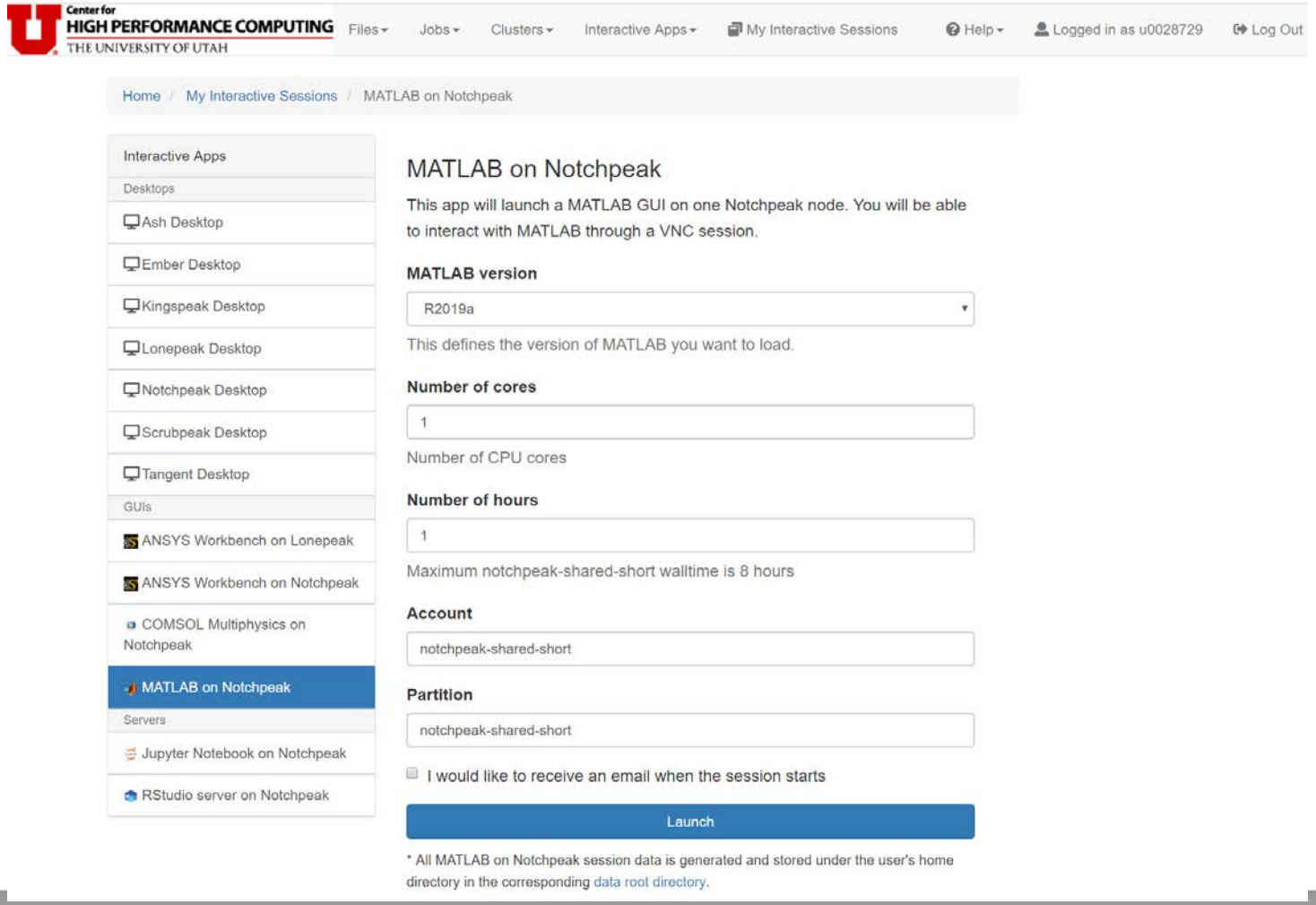
Running Matlab

- Interactive - Open OnDemand Matlab app



Running Matlab

- Batch - serial job script

```
#!/bin/tcsh
#SBATCH --time=1:00:00 # walltime, abbreviated by -t
#SBATCH --nodes=1      # number of cluster nodes, abbreviated by -N
#SBATCH -o slurm-%j.out-%N # name of the stdout, using the job number (%j) and the
first node (%N)
#SBATCH --ntasks=1    # number of MPI tasks, abbreviated by -n
# additional information for allocated clusters
#SBATCH --account=notchpeak-shared-short     # account - abbreviated by -A
#SBATCH --partition=notchpeak-shared-short  # partition, abbreviated by -p

# just in case purge the old modules and load Matlab module
module purge
module load matlab

# run matlab program via the run_matlab script
matlab -nodisplay -r run_matlab_serial -logfile matlab_serial.log
```

- Submit as `sbatch run_matlab_serial.slr`

Running Matlab

- Batch - helper script

```
% path where is the matlab program we want to run
% addpath path_to_my_matlab_script
% execute the matlab program
loop_serial
% exit from Matlab - if we don't exit Matlab the job sits around idle and wasting time till it runs out of walltime
exit
```

- Actual serial Matlab code

```
tic
n = 400;
A = 1000;
a = zeros(1,n);
for i = 1:n
    a(i) = max(abs(eig(rand(A))));
end
toc
```

- NOTE - code like this does not run in parallel so it may not run efficiently - more on this later

Introduction to Parallel Computing

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Overview

- Types of parallel computers.
- Parallel programming options.
- OpenMP, OpenACC, MPI
- Debugging, profiling and libraries
- Higher level languages
- Summary, further learning.

