Debugging, benchmarking, tuning i.e. software development tools

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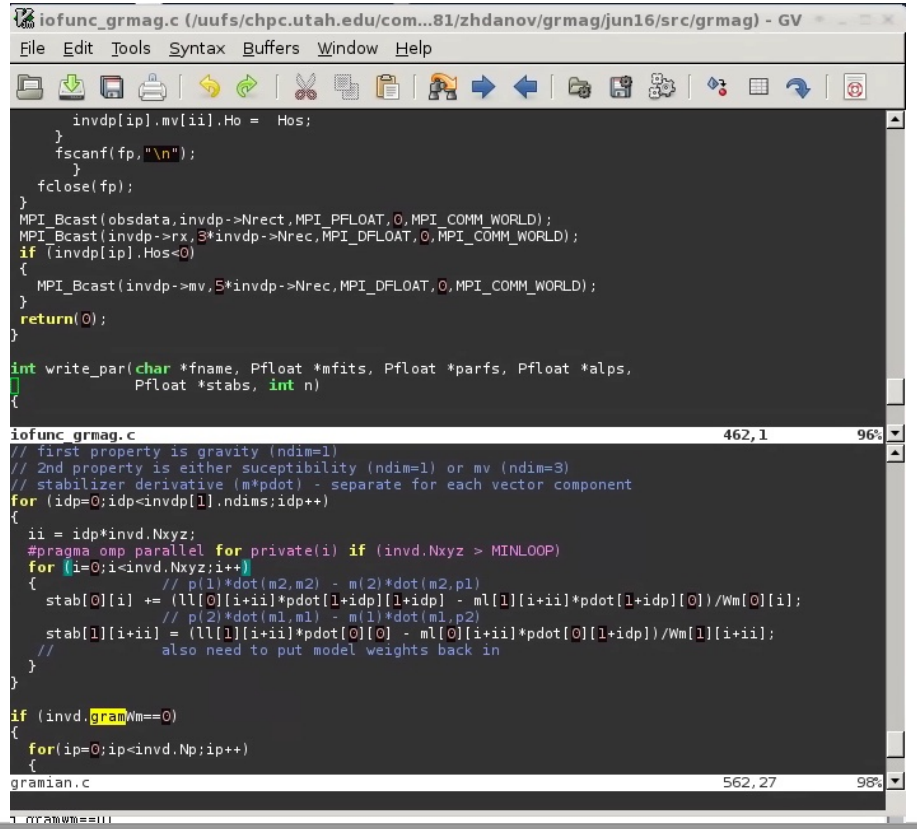
SW development tools

- Development environments
- Compilers
- Version control
- Debuggers
- Profilers
- Runtime monitoring
- Benchmarking

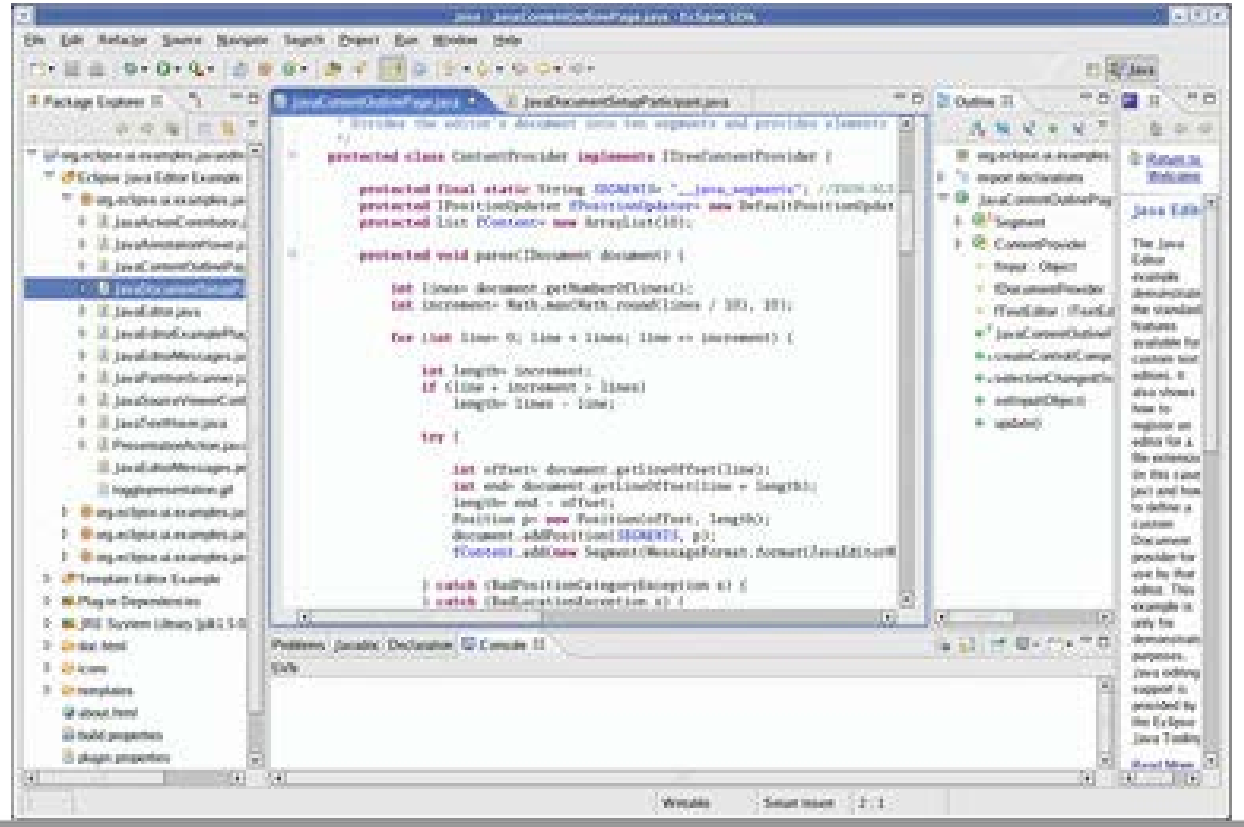
PROGRAMMING TOOLS

Program editing

- Text editors
  - vim, emacs, atom



- IDEs
  - Visual *, Eclipse



Compilers

- Open source
  - GNU
  - Open64, clang
- Commercial
  - Intel
  - Portland Group (PGI, owned by Nvidia)
  - Vendors (IBM XL, Cray)
  - Others (Absoft, CAPS, PathScale)

Language support

- Languages
  - C/C++ - GNU, Intel, PGI
  - Fortran – GNU, Intel, PGI
- Interpreters
  - Matlab – has its own ecosystem
  - Java – reasonable ecosystem, not so popular in HPC, popular in HTC
  - Python – attempts to have its own ecosystem, some tools can plug into Python (e.g. Intel VTune)

Language/library support

- Language extensions
  - OpenMP (4.0+*) – GNU, Intel*, PGI
  - OpenACC – PGI, GNU very experimental
  - CUDA – Nvidia GCC, PGI Fortran
- Libraries
  - Intel Math Kernel Library (MKL)
  - PGI packages open source (OpenBLAS?).

