Introduction to Parallel Programming

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Overview

- Types of parallel computers.
- Parallel programming options.
- How to write parallel applications.
- How to compile.
- How to debug/profile.
- Summary, future expansion.

Parallel architectures

Single processor:

- SISD – single instruction single data.

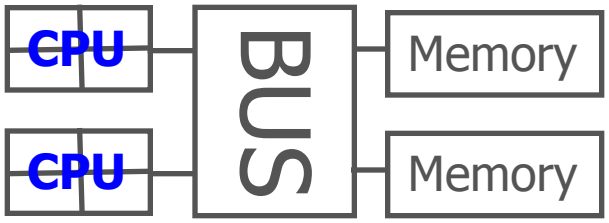
Multiple processors:

- SIMD - single instruction multiple data.
- MIMD – multiple instruction multiple data.
  - Shared Memory
  - Distributed Memory

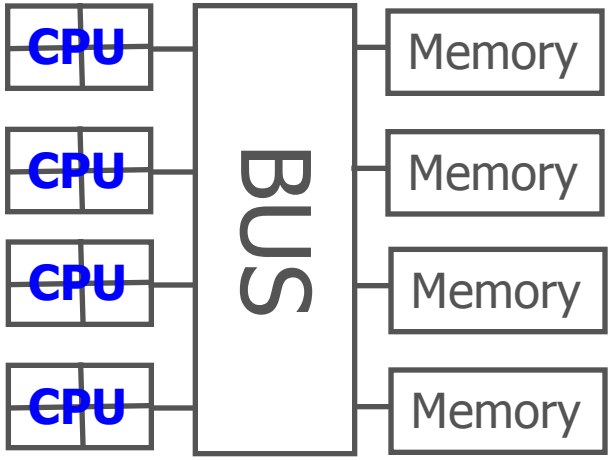
Shared memory

- All processors have access to local memory
- Simpler programming
- Concurrent memory access
- More specialized hardware
- CHPC :
  Linux clusters, 2, 4, 8, 12, 16 core nodes
  GPU nodes

Dual quad-core node

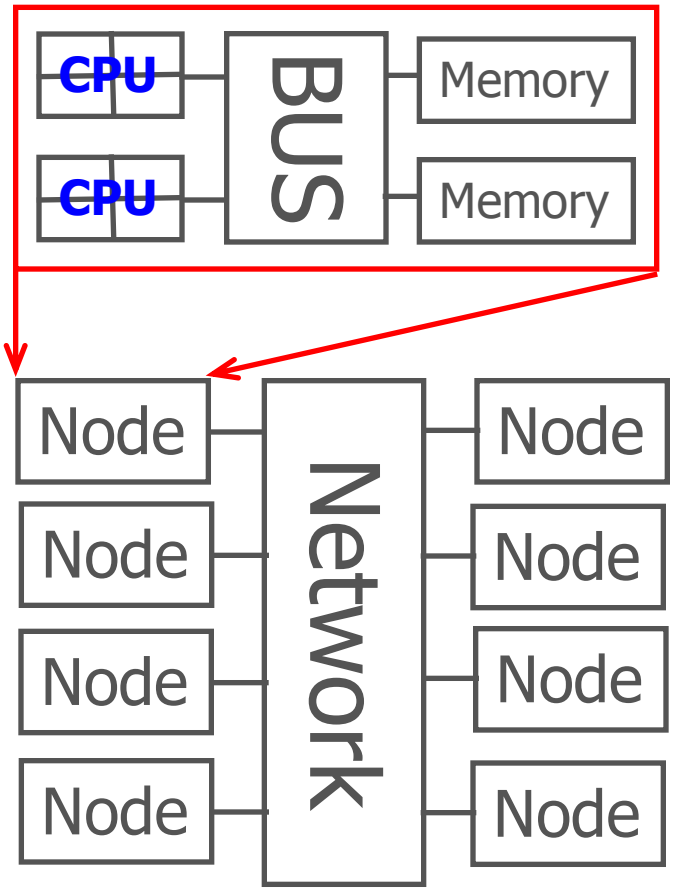


Many-core node (e.g. SGI)



Distributed memory

- Process has access only to its local memory
- Data between processes must be communicated
- More complex programming
- Cheap commodity hardware
- CHPC: Linux clusters



8 node cluster (64 cores)

