703308 VO High-Performance Computing
Debugging Parallel Programs

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Overview

- functional debugging
  - generic guidelines
  - serial debugging
  - parallelism-specific debugging

- performance debugging
  - generic guidelines
  - serial debugging
  - parallelism-specific debugging

Motivation: first Ariane-5 flight, 1996

- Debugging Ariane-5's maiden flight
  - booster nozzles adjusted for a 20% angle of attack, causing vehicle separation, triggering self-destruction
  - because a diagnostic bit pattern was sent to on-board computer as flight data
  - because a data conversion from 64 bit float to 16 bit signed int overflowed
  - because they used Ariane 4 inertial code for Ariane 5, which has larger possible value ranges (velocities)
    - and only protected 4 out of 7 critical variables against overflow and not this one because in Ariane 4 velocities were lower
    - also, this software component serves no purpose after lift-off (only used for inertial platform alignment before launch)

https://www.youtube.com/watch?v=gp_D8r-2hwk

Motivation: first Ariane-5 flight, 1996

- Debugging Ariane-5's maiden flight
  - booster nozzles adjusted for a 20% angle of attack, causing vehicle separation, triggering self-destruction
  - because a diagnostic bit pattern was sent to on-board computer as flight data → bad choice of sentinel values
  - because a data conversion from 64 bit float to 16 bit signed int overflowed → compiler warnings!
  - because they used Ariane 4 inertial code for Ariane 5, which has larger possible value ranges (velocities) → lack of proper requirement analysis
    - and only protected 4 out of 7 critical variables against overflow and not this one because in Ariane 4 velocities were lower → lack of proper requirement analysis
    - also, this software component serves no purpose after lift-off (only used for inertial platform alignment before launch) → debugging code active in release

Motivation

- Why do we need debugging?
  - Because we make mistakes!
- Why do we need a lecture about this?
  - OpenMPI FAQ "Debugging applications in parallel", first question:
    Q: "How do I debug OpenMPI processes in parallel?"
    A: "This is a difficult question. […] This FAQ section does not provide any definite solutions to debugging in parallel. […]"

Functional Debugging

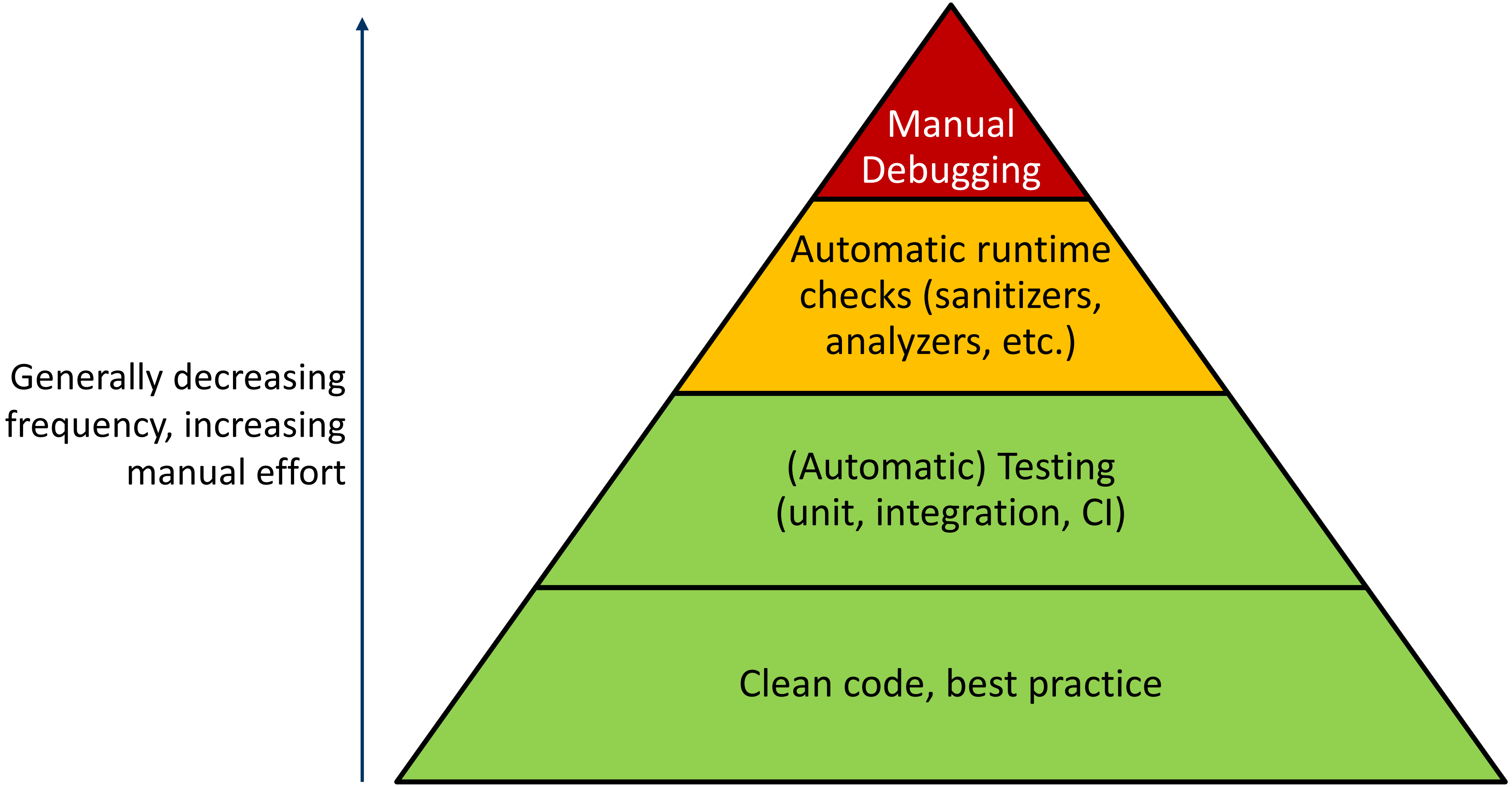
Functional debugging

- Dealing with everything that results in not getting the correct program output
  - program crashes (e.g. segmentation faults, undefined behavior, race conditions)
  - program not finishing (deadlocks, infinite loops)
  - incorrect output (e.g. undefined behavior, race conditions, arithmetic errors)

- errors can be deterministic or non-deterministic

- all that applies to debugging serial programs is <u>crucial</u> for parallel ones
  - If you can’t trust the serial implementation, why would you in a parallel context?
  - parallel programming models are just different means to cause the same issues

Debugging effort pyramid



Coding guidelines

- write clean code that prevents bugs or facilitates their detection, e.g.
  - use meaningful identifiers
  - minimize vertical distance of variables
  - don’t use OpenMP’s `private`
  - follow the <u>D</u>on’t <u>R</u>epeat <u>Y</u>ourself (DRY) principle (single component per feature)
  - …
- The toolchain you must use!
  - read & heed compiler warnings
  - write and regularly run unit and/or integration tests, especially aimed at (varying degrees of) parallelism
  - use code coverage tests
  - use continuous integration
  - use source version control

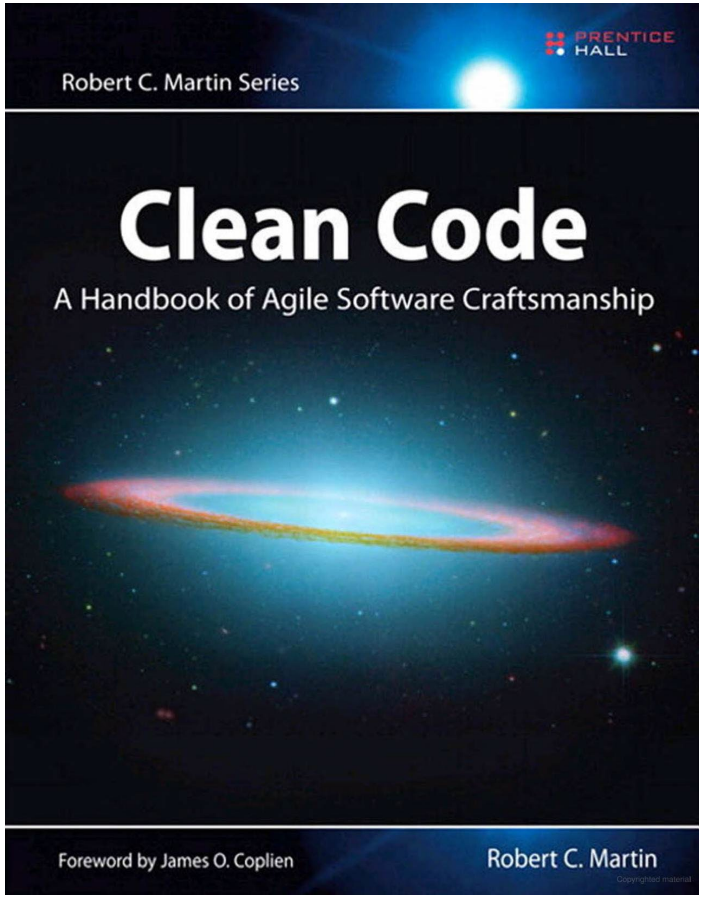
“Best of” real commit messages encountered in the past

