

Profiling for the APinTA-PDEs project

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To do

1. Write up ITAC examples
2. Builds on Isca: GCC reference, Intel MPI+GCC for profiling, Platform optimised Intel toolchain
3. Firedrake example on Isca
4. Firedrake example with Performance Reports
5. Add examples using ARM MAP
6. Add examples using Cray PAT perftools-lite
7. Describe other capabilities of Cray PAT in addition to perftools-lite including rank re-ordering
8. Write conclusions and recommendations section: include the next steps e.g. how to switch to reference BLAS/Lapack to test the impact of maths libraries

1 Introduction

In order to understand the performance characteristics of numerical schemes, and the impact of potential optimisations it is necessary to gather information beyond simple measures of elapsed run times. A number of profiling tools exist which are capable of gathering performance information from applications parallelised using MPI. This enables information to be gathered about the application for example the time spent in MPI calls and the identification of performance problems such as load imbalance. This document gives an overview of the profiling tools available to the APinTA-PDEs project focussing on tools which can provide information about MPI and related performance issues. Although this report primarily focusses on Firedrake the profiling tools evaluated could be used for profiling other codes used by the project.

Section 2 presents the target platforms being considered in this report and reviews the hardware and software available on these systems.

2 Target platforms

An overview of the hardware in the target platforms for this project is shown in Table 1. The target HPC platforms are Archer-2 (national tier-1), Isambard (national tier-2) and Isca (local tier-3). Isambard has two separate systems based on the ARM64 architecture: the XCI system which is an established production system, and the A64FX system which is a newer system. The A64FX system should be considered a stretch objective as the hardware and software are relatively new and less well tested. We have also purchased a local server which is designed to be similar to an Archer compute node, although it will run Ubuntu which will make it easier to build Firedrake. The server can function as a reference installation as it will use an unmodified Firedrake install script, rather than the more customised installations on the HPC platforms which will use non-standard components, for example MPI libraries and maths libraries.

An overview of the software stacks on the target platforms is shown in Table 2. Each HPC platform has the GNU compilers, a compiler from the processor vendor (AMD, Intel, ARM and Fujitsu) and Cray systems also have the Cray compiler¹. The GNU compilers are the one compiler family which is available on all the target platforms.

On the Cray systems compilation is handled by wrapper scripts from the Cray Programming Environment. The wrapper script can run different compilers depending on which programming environment module is loaded at compile time (e.g. if `PrgEnv-cray` is loaded then `cc` calls the Cray C compiler and if `PrgEnv-gnu` is loaded `cc` calls the GNU C compiler). The MPI library and maths library (Cray libsci) are then linked by the wrapper script. On Cray systems the standard

¹On Isambard A64FX run `module use /lustre/software/aarch64/modulefiles` to make extra modules available

System	Processor	Cores/node	Memory/node	Interconnect
Archer-2	AMD x86_64	128	256 GB DRAM	HPE Cray Slingshot
Isambard XCI	Thunder X2 ARM64	64	256 GB DRAM	Cray Aries
Isambard A64FX	Fujitsu A64FX ARM64	48	32 GB HBM	Mellanox Infiniband
Isca	Intel x86_64	16/20	128 GB DRAM	Mellanox Infiniband
Server	AMD x86_64	128	256 GB DRAM	None

Table 1: Target platform hardware specifications. The Isambard A64FX platform has high bandwidth memory (HBM) which should give better performance than DRAM but has a smaller capacity.

System	Compilers	MPI libraries	Maths lib.	Profilers
Archer-2	Cray, GNU, AOCC	Cray MPICH2	Cray libsci	Cray
Isambard XCI	Cray, GNU, ARM	Cray MPICH2	Cray libsci	Cray, ARM
Isambard A64FX	Cray, GNU, ARM, Fujitsu	Cray MVAPICH2	Cray libsci	ARM
Isca (GCC)	GNU	OpenMPI	OpenBLAS	None
Isca (Intel)	Intel	Intel	Intel MKL	Intel
Server	GNU	MPICH?	???	None

Table 2: Software stacks on target platforms. AOCC is the AMD Optimizing Compiler Collection. Intel MPI and MVAPICH are MPICH derivatives which support an Infiniband interconnect. The Cray profiler is Cray Performance Analysis Tools (PAT), the ARM profilers are part of the ARM Forge tool suite and the Intel profilers are part of the Intel Parallel Studio suite. The A64FX system did not appear to have a perftools module.

profiling tool is Cray Performance Analysis Tools (PAT) but on Isambard the profiling tools from the ARM Forge suite² are also available.

The software environment on Isca is managed using Easybuild which has the concept of a toolchain. There are two toolchains on Isca: the GCC-foss toolchain and the Intel toolchain. Each toolchain has a different MPI library and maths library. Intel Parallel Studio has an MPI profiling tool called Intel Trace Analyzer and Collector (ITAC) which needs to use Intel MPI. However the Intel toolchain can be used with GNU compilers such that the Intel MPI library wrapper scripts call the GNU compilers; the wrapper script `mpiicc` is the MPI-enabled wrapper for the Intel C compiler with Intel MPI, whereas `mpicc` is the MPI-enabled wrapper for the GNU C compiler with Intel MPI. Hence is it possible to use the GNU compilers with the Intel MPI library which allows profiling with Intel Trace Analyzer and Collector.

The server does not currently have any profiling software but Intel’s Parallel Studio product is now available for free download as part of the HPC toolkit from the newer OneAPI product³. There is also the option of obtaining an evaluation licence for ARM Forge to test these tools on the server.

Recommendation: standardise on the GNU compilers for all platforms to avoid having to manage too many different builds. This also takes the compiler out of the performance equation (different GCC versions notwithstanding).

3 Test cases

The profilers will be tested using three different versions of a Mandelbrot set calculation. The different versions parallelise the calculation in different ways and have different performance characteristics:

- Version 1: divides the computational domain into equal sized chunks along the real axis. This introduces a load imbalance.

²ARM Forge was previously known as Allinea Forge

³<https://software.intel.com/content/www/us/en/develop/tools/oneapi/all-toolkits.html>

- Version 2: similar to version 1 but interleaves the iterations on the real axis to fix the load balance. This version (and version 1) pack a 2D array into a 1D buffer which is communicated using an `MPI_Reduce` and constitutes an overhead.
- Version 3: implements a manager-worker pattern for distributing the iterations to ensure load balancing. This replaces the `MPI_Reduce` with point-to-point communication between the manager-process and the worker processes. One process (the manager process) does not perform any calculations which adversely affects performance with small numbers of MPI processes. However this version scales better to larger numbers of MPI processes.

