703308 VO High-Performance Computing WS2021/2022
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

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

- everything that results in not getting the correct program output
  - program crashes
  - program not finishing (freezes, infinite loops)
  - incorrect output

- errors can be deterministic or non-deterministic
  - ensure/maximize reproducibility during testing (e.g. fix random seeds, process/thread numbers, affinities, …)

- 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?

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

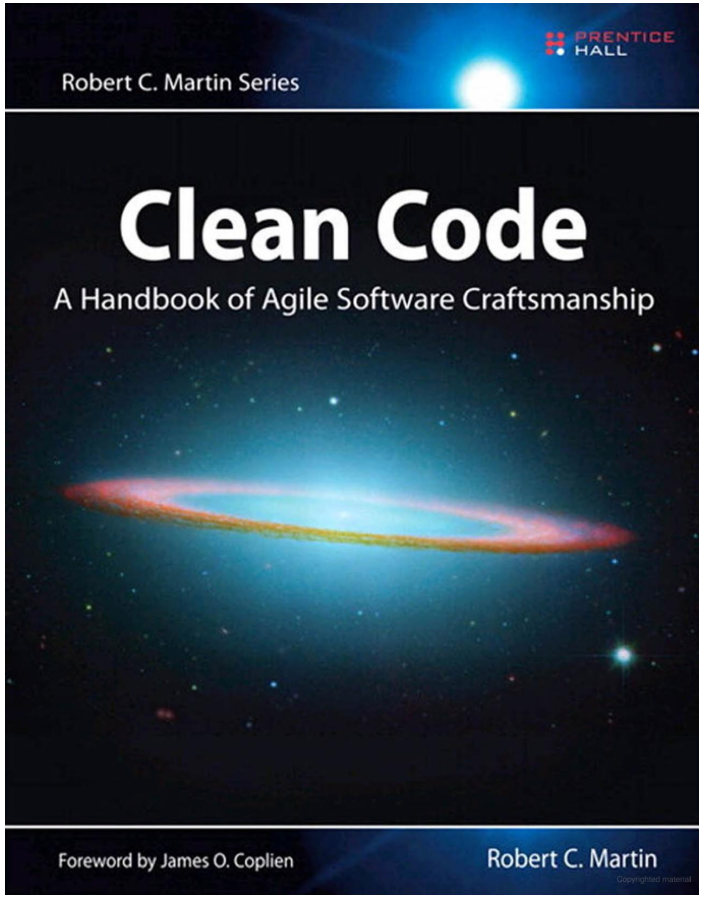
“Best of” Real Commit Messages Encountered in the Past

- 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

- "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
  - 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 this
  - 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 a single MPI process among many
    - `mpiexec -n 1 gdb ./a.out : -n X-1 ./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 no parallel execution!)
  - can yield some false positives e.g. for OpenMP related to thread-local storage