- stufF
- manager stuff
- more manager stuff
- Make things work
- ::w
  :q
  Merge branch 'master’
- dl;adlwa
- Added performance fix for DataItemManager::get() by caching fragment result in reference
- Removed debug print statement
- Fixed a linking issue of the unwrap_tuple function
- Redirected runtime system output to error stream
- fixing typos

Recommended reading/reference material example

- “Clean Code” by Robert Martin, Prentice Hall 2008
  - ISBN 9780132350884
  - also available in German

- naming, functions, commenting, formatting, data structures, error handling, unit tests, classes, concurrency, refinement & refactoring, …



Generic debugging guidelines

- create a **<u>M</u>**inimal **<u>W</u>**orking **<u>E</u>**xample (MWE)
  - minimize problem size
  - minimize software components/features involved
  - ensure/increase reproducibility (e.g. fix random seeds, thread/process mapping/binding, …)
  - if parallel
    - minimize machine size (number of threads and/or ranks)
    - minimize complexity of parallel interaction (e.g. communication patterns, …)

- minimizes debugging feedback cycles times, amount of memory to inspect, amount of code to consider, overall degree of complexity of component & parallel interaction
  - sounds simple, but don't underestimate its significance
  - every change along the way to an MWE gives you more information about the problem

Serial debuggers

- gdb
  - useful for inspecting memory contents and getting call stacks
  - can work with multi-threaded programs and also MPI
    - `mpiexec -n X gdb –ex ‘run’ –ex ‘bt’ –ex ‘quit’ ./a.out`
  - can be used to debug e.g. a single MPI process among many
    - `mpiexec -n 1 gdb ./a.out : -n 7 ./a.out`
  - can be attached to already-running processes
    - `gdb –pid 12345`

- valgrind
  - mostly used for finding memory leaks (can also simulate cache or generate call graph)
  - can work with multi-threaded programs (but only concurrent execution!)
  - can yield some false positives e.g. for OpenMP related to thread-local storage
  - there is a dedicated `valgrind4hpc` (mainly handles output redirection from multiple ranks)

Sanitizers (still mostly serial)

- tools that instrument code at compile time to perform checks at runtime
  - often lower overhead compared to external tools such as valgrind
  - if in doubt, check same issue with multiple tools (e.g. address sanitizers of multiple compilers and valgrind)

- depending on compiler, several sanitizers available, e.g.
  - address: buffer overflows, use-after-free, stack corruption, etc.
  - undefined behavior: signed integer overflow, float division by zero, negative shift operands, etc.
  - thread: detects data races
  - leak: detects memory leaks

Example 1: wrong order of arguments in MPI call

```
MPI_Send(&A_local[0], MPI_DOUBLE, N, rank - 1, 0, MPI_COMM_WORLD);
```

- Compile with –Wall –Wextra –pedantic:

Example 2: Incorrect array indexing
"program hangs" or "receiving garbage in ghost cells"

```
(JobID 12100)[c703429@n011.intern.lcc3 debugging_tests]$ mpicc heat_2D_mpi.c -o heat_2D_mpi -O3 -fsanitize=undefined,address -g
(JobID 12100)[c703429@n011.intern.lcc3 debugging_tests]$ mpiexec -n 2 ./heat_2D_mpi
==1510386==ERROR: AddressSanitizer: heap-buffer-overflow on address 0x61f000002880 at pc 0x14f80355538b bp 0x7ffc8a704810 sp 0x7ffc8a703fc0
READ of size 6144 at 0x61f000002880 thread T0
    #0 0x14f80355538a in __interceptor_memcpy /tmp/hpc-inst/spack-v0.19-lcc3-20230919-stage/spack-stage-gcc-12.2.0-p4pe45vebc7w5leppo2eeesyakewpbxf/spack-src/libsanitizer/sanitizer_common/sanitizer_common_interceptors.inc:827
    #1 0x14f80104b8a2 in ucp_dt_pack (/lib64/libucp.so.0+0x248a2)
    #2 0x14f801055403 in ucp_tag_pack_eager_only_dt (/lib64/libucp.so.0+0x2e403)
    #3 0x14f800e0f8e8 in uct_mm_ep_am_bcopy (/lib64/libuct.so.0+0x148e8)
    #4 0x14f8010557ca in ucp_tag_eager_bcopy_single (/lib64/libucp.so.0+0x2e7ca)
    #5 0x14f801061a0d in ucp_tag_send_nbr (/lib64/libucp.so.0+0x3aa0d)
    #6 0x14f8032318b0 in mca_pml_ucx_send (/usr/site/hpc/spack/v0.19-lcc3-20230919/opt/spack/linux-rocky8-westmere/gcc-12.2.0/openmpi-3.1.6-d2gmn55g7hoinwfuk2lc3ibz6odzujak/lib/libmpi.so.40+0x1a68b0)
    #7 0x14f80313d64a in PMPI_Send (/usr/site/hpc/spack/v0.19-lcc3-20230919/opt/spack/linux-rocky8-westmere/gcc-12.2.0/openmpi-3.1.6-d2gmn55g7hoinwfuk2lc3ibz6odzujak/lib/libmpi.so.40+0xb264a)
    #8 0x402ab6 in main /scratch/c703429/debugging_tests/heat_2D_mpi.c:116
    #9 0x14f8022add84 in __libc_start_main (/lib64/libc.so.6+0x3ad84)
    #10 0x4046bd in _start (/gpfs/gpfs1/scratch/c703429/debugging_tests/heat_2D_mpi+0x4046bd)
```

Example 2: Incorrect array indexing
“program hangs” or “receiving garbage in ghost cells”

```
if (rank > 0) {

 MPI_Send(&A_local[0], N, MPI_DOUBLE, rank - 1, 0, MPI_COMM_WORLD);
 MPI_Recv(ghost_vec_upper, N, MPI_DOUBLE, rank - 1, 1, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
if (rank < size - 1) {
  // printf("A_N\n");
  // printVec((A_local[rows_local-1]),N);
  MPI_Send(&A_local[rows_local-1], N, MPI_DOUBLE, rank + 1, 1, MPI_COMM_WORLD);
  MPI_Recv(ghost_vec_lower, N, MPI_DOUBLE, rank + 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

Example 3: MPI Send/Recv deadlock

Live Demo with MUST (https://itc.rwth-aachen.de/must/)!

