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

- 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

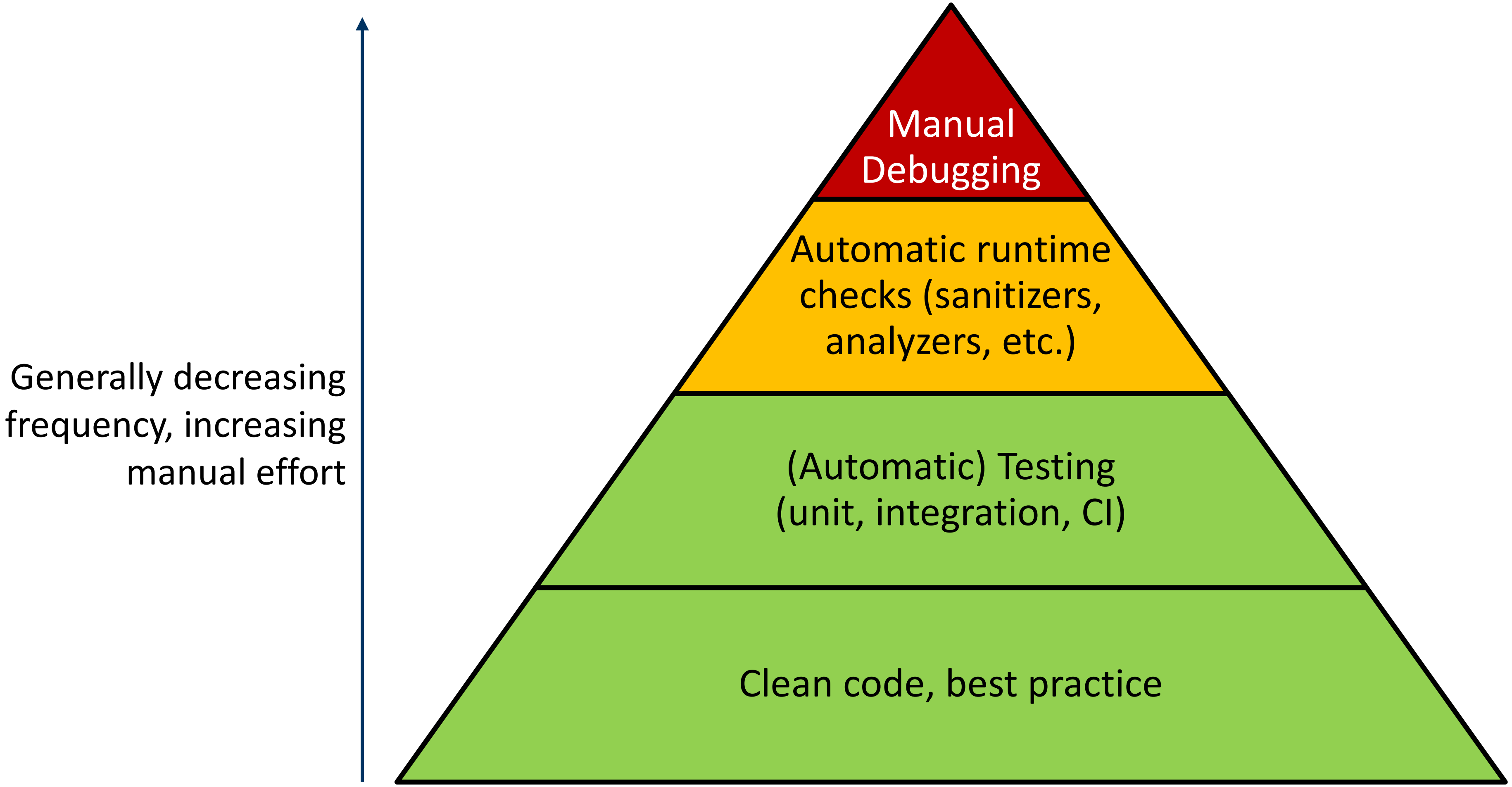
Functional debugging

- 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 **D**on't **R**epeat **Y**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

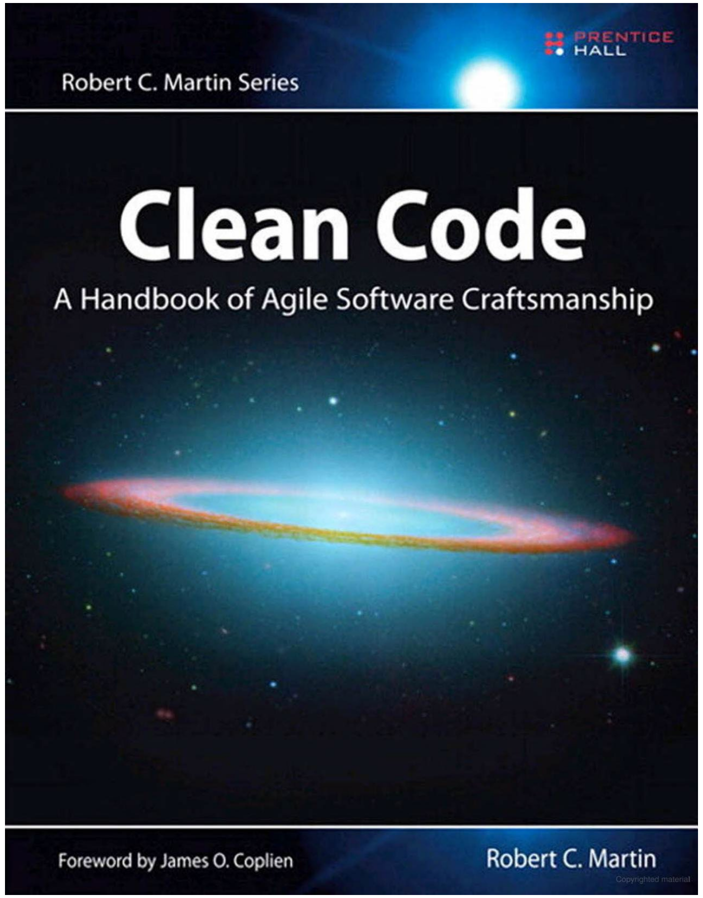
“Best of” real commit messages encountered in the past