The following tests will be used to demonstrate the profiling tools:

- Test 1: version 1, no I/O, 4 MPI processes
- Test 2: version 1, with I/O, 4 MPI processes
- Test 3: version 2, no I/O, 4 MPI processes
- Test 4: version 3, no I/O, 4 MPI processes
- Test 5: version 3, no I/O, 16 MPI processes

These examples show the load imbalance vs. overhead (version 1 vs. version 2) and can the difference between collectives and point-to-point communication (version 2 vs version 3). The I/O is performed by writing to an ASCII file which causes a substantial overhead compared to the case without I/O.

Test with a Firedrake example e.g. high resolution DG advection. This will show point-to-point communication pattern from domain decomposition.

4 Profiling tools

Within Firedrake itself performance information can be obtained from PETSc by adding the `-log_view` flag when running Firedrake. There is also the ability to time sections of code by adding a PyOP2 timed stage. These options will be available on all platforms when Firedrake is the target application but the rest of this report will look at how external profilers can be used to obtain extra information. There are external profilers already installed on the target platforms with different platforms having different profiling tool available:

- ARM Forge (currently only licensed on Isambard)
- Intel Parallel Studio (Intel MPI only)
- Cray PAT (Cray systems only)

Each of these products is a suite of tools and this report will focus on the tools appropriate for understanding the performance of MPI applications.

4.1 Intel Parallel Studio

The MPI profiler in Intel Parallel Studio is called Intel Trace Analyzer and Collector (ITAC). Other profiling tools are available which provide information node-level performance.

4.1.1 Intel Trace Analyzer and Collector

In this example the Mandelbrot executable will be build with MPI tracing enabled. Firstly load the modules for the Intel compilers and the ITAC tool.

```
> module load intel/2017b
> module load itac/2017.1.024
```

Then compile the executable with `-trace` flag:

```
> mpicc -trace -o mandelbrot mandelbrot_mpi.c
```

The `intel` and `itac` modules need to be loaded in the job script but no other modifications are required to the job script. When the job runs a number of additional files are generated, including a file with a `.stf` extension which is the trace file. The profiling output can be viewed opening the trace file with the Trace Analyzer GUI:

```
> traceanalyzer.bin mandelbrot_mpi.stf &
```

Test 1: Figure 1 (top) shows the opening summary page for test 1 (Mandelbrot version 1, no I/O, 4 MPI processes). This test has a load imbalance which is seen as a large fraction of time spent in `MPI_Reduce`. The reduce itself is not time consuming (all communication takes place on the same compute node) but this is the blocking collective where the MPI processes synchronise. This can be seen more clearly in the lower panel of figure 1 which shows the event timeline. To view the event timeline as seen in this figure:

- Click the continue button on the summary page
- Select **Charts** → **Event Timeline** to open a new pane showing process activity over time.
- In the lower left pane select the **Load Balance** tab and click the **Show pies** button.
- Right click on a red MPI section in the timeline and choose **Ungroup MPI** from the drop down menu

The timeline shows that process 2 is taking much longer to complete its than the other processes which has resulted in processes 0, 1 and 3 waiting at the `MPI_Reduce` call.

Test 2: this test is similar to test 1 but has I/O enabled. The summary page (see figure 2) shows a significantly longer runtime (450s vs. 250s) and significant time spent in `MPI_Barrier`. The I/O is carried by process 0 which causes all the other processes to wait at a barrier at the end of the program (processes are synchronised before a final run time is reported by process 0). The effect of switching on I/O has been to introduce another load imbalance, this time with process 0 working and all other processes waiting. This can be seen clearly in the timeline where there are two distinct phases both of which have a load imbalance, but is less clear from the summary or pie charts alone.

Test 3:

Test 4: Charts → message profile

Test 5:

4.1.2 Firedrake

Previously working on Isca with the Intel build.

4.2 ARM Forge

The ARM Forge suite of development tools is available on the Isambard system. ARM Forge includes two performance tools: “Performance Reports” and “MAP”. ARM MAP is a profiler which is part of the ARM Forge suite and it can profile C++, C, Fortran and Python⁴.

4.2.1 Performance Reports

The documentation for Performance Reports says that on Cray systems dynamic linking or explicit linking with the profiling libraries is required⁵. However in the latest Cray compilers dynamic linking is the default so no changes are required to the build process. The following shows an example session and output from Performance Reports on the Isambard XCI system.

No changes are required at compile time so simply compile the executable as normal. For this example the GCC compiler will be used:

⁴<https://www.arm.com/products/development-tools/server-and-hpc/forgemap>

⁵<https://developer.arm.com/documentation/101136/2102/Performance-Reports/Get-started-with-Performance-Reports/Compile-on-Cray-X-series-systems>