How to compute faster

- Faster CPU clock speed
  - Higher voltage = more heat – not sustainable
- Work distribution
  - Vectorization – process more than one value at a time
  - Parallelization – spread work over multiple processing elements
  - Specialization – application specific processors (ASIC), programmable logic (FPGA)

Parallel architectures

Single processor:

- SISD – single instruction single data.

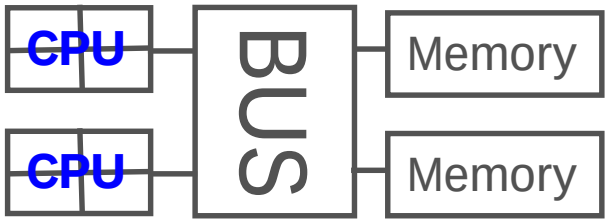
Multiple processors:

- SIMD - single instruction multiple data.
- MIMD – multiple instruction multiple data.
  - Shared Memory
  - Distributed Memory
- Current processors combine SIMD and MIMD
  - Multi-core CPUs w/ SIMD instructions (AVX, SSE)
  - GPUs with many cores and SIMT

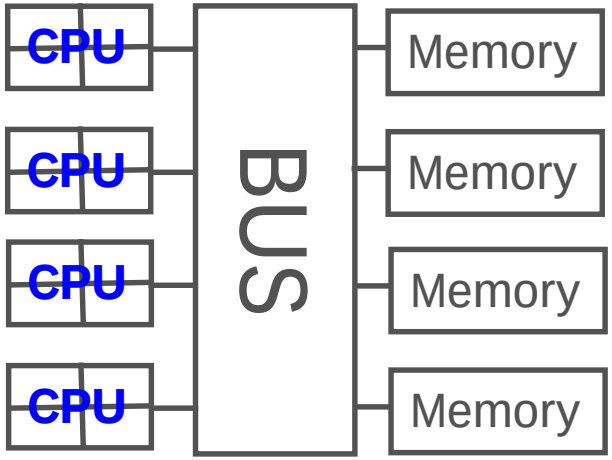
Shared memory

- All processors have access to local memory
- Simpler programming
- Concurrent memory access
- More specialized hardware
- Representatives:
  Linux clusters nodes 8-32 core GPU nodes

Dual quad-core node

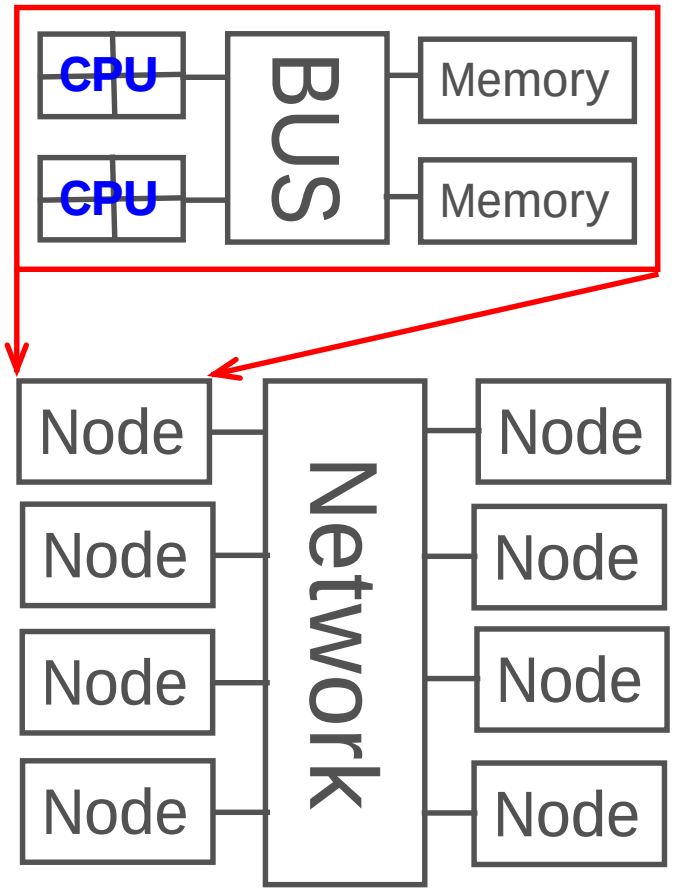


Many-CPU node (e.g. SGI)



Distributed memory

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



8 node cluster (64 cores)

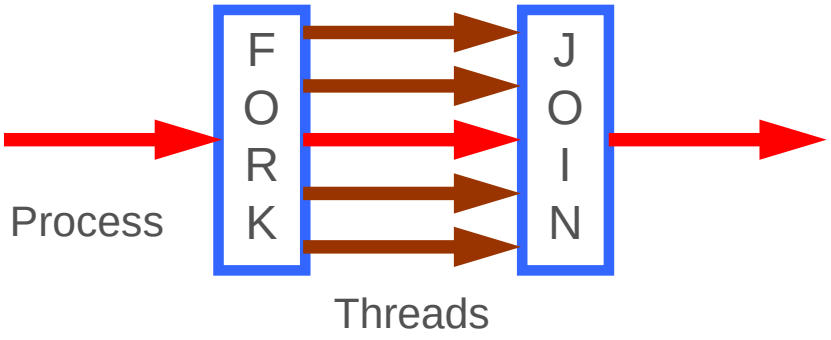
Ways of program execution

- Process (task)

  Entity that executes a program – has its own memory space, execution sequence, is independent from other processes

- Thread

  Has own execution sequence but shares memory space with the original process - a process may have many threads



Parallel programming options

Shared Memory

- Threads
  - POSIX Pthreads, OpenMP (CPU, MIC), OpenACC, CUDA (GPU)
- Processes
  - message passing, independent processes

