Profiling Firedrake for the APinTA-PDEs project

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Contents

1	Introduction	3
2	Target platforms	3
3	Test cases	4
4	Profiling tools 4.1 Intel Parallel Studio 4.2 ARM Forge 4.3 Cray PAT	6 8 14
5	Builds	14
6	Profiling Firedrake	19
7	Conclusions and recommendations	19

To do

- 1. Write up ITAC examples
- 2. Add examples using ARM MAP
- 3. Builds on Isca: GCC reference, platform optimised Intel toolchain. Describe how to use Easybuild to set up the Intel build if this works.
- 4. Firedrake example with Performance Reports and MAP
- 5. Add examples using Cray PAT perftools-lite
- 6. Describe other capabilities of Cray PAT in addition to perftools-lite including rank re-ordering
- 7. Write conclusions and recommendations section: include the next steps

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, 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 with a focus on tools which can provide information about MPI communication and related performance issues.

The Firedrake will be used extensively for development and rapid prototyping work in the course of the project. Firedrake is python-based domain specific language which generates code at run time. These characteristics make integrating Firedrake with profilers more complex than for traditional HPC applications written using C/C++/Fortran which are compiled then run. Although this report primarily focusses on Firedrake the profiling tools evaluated could be used for profiling other codes used by the project even if those tools are not currently suitable for use with Firedrake.

Section 2 presents the target platforms being considered in this report and reviews the hardware and software available on these systems. Section 3 describes the test cases which will be used to demonstrate the profilers. The profiling tools available to the project are discussed in section 4 and their capabilities demonstrated with the test cases from section 3. Section 5 discusses how to build Firedrake on the target platforms and which profilers the successful builds can be used with. Proof-of-concept results from these profilers are shown in section 6. Finally section 7 presents conclusions and recommendations.

2 Target platforms

An overview of the hardware in the target platforms for this project is shown in Table 1. The

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
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.

target HPC platforms are Archer-2 (national tier-1), Isambard (national tier-2) and Isca (local tier-3). Isambard comprises multiple systems and for this project we will focus on the the XCI system which is an established production system based on the ARM64 processor architecture. The project has 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 provide a reference installation as it will use an unmodified Firedrake installation, 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, compilers from the processor vendor (AMD, Intel, or ARM) and Cray systems also have the Cray compiler. 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 profiling tool is Cray Performance Analysis Tools (PAT) but on Isambard the profiling tools from

System	Compilers	MPI libraries	Maths lib.	Profilers
Archer-2	GNU, Cray, AOCC	Cray MPICH2	Cray libsci	Cray
Isambard XCI	GNU, Cray, ARM	Cray MPICH2	Cray libsci	Cray, ARM
Isca (GCC-foss)	GNU	OpenMPI	OpenBLAS	None
Isca (Intel)	Intel	Intel	Intel MKL	Intel
Server	GNU	MPICH	OpenBLAS	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 ARM Forge suite¹ 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 works with Intel MPI.

The server does not currently have any profiling software. However the profiling tools from Intel's Parallel Studio product are now available for free as part of the HPC toolkit from the newer OneAPI product² and these could be installed on the server. There is also the option of obtaining an evaluation licence for ARM Forge to test these tools on the server. A server licence for the ARM Forge product costs \$USD 425 for a one year academic licence which allows profiling with up to 64 MPI processes³.

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, have different performance characteristics and display different performance issues:

- Version 1: divides the computational domain into equal sized chunks along the real axis. Dividing the workload in this manner causes a load imbalance as some sub-domains will complete significantly more iterations than other (see figure 1)
- Version 2: similar to version 1 but interleaves the iterations on the real axis to improve the load balance. Both version 2 and version 1 pack a 2D array into a 1D buffer which is communicated using an MPI_Reduce. Even when the program is run on a single compute node (where MPI communication is quick) there will be an overhead from packing and unpacking the buffer.
- Version 3: implements a manager-worker pattern for distributing the iterations to ensure good load balancing. This version also 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 than the other versions and avoids calling MPI_Reduce.