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

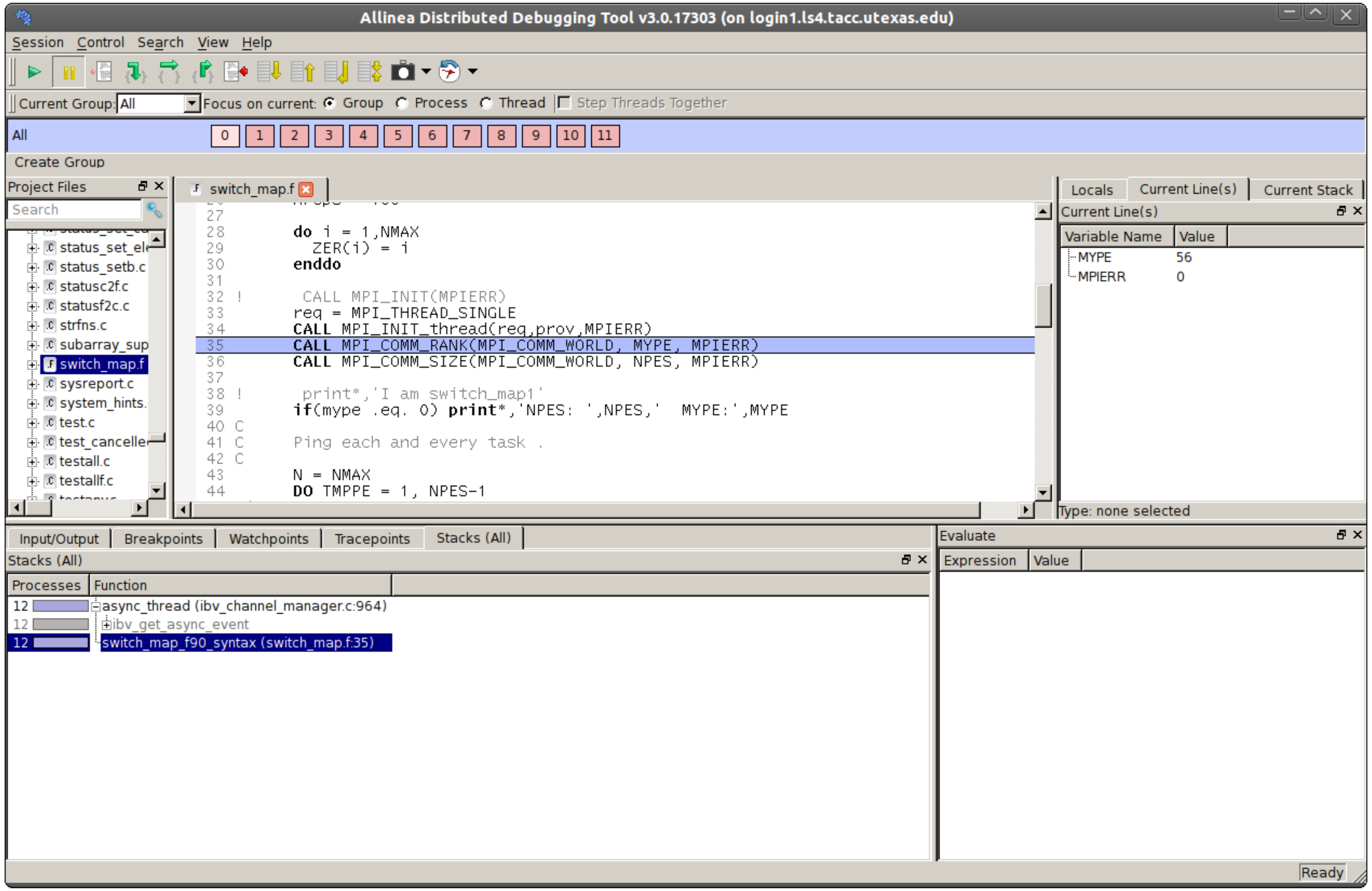
Call Graph Generators

- many tools available for generating call graphs
- static (at compile time)
  - doxygen, opt (llvm), cflow (gcc), etc.
- dynamic (at runtime)
  - gprof, callgrind, OpenPAT, pprof, CodeAnalyst, etc.
  - most performance analysis tools offer some form of call graph generation