```
[c703429@login.lcc3 debugging_tests]$ mustrun -np 2 ./heat_stencil_2D_mpi --must:output stdout
Using prebuild /home/c703/c703429/.cache/must/prebuilds/b62ed64425437f6c696454be27e2071b
Using prebuild /home/c703/c703429/.cache/must/prebuilds/b62ed64425437f6c696454be27e2071b
[MUST] MUST configuration ... centralized checks with fall-back application crash handling (very slow)
[MUST] Information: overwritting old intermediate data in directory "/scratch/c703429/debugging_tests/must_temp"!
[MUST] Using prebuilt infrastructure at /home/c703/c703429/.cache/must/prebuilds/b62ed64425437f6c696454be27e2071b
[MUST] Search for linked P^nMPI ... not found ... using LD_PRELOAD to load P^nMPI ... success
[MUST] Executing application:
[MUST-RUNTIME] ============MUST===============
[MUST-RUNTIME] ERROR: MUST detected a deadlock, detailed information is available in the MUST output file. You should either investigate details with a
debugger or abort, the operation of MUST will stop from now.
[MUST-RUNTIME] ===============================
[MUST-REPORT] Error global: The application issued a set of MPI calls that can cause a deadlock! A graphical representation of this situation is available
in a <a href="./MUST_Output-files/MUST_Deadlock.html" title="detailed deadlock view"> detailed deadlock view (./MUST_Output-files/MUST_Deadlock.html)</a>.
References 1-1 list the involved calls (limited to the first 5 calls, further calls may be involved). The application still runs, if the deadlock
manifested (e.g. caused a hang on this MPI implementation) you can attach to the involved ranks with a debugger or abort the application (if necessary).
References of a representative process:
[MUST-REPORT] Reference 1: call MPI_Send@rank 0, threadid 0;
[MUST-REPORT] Stacktrace:
[MUST-REPORT] #0  main@/scratch/c703429/debugging_tests/heat_stencil_2D_mpi.c:83
```

Example 3: MPI Send/Recv deadlock cont'd

MUST Deadlock Details, date: Mon Nov 20 17:18:38 2023.

Back to MUST error report

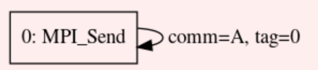
Message

The application issued a set of MPI calls that can cause a deadlock! The graphs below show details on this situation. This includes a wait-for graph that shows active wait-for dependencies between the processes that cause the deadlock. Note that this process set only includes processes that cause the deadlock and no further processes. A legend details the wait-for graph components in addition , while a parallel call stack view summarizes the locations of the MPI calls that cause the deadlock . Below these graphs, a message queue graph shows active and unmatched point-to-point communications. This graph only includes operations that could have been intended to match a point-to-point operation that is relevant to the deadlock situation. Finally, a parallel call stack shows the locations of any operation in the parallel call stack. The leafs of this call stack graph show the components of the message queue graph that they span. The application still runs, if the deadlock manifested (e.g. caused a hang on this MPI implementation) you can attach to the involved ranks with a debugger or abort the application (if necessary).

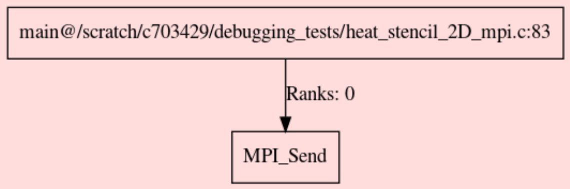
Active Communicators

Comm:	A
MPI_COMM_WORLD	

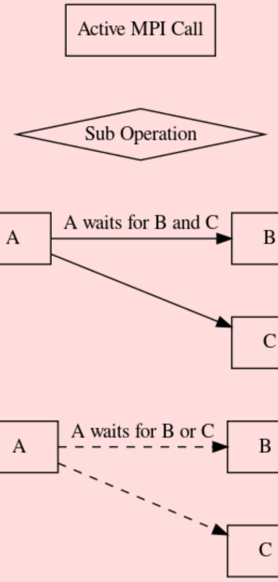
Wait-for Graph



Call Stack



Legend



Active and Relevant Point-to-Point Messages: Overview

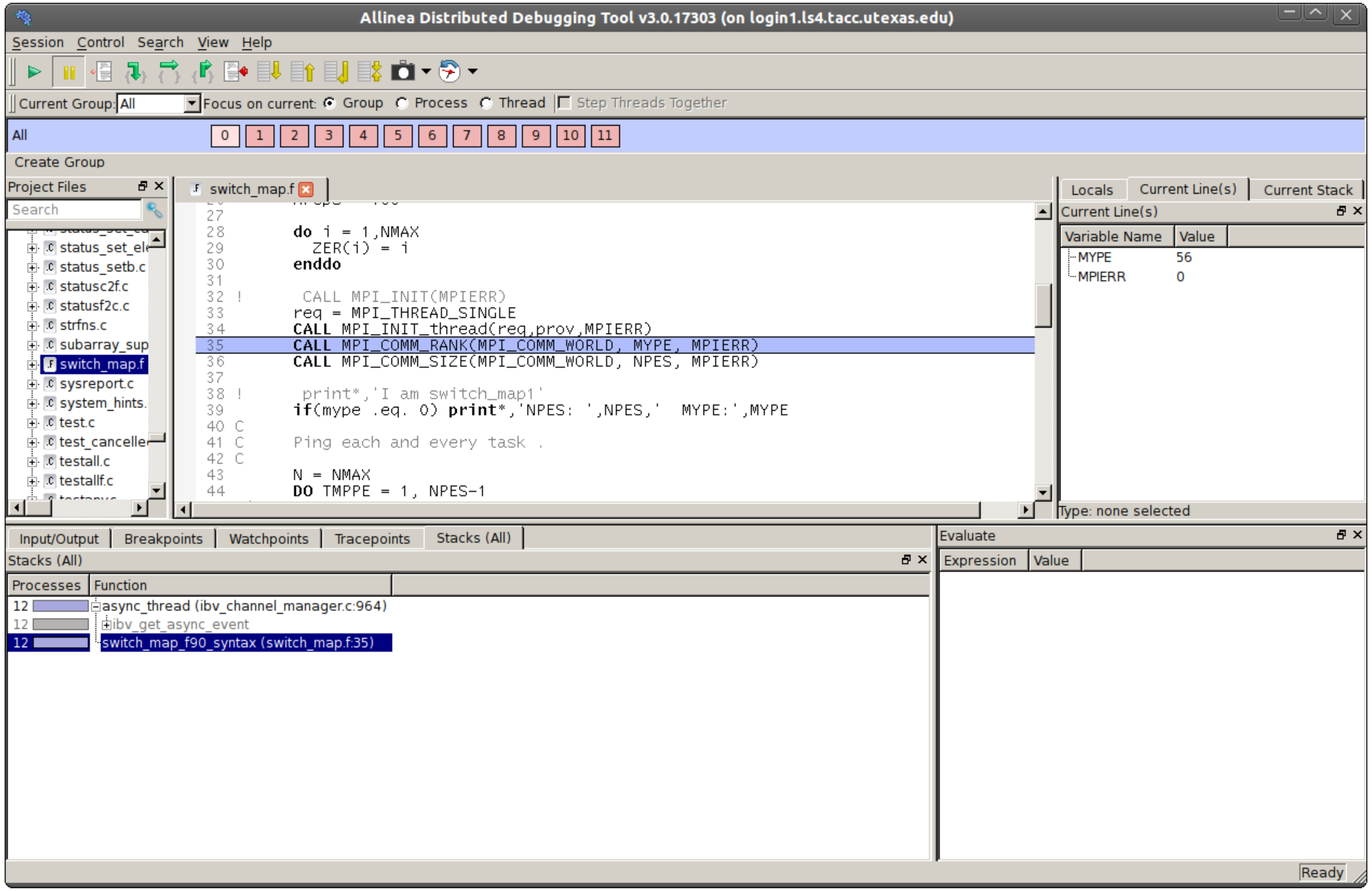
Active and Relevant Point-to-Point Messages: Callstack-view

Parallel debuggers

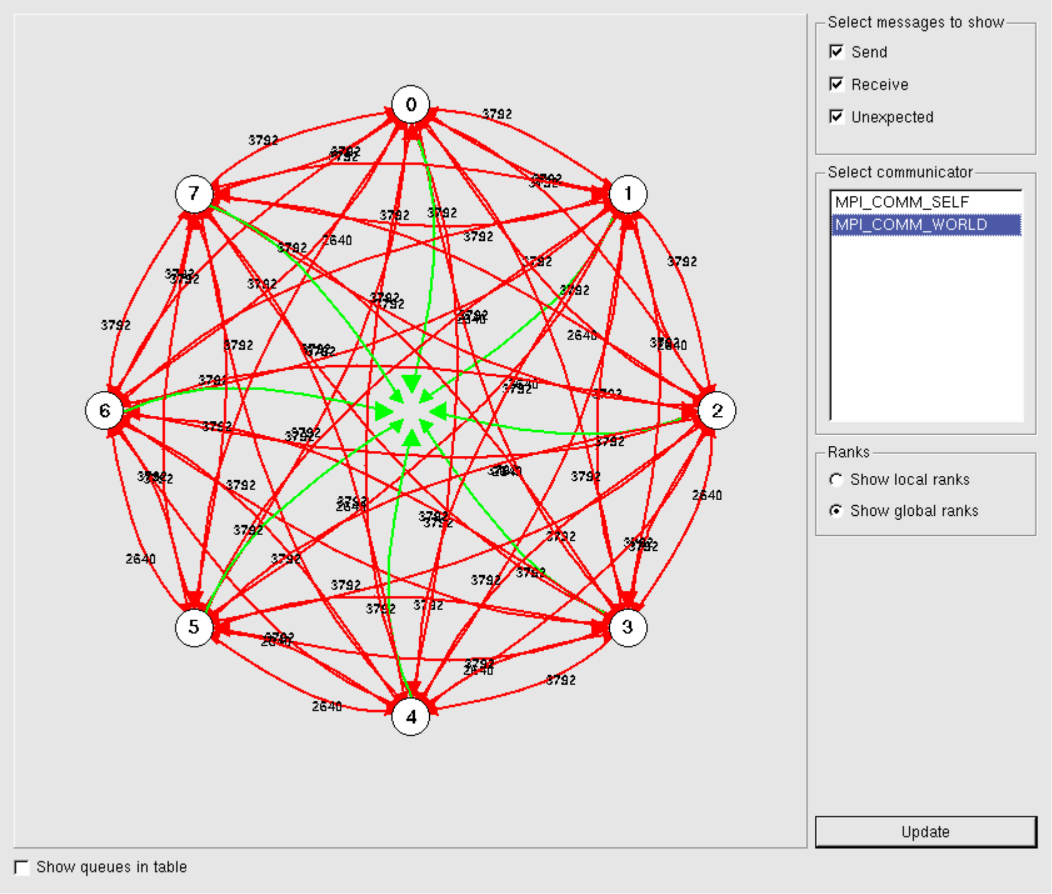
- very little free software
- two commercial top dogs: DDT (Linaro) and TotalView (Perforce Software)
- support OpenMP, MPI, CUDA, etc.
- several features centered around parallelism
  - examine variables per rank/thread, examine send/receive queues of MPI libraries, etc.
  - still, limited usefulness

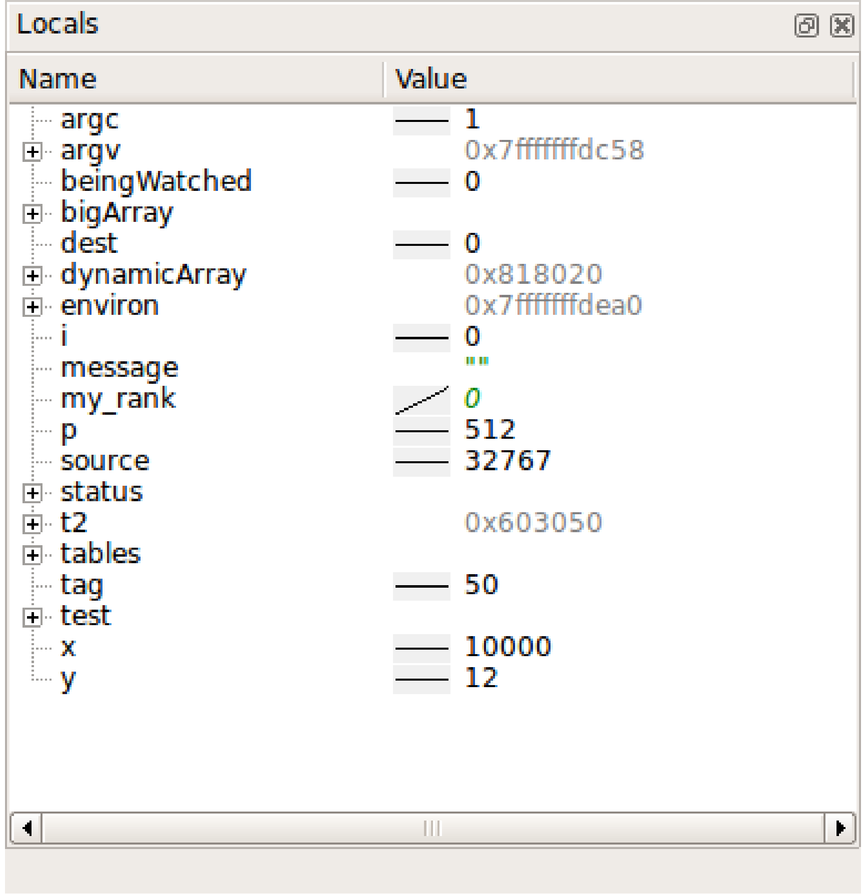
- Several other software packages
  - MUST: MPI runtime error checking tool
  - Visual Studio: supports debugging MPI-Programs in Windows
  - Intel Inspector: data race detector for multi-threaded programs
