/macro. Some are thoroughly tested. Others have undergone some testing, but are still considered Beta. Others have been implemented, but are relatively untested.

Fully tested

- Call graph: Generates callgrind.out file that can be visualized in either KCacheGrind or QCacheGrind. More details are given in 3.9.
- Spyplot: Generates .csv data files tabulating the number of messages and number of bytes sent between MPI ranks. SST/macro can also directly generate a PNG file. Otherwise, the .csv files can be visualized in the plotting program Scilab. More details are given in 3.10.
- Fixed-time quanta (FTQ): Generates a .csv data tabulating the amount of time spent doing computation/communication as the application progresses along with a Gnuplot script for visualization as a histogram. More details are given in 3.11

1.3 Known Issues and Limitations

1.3.1 Global Variables

The use of global variables in SST/macro inherently creates a false-sharing scenario because of the use of user-space threads to model parallel processes. While we do have a mechanism for supporting them (see 5.1 for more information), the file using them must be compiled with C++. This is somewhat unfortunate, because many C programs will use global variables as a convenient means of accessing program data. In almost every case, though, a C program can simply be compiled as C++ by changing the extension to .cc or .cpp.

1.3.2 MPI

Everything from MPI 2 is implemented with a few exceptions noted below. The following are *not* implemented (categorized by MPI concepts):

Communicators

- Anything using or having to do with Inter-communicators (`MPI_Intercomm_create()`)
- Topology communicators

Datatypes and Addressing

- Complicated use of `MPI_LB` and `MPI_UB` to define a struct, and collections of structs (MPI test 138).
- Changing the name of built-in datatypes with `MPI_Type_set_name()` (MPI test 171).
- `MPI_Create_darray()`, `MPI_Create_subarray()`, and `MPI_Create_resized()`
- `MPI_Pack_external()`, which is only useful for sending messages across MPI implementations apparently.
- `MPI_Type_match_size()` - extended fortran support
- Use of `MPI_BOTTOM` (relative addressing). Use normal buffers.
- Using Fortran types (*e.g.*`MPI_COMPLEX`) from C.

Info and Attributes

No `MPI_Info_*`, `MPI_*_keyval`, or `MPI_Attr_*` functions are supported.

Point-to-Point

- `MPI_Grequest_*` functions (generalized requests).
- Use of testing non-blocking functions in a loop, such as:

```
1 while(!flag)
2 {
3   MPI_Iprobe( 0, 0, MPI_COMM_WORLD, &flag, &status );
4 }
```

  For some configurations, simulation time never advances in the MPI_Iprobe call. This causes an infinite loop that never returns to the discrete event manager. Even if configured so that time progresses, the code will work but will take a very long time to run.

Collectives

- There seems to be a problem with using `MPI_FLOAT` and `MPI_PROD` in `MPI_Allreduce()` (MPI test 22)
- There seems to be a problem with using non-commutative user-defined operators in `MPI_Reduce()` and `MPI_Allreduce()`.
- `MPI_Alltoallw()` is not implemented
- `MPI_Exscan()` is not implemented
- `MPI_Reduce_Scatter_block()` is not implemented.
- `MPIX_*` functions are not implemented (like non-blocking collectives).
- Calling MPI functions from user-defined reduce operations (MPI test 39; including `MPI_Comm_rank`).

1.3.3 Fortran

SST/macro previously provided some experimental support for Fortran90 applications. This has been discontinued for the foreseeable future. For profiling existing apps written with Fortran, DUMPI traces can still be generated.

Chapter 2

Building and Running SST/macro

2.1 Build and Installation of SST/macro

2.1.1 Downloading

SST/macro is available at `https://github.com/sstsimulator/sst-macro`

```
shell> git clone https://github.com/sstsimulator/sst-macro.git
```

or for ssh

```
shell> git clone ssh://git@github.com/sstsimulator/sst-macro.git
```

If you'd like to use ssh for convenience, make sure you have added a public key for your GitHub account.

2.1.2 Dependencies

The most critical change is that C++11 is now a strict prerequisite. Workarounds had previously existed for older compilers. These are no longer supported. The following are dependencies for SST/macro.

- (optional) Git is needed in order to clone the source code repository, but you can also download a tar (Section 2.1.1).
- (optional, recommended) Autoconf and related tools are needed unless you are using an unmodified release or snapshot tar archive.
- Autoconf: 2.68 or later
- Automake: 1.11.1 or later
- Libtool: 2.4 or later
- A C/C++ compiler is required with C++11 support. gcc 4.8 and onward is known to work.
- (optional) Doxygen and Graphviz are needed to build the documentation.
- (optional) Graphviz is needed to collect call graphs.

2.1.3 Configuration and Building

SST/macro is an SST element library, proving a set of simulation components that run on the main SST core. The SST core provides the parallel discrete event simulation manager that manages time synchronization and sending events in serial, MPI parallel, multi-threaded, or MPI + threaded mode. The core does not provide any simulation components like node models, interconnect models, MPI trace readers, etc. The actual simulation models are contained in the element library.

The SST core is a standalone executable that dynamically loads shared object files containing the element libraries. For many element libraries, a Python input file is created that builds and connects the various simulation components. For maximum flexibility, this will become the preferred mode. However, SST/macro has historically had a text-file input `parameters.ini` that configures the simulation. To preserve that mode for existing users, a wrapper Python script is provided that processes SST/macro input files.

The workflow for installing and running is therefore:

- Build and install SST core
- Build and install the SST/macro element library `libmacro.so`
- Make sure paths are properly configured for `libmacro.so` to be visible to the SST core
- Run the `sstmac` wrapper Python script that runs SST/macro-specific parameters OR
- Write a custom Python script

Build SST core

The recommended mode for maximum flexibility is to run using the SST core downloadable from `http://sst-simulator.org/SSTPages/SSTMainDownloads/`. Building and installing sets up the discrete event simulation core required for all SST elements. SST core still has a few Boost dependencies, which should be the only complication in building. For building Boost, we recommend two files: `user-config.jam` to configure the Boost compiler flags and a `runme.sh` that bootstraps, compiles, and installs the prerequisite Boost libraries. For GCC, the `user-config.jam` should go in the top-level home directory and the file should contain the line:

```
using gcc : : $PATH_TO_MPIC++  : <compileflags>-std=c++1y ;
```

For Clang on Mac, use:

```
using clang : : $PATH_TO_CLANG_MPIC++  : <compileflags>-std=c++1y <linkflags>-stdlib=libc++
```

We recommend Boost 1.59. Other Boost versions should work as well, but this seems the most stable. In the top-level Boost directory, make a script `runme.sh` that contains:

```
./bootstrap.sh \
  --with-libraries=program_options,serialization,filesystem \
  --with-toolset=gcc

./b2 ---prefix=$INSTALL
./b2 --layout=tagged --prefix=$INSTALL
```

The toolset can be changed from gcc to clang, as needed. For maximum safety, Boost should install both "tagged" versions of libraries and un-tagged versions. Once Boost is installed with these options, configuration and installation of SST core should be straightforward following documentation in the core library.

Build SST/macro element library

Once SST/macro is extracted to a directory, we recommend the following as a baseline configuration, including building outside the source tree:

```
sst-macro> ./bootstrap.sh
sst-macro> mkdir build
sst-macro> cd build
sst-macro/build> ../configure --prefix=/path-to-install --with-sst=$PATH_TO_SST_CORE CC=$MPICC CXX=$MPICXX
```

`PATH_TO_SST_CORE` should be the prefix install directory used when installing the core. The MPI compilers should be the same compilers used for building Boost and SST core.

SST/macro can still be built in standalone mode for a select set of features that have not been fully migrated to the SST core. The installation and running are the same for both modes - simply remove the `--with--sst` parameter. A complete list of options for standalone building can be seen by running `../configure --help`. Some common options include:

- –(dis|en)able-graphviz : Enables the collection of simulated call graphs, which can be viewed with graphviz. Enabled by default. Disable if not using Boost or C++11. Ordered maps can be used as a replacement, but with lower performance.
- –(dis|en)able-regex : Regular expressions can be used to proofread input files, but this requires either Boost or C++11. Enabled by default. Disable if not using Boost or C++11.
- –(dis|en)able-custom-new : Memory is allocated in larger chunks in the simulator, which can speed up large simulations.
- –(dis|en)able-multithread : This configures for thread-level parallelism for (hopefully) faster simulation

Once configuration has completed, printing a summary of the things it found, simply type `make`.

2.1.4 Post-Build

If the build did not succeed, check 2.1.5 for known issues, or contact SST/macro support for help (sstmacro-support@googlegroups.com).

If the build was successful, it is recommended to run the range of tests to make sure nothing went wrong. To do this, and also install SST/macro to the install path specified during installation, run the following commands:

```
sst-macro/build> make -j8 check
sst-macro/build> make install
sst-macro/build> make -j8 installcheck
```

Make check runs all the tests we use for development, which checks all functionality of the simulator. Make installcheck compiles some of the skeletons that come with SST/macro, linking against the installation.

> Important: Applications and other code linking to SST/macro use Makefiles that use the sst++/sstcc compiler wrappers that are installed there for convenience to figure out where headers and libraries are. Make sure your path is properly configured.

2.1.5 Known Issues

- Any build or runtime problems should be reported to sstmacro-devel@googlegroups.com. We try to respond as quickly as possible.
- make -j: When doing a parallel compile dependency problems can occur. There are a lot of interrelated libraries and files. Sometimes the Makefile dependency tracker gets ahead of itself and you will get errors about missing libraries and header files. If this occurs, restart the compilation. If the error vanishes, it was a parallel dependency problem. If the error persists, then it's a real bug.
- Ubuntu: The Ubuntu linker performs too much optimization on dynamically linked executables. Some call it a feature. I call it a bug. In the process it throws away symbols it actually needs later. When compiling with Ubuntu, make sure that '-Wl,–no-as-needed' is always given in LDFLAGS.

  The problem occurs when the executable depends on libA which depends on libB. The executable has no direct dependence on any symbols in libB. Even if you add `-lB` to the `LDFLAGS` or `LDADD` variables, the linker ignores them and throws the library out. It takes a dirty hack to force the linkage. If there are issues, contact the developers at sstmacro-devel@googlegroups.com and report the problem. It can be fixed easily enough.
- Compilation with clang should work, although the compiler is very sensitive. In particular, template code which is correct and compiles on several other platforms can mysteriously fail. Tread with caution.

2.2 Building DUMPI

By default, DUMPI is configured and built along with SST/macro with support for reading and parsing DUMPI traces, known as libundumpi. DUMPI binaries and libraries are also installed along with everything for SST/macro during make install. DUMPI can be used as it's own library within the SST/macro source tree by changing to `sst-macro/sst-dumpi`, where you can change its configuration options. It is not recommended to disable libundumpi support, which wouldn't make much sense anyway.

DUMPI can also be used as stand-alone tool/library if you wish (*e.g.* for simplicity if you're only tracing). To get DUMPI by itself, either copy the `sstmacro/dumpi` directory somewhere else or visit `https://github.com/sstsimulator/sst-dumpi` and follow similar instructions for obtaining SST/macro.

To see a list of configuration options for DUMPI, run `./configure --help`. If you're trying to configure DUMPI for trace collection, use `--enable-libdumpi`. Your build process might look like this (if you're building in a separate directory from the dumpi source tree) :

```
sst-dumpi/build> ../configure --prefix=/path-to-install --enable-libdumpi
sst-dumpi/build> make -j8
sst-dumpi/build> sudo make install
```

2.2.1 Known Issues

- When compiling on platforms with compiler/linker wrappers, e.g. ftn (Fortran) and CC (C++) compilers at NERSC, the libtool configuration can get corrupted. The linker flags automatically added by the wrapper produce bad values for the predeps/postdeps variable in the libtool script in the top

level source folder. When this occurs, the (unfortunately) easiest way to fix this is to manually modify the libtool script. Search for predeps/postdeps and set the values to empty. This will clear all the erroneous linker flags. The compilation/linkage should still work since all necessary flags are set by the wrappers.

2.3 Running an Application

2.3.1 SST Python Scripts

Full details on building SST Python scripts can be found at `http://sst-simulator.org`. To preserve the old parameter format in the near-term, SST/macro provides the `pysstmac` script:

```
1 export PYTHONPATH=$PYTHONPATH:$SSTMAC_PREFIX/include/python:$SSTMAC_PREFIX/lib
2 export SST_LIB_PATH=$SST_LIB_PATH:$SSTMAC_PREFIX/lib
3
4 options="$@"
5 $SST_PREFIX/bin/sst $SSTMAC_PREFIX/include/python/default.py --model-options="$options"
```

The script configures the necessary paths and then launches with a Python script `default.py`. Interested users can look at the details of the Python file to understand how SST/macro converts parameter files into a Python config graph compatible with SST core. Assuming the path is configured properly, users can run

```
pysstmac -f parameters.ini
```

with a properly formatted parameter file. If running in standalone mode, the command would be similarly (but different)

```
sstmac -f parameters.ini
```

since there is no Python setup involved.

2.3.2 Building Skeleton Applications

To demonstrate how an external skeleton application is run in SST/macro, we'll use a very simple send-recv program located in `skeletons/sendrecv`. We will take a closer look at the actual code in Section 3.3. After SST/macro has been installed and your PATH variable set correctly, run:

```
sst-macro> cd skeletons/sendrecv
sst-macro/skeleton/sendrecv> make
sst-macro/skeleton/sendrecv> ./runsstmac -f parameters.ini
```

You should see some output that tells you 1) the estimated total (simulated) runtime of the simulation, and 2) the wall-time that it took for the simulation to run. Both of these numbers should be small since it's a trivial program.

This is how simulations generally work in SST/macro: you build skeleton code and link it with the simulator to produce a binary. Then you run that binary and pass it a parameter file which describes the machine model to use.

2.3.3 Makefiles

We recommend structuring the Makefile for your project like the one seen in `skeletons/sendrecv/Makefile` :

```
TARGET := runsstmac
SRC := $(shell ls *.c)

CXX :=        $(PATH_TO_SST)/bin/sst++
CC :=          $(PATH_TO_SST)/bin/sstcc
CXXFLAGS :=  ...
CPPFLAGS :=  ...
LIBDIR :=   ...
PREFIX :=    ...
LDFLAGS :=  -Wl,-rpath,$(PREFIX)/lib
...
```

The SST compiler wrappers `sst++` and `sstcc` automagically configure and map the code for simulation. More details are given in Section 5.2. If using external skeleton applications, the default Python script for SST/macro will not work and a small modification will be required.