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

¹ARM Forge was previously known as Allinea Forge

²https://software.intel.com/content/www/us/en/develop/tools/oneapi/all-toolkits.html

 $^{^3 \}verb|https://store.developer.arm.com/store/high-performance-computing-hpc-tools/arm-forge$

Mandelbrot example with 4 MPI processes

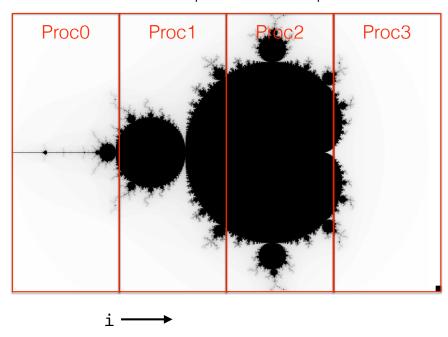


Figure 1: Domain decomposition in version 1 of the Mandelbrot program with four MPI processes. Darker colours show regions of the domain where more iterations are required illustrating the load-imbalance from this decomposition (e.g. process 2 will carry out many more iterations than process 0 or 3).

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

Comparing test 1 and test 2 shows the impact of I/O. The I/O comprises process 0 writing values to an ASCII file which adds a significant overhead which will show up in the profiling output. Comparing tests 1 and test 3 and shows the impact of load imbalance, as the only difference between these tests is the distribution of the workload. Tests 4 and 5 have been designed to illustrate a different communication pattern (manager-worker) and a different type of MPI call (point-to-point rather than collectives). The manager-worker pattern is relatively inefficient with 4 MPI processes (as one process is the manager which does not participate in the calculation) but shows good efficiency with 16 MPI processes.

4 Profiling tools

Some performance information can be obtained from within Firedrake itself. Performance information can be obtained from PETSc (by adding the -log_view flag when running Firedrake⁴) and there is also the ability to time sections of code by adding a PyOP2 timed stage⁵. 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:

- Intel Parallel Studio: Isca only (requires Intel MPI)
- ARM Forge: Isambard only (currently only licensed on Isambard)
- Cray PAT: Isambard and Archer (Cray systems only)

Each of these products is a suite of tools with a range of capabilities. This report will focus on the tools appropriate for understanding the performance of parallel applications which use MPI.

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, but the focus of this report is on MPI performance.

In the following examples the Mandelbrot executable will be build with MPI tracing enabled as follows. 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 itac module needs to be loaded in the job script (in addition to the intel module) 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 2 (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 (56%) 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 in the lower panel of figure 2 which shows the event timeline. To view the event timeline as seen in this figure:

⁴https://petsc.org/release/documentation/manual/profiling/

⁵https://op2.github.io/PyOP2/profiling.html

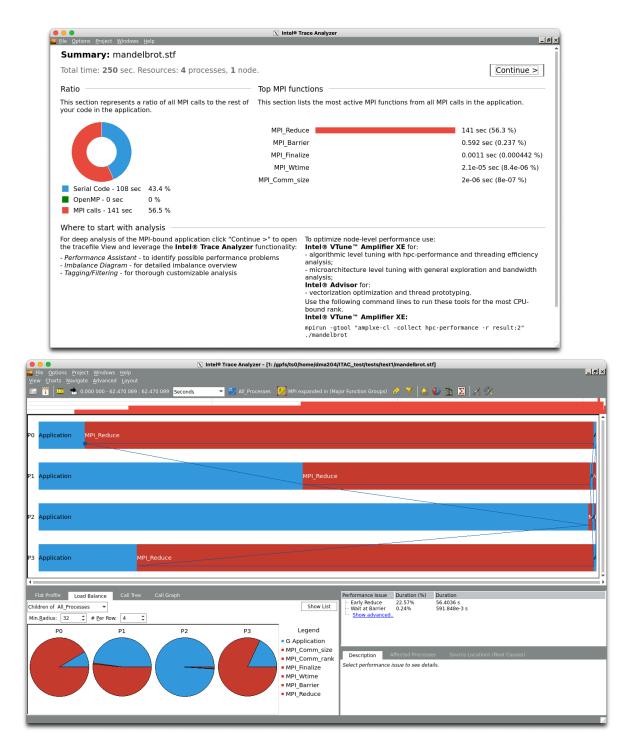


Figure 2: Intel Trace Analyzer plots for test 1. On the summary page (top) the load imbalance shows up as a large fraction of time spent in MPI_Reduce. The event timeline (bottom) shows that process 2 takes longer than the other processes to complete its iterations which results in the other processes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