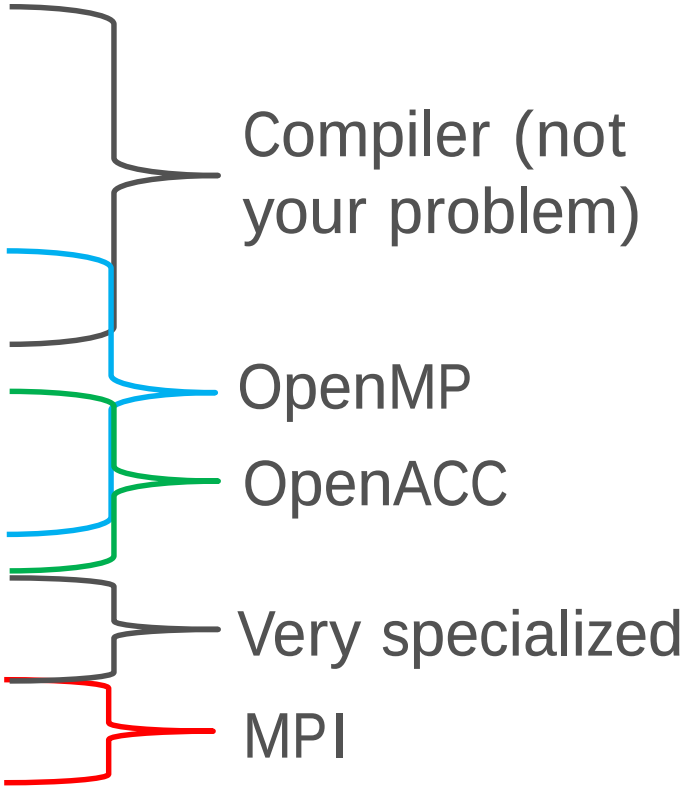
Distributed Memory

- Independent processes
- Message passing libraries
  - General – MPI, PVM, language extensions (Co-array Fortran, UPC. …)

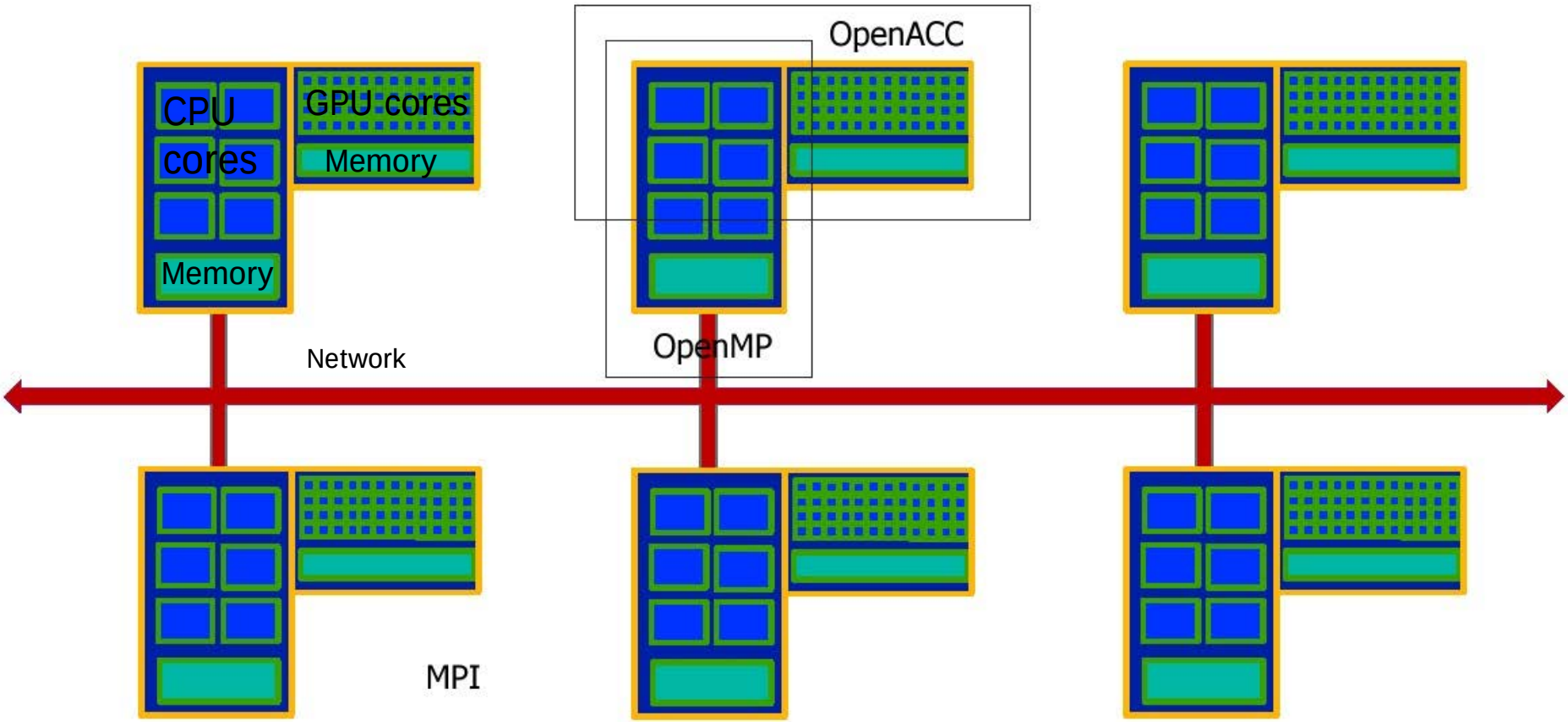
Higher level programming languages (Python, R, Matlab) do a combination of these approaches under the hood.

