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Debugging and Profiling HPC Applications

ATPESC

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Ryan Hulguin
ryan.hulguin@arm.com
HPC Senior Applications Engineer

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Agenda

- General Debugging and Profiling Advice
- Arm Software for Debugging and Profiling
- Debugging with DDT
- Profiling with MAP
- Theta Specific Settings

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Debugging

Transforming a broken program to a working one

How? TRAFFIC!

- **T**rack the problem
- **R**eproduce
- **A**utomate - (and simplify) the test case
- **F**ind origins – where could the “infection” be from?
- **F**ocus – examine the origins
- **I**solate – narrow down the origins
- **C**orrect – fix and verify the test case is successful

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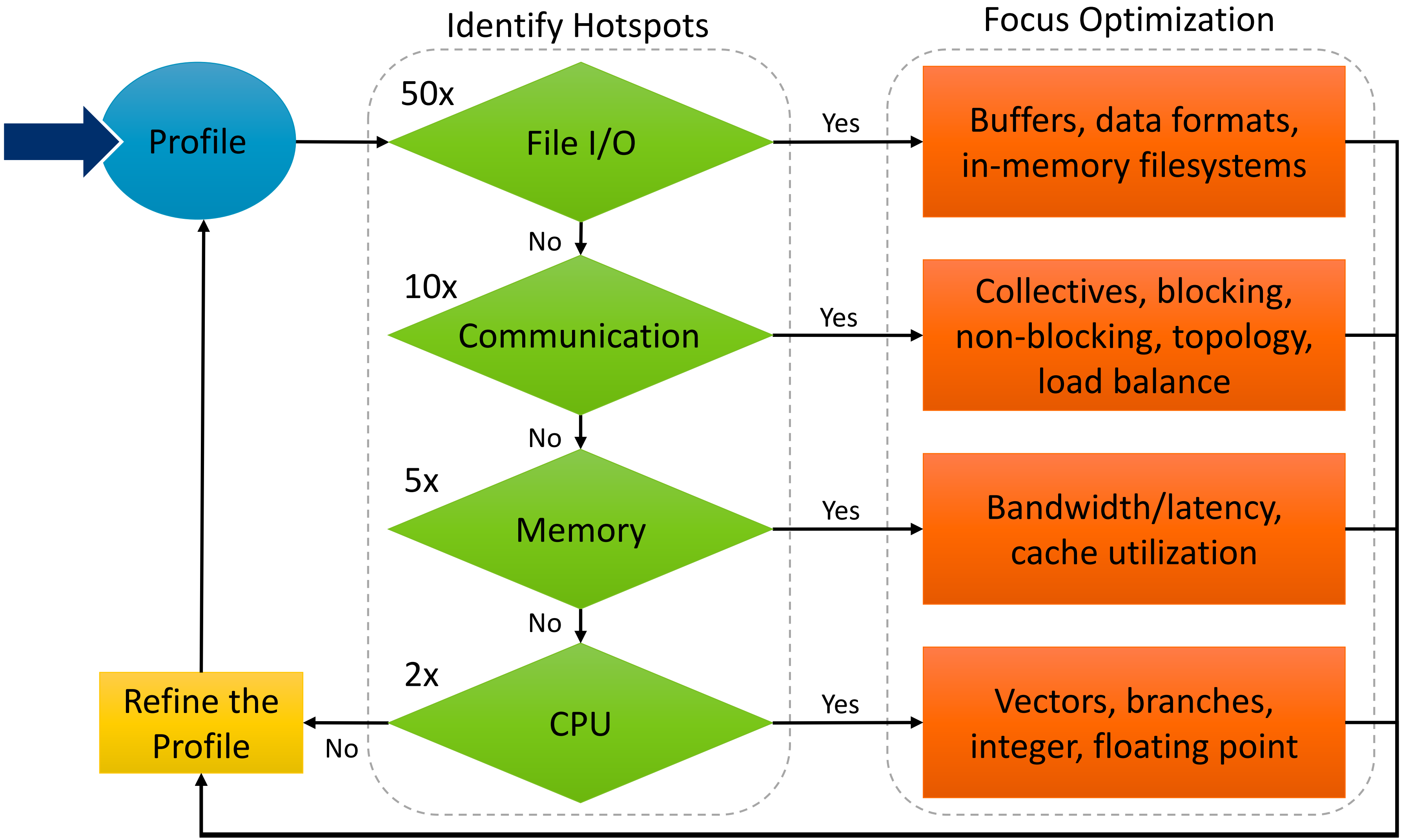
Profiling

Profiling is central to understanding and improving application performance.



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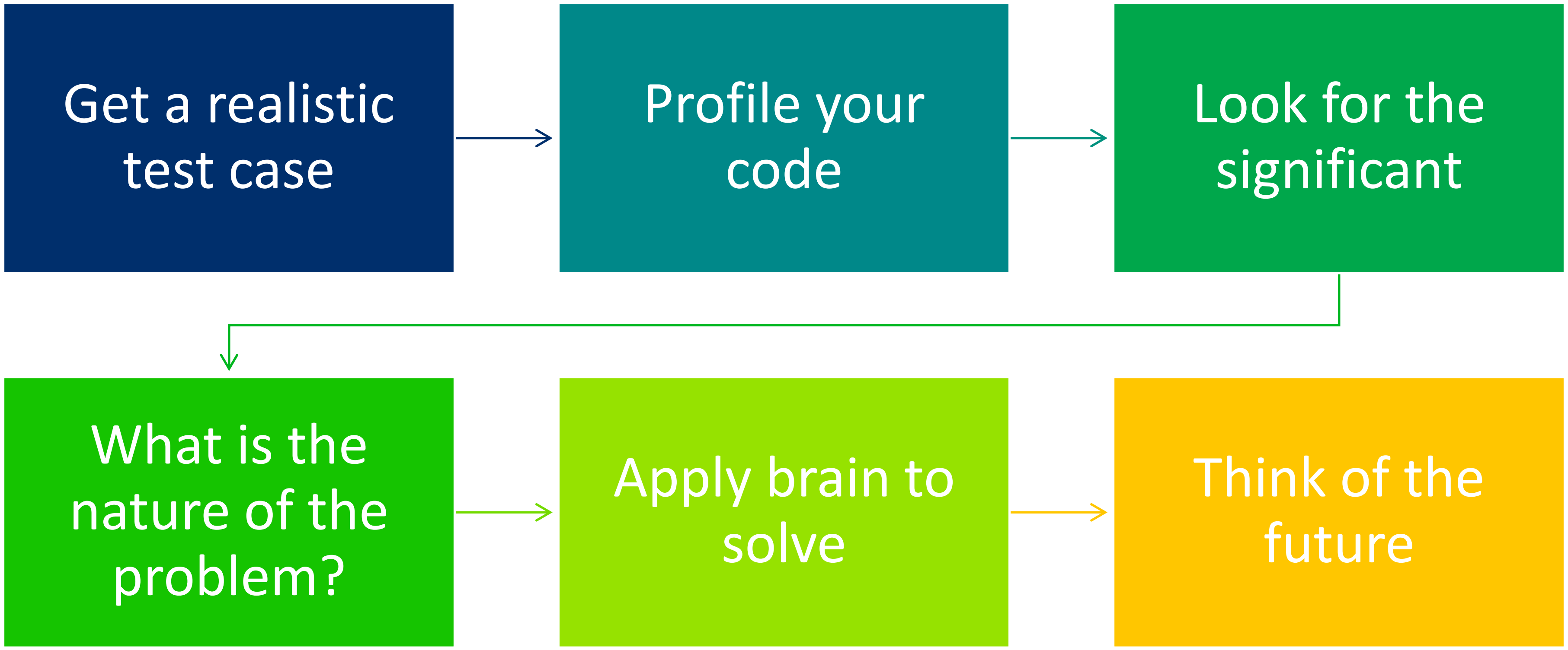
Performance Improvement Workflow



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Arm Software

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Arm Forge

An interoperable toolkit for debugging and profiling

Commercially supported by Arm

Fully Scalable

Very user-friendly

The de-facto standard for HPC development

- Available on the vast majority of the Top500 machines in the world
- Fully supported by Arm on x86, IBM Power, Nvidia GPUs, etc.

State-of-the art debugging and profiling capabilities

- Powerful and in-depth error detection mechanisms (including memory debugging)
- Sampling-based profiler to identify and understand bottlenecks
- Available at any scale (from serial to parallel applications running at petascale)

Easy to use by everyone

- Unique capabilities to simplify remote interactive sessions
- Innovative approach to present quintessential information to users

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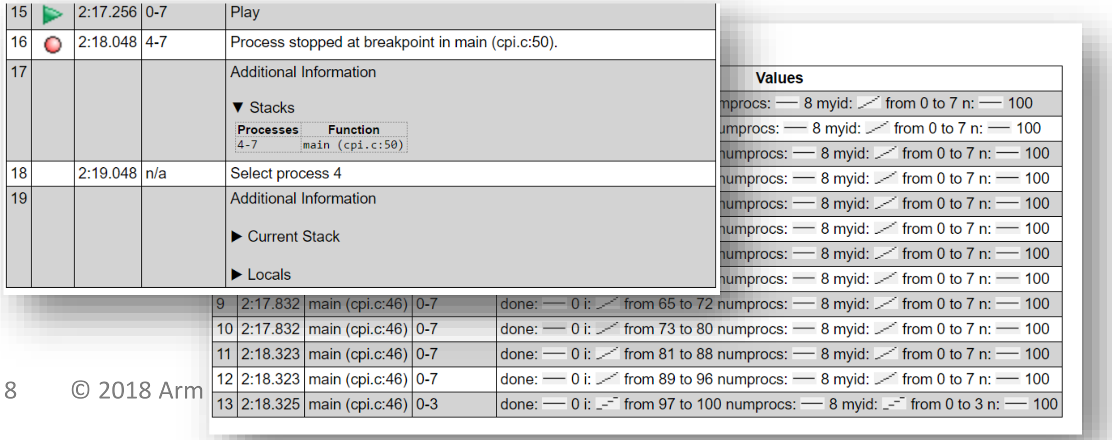
Run and ensure application correctness

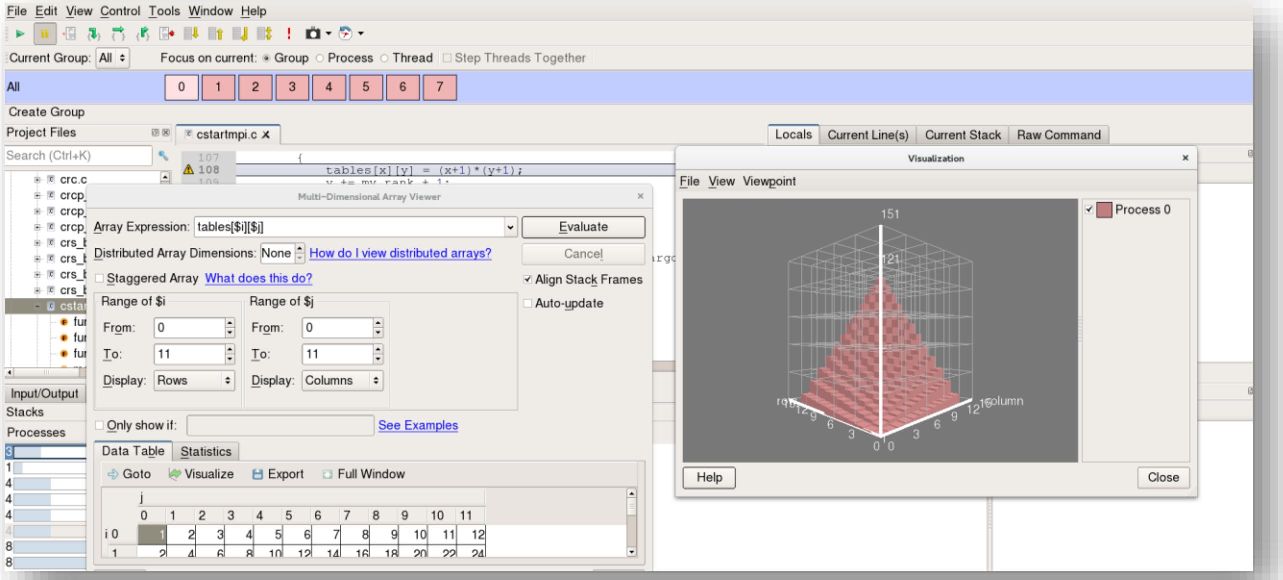
Combination of debugging and re-compilation

- Ensure application correctness with **Arm DDT scalable debugger**
- Integrate with continuous integration system.
- Use version control to track changes and leverage Forge’s built-in VCS support.