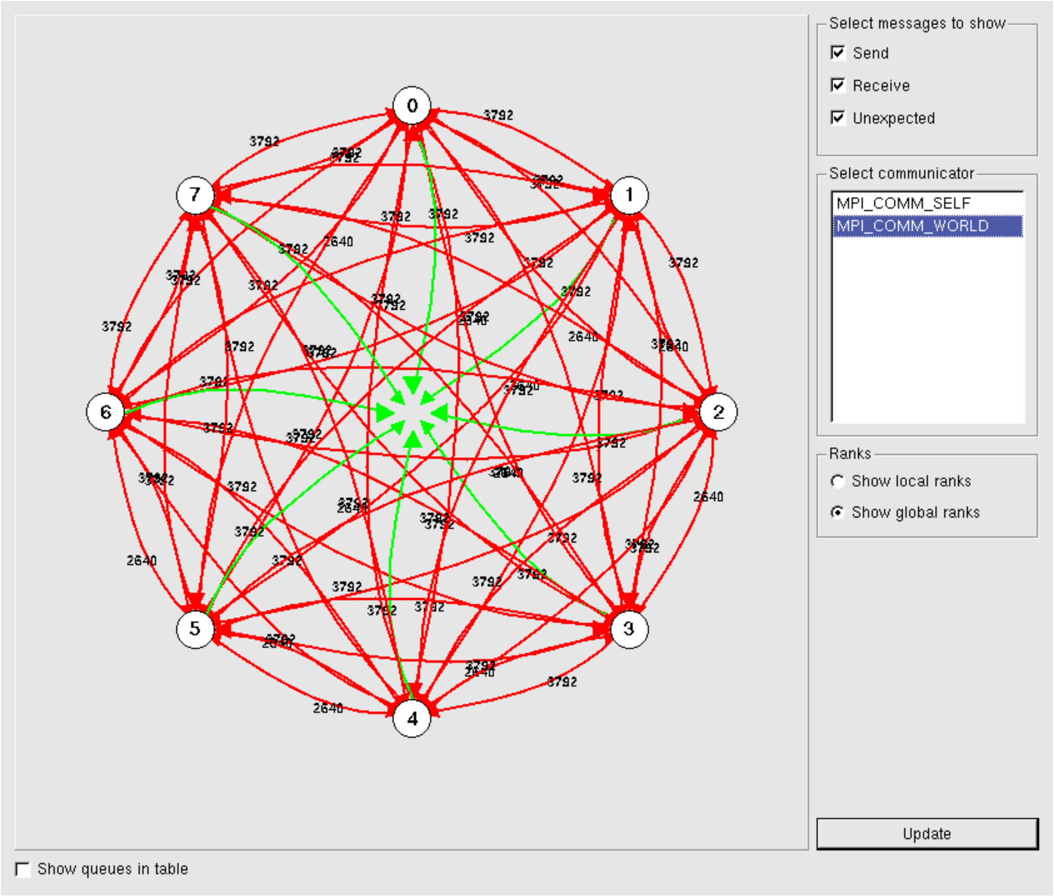
Parallel Debuggers

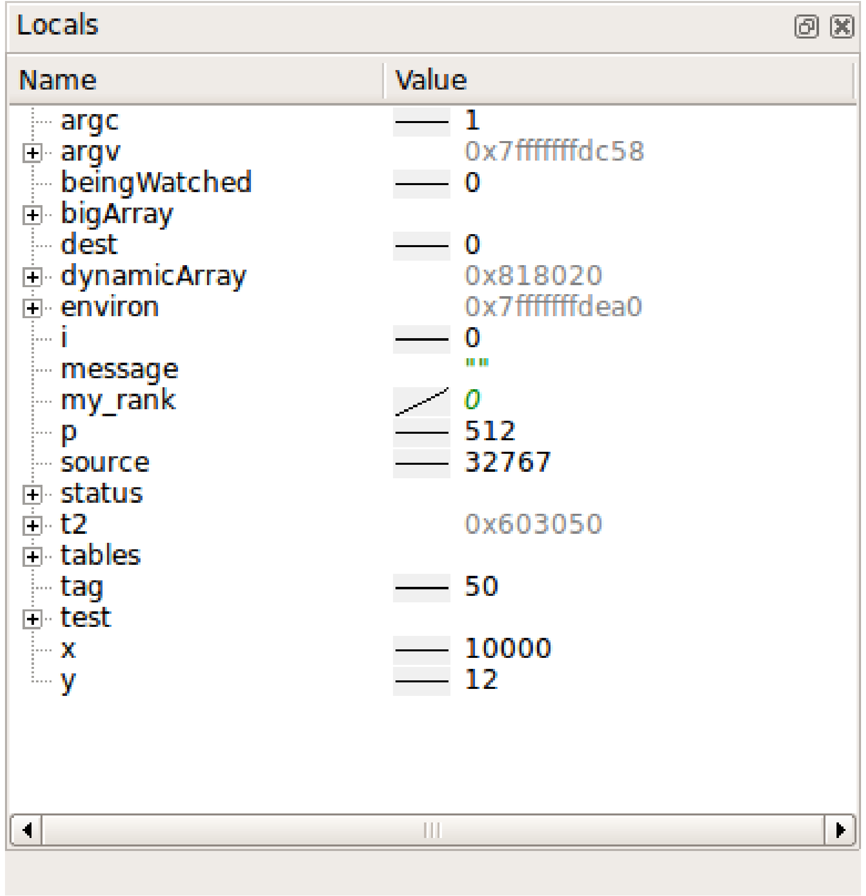
- very little free software
- two commercial top dogs: DDT (ARM) and TotalView (Rogue Wave Software)
- support OpenMP, MPI, CUDA, etc.
- several features centered around parallelism
  - examine variables per rank/thread, examine send/receive queues of MPI libraries, etc.
  - still, limited usefulness

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 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