Version control

- Copies of programs
  - Good enough for simple code and quick tests/changes
- Version control software
  - Allow code merging, branching, etc
  - Essential for collaborative development
  - RCS, CVS, SVN
  - Git – integrated web services, free for open source, can run own server for private code

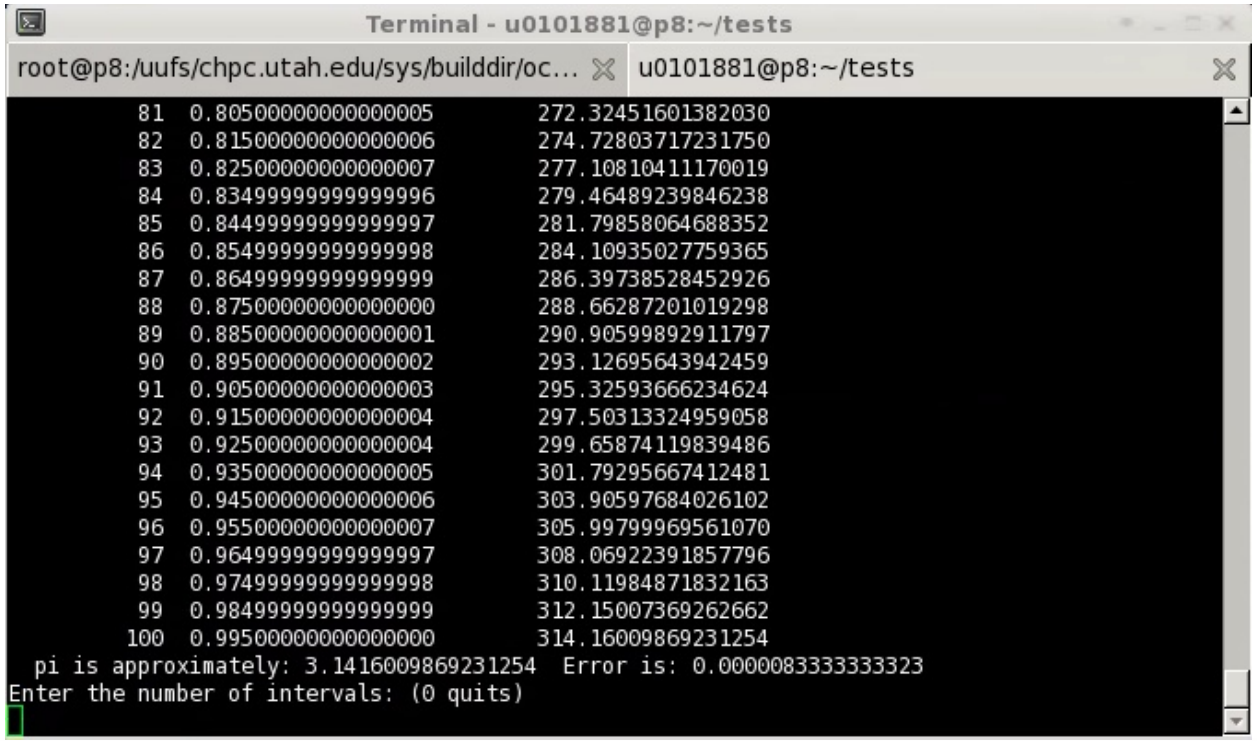
DEBUGGING

Program errors

- Crashes
  - Segmentation faults (bad memory access)
    - often writes core file – snapshot of memory at the time of the crash
  - Wrong I/O (missing files)
  - Hardware failures
- Incorrect results
  - Reasonable but incorrect results
  - NaNs – not a numbers – division by 0, …

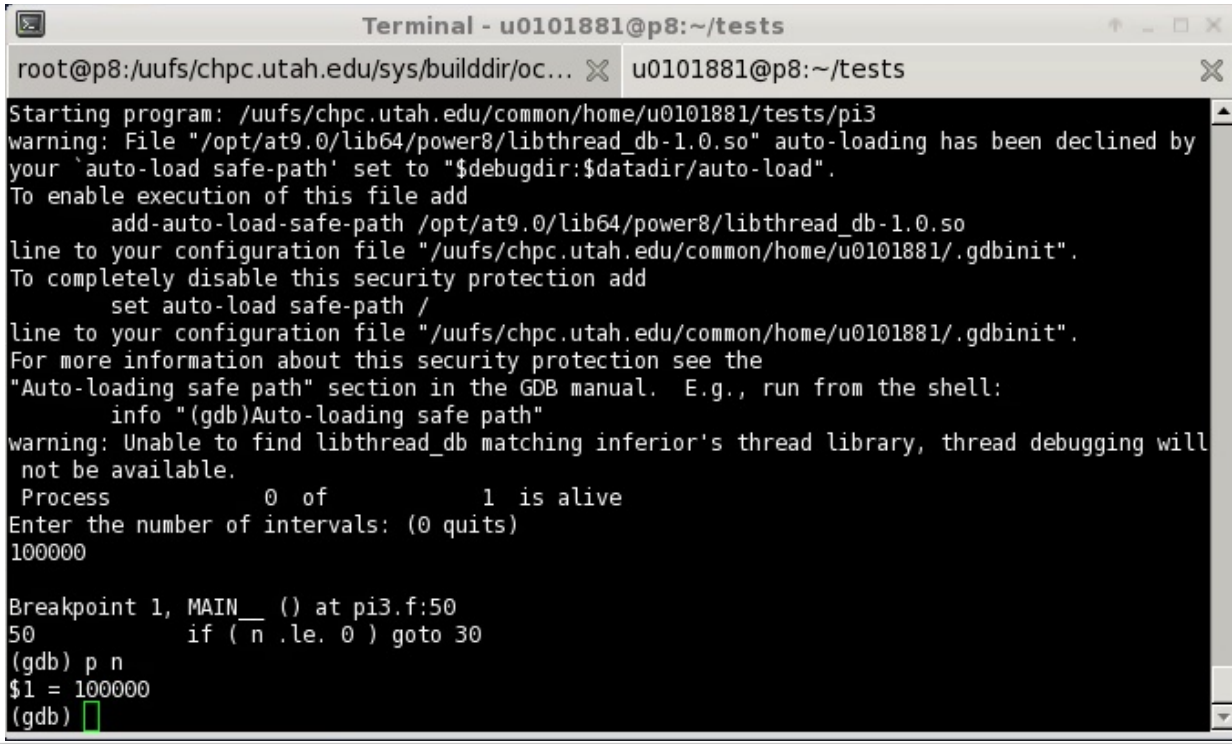
write/printf

- Write variables of interest into the stdout or file
- Simplest but cumbersome
  - Need to recompile and rerun
  - Need to browse through potentially large output



Terminal debuggers

- Text only, e.g. gdb, idb
- Need to remember commands or their abbreviations
- Need to know lines in the code (or have it opened in other window)
- Useful for quick code checking on compute nodes and core dump analysis



GUI debuggers

- Have graphical user interface
- Some free, mostly commercial
- Eclipse CDT (C/C++ Development Tooling), PTP (Parallel Tools Platform) - free
- PGI's pdbg – part of PGI compiler suite
- Intel development tools
- Rogue Wave Totalview - commercial
- Allinea DDT - commercial

Totalview and DDT

- The only real alternative for parallel or accelerator debugging
- Cost a lot of money (thousands of $), but, worth it
- We have Totalview license (for historical reasons), 32 tokens enough for our needs (renewal ~$1500/yr).
- XSEDE systems have DDT.