- 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 **M**inimal **W**orking **E**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], N, MPI_DOUBLE, rank - 1, 0, MPI_COMM_WORLD);
```

- Compile with –Wall –Wextra –pedantic:

```
In file included from heat_2D.c:4:
heat_2D.c: In function ‘main’:
/usr/lib/x86_64-linux-gnu/openmpi/include/mpi.h:402:47: warning: passing argument 2 of ‘MPI_Send’ makes integer from pointer without a cast [-Wint-conversion]
402 | #define OMPI_PREDEFINED_GLOBAL(type, global) ((type) ((void *) &(global)))
    |                                               ~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~
    |                                                |
    |                                                struct ompi_datatype_t *
/usr/lib/x86_64-linux-gnu/openmpi/include/mpi.h:1171:20: note: in expansion of macro ‘OMPI_PREDEFINED_GLOBAL’
1171 | #define MPI_DOUBLE OMPI_PREDEFINED_GLOBAL(MPI_Datatype, ompi_mpi_double)
    | ^~~~~~~~~~~~~~~~~~~~~~
heat_2D.c:110:25: note: in expansion of macro ‘MPI_DOUBLE’
110 | MPI_Send(&A_local[0], MPI_DOUBLE, N, rank - 1, 0, MPI_COMM_WORLD);
    | ^~~~~~~~~~
/usr/lib/x86_64-linux-gnu/openmpi/include/mpi.h:1784:50: note: expected ‘int’ but argument is of type ‘struct ompi_datatype_t *’
1784 | OMPI_DECLSPEC int MPI_Send(const void *buf, int count, MPI_Datatype datatype, int dest,
heat_2D.c:110:37: warning: passing argument 3 of ‘MPI_Send’ makes pointer from integer without a cast [-Wint-conversion]
110 | MPI_Send(&A_local[0], MPI_DOUBLE, N, rank - 1, 0, MPI_COMM_WORLD);
    |                                   ^
    |                                   |
    |                                   int
In file included from heat_2D.c:4:
/usr/lib/x86_64-linux-gnu/openmpi/include/mpi.h:1784:70: note: expected ‘MPI_Datatype’ {aka ‘struct ompi_datatype_t *’} but argument is of type ‘int’
1784 | OMPI_DECLSPEC int MPI_Send(const void *buf, int count, MPI_Datatype datatype, int dest,
    | ~~~~~~~~~~~~~^~~~~~~~
```

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

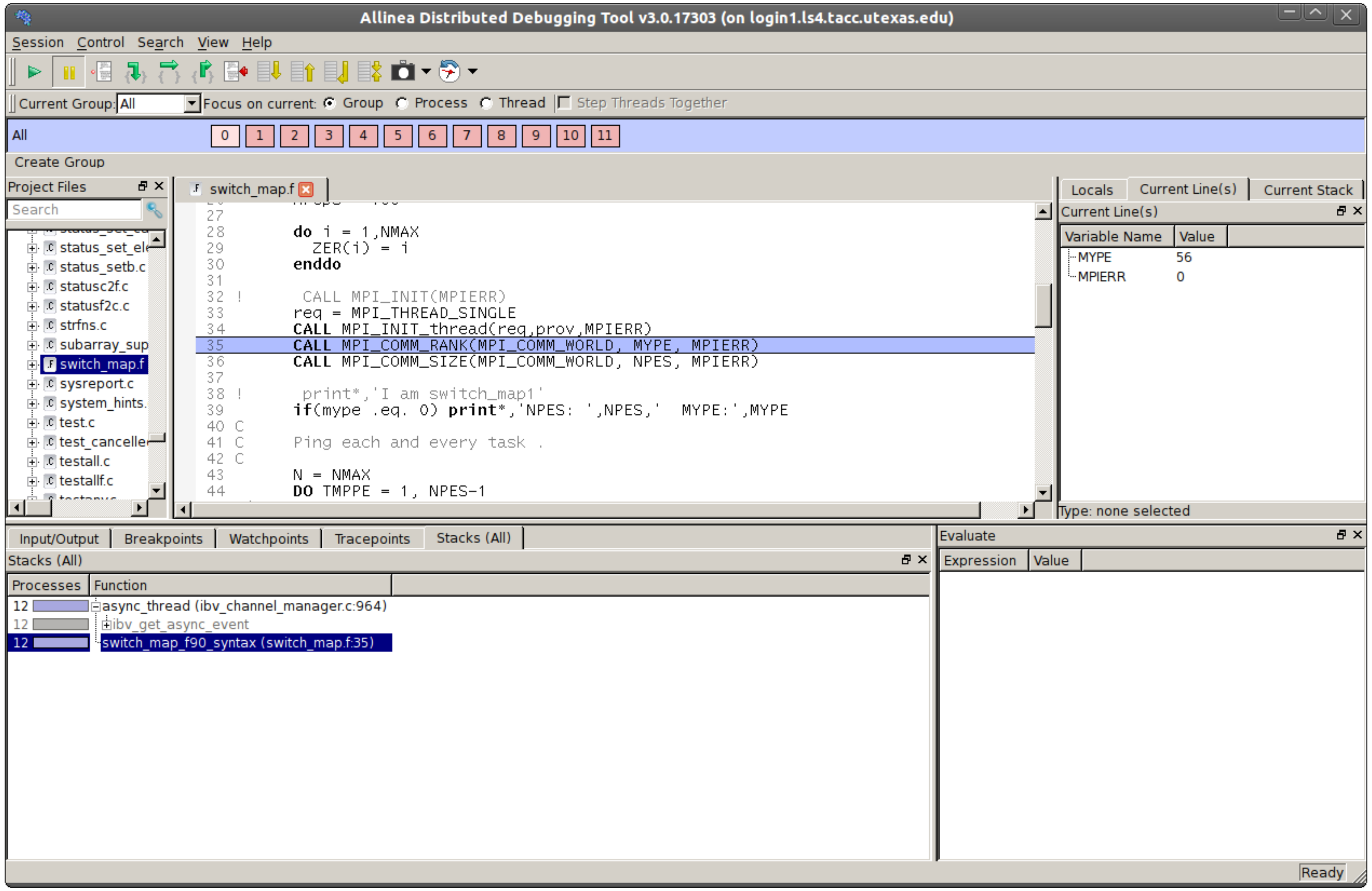
- Live Demo with MUST (https://itc.rwth-aachen.de/must/)!

Parallel debuggers

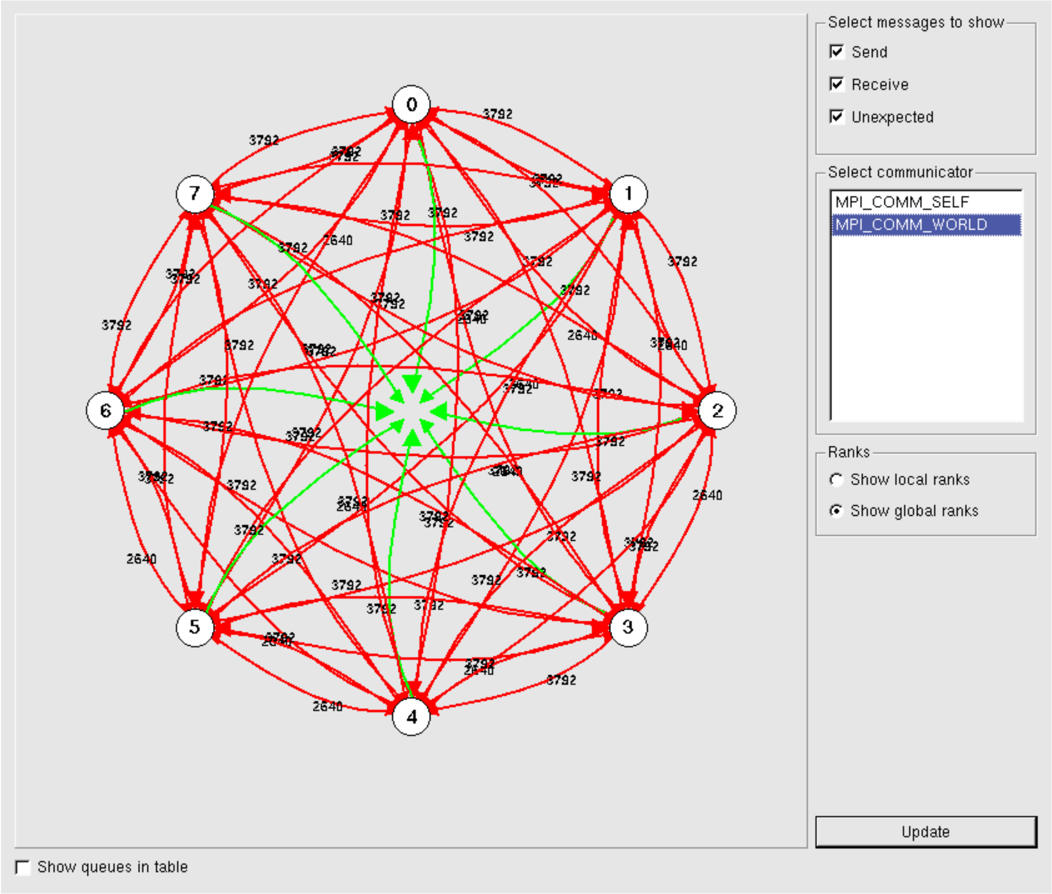
- very little free software
- two commercial top dogs: DDT (ARM) and TotalView (Perforce Software)
- support OpenMP, MPI, CUDA, etc.
- several features centered around parallelism
  - examine variables per rank/thread, examine send/receive queues of MPI libraries, etc.
  - still, limited usefulness

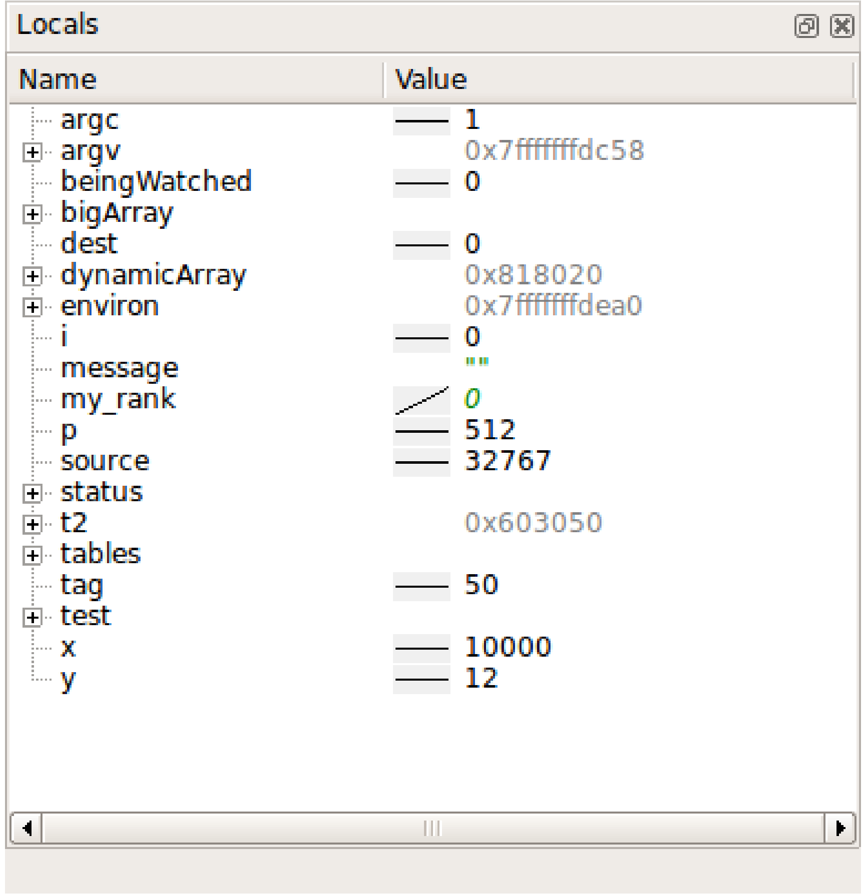
- Several other software packages
  - MUST: MPI runtime error checking tool
  - Visual Studio: supports debugging MPI-Programs in Windows
  - Intel Inspector: data race detector for multi-threaded programs
  - ARCHER: data race detector for OpenMP
  - STAT: trace analysis tool to group ranks with similar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

Intel Inspector

- features
  - free
  - Linux & Windows version
  - automatically finds bugs in multi-threaded programs
    - deadlocks
    - memory corruption
    - race conditions
    - vulnerabilities
  - supports OpenMP, TBB, Pthreads, Windows threads

- limitations & issues
  - slowdown by 1-2 orders of magnitude!
  - explicit support only for Intel OpenMP runtime
  - error detection only at runtime, only in executed control flow branches
  - false positives and negatives possible

OpenMP data race example 1