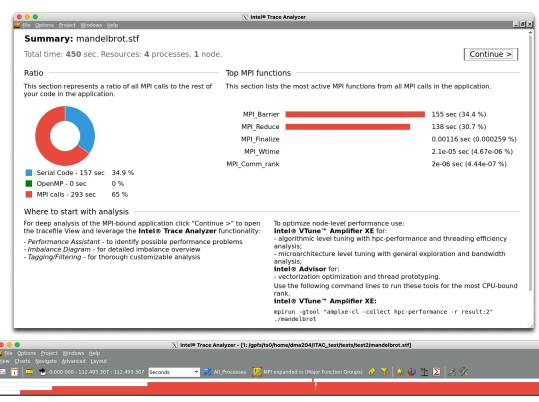
- Click the continue button on the summary page
- Select Charts → Event Timeline to open a new pane showing process activity over time.
- In the lower left pane select the Load Balance tab and click the Show pies button.
- Right click on a red MPI section in the timeline and choose Ungroup MPI from the 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 3) 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 an MPI_barrier at the end of the program (processes are synchronised at a barrier 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: this test uses version 2 of the program which has corrected the load imbalance and the profiling results are shown in figure 4. The run time is now significantly reduced (108 seconds vs. 250 seconds) and the time line shows the MPI processes reaching the MPI_Reduce together. At the end of the time line we can see some time spent carrying out the MPI_Reduce and some application time (blue) as the buffer is unpacked (if required the time line can be zoomed-in to show more detail in a selected region).

Test 4: Charts \rightarrow message profile Test 5:



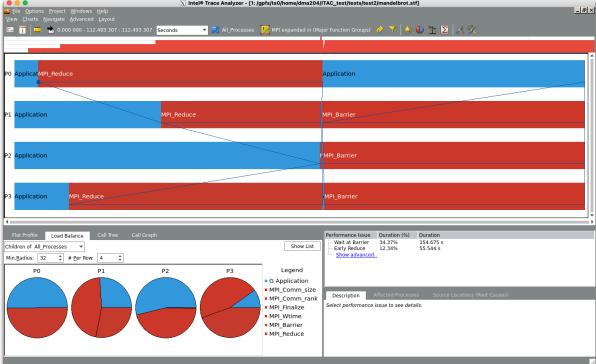


Figure 3: Intel Trace Analyzer plots for test 2 which is like test 1 but with I/O enabled. There are two distinct phases to the time line: firstly the calculation and secondly the I/O. Both phases have a load imbalance with the second phase showing processes waiting at a barrier as the rank zero process performs I/O.

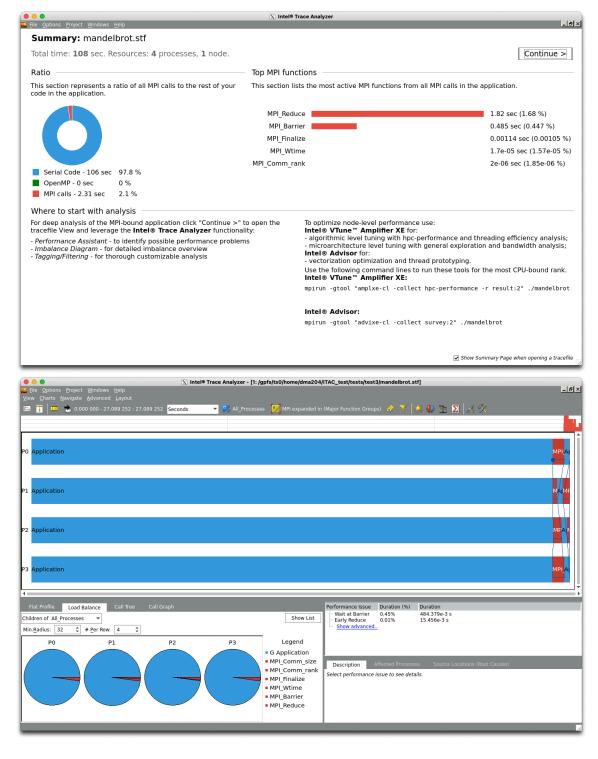


Figure 4: Intel Trace Analyzer plots for test 3. This test uses version 2 of the program which has corrected the load imbalance presence in version 1 resulting in all MPI processes reaching the MPI_Reduce together.