Parallel programming options

Shared Memory

- Threads – POSIX Pthreads, OpenMP (CPU, MIC), OpenACC, CUDA (GPU)
  - Thread – own execution sequence but shares memory space with the original process
- Message passing – processes
  - Process – entity that executes a program – has its own memory space, execution sequence

Distributed Memory

- Message passing libraries
- Vendor specific – non portable
- General – MPI, PVM

OpenMP basics

- Compiler directives to parallelize
- Fortran – source code comments

  `!$omp parallel/!$omp end parallel`
- C/C++ - #pragmas

  `#pragma omp parallel`
- Small set of subroutines
- Degree of parallelism specification
- `OMP_NUM_THREADS` or `omp_set_num_threads(INTEGER n)`

MPI Basics

- Communication library
- Language bindings:
  - C/C++ - `int MPI_Init(int argv, char* argc[])`
  - Fortran - `MPI_Init(INTEGER ierr)`
- Quite complex (100+ subroutines)

  but only small number used frequently
- User defined parallel distribution

MPI vs. OpenMP

- Complex to code
- Slow data communication

- Ported to many architectures
- Many tune-up options for parallel execution

- Easy to code
- Fast data exchange

- Memory access (thread safety)
- Limited usability
- Limited user's influence on parallel execution

Program example

- saxpy – vector addition: $\bar{z} = a\bar{x} + \bar{y}$
- simple loop, no cross-dependence, easy to parallelize

```
subroutine saxpy_serial(z, a, x, y, n)
integer i, n
real z(n), a, x(n), y(n)

do i=1, n
   z(i) = a*x(i) + y(i)
enddo
return
```

OpenMP program example

```
subroutine saxpy_parallel_omp(z, a, x, y, n)
integer i, n
real z(n), a, x(n), y(n)

!$omp parallel do
do i=1, n
   z(i) = a*x(i) + y(i)
enddo
return
```

setenv OMP_NUM_THREADS 4

MPI program example

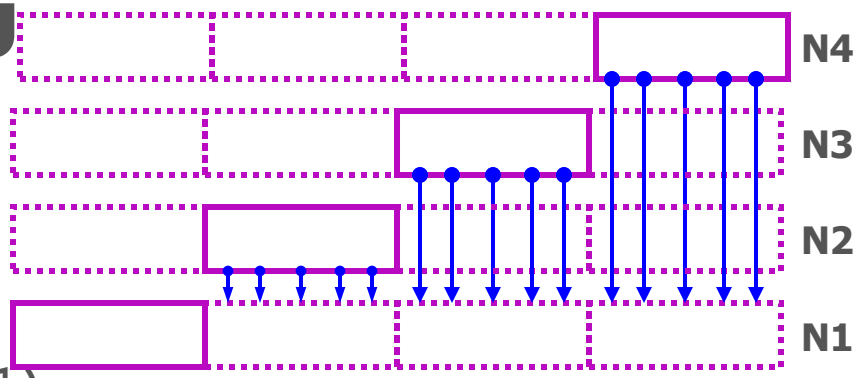
```
subroutine saxpy_parallel_mpi(z, a, x, y, n)
integer i, n, ierr, my_rank, nodes, i_st, i_end
real z(n), a, x(n), y(n)

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD,my_rank,ierr)
call MPI_Comm_size(MPI_COMM_WORLD,nodes,ierr)
i_st = n/nodes*my_rank+1
i_end = n/nodes*(my_rank+1)

do i=i_st, i_end
   z(i) = a*x(i) + y(i)
enddo
call MPI_Finalize(ierr)
return
```

z(i) operation on 4 processes

z(1 ... n/4)	z(n/4+1 ... 2*n/4)	z(2*n/4+1 ... 3*n/4)	z(3*n/4+1 ... n)

MPI program example

- **Result on the first CPU**




```
include "mpif.h"
integer status(MPI_STATUS_SIZE)
if (my_rank .eq. 0 ) then
  do j = 1, nodes-1
    do i= n/nodes*j+1, n/nodes*(j+1)
      call MPI_Recv(z(i),1,MPI_REAL,j,0,MPI_COMM_WORLD,
&     status,ierr)
    enddo
  enddo
else
  do i=i_st, i_end
    call MPI_Send(z(i),1,MPI_REAL,0,0,MPI_COMM_WORLD,ierr)
  enddo
endif
```