```
int counter = 0;

#pragma omp parallel for
for(int i = 0; i < 10; ++i) {
  counter++;
}
```

Description	Source	Function	Module
Read	ConsoleApplication1.cpp:9	main	consoleapplication1.exe

```
7      #pragma omp parallel for
8      for (int i = 0; i < 10; ++i) {
9          counter++;
10     }
11
```

Description	Source	Function	Module
Write	ConsoleApplication1.cpp:9	main	consoleapplication1.exe

```
7      #pragma omp parallel for
8      for (int i = 0; i < 10; ++i) {
9          counter++;
10     }
11
```

OpenMP data race example 2

```
int sum = 0;

#pragma omp parallel for
for(int i = 0; i < 10; i++) {
  int tmp = sum;
  tmp = tmp + 1;
  sum = tmp;
}
```

Description	Source	Function	Module
Read	ConsoleApplication1.cpp:17	main	consoleapplication1.exe

```
15      #pragma omp parallel for
16      for (int i = 0; i < 10; i++) {
17          int tmp = sum;
18          tmp = tmp + 1;
19          sum = tmp;
```

Description	Source	Function	Module
Write	ConsoleApplication1.cpp:19	main	consoleapplication1.exe

```
17          int tmp = sum;
18          tmp = tmp + 1;
19          sum = tmp;
20      }
21
```

OpenMP data race example 2: wrong fix

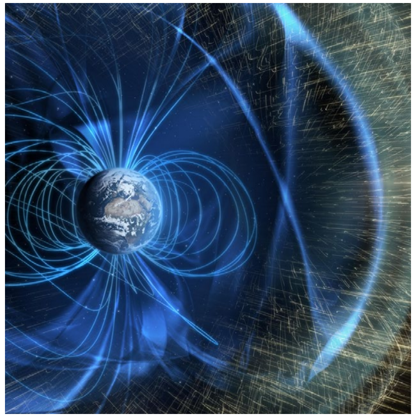
```
int sum = 0;

#pragma omp parallel for
for(int i = 0; i < 10; i++) {
  int tmp;
  #pragma omp critical
  tmp = sum;
  tmp = tmp + 1;
  #pragma omp critical
  sum = tmp;
}
```

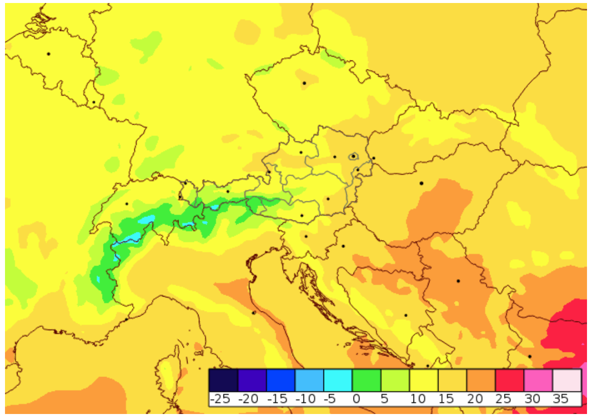
☹

(not detected by Intel Inspector 2020)

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, 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

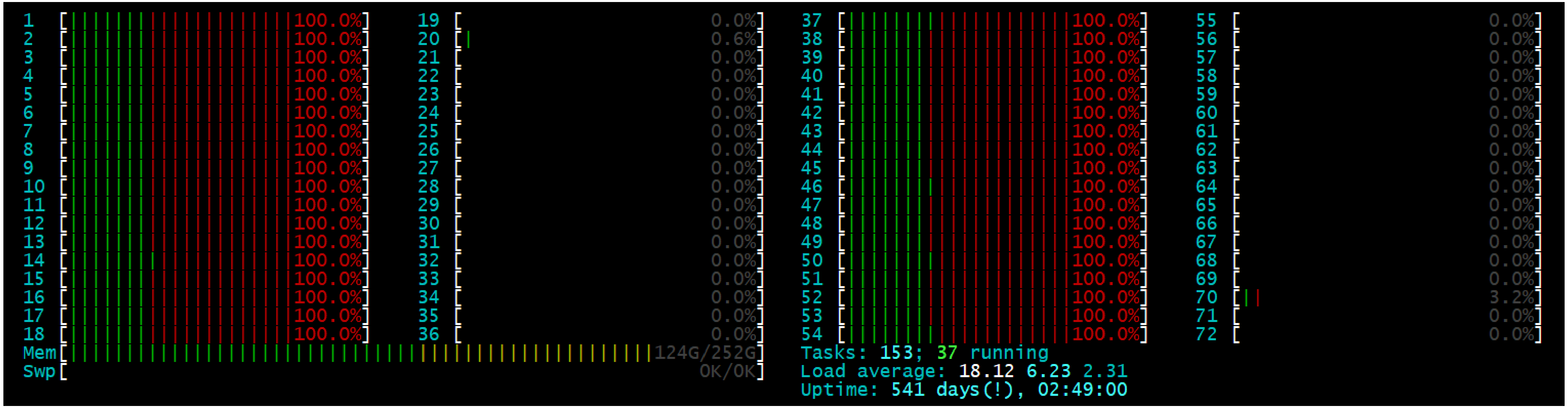
`(h)top`

- 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?



Recap: 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
  - 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
```

