



# 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

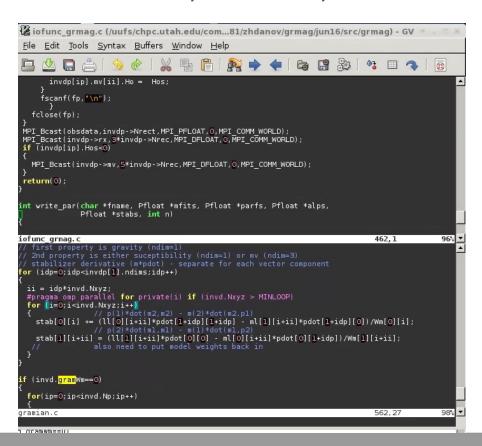
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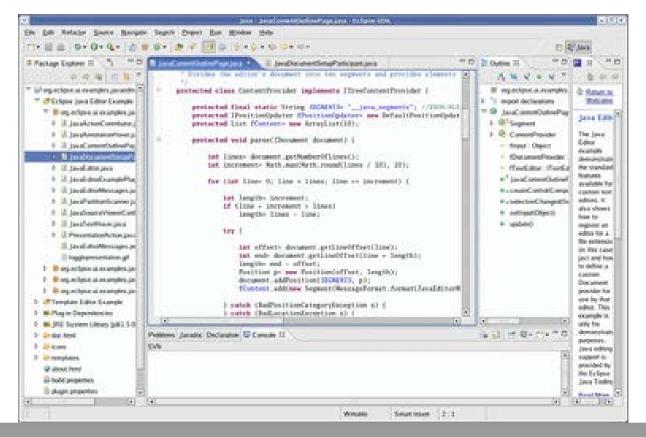
# Program editing



- Text editors
  - vim, emacs, atom



- IDEs
  - Visual \*, Eclipse





# Compilers



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



#### Language support



#### Languages

- C/C++ GNU, Intel, PGI
- Fortran GNU, Intel, PGI

#### Interpreters

- Matlab has its own ecosystem (debugger, profiler)
- Java reasonable ecosystem, not so popular in HPC, popular in HTC
- Python ecosystem improving, 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 (gitlab)





### **DEBUGGING**

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#### Program errors



#### Crashes

- Segmentation faults (bad memory access)
  - often writes core file snapshot of memory at the time of the crash

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- 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 - u0101881@p8:~/tests
root@p8:/uufs/chpc.utah.edu/sys/builddir/oc... 💥 u0101881@p8:~/tests
         81 0.805000000000000005
                                         272.32451601382030
                                         274.72803717231750
             0.8150000000000000006
                                         277.10810411170019
             0.8250000000000000007
             0.8349999999999996
                                         279.46489239846238
                                         281.79858064688352
                                         284.10935027759365
                                         286.39738528452926
                                         288.66287201019298
             0.875000000000000000
                                         290.90599892911797
                                         293.12695643942459
             0.905000000000000003
                                         295.32593666234624
                                         297.50313324959058
             0.9150000000000000004
                                         299.65874119839486
             0.9250000000000000004
                                         301.79295667412481
             0.945000000000000006
                                         303.90597684026102
             0.955000000000000007
                                         305.99799969561070
                                         308.06922391857796
                                         310.11984871832163
             0.9849999999999999
                                         312.15007369262662
        100 0.995000000000000000
                                         314.16009869231254
 pi is approximately: 3.1416009869231254 Error is: 0.0000083333333323
Enter the number of intervals: (0 quits)
```

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#### 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