Types of parallelism in a nutshell

- Instruction level (ILP)
  - Instruction pipelining, speculative execution, branch prediction, …
- Vector (SIMD)
- Multi-core/Multi-socket SMP
- Accelerators (GPU, MIC)
- FPGA, ASIC
- Distributed clusters



Mapping onto the hardware



OpenMP basics

- Compiler directives to parallelize (CPU or GPU)
- 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)`

OpenACC Basics

- Compiler directives to offload to GPU
- Fortran – source code comments
  `!$acc kernels/!$acc end kernels`
- C/C++ - #pragmas
  `#pragma acc kernels`
- 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, data dependencies)
- Limited usability
- Limited user's influence on parallel execution

Program example

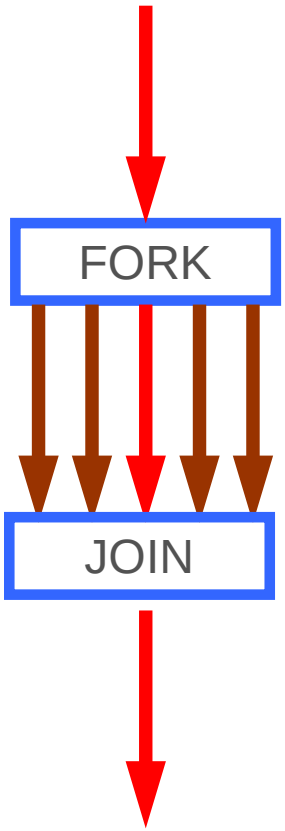
- saxpy – vector addition: $\bar{z} = a\bar{x} + \bar{y}$
- simple loop, no cross-dependence, easy to parallelize

```
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
```

```
$ gcc –fopenmp saxpy.f
$ export OMP_NUM_THREADS=16
$ ./a.out
```



OpenMP caveats

- Data dependencies
  - Private (thread-local) variables
  - Flow dependence – rearrangement
  - Reduction (sum over threads)

```
x = a(i)
b(i) = c + x
```

```
a(i) = a(i+1) + x
```

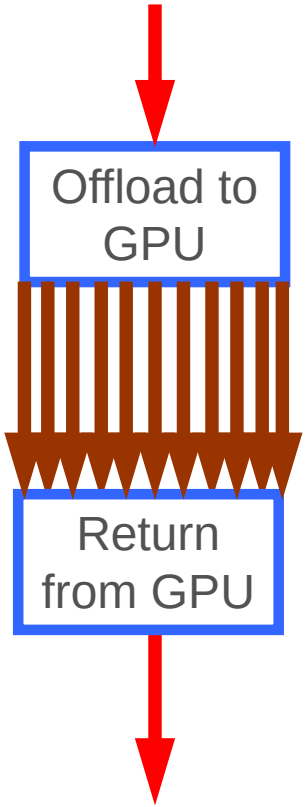
```
x += a(i)
```

- Scheduling
  - What runs on what thread – schedule, task,…
- Advanced features
  - Thread affinity (to CPU core)
  - Vectorization
  - Accelerator offload

OpenACC program example

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

!$acc kernels datain(x,y) dataout(z)
do i=1, n
  z(i) = a*x(i) + y(i)
enddo
return
```

```
$ pgcc –acc –Minfo=accel saxpy.f
$ pgaccelinfo To verify that GPU is available
$ ./a.out
```



OpenACC caveats

- Data dependencies (Like in OpenMP)
- Data locality
  - Transfers from host to GPU and back take time
  - need to minimize them

```
#pragma acc data [copyin, copyout, create,...]
```

- Parallel regions
  - More explicit execution control (warps, threads)

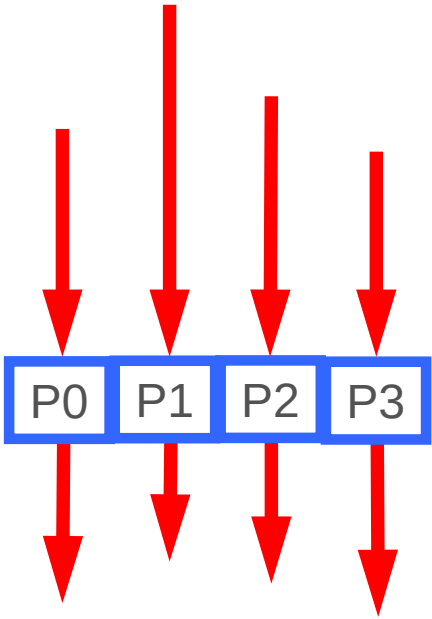
```
#pragma acc parallel
```

- Procedure calls
  - If procedure is executed on the GPU

```
#pragma acc routine
```

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
```

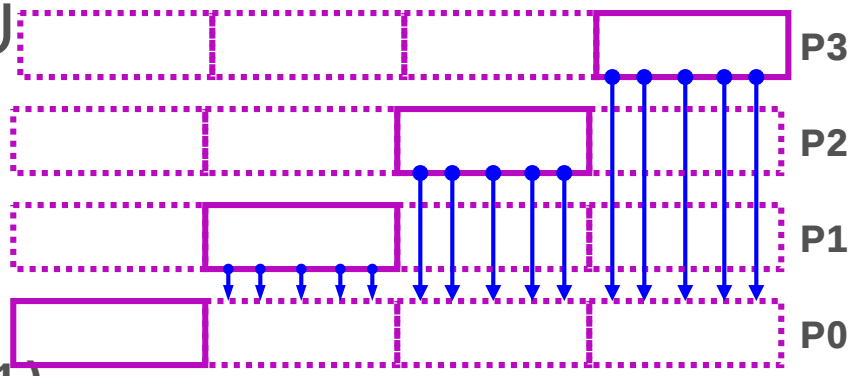


z(i) operation on 4 processes (tasks)