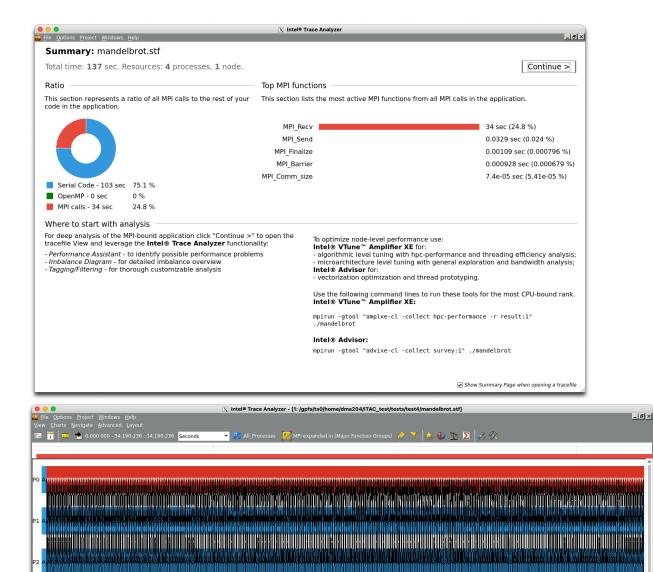


Figure 5: Intel Trace Analyzer plots for test 4.

Legend

P1

P2

Р3

Sum

G Application

MPI_Finalize

MPI_Recv
MPI_Wtime

MPI Send

MPI_Comm_sizeMPI_Comm_rank

P0 P1 P2 P3 Sum Mean itdDe

0

0

0

25.4e-3

22.8e-3

20.2e-3

17.6e-3

15e-3

Flat Profile Load Balance
Children of All_Processes

Min.Radius: 32

\$ # Per Row: 4

Р1

P2

ЬЗ

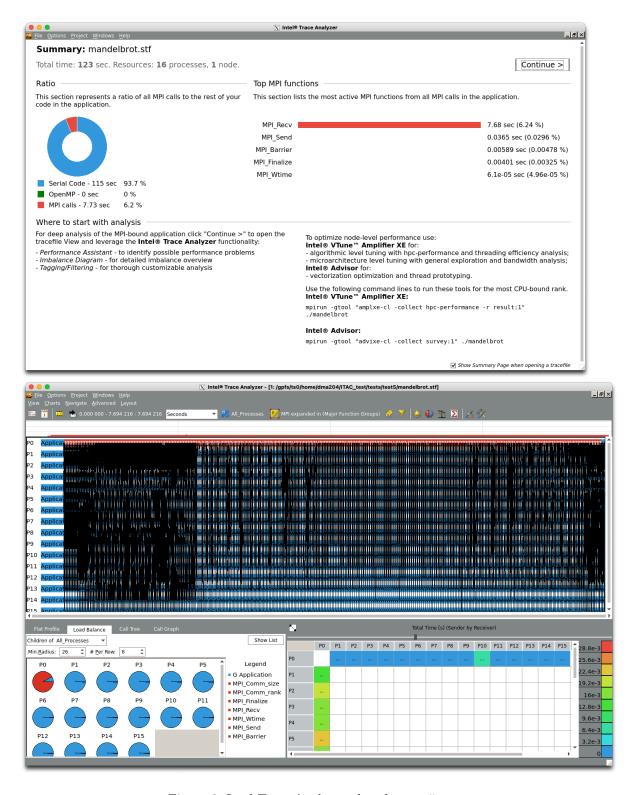


Figure 6: Intel Trace Analyzer plots for test 5.

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 Python⁶.