Examples:

```
$> ddt --offline mpirun -n 48 ./example
$> ddt mpirun -n 48 ./example
```





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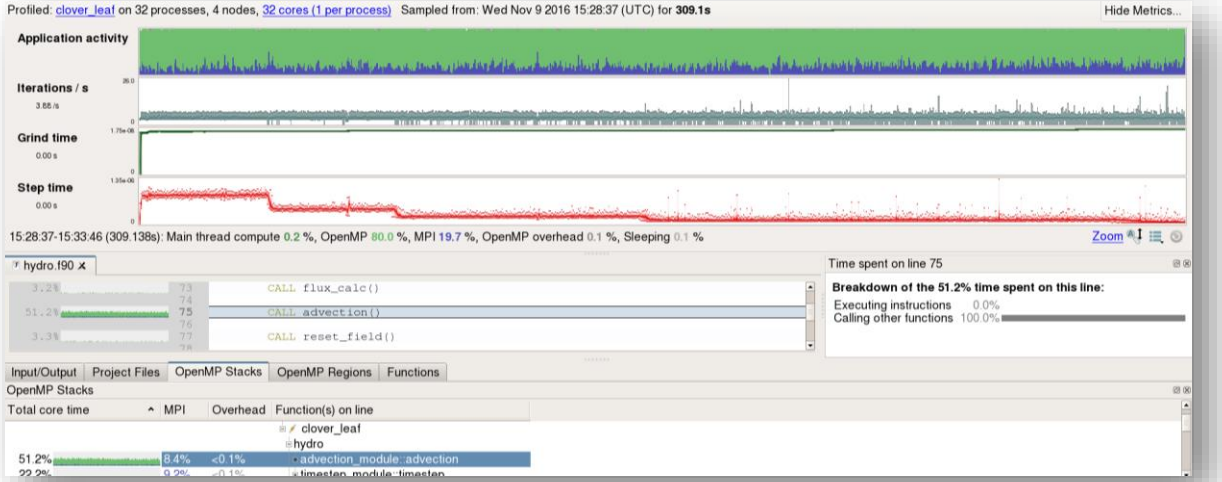
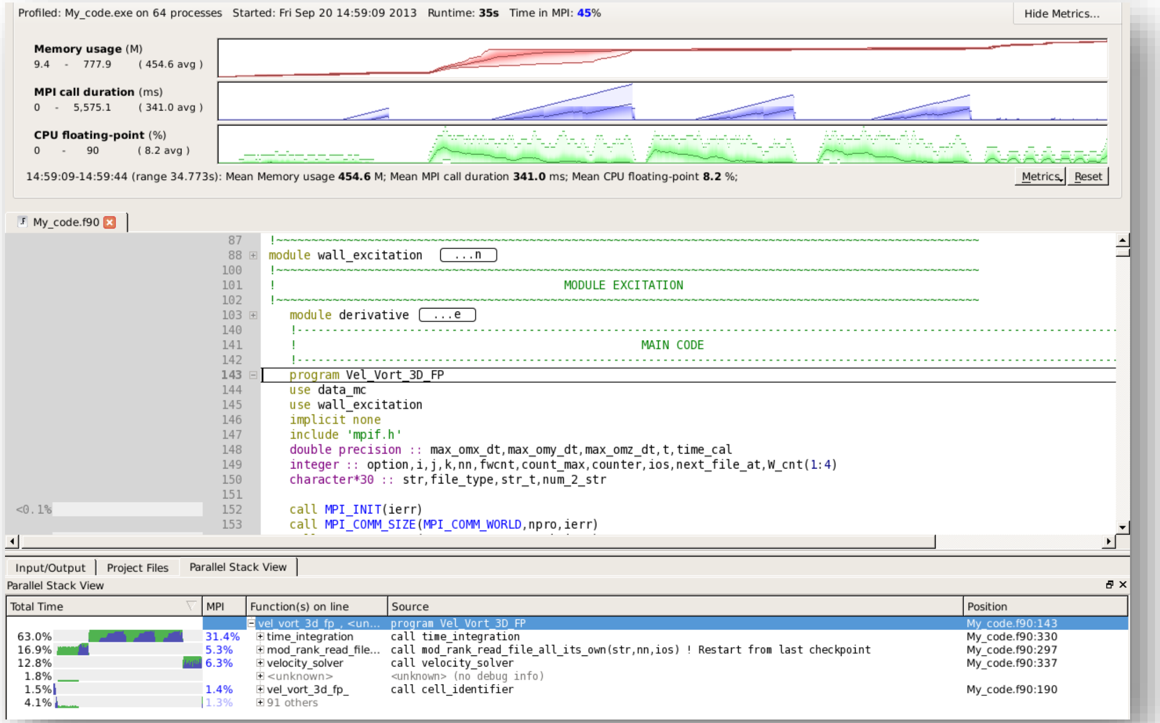
Visualize the performance of your application

- Measure all performance aspects with **Arm MAP parallel profiler**
- Identify bottlenecks and rewrite some code for better performance

Examples:

```
$> map --profile mpirun -n 48 ./example
```





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Debugging with DDT

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Arm DDT – The Debugger

Who had a rogue behaviour ?

- Merges stacks from processes and threads

Where did it happen?

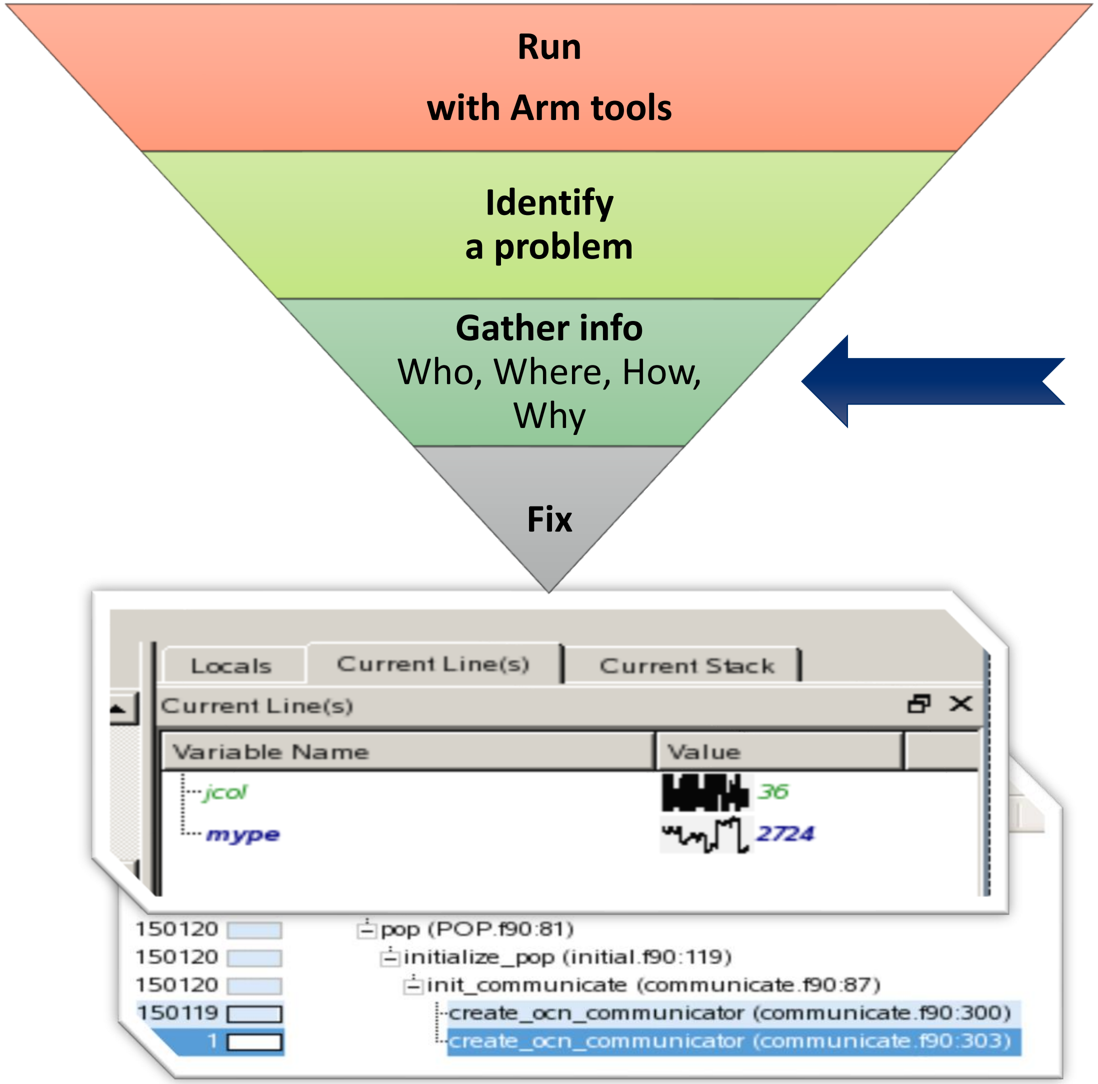
- leaps to source

How did it happen?

- Diagnostic messages
- Some faults evident instantly from source

Why did it happen?

- Unique "Smart Highlighting"
- Sparklines comparing data across processes



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Preparing Code for Use with DDT

As with any debugger, code must be compiled with the debug flag typically **`-g`**

It is recommended to turn off optimization flags i.e. **`-O0`**

Leaving optimizations turned on can cause the compiler to *optimize out* some variables and even functions making it more difficult to debug

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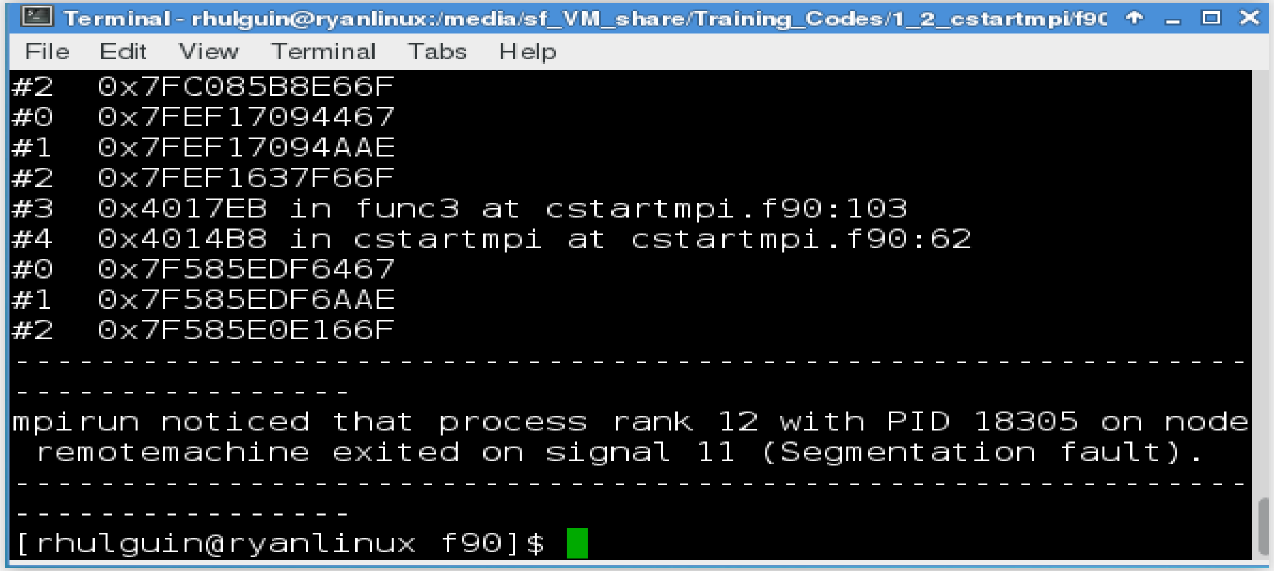
Segmentation Fault

In this example, the application crashes with a segmentation error outside of DDT.