```
Terminal - u0101881@p8:~/tests
 root@p8:/uufs/chpc.utah.edu/sys/builddir/oc... × u0101881@p8:~/tests
Starting program: /uufs/chpc.utah.edu/common/home/u0101881/tests/pi3
warning: File "/opt/at9.0/lib64/power8/libthread db-1.0.so" auto-loading has been declined by
your `auto-load safe-path' set to "$debugdir:$datadir/auto-load".
To enable execution of this file add
        add-auto-load-safe-path /opt/at9.0/lib64/power8/libthread_db-1.0.so
line to your configuration file "/uufs/chpc.utah.edu/common/home/u0101881/.gdbinit".
To completely disable this security protection add
        set auto-load safe-path /
line to your configuration file "/uufs/chpc.utah.edu/common/home/u0101881/.gdbinit".
For more information about this security protection see the
"Auto-loading safe path" section in the GDB manual. E.g., run from the shell:
        info "(qdb)Auto-loading safe path"
warning: Unable to find libthread db matching inferior's thread library, thread debugging will
 not be available.
 Process
                                     1 is alive
Enter the number of intervals: (0 quits)
Breakpoint 1, MAIN () at pi3.f:50
              if (n .le. 0) goto 30
 (adb) p n
$1 = 100000
```



#### 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 had Totalview license (for historical reasons), 32 tokens enough for our needs (renewal ~\$1500/yr)
- In 2017 we switched to DDT which gave us competitive upgrade
- XSEDE systems have DDT