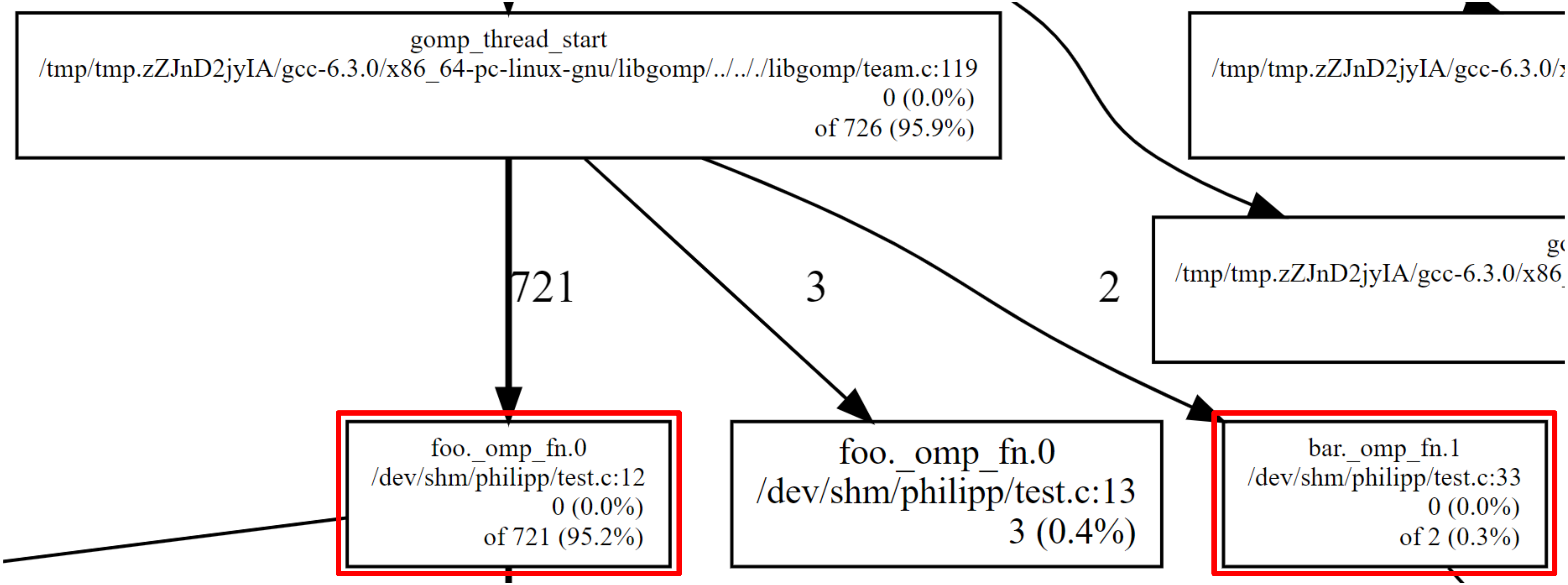
gperftools

- 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



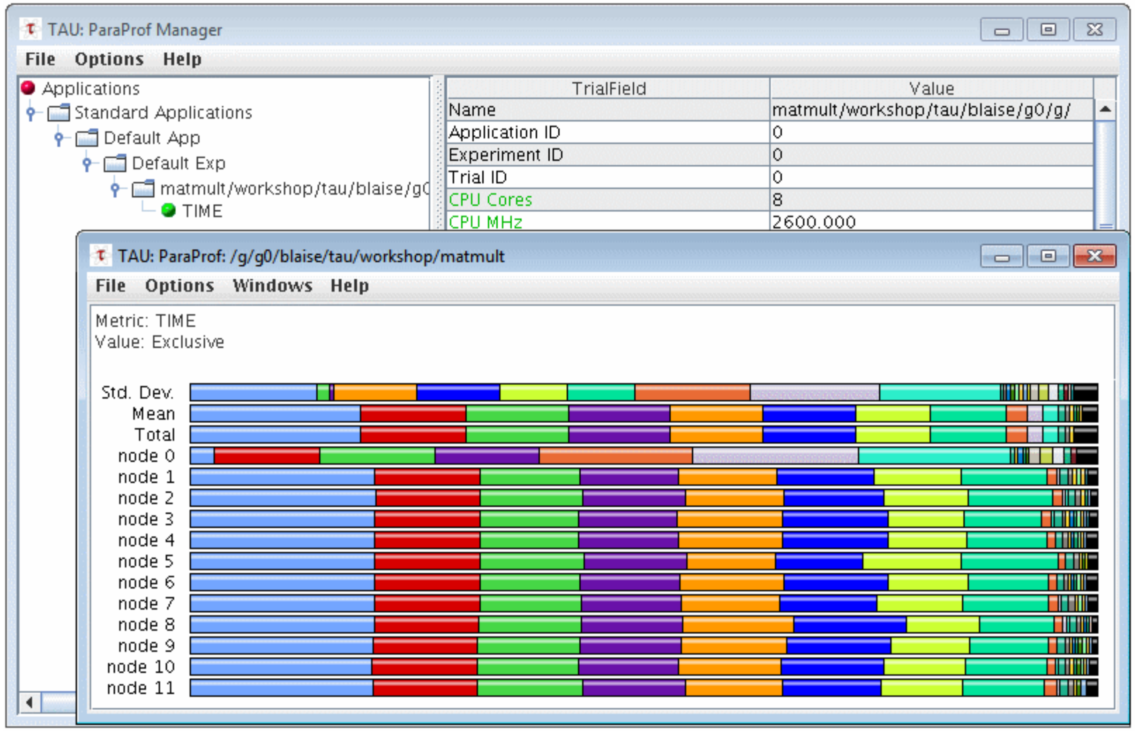
Performance analysis tools for parallel programs