  - ARCHER: data race detector for OpenMP
  - STAT: trace analysis tool to group ranks with similar behavior for easier analysis
  - AutomaDeD: uses heuristics to find dissimilarities in rank behaviors

DDT screenshot (overview)



DDT screenshots (communication patterns, data across ranks)





Automatic race condition debugging

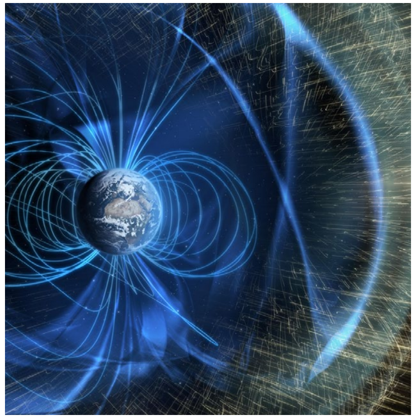
- difficult to do automatically and exactly
  - statically detecting race conditions is NP-hard
  - dynamically detecting race conditions incurs large runtime overhead (every memory access and synchronization action must be logged and checked)

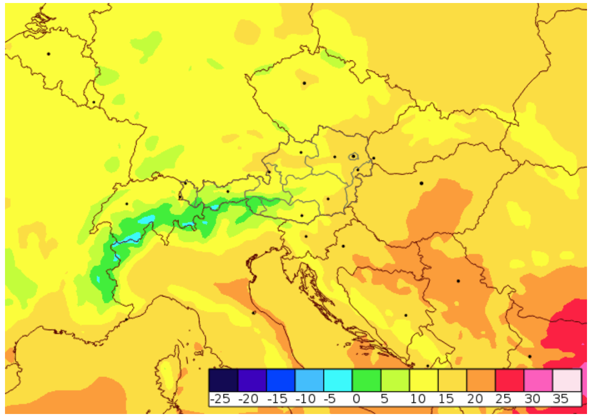
- most solutions resort to simulation and/or heuristics
  - several experimental tools available in research
  - many issues: limited scope, only apply to a subset of programming language, etc.
  - few “mature” tools, e.g. Intel Inspector

Domain-specific debugging

- Visualize the output using appropriate tools
  - gnuplot
  - matplotlib
  - ParaView
  - …

- note that this usually prohibits automatic checking
  - whenever feasible, unit and integration tests are preferred





Best approach to debugging parallel programs

- know your algorithm and implementation
  - e.g. “a structured grid problem with 2 ghost cells in every direction”
- know your programming models and languages, and their semantics
  - “reading the send buffer during an `MPI_Isend(…)` is illegal”
  - “this C++ object’s destructor will be called at the end of the full-expression”
- Don’t trust (seemingly) automatic analysis tools too much (ChatGPT!!!), read and understand the source code when available!

Supercomputer-specific information

- Check available SLURM QOS and partitions
  - e.g. VSC5 shown on the right
- Use interactive jobs
  - e.g. LCC3: `srun --nodes=1 --ntasks-per-node=12 --pty bash –i`
- General good practices
  - SLURM’s resource limits, even in production (wall time, RAM)
  - e-mail notifications for (some) job state changes
  - Don’t run anything parallel on the login node that has even a remote chance of running >1 second!

QOS name	Gives access to Partition	Hard run time limits	Description
zen3_0512	zen3_0512	72h (3 days)	Default
zen3_1024	zen3_1024	72h (3 days)	High Memory
zen3_2048	zen3_2048	72h (3 days)	Higher Memory
cascadelake_0384	cascadelake_0384	72h (3 days)	
zen2_0256_a40x2	zen2_0256_a40x2	72h (3 days)	GPU Nodes
zen3_0512_a100x2	zen3_0512_a100x2	72h (3 days)	GPU Nodes
zen3_0512_devel	5 nodes on zen3_0512	10min	Fast Feedback

https://wiki.vsc.ac.at/doku.php?id=doku:vsc5_queue

Performance Debugging

Performance debugging

- also sometimes known as *“non-functional”* debugging (not related to functional output)
  - short execution time not necessarily but most often the only goal
  - much more tricky than functional debugging
    - How do you know the performance “bug” was fixed? Because it’s “fast” now?

- most aspects of functional debugging or sequential programs still apply
  - coding guidelines & best practice
  - + reproducibility (e.g. fix random seeds, scheduling affinities, …)
  - + if required, performance unit tests, performance regression checks
  - + performance tools (the ones for sequential programs can also be useful)
  - + a lot more knowledge about hardware required

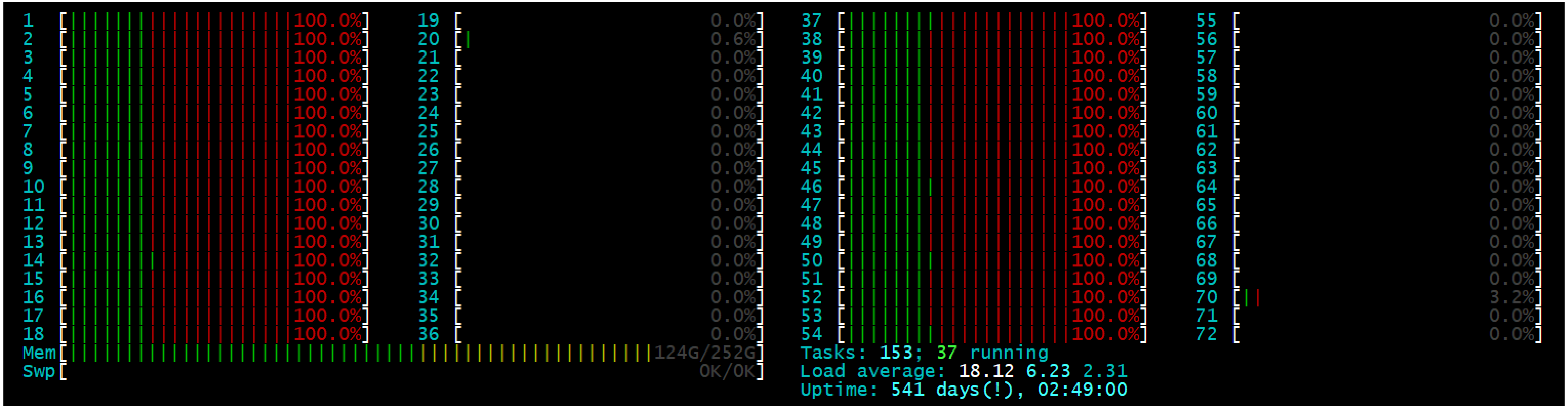
(h)top

- Don’t underestimate the power of `top` or `htop`!

- Get a high-level overview of the workload on the system (and it’s components) and compare to what you expected!
  - What’s the ratio between user time and system time?
    - high system time could be caused by inefficient I/O, high amount of context switching, etc.
  - Which CPU cores am I <u>really</u> using?
    - the only way to verify affinity policies
  - What is the actual memory footprint vs. what it should be?
    - detect e.g. memory leaks or inefficient memory management without any additional analysis tools

htop & affinity

- 2x Intel E5-2699 v3 (18 cores per CPU) in a single node
- htop shows cores 1-18 and 37-54 busy, hence 36 cores total – right?



Performance Counters via `perf`