#### How to use Totalview/DDT

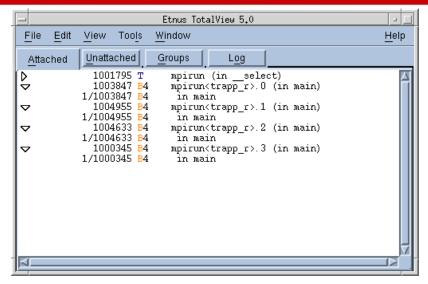


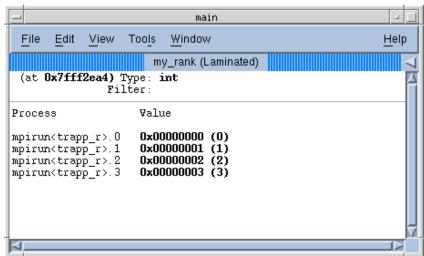
- 1. Compile binary with debugging information
- flag -g
  gcc -g test.f -o test
- 2. Load module and run Totalview or DDT module load totalview; module load ddt
- TV/DDT + executable totalview executable; ddt executable
- TV/DDT + core file totalview executable core\_file; ddt executable corefile
- Run TV/DDT and choose what to debug in a startup dialog totalview; ddt

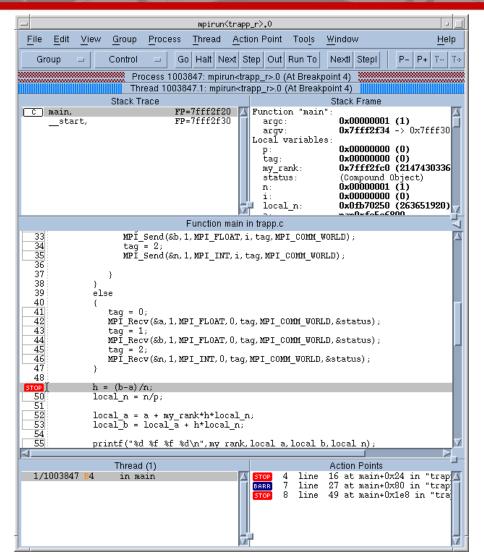


## Totalview windows





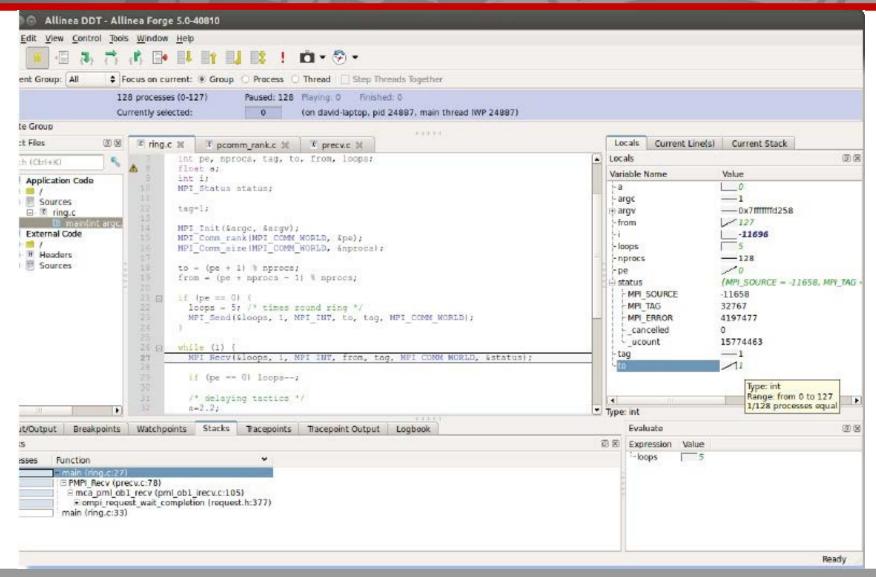






#### DDT screenshot





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# 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



# 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 + 2 just for compilers
  - One license locks all the tools
  - Cost ~\$4000/year + ~\$1000 for the compilers
  - Free for students, open source developers, educators
- 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 or DDT
- Standalone or GUI integration
- More info

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

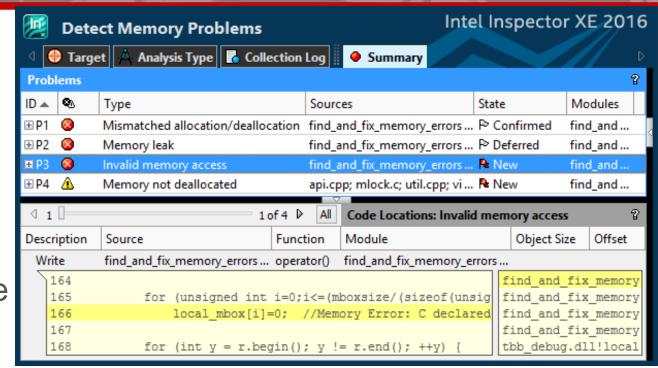


# Intel Inspector



- 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

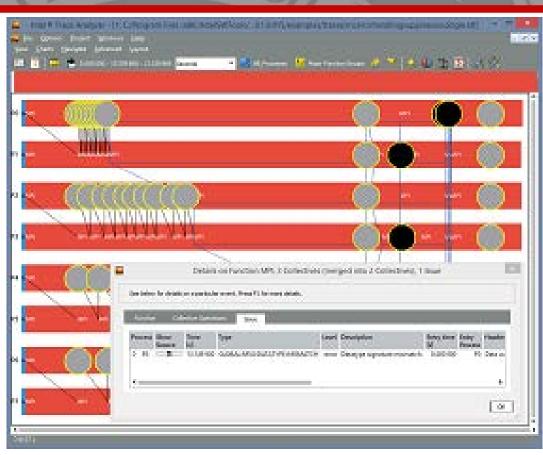


- MPI profiler and correctness checker
- Detects violations of MPI standard and errors in execution environment
- To use correctness checker