2.3.4 Command-line arguments

There are only a few basic command-line arguments you'll ever need to use with SST/macro, listed below

- -h/–help: Print some typical help info
- -f [parameter file]: The parameter file to use for the simulation. This can be relative to the current directory, an absolute path, or the name of a pre-set file that is in sstmacro/configurations (which installs to /path-to-install/include/configurations, and gets searched along with current directory).
- –dumpi: If you are in a folder with all the DUMPI traces, you can invoke the main `sstmac` executable with this option. This replays the trace in a special debug mode for quickly validating the correctness of a trace.
- -d [debug flags]: A list of debug flags to activate as a comma-separated list (no spaces) - see Section 2.5
- -p [parameter]=[value]: Setting a parameter value (overrides what is in the parameter file)
- -t [value]: Stop the simulation at simulated time [value]
- -c: If multithreaded, give a comma-separated list (no spaces) of the core affinities to use - see Section 2.4.2

2.4 Parallel Simulations in Standalone Mode

SST/macro supports running parallel discrete event simulation (PDES) in distributed memory (MPI), threaded shared memory (pthreads) and hybrid (MPI+pthreads) modes. Running these in standalone mode is generally discouraged as parallel simulations should use the unified SST core.

2.4.1 Distributed Memory Parallel

In order to run distributed memory parallel, you must configure the simulator with the `--enable-mpiparallel` flag. Configure will check for MPI and ensure that you're using the standard MPI compilers. Your configure should look something like:

```
sst-macro/build> ../configure --enable-mpiparallel CXX=mpicxx CC=mpicc ...
```

SST/macro can now run parallel jobs without any graph partitioning packages. In previous versions, SST/macro required METIS for partitioning the workload amongst parallel processes. With the above options, you can just compile and go. SST/macro is run exactly like the serial version, but is spawned like any other MPI parallel program. Use your favorite MPI launcher to run, e.g. for OpenMPI

```
mysim> mpirun -n 4 sstmac -f parameters.ini
```

or for MPICH

```
mysim$ mpiexec -n 4 sstmac -f parameters.ini
```

Even if you compile for MPI parallelism, the code can still be run in serial with the same configuration options. SST/macro will notice the total number of ranks is 1 and ignore any parallel options. When launched with multiple MPI ranks, SST/macro will automatically figure out how many partitions (MPI processes) you are using, partition the network topology into contiguous blocks, and start running in parallel.

2.4.2 Shared Memory Parallel

In order to run shared memory parallel, you must configure the simulator with the `--enable-multithread` flag. Partitioning for threads is currently always done using block partitioning and there is no need to set an input parameter. Including the integer parameter `sst_nthread` specifies the number of threads to be used (per rank in MPI+pthreads mode) in the simulation. The following configuration options may provide better threaded performance.

- `--enable-spinlock` replaces pthread mutexes with spinlocks. Higher performance and recommended when supported.
- `--enable-cpu-affinity` causes SST/macro to pin threads to specific cpu cores. When enabled, SST/macro will require the `cpu_affinity` parameter, which is a comma separated list of cpu affinities for each MPI task on a node. SST/macro will sequentially pin each thread spawned by a task to the next next higher core number. For example, with two MPI tasks per node and four threads per MPI task, `cpu_affinity = 0,4` will result in MPI tasks pinned to cores 0 and 4, with pthreads pinned to cores 1-3 and 5-7. For a threaded only simulation `cpu_affinity = 4` would pin the main process to core 4 and any threads to cores 5 and up. The affinities can also be specified on the command line using the `-c` option. Job launchers may in some cases provide duplicate functionality and either method can be used.

2.4.3 Warnings for Parallel Simulation

- Watch your `LD_LIBRARY_PATH` if you have multiple different builds. If your paths get scrambled and the wrong libraries are being read, you will get bizarre, inscrutable errors.
- If the number of simulated processes specified by e.g. `aprun -n 100` does not match the number of nodes in the topology (i.e. you are not space-filling the whole simulated machine), parallel performance will suffer. SST/macro partitions nodes, not processes.
- Furthermore, if you don't space-fill the simulated machine, you might even get weird errors. Some MPI ranks might have zero virtual processes, which leads to undefined behavior.
- If running an MPI program, you should probably be safe and use the mpicheck debug flag (see below) to ensure the simulation runs to completion. The flag ensures `MPI_Finalize` is called and the simulation did not "deadlock." While the PDES implementation should be stable, it's best to treat it as Beta++ to ensure program correctness.

> Parallel simulation speedups are likely to be modest for small runs. Speeds are best with serious congestion or heavy interconnect traffic. Weak scaling is usually achievable with 100-500 simulated MPI ranks per logical process. Even without speedup, parallel simulation can certainly be useful in overcoming memory constraints, expanding the maximum memory footprint.

2.5 Debug Output

SST/macro defines a set of debug flags that can be specified in the parameter file to control debug output printed by the simulator. To list the set of all valid flags with documentation, the user can run

```
bin> ./sstmac --debug-flags
```

which will output something like

```
    mpi
        print all the basic operations that occur on each rank - only API calls are
        logged, not any implementation details
    mpi_check
        validation flag that performs various sanity checks to ensure MPI application
        runs and terminates cleanly
    mpi_collective
        print information about MPI collective calls as well as implementation details
    mpi_pt2pt
        print information about MPI point-to-point calls as well as implementation
        details
     ....
```

The most important flag for validating simulations is the `mpi_check` flag, which causes special sanity checks and a final validation check to ensure the simulation has finished cleanly. Some of the debug flags can generate information overload and will only be useful to a serious developer, rather than a user.

To turn on debug output, add the following to the input file

```
debug = mpi  mpi_check
```

listing all flags you want separated by spaces. Note: this is a major shift from the previous (and really tedious, unfriendly) debug system of past versions. The new system allows much finer-grained, simpler printing of debug output. Additionally, it allows new debug flags to very easily defined. More info on declaring new debug flags in your own code can be found in the developer's reference.

Chapter 3

Basic Tutorials

3.1 SST/macro Parameter files

A minimal parameter file setting up a 2D-torus topology is shown below. The preferred (current) version uses namespaces (ns.param syntax). However, we also show the deprecated parameters used by previous versions.

```
# Launch parameters
app1.launch_indexing = block
app1.launch_allocation = first_available
app1.launch_cmd = aprun -n2 -N1
app1.name = user_app_cxx
app1.argv =
# Application parameters
app1.sendrecv_message_size = 128
# Network parameters
interconnect = simple
switch.bandwidth = 1.0GB/s
switch.hop_latency = 100ns
# Topology - Ring of 4 nodes
topology.name = hdtorus
topology.geometry = 4,4
# Node parameters
node.ncores = 1
node.model = null
node.memory.model = null
nic.model = null
```

The input file follows a basic syntax of `parameter = value`. Parameter names follow C++ variable rules (letters, numbers, underscore) while parameter values can contain spaces. Trailing and leading whitespaces are stripped from parameters. Comments can be included on lines starting with #.

The input file is broken into sections via comments. First, application launch parameters must be chosen determining what application will launch, how nodes will be allocated, how ranks will be indexed, and finally what application will be run. Additionally, you must specify how many processes to launch and how many to spawn per node. We currently recommend using aprun syntax (the launcher for Cray machines), although support is being added for other process management systems. SST/macro can simulate command line parameters by giving a value for `app1.argv`.

A network must also be chosen. In the simplest possible case, the network is modeled via a simple latency/bandwidth formula. For more complicated network models, many more than two parameters will be required. See 3.6 for a brief explanation of SST/macro network congestion models. A topology is also needed for constructing the network. In this case we choose a 2-D 4×4 torus (16 switches). The `topology_geometry` parameter takes an arbitrarily long list of numbers as the dimensions to the torus.

Finally, we must construct a node model. In this case, again, we use the simplest possible models (null model) for the node, network interface controller (NIC), and memory. The null model is essentially a no-op, generating the correct control flow but not actually simulating any computation. This is useful for validating program correctness or examining questions only related to the network. More accurate (and complicated) models will require parameters for node frequency, memory bandwidth, injection latency, etc.

Parameter files can be constructed in a more modular way through the `include` statement. An alternative parameter file would be:

```
include machine.ini
# Launch parameters
app1.launch_indexing = block
app1.launch_allocation = first_available
app1.launch_cmd = aprun -n2 -N1
app1.name = user_mpiapp_cxx
app1.argv =
# Application parameters
app1.sendrecv_message_size = 128
```

where in the first line we include the file `machine.ini`. All network, topology, and node parameters would be placed into a `machine.ini` file. In this way, multiple experiments can be linked to a common machine. Alternatively, multiple machines could be linked to the same application by creating and including an `application.ini`.

Using the deprecated (non-namespace) parameters the file would be:

```
# Launch parameters
launch_indexing = block
launch_allocation = first_available
launch_app1_cmd = aprun -n2 -N1
launch_app1 = user_mpiapp_cxx
launch_app1_argv =
# Network parameters
network_name = simple
network_bandwidth = 1.0GB/s
network_hop_latency = 100ns
# Topology - Ring of 4 nodes
topology_name = hdtorus
topology_geometry = 4,4
# Node parameters
node_cores = 1
node_name = null
node_memory_model = null
nic_name = null
# Application parameters
sendrecv_message_size = 128
```

3.2 Abstract Machine Models

The preferred mode for usage of SST/macro will be through specifying parameters for well-defined abstract machine models. This represents an intermediate-level mode that should cover the vast majority of use cases.

The highly configurable, detailed parameter files will remain valid but will represent advanced usage mode for corner cases. The primary advantage of the abstract machine models is a uniform set of parameters regardless of the underlying congestion model or accuracy level (e.g. packet, flow, train, packet-flow, LogGOPSim). Each input file requires the usual set of software parameters given in 3.1. For hardware parameters, two initial parameters are required and one is optional.

```
congestion_model = packet_flow
amm_model = amm1
accuracy_parameter = 1024
```

Here we indicate the congestion model to be used (the packet-flow) and the overall machine model (abstract machine model #1). Currently valid values for the congestion model are `packet_flow` (most accurate, slowest) and `simple` (least accurate, fastest), but more congestion models should be supported in future versions. Currently valid values for the abstract machine model are `amm1`, `amm2`, `amm3`, see details below. Another model, `amm4`, that adds extra detail to the NIC is pending and should be available soon. The details of individual abstract machine models are given in the following sections. The optional accuracy parameter is less well-defined and the exact meaning varies considerably between congestion models. In general, the accuracy parameter represents how coarse-grained the simulation is in bytes. It basically corresponds to a packet-size. How many bytes are modeled moving through the machine separately at a time? If the parameter is set to 8 bytes, e.g., that basically means we are doing flit-level modeling. If the parameter is set to 8192 bytes, e.g. that means we are doing very coarse-grained modeling which only really affects large messages. If the parameter is set to 100-1000 bytes, e.g., that means we are doing more fine-grained modeling on real packet sizes, but we are ignoring flit-level details.

3.2.1 Common Parameters

The following parameters define the CPU and compute power of the node (independent of memory subsystem). They are universal and are valid for all abstract machine models.

Using the preferred (current) namespace parameters:

```
node.model = simple
node.frequency = 2.1ghz
node.ncores = 24
node.nsockets = 4
```

or using the deprecated parameters:

```
node_name = simple
node_frequency = 2.1ghz
node_ccores = 24
node_sockets = 4
```

3.2.2 AMM1

This is simplest abstract machine model and incorporates three basic components (i.e. congestion points). Each node has a memory subsystem and NIC (injection/ejection). Once packets are injected, they traverse a series of network switches. The memory, injection, and network are all defined by a bandwidth/latency parameter pair.

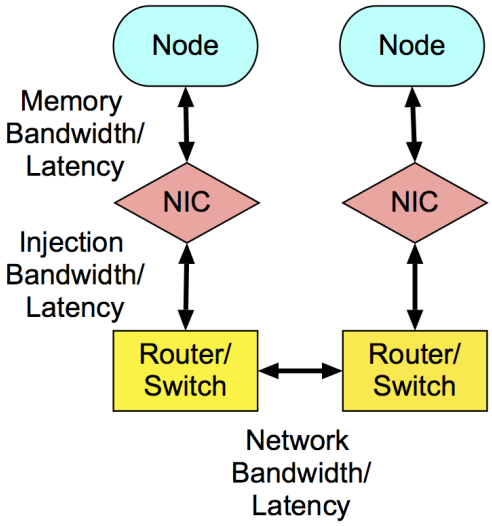


Figure 3.1: AMM1: Used when focusing on network traffic only

```
network_bandwidth = 6GB/s
network_hop_latency = 100ns
injection_bandwidth = 10GB/s
injection_latency = 1us
memory_bandwidth = 10GB/s
memory_latency = 15ns
```

These are special parameters used by the AMM configurations. They can be by-passed by directly using fully namespaced parameters (not shown).

NOTE: there is no parameter `network_latency`. The parameter is `network_hop_latency`. This is the latency required for a single packet to traverse one switch and hop to the next one in the network. Thus, even in the most basic of network models, there is a still a notion of topology that affects the number of hops and therefore the latency. To compute the total network network latency as one would observe in an MPI ping-ping benchmark, one would compute

$$lat = n_{hops} * lat_{hop} + 2 * lat_{inj}$$

using the hop latency and the injection latency.

This abstract machine model is a good place to start for getting a "lay of the land" for simulations - and the simplest to configure. However, it has a few deficiencies that can cause problems when there is serious memory or network congestion. More details (and their fixes) are given in the next abstract machine models.

3.2.3 AMM2

A major deficiency of AMM1 is that it grants exclusive access to memory resources. Two CPUs or the NIC cannot be using the memory subsystem in parallel. This is particularly problematic for large memory

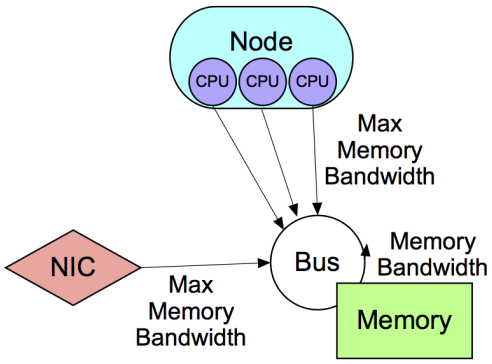


Figure 3.2: AMM2: Adds extra memory model details to AMM1

transfers (1 MB or greater). The memory system might be blocked for approx 1 ms, creating unphysical delays while other resources wait for access. A more realistic model allows multiple resources to access the memory, albeit with reduced bandwidth when congestion is observed. In many cases, multiple memory links or management units are connect to a shared bus. The bus determines to the total, aggregate memory bandwidth. However, the individual links determine the maximum observed bandwidth by any single component. AMM2 has all the same parameters as AMM1, but now allows an additional parameter for memory. These are special parameters used by the AMM configurations. They can be by-passed by directly using fully namespaced parameters (not shown).

```
1 max_memory_bandwidth = 5GB/s
2 memory_bandwidth = 10GB/s
3 memory_latency = 15ns
```

The new parameter `max_memory_bandwidth` now defines the maximum bandwidth any single component is allowed. Thus, even if the CPU is doing something memory intensive, 5 GB/s is still available to the NIC for network transfers. We remark here that the memory parameters might be named something slightly more descriptive. However, as a rule, we want the AMM1 parameters to be a proper subset of the AMM2 parameters. Thus parameter names should not change - only new parameters should be added.