```
[c703429@login.lcc2 ~]$ perf stat ./heat_stencil_1D_seq
                               ...
28,826,239,136 cycles:u             #   2.471 GHz
35,220,856,783 instructions:u       #   1.22  insn per cycle
 6,711,849,029 branches:u           # 575.356 M/sec
     1,295,209 branch-misses:u      #   0.02% of all branches
         1,044 LLC-load-misses:u
            26 LLC-store-misses:u
    15,312,122 L1-dcache-load-misses:u
   476,440,489 L1-dcache-store-misses:u
```

Terminology

- instrumentation
  - add source/machine code that will measure something when executed
  - can happen manually, automatically, during compilation, linking, runtime, …
  - do not confuse with “measurement”
- inclusive/exclusive measurements
  - do measurements include data for nested code regions (e.g. functions)?

```
int outside() {
  for(int i = 0; i < N; ++i) {
    // work
  }
  inside();
  for(int j = 0; j < M; ++j) {
    // more work
  }
}
```

exclusive

exclusive

inclusive

More terminology: sample- vs. trace-based profiling

- Sampling
  - gives aggregated information of how much time spent where in the code
  - based on statistics: does not provide information on the order of events, their time interval or exact numbers
  - easy to accomplish, comparatively low overhead, often no code changes required
    - e.g. stop program periodically and read program counter register of the CPU core
    - build histogram at the end
- Tracing
  - produces a detailed log of which event happened at what point in time
  - allows to establish order of events, even across processes/nodes if clocks are in sync
  - often requires code changes/instrumentation
    - e.g. wrap every function call with

```
get_timestamp();
func_call();
get_timestamp();
```

`gprof`

- sample-based profiler
  - also limited code instrumenter for call graph generation and call counts
  - very simplistic, not always accurate
- available with every GCC installation
- very simple in its use
  - compile with debug symbols (`-g`) and gprof support (`-pg`)
  - run binary as usual
  - run `gprof binary gmon.out` to view results
  - use `--line` to get more detailed, line-based results

gprof example: global sum vs. thread-local sum

```
int foo() {
  long long counter = 0;
  #pragma omp parallel for
  for(int i = 0; i < N; ++i) {
    #pragma omp critical
    counter++;
  }
  return counter;
}
```

```
int bar() {
  long long partSum[MAX_NUM_THREADS][8];
  long long counter = 0;
  #pragma omp parallel
  {
    int tid = omp_get_thread_num();
    partSum[tid][0] = 0;
    #pragma omp for
    for(int i=0; i<N; ++i) partSum[tid][0]++;
    #pragma omp critical
    counter += partSum[tid][0];
  }
  return counter;
}
```

gprof example cont'd

```
Flat profile:

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  Ts/call  Ts/call  name
100.71      0.02     0.02                             foo._omp_fn.0 (test.c:13 @ 400a3d)
  0.00      0.02     0.00        1     0.00     0.00  bar (test.c:19 @ 40092c)
  0.00      0.02     0.00        1     0.00     0.00  foo (test.c:8 @ 4008e6)
```

perf record/report

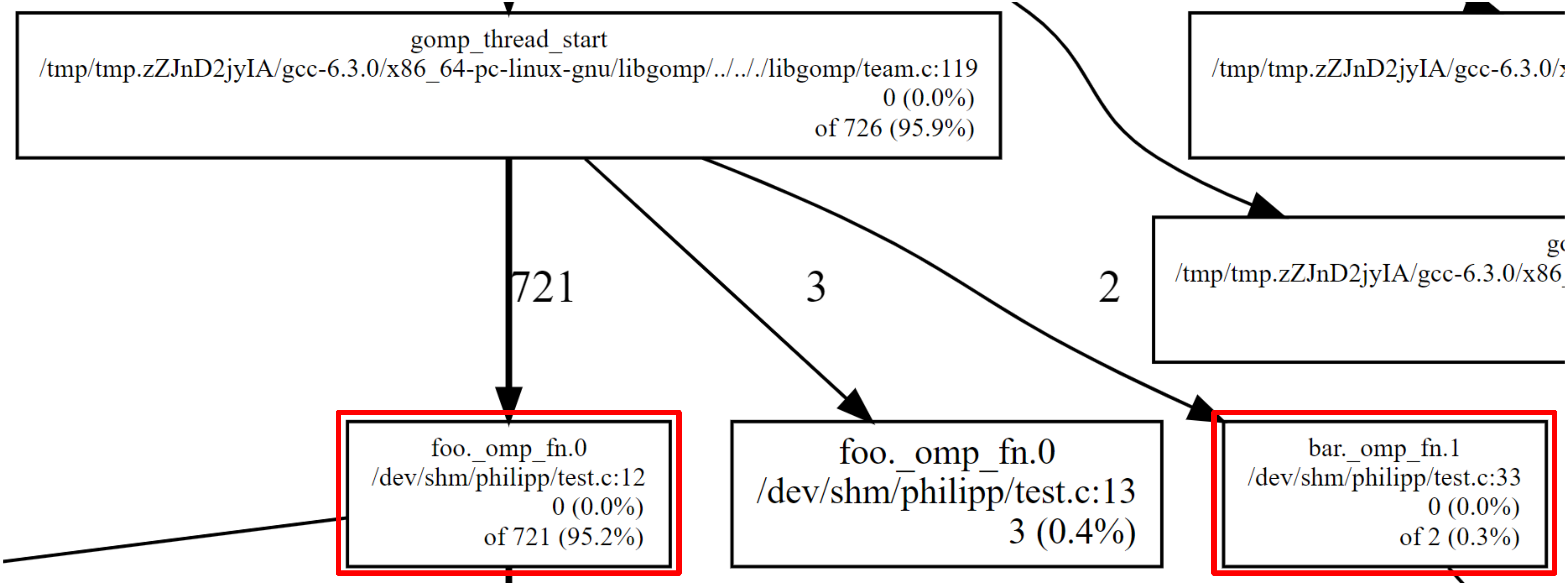
- Perf also supports profiling
  - `perf record ./application`
  - `perf report –s sym,srcline`
- Supports time as well as performance counters
- Also records a lot of platform information
  - `perf report --header-only`
    - CPU type, OS version, date & time of record, etc.
  - `perf report --header-only –I`
    - includes NUMA topology, cache info, etc.