What happens when it runs under DDT?

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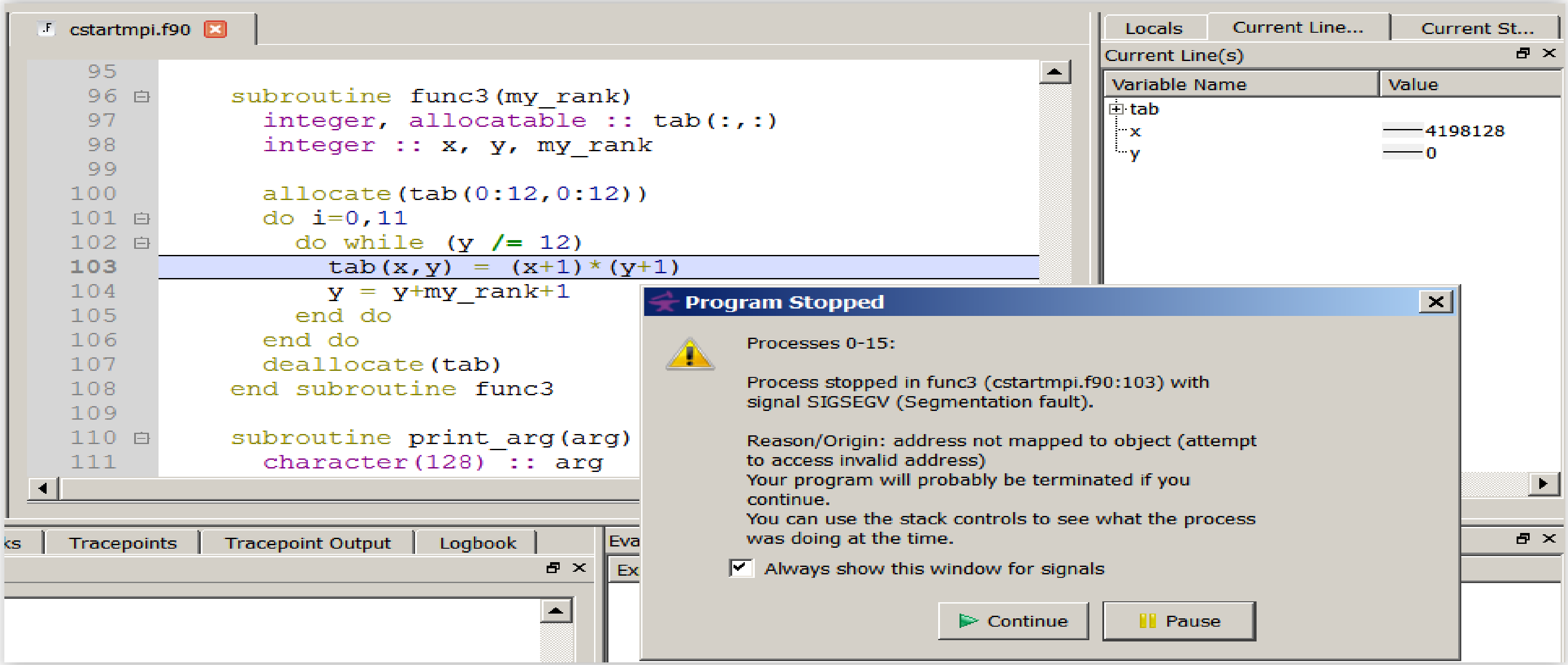
Segmentation Fault in DDT



DDT takes you to the exact line where Segmentation fault occurred, and you can pause and investigate

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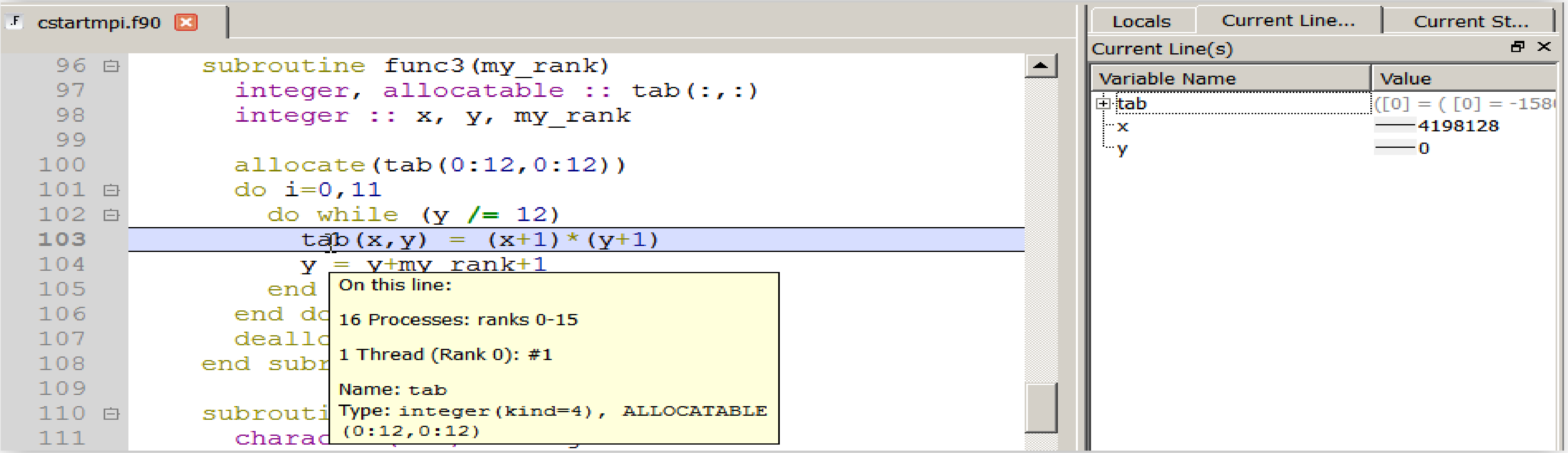
Invalid Memory Access



The array tab is a 13x13 array, but the application is trying to write a value to tab(4198128,0) which causes the segmentation fault.

`i` is not used, and **`x`** and **`y`** are not initialized

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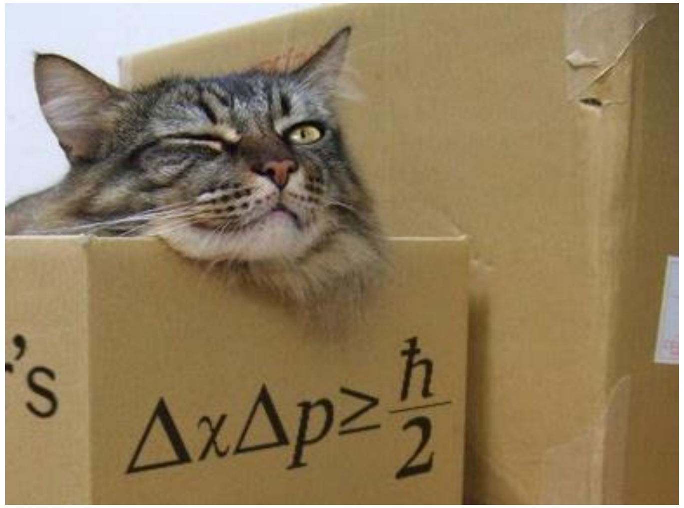
It works… Well, most of the time



SCHRODIN BUG

!

A strange behaviour where the application “sometimes” crashes is a typical sign of a memory bug

Arm DDT is able to force the crash to happen

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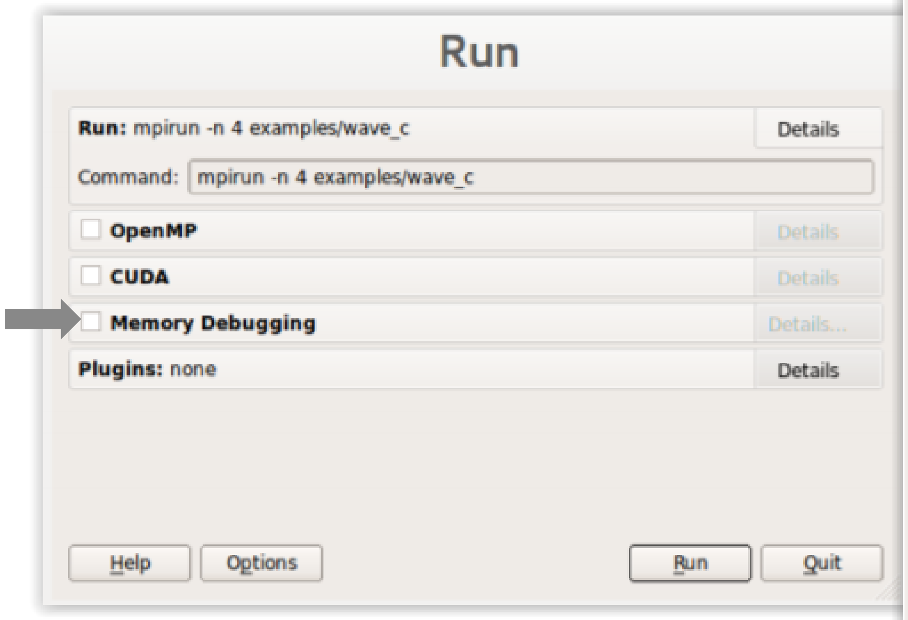
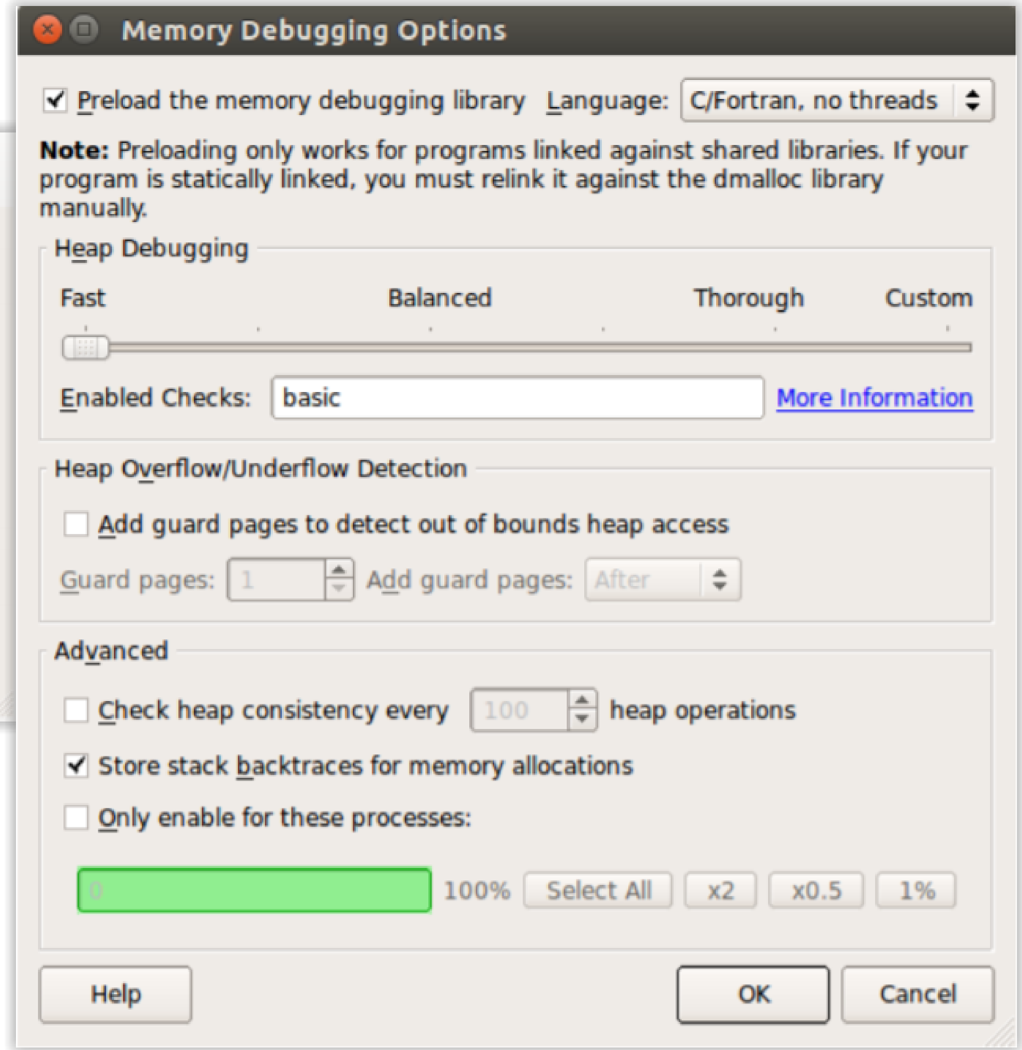
Advanced Memory Debugging