Data | Count

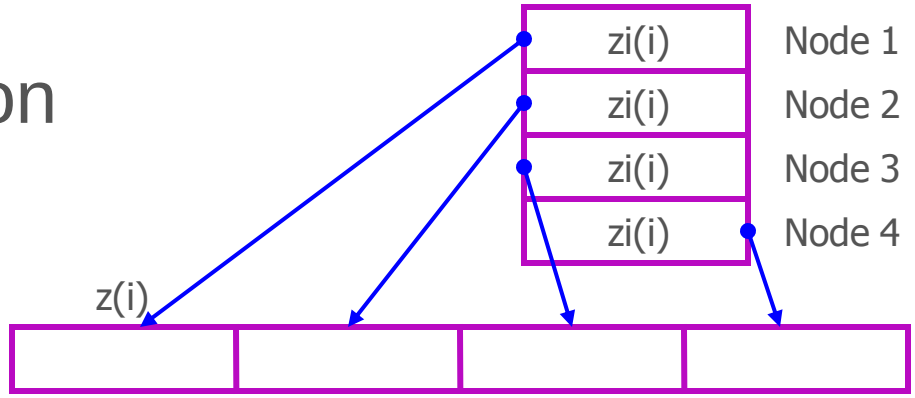
Sender

Recipient

MPI program example

- Collective communication

```
real zi(n)
j = 1
do i=i_st, i_end
   zi(j) = a*x(i) + y(i)
   j = j +1
enddo
```



Send data

Receive data

```
call MPI_Gather(zi,n/nodes,MPI_REAL,z,n/nodes,MPI_REAL,
&                0,MPI_COMM_WORLD,ierr)
```

Root process

- Result on all nodes

```
call MPI_AllGather(zi,n/nodes,MPI_REAL,z,n/nodes,
&                  MPI_REAL,MPI_COMM_WORLD,ierr)
```

No root process

Arches - login

- First log into one of the clusters
  `ssh sanddunearch.chpc.utah.edu` – Ethernet, InfiniBand
  `ssh updraft.chpc.utah.edu` – Ethernet, InfiniBand
  `ssh ember.chpc.utah.edu` – Ethernet, InfiniBand
  `ssh kingspeak.chpc.utah.edu` – Ethernet, InfiniBand

- Then submit a job to get compute nodes
  ```
  qsub -I -l nodes=2:ppn=4,walltime=1:00:00
  qsub script.pbs
  ```

- Useful scheduler commands
  `qsub` – submit a job
  `qdel` – delete a job
  `showq` – show job queue

Security Policies

- No clear text passwords use ssh and scp
- You may not share your account under any circumstances
- Don't leave your terminal unattended while logged into your account
- Do not introduce classified or sensitive work onto CHPC systems
- Use a good password and protect it

Security Policies

- Do not try to break passwords, tamper with files etc.
- Do not distribute or copy privileged data or software
- Report suspicions to CHPC (security@chpc.utah.edu)
- Please see http://www.chpc.utah.edu/docs/policies/security.html for more details

Compilation - OpenMP

Arches

- Supported by most compilers, –openmp, –fopenmp or –mp switch

  e.g. `pgf77 -mp source.f -o program.exe`
- Dual-processor and quad-processor (Sanddunearch) nodes
- Further references:

  Compilers man page – `man ifort`

  Compilers websites

  http://www.intel.com/software/products/compilers

  http://gcc.cnu.org

  http://www.pgroup.com/doc/

  http://www.pathscale.com/node/70

Compilation - MPI

- Three common network interfaces
  - Ethernet, Myrinet, InfiniBand
- Different MPI implementations
  - MPICH2 - Ethernet, shmem
  - OpenMPI – Ethernet, InfiniBand
  - MVAPICH2 - InfiniBand
  - Intel MPI, Scali MPI - commercial

Compilation - MPI

- **Clusters** – MPICH2, OpenMPI, MVAPICH2

```
/MPI-path/bin/mpixx source.x -o program.exe
```

- `MPI-path` = location of the distribution

  `/uufs/chpc.utah.edu/sys/pkg/mpich2/std` MPICH2 TCP-IP

  `/uufs/$UUFSCELL.arches/sys/pkg/openmpi/std` OpenMPI InfiniBand

  `/uufs/$UUFSCELL.arches/sys/pkg/mvapich2/std` MVAPICH2 InfiniBand

  = must specify full path to `mpixx` (`/MPI-path/bin`) or add this path to `PATH` environment variable