```
Samples: 262K of event 'cache-misses:u', Event
count (approx.): 1072111977
Overhead  Symbol        Source:Line
  98.87%  [.] main      02_matrix_mul.c:68
   1.10%  [.] main      02_matrix_mul.c:69
   0.01%  [.] vfprintf  vfprintf+15272
   0.01%  [.] vfprintf  vfprintf+15262
   0.00%  [.] vfprintf  vfprintf+15292
   0.00%  [.] vfprintf  vfprintf+15255
```

gperftools

- sample-based profiler
  - formerly Google Performance Tools
- actually a collection of performance analysis tools and high-performance multi-threaded memory allocators
- very simple in its use
  - install gperftools library
  - link with `-lprofiler`
  - run with environment variable `CPUPROFILE=prof.out`
  - run `pprof binary prof.out` to view results (`--gv` for graphical visualization)

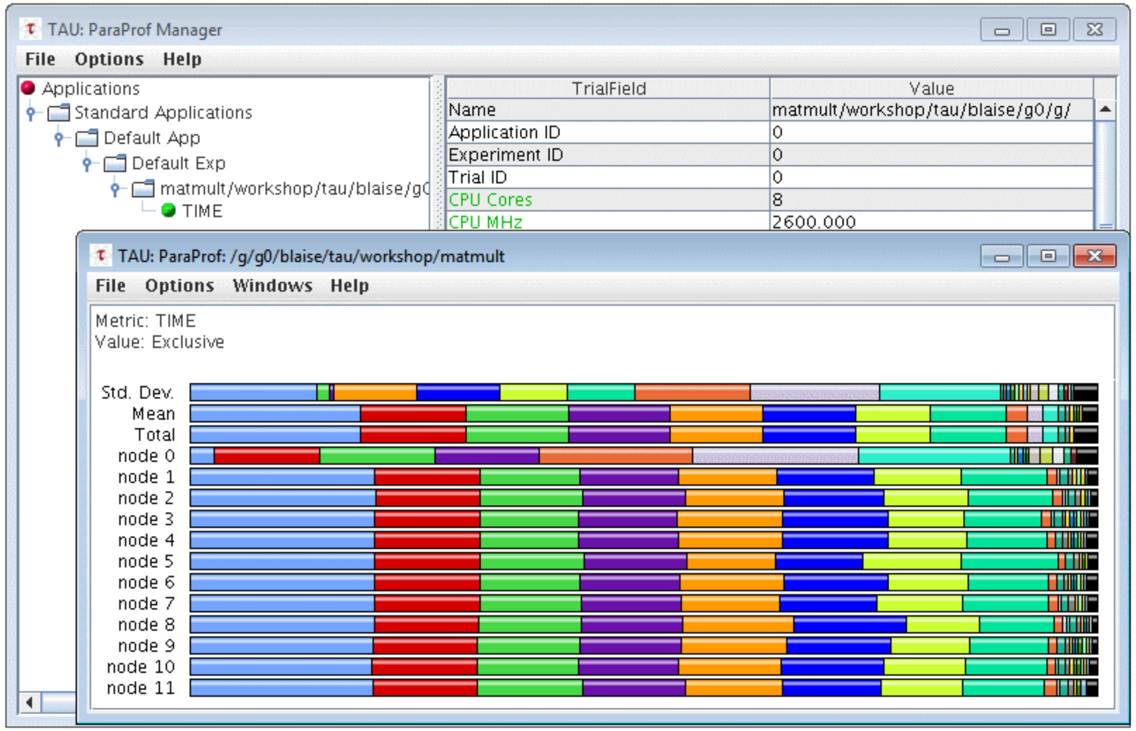
gperftools example

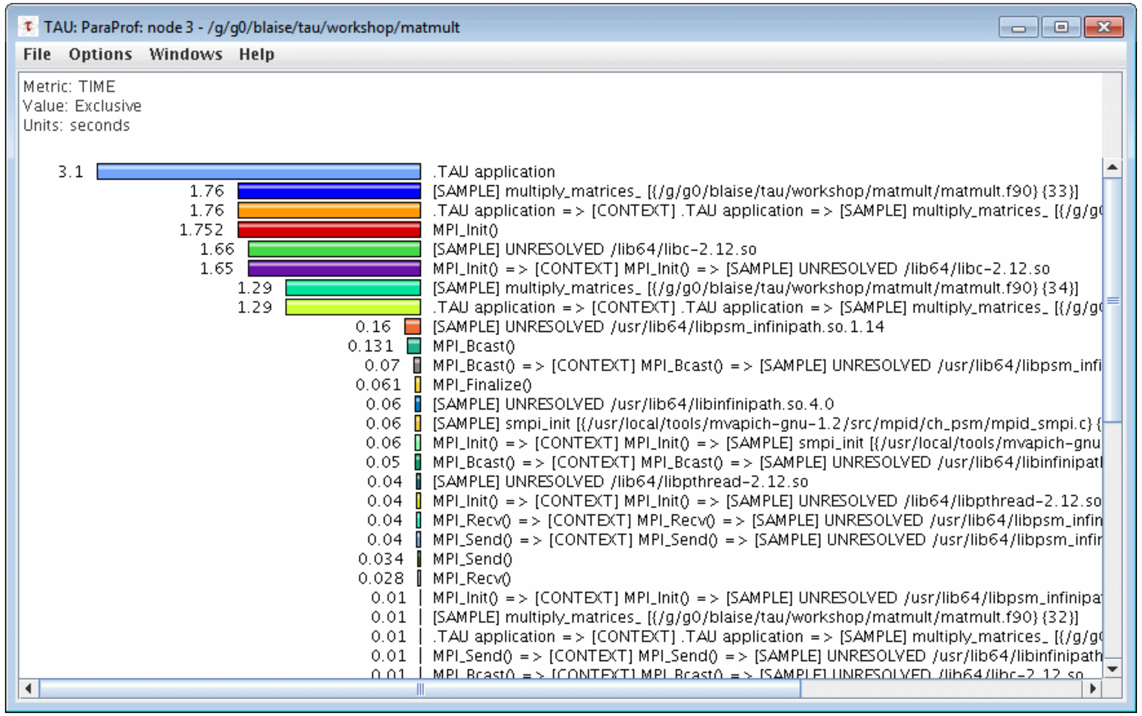


Performance analysis tools for parallel programs

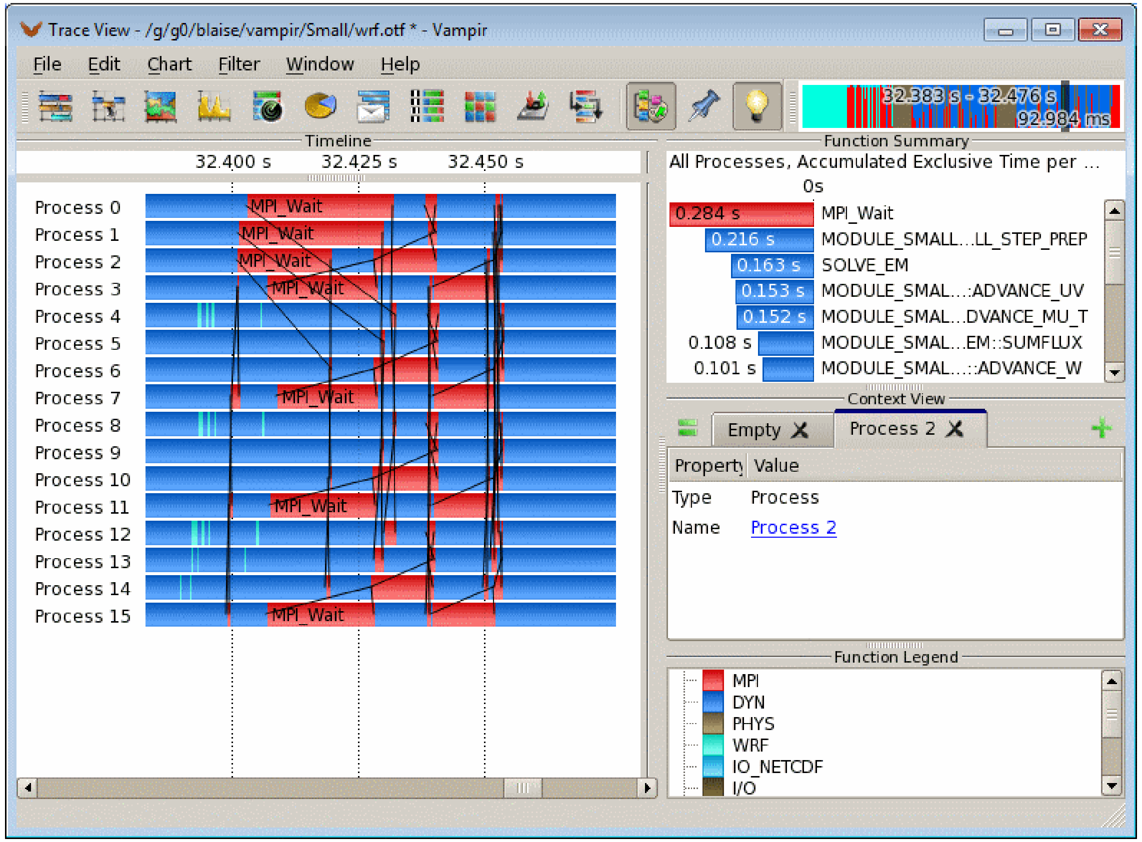
- profiling and analysis software
  - Intel Pin: dynamic binary instrumentation
  - Intel VTune: performance analysis for multi-threaded programs
  - Intel Advisor: dependency, vectorization and cache analysis tool
  - AMD CodeXL / NVIDIA Nsight: profiler and debugger for GPUs
  - TAU: profiling and tracing suite
  - HPCToolkit: profiling and tracing suite, includes GUI tools and tools for mapping binary code to source code
  - PAPI: library for access to hardware performance counters
  - OProfile: sampling-based profiler with hardware performance counter support
  - also, some software built into your IDE, e.g. MS Visual Studio
- analysis and visualization/reporting tools
  - Scalasca, Vampir, Paraver, JumpShot, paraprof, CUBE, etc.
- These lists are by far not complete!

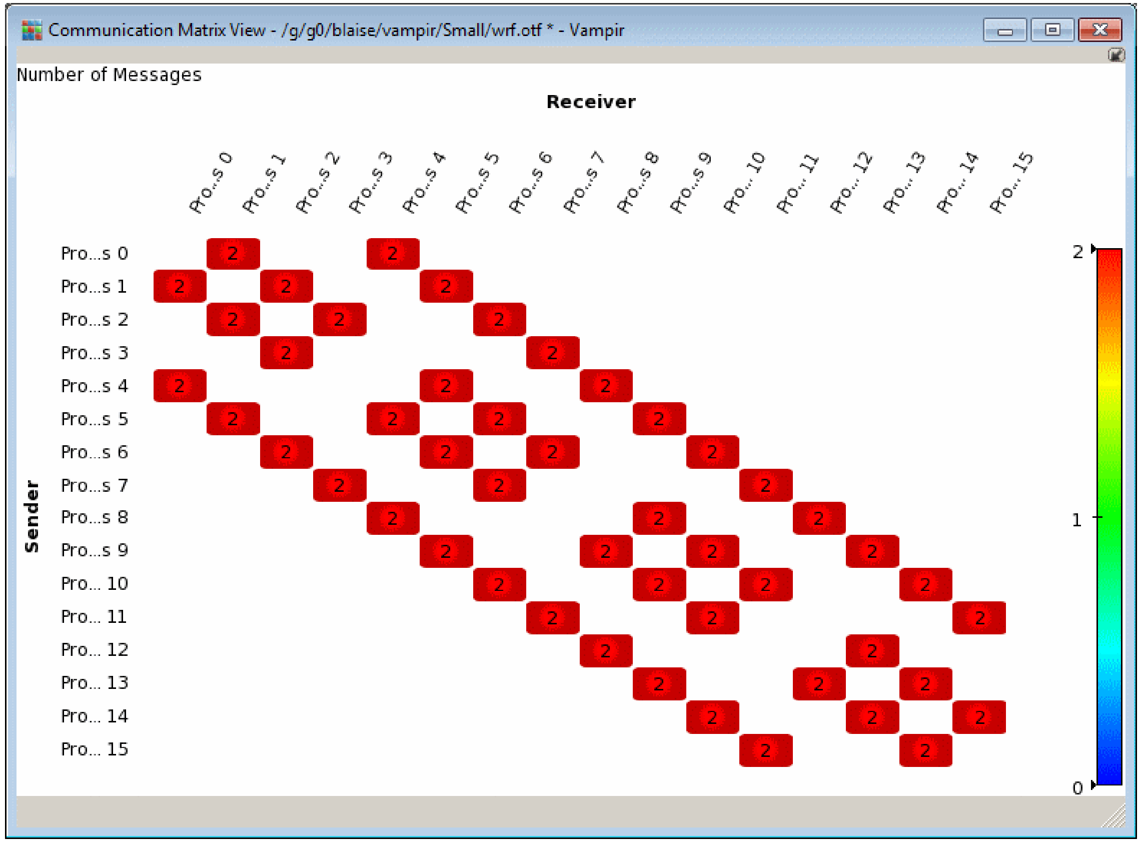
TAU & ParaProf



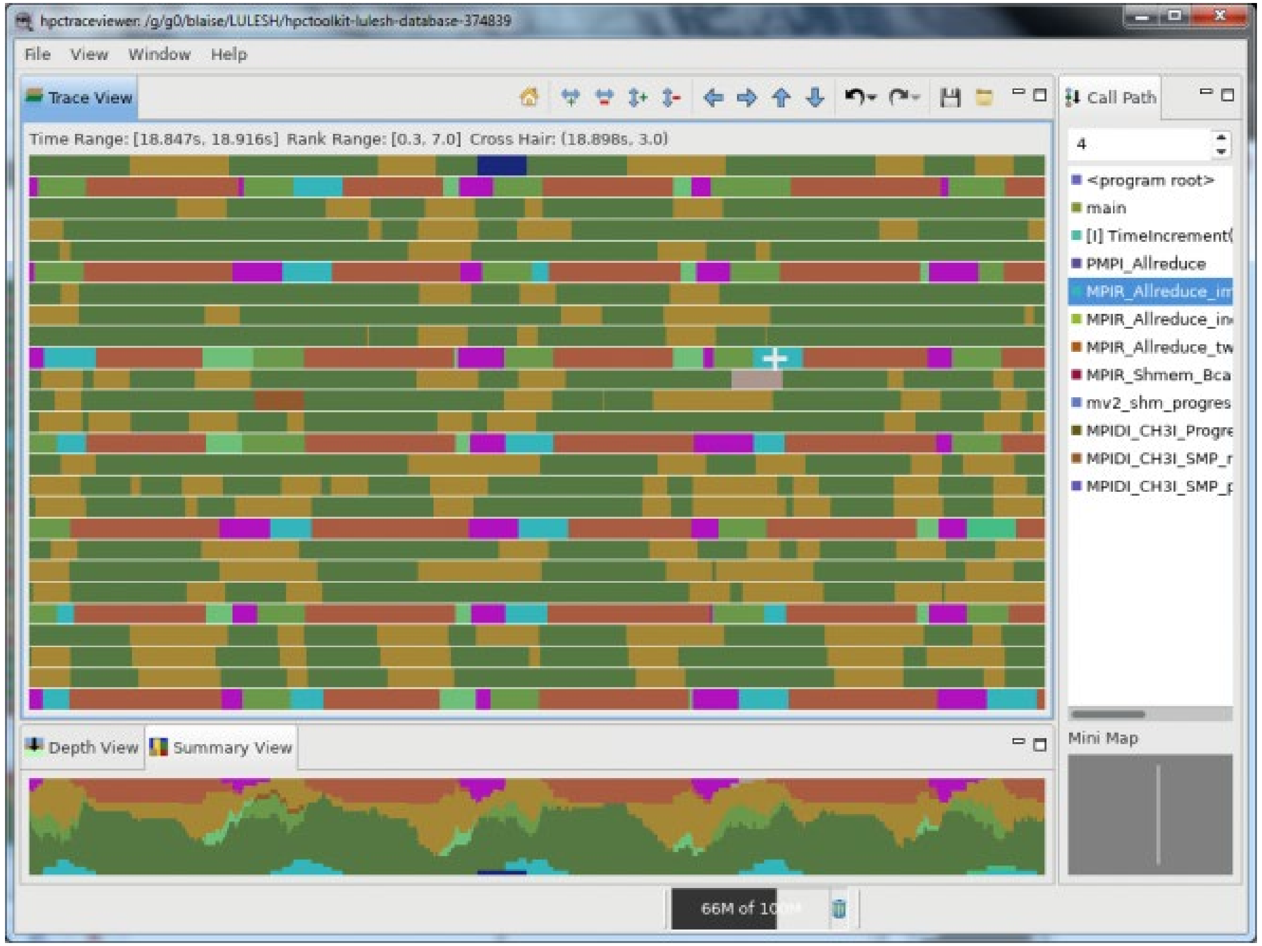


Vampir

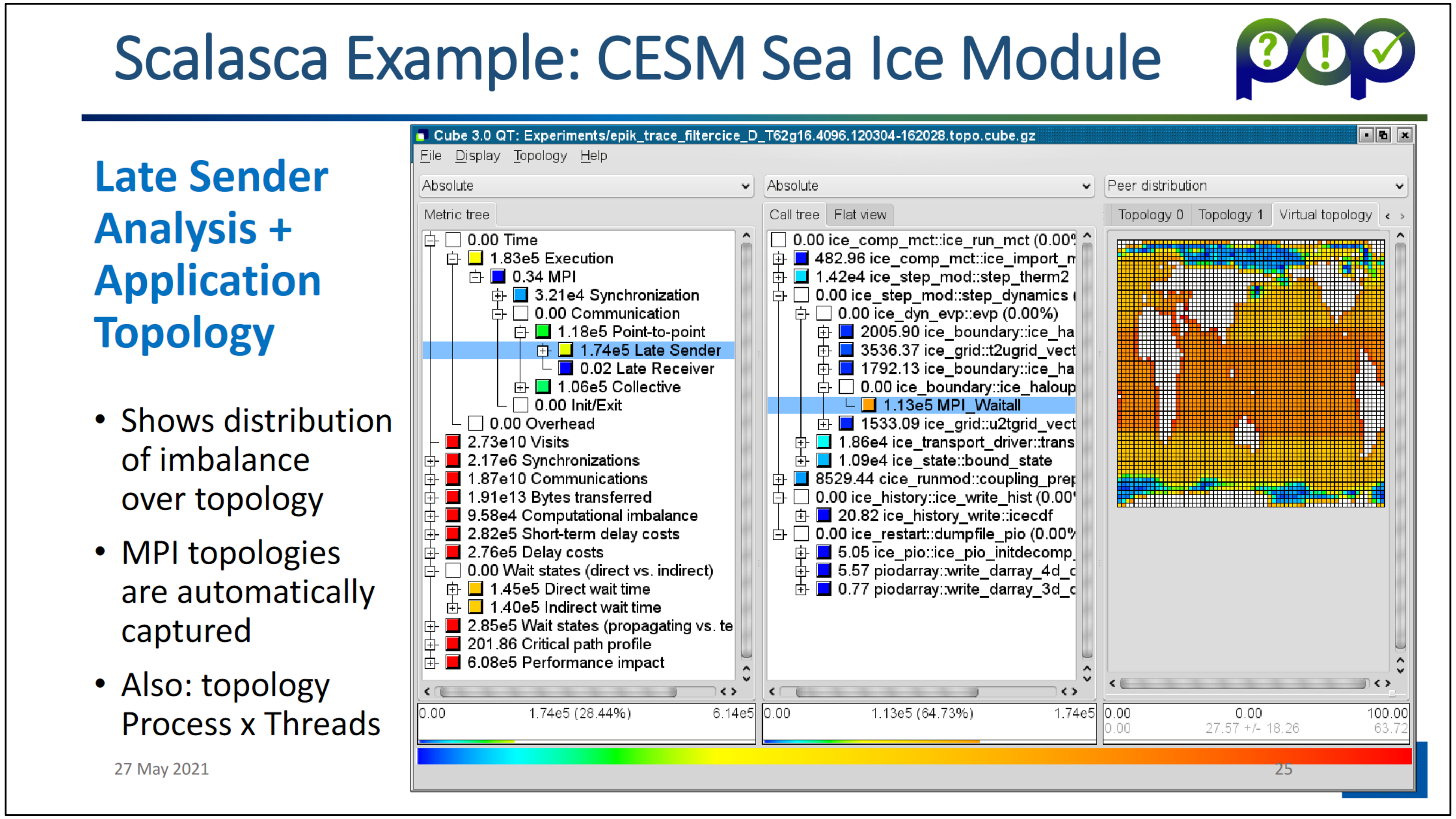

Trace View - /g/g0/blaise/vampir/Small/wrf.otf * - Vampir