How to use Totalview

1. Compile binary with debugging information

- flag -g

```
gcc -g test.f -o test
```

2. Load module and run Totalview

```
module load totalview
```

- TV + executable

```
totalview executable
```

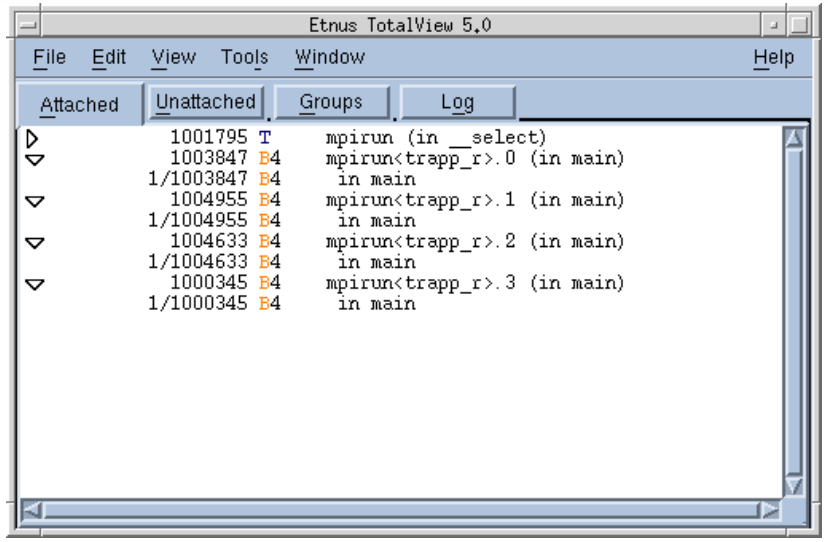
- TV + core file

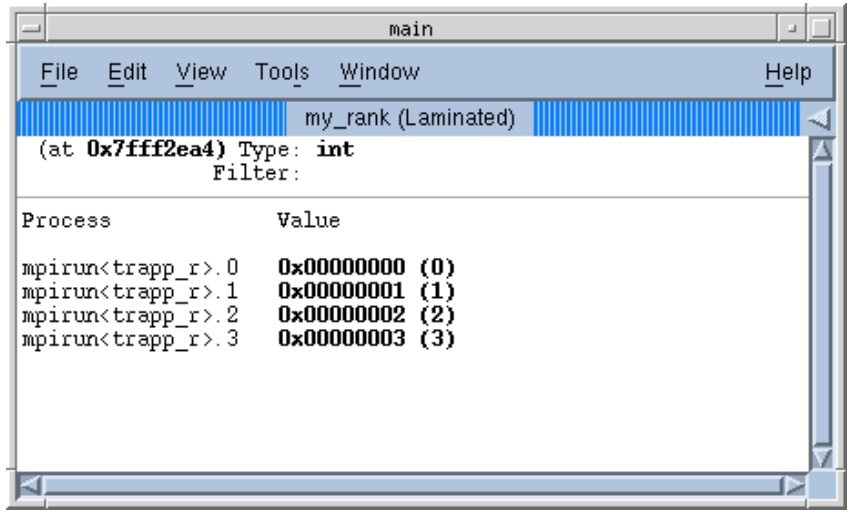
```
totalview executable core_file
```

- Run TV and choose what to debug in a startup dialog

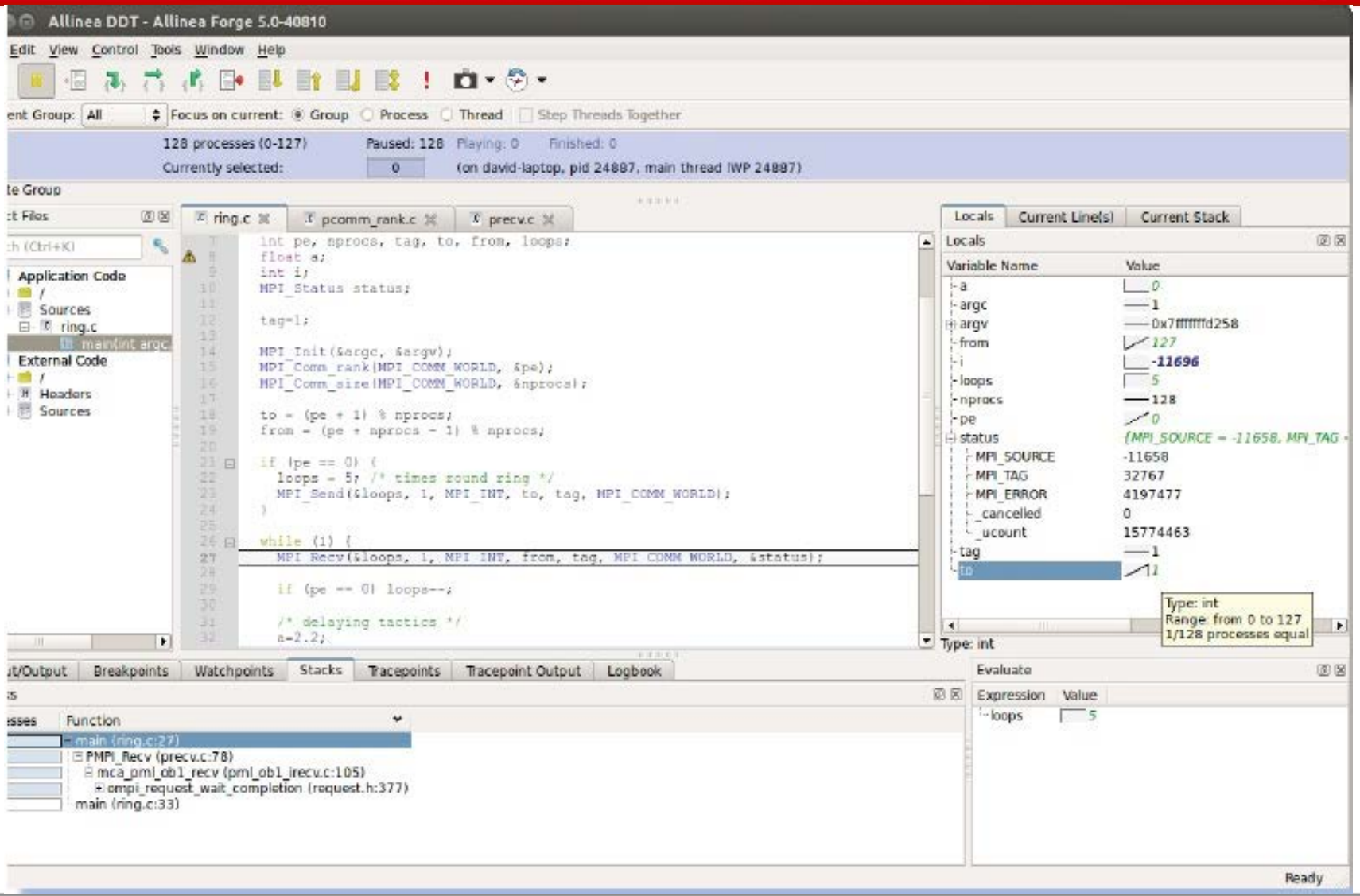
```
totalview
```

Totalview windows





DDT screenshot



Debugger basic operations

- Data examination
  - view data in the variable windows
  - change the values of variables
  - modify display of the variables
  - visualize data
- Action points
  - breakpoints and barriers (static or conditional)
  - watchpoints
  - evaluation of expressions