The documentation for Performance Reports says that on Cray systems dynamic linking or explicit linking with the profiling libraries is required. 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:

```
> 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 7. 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 8. 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 10 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 increases to 16 (see figure 11) 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.

4.3 Cray PAT

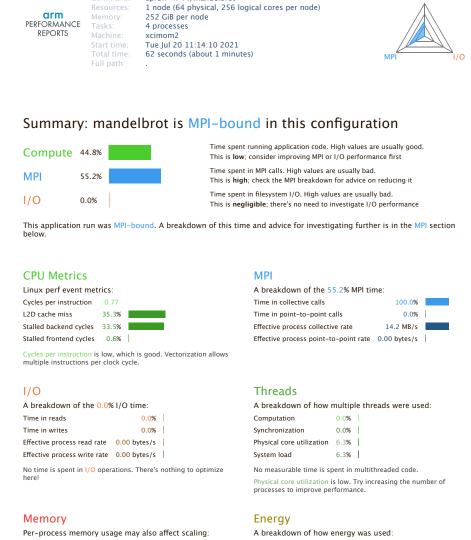
Although this is a Cray tool it does work with compilers other than Cray (the other PrgEnv modules load perftools-base). Experience building SWIFT showed that the perftools-lite module can confuse autogen and configure so only load the module prior to the make command.

- Cray PAT has two modes: standard and "lite"
- There is a graphical viewer (Apprentice 2) which reads the profiling output

⁶https://www.arm.com/products/development-tools/server-and-hpc/forge/map

⁷https://developer.arm.com/documentation/101136/2102/Performance-Reports/

Compute



CPII

Peak node power

not supported %

0.00 W

Mean node power not supported W

Energy metrics are not available on this system.

aprun -n 4 ./mandelbrot

Figure 7: 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.

Mean process memory usage 677 MiB

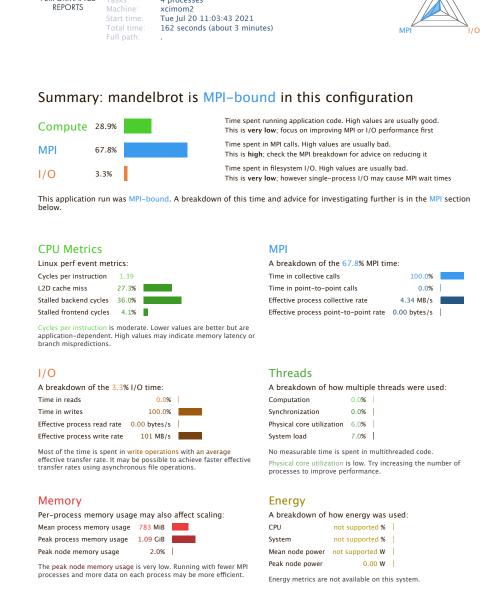
Peak process memory usage 1.09 GiB

2.0%

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.

Peak node memory usage

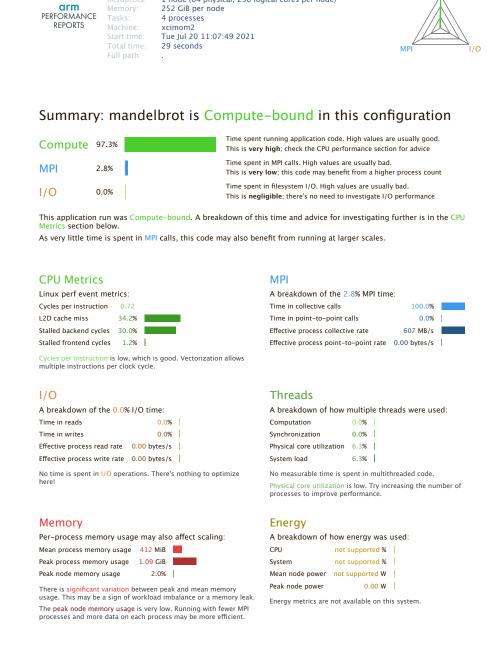


aprun -n 4 ./mandelbrot 1 node (64 physical, 256 logical cores per node)

252 GiB per node 4 processes

arm PERFORMANCE

Figure 8: 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.



aprun -n 4 ./mandelbrot

1 node (64 physical, 256 logical cores per node)

Figure 9: ARM Performance Report from the Mandelbrot version 2 example. This version has fixed the load imbalance by interleaving iterations on the real axis.

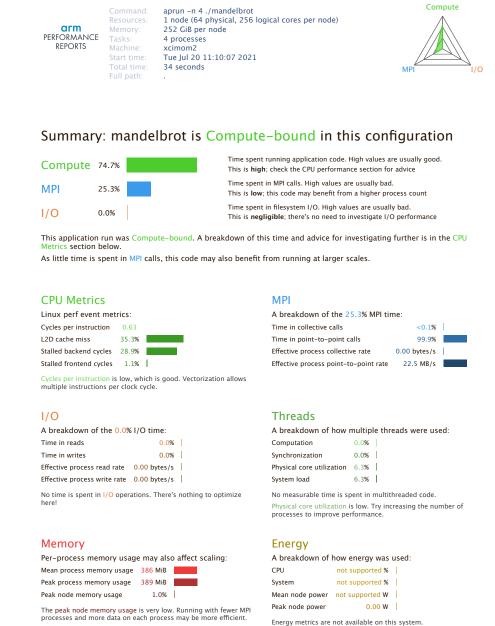
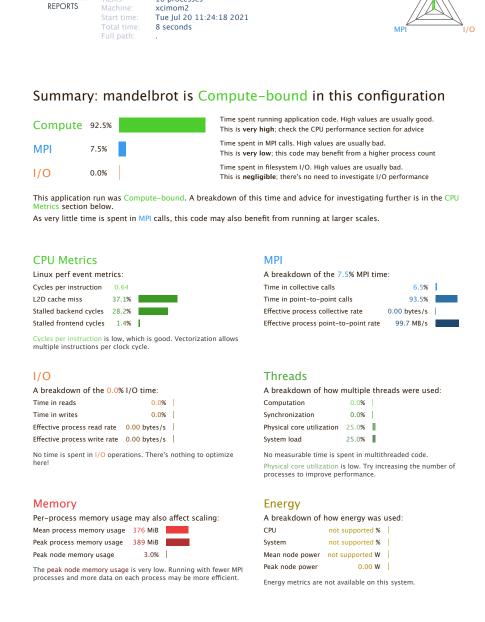


Figure 10: ARM Performance Report from the Mandelbrot version 3 example with 4 MPI processes. In the manager-worker pattern only 3 out of 4 MPI processes carry out the calculation and the fourth process is the manager which does not compute any points.



aprun -n 16 ./mandelbrot