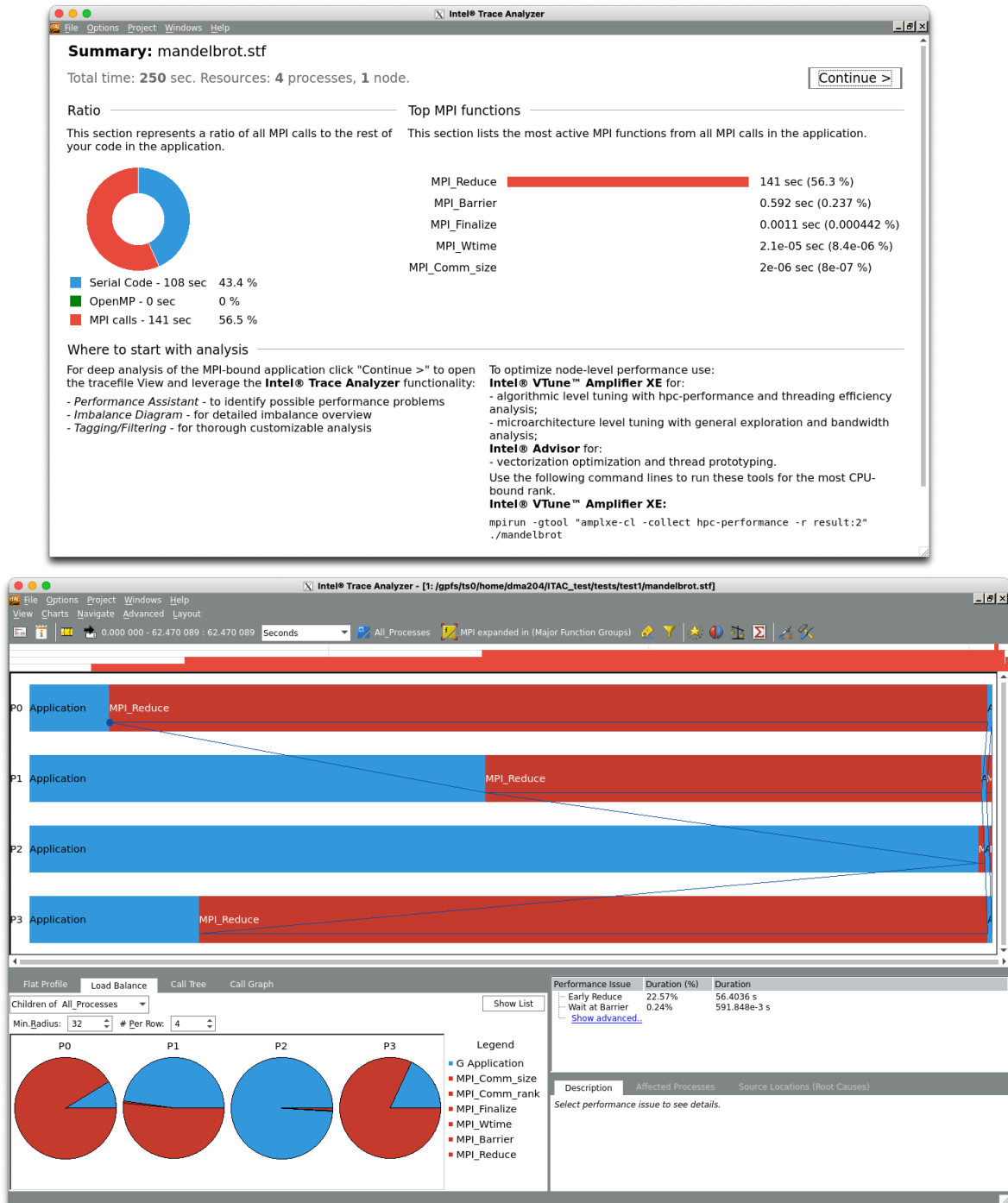


Figure 1: Intel Trace Analyzer plots for test 1. On the summary page (top) the load imbalance shows up as a large fraction of time spent in MPI.Reduce. The event timeline (bottom) shows that process 2 takes longer than the other processes to complete its iterations which results in the other processes waiting at the MPI.Reduce call.

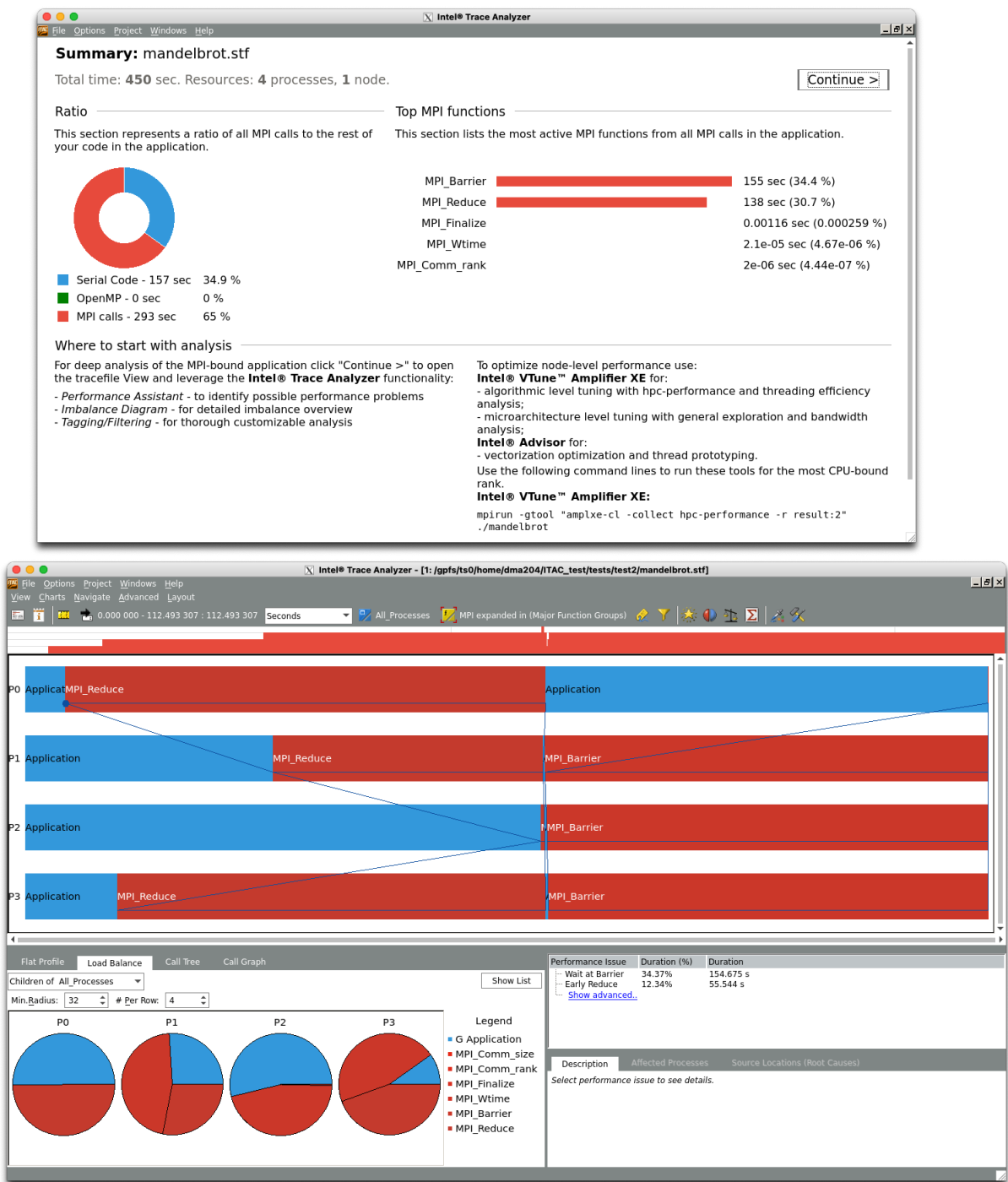


Figure 2: Intel Trace Analyzer plots for test 2.