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Heap debugging options available

Fast

basic

- Detect invalid pointers passed to memory functions (e.g. malloc, free, ALLOCATE, DEALLOCATE,...)

check-fence

- Check the end of an allocation has not been overwritten when it is freed.

free-protect

- Protect freed memory (using hardware memory protection) so subsequent read/writes cause a fatal error.

Added goodiness

- Memory usage, statistics, etc.

Balanced

free-blank

- Overwrite the bytes of freed memory with a known value.

alloc-blank

- Initialise the bytes of new allocations with a known value.

check-heap

- Check for heap corruption (e.g. due to writes to invalid memory addresses).

realloc-copy

- Always copy data to a new pointer when re-allocating a memory allocation (e.g. due to realloc)

Thorough

check-blank

- Check to see if space that was blanked when a pointer was allocated/freed has been overwritten.

check-funcs

- Check the arguments of addition functions (mostly string operations) for invalid pointers.

See user-guide:

Chapter 12.3.2

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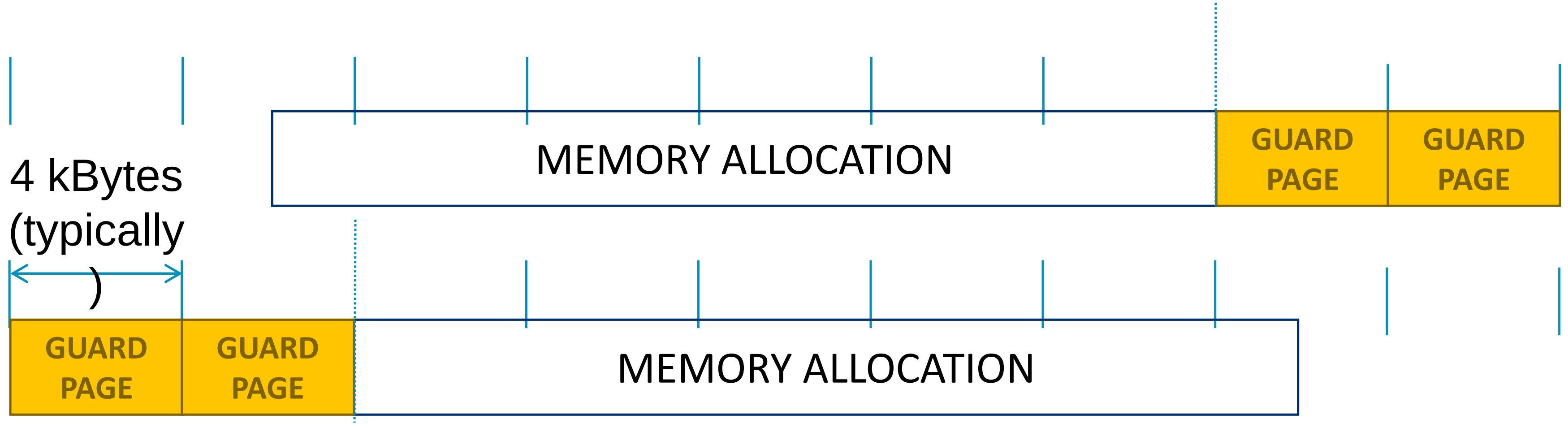
Guard pages (aka “Electric Fences”)



- **A powerful feature…:**
  - Forbids read/write on guard pages throughout the whole execution

    (because it overrides C Standard Memory Management library)
- **… to be used carefully:**
  - Kernel limitation: up to 32k guard pages max (“mprotect fails” error)
  - Beware the additional memory usage cost

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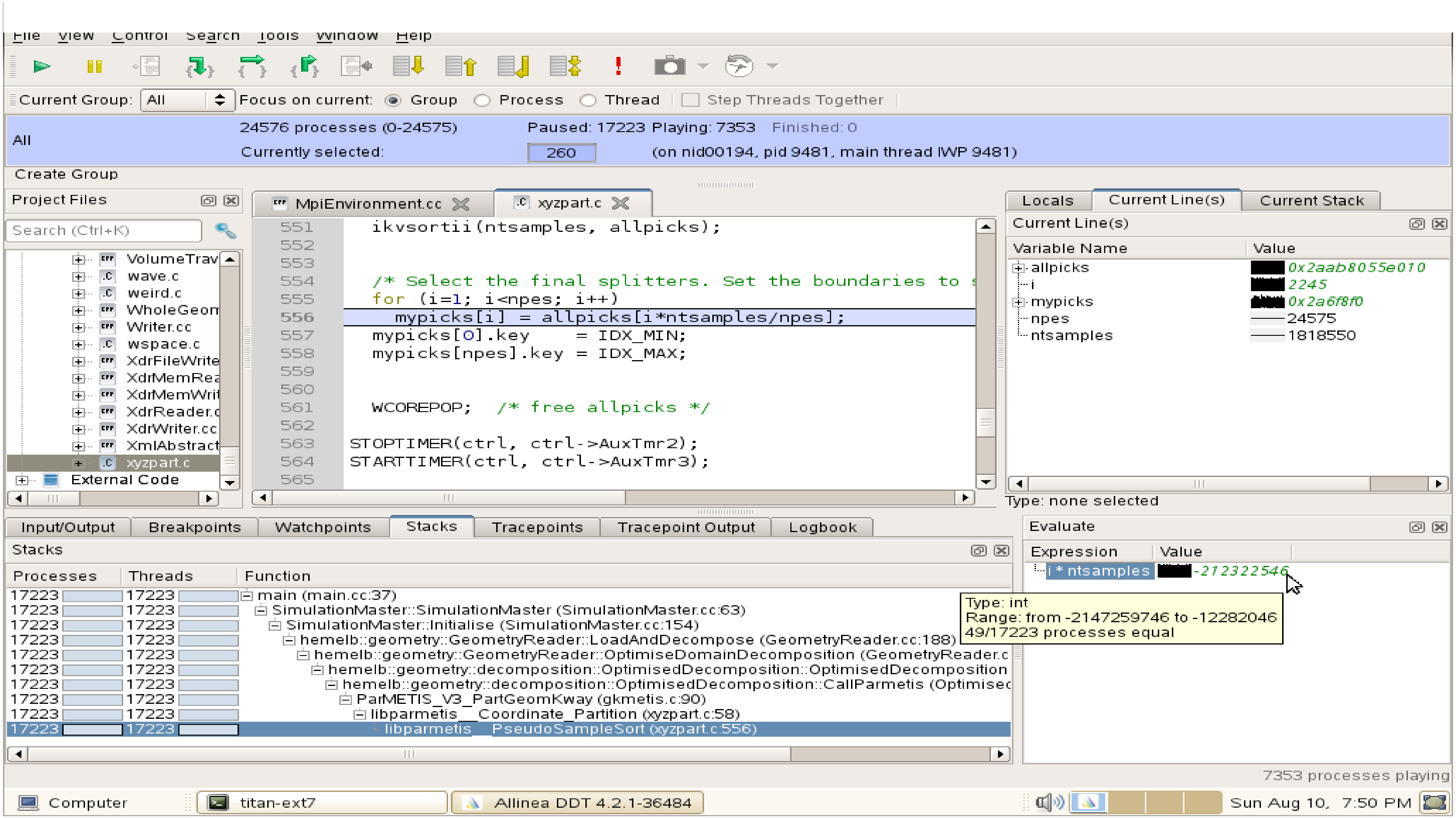
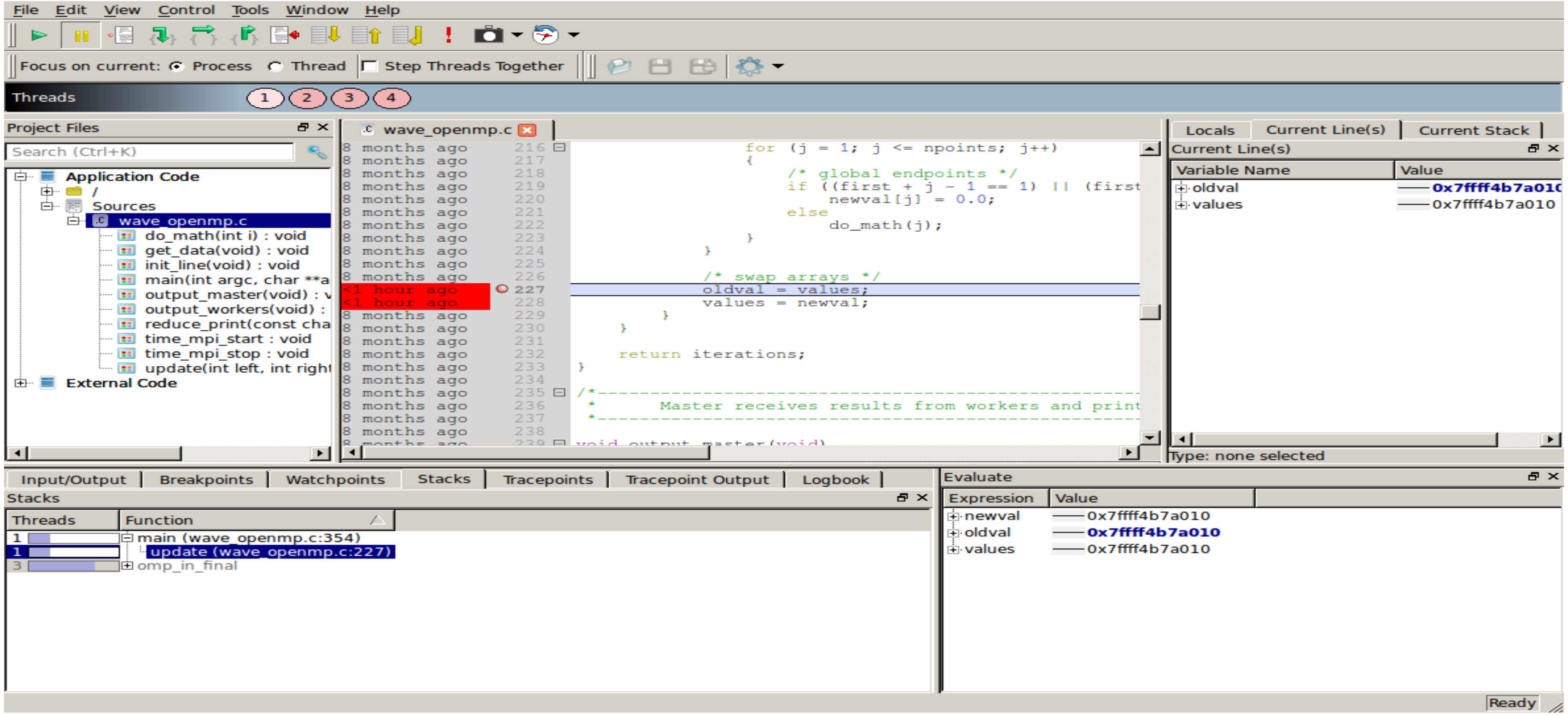