3.2.4 AMM3

A major deficiency of AMM2 is its inability to distinguish between the network link bandwidth (associated with the outport port serializer/deserializer) and the switch bandwidth (associated with the crossbar that arbitrates packets). Only packets traveling the same path cause congestion on the network links in AMM1 and AMM2. However, packets "intersecting" at a switch - even if following separate paths - can cause congestion through sharing the switching fabric. AMM3 generalize the network parameters by adding a switch bandwidth. We note again here that AMM3 has all the same parameters as AMM2, plus the additional switch bandwidth parameter. Thus, higher-numbered abstract machine models always add more detail. These are special parameters used by the AMM configurations. They can be by-passed by directly using fully namespaced parameters (not shown) for more detailed configurations.

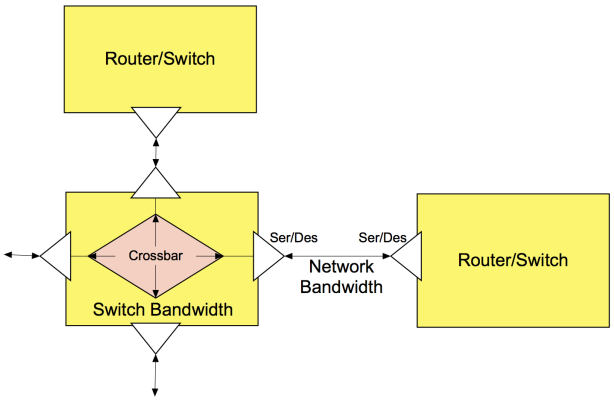


Figure 3.3: AMM3: Adds extra router (switch) details to AMM2

```
network_switch_bandwidth = 12GB/s
network_bandwidth = 6GB/s
network_hop_latency = 100ns
```

3.3 Basic MPI Program

Let us go back to the simple send/recv skeleton and actually look at the code. This code should be compiled with SST compiler wrappers installed in the `bin` folder.

```
#include <stdlib.h>
#include <stdio.h>
#include <mpi.h>

#define sstmac_app_name "simple_test"

int main(int argc, char **argv)
{
  int message_size = 128;
  int me, nproc;
  int tag = 0;
  int dst = 1;
  int src = 0;
  MPI_Status stat;

  MPI_Init(&argc,&argv);
  MPI_Comm world = MPI_COMM_WORLD;
  MPI_Comm_rank(world,&me);
  MPI_Comm_size(world,&nproc);
```

The starting point is creating a main routine for the application. The simulator itself already provides a `main` routine. The SST compiler automatically changes the function name to `user_skeleton_main`, which provides an entry point for the application to actually begin. When SST/macro launches, it will invoke this routine and pass in any command line arguments specified via the `app1.argv` parameter. Upon entering the

main routine, the code is now indistinguishable from regular MPI C++ code. In the parameter file to be used with the simulation, you must set

```
app1.name = simple_test
```

The name associated to the application is given by the `sstmac_app_name` macro. This macro must be defined to a unique string name in the source file containing `main`. SST/macro will automatically associate the given main routine with the string internally. That application can then be selected in the input file with `app1.name`.

At the very top of the file, the `mpi.h` header is actually mapped by the SST compiler to an SST/macro header file. This header provides the MPI API and configures MPI function calls to link to SST/macro instead of the real MPI library. The code now proceeds:

```
    if (nproc != 2) {
        fprintf(stderr, "sendrecv only runs with two processors\n");
        abort();
    }
    if (me == 0) {
        MPI_Send(NULL, message_size, MPI_INT, dst, tag, world);
        printf("rank %i sending a message\n", me);
    }
    else {
        MPI_Recv(NULL, message_size, MPI_INT, src, tag, world, &stat);
        printf("rank %i receiving a message\n", me);
    }
    MPI_Finalize();
    return 0;
}
```

Here the code just checks the MPI rank and sends (rank 0) or receives (rank 1) a message.

3.4 Network Topologies and Routing

We here give a brief introduction to specifying different topologies and routing strategies. We will only discuss one basic example (torus). A more thorough introduction covering all topologies is planned for future releases. Excellent resources are "Principles and Practices of Interconnection Networks" by Brian Towles and William Dally published by Morgan Kaufman and "High Performance Datacenter Networks" by Dennis Abts and John Kim published by Morgan and Claypool.

3.4.1 Topology

Topologies are determined by two mandatory parameters.

```
topology.name = torus
topology.geometry = 4 4
```

Here we choose a 2D-torus topology with extent 4 in both the X and Y dimensions for a total of 16 nodes (Figure 3.4) The topology is laid out in a regular grid with network links connecting nearest neighbors. Additionally, wrap-around links connect the nodes on each boundary.

The figure is actually an oversimplification. The `topology_geometry` parameter actually specifies the topology of the *network switches*, not the compute nodes. A torus is an example of a direct network in which each

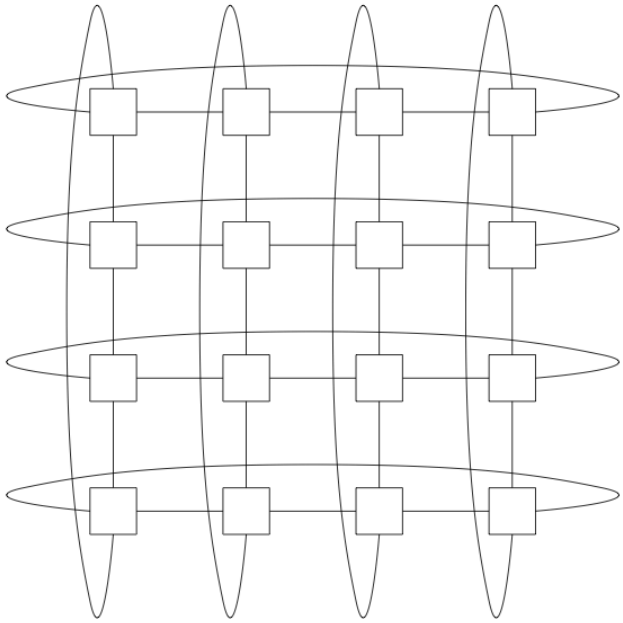


Figure 3.4: 4 x 4 2D Torus

switch has one or more nodes "directly" connected to it. A more accurate picture of the network is given in Figure 3.5. While in many previous architectures there was generally a one-to-one correspondence between compute nodes and switches, more recent architectures have multiple compute nodes per switch (e.g. Cray Gemini with two nodes). Multinode switches can be specified via

```
1 topology.name = torus
2 topology.geometry = 4 4
3 topology.concentration = 2
```

which would now generate a torus topology with 16 switches and 32 compute nodes.

Another subtle modification of torus (and other networks) can be controlled by giving the X, Y, and Z directions different bandwidth. The above network could be modified as

```
1 topology.name = torus
2 topology.geometry = 4 4
3 topology.redundant = 2 1
```

giving the the X-dimension twice the bandwidth of the Y-dimension. This pattern DOES exist in some interconnects as a load-balancing strategy. A very subtle point arises here. Consider two different networks:

```
1 topology.name = torus
2 topology.geometry = 4 4
3 topology.redundant = 1 1
4 network_bandwidth = 2GB/s
```

```
1 topology.name = torus
2 topology.geometry = 4 4
```

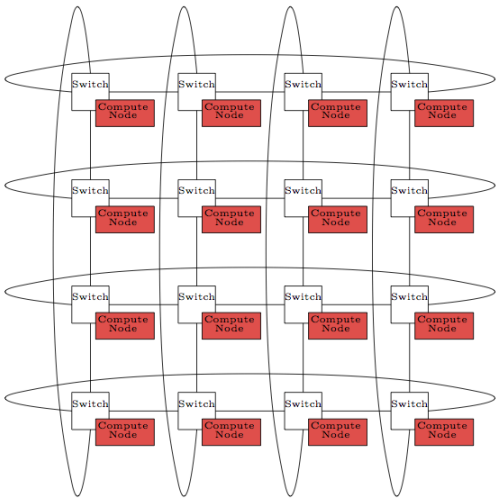


Figure 3.5: 4 x 4 2D Torus of Network Switches with Compute Nodes

```
3 topology.redundant = 2 2
4 network_bandwidth = 1GB/s
```

For some coarse-grained models, these two networks are exactly equivalent. In more fine-grained models, however, these are actually two different networks. The first network has ONE link carrying 2 GB/s. The second network has TWO links each carrying 1 GB/s.

3.4.2 Routing

By default, SST/macro uses the simplest possible routing algorithm: dimension-order minimal routing (Figure 3.6). In going from source to destination, the message first travels along the X-dimension and then travels along the Y-dimension. The above scheme is entirely static, making no adjustments to avoid congestion in the network. SST/macro supports a variety of adaptive routing algorithms. This can be specified:

```
1 router = min_ad
```

which specifies minimal adaptive routing. There are now multiple valid paths between network endpoints, one of which is illustrated in Figure 3.7. At each network hop, the router chooses the *productive* path with least congestion. In some cases, however, there is only one minimal path (node $(0, 0)$ sending to $(2, 0)$ with only X different). For these messages, minimal adaptive is exactly equivalent to dimension-order routing. Other supported routing schemes are valiant and UGAL. More routing schemes are scheduled to be added in future versions. A full description of more complicated routing schemes will be given in its own chapter in future versions. For now, we direct users to existing resources such as "High Performance Datacenter Networks" by Dennis Abts and John Kim.

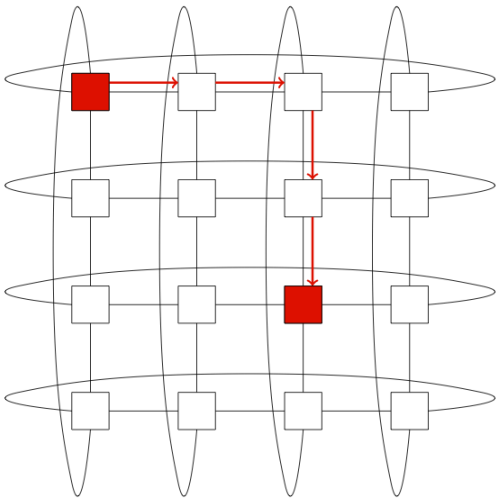


Figure 3.6: Dimension-Order Minimal Routing on a 2D Torus

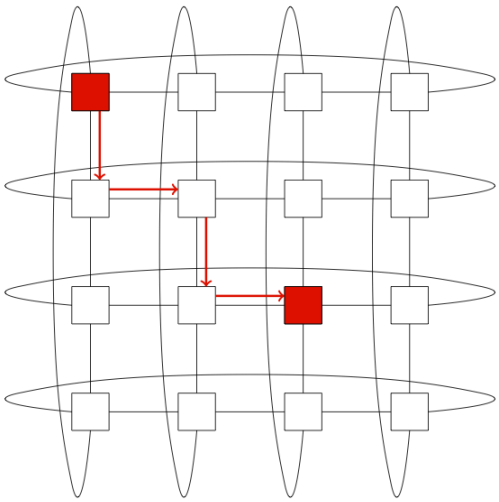


Figure 3.7: Adaptive Minimal Routing on a 2D Torus

3.5 Discrete Event Simulation

Although not necessary for using the simulator, a basic understanding of discrete event simulation can be helpful in giving users an intuition for network models and parameters. Here we walk through a basic program that executes a single send/recv pair. SST/macro simulates many parallel processes, but itself runs as a single process with only one address space (SST/macro can actually run in parallel mode, but we ignore that complication here). SST/macro manages each parallel process as a user-space thread (application thread), allocating a thread stack and frame of execution. User-space threading is necessary for large simulations

since otherwise the kernel would be overwhelmed scheduling thousands of threads.

SST/macro is driven by a simulation thread which manages the user-space thread scheduling (Figure 3.8). In the most common (and simplest) use case, all user-space threads are serialized, running one at a time. The main simulation thread must manage all synchronizations, yielding execution to process threads at the appropriate times. The main simulation thread is usually abbreviated as the DES (discrete event simulation) thread. The simulation progresses by scheduling future events. For example, if a message is estimated to take 5 μs to arrive, the simulator will schedule a MESSAGE ARRIVED event 5 μs ahead of the current time stamp. Every simulation starts by scheduling the same set of events: launch process 0, launch process 1, etc.

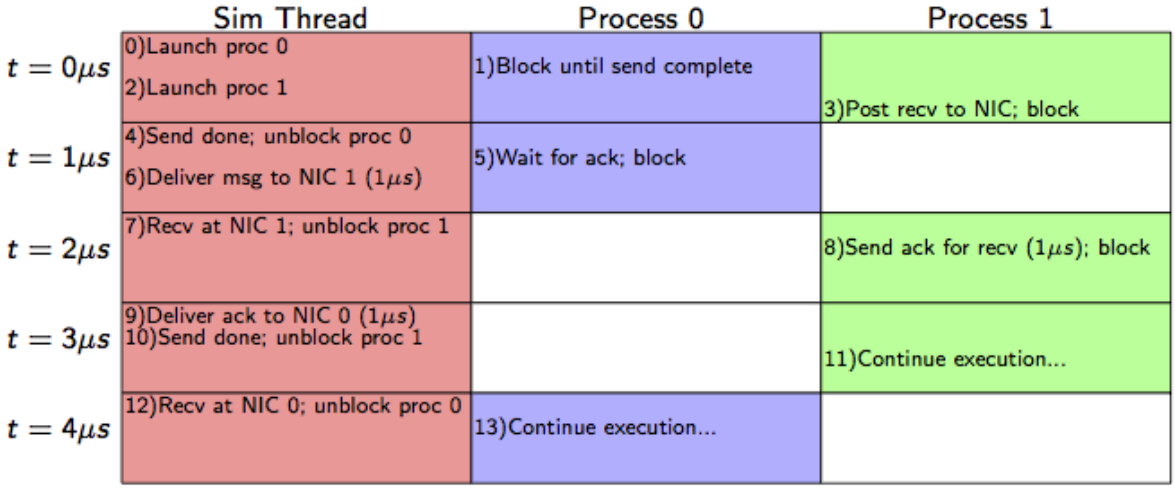


Figure 3.8: Progression of Discrete Event Simulation for Simple Send/Recv Example

The simulation begins at time $t = 0\mu s$. The simulation thread runs the first event, launching process 0. The context of process 0 is switched in, and SST/macro proceeds running code as if it were actually process 0. Process 0 starts a blocking send in Event 1. For process 0 to perform a send in the simulator, it must *schedule* the necessary events to simulate the send. Most users of SST/macro will never need to explicitly schedule events. Discrete event details are always hidden by the API and executed inside library functions. In this simple case, the simulator estimates the blocking send will take 1 μs. It therefore schedules a SEND DONE (Event 4) 1 μs into the future before blocking. When process 0 blocks, it yields execution back to the main simulation.