Multiprocess debugging

- Automatic attachment of child processes
- Create process groups
- Share breakpoints among processes
- Process barrier breakpoints
- Process group single-stepping
- View variables across procs/threads
- Display MPI message queue state

Additional Totalview tools

- Memoryscape
  - Dynamic memory debugging tool
- Replay Engine
  - Allows to reversely debug the code
- Accelerator debugging
  - CUDA and OpenACC

Code checkers

- Compilers check for syntax errors
  - lint based tools
  - Runtime checks through compiler flags (-fbounds-check, -check*, -Mbounds)
- DDT has a built in syntax checker
  - Matlab does too
- Memory checking tools - many errors are due to bad memory management
  - valgrind – easy to use, many false positives
  - Intel Inspector – intuitive GUI

Intel software development products

- We have a 2 concurrent user license
  - One license locks all the tools
  - Cost ~$2000/year
- Tools for all stages of development
  - Compilers and libraries
  - Verification tools
  - Profilers
- More info

https://software.intel.com/en-us/intel-parallel-studio-xe

Intel Inspector

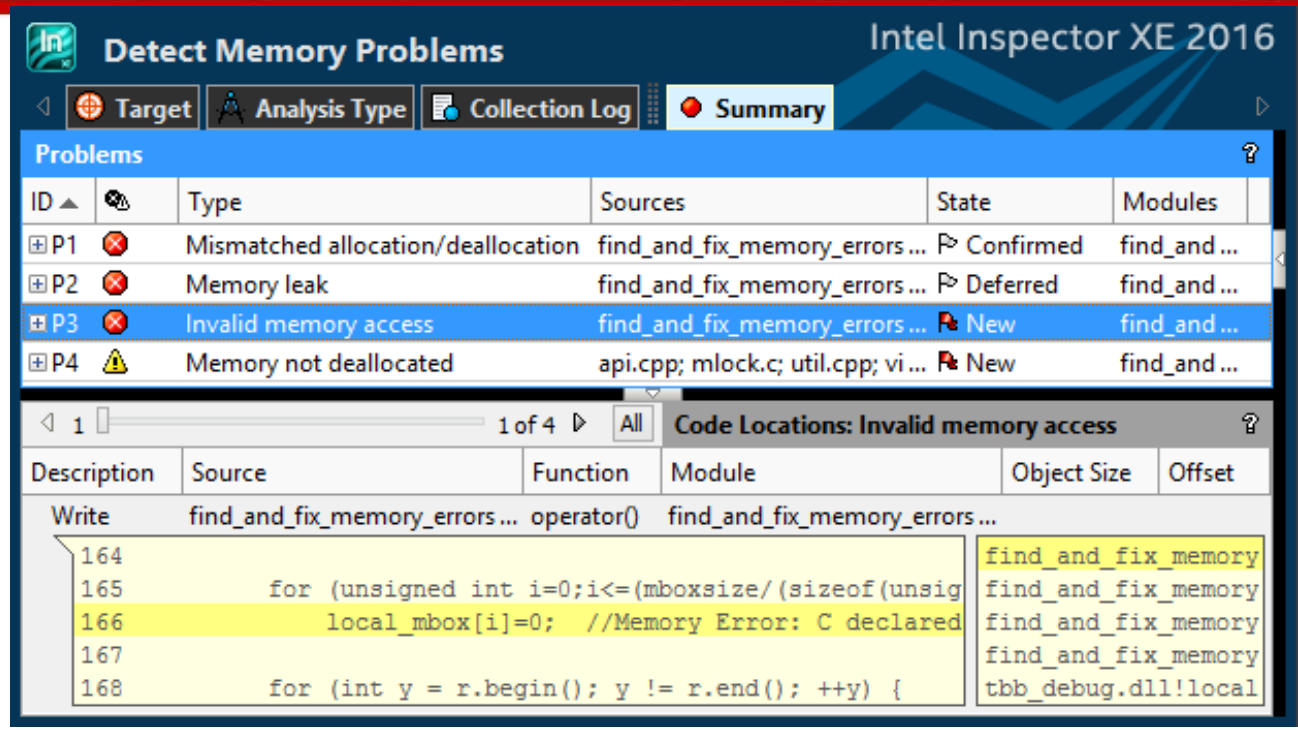
- Thread checking
  - Data races and deadlocks
- Memory checker
  - Like leaks or corruption
  - Good alternative to Totalview MemoryScape
- Standalone or GUI integration
- More info

http://software.intel.com/en-us/intel-inspector-xe/

Intel Inspector

- Source the environment
  `module load inspectorxe`
- Compile with `-tcheck -g`
  `ifort -openmp -tcheck -g trap.f`
- Run tcheck
  `inspxe-gui` – graphical user interface
  `inspxe-cl` – command line
- Tutorial

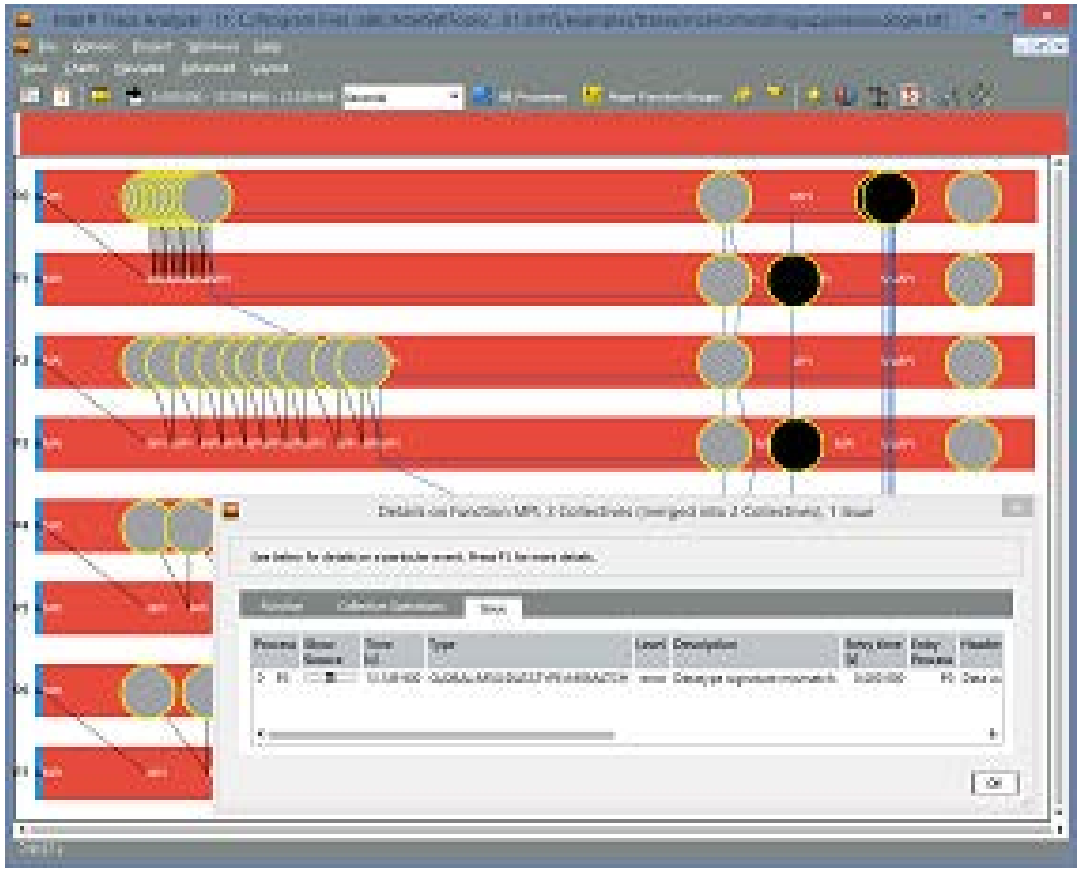
`https://software.intel.com/en-us/articles/inspectorxe-tutorials`