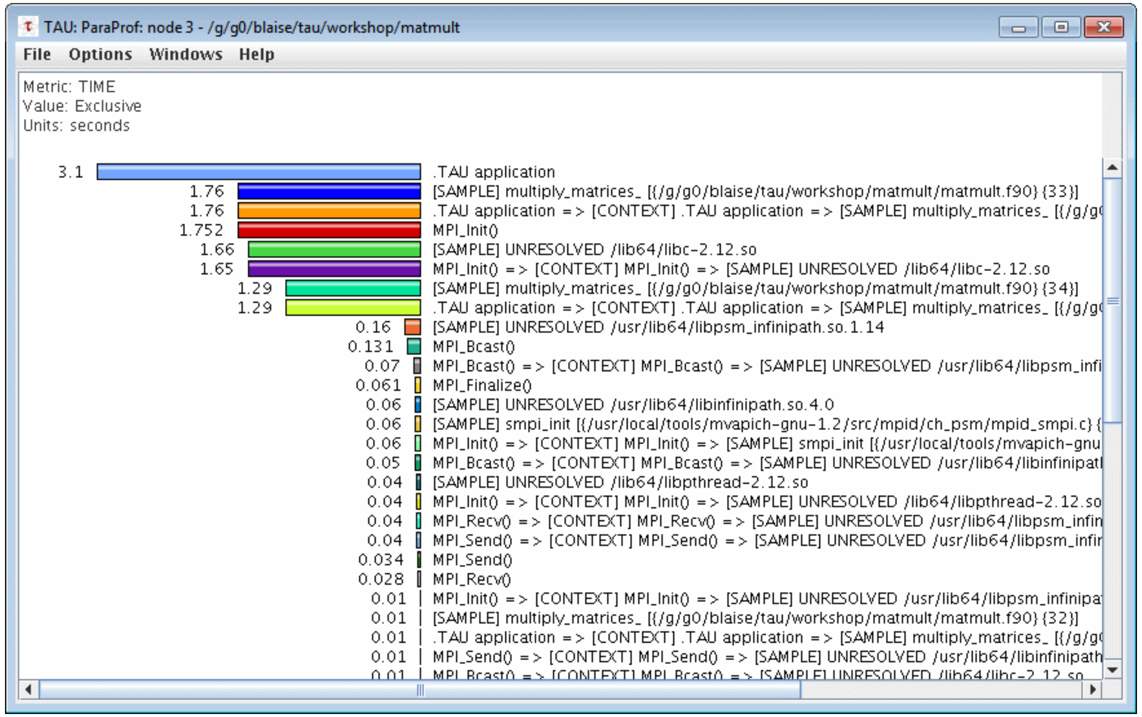
- profiling and analysis software
  - Intel Pin: dynamic binary instrumentation
  - Intel VTune: performance analysis for multi-threaded programs
  - Intel Advisor: dependency, vectorization and cache analysis tool
  - AMD CodeXL / NVIDIA Nsight: profiler and debugger for GPUs
  - TAU: profiling and 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.

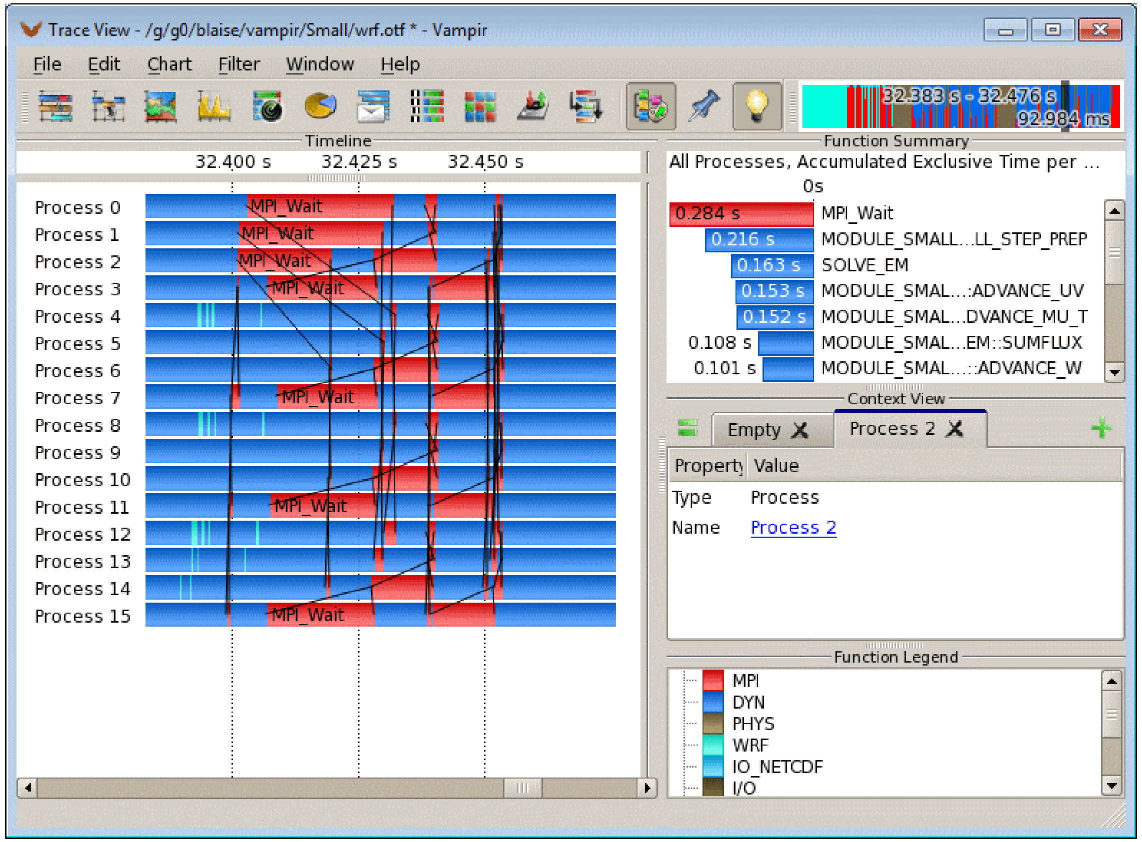
- These lists are by far not complete!