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

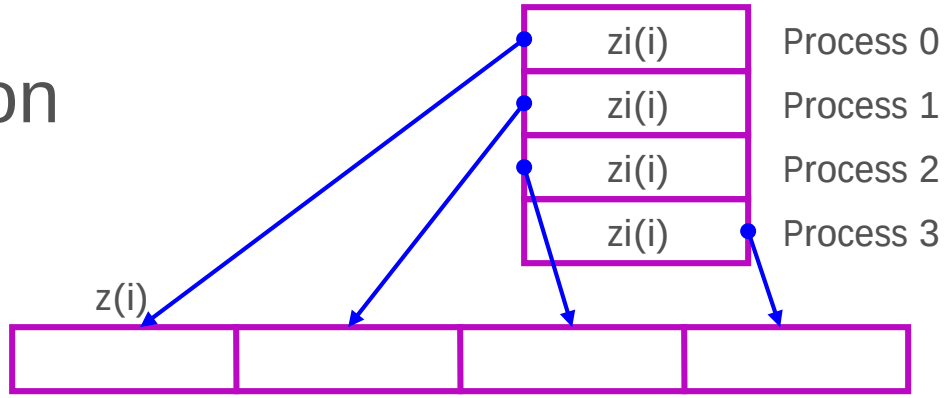
Sender

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

MPI distributions

- Different networks
  - Ethernet
  - InfiniBand
  - Intel OmniPath
  - most MPI distributions now come with multiple networks support
- Several distributions follow the MPI standard
  - MPICH, MVAPICH2
  - Intel MPI, Cray MPI,…
  - OpenMPI
  - Ensure that build and run is done with the same distribution (ABI compatibility)

But wait, my program is not in C or Fortran

Interpreted languages are popular

- Matlab, Python, R

Each has some sort of parallel support, but most likely it will not perform as well as using OpenMP or MPI with C/Fortran.

Try to parallelize (and optimize) your Matlab/Python/R code and if it's still not enough consider rewriting in C++ or Fortran.

Cluster running options for Matlab, Python, R

- Using parallelization in the program run through interactive or batch job
  - multi-threading and/or multi-processing packages (parfor, mpi4py, R parallel, Rmpi, …)
- Using built in job submission
  - Matlab Parallel Server, rslurm, python Dask, snakemake
- Independent calculations in parallel
  - launching concurrent calculations in a job

Matlab

Threads

- Built in Matlab functions. Vector/matrix operations threaded (and vectorized) through Intel MKL library, many other functions also threaded

Tasks (processes)

- *Parallel Computing Toolbox* allows for task based parallelism
- *Parallel Server* can distribute tasks to multiple nodes
- Great for independent calculations, when communication is needed uses MPI under the hood

https://www.chpc.utah.edu/documentation/software/matlab.php

Matlab tasks

- Parallel program

```
function t = parallel_example
parfor idx = 1:16
  A(idx) = idx;
end
```

Will launch loop iterations on multiple workers

- Parallel worker pool on a single machine

```
poolobj=parpool('local',8);
parallel_example;
delete(poolobj);
```

Starts multiple workers pool

- Parallel pool on a cluster

```
c = parcluster;
c.AdditionalProperties.QueueName = 'kingspeak';
...
j = c.batch(@parallel_example, 1, {}, 'Pool', 4);
j.State
j.fetchOutputs{:}
```

Submits cluster job

Matlab examples

- Parallel worker pool on a single node
  - best run from a SLURM job
    loop_parallel_onenode.m, run_matlab_onenode.m, run_matlab_onenode.slr - https://github.com/CHPC-UofU/USU-lectures
  - `sbatch run_matlab_onenode.slr`
- Parallel worker pool on a multiple nodes
  - must run from inside of Matlab
  - start Matlab on interactive node inside of a FastX session

```
ml matlab
matlab &
```

  - loop_parallel.m, parallel_multinode.m

```
parallel_multinode
```

R

Threads

- Under the hood threading with specially built (or Microsoft) R for vector/matrix operations using MKL
- *parallel* R library

Tasks (processes)

- *parallel* R library (uses *multicore* for shared and *snow* for distributed parallelism)
- Parallelized **apply* functions, e.g. *mclapply*
- *Rmpi* library provides MPI like functionality
- Many people run multiple independent R instances in parallel

https://www.chpc.utah.edu/documentation/software/r-language.php

Parallel R on a cluster

- Load libraries

```
library(parallel)
library(foreach)
library(doParallel)
```

`hostlist.txt` comes from a job script

```
srun -n $SLURM_NTASKS > hostlist.txt
```

- Start R cluster

```
hostlist <- paste(unlist(read.delim(file="hostlist.txt",
header=F, sep =" ")))
cl <- makeCluster(hostlist)
registerDoParallel(cl)
clusterEvalQ(cl,.libPaths("/uufs/chpc.utah.edu/sys/installdir/
RLibs/3.5.2i"))
```

this is only needed if running on multiple nodes

- Run parallel loop

```
r <- foreach(icount(trials), .combine=rbind) %dopar% {}
```

- Stop R cluster

```
stopCluster(cl)
```

R examples

- Parallel R on one node
  - best run from a SLURM job
    parallel-onenode-iris.R, R-parallel-onenode-iris.slr-
    https://github.com/CHPC-UofU/USU-lectures
  - `sbatch R-parallel-onenode-iris.slr`
- Parallel R multiple nodes
  - must specify list of nodes where R workers run
    parallel-multinode-iris.R, R-parallel-multinode-iris.slr-
  - `sbatch R-parallel-onenode-iris.slr`
- Submit SLURM job directly from R - rslurm
  - SLURM-aware apply function, some issues with results collection
  - rslurm-example.R