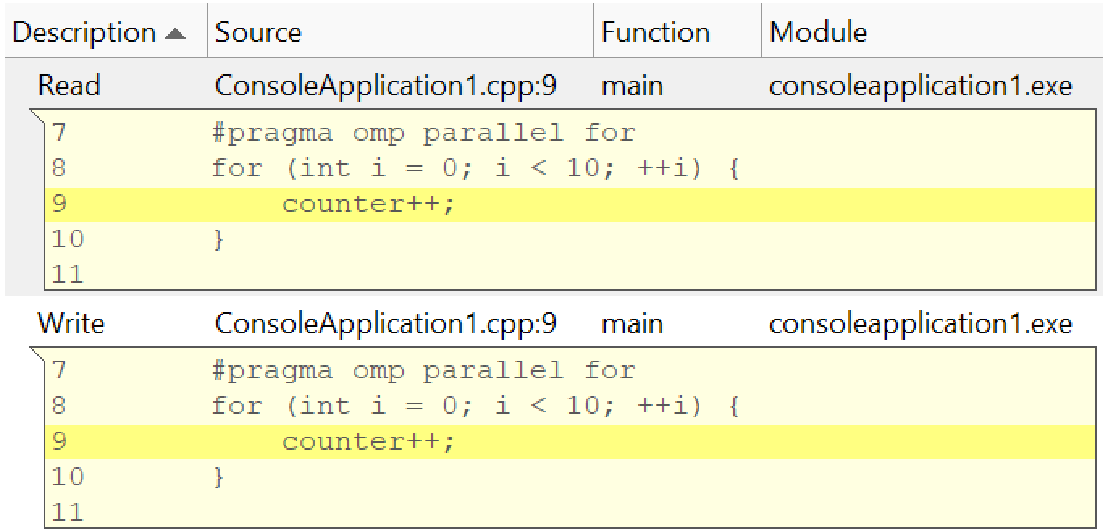
Intel Inspector

- 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

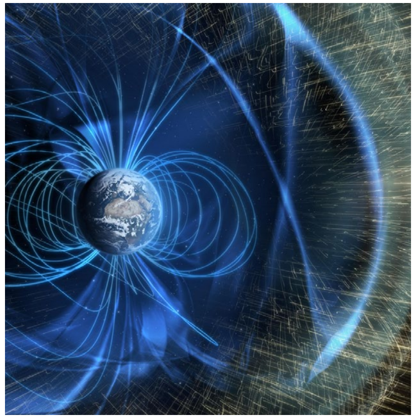
```
int sum = 0;

#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;
}
```

☹

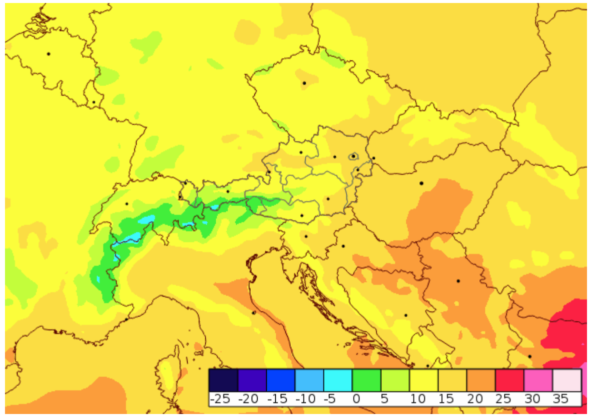
(not detected by Intel Inspector 2020)

Domain-specific Debugging

- Visualize the output using appropriate tools
  - gnuplot
  - 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. “an n-body simulation using Barnes-Hut”

- know your programming models and languages, and their semantics
  - “OpenMP threadprivates persist per thread between parallel regions with the same number of threads and affinity policies”
  - “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!

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 "faster" 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