Intel Trace Analyzer and Collector

- MPI profiler and correctness checker
- Detects violations of MPI standard and errors in execution environment
- To use correctness checker

```
module load intel impi itac
setenv VT_CHECK_TRACING 0
mpirun –check-mpi –n 4 ./myApp
```



- ITAC documentation

`https://software.intel.com/en-us/intel-trace-analyzer-support/documentation`

PROFILING

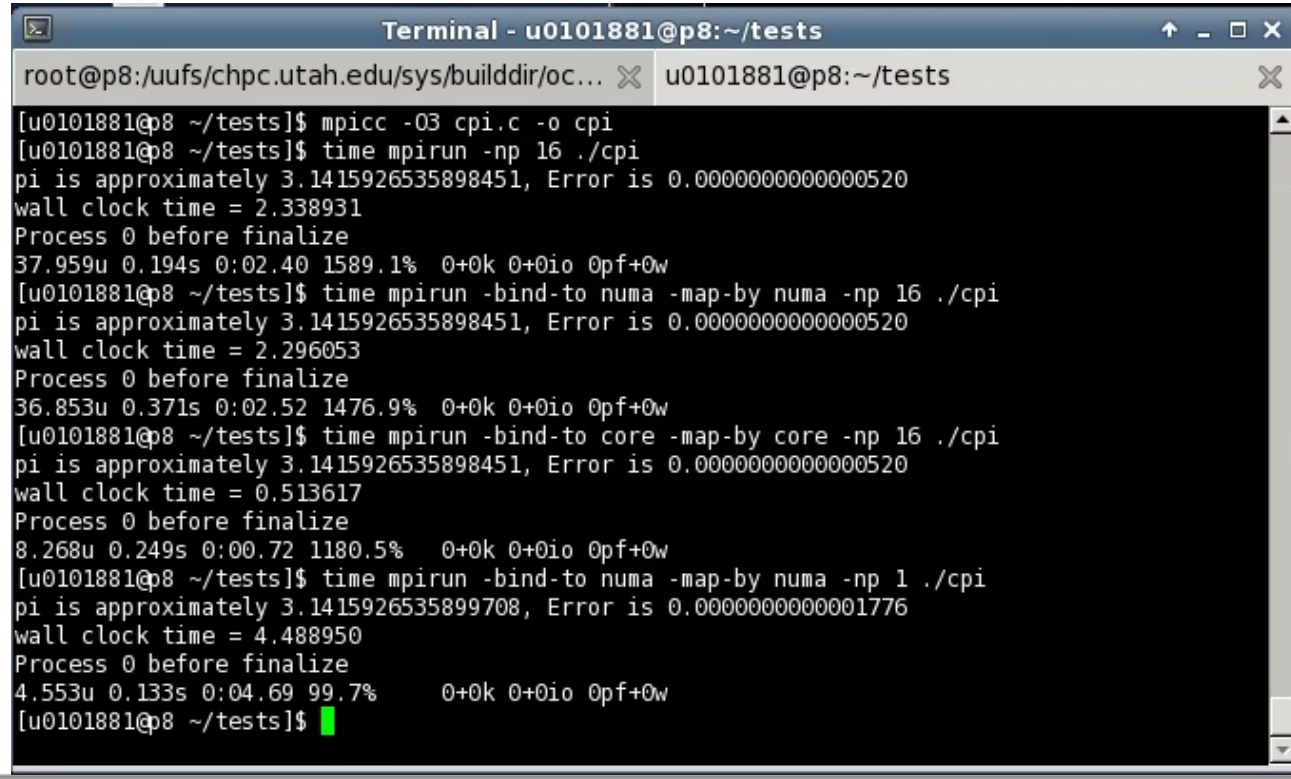
Why to profile

- Evaluate performance

- Find the performance bottlenecks
  - Inefficient programming
  - Memory or I/O bottlenecks
  - Parallel scaling

Program runtime

- Time program runtime
  - get an idea on time to run and parallel scaling
- Many programs include benchmark problems
  - Some also accessible via "make test"
- Consider scripts, especially if doing parallel performance evaluation