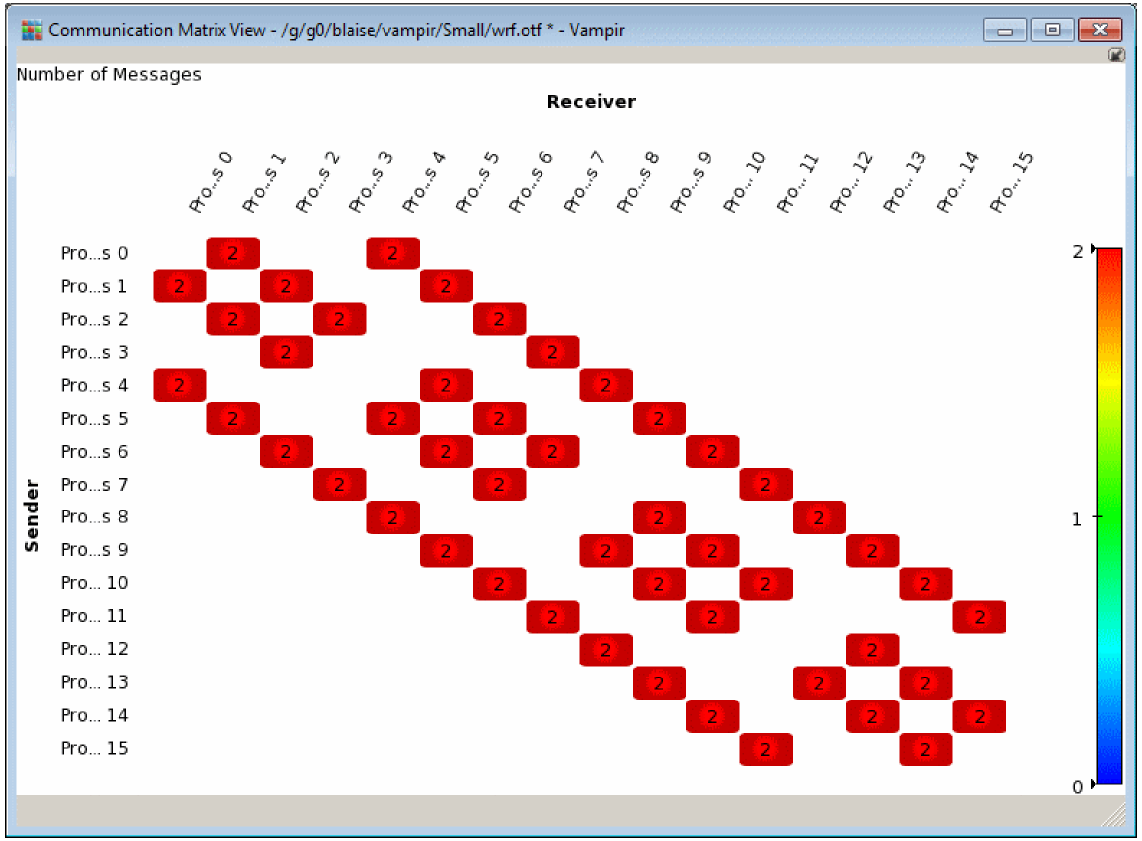
TAU & ParaProf



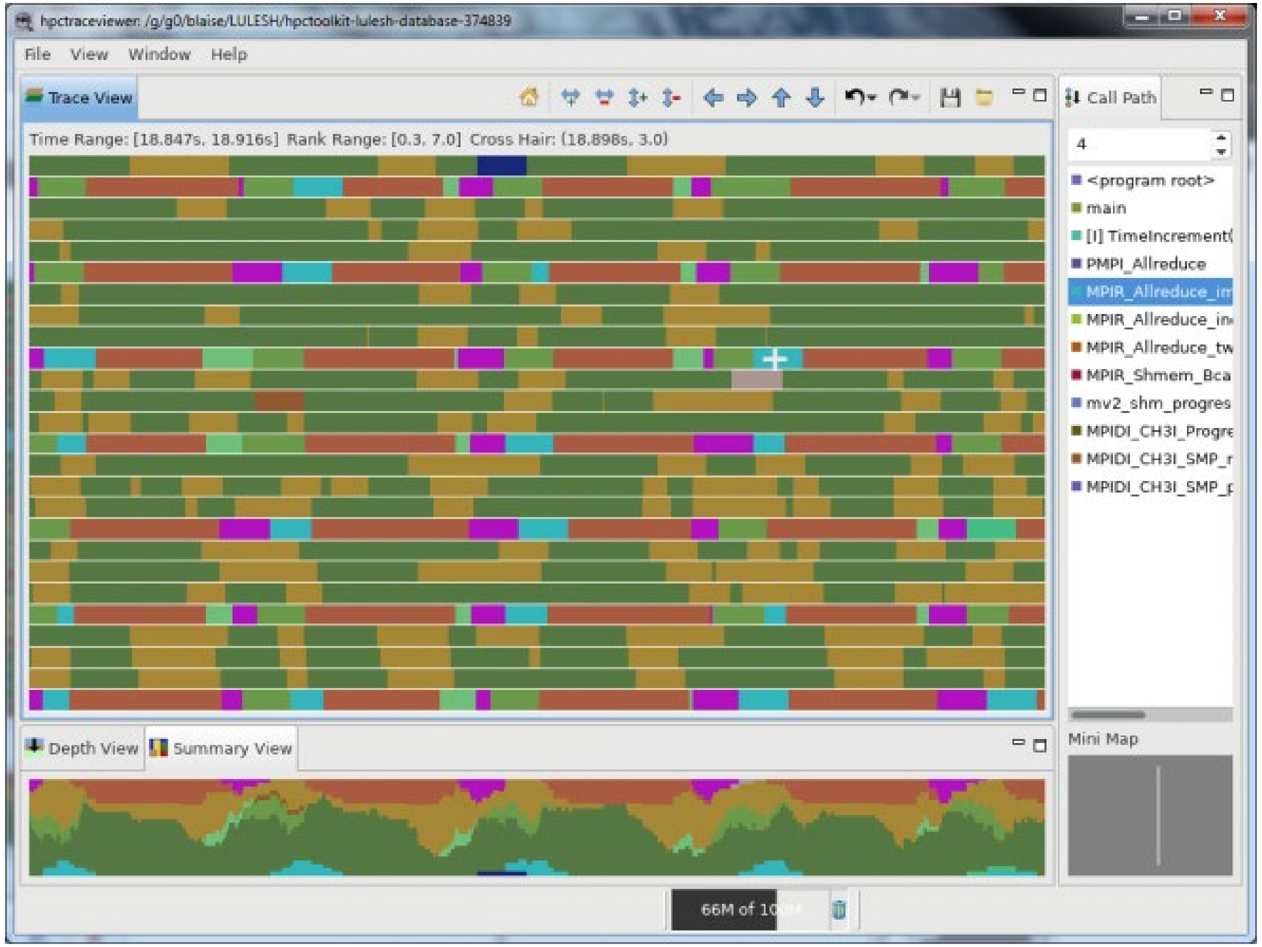


Vampir

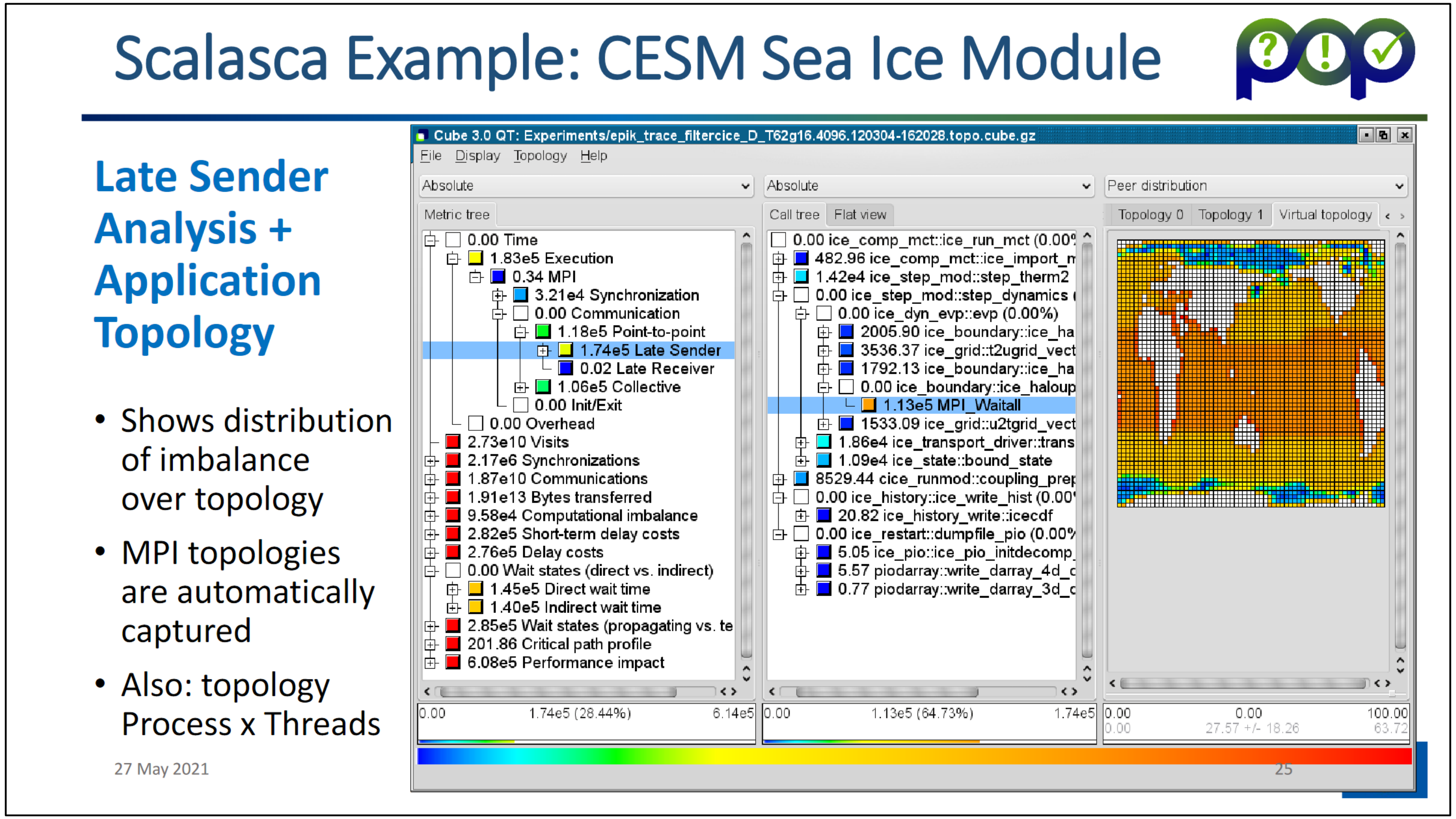

Trace View - /g/g0/blaise/vampir/Small/wrf.otf * - Vampir
File Edit Chart Filter Window Help
32.383 s - 32.476 s
92.984 ms
Timeline
32.400 s 32.425 s 32.450 s
Process 0
Process 1
Process 2
Process 3
Process 4
Process 5
Process 6
Process 7
Process 8
Process 9
Process 10
Process 11
Process 12
Process 13
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
PMPI_Allreduce
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 != -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