Running a parallel job – Clusters

- MPICH Interactive batch (incl. Updraft)

```
qsub -I -l nodes=2:ppn=2,walltime=1:00:00
… wait for prompt …
/MPI-path/bin/mpirun -np 4 -machinefile
$PBS_NODEFILE program.exe -
```

Updraft, Ember, Kingspeak

```
/MPI-path/bin/mpirun -launcher rsh -np 4
-machinefile $PBS_NODEFILE program.exe -
```

sanddunearch

- MPICH Batch

```
#PBS -l nodes=2:ppn=2,walltime=1:00:00
```

- OpenMP Batch

```
#PBS -l nodes=1:ppn=2,walltime=1:00:00
setenv OMP_NUM_THREADS 2
program.exe
```

Debuggers

- Useful for finding bugs in programs
- Several free
  - `gdb` – GNU, text based, limited parallel
  - `ddd` – graphical frontend for gdb
- Commercial that come with compilers
  - `pgdbg` – PGI, graphical, parallel but not intuitive
  - `pathdb, idb` – Pathscale, Intel, text based
- Specialized commercial
  - `totalview` – graphical, parallel, CHPC has a license
  - `ddt` - Distributed Debugging Tool
- How to use:
- `http://www.chpc.utah.edu/docs/manuals/software/par_devel.html`

Debuggers - parallel

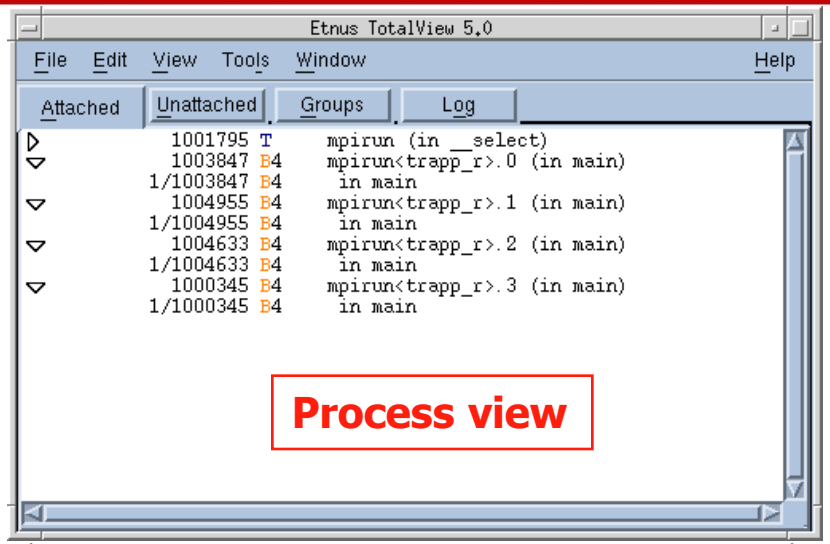
- Parallel debugging more complex due to interaction between processes
- Totalview is the debugger of choice at CHPC
- Expensive but academia get discount
- How to run it:
  - compile with `-g` flag
  - automatic attachment to OpenMP threads
  - extra flag (`-tv`) to mpirun/mpiexec
- Details:

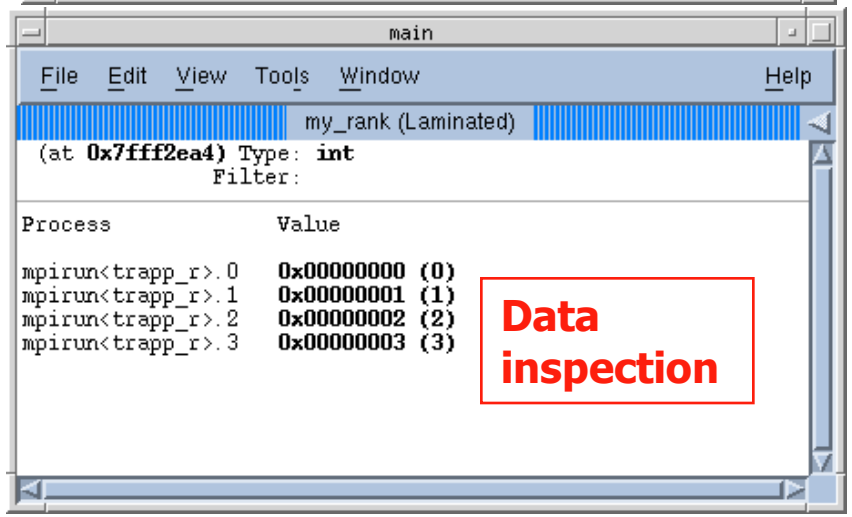
`http://www.chpc.utah.edu/docs/manuals/software/totalview.html`