16 processes

arm PERFORMANCE

REPORTS

1 node (64 physical, 256 logical cores per node) 252 GiB per node

Figure 11: 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.

• 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.

5 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 to avoid duplication of effort.

For each target platform there is a build using the reference BLAS/Lapack implementation (fblaslapack) and optimised builds which use optimised maths libraries appropriate for the platform. The status of the builds is shown in table 3

Platform	Build	Status	Profiler
Isca	GCC-OpenMPI-fblaslapack	✓	-
Isca	GCC-OpenMPI-OpenBLAS	✓	_
Isambard XCI	GCC-CrayMPI-fblaslapack	✓	perf-report
Isambard XCI	GCC-CrayMPI-CrayLibsci	✓	perf-report

Table 3: Status of Firedrake builds and profiling for the Isca and Isambard

- Flag to PETSc can be used to switch to reference version of BLAS/Lapack
- To see how PETSc was configured see the end of the file firedrake/src/petsc/configure.log
- Vendor supplied maths libraries often have support for multi-threading which needs to be switched off when using Firedrake. Newer Firedrake versions warn about this.
- Building Firedrake on Isca with the Intel compilers is not working because pybind11 requires Intel C++ compiler v18 or newer. Try pip installing pybind11 before running the Firedrake install script.
- $\bullet \ \ {\it The Isca build scripts are named install_firedrake_isca_COMPILER_MPI_MATHLIB.sh}$

6 Profiling Firedrake

ITAC was previously working on Isca with the Intel Say how to modify the mpirun command. Can build problems be fixed with newer compiler versions?

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 exit⁸ (this appears to be specific to the ARM64 architecture).

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

7 Conclusions and recommendations

Carry out initial performance studies using Firedrake for rapid prototyping. Use ARM Forge to profile Firedrake on Isambard which enables profiling up to the $20\,992$ cores. Once the scalability

 $^{^8}$ https://developer.arm.com/documentation/101136/2102/Appendix/Known-issues/Arm-MAP

of the algorithm has been established on Isambard implement the algorithm in FRric and run on Archer-2 with profiling using Cray PAT. This will enable performance studies beyond 20 000 cores. Describe the next steps with reference to the proposal document.