File Edit Chart Filter Window Help
32.383 s - 32.476 s
92.984 ms
Timeline
32.400 s
32.425 s
32.450 s
Process 0
Process 1
Process 2
Process 3
Process 4
Process 5
Process 6
Process 7
Process 8
Process 9
Process 10
Process 11
Process 12
Process 13
Process 14
Process 15
MPI_Wait
Function Summary
All Processes, Accumulated Exclusive Time per ...
0s
0.284 s MPI_Wait
0.216 s MODULE_SMALL...LL_STEP_PREP
0.163 s SOLVE_EM
0.153 s MODULE_SMAL...:ADVANCE_UV
0.152 s MODULE_SMAL...DVANCE_MU_T
0.108 s MODULE_SMAL...EM::SUMFLUX
0.101 s MODULE_SMAL...::ADVANCE_W
Context View
Empty
Process 2
Property Value
Type Process
Name Process 2
Function Legend
MPI
DYN
PHYS
WRF
IO_NETCDF
I/O


Communication Matrix View - /g/g0/blaise/vampir/Small/wrf.otf * - Vampir
Number of Messages
Receiver
Sender
Pro...s 0
Pro...s 1
Pro...s 2
Pro...s 3
Pro...s 4
Pro...s 5
Pro...s 6
Pro...s 7
Pro...s 8
Pro...s 9
Pro... 10
Pro... 11
Pro... 12
Pro... 13
Pro... 14
Pro... 15
2
1
0

HPCToolkit


hpctraceviewer: /g/g0/blaise/LULESH/hpctoolkit-lulesh-database-374839
File View Window Help
Trace View
Time Range: [18.847s, 18.916s] Rank Range: [0.3, 7.0] Cross Hair: (18.898s, 3.0)
Call Path
4
<program root>
main
[I] TimeIncrement(
PMPI_Allreduce
MPIR_Allreduce_in
MPIR_Allreduce_in
MPIR_Allreduce_tw
MPIR_Shmem_Bca
mv2_shm_progres
MPIDI_CH3I_Progre
MPIDI_CH3I_SMP_r
MPIDI_CH3I_SMP_
Depth View
Summary View
Mini Map

Cube (from Scalasca suite)



Source: Bernd Mohr, https://pop-coe.eu/sites/default/files/pop_files/pop-webinar-scalasca.pdf

General hints when working with debuggers

- −g when compiling if source code locations are required
  - Has **nothing** to do with optimization levels/flags! You can often use −O3 −g!
  - usually negligible performance impact
- careful with optimization levels/flags, especially −O#
  - function inlining, loop fusion/fission, …
  - likely to obfuscate source code locations
  - if required and feasible, work in −O0 or temporarily disable conflicting flags