Python

Threads

- No threads in Python code because of GIL (Global Intepreter Lock)
- C/Fortran functions can be threaded (e.g. *NumPy* - Anaconda)

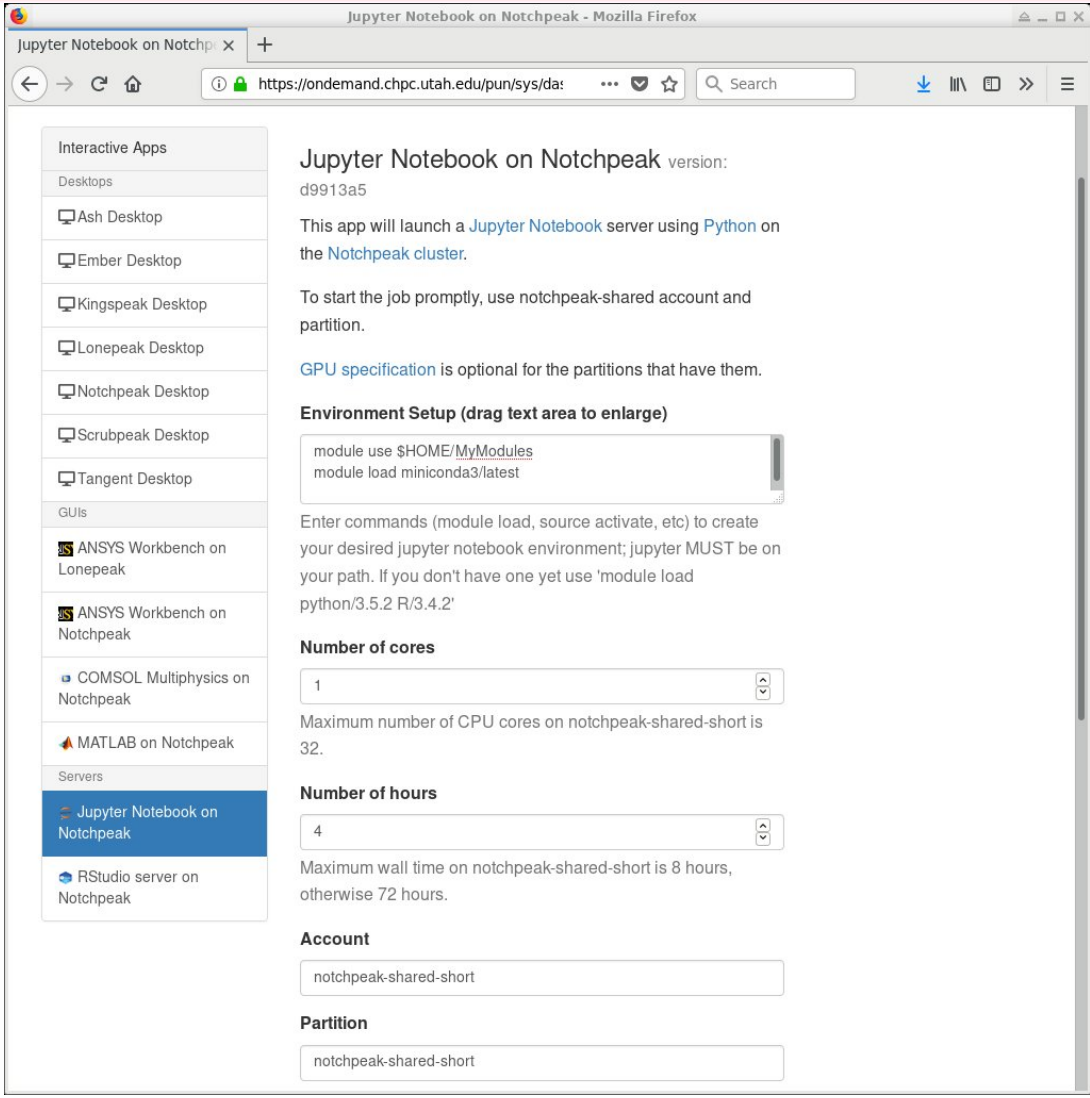
Tasks (processes)

- Several libraries that use MPI under the hood, most popular is *mpi4py*
- More-less MPI function compatibility, but slower communication because of the extra overhead
- Also many other data-parallel libraries, e.g. *Dask*

https://www.chpc.utah.edu/documentation/software/python.php

Python - Jupyter

- Several options listed at https://www.chpc.utah.edu/documentation/software/jupyterhub.php
- The easiest is to use Open OnDemand



Python tasks

- Our personal favorite is to ignore all the Python parallel efforts, divide the data into independent parts and run multiple Python processes on parts of the data concurrently
- Only works if data can be split
- Use various approaches for independent parallel calculations listed at https://www.chpc.utah.edu/documentation/software/serial-jobs.php
- More on this later

Python- Dask

- With relatively small effort one can use Dask
- Install Miniconda

```
wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
bash ./Miniconda3-latest-Linux-x86_64.sh -b -p $HOME/software/pkg/miniconda3
mkdir -p $HOME/MyModules/miniconda3
cp /uufs/chpc.utah.edu/sys/installdir/python/modules/miniconda3/latest.lua $HOME/MyModules/miniconda3
```

- Install Jupyter and Dask

```
module use $HOME/MyModules
module load miniconda3/latest
conda install dask
```

- Start Open OnDemand Jupyter notebook
  - log into ondemand.chpc.utah.edu with CHPC credentials

Python- Dask

- Go to Interactive Apps - Jupyter Notebook on notchpeak
- In the Environment Setup text box, put:

```
module use $HOME/MyModules
module load miniconda3/latest
```