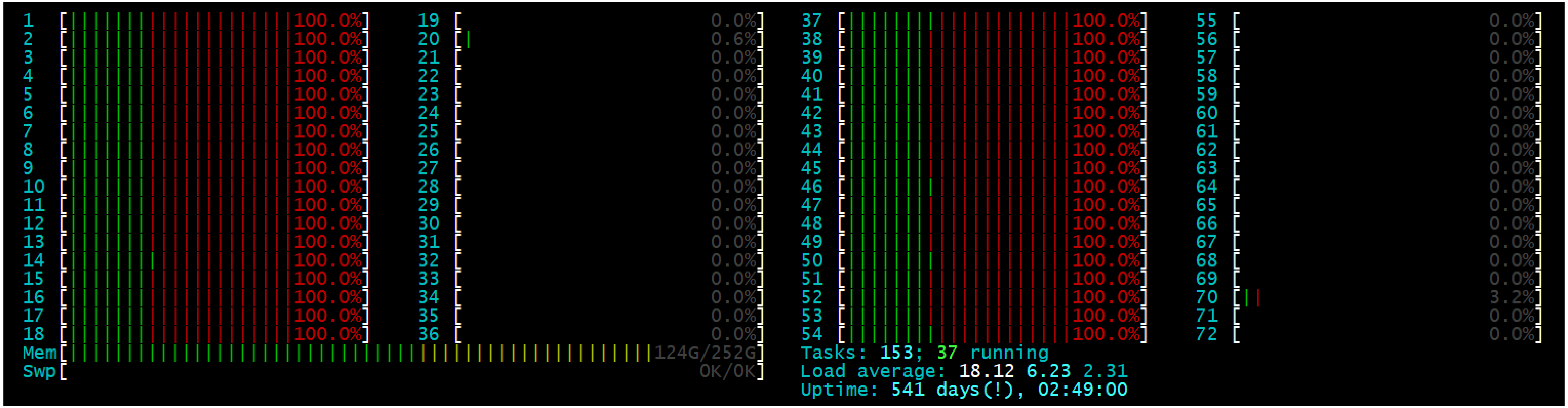
`(h)top`

- 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 existence of memory leaks 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, no code changes required
    - stop program periodically and read program counter of CPU
    - 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

```
start_timer();
func_call();
end_timer();
```

`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

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

```c
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)
```