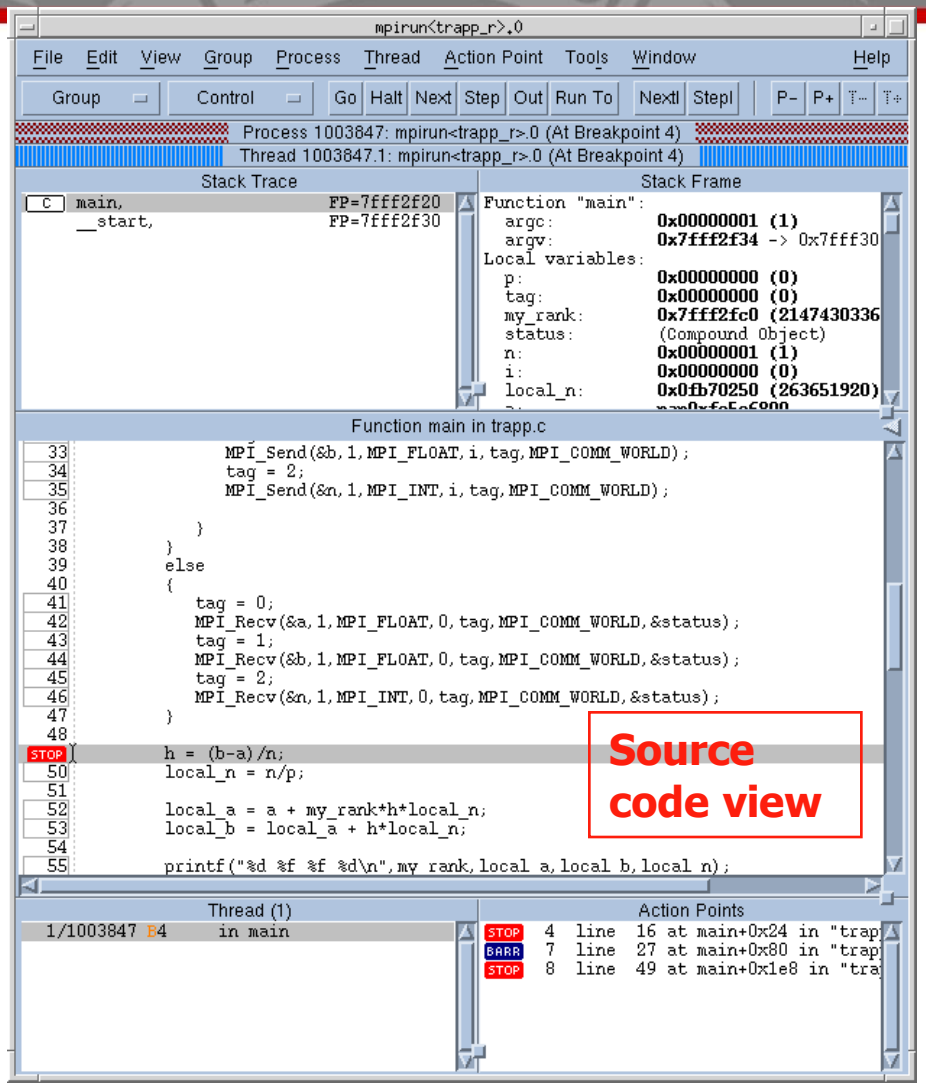
- Further information

`http://www.totalviewtech.com/alltvdocs.htm`

Debuggers – parallel



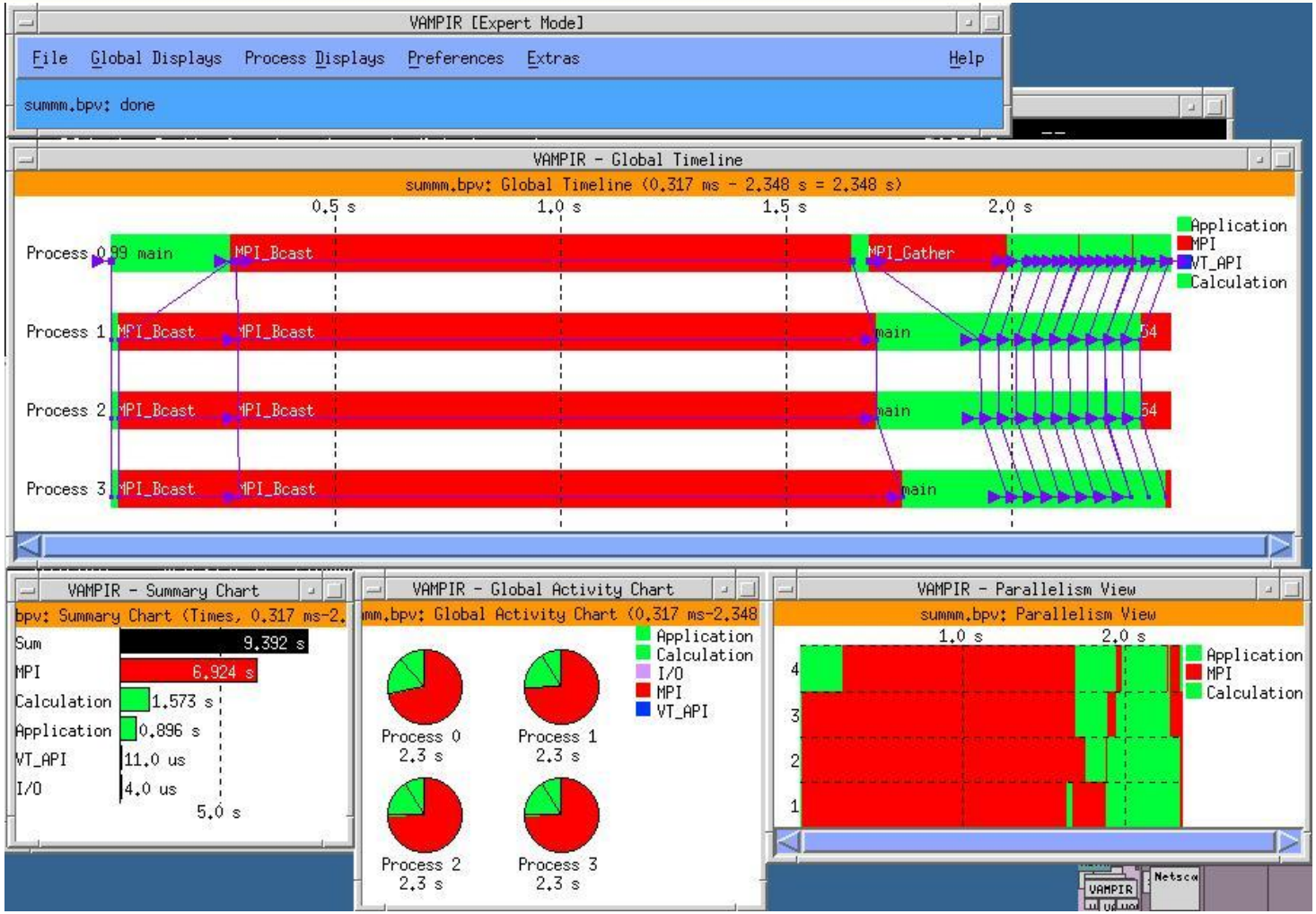




Profilers

- Measure performance of the code
- Serial profiling
  - discover inefficient programming
  - computer architecture slowdowns
  - compiler optimizations evaluation
  - gprof, pgprof, pathopt2
- Parallel profiling
  - target is inefficient communication
  - Intel Trace Collector and Analyzer

Profilers - parallel



Summary

- Shared vs. Distributed memory
- OpenMP
  - limited on Arches
  - Simple parallelization
- MPI
  - Arches
  - Must use communication

`http://www.chpc.utah.edu/docs/presentations/intro_par`

References

- OpenMP

  `http://www.openmp.org/`

  Chandra, et. al. - Parallel Programming in OpenMP

  Chapman, Jost, van der Pas – Using OpenMP
- MPI

  `http://www-unix.mcs.anl.gov/mpi/`

  Pacheco - Parallel Programming with MPI

  Gropp, Lusk, Skjellum - Using MPI 1, 2
- MPI and OpenMP

  Pacheco – An Introduction to Parallel Programming

Future Presentations

- Introduction to MPI
- Introduction to OpenMP
- Debugging with Totalview
- Profiling with TAU/Vampir
- Intermediate MPI and MPI-IO
- Mathematical Libraries at the CHPC