At this point, no time has yet progressed in the simulator. The DES thread runs the next event, launching process 1, which executes a blocking receive (Event 3). Unlike the blocking send case, the blocking receive does not schedule any events. It cannot know when the message will arrive and therefore blocks without scheduling a RECV DONE event. Process 1 just registers the receive and yields back to the DES thread.

At this point, the simulator has no events left at t=0 μs and so it must progress its time stamp. The next event (Event 4) is SEND DONE at t=1 μs. The event does two things. First, now that the message has been injected into the network, the simulator estimates when it will arrive at the NIC of process 1. In this case, it estimates 1 μs and therefore schedules a MESSAGE ARRIVED event in the future at t=2 μs (Event

7). Second, the DES thread unblocks process 0, resuming execution of its thread context. Process 0 now posts a blocking receive, waiting for process 1 to acknowledge receipt of its message.

The simulator is now out of events at t=1 μs and therefore progresses its time stamp to t=2 μs. The message arrives (Event 7), allowing process 1 to complete its receive and unblock. The DES thread yields execution back to process 1, which now executes a blocking send to ack receipt of the message. It therefore schedules a SEND DONE event 1 μs in the future (Event 10) and blocks, yielding back to the DES thread. This flow of events continues until all the application threads have terminated. The DES thread will run out of events, bringing the simulation to an end.

3.6 Network Model

3.6.1 Packet

The packet model is the simplest and most intuitive of the congestion models for simulating network traffic. The physics correspond naturally to a real machine: messages are broken into small chunks (packets) and routed individually through the network. When two messages compete for the same channel (Figure 3.9A), arbitration occurs at regular intervals to select which packet has access. Packets that lose arbitration are delayed, leading to network congestion. In SST/macro, the packet model is still *coarse-grained*. In a real machine, packet sizes can be very small (100 B). Additionally, arbitration can happen on flits (flow control units), an even smaller unit than the packet. Flit-level arbitration or even 100B packet arbitration is far too fine-grained to do system-level simulation. While packet size is tunable in SST/macro, the simulator is designed for coarse-grained packet sizes of 1 KB to 8 KB. The same flow control (routing, arbitration, congestion avoidance) is performed on coarse-grained packets, but some accuracy is lost.

The coarse-grained packet model has two main sources of error. First, coarse-grained packets systematically overestimate (de)serialization latency. Before a packet can be forwarded to its next destination, it must be completely deserialized off the network link into a buffer. In a real machine, data can be forwarded on a flit-by-flit basis, efficiently pipelining packets. Flits that would send in a real system are artificially delayed until the rest of the coarse-grained packet arrives. Second, coarse-grained packets exclusively reserve network links for the entire length of the packet. In a real machine, two packets could multiplex across a link on a flit-by-flit basis.

3.6.2 Flow

The flow model, in simple cases, corrects the most severe problems of the packet model. Instead of discrete chunks, messages are modeled as fluid flows moving through the network (Figure 3.9B). Congestion is treated as a fluid dynamics problem, sharing bandwidth between competing flows. Without congestion, a flow only requires a FLOW START and FLOW STOP event to be modeled (see tutorial on discrete event simulation in 3.5). While the packet model would require many, many events to simulate a 1 MB message, the flow model might only require two. With congestion, flow update events must be scheduled whenever congestion changes on a network link. For limited congestion, only a few update events must occur. The flow model also corrects the latency and multiplexing problems in the packet model, providing higher-accuracy for coarse-grained simulation.

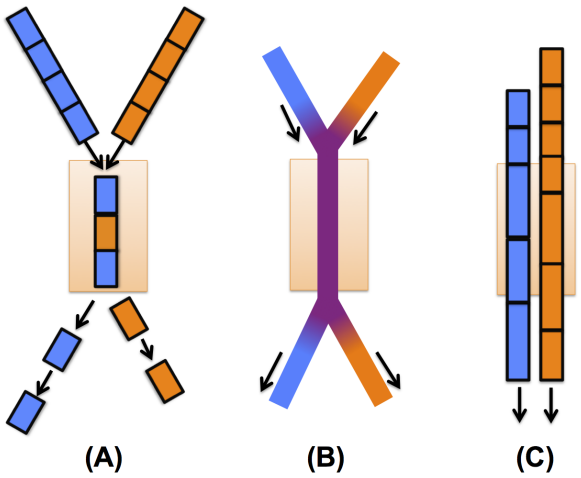


Figure 3.9: Schematic of two messages competing for same channel in the different SST/macro congestion models. (A) Packet Model (B) Flow Model (C) Packet-flow Model

The flow model starts to break down for large systems or under heavy congestion. In the packet model, all congestion events are "local" to a given router. The number of events is also constant in packet models regardless of congestion since we are modeling a fixed number of discrete units. In flow models, flow update events can be "non-local," propagating across the system and causing flow update events on other routers. When congestion occurs, this "ripple effect" can cause the number of events to explode, overwhelming the simulator. For large systems or heavy congestion, the flow model is actually much slower than the packet model. Support for this model has been completely removed.

3.6.3 Packet-flow

Packet-flow is a hybrid-model of flow and packet, trying to correct the latency errors in the packet model while avoiding the ripple effect of the flow model. Much like packets, the packet-flow model begins by converting messages into many discrete chunks of fixed size. In contrast to the packet model, channel arbitration is not exclusive. When multiple packets compete for a channel, each packet "samples" the current congestion (Figure 3.9C). Based on congestion, the packets estimates its bandwidth and latency. If low congestion is sampled, high-bandwidth is assigned (short packet in the figure). If high congestion is sampled, low-bandwidth is assigned (long packet in the figure).

The packet-flow model corrects the two most important packet model errors. Once bandwidth has been assigned, the packet can immediately be forwarded to the next router, producing accurate latencies. The sampling procedure also allows two packets to multiplex across a channel. Because messages are broken into discrete chunks, the number of events per message is constant regardless of congestion, avoiding the ripple effect.

For more details on packet-flow parameters, see the `hopper_amm.ini` files in the `configurations` folder in the SST/macro source.

3.7 Launching, Allocation, and Indexing

3.7.1 Launch Commands

Just as jobs must be launched on a shared supercomputer using Slurm or aprun, SST/macro requires the user to specify a launch command for the application. Currently, we encourage the user to use aprun from Cray, for which documentation can easily be found online. In the parameter file you specify, e.g.

```
app1.name = user_mpiapp_cxx
app1.launch_cmd = aprun -n 8 -N 2
```

which launches an external user C++ application with eight ranks and two ranks per node. The aprun command has many command line options (see online documentation), some of which may be supported in future versions of SST/macro. In particular, we are in the process of adding support for thread affinity, OpenMP thread allocation, and NUMA containment flags. Most flags, if included, will simply be ignored.

3.7.2 Allocation Schemes

In order for a job to launch, it must first allocate nodes to run on. Here we choose a simple 2D torus

```
topology.name = torus
topology.geometry = 3 3
topology.concentration = 1
```

which has 9 nodes arranged in a 3x3 mesh. For the launch command `aprun -n 8 -N 2`, we must allocate 4 compute nodes from the pool of 9. Our first option is to specify the first available allocation scheme (Figure 3.10)

```
app1.launch_allocation = first_available
```

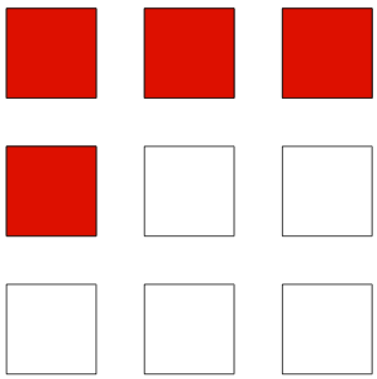


Figure 3.10: First available Allocation of 4 Compute Codes on a 3x3 2D Torus

In first available, the allocator simply loops through the list of available nodes as they are numbered by the topology object. In the case of a 2D torus, the topology numbers by looping through columns in a row. In general, first available will give a contiguous allocation, but it won't necessarily be ideally structured.

To give more structure to the allocation, a Cartesian allocator can be used (Figure 3.11).

```
app1.launch_allocation = cartesian
app1.cart_launch_sizes = 2 2
app1.cart_launch_offsets = 0 0
```

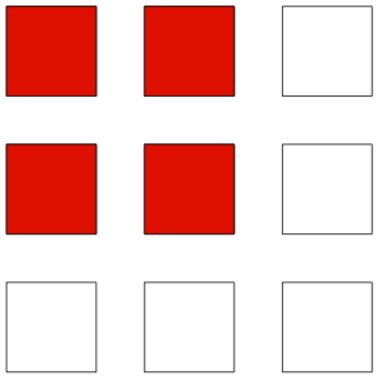


Figure 3.11: Cartesian Allocation of 4 Compute Codes on a 3x3 2D Torus

Rather than just looping through the list of available nodes, we explicitly allocate a 2x2 block from the torus. If testing how "topology agnostic" your application is, you can also choose a random allocation.

```
app1.launch_allocation = random
```

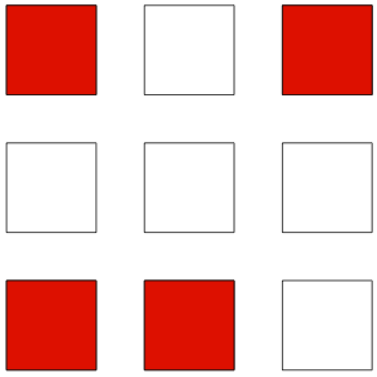


Figure 3.12: Random Allocation of 4 Compute Codes on a 3x3 2D Torus

In many use cases, the number of allocated nodes equals the total number of nodes in the machine. In this case, all allocation strategies allocate the same *set* of nodes, i.e. the whole machine. However, results may still differ slightly since the allocation strategies still assign an initial numbering of the node, which means a random allocation will give different results from Cartesian and first available.

Indexing Schemes

Once nodes are allocated, the MPI ranks (or equivalent) must be assigned to physical nodes, i.e. indexed. The simplest strategies are block and round-robin. If only running one MPI rank per node, the two strategies are equivalent, indexing MPI ranks in the order received from the allocation list. If running multiple MPI ranks per node, block indexing tries to keep consecutive MPI ranks on the same node (Figure 3.13).

```
app1.launch_indexing = block
```

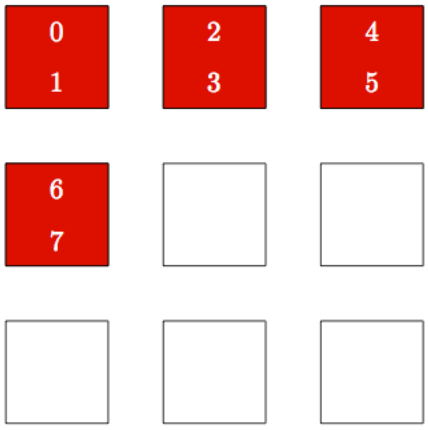


Figure 3.13: Block Indexing of 8 MPI Ranks on 4 Compute Nodes

In contrast, round-robin spreads out MPI ranks by assigning consecutive MPI ranks on different nodes (Figure 3.14).

```
app1.launch_indexing = round_robin
```

Finally, one may also choose

```
app1.launch_indexing = random
```

Random allocation with random indexing is somewhat redundant. Random allocation with block indexing is *not* similar to Cartesian allocation with random indexing. Random indexing on a Cartesian allocation still gives a contiguous block of nodes, even if consecutive MPI ranks are scattered around. A random allocation (unless allocating the whole machine) will not give a contiguous set of nodes.

3.8 Using DUMPI

3.8.1 Building DUMPI

As noted in the introduction, SST/macro is primarily intended to be an on-line simulator. Real application code runs, but SST/macro intercepts calls to communication (MPI) and computation functions to simulate

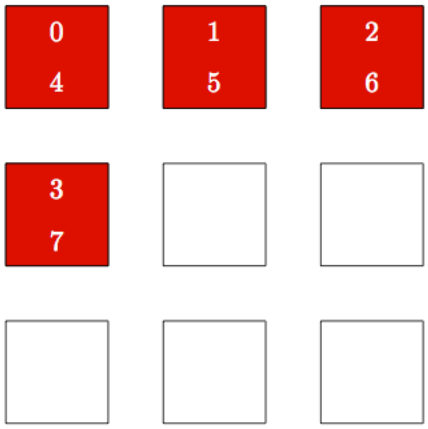


Figure 3.14: Round-Robin Indexing of 8 MPI Ranks on 4 Compute Nodes

time passing. However, SST/macro can also run off-line, replaying application traces collected from real production runs. This trace collection and trace replay library is called DUMPI.

Although DUMPI is automatically included as a subproject in the SST/macro download, trace collection can be easier if DUMPI is built independently from SST/macro. The code can be downloaded from `https://bitbucket.org/sst-ca/dumpi`. If downloaded through Mercurial, one must initialize the build system and create the configure script.

```
dumpi> ./bootstraps.h
```

DUMPI must be built with an MPI compiler.

```
dumpi/build> ../configure CC=mpicc CXX=mpicxx \
               --enable-libdumpi --prefix=$DUMPI_PATH
```

The `--enable-libdumpi` flag is needed to configure the trace collection library. After compiling and installing, a `libdumpi.$prefix` will be added to `$DUMPI_PATH/lib`.

Collecting application traces requires only a trivial modification to the standard MPI build. Using the same compiler, simply add the DUMPI library path and library name to your project's `LDFLAGS`.

```
your_project/build> ../configure CC=mpicc CXX=mpicxx \
                                 LDFLAGS=‘‘-L$DUMPI_PATH/lib -ldumpi"
```

Trace Collection

DUMPI works by overriding *weak symbols* in the MPI library. In all MPI libraries, functions such as `MPI_Send` are only weak symbol wrappers to the actual function `PMPI_Send`. DUMPI overrides the weak symbols by implementing functions with the symbol `MPI_Send`. If a linker encounters a weak symbol and regular symbol with the same name, it ignores the weak symbol. DUMPI functions look like

```c
int MPI_Send(...)
{
  /** Start profiling work */
  ...
  int rc = PMPI_Send(...);
  /** Finish profiling work */
  ...
  return rc;
}
```

collecting profile information and then directly calling the PMPI functions.