File View Control Search Tools Window Help
Current Group: All
Focus on current: Group Process Thread
Step Threads Together
All
24576 processes (0-24575)
Paused: 17223 Playing: 7353 Finished: 0
Currently selected: 260
(on nid00194, pid 9481, main thread LWP 9481)
Create Group
Project Files
Search (Ctrl+K)
VolumeTrav
wave.c
weird.c
WholeGeom
Writer.cc
wspace.c
XdrFileWrite
XdrMemRea
XdrMemWrit
XdrReader.c
XdrWriter.cc
XmlAbstract
xyzpart.c
External Code
MpiEnvironment.cc
xyzpart.c
551 ikvsortii(ntsamples, allpicks);
554 /* Select the final splitters. Set the boundaries to s
555 for (i=1; i<npes; i++)
556 mypicks[i] = allpicks[i*ntsamples/npes];
557 mypicks[0].key = IDX_MIN;
558 mypicks[npes].key = IDX_MAX;
561 WCOREPOP; /* free allpicks */
563 STOPTIMER(ctrl, ctrl->AuxTmr2);
564 STARTTIMER(ctrl, ctrl->AuxTmr3);
Locals
Current Line(s)
Current Stack
Variable Name
Value
allpicks 0x2aab8055e010
i 2245
mypicks 0x2a6f8f0
npes 24575
ntsamples 1818550
Type: none selected
Input/Output
Breakpoints
Watchpoints
Stacks
Tracepoints
Tracepoint Output
Logbook
Processes
Threads
Function
17223 17223 main (main.cc:37)
17223 17223 SimulationMaster::SimulationMaster (SimulationMaster.cc:63)
17223 17223 SimulationMaster::Initialise (SimulationMaster.cc:154)
17223 17223 hemelb::geometry::GeometryReader::LoadAndDecompose (GeometryReader.cc:188)
17223 17223 hemelb::geometry::GeometryReader::OptimiseDomainDecomposition (GeometryReader.c
17223 17223 hemelb::geometry::decomposition::OptimisedDecomposition::OptimisedDecomposition
17223 17223 hemelb::geometry::decomposition::OptimisedDecomposition::CallParmetis (Optimisec
17223 17223 ParMETIS_V3_PartGeomKway (gkmetis.c:90)
17223 17223 libparmetis__Coordinate_Partition (xyzpart.c:58)
17223 17223 libparmetis__PseudoSampleSort (xyzpart.c:556)
Evaluate
Expression
Value
i * ntsamples -212322546
Type: int
Range: from -2147259746 to -12282046
49/17223 processes equal
7353 processes playing
Computer
titan-ext7
Allinea DDT 4.2.1-36484
Sun Aug 10, 7:50 PM

New Bugs from Latest Changes



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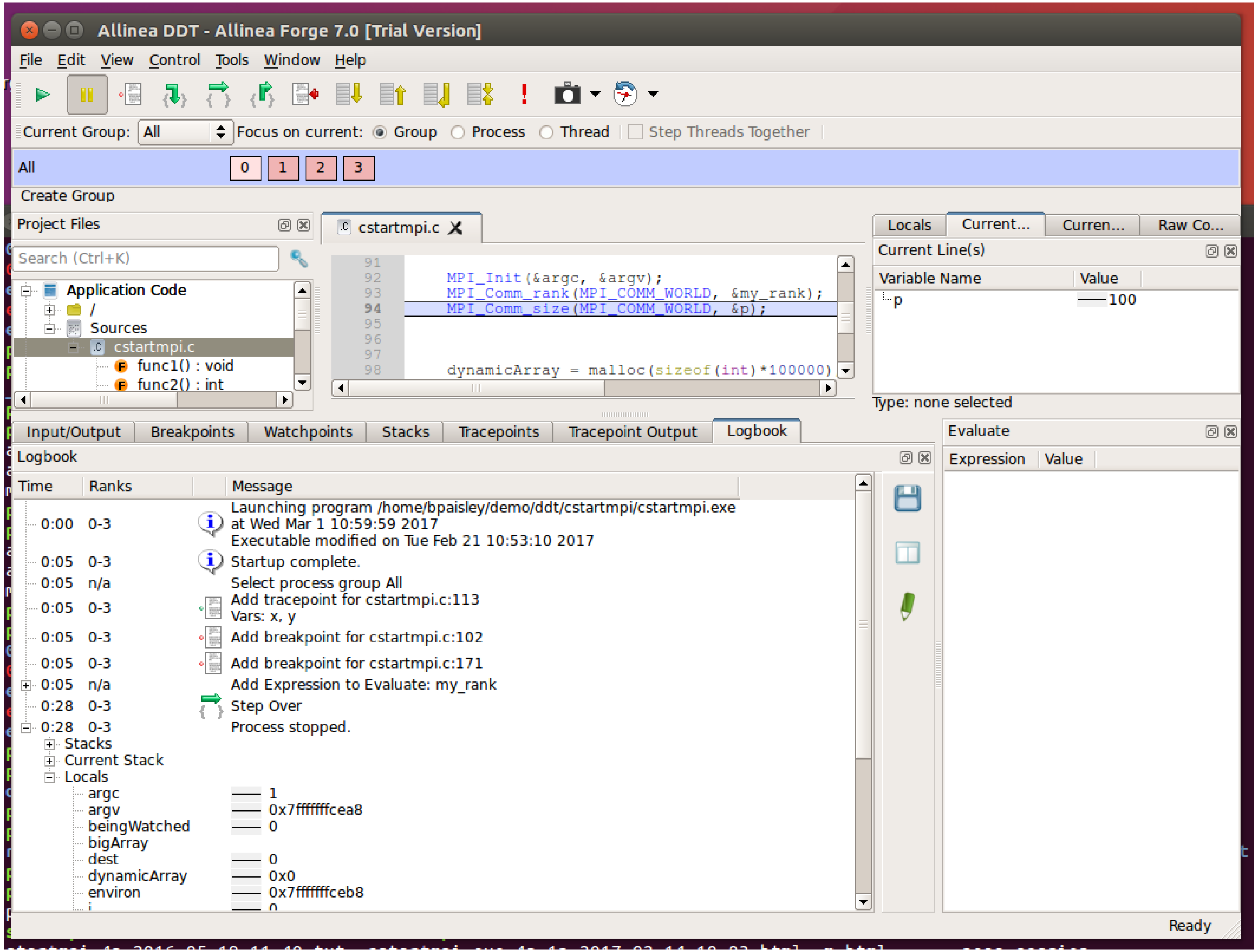
Track Your Changes in a Logbook



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Arm DDT Demo

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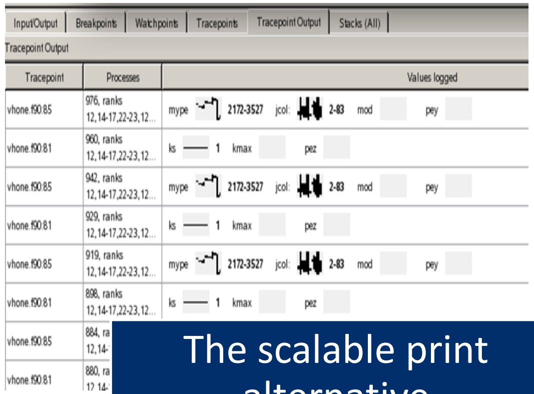
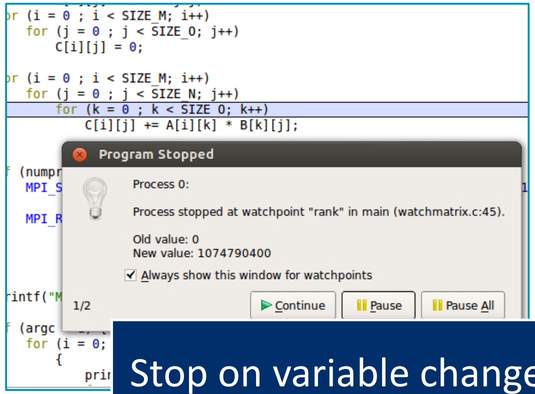
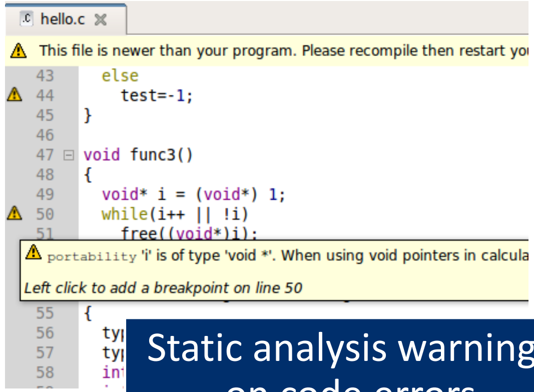
Five great things to try with Allinea DDT