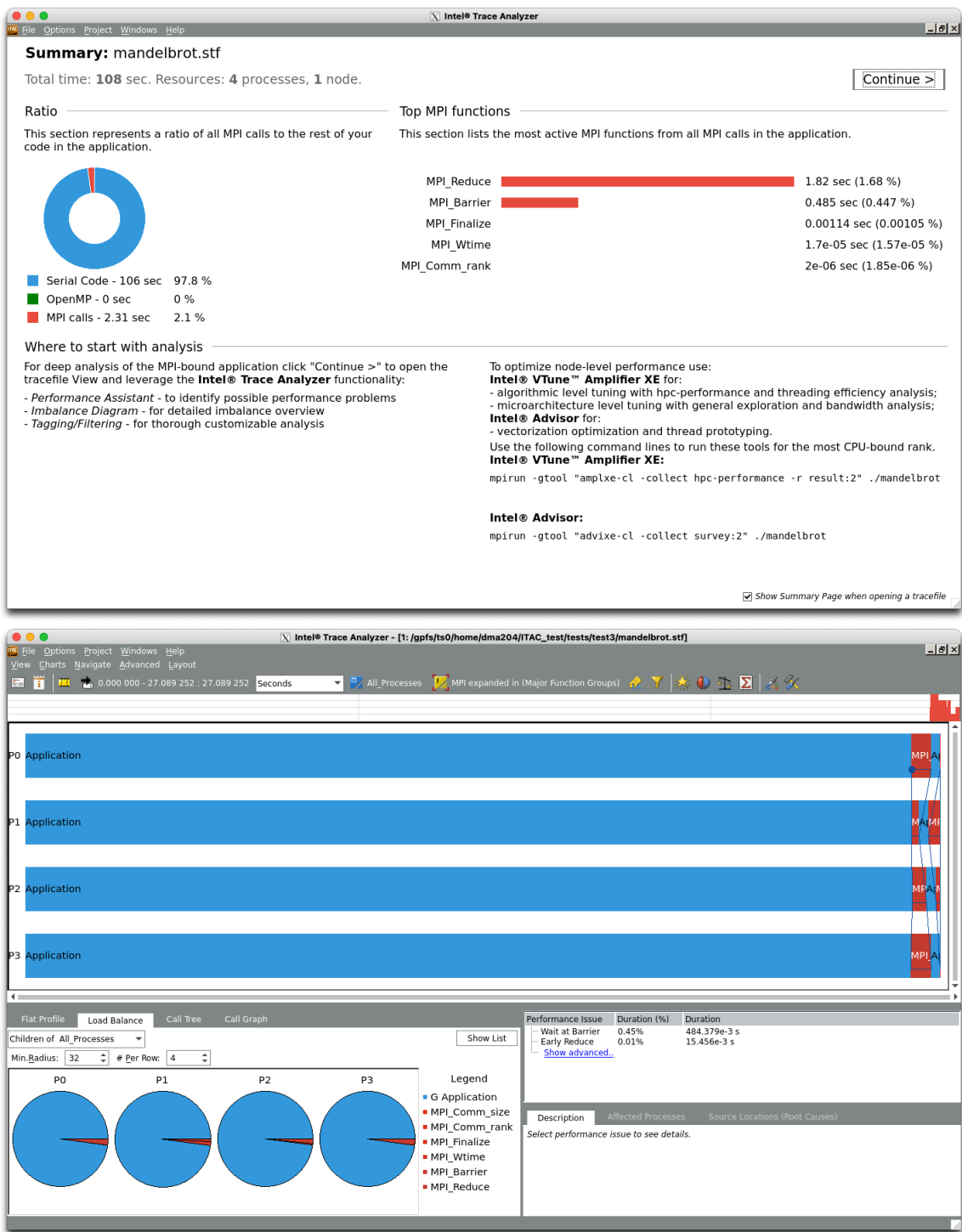


Figure 3: Intel Trace Analyzer plots for test 3.

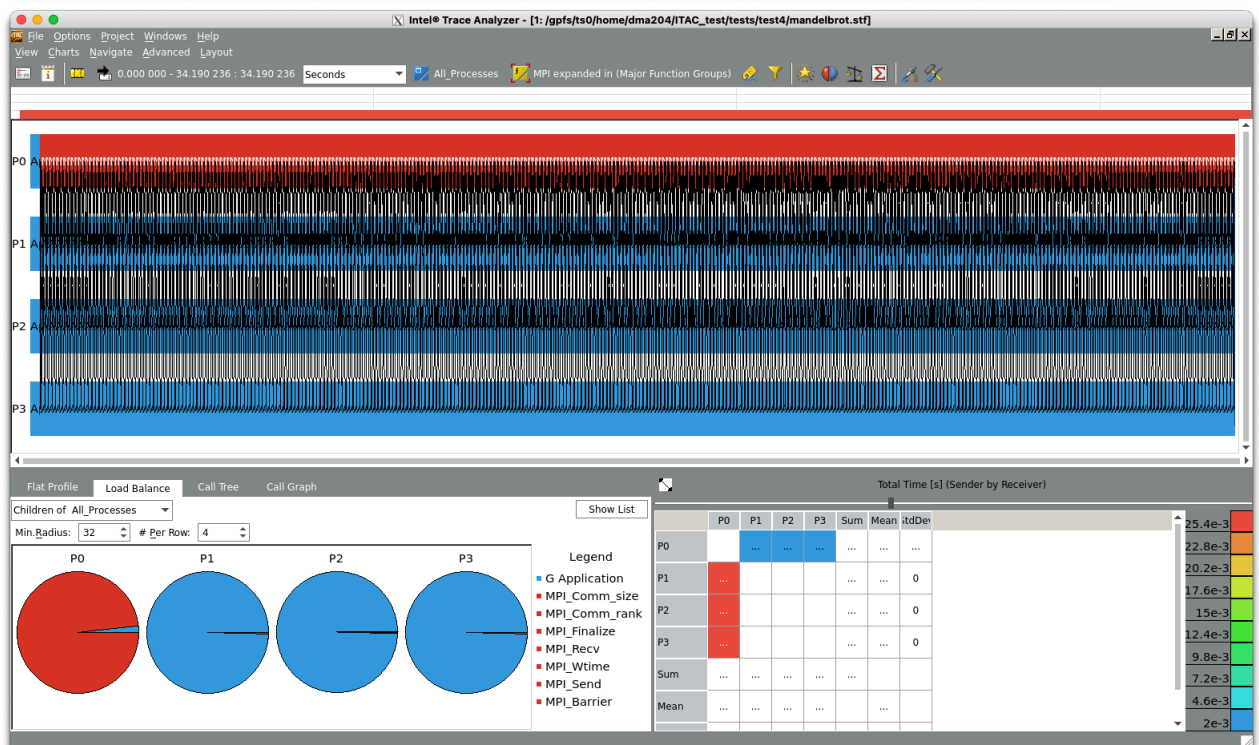
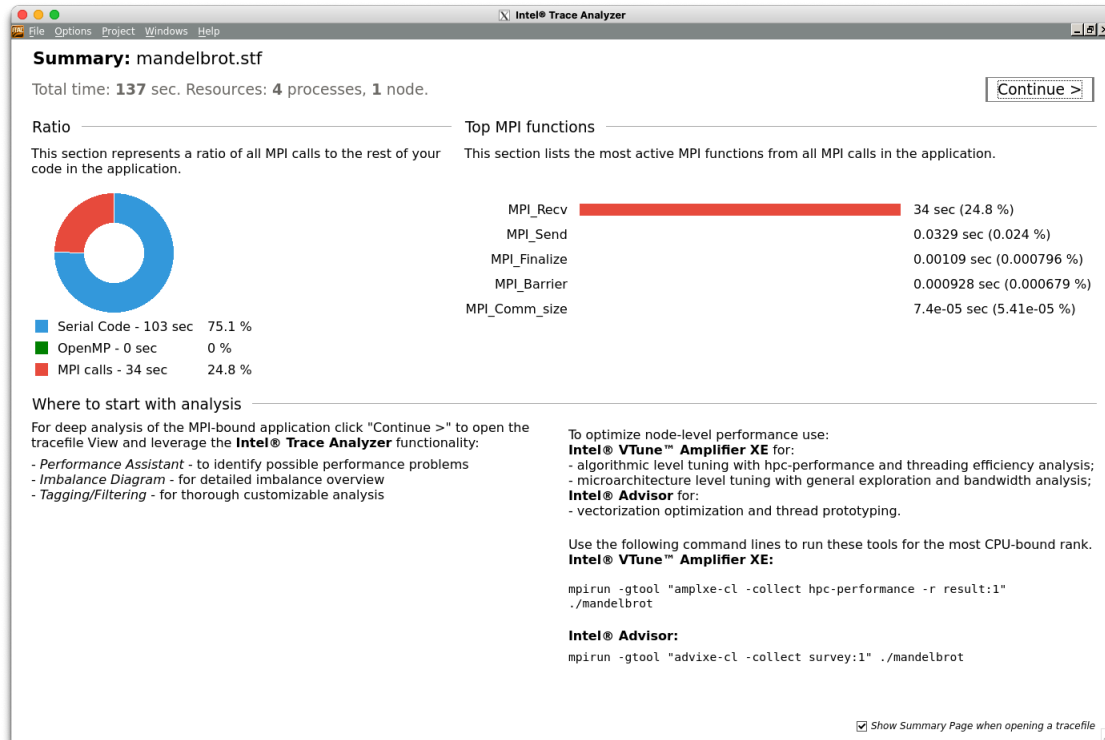