We examine DUMPI using a very basic example program.

```c
#include <mpi.h>
int main(int argc, char** argv)
{
    MPI_Init(&argc, &argv);
    MPI_Finalize();
    return 0;
}
```

After compiling the program named `test` with DUMPI, we run MPI in the standard way.

```
example> mpiexec -n 2 ./test
```

After running, there are now three new files in the directory.

```
example> ls dumpi*
dumpi-2013.09.26.10.55.53-0000.bin
dumpi-2013.09.26.10.55.53-0001.bin
dumpi-2013.09.26.10.55.53.meta
```

DUMPI automatically assigns a unique name to the files from a timestamp. The first two files are the DUMPI binary files storing separate traces for MPI rank 0 and rank 1. The contents of the binary files can be displayed in human-readable form by running the `dumpi2ascii` program, which should have been installed in `$DUMPI_PATH/bin`.

```
example> dumpi2ascii dumpi-2013.09.26.10.55.53-0000.bin
```

This produces the output

```
MPI_Init entering at walltime 8153.0493, cputime 0.0044 seconds in thread 0.
MPI_Init returning at walltime 8153.0493, cputime 0.0044 seconds in thread 0.
MPI_Finalize entering at walltime 8153.0493, cputime 0.0045 seconds in thread 0.
MPI_Finalize returning at walltime 8153.0498, cputime 0.0049 seconds in thread 0.
```

The third file is just a small metadata file DUMPI used to configure trace replay.

```
hostname=deepthought.magrathea.gov
numprocs=2
username=slartibartfast
startime=1380218153
fileprefix=dumpi-2013.09.26.10.55.53
version=1
subversion=1
subsubversion=0
```

Trace Replay

It is often useful to validate the correctness of a trace. Sometimes there can be problems with trace collection. There are also a few nooks and crannies of the MPI standard left unimplemented. To validate the trace, you can run in a special debug mode that runs the simulation with a very coarse-grained model to ensure as quickly as possible that all functions execute correctly. This can be done straightforwardly by running the executable with the dumpi flag: `sstmac --dumpi`.

To replay a trace in the simulator, a small modification is required to the example input file in 3.1. We have two choices for the trace replay. First, we can attempt to *exactly* replay the trace as it ran on the host machine. Second, we could replay the trace on a new machine or different layout.

For exact replay, the key issue is specifying the machine topology. For some architectures, topology information can be directly encoded into the trace. This is generally true on Blue Gene, but not Cray. When topology information is recorded, trace replay is much easier. The parameter file then becomes, e.g.

```
app1.launch_type = dumpi
app1.launch_indexing = dumpi
app1.launch_allocation = dumpi
app1.name = parsedumpi
app1.launch_dumpi_metaname = testbgp.meta
```

We have a new parameter `launch_type` set to `dumpi`. This was implicit before, taking the default value of `skeleton`. We also set indexing and allocation parameters to read from the DUMPI trace. The application name is a special app that parses the DUMPI trace. Finally, we direct SST/macro to the DUMPI metafile produced when the trace was collected. To extract the topology information, locate the `.bin` file corresponding to MPI rank 0. To print topology info, run

```
traces> dumpi2ascii -H testbgp-0000.bin
```

which produces the output

```
version=1.1.0
starttime=Fri Nov 22 13:53:58 2013
hostname=R00-M1-N01-J01.challenger
username=<none>
meshdim=3
meshsize=[4, 2, 2]
meshcrd=[0, 0, 0]
```

Here we see that the topology is 3D with extent 4,2,2 in the X,Y,Z directions. At present, the user must still specify the topology in the parameter file. Even though SST/macro can read the topology *dimensions* from the trace file, it cannot read the topology *type*. It could be a torus, dragonfly, or fat tree. The parameter file therefore needs

```
topology_name = hdtorus
topology_geometry = 4 2 2
```

Beyond the topology, the user must also specify the machine model with bandwidth and latency parameters. Again, this is information that cannot be automatically encoded in the trace. It must be determined via small benchmarks like ping-pong. An example file can be found in the test suite in `tests/test_configs/testdumpibgp.ini`.

If no topology info could be recorded in the trace, more work is needed. The only information recorded in the trace is the hostname of each MPI rank. The parameters are almost the same, but with allocation now

set to `hostname`. Since no topology info is contained in the trace, a hostname map must be put into a text file that maps a hostname to the topology coordinates. The new parameter file, for a fictional machine called deep thought

```
# Launch parameters
app1.launch_type = dumpi
app1.launch_indexing = dumpi
app1.launch_allocation = hostname
app1.name = parsedumpi
app1.launch_dumpi_metaname = dumpi-2013.09.26.10.55.53.meta
app1.launch_dumpi_mapname = deepthought.map
# Machine parameters
topology_name = torus
topology_geometry = 2 2
```

In this case, we assume a 2D torus with four nodes. Again, DUMPI records the hostname of each MPI rank during trace collection. In order to replay the trace, the mapping of hostname to coordinates must be given in a node map file, specified by the parameter `launch_dumpi_mapname`. The node map file has the format

```
4 2
nid0 0 0
nid1 0 1
nid2 1 0
nid3 1 1
```

where the first line gives the number of nodes and number of coordinates, respectively. Each hostname and its topology coordinates must then be specified. More details on building hostname maps are given below.

We can also use the trace to experiment with new topologies to see performance changes. Suppose we want to test a crossbar topology.

```
# Launch parameters
app1.launch_indexing = block
app1.launch_allocation = first_available
app1.launch_dumpi_metaname = dumpi-2013.09.26.10.55.53.meta
app1.name = parsedumpi
app1.size = 2
# Machine parameters
topology.name = crossbar
topology.geometry = 4
```

We no longer use the DUMPI allocation and indexing. We also no longer require a hostname map. The trace is only used to generate MPI events and no topology or hostname data is used. The MPI ranks are mapped to physical nodes entirely independent of the trace.

3.9 Call Graph Visualization

Generating call graphs requires a special build of SST/macro.

```
build$ ../configure --prefix=$INSTALL_PATH --enable-graphviz
```

The `--enable-graphviz` flag defines an instrumentation macro throughout the SST/macro code. This instrumentation must be *compiled* into SST/macro. In the default build, the instrumentation is not added since the instrumentation has a high overhead. However, SST/macro only instruments a select group of the most important functions so the overhead should only be 10-50%. After installing the instrumented version of SST/macro, a call graph is collected by adding a simple filename to the parameter file.

```
1 call_graph = <fileroot>
```

After running, a `<fileroot>.callgrind.out` file should appear in the folder.

To visualize the call graph, you must download KCachegrind: `http://kcachegrind.sourceforge.net/html/Download.html`. KCachegrind is built on the KDE environment, which is simple to build for Linux but can be very tedious for Mac. The download also includes a QCachegrind subfolder, providing the same functionality built on top of Qt. This is highly recommended for Mac users.

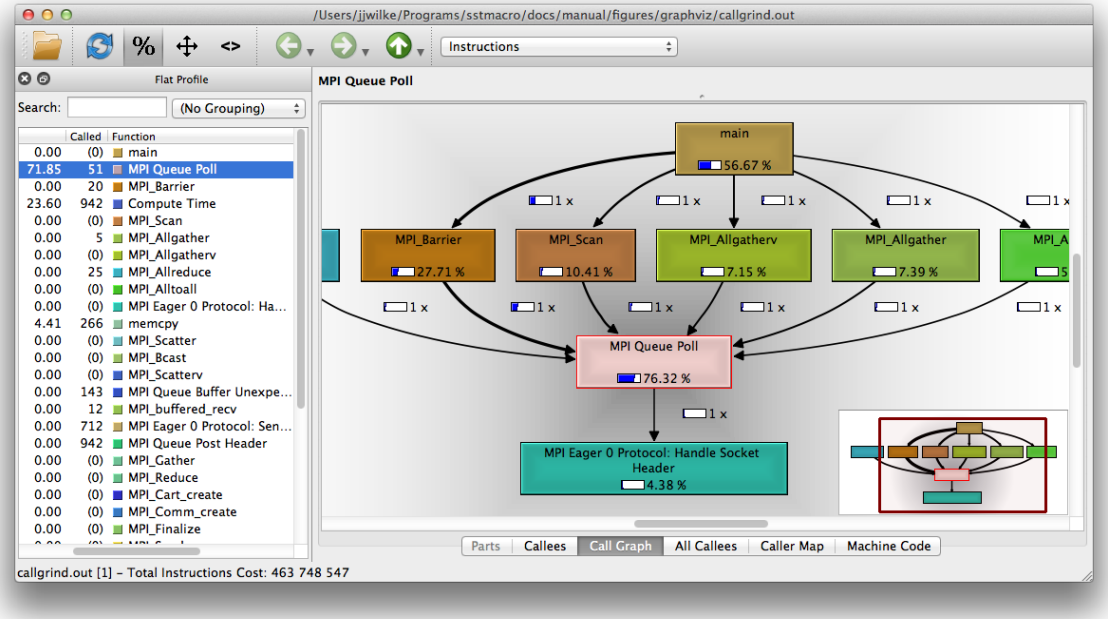


Figure 3.15: QCachegrind GUI

The basic QCachegrind GUI is shown in Figure 3.15. On the left, a sidebar contains the list of all functions instrumented with the percent of total execution time spent in the function. In the center pane, the call graph is shown. To navigate the call graph, a small window in the bottom right corner can be used to change the view pane. Zooming into one region (Figure 3.16), we see a set of MPI functions (Barrier, Scan, Allgatherv). Each of the functions enters a polling loop, which dominates the total execution time. A small portion of the polling loop calls the "Handle Socket Header" function. Double-clicking this node unrolls more details in the call graph (Figure 3.17). Here we see the function splits execution time between buffering messages (memcpy) and posting headers (Compute Time).

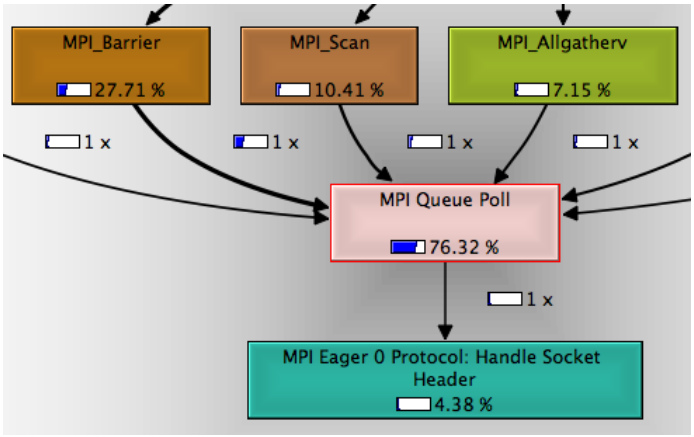


Figure 3.16: QCachegrind Call Graph of MPI Functions

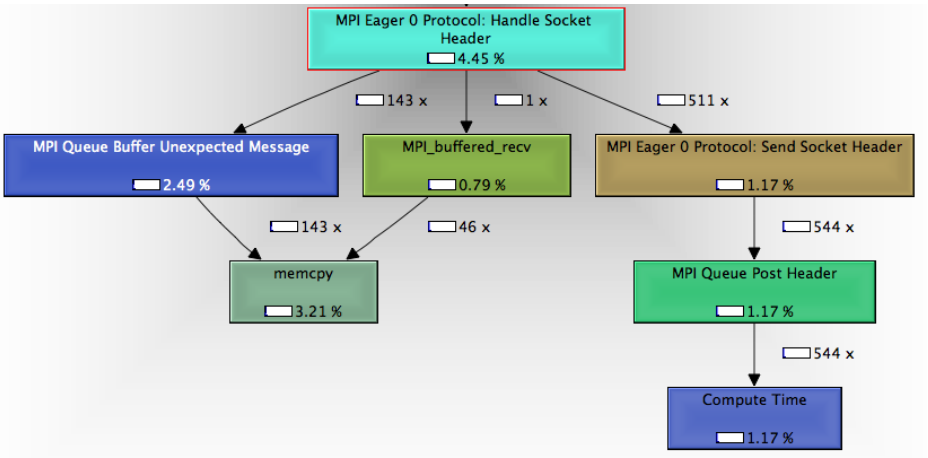


Figure 3.17: QCachegrind Expanded Call Graph of Eager 0 Function

3.10 Spyplot Diagrams

Spyplots visualize communication matrices, showing either the number of messages or number of bytes sent between two network endpoints. They are essentially contour diagrams, where instead of a continuous function $F(x, y)$ we are plotting the communication matrix $M(i, j)$. An example spyplot is shown for a simple application that only executes an MPI_Allreduce (Figure 3.18). Larger amounts of data (red) are sent to nearest neighbors while decreasing amounts (blue) are sent to MPI ranks further away.

Various spyplots can be activated by boolean parameters in the input file. The most commonly used are the MPI spyplots, for which you must add

```
1 mpi_spyplot = <fileroot>
```

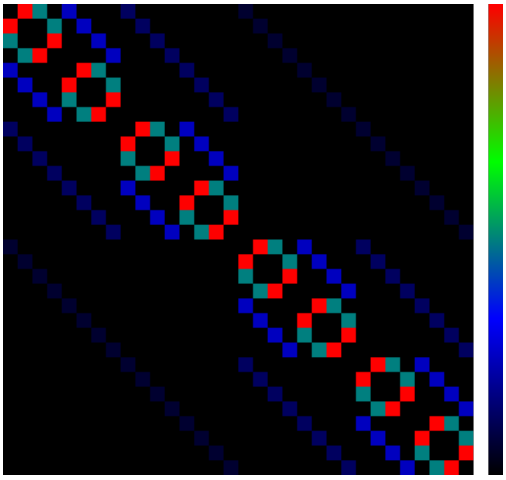


Figure 3.18: Spyplot of Bytes Transferred Between MPI Ranks for MPI_Allreduce

After running there will be a .csv and .png file in the folder, with e.g. `fileroot = test`

```
example> ls
test.png
test.csv
```

`test.png` shows the number of bytes exchanged between MPI ranks. To extend the analysis you can specify

```
1 network_spyplot = <fileroot>
```

A new csv/png will appear showing the number of bytes exchanged between physical nodes, accumulating together all MPI ranks sharing the same node. This gives a better sense of spatial locality when many MPI ranks are on the same node.

3.11 Fixed-Time Quanta Charts

Another way of visualizing application activity is a fixed-time quanta (FTQ) chart. While the call graph gives a very detailed profile of what code regions are most important for the application, they lack temporal information. The FTQ histogram gives a time-dependent profile of what the application is doing (Figure 3.19). This can be useful for observing the ratio of communication to computation. It can also give a sense of how "steady" the application is, i.e. if the application oscillates between heavy computation and heavy communication or if it keeps a constant ratio. In the simple example, Figure 3.19, we show the FTQ profile of a simple MPI test suite with random computation mixed in. In general, communication (MPI) dominates. However, there are a few compute-intensive and memory-intensive regions.

The FTQ visualization is activated by another input parameter

```
1 ftq = <fileroot>
```

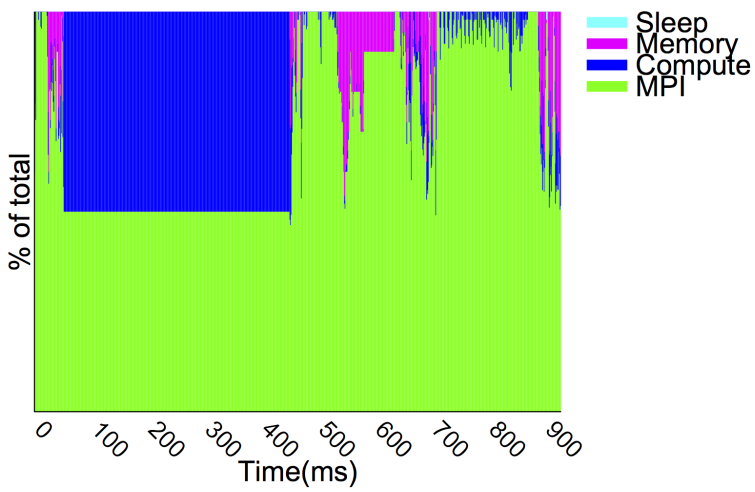


Figure 3.19: Application Activity (Fixed-Time Quanta; FTQ) for Simple MPI Test Suite

where the `fileroot` parameter gives a unique prefix for the output files.