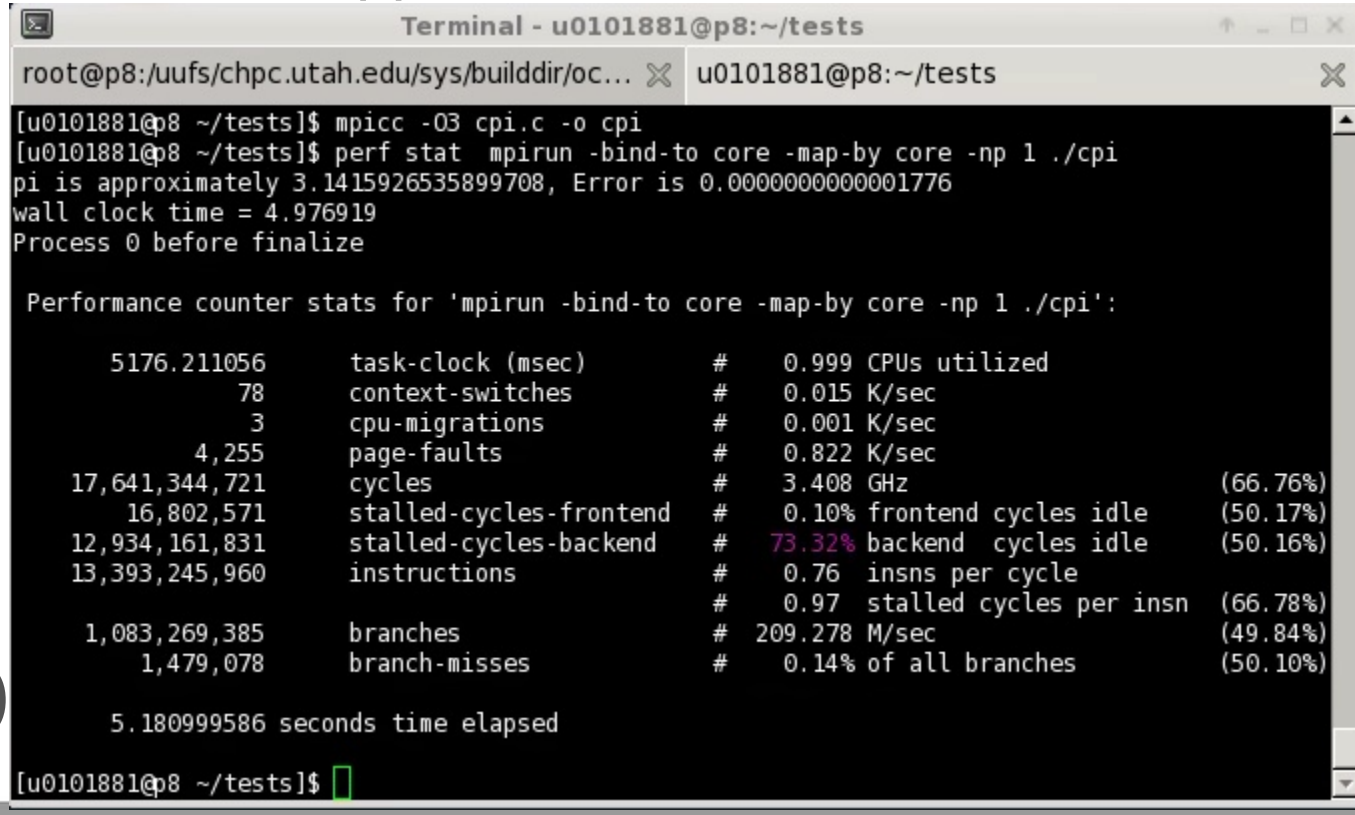


Profiling categories

- Hardware counters
  - count events from CPU perspective (# of flops, memory loads, etc)
  - usually need Linux kernel module installed (>2.6.31 has it)
- Statistical profilers (sampling)
  - interrupt program at given intervals to find what routine/line the program is in
- Event based profilers (tracing)
  - collect information on each function call

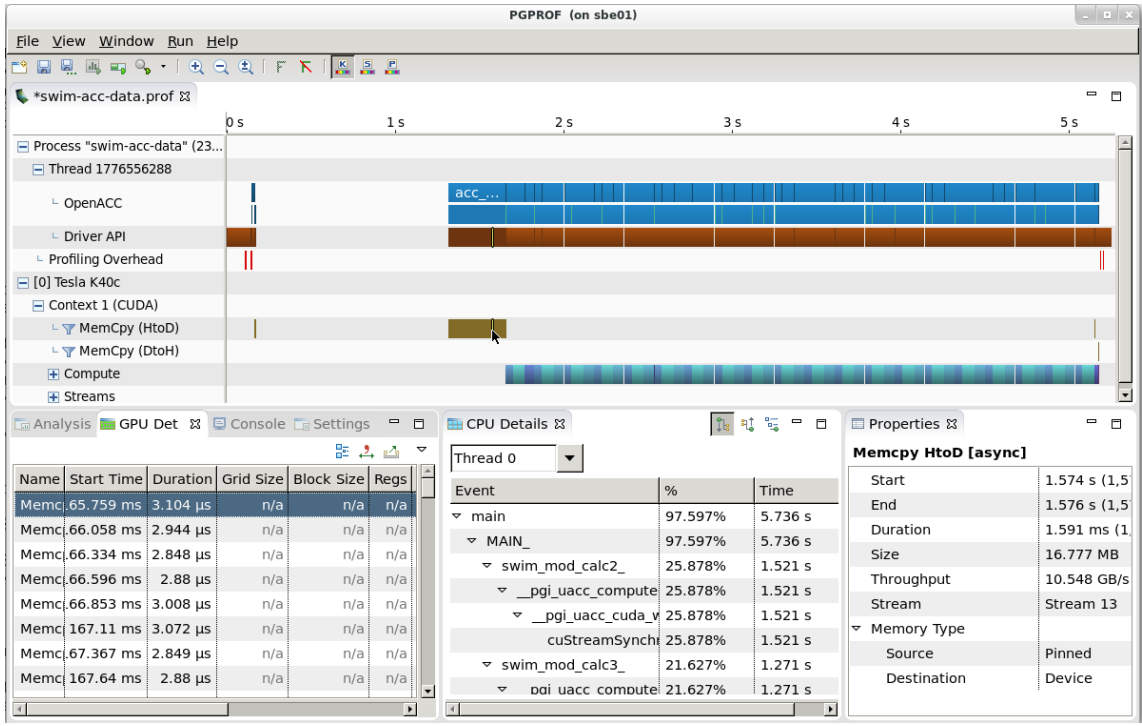
Hardware counters

- CPUs include counters to count important events
  - Flops, instructions, cache/memory access
  - Access through kernel or PAPI (Performance Application Programming Interface)
- Tools to analyze the counters
  - perf - hardware counter collection, part of Linux
  - oprofile – profiler + hw counters
  - Intel VTune
- Drawback – harder to analyze the profiling results (exc. VTune)



Serial profiling

- Discover inefficient programming
- Computer architecture slowdowns
- Compiler optimizations evaluation
- gprof
- Compiler vendor supplied (e.g. pgprof, nvvp)
- Intel tools on serial programs
  - AdvisorXE, VTune



HPC open source tools

- HPC Toolkit
  - A few years old, did not find it as straightforward to use
- TAU (Tuning and Analysis Utilities)
  - Lots of features, which makes the learning curve slow
- Scalasca
  - Developed by European consortium, did not try yet

Intel tools

- Intel Parallel Studio XE 2016 Cluster Edition
  - Compilers (C/C++, Fortran)
  - Math library (MKL)
  - Threading library (TBB)
  - Thread design and prototype (Advisor)
  - Memory and thread debugging (Inspector)
  - Profiler (VTune Amplifier)
  - MPI library (Intel MPI)
  - MPI analyzer and profiler (ITAC)

Intel VTune Amplifier

- Serial and parallel profiler
  - Multicore support for OpenMP and OpenCL on CPUs, GPUs and Xeon Phi
- Quick identification of performance bottlenecks
  - Various analyses and points of view in the GUI
  - Makes choice of analysis and results inspection easier
- GUI and command line use
- More info