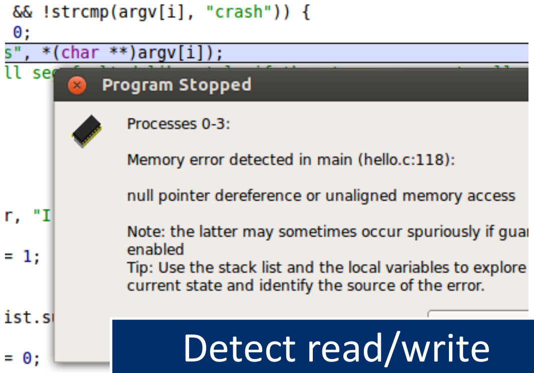
The scalable print alternative



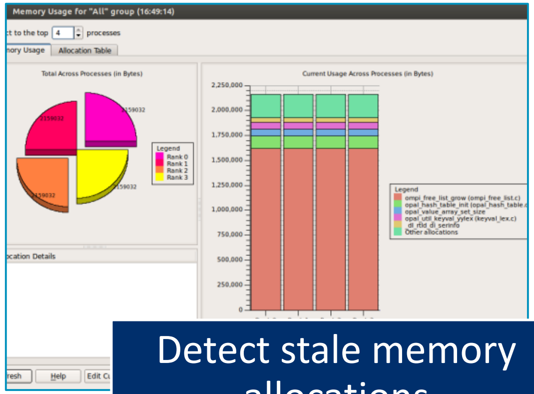
Stop on variable change



Static analysis warnings on code errors



Detect read/write beyond array bounds



Detect stale memory allocations

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Arm DDT cheat sheet

Load the environment module

- $ module load **forge/19.0.2**

Prepare the code

- $ cc **-O0 -g** myapp.c -o myapp.exe

Start Arm DDT in interactive mode

- $ **ddt** aprun -n 8 ./myapp.exe arg1 arg2

Or use the reverse connect mechanism

- On the login node:
  - $ ddt &
- (or use the remote client) **<- Preferred method**
- Then, edit the job script to run the following command and submit:
  - **ddt --connect** aprun -n 8 ./myapp.exe arg1 arg2

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Profiling with MAP

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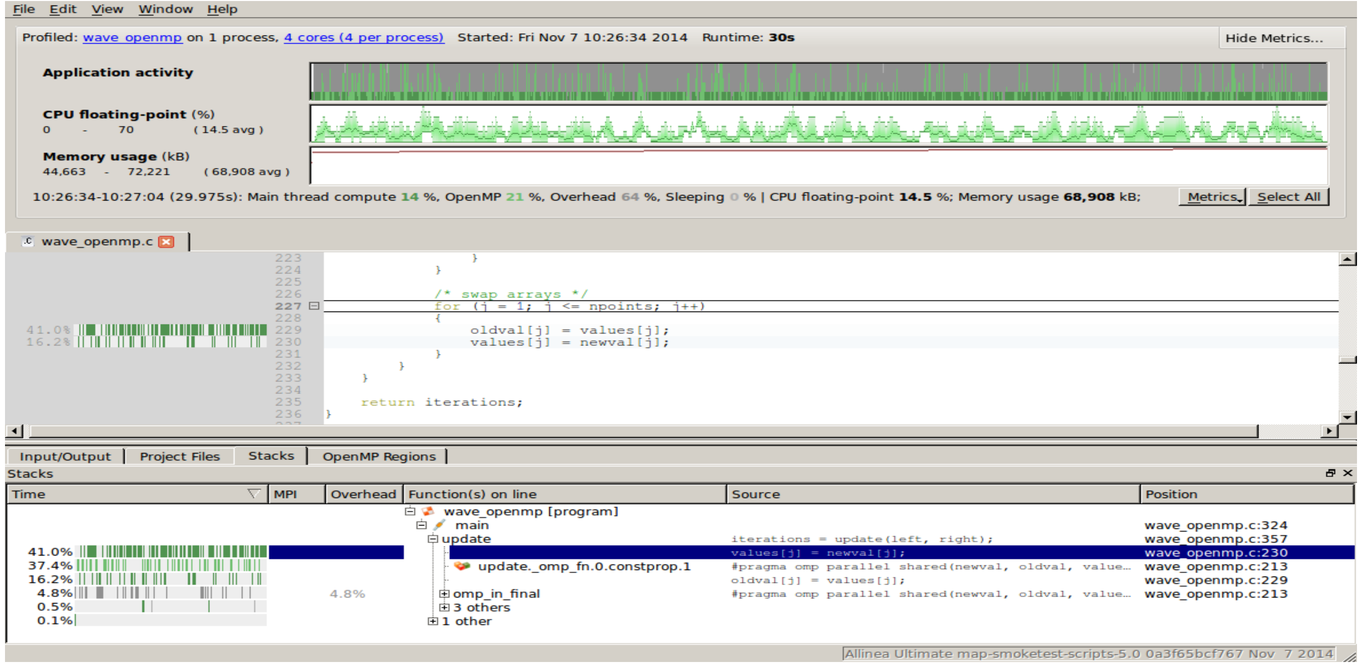
Arm MAP – The Profiler

- Small data files
- <5% slowdown
- No instrumentation
- No recompilation



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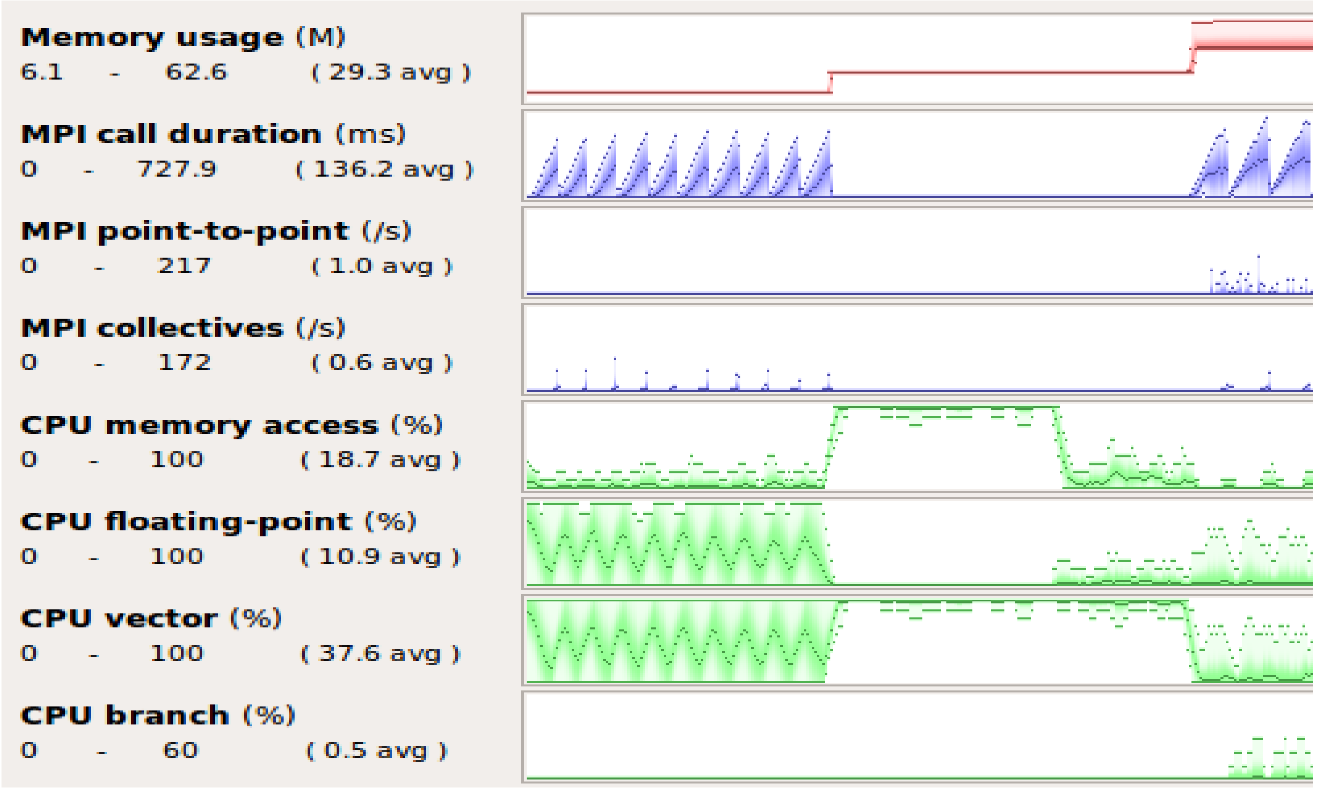
Glean Deep Insight from our Source-Level Profiler



Track memory usage across the entire application over time

Spot MPI and OpenMP imbalance and overhead

Optimize CPU memory and vectorization in loops

Detect and diagnose I/O bottlenecks at real scale

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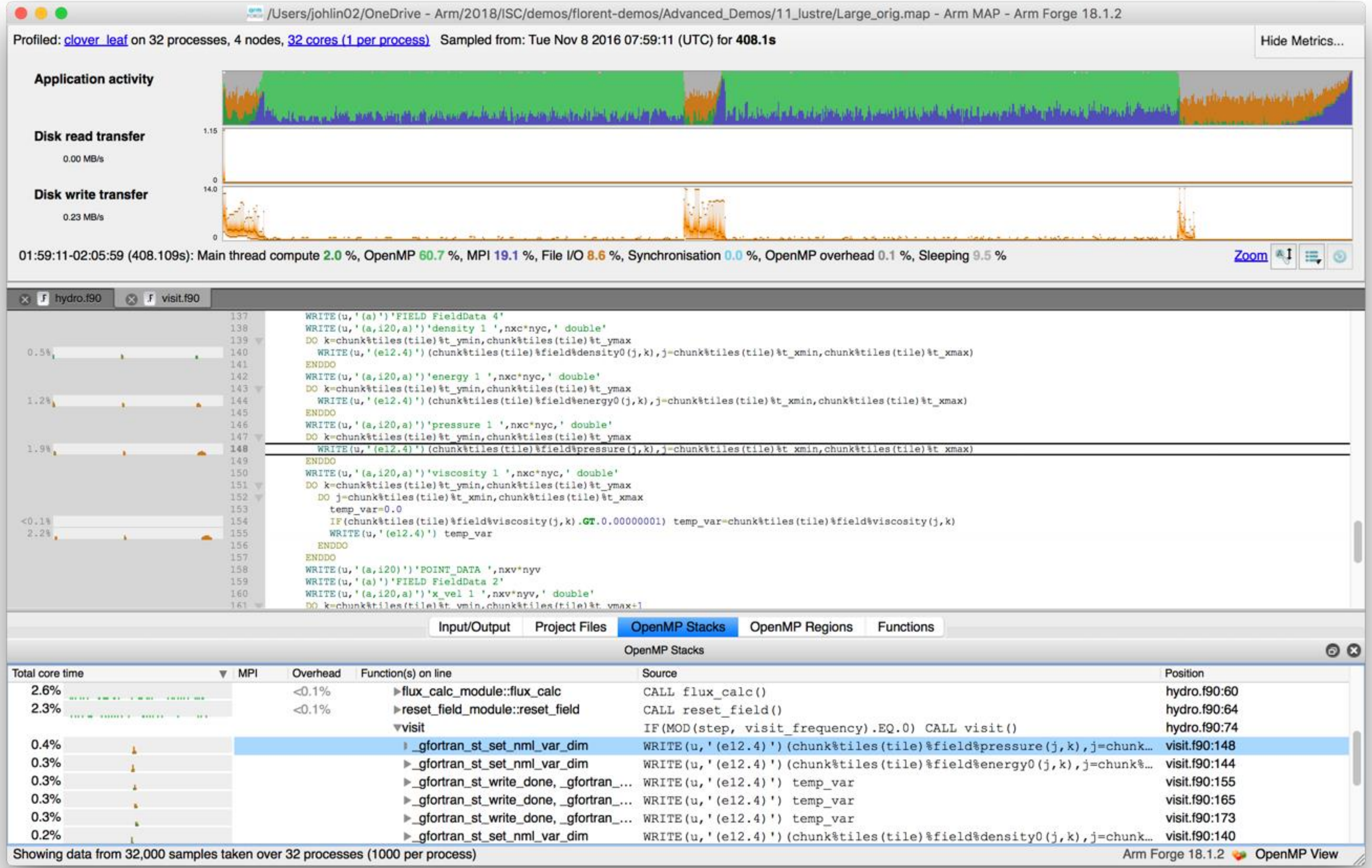
Initial profile of CloverLeaf shows surprisingly unequal I/O

Each I/O operation should take about the same time, but it's not the case.