```
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**

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#### Why to profile



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Evaluate performance

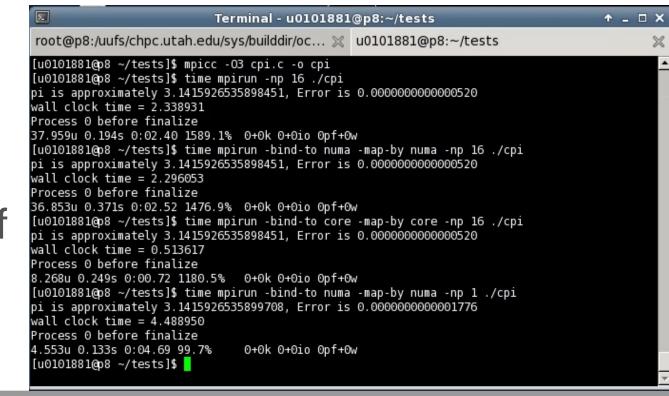
- Find the performance bottlenecks
  - Inefficient programming
    - Array data access, optimized functions, vectorization
  - Memory or I/O bottlenecks
  - Parallel scaling
    - Inefficient parallel decomposition, communication



# 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)

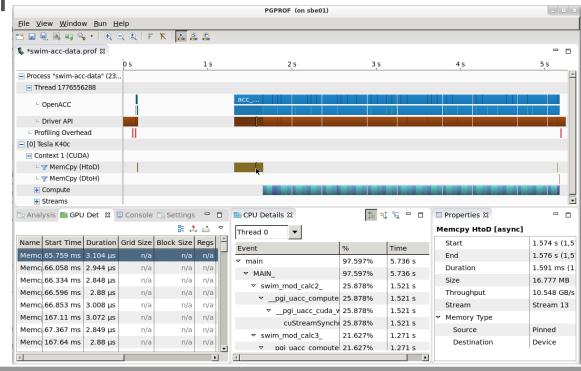
```
Terminal - u0101881@p8:~/tests
 root@p8:/uufs/chpc.utah.edu/sys/builddir/oc... 💥 u0101881@p8:~/tests
[u0101881@p8 ~/tests]$ mpicc -03 cpi.c -o cpi
 [u0101881@p8 ~/tests]$ perf stat mpirun -bind-to core -map-by core -np 1 ./cpi
pi is approximately 3.1415926535899708, Error is 0.0000000000001776
wall clock time = 4.976919
Process O before finalize
 Performance counter stats for 'mpirun -bind-to core -map-by core -np 1 ./cpi':
       5176.211056
                        task-clock (msec)
                                                       0.999 CPUs utilized
                        context-switches
                                                       0.015 K/sec
                        cpu-migrations
                                                       0.001 K/sec
                        page-faults
             4,255
                                                       0.822 K/sec
                        cycles
    17,641,344,721
                                                                                       (66.76\%)
                                                       3.408 GHz
                        stalled-cycles-frontend
        16,802,571
                                                       0.10% frontend cycles idle
                                                                                       (50.17%)
                        stalled-cycles-backend
    12,934,161,831
                                                      73.32% backend cycles idle
                                                                                       (50.16\%)
    13,393,245,960
                                                       0.76 insns per cycle
                        instructions
                                                       0.97 stalled cycles per insn
                                                                                       (66.78%)
     1,083,269,385
                        branches
                                                      209.278 M/sec
                                                                                       (49.84\%)
         1,479,078
                        branch-misses
                                                       0.14% of all branches
                                                                                       (50.10\%)
       5.180999586 seconds time elapsed
[u0101881@p8 ~/tests]$
```



# 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
- Score-P/Scalasca
  - Developed by European consortium, did not try yet



#### Intel tools



- Intel Parallel Studio XE 2017 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

Basic Hotspots Hotspots by CPU Usage viewpoint (change) ②



Intel VTune Amplifier XE 2016

- 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

🔛 Collection Log | 🕀 Analysis Target | 🛕 Analysis Type | 🛍 Summary | 🗞 Bottom-up 🚱 Caller/Callee 🥵 Top-down Tree 🔣 Platforr Data Of Interest (CPU Metrics) Function / Call Stack ★Viewing 4 1 of 56 ▶ selected stack(s) CPU Timey 26.6% (2.038s of 7.650s) Function / Call Stack Effective Time by Utilization Spin Overhead 🔳 Idle 📕 Poor 📋 Ok 📳 Ideal 📋 Over SystemProceduralFire....ion - fireobject.cpp SystemProceduralFire... fireobject.cpp:1459 ⊕ func@0x1000e190 3.318s 2.020s SystemProceduralFire... fireobject.cpp:1377 □ FireObject::ProcessFireCollisionsRange 5.013s Smoke.exe!ParallelF...managertbb.cpp:573 4.025s 0s Smoke.exe![TBB parall... - parallel\_for.h:212 0.988s 0s func@0x7545a064 0.675s Smoke.exe!tbb::intern...- parallel\_for.h:150 7.650s Selected 1 row(s): 0s Smoke.exe!TaskMan...anagertbb.cpp:606 31.5s 32s 32.5s ▼ Thread Running Frame Rate CPU Time wWinMainCRTStartup (TID: 3496) ✓ W Spin and Overhead Time func@0x7854345e (TID: 9332) □ ▼ CPU Sample func@0x7854345e (TID: 12704) ▼ Tasks func@0x7854345e (TID: 10792) CPU Usage CPU Usage ✓ Audi CPU Time Spin and Overhead Time No filters are applied. Any Thread Any Module Any Utilization Call Stack Mode: User functions + 1 ✓ Inline Mode: on ∨ Loop Mode: Functions only

https://software.intel.com/en-us/articles/processor-specificperformance-analysis-papers



# Intel Advisor



- Vectorization advisor
  - Identify loops that benefit from vectorization, find what is blocking efficient vectorization
  - Useful for speeding up loop performance
- Thread design and prototyping
  - Analyze, design, tune and check threading design
  - Useful for implementing OpenMP in serial code
- 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