After running, two new files appear in the folder: `<fileroot>_app1.p` and `<fileroot>_app1.dat`. `plot_app1.p` is a Gnuplot script that generates the histogram as a postscript file.

```
your_project$ gnuplot plot_app1.p > output.ps
```

Gnuplot can be downloaded from `http://www.gnuplot.info` or installed via MacPorts. We recommend version 4.4, but at least 4.2 should be compatible.

The granularity of the chart is controlled by the `ftq_epoch` parameter in the input file. The above figure was collected with

```
1 ftq_epoch=5us
```

Events are accumulated into a single data point per "epoch." If the timestamp is too small, too little data will be collected and the time interval won't be large enough to give a meaningful picture. If the timestamp is too large, too many events will be grouped togther into a single data point, losing temporal structure.

Using fully namespace parameters, this would be specified as:

```
1 node.os.ftq.fileroot=<fileroot>
2 node.os.ftq.epoch=5us
```

Chapter 4

Topologies

The torus topology is straightforward and easy to understand. Here we introduce the basics of other topologies within SST that are more complex and require extra documentation to configure properly. These are generally higher-radix or path-diverse topologies like fat tree, dragonfly, and flattened butterfly. As noted in 3.4, a more thorough and excellent discussions of these topologies is given in "High Performance Datacenter Networks" by Dennis Abts and John Kim.

4.1 Topology Query Utility

Understanding topology inputs and geometries can sometimes be challenging. SST/macro provides an executable for testing topology inputs and doing example coordinate computations. After making and installing, an executable `sstmac_top_info` will appear in the `bin` folder. The invocation of `sstmac_top_info` is exactly the same as the main `sstmac` executable. For the example parameter file named `machine.ini`:

```
1 topology.name = fattree
2 topology.geometry = 4 3
```

we run

```
bin> sstmac_top_info -f machine.ini
```

which produces the output

```
1 Number of nodes:          81
2 Number of leaf switches: 27
3 Number of switches:       94
```

detailing the produced geometry. Here the fat tree has a total of 94 switches, 27 of which are "leaf" switches directly connected to compute nodes. The output is followed by the prompt

```
NextInput:
```

One can either enter a single number (switch ID) or set of coordinates. If given a switch ID, the coordinates are computed. If coordinates are given, the switch ID is computed.

```
NextInput: 32
Switch ID maps to coordinates [ 2 0 1 2 ]
NextInput: 2 0 1 2
Coordinates map to switch ID 32
```

The program is just exited with Ctrl-C. The meaning of the above coordinates is detail below for fat tree (Section 4.4).

4.2 Torus

The torus is the simplest topology and fairly easy to understand. We have already discussed basic indexing and allocation as well as routing. More complicated allocation schemes with greater fine-grained control can be used such as the coordinate allocation scheme (see hypercube below for examples) and the node ID allocation scheme (see fat tree below for examples). More complicated Valiant and UGAL routing schemes are shown below for hypercube and dragonfly, but apply equally well to torus.

For torus we illustrate here the Cartesian allocation for generating regular Cartesian subsets. For this, the input file would look like

```
1 topology.name = torus
2 topology.geometry = 4 4 4
3 app1.launch_cmd = aprun -n 8
4 app1.launch_indexing = block
5 app1.launch_allocation = cartesian
6 app1.launch_cart_sizes = 2 2 2
7 app1.launch_cart_offsets = 0 0 0
```

This allocates a 3D torus of size 4x4x4. Suppose we want to allocate all 8 MPI ranks in a single octant? We can place them all in a 2x2x2 3D sub-torus by specifying the size of the sublock (`launch_cart_sizes`) and which octant (`launch_cart_offsets`). This applies equally well to higher dimensional analogs. This is particularly useful for allocation on Blue Gene machines which always maintain contiguous allocations on a subset of nodes.

This allocation is slightly more complicated if we have multiple nodes per switch. Even though we have a 3D torus, we treat the geometry as a 4D coordinate space with the 4th dimension referring to nodes connected to the same switch, i.e. if two nodes have the 4D coordinates [1 2 3 0] and [1 2 3 1] they are both connected to the same switch. Consider the example below:

```
1 topology.name = torus
2 topology.geometry = 4 4 4
3 topology.concentration = 2
4 app1.launch_cmd = aprun -n 8
5 app1.launch_indexing = block
6 app1.launch_allocation = cartesian
7 app1.launch_cart_sizes = 2 2 1 2
8 app1.launch_cart_offsets = 0 0 0 0
```

We allocate a set of switches across an XY plane (2 in X, 2 in Y, 1 in Z for a single plane). The last entry in `launch_cart_sizes` indicates that both nodes on each switch should be used.

4.3 Hypercube

Although never used at scale in a production system, the generalized hypercube is an important topology to understand, particularly for flattened butterfly and dragonfly. The (k,n) generalized hypercube is geometrically an N-dimensional torus with each dimension having size k (although dimension sizes need not be equal). Here we show a (4,2) generalized hypercube (Figure 4.1). This would be specified in SST as:

```
1 topology.name = hypercube
2 topology.geometry = 4 4
```

indicating size 4 in two dimensions.

While a torus only has nearest-neighbor connections, a hypercube has full connectivity within a row and column (Figure 4.1). Any switches in the same row or same column can send packets with only a single hop.

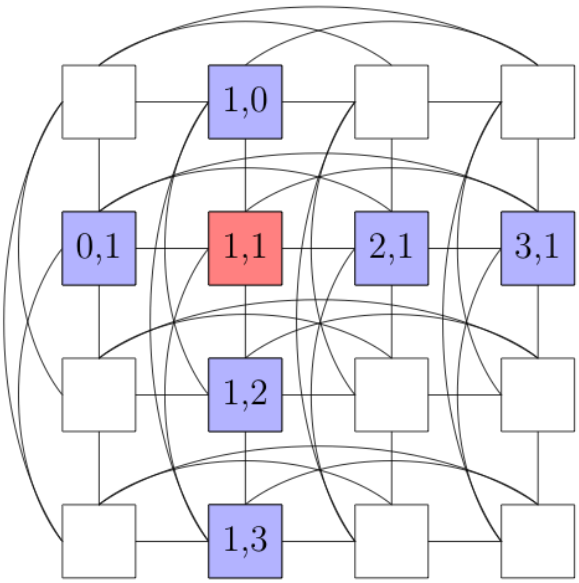


Figure 4.1: Hypercube with links and connections within a row/column

This extra connectivity leads to greater path diversity and higher radix switches. The cost tradeoff is that each link has lower bandwidth than a torus. Whereas a torus has a few fat links connecting switches, a hypercube has many thin links. A hypercube can have more dimensions and be asymmetric, e.g.

```
1 topology.name = hypercube
2 topology.geometry = 4 5 6
```

where now we have full connections within horizontal rows, horizontal columns, and vertical columns. Here each switch has radix 12 (3 connections in X, 4 connections in Y, 5 connections in Z).

4.3.1 Allocation and indexing

A hypercube has the same coordinate system as a torus. For example, to create a very specific, irregular allocation on a hyerpcube:

```
app1.launch_cmd = aprun -n 5
app1.launch_indexing = coordinate
app1.launch_allocation = coordinate
app1.launch_coordinate_file = coords.txt
```

and then a coordinate file named `coords.txt`

```
5 2
0 0
0 1
1 1
2 0
3 3
```

The first line indicates 5 entries each with 2 coordinates. Each line then defines where MPI ranks 0-4 will be placed

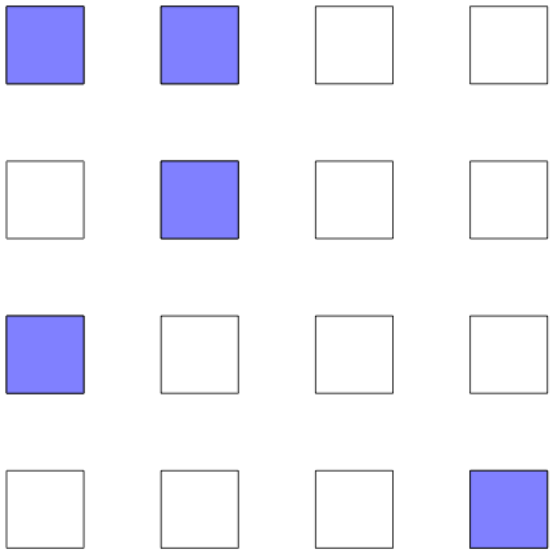


Figure 4.2: Hypercube allocation for given set of coordinates

4.3.2 Routing

Hypercubes allow very path-diverse routing because of its extra connections. In the case of minimal routing (Figure 4.3), two different minimal paths from blue to red are shown. While dimension order routing would rigorously go X then Y, you can still route minimally over two paths either randomly selecting to balance load or routing based on congestion.

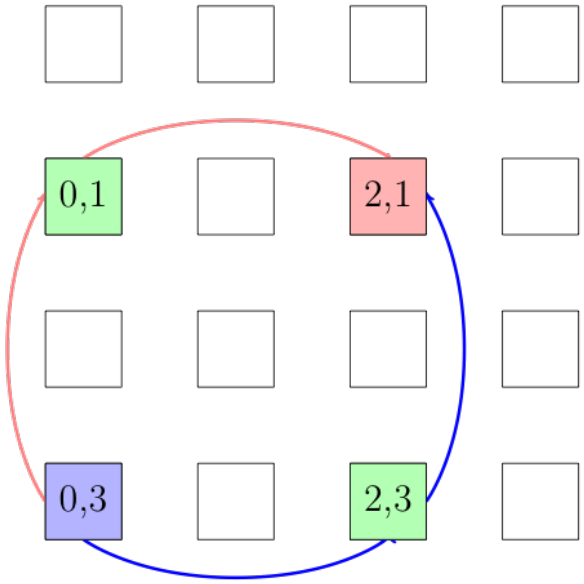


Figure 4.3: Minimal routing within a hypercube showing path diversity. Packet travels from blue to red, passing through green intermediate switches.

To fully maximize path diversity on adversarial traffic patterns, though, path-diverse topologies can benefit from Valiant routing. Here, rather than directly routing to the final destination, packets first route to random intermediate switches on a minimal path. Then they route again from the intermediate switch to the final destination also on a minimal path (Figure 4.4). Although it increases the hop count and therefore the point-to-point latency, it utilizes more paths and therefore increases the effective point-to-point bandwidth.

4.4 Fat Tree

Within SST, a fat tree is defined by the following parameters:

```
1 topology.name = fattree
2 topology.geometry = 4 2
```

The first number, 4, indicates the number of levels in the fat tree. The second number, 2, indicates the radix or branching factor of the tree. The number of compute nodes in this topology is $2^4 = 16$. This is illustrated conceptually in Figure 4.5. The color coding will become clear later. We note this is somewhat confusing since the fat tree appears to have 5 levels. Here the topology is defined by the number of levels containing switches or the number of branches. This is done for a very specific reason. At the final level, you may wish to have a different branching fraction for the compute nodes, e.g.

```
1 topology.concentration = 1
```

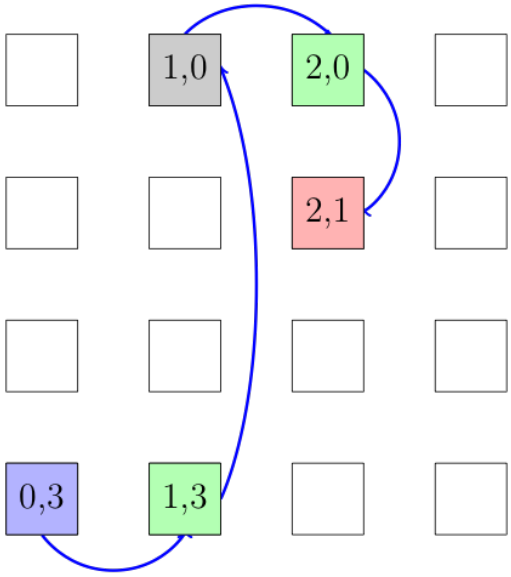


Figure 4.4: Valiant routing within a hypercube. Packet travels from blue to red via a random intermediate destination shown in gray. Additional intermediate switches are shown in green.

This loads the injection bandwidth for the compute node dedicating its own injection switch. If the parameter `network_nodes_per_switch` is omitted, it defaults to the fat tree radix. This case is shown in Figure 4.5 where there are two nodes injecting to the same switch. Higher radix fat trees can be specified, e.g.

```
1 topology.name = fattree
2 topology.geometry = 3 4
```

which would have $4^3 = 64$ compute nodes.

In reality, it is not practical to implement a fat tree exactly as shown in Figure 4.5. One would need to buy many non-standard, high capacity switches for the higher levels in the fat-tree. The simple model is available by specifying `simple_fattree` as the topology, and SST will construct special large switches at higher levels. The best practical implementation employs all uniform, commodity switches (Figure 4.6). The fat tree is "virtual" with several commodity switches grouped together to simulate a heavy-weight, high capacity switch at higher levels of the fat tree. The connection between the physical implementation and the conceptual fat tree can easily be seen by the color coding. For example, the second row contains eight switches, but only two virtual switches. Each virtual switch is composed of four commodity switches.

Within SST, each switch is assigned a unique ID, starting from zero in the bottom row and proceeding through the top level. In addition, each compute node is also assigned a unique ID from 0 to 15. The switches can also be defined by a set of coordinates. While the choice of coordinate system for a 3D torus is obvious, the coordinate system for the fat tree is less clear. In SST, we define a 2D mesh coordinate system for the row (level) and column of the switch.