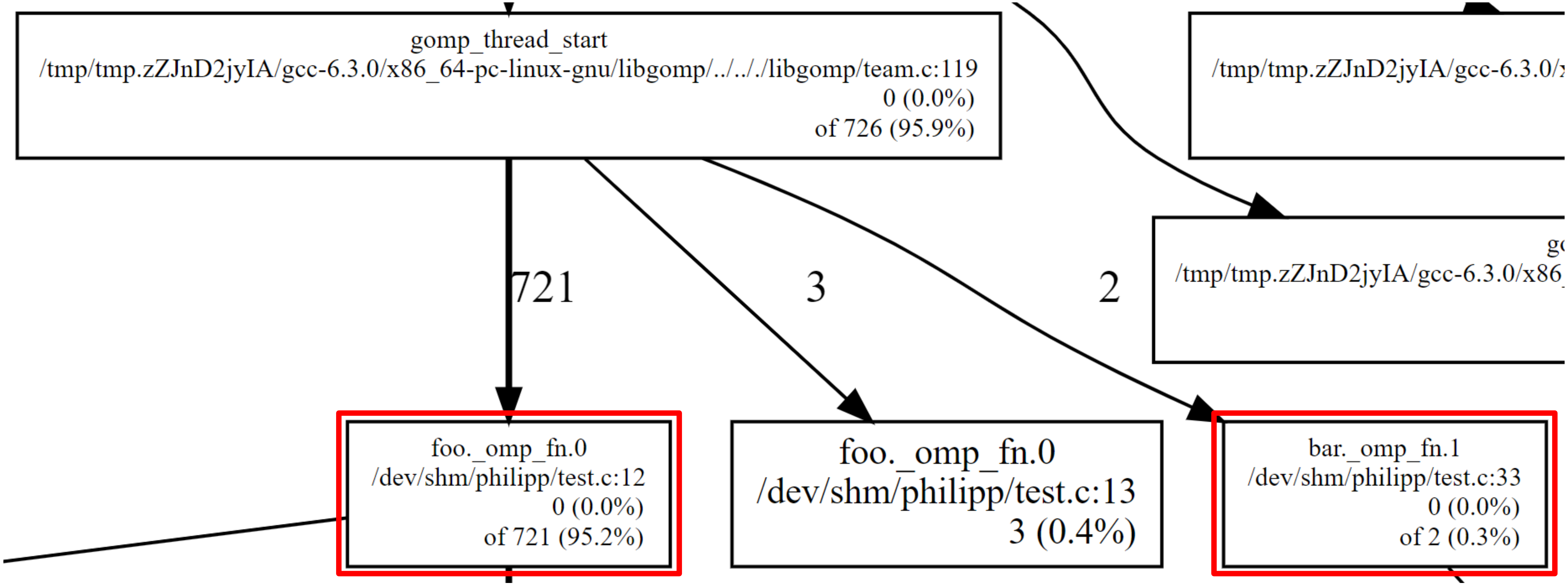
gperftools

- 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



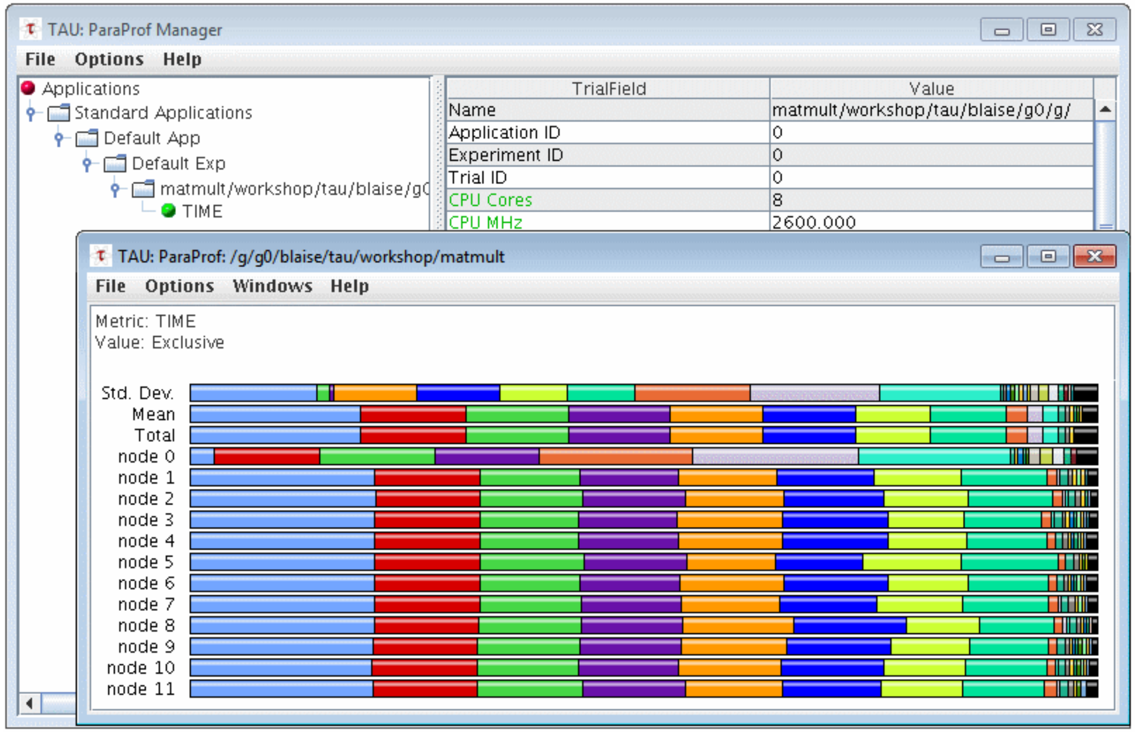
Performance Analysis Tools for Parallel Programs

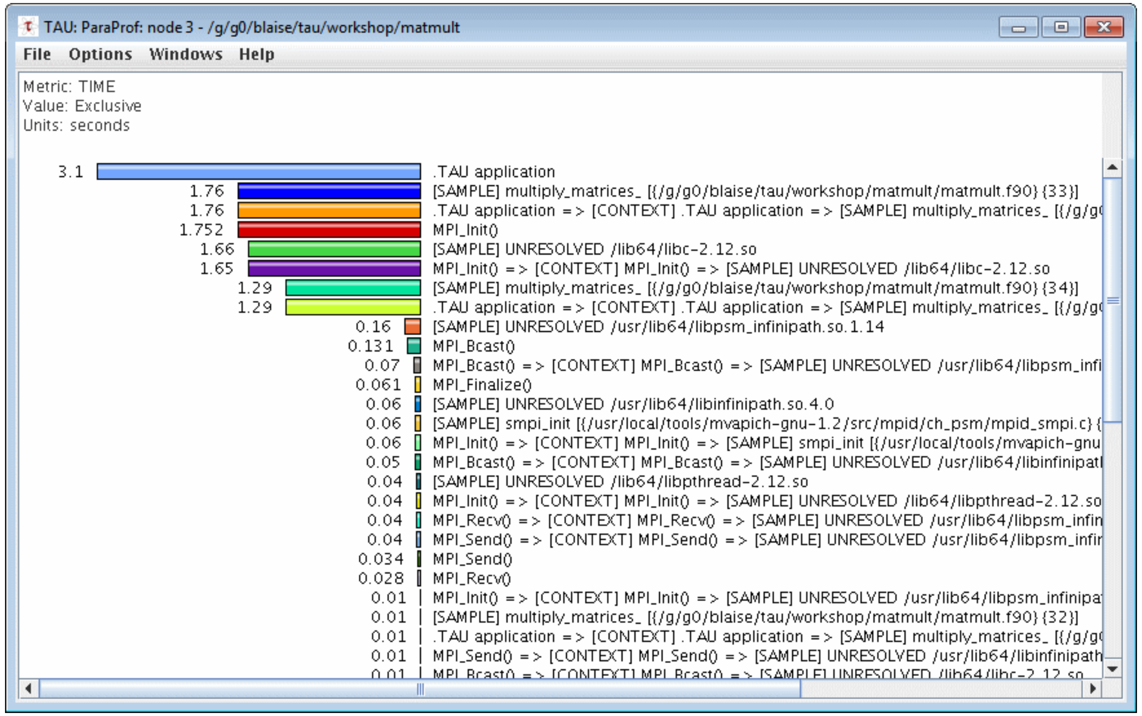
- profiling and analysis software
  - Intel Pin: dynamic binary instrumentation
  - Intel VTune: performance analysis for multi-threaded programs
  - Intel Advisor: dependency, vectorization and cache analysis tool
  - AMD CodeXL / NVIDIA Nsight: profiler and debugger for GPUs
  - TAU: profiling and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