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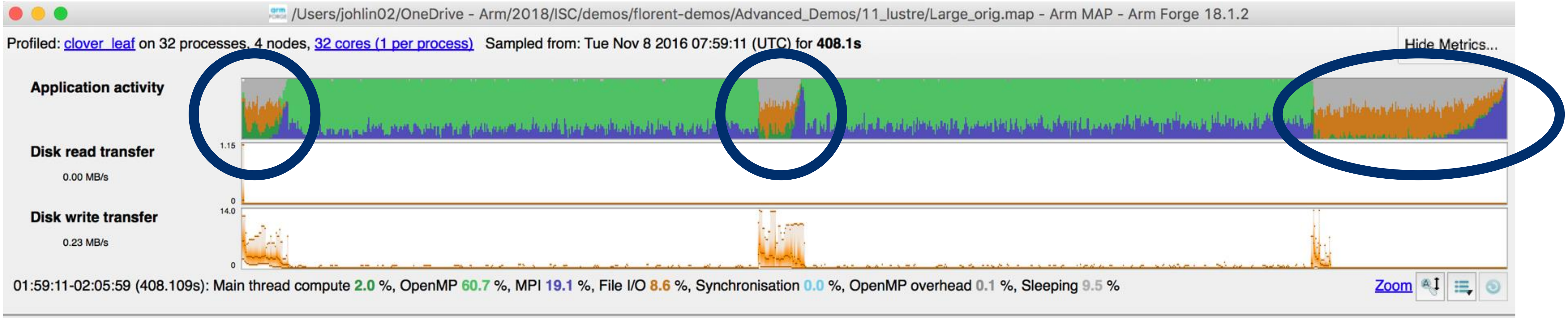
Symptoms and causes of the I/O issues

Sub-optimal file format and surprise buffering.



- Write rate is less than 14MB/s.
- Writing an ASCII output file.
- Writes not being flushed until buffer is full.
  - Some ranks have much less buffered data than others.
  - Ranks with small buffers wait in barrier for other ranks to finish flushing their buffers.

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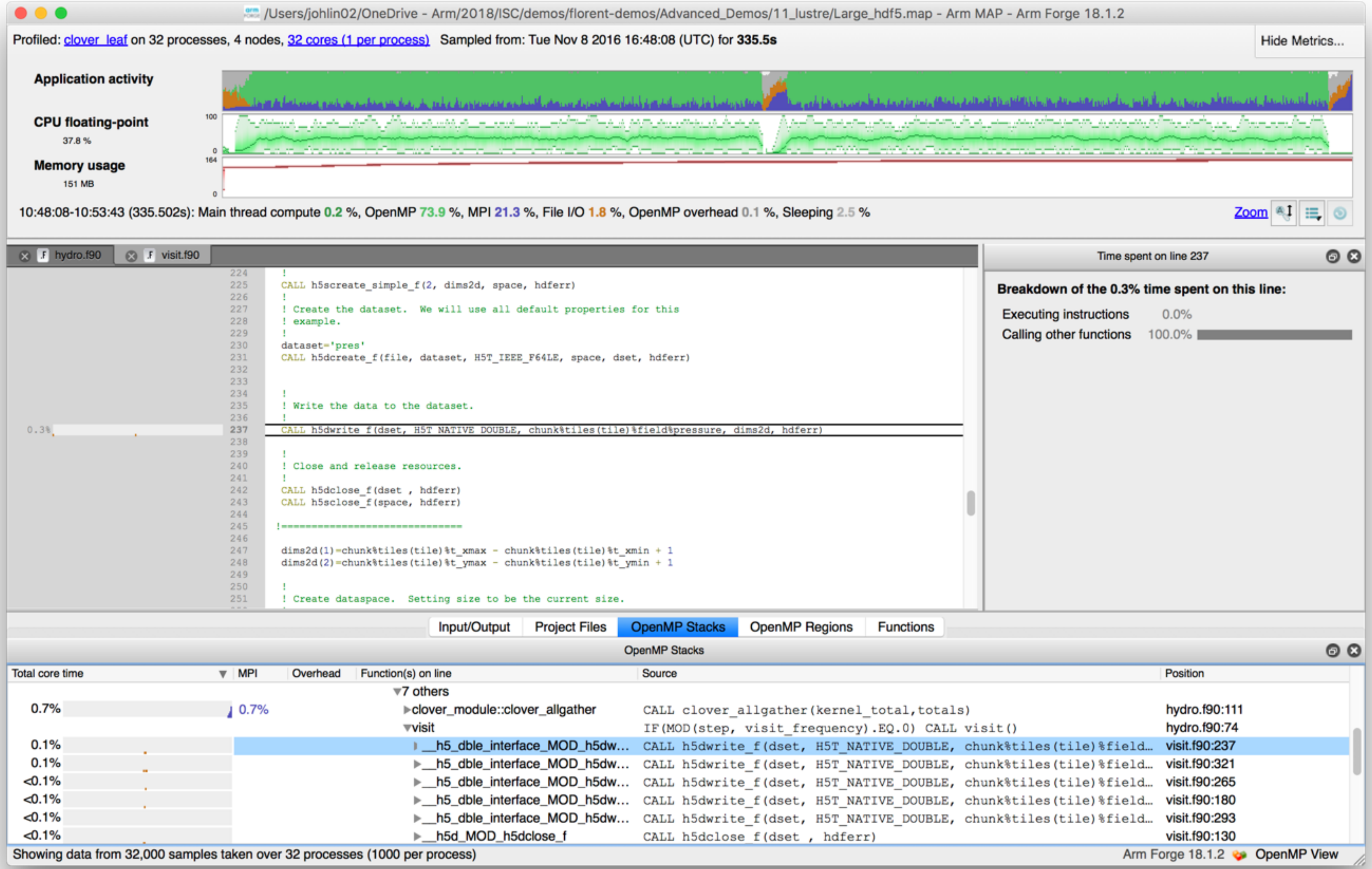
Solution: use HDF5 to write binary files

Using a library optimized for HPC I/O improves performance and portability.



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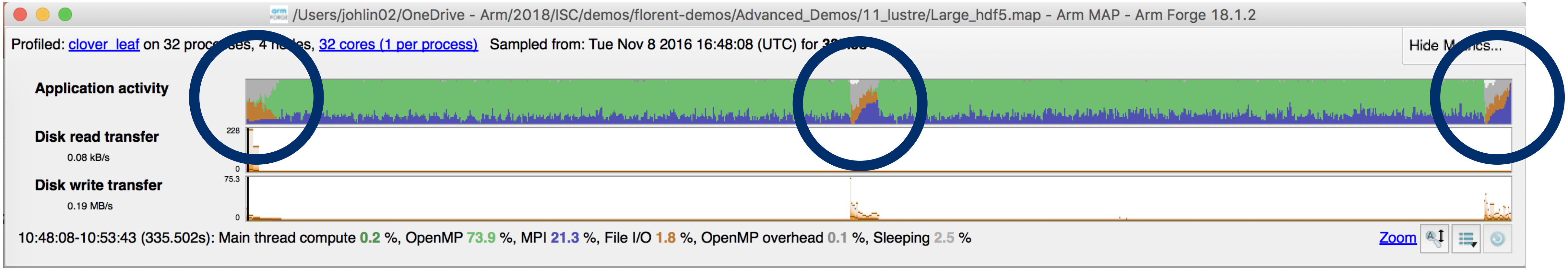
Solution: use HDF5 to write binary files

Using a library optimized for HPC I/O improves performance and portability.



- Replace Fortran write statements with HDF5 library calls.
  - Binary format reduces write volume and can improve data precision.
  - Maximum transfer rate now 75.3 MB/s, over 5x faster.
- Note MPI costs (blue) in the I/O region, so room for improvement.

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Arm MAP: Python profiling

- Launch command
  - $ **python** ./laplace1.py slow 100 100
- Profiling command
  - $ **map --profile python** ./laplace1.py slow 100 100
  - --profile: non-interactive mode
  - --output: name of output file
- Display profiling results
  - $ **map** laplace1.map

Laplace1.py

```
[…]
err = 0.0
for i in range(1, nx-1):
  for j in range(1, ny-1):
    tmp = u[i,j]
    u[i,j] = ((u[i-1, j] + u[i+1, j])*dy2 +
      (u[i, j-1] + u[i, j+1])*dx2)*dnr_inv
    diff = u[i,j] - tmp
    err += diff*diff
return numpy.sqrt(err)
[…]
```


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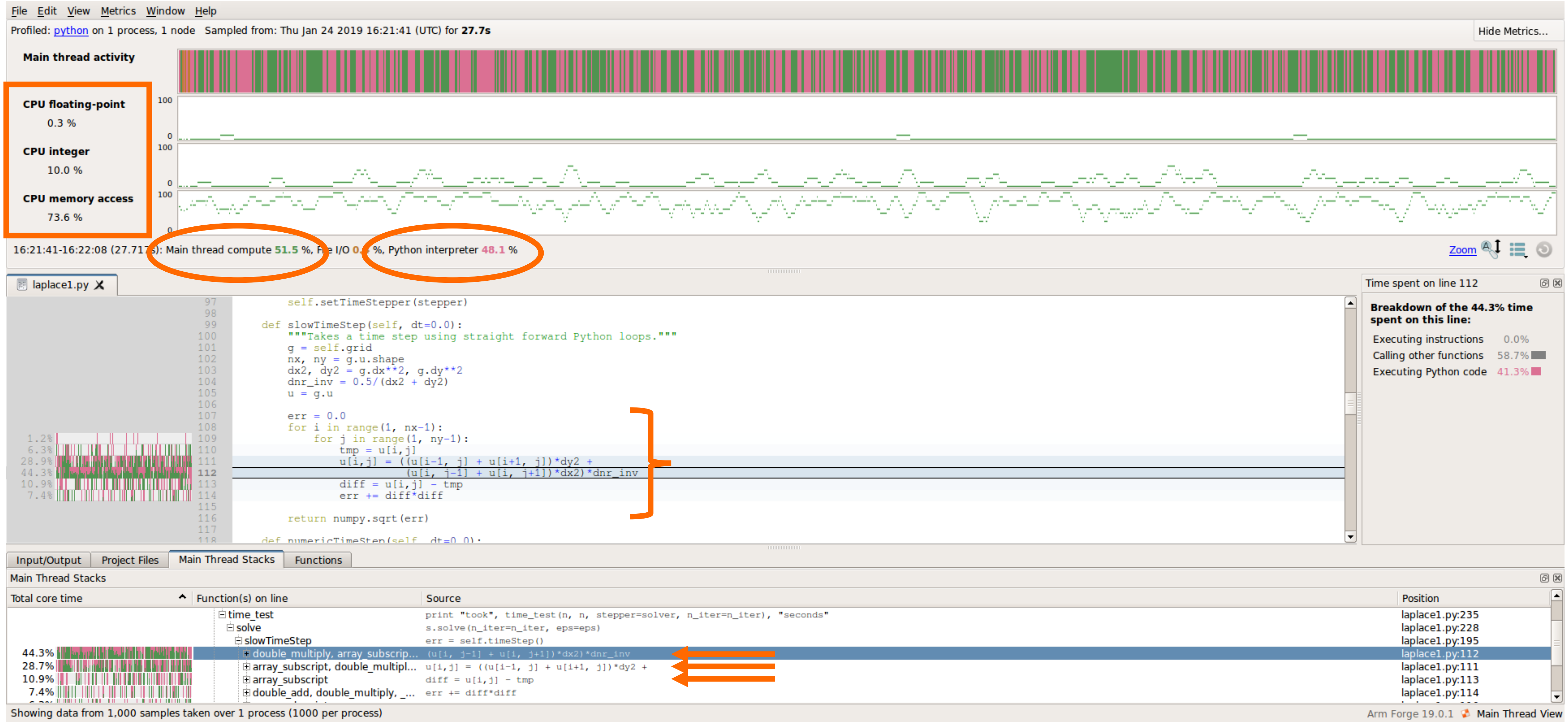
Naïve Python loop (laplace1.py slow 100 1000)