- Use notchpeak-shared-short for account and partition, and select your choice of CPU cores and walltime hours (within the listed limits). Then hit Launch to submit the job.
- Once the job starts, hit the blue Connect to Jupyter button
- Open one of the following notebooks: dask_embarrass.ipynb, dask_slurmcluster.ipynb, dask_slurm_xarray.ipynb
- DASK also allows to submit jobs to SLURM (last 2 examples)

Independent calculations

- Different approaches based on the nature of the calculations
  - Runtime length, variability, number of calculations
- Similar runtime, small calculation count
  - Shell script in a SLURM job

```
#!/bin/bash
for (( i=0; i < $SLURM_NTASKS ; i++ )); do
  /path_to/myprogram $i &
done
wait
```

  - srun –multi-prog

```
srun --multi-prog my.conf
cat my.conf
0-11 ./example.sh %t
```

https://www.chpc.utah.edu/documentation/software/serial-jobs.php

Variable runtime

- Mini-scheduler inside of a job
  - to launch calculations till all are done
  - GNU Parallel - https://www.gnu.org/software/parallel/
  - TACC Launcher - https://www.tacc.utexas.edu/research-development/tacc-software/the-launcher
  - CHPC Submit - https://www.chpc.utah.edu/documentation/software/serial-jobs.php#submit
- Workflow managers
  - More on this later
  - Makeflow, Swift, Snakemake, Pegasus
- Distributed computing resources
  - Open Science Grid - https://opensciencegrid.org/

Single executable across desktops and clusters

- MPICH, MVAPICH2 and Intel MPI are cross-compatible using the same ABI
  - Can e.g. compile with MPICH on a desktop, and then run on the cluster using MVAPICH2 and InfiniBand
- Intel and PGI compilers allow to build "unified binary" with optimizations for different CPU platforms
  - But in reality it only works well under Intel compilers
- On a desktop

```
module load intel mpich
mpicc –axCORE-AVX512,CORE-AVX2,AVX program.c –o program.exe
mpirun –np 4 ./program.exe
```

- On a cluster

```
srun –N 2 –n 24 ...
module load intel mvapich2
mpirun –np $SLURM_NTASKS ./program.exe
```

- https://www.chpc.utah.edu/documentation/software/single-executable.php

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
  - **Intel Inspector XE** – memory and threading error checker
- How to use:
- `http://www.chpc.utah.edu/docs/manuals/software/par_devel.html`

Debuggers - parallel

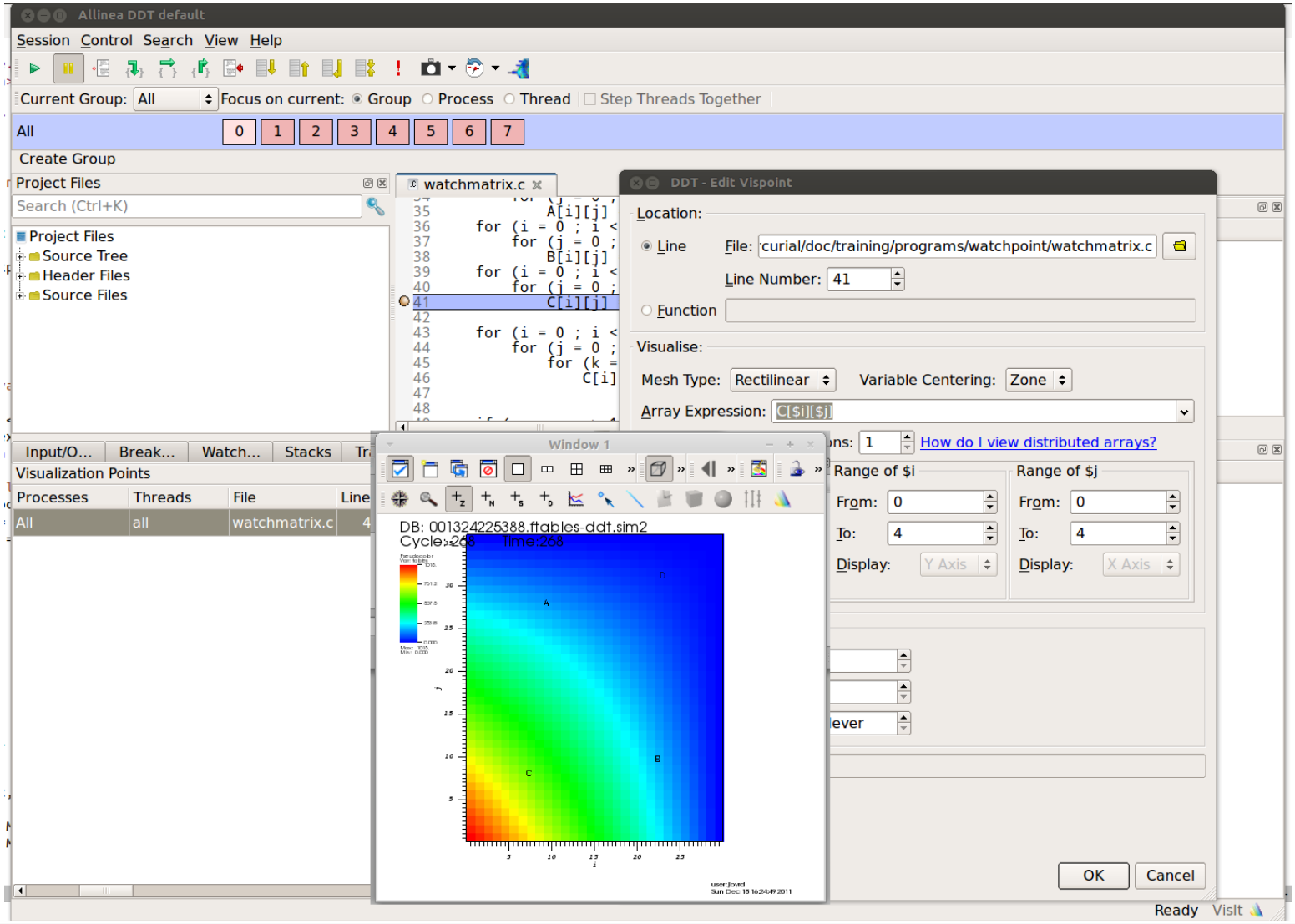
- Parallel debugging more complex due to interaction between processes
- DDT is the debugger of choice at CHPC
- Expensive but academia get discount
- How to run it:
  - compile with `-g` flag
  - run `ddt` command
  - fill in information about executable, parallelism, …
- Details:

`https://www.chpc.utah.edu/documentation/software/debugging.php`

- Further information

`https://www.allinea.com/products/ddt`

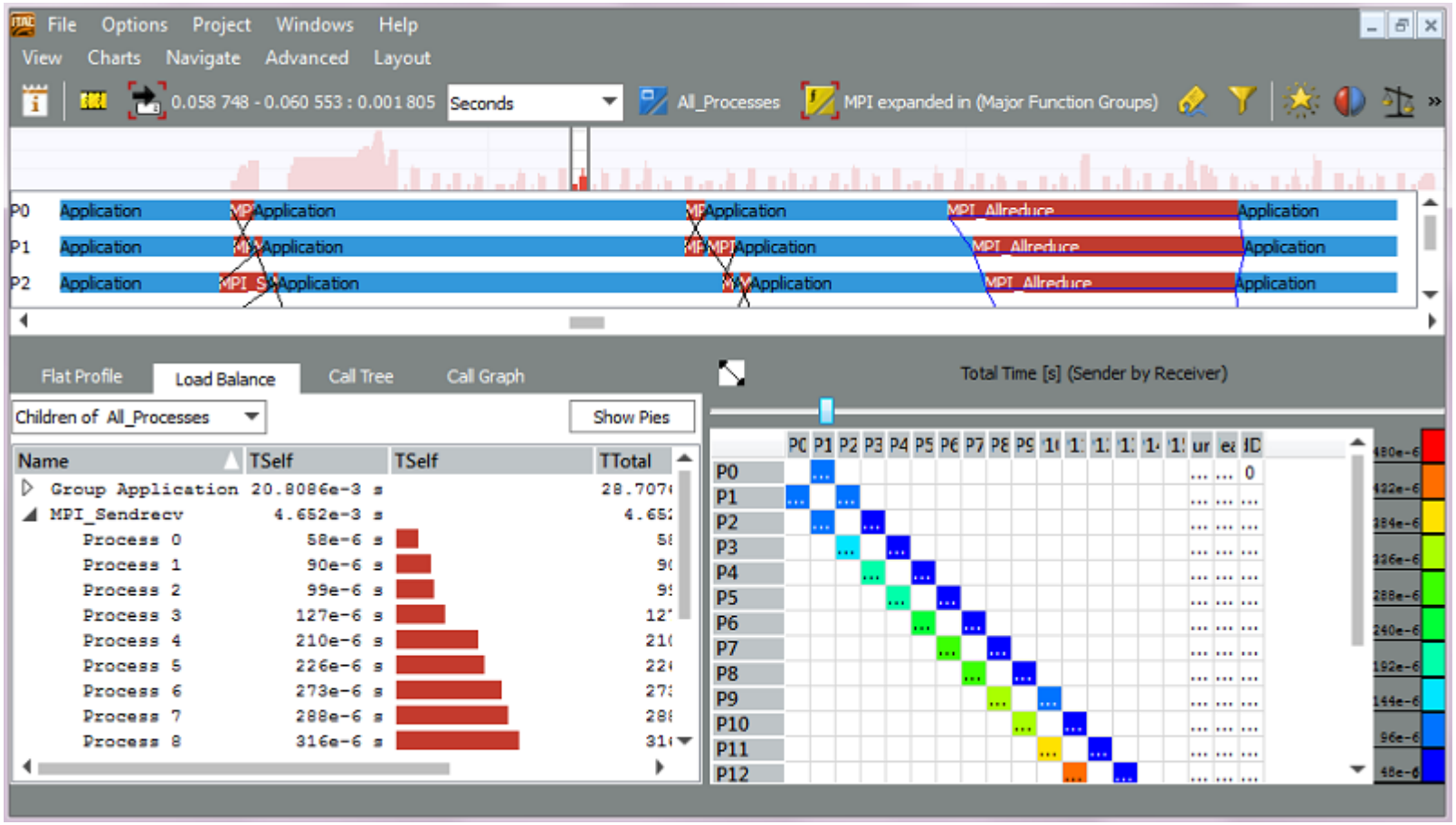
Debuggers – parallel



Profilers

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

Profilers - parallel



Libraries

- Use libraries for common operationsSerial
  - BLAS, LAPACK – linear algebra routines
  - MKL, ACML – hardware vendor libraries
- Parallel
  - ScaLAPACK, PETSc, FFTW
  - MKL – dense and sparse matrices
- Design a new code around existing library
  - PETSc, Trilinos,…

Summary

- Shared vs. Distributed memory parallelism
- OpenMP, OpenACC and MPI for low level parallelism
- There are tools for debugging, profiling
- Different approaches for higher level languages
- Many ways to run independent calculations in parallel

To learn more

- Videos of recent workshops
- XSEDE HPC Summer Boot Camp
  - OpenMP, OpenACC, MPI
  - https://www.youtube.com/XSEDETraining
- Petascale Computing Institute
  - Wide range of parallel programming topics
  - https://bluewaters.ncsa.illinois.edu/bw-petascale-computing-2019/agenda