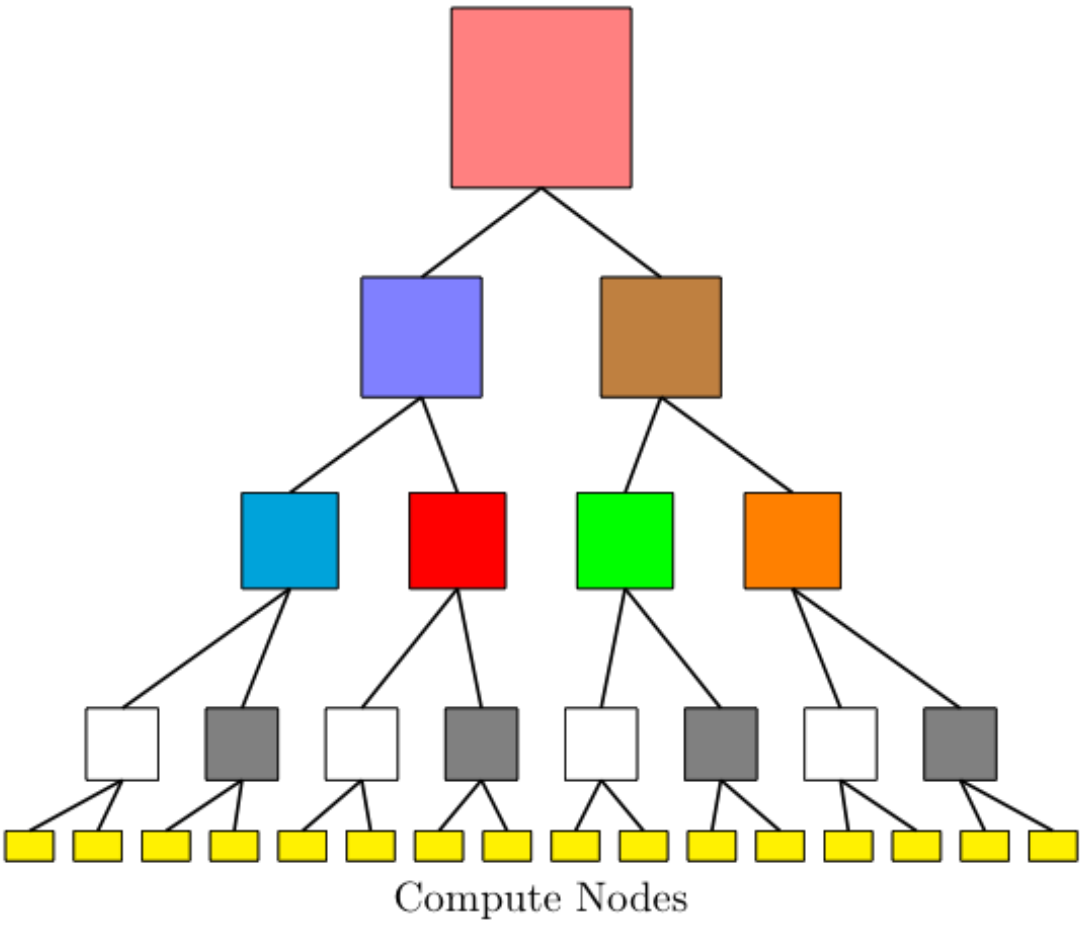


Figure 4.5: Abstract, conceptual picture of Fat Tree topology

4.4.1 Allocation and indexing

The numbering of compute nodes is shown in Figure 4.6. Consider the case

```
1 app1.launch_cmd = aprun -n 4 -N 1
```

which launches four processes all on distinct nodes. In the simplest allocation and indexing scheme (first available), processes would be placed in order on 0,1,2,3. An alternative allocation/indexing scheme uses the

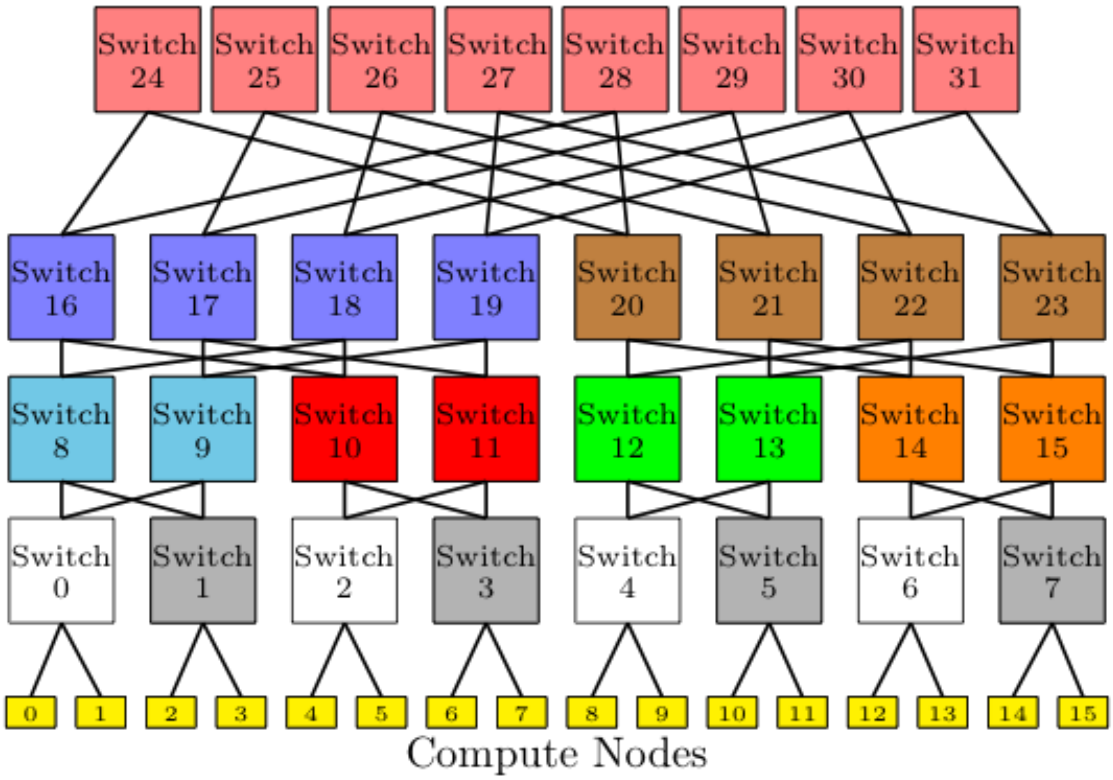


Figure 4.6: Physical implementation of Fat Tree with commodity switches showing ID numbering

Node ID allocator.

```
app1.launch_allocation = node_id
app1.launch_indexing = node_id
app1.launch_node_id_file = nodes.txt
```

Here `nodes.txt` would contain the number of nodes on the first line, followed by the list of Node IDs, in order, of where to place MPI ranks. For the file

```
4
0
4
8
12
```

Four MPI ranks would be placed in spatially distant parts of the machine.

If indexing differs from allocation (usually because there are multiple MPI ranks per node), both an allocation and an indexing file are needed. Suppose we have:

```
app1.launch_cmd = aprun -n 4 -N 2
```

We then need:

```
app1.launch_allocation = node_id
app1.launch_indexing = node_id
app1.launch_node_id_allocation_file = alloc.txt
app1.launch_node_id_indexing_file = index.txt
```

where the contents of `alloc.txt` are, e.g.

```
2
0
1
```

choosing nodes 0 and 1 in the allocation and then `index.txt` would be, e.g.

```
4
0
1
0
1
```

which round-robin assigns rank 0 to node, rank 1 to node 1, rank 2 to node 0, and so on.

4.4.2 Routing

Fat tree routing is actually straightforward, but can employ path diversity. Suppose you are routing from Node 0 to Node 2 (Figure 4.6). At the first stage, you have no choice. You must route to Switch 1. At the second stage, you can either route to Switch 8 or Switch 9. Suppose you branch to Switch 9. At this point, you are done moving up. The packet now proceeds down the fat-tree. On the downward routing, there is no path diversity. Only a single, minimal route exists to the destination node. In the simplest case, Switch 1 alternates between selecting Switch 8 and Switch 9 to distribute load. In a more complicated scheme, Switch 1 could adaptively route selecting either Switch 8 or Switch 9 based on congestion information.

4.5 Dragonfly

As bandwidth per pin increases, arguments can be made that optimal topologies should be higher radix. A 3D torus is on the low-radix extreme while a hypercube is a high-radix extreme. Unfortunately a hypercube topology is not scalable and the radix quickly becomes too high to efficiently implement. A dragonfly is sometimes viewed as a generalization of flattened butterfly and hypercube topologies with "virtual" switches of very high radix, not dissimilar from the fat-tree implementation with many physical commodity switches composing a single virtual switch. The dragonfly topology (Figure 4.7) is actually quite simple. Small groups are connected as a generalized hypercube with full connectivity within a row or column. Intergroup connections (global links) provide pathways for hopping between groups. A dragonfly is usually understood through three parameters:

- p: number of nodes connected to each router
- a: number of routers in a group
- h: number of global links that each switch has

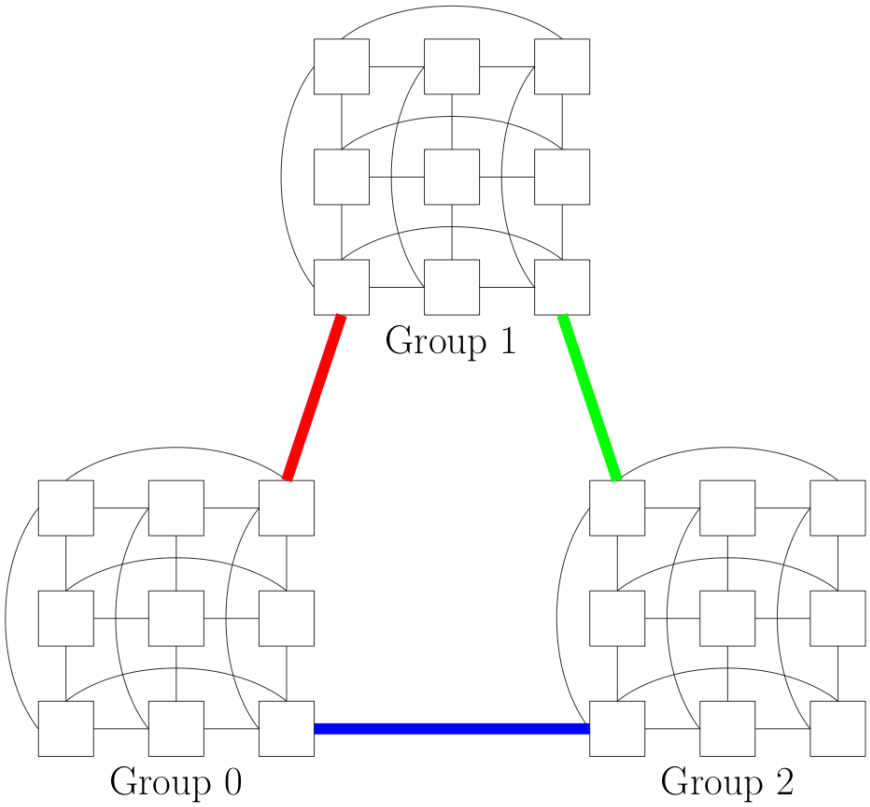


Figure 4.7: Schematic of dragonfly with three groups showing hypercube intragroup links and high bandwidth intergroup global links

For simplicity, only three example global links are show for clarity in the picture. For the Cray X630, $a = 96$, $h = 10$, and $p = 4$ so that each router is connected to many other ($h = 10$) groups. The caveat is that in many implementations global links are grouped together for $h = 2$ or 3 fat global links. These demonstrate well-balanced ratios. In general, scaling out a dragonfly should not increase the size of a group, only the number of groups.

4.5.1 Allocation and indexing

The dragonfly coordinate system is essentially the same as a 3D torus. The group 2D hypercube layout defines X and Y coordinates. The group number defines a Z or G coordinate. Thus the topology in Figure 4.7 would be specified as

```
1 topology.name = dragonfly
2 topology.geometry = 3 3 3
```

for groups of size 3×3 with a total of 3 groups. To complete the specification, the number of global links (h) for each router must be given

```
topology.group_connections = 10
```

4.5.2 Routing

It is important to understand the distinction between link bandwidth, channel bandwidth, and pin bandwidth. All topologies have the same pin bandwidth and channel bandwidth (assuming they use the same technology). Each router in a topology is constrained to have the same number of channels (called radix, usually about $k = 64$). The number of channels per link changes dramatically from topology to topology. Low radix topologies like 3D torus can allocate more channels per link, giving higher bandwidth between adjacent routers. Dragonfly is higher radix, having many more connections but having lower bandwidth between adjacent routers. While minimal routing is often sufficient on torus topologies because of the high link bandwidth, dragonfly will exhibit very poor performance with minimal routing. To effectively utilize all the available bandwidth, packets should have a high amount of path diversity. Packets sent between two routers should take as many different paths as possible to maximize the effective bandwidth point-to-point.

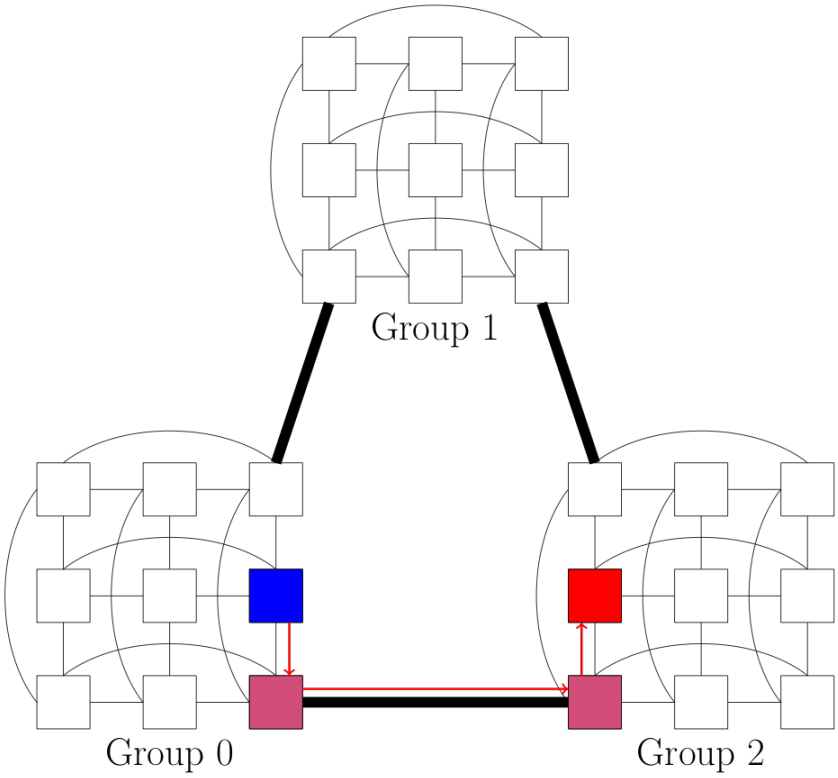


Figure 4.8: Schematic of dragonfly showing minimal route. Traveling between groups requires routing to the correct global link, hopping the global link, then routing within a group to the correct final node.

Minimal routing itself has a few complications (Figure 4.8). Each router only has a few global links. Thus, traveling from e.g. the blue router at X=3,Y=2,G=0 to the red router at X=1,Y=2,G=2, there is no direct link between the routers. Furthermore, there is no direct link between Groups 0 and 2. Thus packets must route through the purple intermediate nodes. First, the packet hops to X=3,Y=3, G=0. This router has a global link to Group 2, allowing the packet to hop to the next intermediate router at X=1, Y=3, G=2. Finally, the minimal route completes by hopping within Group 2 to the final destination.