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Optimizing computation on NumPy arrays

Naïve Python loop

```
err = 0.0
for i in range(1, nx-1):
  for j in range(1, ny-1):
    tmp = u[i,j]
    u[i,j] = ((u[i-1, j] + u[i+1, j])*dy2 +
    (u[i, j-1] + u[i, j+1])*dx2)*dnr_inv
    diff = u[i,j] - tmp
    err += diff*diff
return numpy.sqrt(err)
```

NumPy loop

```
u[1:-1, 1:-1] =
    ((u[0:-2, 1:-1] + u[2:, 1:-1])*dy2 +
     (u[1:-1,0:-2] + u[1:-1, 2:])*dx2)*dnr_inv

return g.computeError()
```


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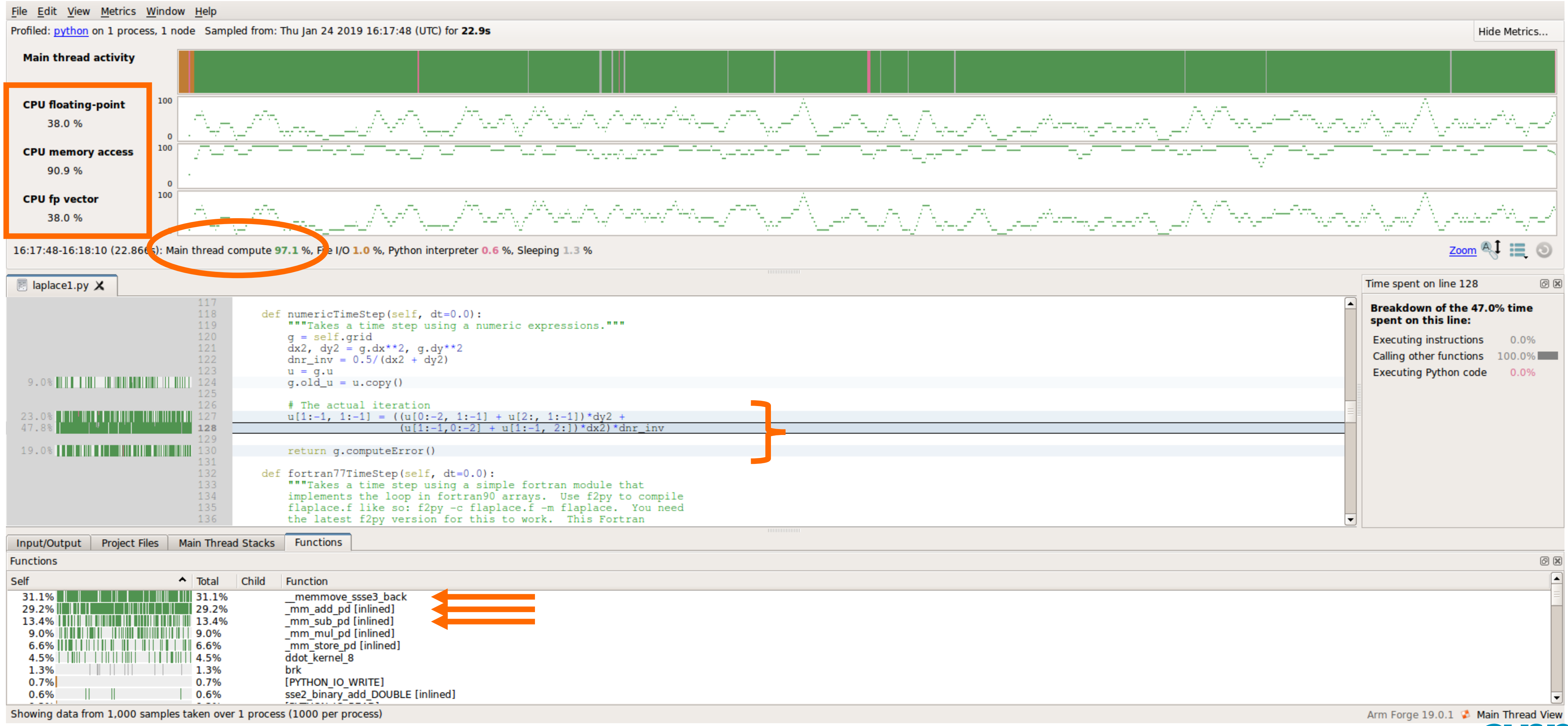
NumPy array notation (laplace1.py numeric 1000 1000)

This is 10 times more iterations than was computed in the previous profile



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Arm MAP cheat sheet

Load the environment module (manually specify version)

- $ module load **forge/19.0.2**

Generate the wrapper libraries (static is default on Theta)

- $ make-profiler-libraries --lib-type=static

Unload Darshan module (It wraps MPI calls which cannot be used with MAP)

- $ module unload darshan

Follow the instructions displayed to prepare the code

- $ cc -O3 **-g** myapp.c -o myapp.exe **-Wl,@/path/to/profiler_wrapper_libraries/allinea-profiler.ld**
- Edit the job script to run Arm MAP in “profile” mode
- $ **map --profile** aprun -n 8 ./myapp.exe arg1 arg2

Open the results

- On the login node:
  - $ map myapp_Xp_Yn_YYYY-MM-DD_HH-MM.map
- (or load the corresponding file using the remote client connected to the remote system or locally)

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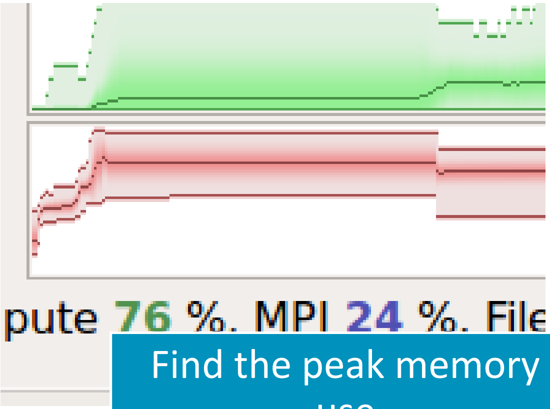
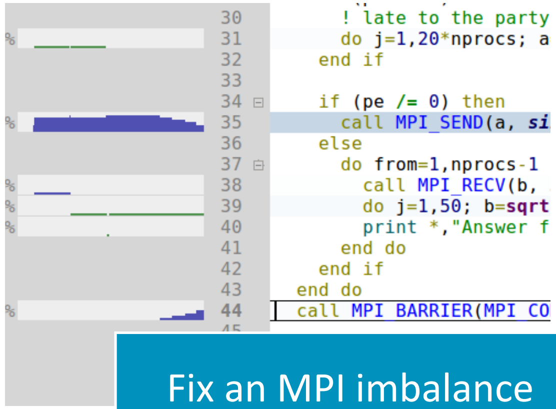
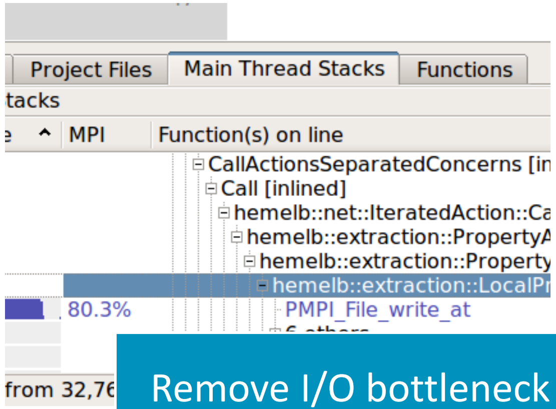
Six Great Things to Try with Allinea MAP



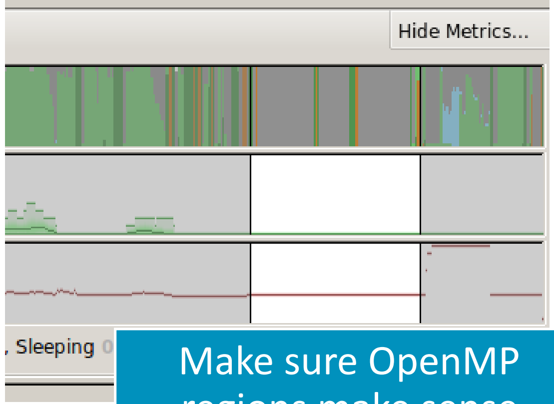
Find the peak memory use



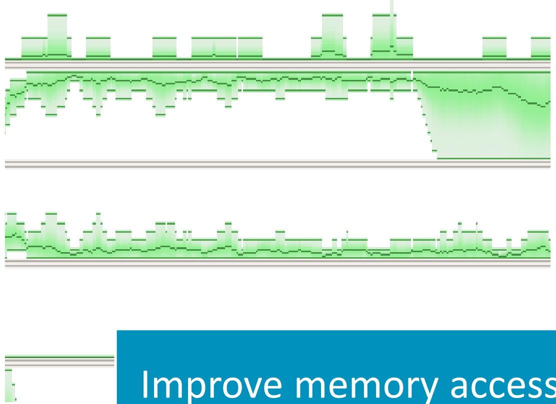
Fix an MPI imbalance



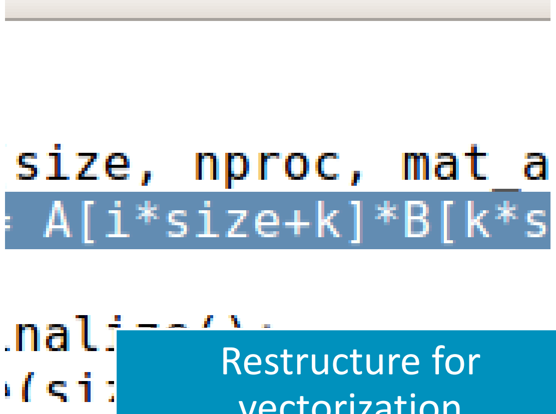
Remove I/O bottleneck



Make sure OpenMP regions make sense



Improve memory access



Restructure for vectorization

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Theta Specific Settings

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Configure the remote client

Install the Arm Remote Client

- Go to : https://developer.arm.com/products/software-development-tools/hpc/downloads/download-arm-forge

Connect to the cluster with the remote client

- Open your Remote Client
- Create a new connection: Remote Launch ➔ Configure ➔ Add
  - Hostname: `<username>@theta.alcf.anl.gov`
  - Remote installation directory:

    `/soft/debuggers/forge`
- ALCF Documentation available at https://tinyurl.com/debugging-cpw-2018-05

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Static Linking Extra Steps

To enable advanced memory debugging features, you must link explicitly against our memory libraries

Simply add the link flags to your Makefile, or however appropriate

lflags = -L/soft/debuggers/ddt/lib/64 -Wl,--undefined=malloc -ldmalloc -Wl,--allow-multiple-definition

In order to profile, static profiler libraries must be created with the command
make-profiler-libraries --lib-type=static

Instructions to link the libraries will be provided after running the above command

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Questions?

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Thank You!

Danke!

Merci!

谢谢!

ありがとう!

Gracias!

Kiitos!

감사합니다

धन्यवाद

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