Figure 4: Intel Trace Analyzer plots for test 4.

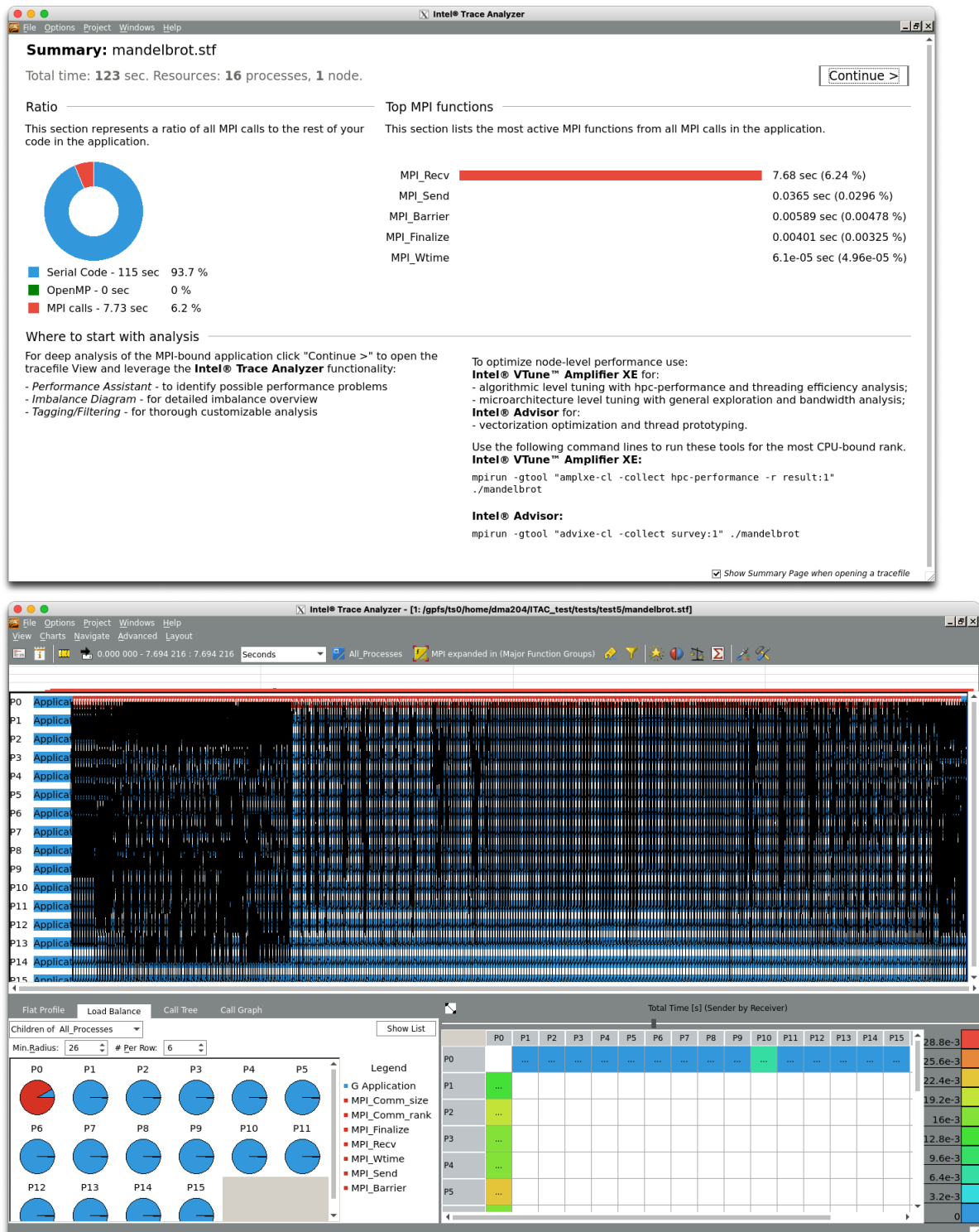


Figure 5: Intel Trace Analyzer plots for test 5.

```
> module switch PrgEnv-cray PrgEnv-gnu
> cc -o mandelbrot mandelbrot_mpi.c
```

Two changes are required in the job script in order to activate performance reports. The first change is to load the `arm-forge` module:

```
module load tools/arm-forge
```

and the second change is to add the `perf-report` command before the `aprun` command:

```
perf-report aprun -n ${nprocs} ./mandelbrot
```

This method of launching a job under `perf-report` is referred to as Express Launch mode. When the job runs two extra files are generated which contain the output from the performance report in text and HTML formats. The output from running a performance report on the Mandelbrot version 1 example using 4 MPI processes is shown in figure 6. In this example the I/O has been switched off to highlight the performance issue caused by the load imbalance. The tool correctly identifies that there is excessive time spent in MPI calls but does not identify load imbalance as the performance issue.