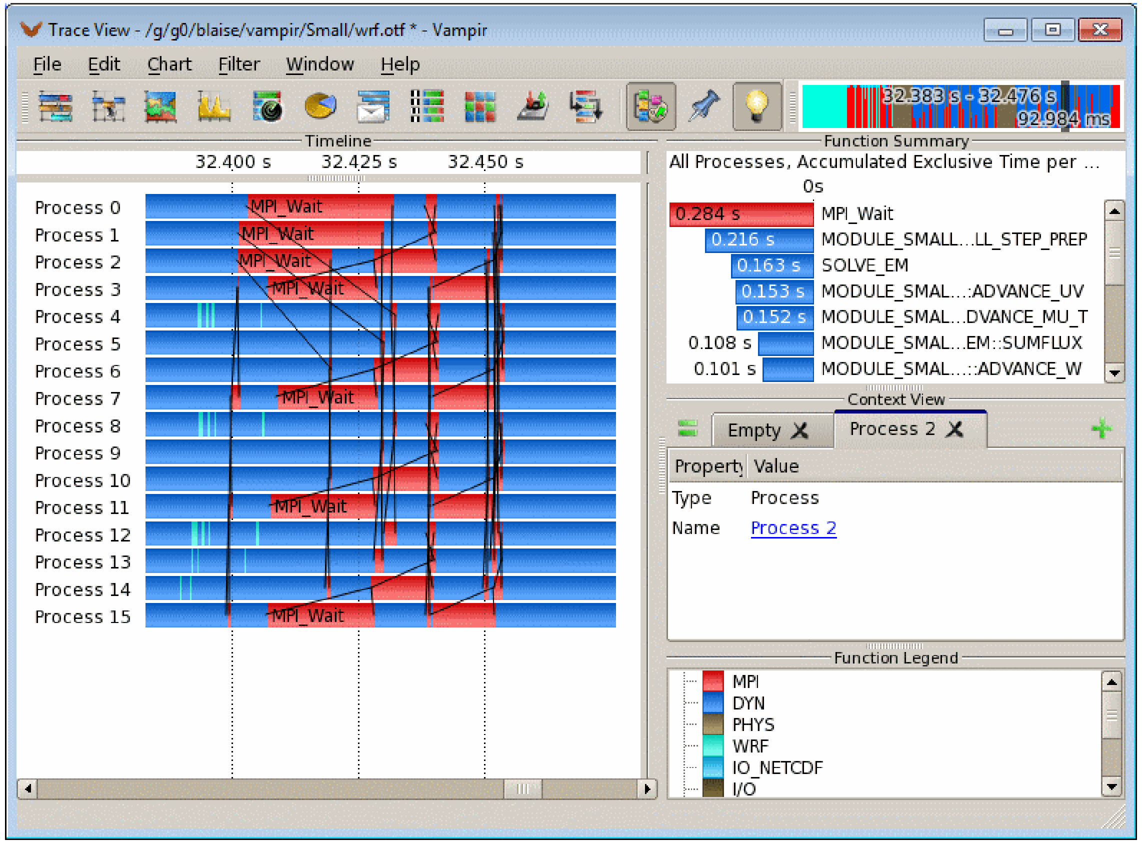


Tau Instrumentation Files

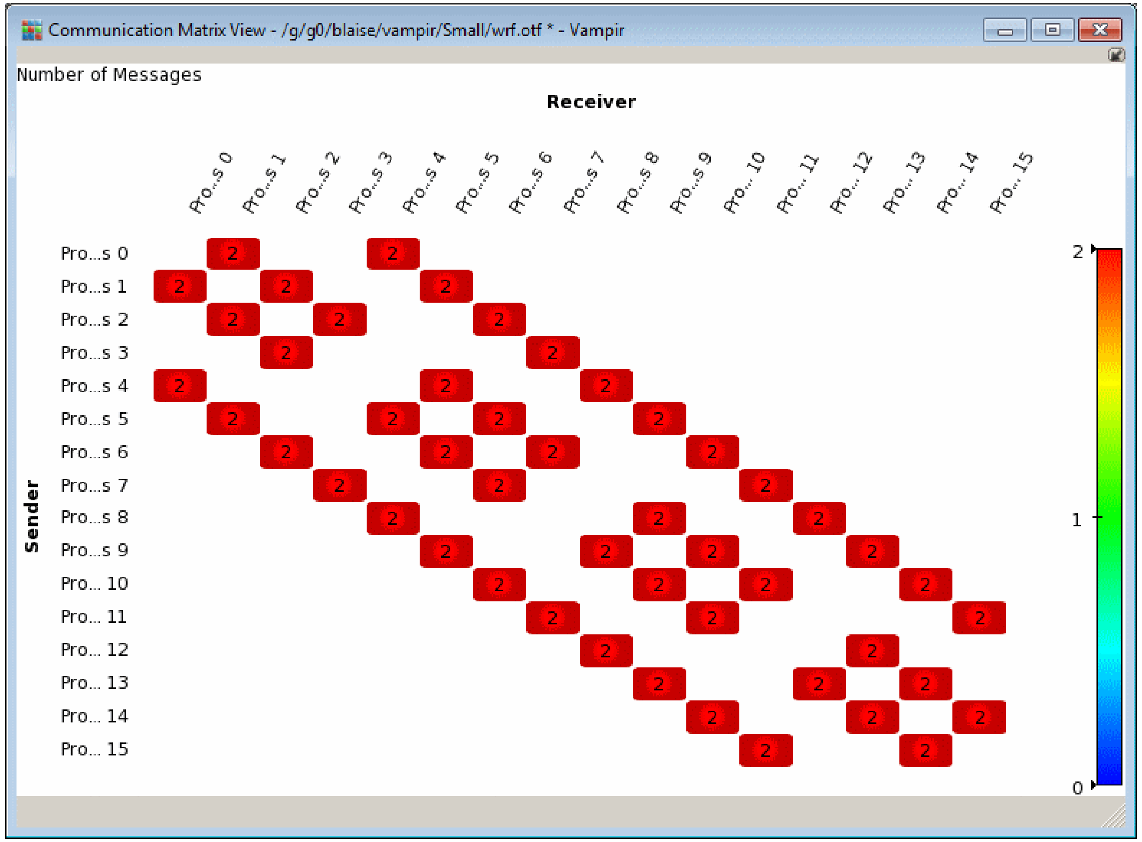
- allows to control the scope of instrumentation
  - reduces measurement overhead
  - reduces collected data to relevant content
- allows to select function patterns, loops, code lines, etc.

```
BEGIN_INSTRUMENT_SECTION

loops file="foo.cpp" routine="int
  bar(int*, double)"

END_INSTRUMENT_SECTION
```

Vampir



Trace View - /g/g0/blaise/vampir/Small/wrf.otf * - Vampir
File Edit Chart Filter Window Help
Timeline
Function Summary
All Processes, Accumulated Exclusive Time per ...
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

General Hints When Working With Debuggers

- –g when compiling if source locations are required
- careful with optimization flags, especially –O#
  - function inlining, loop fusion/fission, …
  - likely to obfuscate source code locations
  - if feasible, work in –O0 or temporarily disable conflicting flags
- check whether child processes are included in analysis/reports
- check whether threads are included in analysis/reports
- if tracing or otherwise large-overhead instrumentation required, restrict to code regions of interest

Points 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 guideline and best practices 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