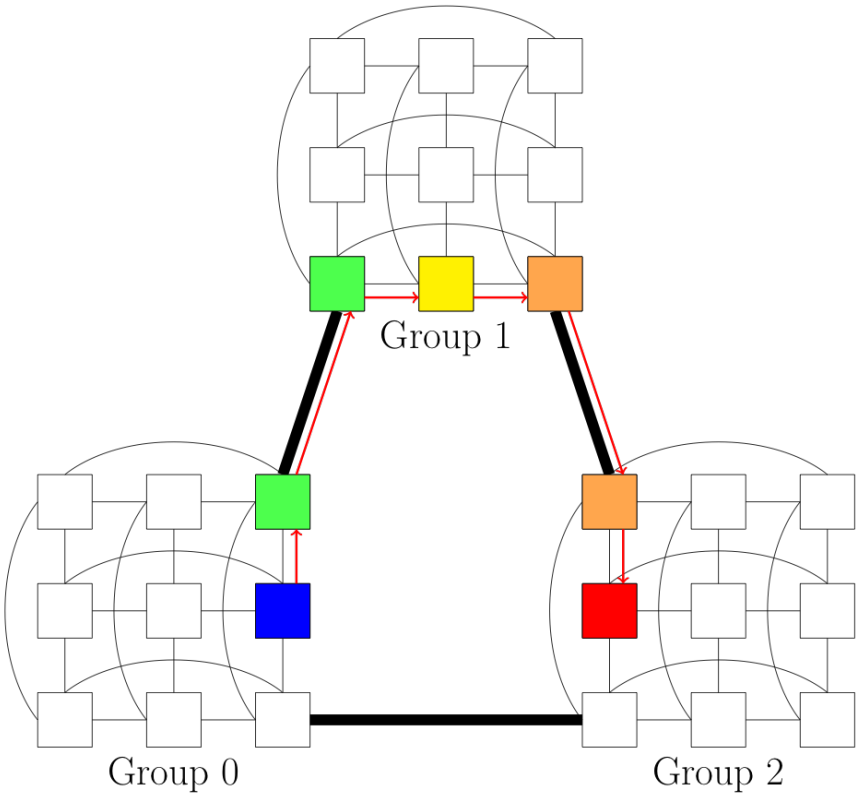


Figure 4.9: Schematic of dragonfly showing Valiant route. Traveling between groups requires routing to a random intermediate node, then routing minimally to the final destination.

To improve on minimal routing, global routing strategies are required (global routing is distinguished here from adaptive routing). Global essentially means "not minimal" and spreads packets along many different paths. The simplest global routing strategy is Valiant routing, which falls in the global, oblivious category (Figure 4.9). Oblivious simply means packets are scattered randomly without measuring congestion. In Valiant routing, each packet does the following:

- Pick a random intermediate node
- Route minimally to random node
- Route minimally from random node to destination node

This is somewhat counterintuitive at first. Rather than go directly to the destination node, packets go out of their way to a random node, shown in Figure 4.9 as the yellow router. Thus, routing from the blue router in Group 0 to the red router in Group 2 first follows the minimal path (green routers) to the randomly selected yellow router in Group 1. From there, a second minimal path is taken through the orange routers to the final destination. In cases with high congestion or even for large messages on a quiet network, this actually improves performance. If a point-to-point message is composed of ten packets, all ten packets will follow different paths to the final destination. This essentially multiplies the maximum bandwidth by a factor of ten. Valiant routing can be specified as

```
router = valiant
```

In contrast, UGAL routing is a global, adaptive strategy, making decisions based on congestion. Because Valiant is oblivious, it often sends too many packets to far away random nodes. Following a Valiant path is only relevant when enough packets fill up router queues, creating congestion. UGAL does the following steps:

- Start routing minimally
- On each step, check congestion (buffer queue depth)
- If congestion is too heavy, switch to Valiant and re-route to random intermediate node. Otherwise stay on minimal path.

UGAL packets stay on a minimal path until congestion forces them to use a Valiant strategy. This routing can be specified as:

```
router = ugal
```

Chapter 5

Applications and Skeletonization

5.1 Basic Application porting

There are three parts to successfully taking a C++ code and turning it into a running application.

- Redirected linkage: Rather than linking to MPI, pThreads, or other parallel libraries (or even calling `hostname`), these functions must be redirected to SST/macro rather than actually executing. If you compiled with the `--enable-replacement-headers` flag, you get all redirected linkage for free by using the SST compiler wrappers `sst++` and `sstcc` installed in the `bin` folder.
- Skeletonization: While SST/macro can run in emulation mode, executing your entire application exactly, this is not scalable. To simulate at scale (i.e. 100K or more MPI ranks) you must strip down or "skeletonize" the application to the minimal amount of computation. The energy and time cost of expensive compute kernels are then simulated via models rather than explicitly executed.
- Process encapsulation: Each virtual process being simulated is not an actual physical process. It is instead modeled as a lightweight user-space thread. This means each virtual process has its own stack and register variables, but that is it. Virtual processes share the same address space and the same global variables. Some refactoring may be necessary if you have global variables.

5.2 Redirected linkage

Because of the way libraries are import in the SST core, using external skeleton apps is more complicated than previously. Steps are being taken to re-automate this process, which will hopefully be available in the next subversion. For running the standalone version, this is essentially automatic if using the SST compiler wrappers. The compiler wrappers produce a new executable incorporating your new skeleton.

The wrinkle is external skeletons apps is changing the application's entry point, i.e. `main`. The SST/macro framework has already taken the `main` function, and consequently the user application becomes a sub-routine within the simulation environment. As introduced in Section 3.3, one needs to change the entry function from

`main` to `user_skeleton_main`, which has the same function signature as the `main` function. This refactoring happens automatically in the SST compiler wrappers.

If you need to use more than one application in the simulator at a time, you need multiple application entry points. It is no longer possible to do automatic refactoring. You must explicitly use the macro `sstmac_register_app` and change the name of your `main`. Thus, a code might look like

```
sstmac_register_app(my_app);

int my_app_main(int argc, char** argv)
{
...
```

where the refactored `main` function matches the name of the declared application.

5.2.1 Loading external skeletons with the integrated core

While the main `libmacro.so` provides the bulk of SST/macro functionality, users may wish to compile and run external skeletons. This gets a bit confusing with SST core since you have an external skeleton for an external element. Follow the instructions on `http://sst-simulator.org`. You must create an element info struct name `X_eli` for X your library name. You can still use the `sst++` compiler wrappers for building, but you must now manually create a `libX.so` from the compiled object files. The `sstmacro.py` script installed must also be edited. The top lines was previously

```
import sst.macro
```

This only loads the main components, not the external skeleton. You must add

```
import sst.X
```

where X is the name of your skeleton. This causes the core to also load the shared library corresponding to your external skeleton app.

5.3 Skeletonization

A program skeleton is a simplified program derived from a parent application. The purpose of a skeleton application is to retain the performance characteristics of interest. At the same time, program logic that is orthogonal to performance properties is removed. The rest of this chapter will talk about skeletonizing an MPI program, but the concepts mostly apply regardless of what programming/communication model you're using.

The default method for skeletonizing an application is *manually*. In other words, going through your application and removing all the computation that is not necessary to produce the same communication/parallel characteristics. Essentially, what you're doing is visually backtracing variables in MPI calls to where they are created, and removing everything else.

Skeletonization falls into three main categories:

- *Data structures* - Memory is a precious commodity when running large simulations, so get rid of every memory allocation you can.
- *Loops* - Usually the main brunt of CPU time, so get rid of any loops that don't contain MPI calls or calculate variables needed in MPI calls.
- *Communication buffers* - While you can pass in real buffers with data to SST/macro MPI calls and they will work like normal, it is relatively expensive. If they're not needed, get rid of them.

A decent example of skeletonization is HPCCG_full (the original code) and HPCCG_skel (the skeleton) in sstmacro/skeletons.

5.3.1 Basic compute modeling

By default, even if you don't remove any computation, *simulation time doesn't pass between MPI or other calls implemented by SST/macro* unless you set

```
1 host_compute_modeling = true
```

in your parameter file. In this case, SST/macro will use the wall time that the host takes to run code between MPI calls and use that as simulated time. This only makes sense, of course, if you didn't do any skeletonization and the original code is all there.

If you do skeletonize your application and remove computation, you need to replace it with a model of the time or resources necessary to perform that computation so that SST/macro can advance simulation time properly. These functions are all accessible by using the SST compiler wrappers or by adding `#include <sstmac/compute.h>` to your file.

You can describe the time it takes to do computation by inserting calls to

```
1 void sstmac_compute(double seconds)
```

Usually, this would be parameterized by some value coming from the application, like loop size. You can also describe memory movement with

```
1 void sstmac_memread(long bytes);
2 void sstmac_memwrite(long bytes);
3 void sstmac_memcpy(long bytes);
```

again usually parameterized by something like vector size. Using these two functions is the simplest and least flexible way of compute modeling.

5.3.2 Detailed compute modeling

The basic compute modeling is not very flexible. In particular, simply computing based on time does not account for congestion delays introduced by things like memory contention. The highly recommended route is a more detailed compute model (but still very simple) that uses the operational intensity (essentially bytes/flops ratio) for a given compute kernel. This informs SST/macro how much stress a given code region puts on either the processor or the memory system. If a kernel has a very high operational intensity, then

the kernel is not memory-bound. The means multiple threads can be running the kernel with essentially no memory contention. If a kernel has a very low operational intensity, the kernel is memory bound. A single thread will have good performance, but multiple threads will compete heavily for memory bandwidth. If a kernel has a medium operational intensity, a few concurrent threads may be possible without heavy contention, but as more threads are added the contention will quickly increase.

The function prototype is

```
1 void
2 sstmac_compute_detailed(long nflops, long nintops, long bytes);
```

Here `flops` is the number of floating point operations and `bytes` is the number of bytes that hit the memory controller. `bytes` is *not* simply the number of writes/reads that a kernel performs. This is the number of writes/reads that *miss the cache* and hit the memory system. For now, SST/macro assumes a single-level cache and does not distinguish between L1, L2, or L3 cache misses. Future versions may incorporate some estimates of cache hierarchies. However, given the coarse-grained nature of the simulation, explicit simulation of cache hierarchies is not likely to provide enough improved accuracy or physical insight to justify the increased computational cost. Additional improvements are likely to involve adding parameters for pipelining and prefetching. This is currently the most active area of SST/macro development.

The characterization of a compute kernel must occur outside SST/macro using performance analysis tools like Vtune or PAPI. For the number of flops, it can be quite easy to just count the number of flops by hand. The number of bytes is much harder. For simple kernels like a dot product or certain types of stencil computation, it may be possible to pen-and-paper derive estimates of the number of bytes read/written from memory since every read is essentially a cache miss. In the same way, certain kernels that use small blocks (dense linear algebra), it may be possible to reason *a priori* about the cache behavior. For more complicated kernels, performance metrics might be the only way. Further discussion and analysis of operational intensity and roofline models can be found in "Roofline Model Toolkit: A Practical Tool for Architectural and Program Analysis" by Yung Ju Lo et al. The PDF is available at `http://www.dcs.warwick.ac.uk/~sdh/pmbs14/PMBS14/Workshop_Schedule.html`.

5.3.3 Skeletonization Issues

The main issue that arises during skeletonization is data-dependent communication. In many cases, it will seem like you can't remove computation or memory allocation because MPI calls depend somehow on that data. The following are some examples of how we deal with those:

- *Loop convergence* - In some algorithms, the number of times you iterate through the main loop depends on an error converging to near zero, or some other converging mechanism. This basically means you can't take out anything at all, because the final result of the computation dictates the number of loops. In this case, we usually set the number of main loop iterations to a fixed (parameterized) number. Do we really care exactly how many loops we went through? Most of the time, no, it's enough just to produce the behavior of the application.
- *Particle migration* - Some codes have a particle-in-cell structure, where the spatial domain is decomposed among processes, and particles or elements are distributed among them, and forces between particles are calculated. When a particle moves to another domain/process (because it's moving through space), this usually requires communication that is different from the force calculation, and

thus depends entirely on the data in the application. We can handle this in two ways: 1) *Ignore it* - If it doesn't happen that often, maybe it's not significant anyway. So just remove the communication, recognizing that the behavior of the skeleton will not be fully reproduced or 2) *Approximate it* - If all we need to know is that this migration/communication happens sometimes, then we can just make it happen every so many iterations, or even sample from a probability distribution.

- *AMR* - Some applications, like adaptive mesh refinement (AMR), exhibit communication that is entirely dependent on the computation. In this case, skeletonization is basically impossible, so you're left with a few options

For applications with heavy dynamic data dependence, we have the following strategies:

- *Traces* - revert to DUMPI traces, where you will be limited by existing machine size. Trace extrapolation is also an option here.
- *Run it* - get yourself a few servers with a lot of memory, and run the whole code in SST/macro.
- *Synthetic* - It may be possible to replace communication with randomly-generated data and decisions, which emulate how the original application worked. This hasn't been tried yet.
- *Hybrid* - It is possible to construct meta-traces that describe the problem from a real run, and read them into SST/macro to reconstruct the communication that happens. Future versions of this manual will have more detailed descriptions as we formalize this process.

5.4 Process Encapsulation

As mentioned above, virtual processes are not real, physical processes inside the OS. They are explicitly managed user-space threads with a private stack, but without a private set of global variables. When porting an application to SST/macro, global variables used in C programs will not be mapped to separate memory addresses causing incorrect execution or even segmentation faults. If you have avoided global variables, there is no major issue. If you have read-only global variables with the same value on each machine, there is still no issue. If you have mutable global variables or read-only variables such as `mpi_rank` that differ across processes, there is so minor refactoring that needs to be done.

5.4.1 Manually refactoring global variables

SST/macro provides a complete set of global variable replacements from `#include <sstmac/sstmac_global.h>`, which is automatically included the SST compiler wrappers. Then replace the variable type declaration with the ones that have a `global_` prefix in the header file. To use this file, you must compile your application with a C++ compiler as a C++ program. While most of C++ is backwards-compatible, there are some things that are not, and will require either a compiler flag to relax strictness or quick refactor of some of your syntax.

When printing a global variable with `printf`, the user should explicitly invoke a cast to the primitive type in the function call:

```
1 print("Hello world on rank %d", int(rank));
```

If not explicitly cast, the `va_args` function will be misinterpreted and produce an "Illegal instruction" error. This still follows the "single-source" principle since whether compiling for SST/macro or a real machine, the code is still valid.

5.4.2 Automatically refactoring global variables

Tools are currently in use by developers to automatically refactor codes to use no global variables. This involves running the source code through a compiler tool chain that then creates a `struct` encapsulating all global variables into thread-specific classes. This process is only for advanced users and requires developer help.