For the next test the I/O was switched on and the results are shown in figure 7. The additional time spent in I/O shows up as an exacerbated load imbalance due to I/O being funnelled through the rank zero process which causes all other processes to wait at an MPI barrier. Although slow I/O is the underlying cause the time spent in I/O is only a small fraction of the time breakdown.

Figure 9 shows the Performance Report from the Mandelbrot version 3 example with 4 MPI processes. This version of the program uses a manager-worker pattern which means that only 3 out of 4 MPI processes carry out the calculation and the fourth process is the manager which does not compute any points. The MPI time of 25% is consistent with the manager process waiting for results from the worker processes. If the number of MPI processes is increased to 16 (see figure 10) then the fraction of MPI time decreases as there are now 15 processes actively working on the calculation.

The Performance Report tool has provided a clear overview of the application performance, which highlighted the presence of performance issues, without needing to change the build process. However was not able to distinguish between load imbalance and overhead which would be clearer when viewing a time line.

4.2.2 MAP

4.2.3 Firedrake

ARM Forge can be used to profile python applications. Make sure to add the `-j 1` flag when using ARM profilers on Isambard otherwise there can be a hang on exit⁶ (this appears to be specific to the ARM64 architecture).

4.3 Cray PAT

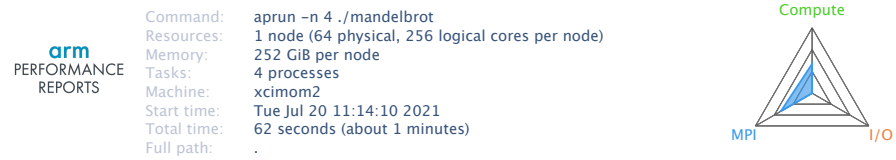
Although this is a Cray tool it does work with compilers other than Cray (the other `PrgEnv` modules load `perftools-base`). Experience building SWIFT showed that the `perftools-lite` module can confuse `autogen` and `configure` so only load the module prior to the `make` command.

- Cray PAT has two modes: standard and “lite”
- There is a graphical viewer (Apprentice 2) which reads the profiling output
- Can view a time line from a full trace

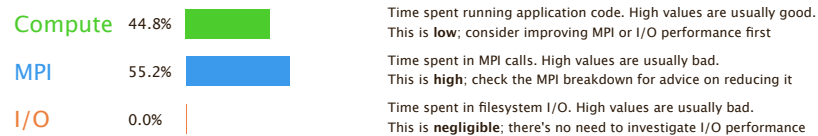
See also <https://docs.nersc.gov/tools/performance/craypat/>.

It's not clear how to use Cray PAT with python/Firedrake. Loading the `perftools-lite` module and using the `python` from the `cray-python` module does not produce any profiling output.

⁶<https://developer.arm.com/documentation/101136/2102/Appendix/Known-issues/Arm-MAP>



Summary: mandelbrot is **MPI-bound** in this configuration



This application run was **MPI-bound**. A breakdown of this time and advice for investigating further is in the **MPI** section below.

CPU Metrics

Linux perf event metrics:

Cycles per instruction	0.77	<div style="width: 0.77%; height: 10px; background-color: #28a745;"></div>
L2D cache miss	35.3%	<div style="width: 35.3%; height: 10px; background-color: #28a745;"></div>
Stalled backend cycles	33.5%	<div style="width: 33.5%; height: 10px; background-color: #28a745;"></div>
Stalled frontend cycles	0.6%	<div style="width: 0.6%; height: 10px; background-color: #28a745;"></div>

Cycles per instruction is low, which is good. Vectorization allows multiple instructions per clock cycle.

I/O

A breakdown of the **0.0%** I/O time:

Time in reads	0.0%	<div style="width: 0.0%; height: 10px; background-color: #ffc107;"></div>
Time in writes	0.0%	<div style="width: 0.0%; height: 10px; background-color: #ffc107;"></div>
Effective process read rate	0.00 bytes/s	<div style="width: 0.0%; height: 10px; background-color: #ffc107;"></div>
Effective process write rate	0.00 bytes/s	<div style="width: 0.0%; height: 10px; background-color: #ffc107;"></div>

No time is spent in I/O operations. There's nothing to optimize here!

Memory

Per-process memory usage may also affect scaling:

Mean process memory usage	677 MiB	<div style="width: 677%; height: 10px; background-color: #dc3545;"></div>
Peak process memory usage	1.09 GiB	<div style="width: 109%; height: 10px; background-color: #dc3545;"></div>
Peak node memory usage	2.0%	<div style="width: 2.0%; height: 10px; background-color: #dc3545;"></div>

There is **significant variation** between peak and mean memory usage. This may be a sign of workload imbalance or a memory leak.
 The **peak node memory usage** is very low. Running with fewer MPI processes and more data on each process may be more efficient.

MPI

A breakdown of the **55.2%** MPI time:

Time in collective calls	100.0%	<div style="width: 100.0%; height: 10px; background-color: #007bff;"></div>
Time in point-to-point calls	0.0%	<div style="width: 0.0%; height: 10px; background-color: #007bff;"></div>
Effective process collective rate	14.2 MB/s	<div style="width: 14.2%; height: 10px; background-color: #007bff;"></div>
Effective process point-to-point rate	0.00 bytes/s	<div style="width: 0.0%; height: 10px; background-color: #007bff;"></div>

Threads

A breakdown of how multiple threads were used:

Computation	0.0%	<div style="width: 0.0%; height: 10px; background-color: #28a745;"></div>
Synchronization	0.0%	<div style="width: 0.0%; height: 10px; background-color: #28a745;"></div>
Physical core utilization	6.3%	<div style="width: 6.3%; height: 10px; background-color: #28a745;"></div>
System load	6.3%	<div style="width: 6.3%; height: 10px; background-color: #28a745;"></div>

No measurable time is spent in multithreaded code.

Physical core utilization is low. Try increasing the number of processes to improve performance.