Where should I add vectorization and/or threading parallelism? Intel Advisor XE 2016 🬳 Summary 🚭 Survey Report 🤌 Refinement Reports 🔥 Annotation Report 🏻 🖞 Suitability Report Elapsed time: 54.44s Vectorized Not Vectorized FILTER: All Modules ✓ All Sources Trip 🔊 Vectorized Loops Total ♠ P Vector Issues Loop Type Function Call Sites and Loops Why No Vectorization? Time▼ Time Counts Vecto... Efficiency > 🖔 [loop at stl\_algo.h:4740 in std::tr... 🔲 📮 non-vectorizable loop ins ... 0.170s I 0.170s I Scalar 0.170s I ~100% 🛮 💯 [loop at loopstl.cpp:2449 in s234\_] 0.170s1 12: 4 Collapse Collapse AVX 🚯 🐸 [loop at loopstl.cpp:2449 in s ... 📗 0.150s1 12 Vectorized (B AVX 0.150s I i> 5 [loop at loopstl.cpp:2449 in s ... ] 0.020s1 0.020s1 4 Remainder 🗈 🍮 [loop at loopstl.cpp:7900 in vas\_] 📗 0.170s I 0.170s1 500 Scalar 📮 vectorization possible but... ~6<mark>9</mark>9 [loop at loopstl.cpp:3509 in s2 ... 0.160s | 12 AVX 💡 1 High vector register ... 0.160s l Expand Expand | 🗄 👅 [loop at loopstl.cpp:3891 in s279\_] ② 2 Ineffective peeled/rem ... 0.150s I 0.150s1 | 125; 4 Expand Expand AVX 🗉 U [loop at loopstl.cpp:6249 in s414 ] 0.150s I 0.150s1 12 AVX ~100° Expand Expand 🗈 🍮 [loop at stl\_numeric.h:247 in std... 🔃 🔐 🛽 Assumed dependency... 0.150s l 📮 vector dependence preve ... 0.150s1 49 Scalar

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

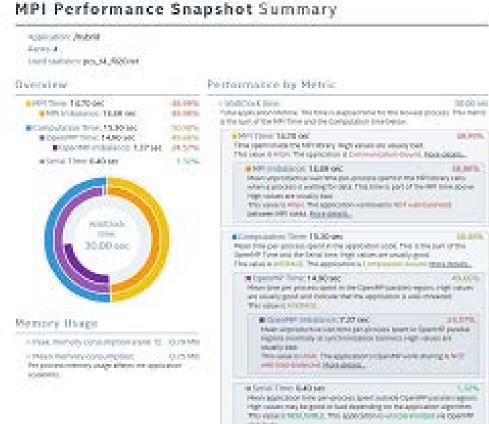
## Intel Trace Analyzer and Collector





- 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

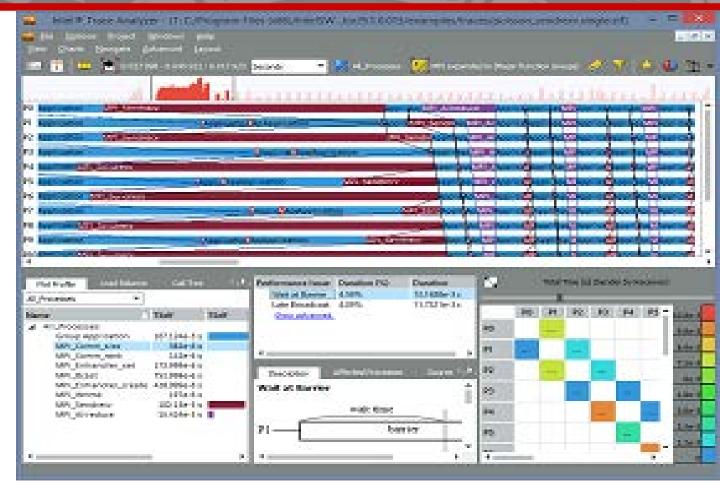


- Source the environment module load itac
- Using Intel compilers, can compile with -trace

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

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#### 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, "dmesg", "taskset", ...
- SLURM (or other scheduler) logs and statistics
- LBNL's Node Health Check (nhc)

#### Tools

- XDMoD XSEDE Metrics on Demand (through SUPReMM module)
- REMORA REsource MOnitoring for Remote Applications





#### BENCHMARKING

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### 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)





# WHAT ELSE DO YOU DO AT YOUR SITE?

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## **BACKUP**

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#### Demos



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- Totalview
- Advisor
- Inspector
- VTune