`https://software.intel.com/en-us/intel-vtune-amplifier-xe`

Intel VTune Amplifier

- Source the environment

  `module load vtune`

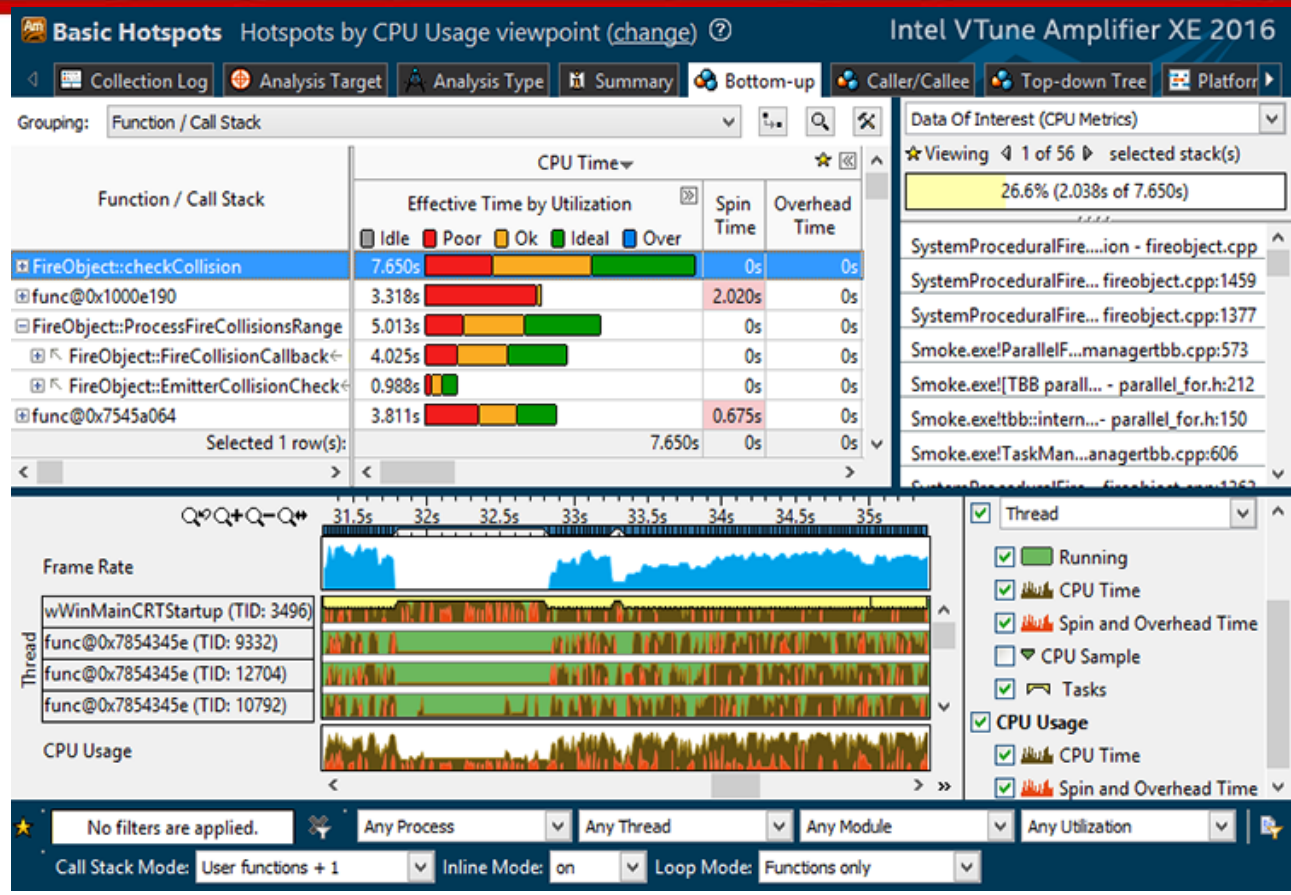
- Run VTune

  `amplxe-gui` – GUI

  `amplxe-cl` – CLI

  Can be used also for remote profiling (e.g. on Xeon Phi)

- Tuning guides for specific architectures



`https://software.intel.com/en-us/articles/processor-specific-performance-analysis-papers`

Intel Advisor

- Vectorization advisor
  - Identify loops that benefit from vectorization, what is blocking efficient vectorization and explore benefit of data reorganization
- Thread design and prototyping
  - Analyze, design, tune and check threading design without disrupting normal development
- More info

`http://software.intel.com/en-us/intel-advisor-xe/`

Intel Advisor

- Source the environment

  `module load advisorxe`

- Run Advisor

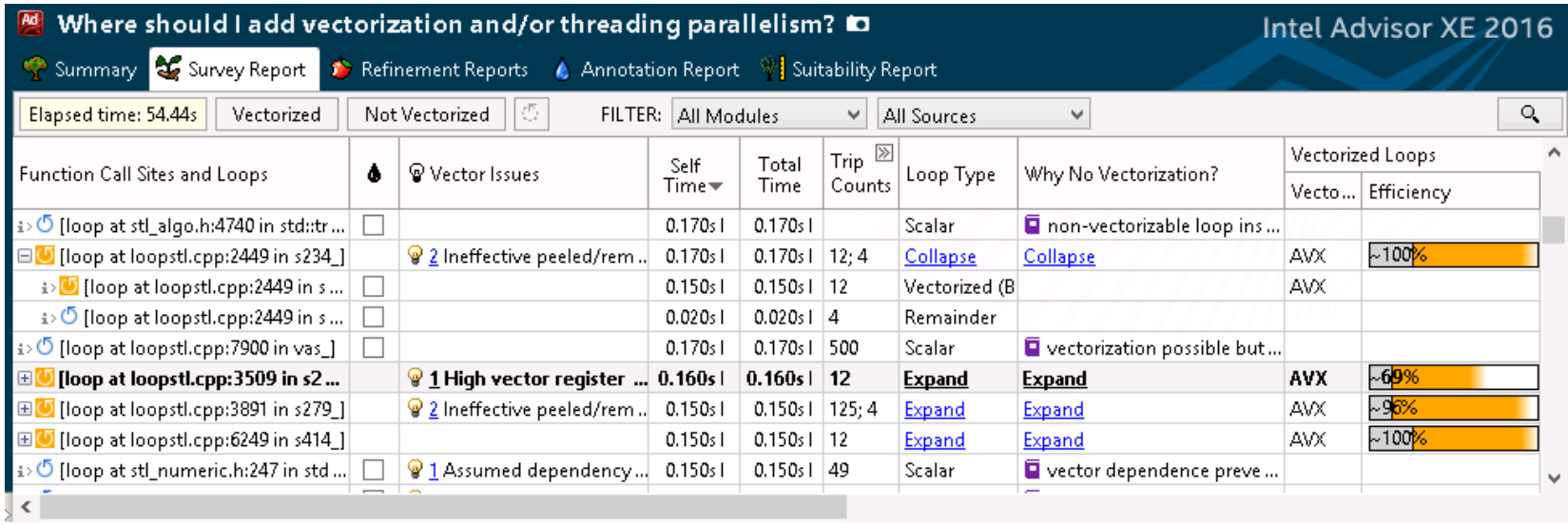
  `advixe-gui` – GUI

  `advixe-cl` – CLI

- Create project and choose appropriate modeling

- Getting started guide

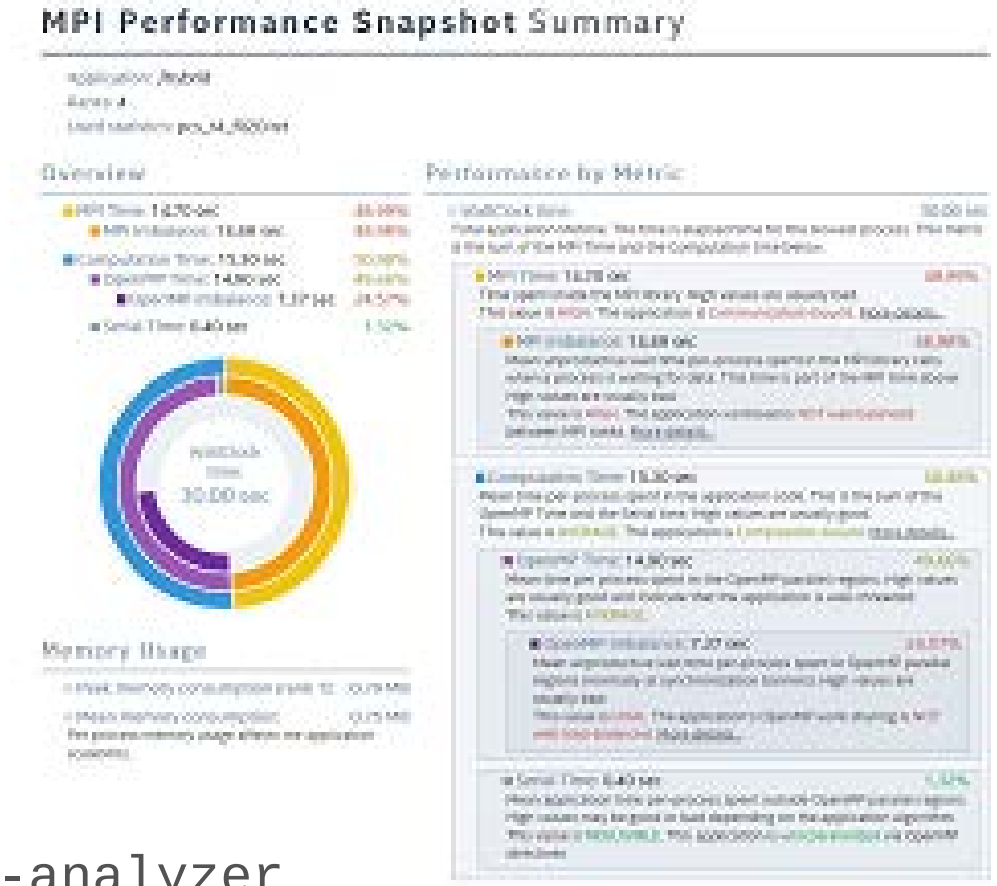
`https://software.intel.com/en-us/get-started-with-advisor`