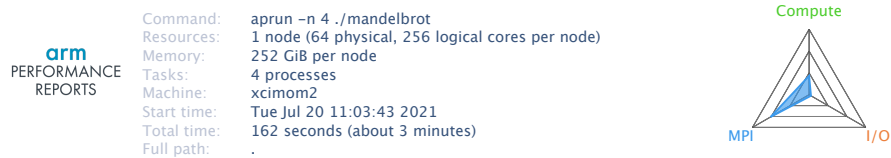
Energy

A breakdown of how energy was used:

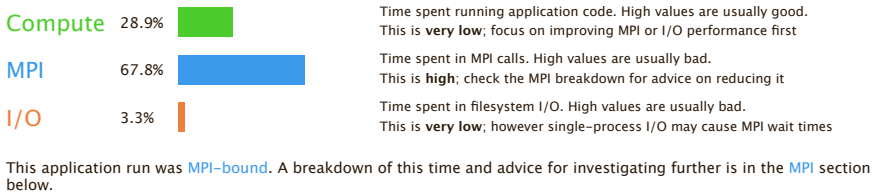
CPU	not supported %	<div style="width: 0%; height: 10px; background-color: #ffc107;"></div>
System	not supported %	<div style="width: 0%; height: 10px; background-color: #ffc107;"></div>
Mean node power	not supported W	<div style="width: 0%; height: 10px; background-color: #ffc107;"></div>
Peak node power	0.00 W	<div style="width: 0%; height: 10px; background-color: #ffc107;"></div>

Energy metrics are not available on this system.

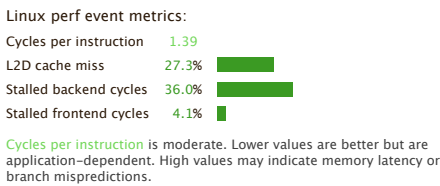
Figure 6: ARM Performance Report from the Mandelbrot version 1 example. The tool correctly identifies that there is excessive time spent in MPI calls but does not identify load imbalance as the performance issue.



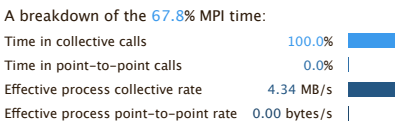
Summary: mandelbrot is **MPI-bound** in this configuration



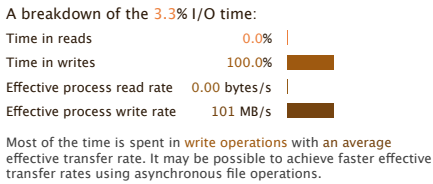
CPU Metrics



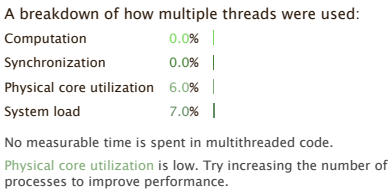
MPI



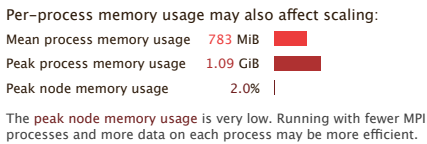
I/O



Threads



Memory



Energy

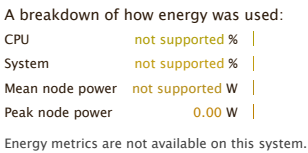
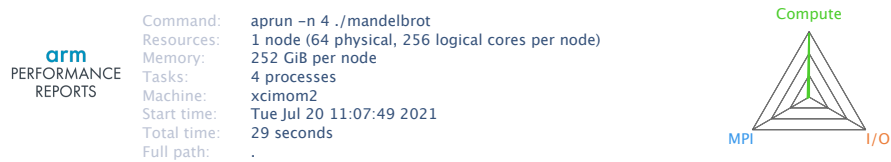
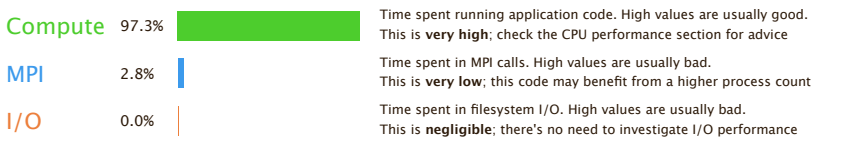


Figure 7: ARM Performance Report from the Mandelbrot version 1 example with I/O switched on. The additional time spent in I/O shows up as an exacerbated load imbalance due to I/O being funnelled through the rank zero process.



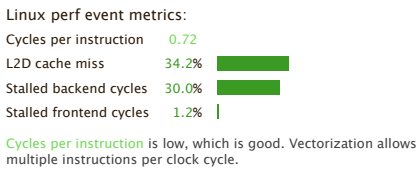
Summary: mandelbrot is **Compute-bound** in this configuration



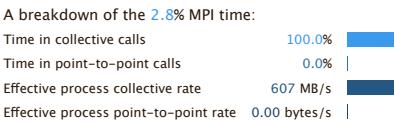
This application run was **Compute-bound**. A breakdown of this time and advice for investigating further is in the **CPU Metrics** section below.

As very little time is spent in **MPI** calls, this code may also benefit from running at larger scales.

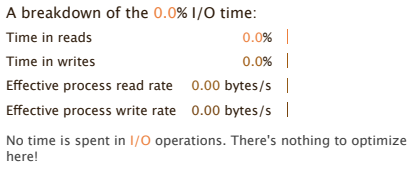
CPU Metrics



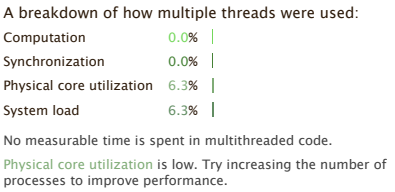
MPI



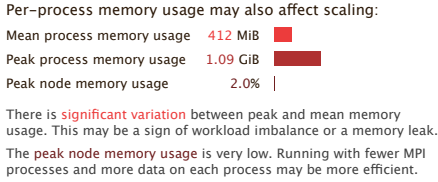
I/O



Threads



Memory



Energy

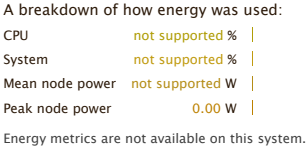
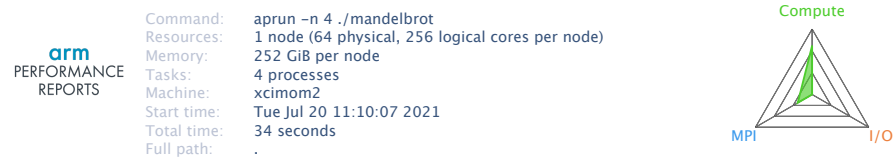
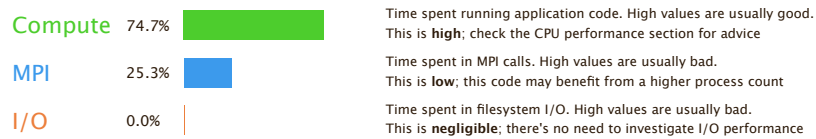


Figure 8: ARM Performance Report from the Mandelbrot version 2 example. This version has fixed the load imbalance by interleaving iterations on the real axis.