  - careful: -O0 performance is very different from -O1/2/3/… performance
- check whether child processes and/or threads are included in analysis/reports
- if tracing or otherwise large-overhead instrumentation required, restrict to code regions of interest

Angles of attack in order of benefit

I/O	• file formats, buffering, distributed I/O, ram disks, data structures
Network	• comm. patterns, non-blocking & one-sided comm., topology mappings, load balancing
Memory	• data structures, NUMA & affinity, cache optimizations (e.g. tiling, alignment, padding)
Compu-tation	• vectorization, data types, intrinsics, load balancing, hardware changes

Summary

- functional debugging
  - adhere to coding guidelines and best practice of software engineering
  - especially relevant for parallelism: know your programming models and semantics, don’t trust automatic tools blindly
- performance debugging
  - don’t underestimate the power of simple tools
  - many more advanced tools out there, but not straight-forward to use
  - know your hardware and your program hotspots

Image sources

- Yoda: https://www.deviantart.com/biggiepoppa/art/Master-Yoda-Star-Wars-395511111
- DDT: https://portal.tacc.utexas.edu/software/ddt, https://www.sharcnet.ca/help/index.php/Parallel_Debugging_with_DDT, https://developer.arm.com/docs/101136/latest/ddt/viewing-variables-and-data
- Domain-specific debugging: https://twitter.com/maven2mars/status/984440044659159040, https://www.nasa.gov/ames/image-feature/nasa-highlights-simulations-at-supercomputing-conference-like-aircraft-landing-gear, ZAMG Wettervorhersage 06.10.2020 12:00
- TAU & ParaProf: https://hpc.llnl.gov/software/development-environment-software/tau-tuning-and-analysis-utilities
- Vampir: https://hpc.llnl.gov/software/development-environment-software/vampir-vampir-server
- HPCToolkit: https://hpc.llnl.gov/software/development-environment-software/hpc-toolkit