Intel Trace Analyzer and Collector

- MPI profiler
  - traces MPI code
  - identifies communication inefficiencies
- Collector collects the data and Analyzer visualizes them
- More info

`https://software.intel.com/en-us/intel-trace-analyzer`



Intel TAC

- Source the environment

```
module load itac
```

- Using Intel compilers, can compile with `-trace`

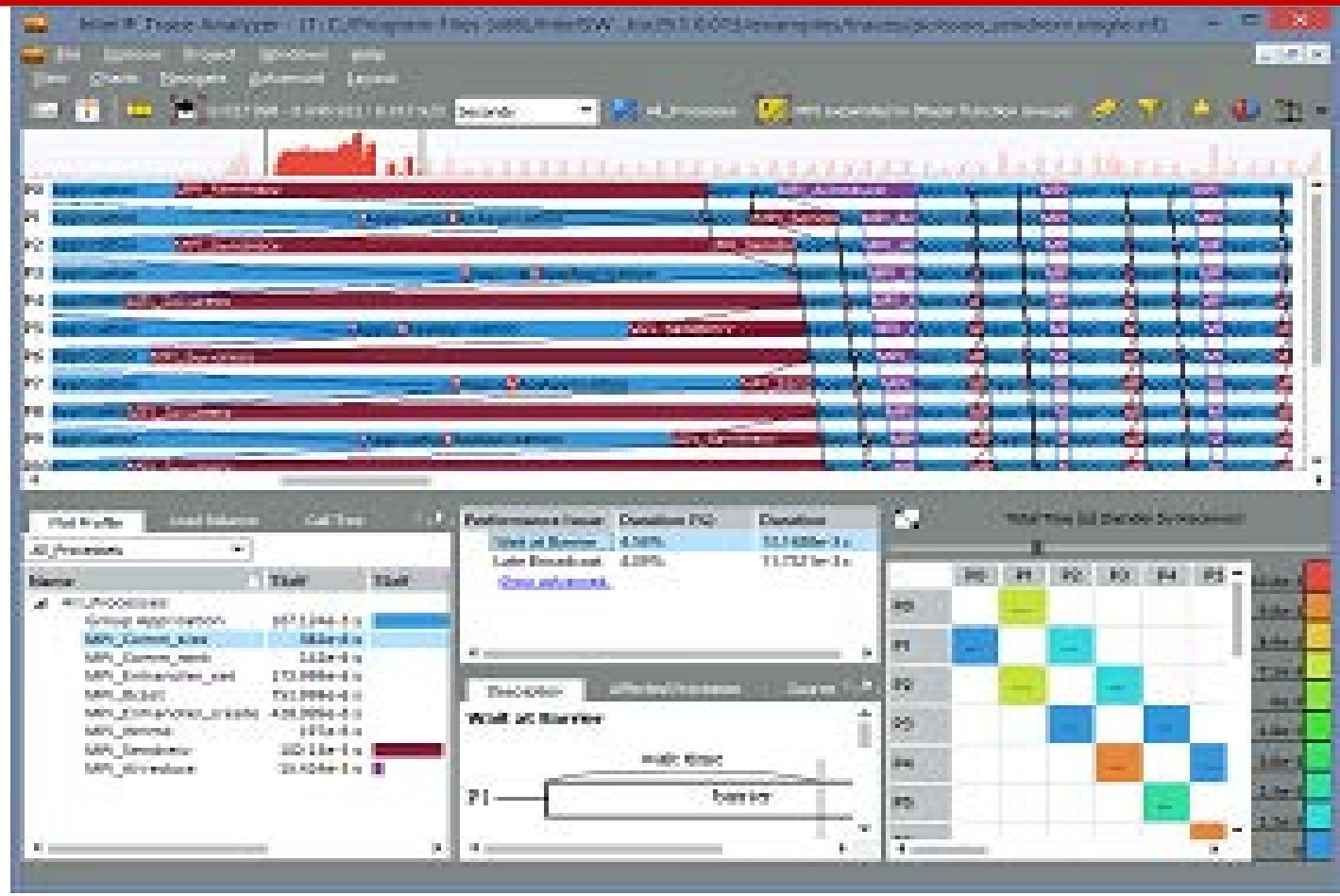
```
mpiifort -openmp –trace trap.f
```

- Run MPI code

```
mpirun –trace –n 4 ./a.out
```

- Run visualizer

```
traceanalyzer a.out.stf &
```



- Getting started guide

```
https://software.intel.com/en-us/get-started-with-itac-for-linux
```

RUNTIME MONITORING

Why runtime monitoring?

- Make sure program is running right
  - Hardware problems
  - Correct parallel mapping / process affinity
- Careful about overhead

Runtime monitoring

- Self checking
  - ssh to node(s), run “top”, or look at “sar” logs
  - SLURM (or other scheduler) logs and statistics
- Tools
  - XDMoD – XSEDE Metrics on Demand (through SUPReMM module)
  - REMORA - REsource MOnitoring for Remote Applications

BENCHMARKING

Why to benchmark?

- Evaluate system's performance
  - Testing new hardware
- Verify correct hardware and software installation
  - New cluster/node deployment
    - There are tools for cluster checking (Intel Cluster Checker, cluster distros, …)
  - Checking newly built programs
    - Sometimes we leave this to the users

New system evaluation

- Simple synthetic benchmarks
  - FLOPS, STREAM
- Synthetic benchmarks
  - HPL – High Performance Linpack – dense linear algebra problems – cache friendly
  - HPCC – HPC Challenge Benchmark – collection of dense, sparse and other (FFT) benchmarks
  - NPB – NAS Parallel Benchmarks – mesh based solvers – OpenMP, MPI, OpenACC implementations

New system evaluation

- Real applications benchmarks
  - Depend on local usage
  - Gaussian, VASP
  - Amber, LAMMPS, NAMD, Gromacs
  - ANSYS, Abaqus, StarCCM+
  - Own codes
- Script if possible
  - A lot of combinations of test cases vs. number of MPI tasks/OpenMP cores

Cluster deployment

- Whole cluster
  - Some vendors have cluster verification tools
  - We have a set of scripts that run basic checks and HPL at the end
- New cluster nodes
  - Verify received hardware configuration, then rack
  - Basic system tests (node health check)
  - HPL – get expected performance per node (CPU or memory issues), or across more nodes (network issues)

BACKUP

Demos

- Totalview
- Advisor
- Inspector
- VTune