Summary: mandelbrot is **Compute-bound** in this configuration

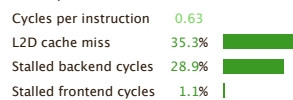


This application run was **Compute-bound**. A breakdown of this time and advice for investigating further is in the **CPU Metrics** section below.

As little time is spent in **MPI** calls, this code may also benefit from running at larger scales.

CPU Metrics

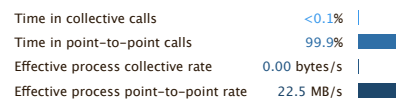
Linux perf event metrics:



Cycles per instruction is low, which is good. Vectorization allows multiple instructions per clock cycle.

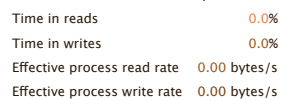
MPI

A breakdown of the **25.3%** MPI time:



I/O

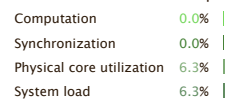
A breakdown of the **0.0%** I/O time:



No time is spent in **I/O** operations. There's nothing to optimize here!

Threads

A breakdown of how multiple threads were used:

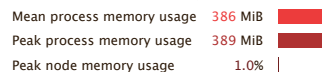


No measurable time is spent in multithreaded code.

Physical core utilization is low. Try increasing the number of processes to improve performance.

Memory

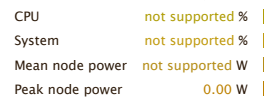
Per-process memory usage may also affect scaling:



The **peak node memory usage** is very low. Running with fewer MPI processes and more data on each process may be more efficient.

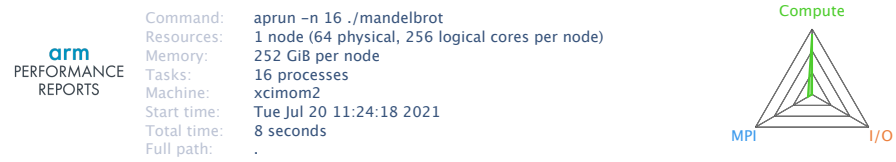
Energy

A breakdown of how energy was used:

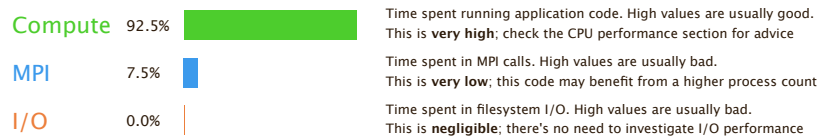


Energy metrics are not available on this system.

Figure 9: ARM Performance Report from the Mandelbrot version 3 example with 4 MPI processes. In the manager-worker pattern only 3 out of 4 MPI processes carry out the calculation and the fourth process is the manager which does not compute any points.



Summary: mandelbrot is **Compute-bound** in this configuration

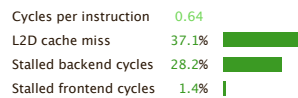


This application run was **Compute-bound**. A breakdown of this time and advice for investigating further is in the **CPU Metrics** section below.

As very little time is spent in **MPI** calls, this code may also benefit from running at larger scales.

CPU Metrics

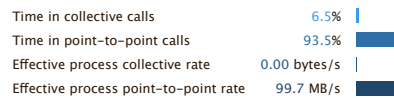
Linux perf event metrics:



Cycles per instruction is low, which is good. Vectorization allows multiple instructions per clock cycle.

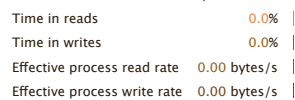
MPI

A breakdown of the 7.5% MPI time:



I/O

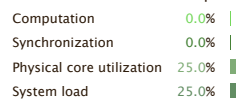
A breakdown of the 0.0% I/O time:



No time is spent in **I/O** operations. There's nothing to optimize here!

Threads

A breakdown of how multiple threads were used:

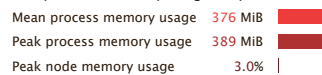


No measurable time is spent in multithreaded code.

Physical core utilization is low. Try increasing the number of processes to improve performance.

Memory

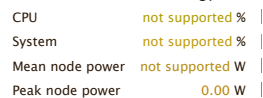
Per-process memory usage may also affect scaling:



The **peak node memory usage** is very low. Running with fewer MPI processes and more data on each process may be more efficient.

Energy

A breakdown of how energy was used:



Energy metrics are not available on this system.

Figure 10: ARM Performance Report from the Mandelbrot version 3 example with 16 MPI processes. The MPI fraction is now reduced as the manager process is only one out of 16 processes.

4.4 Profilers summary

Table 3 summarises the capabilities of the profiling tools reviewed in this section. ARM Forge and

Profiler	C/C++/Fortran	Firedrake
ARM Forge	✓	✓
Intel Parallel Studio	✓	✓
Cray PAT	✓	

Table 3: Summary of profiling tools

Intel Parallel Studio can profile Firedrake on Isambard and Isca respectively.

5 HPC builds

There are three primary HPC platforms for the project: Isca (Exeter university Cluster), Isambard (GW4 tier-2), Archer-2 (national facility). Work on the ARCHER-2 build of Firedrake is supported by an Archer-2 eCSE project (ARCHER2-eCSE04-5 PI: Dr David A Ham (Imperial College) “Scalable and robust Firedrake deployment on ARCHER2 and beyond”) and will not be considered further here.

Plan:

1. Working builds on main target platforms
2. Optimised builds on main target platforms which for this project means using a vendor optimised maths library appropriate for the platform.

Platform	Build status	Profilers
Isca	GCC working	perf-report
Isambard XCI	GCC working	
Archer2	eCSE project	

Table 4: Status of Firedrake builds and profiling for the target HPC platforms

- Isambard build of Firedrake: what’s happening with BLAS/Lapack etc? Scalapack gets built as part of the PETSc build but is also available from `libsci`
- Flag to PETSc can be used to switch to reference version of BLAS/Lapack
- Vendor supplied maths libraries often have support for multi-threading which needs to be switched off when using Firedrake
- Building Firedrake on Isca with the Intel compilers is not working because pybind11 requires Intel C++ compiler v18 or newer.

6 Conclusions and recommendations

Recommendations:

1. Standardise on the GNU compilers for all platforms to avoid having to manage too many different builds. This also takes the compiler out of the performance equation (different GCC versions notwithstanding).
2. Carry out initial performance studies using Firedrake for rapid prototyping. Use ITAC and Performance Reports/MAP to profile Firedrake on Isca and Isambard respectively. This enables profiling up to the 20 992 cores available on Isambard.

3. Once feasibility has been established implement the algorithm in FRric and run on Archer-2 with profiling using Cray PAT. This will enable performance studies beyond 20 000 cores.