VI-HPS VIRTUAL INSTITUTE – HIGH PRODUCTIVITY SUPERCOMPUTING

Tools Guide

June 2025

Introduction

The mission of the Virtual Institute - High Productivity Supercomputing (VI-HPS[1]) is to improve the quality and accelerate the development process of complex simulation codes in science and engineering that are being designed to run on highly-parallel computer systems. For this purpose, the partners of the VI-HPS are developing integrated state-of-the-art programming tools for high-performance computing that assist programmers in diagnosing programming errors and optimizing the performance of their applications.

This Tools Guide offers a brief overview of the technologies and tools developed by the 17 partner institutions of the VI-HPS. It is intended to assist developers of simulation codes in deciding which of the tools of the VI-HPS portfolio is best suited to address their needs with respect to debugging, parallelization, correctness checking, and performance analysis. To simplify navigation and to quickly locate the appropriate tool for a particular use case, an icon list on the left margin of each double page indicates the main characteristics of the corresponding tool. The following paragraphs provide brief definitions of what is meant by each of these icons in the context of this guide.

Focus
single
parallel

Single-node vs. Parallel: These icons indicate whether a tool focuses on either *single-node* or *parallel* characteristics, or both. Here, single-node refers to characteristics of serial, shared-memory or accelerated programs executing on a single system, while *parallel* relates to programs executing on multiple nodes of a cluster using some communication library such as MPI (i.e., using distributed memory parallelism).

Focus
perform
debug
correct
workflow

Performance vs. Debugging vs. Correctness vs. Workflow: *Performance* tools provide information about the runtime behavior of an application and/or inefficient usage of the available hardware resources. This data can be obtained in various ways, e.g., through static code analysis, measurements, or simulation. *Debugging* tools, on the other hand, may be used to investigate a program – either live at execution time or post-mortem – for possible errors by examining the value of variables and the actual control flow. In contrast, a *correctness* checking tool detects errors in the usage of programming models such as MPI against certain error patterns and reports them to the user, usually performing the analysis

[1] https://www.vi-hps.org

right at runtime. Finally, *workflow* tools help to automate certain tasks and workflows and thus improve overall productivity.

Programming models: Over the years, many different programming models, libraries and language extensions have been developed to simplify parallel programming. Unfortunately, tools need to provide specific support for each programming model individually, due to their different characteristics. The corresponding icon list indicates which of the programming models and libraries most-commonly used in the area of high-performance computing are supported by a tool. In particular, these are the de-facto standard for distributed-memory parallelization *MPI*, the shared-memory programming extensions *OpenMP*, *Pthreads* (a.k.a. POSIX threads) and *OmpSs*, the programming models *CUDA*, *HIP*, *OpenCL* and *OpenACC* targeting accelerators, as well as the partitioned global address space (PGAS) languages/libraries *UPC*, *SHMEM*, and *GASPI*. However, it may be possible that a tool supports additional programming models, which will then be indicated in the tool description.

Prog. model

MPI
OpenMP
Pthreads
OmpSs
CUDA
HIP
OpenCL
OpenACC
UPC
SHMEM
GASPI

Languages: Some tools may be restricted with respect to the programming languages they support, for example, if source-code processing is required. Here, we only consider the most commonly used programming languages in HPC, namely *C*, *C++*, *Fortran*, and *Python*. Again, it may be possible that tools support further languages or are even language-independent, which will then be mentioned in the description.

Language

C
C++
Fortran
Python

Processor architectures: Finally, tools may support only certain CPU architectures and/or offer support for GPUs. Others are essentially CPU architecture agnostic, however, may not have tested support for all architectures. Here the most common architectural families are distinguished, and details of variants (such as 32-bit vs 64-bit) may be found in the accompanying text. *x86* includes Intel Xeon Phi (MIC) and AMD x86-compatible processors, *Power* includes PowerPC, and *GPU* covers attached general-purpose graphical processing unit devices from Nvidia, AMD and others. Not all variants within these families may be supported, and additional processor architectures may be mentioned in the description.

Processor

x86
Power
ARM
GPU

Focus

- single
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Prog. model

- MPI
- OpenMP
- Pthreads
- OmpSs
- CUDA
- HIP
- OpenCL
- OpenACC
- UPC
- SHMEM
- GASPI

Language

- C
- C++
- Fortran
- Python

Processor

- x86
- Power
- ARM
- GPU

Archer

Archer is a data race detector for OpenMP programs. Archer builds on open-source tool infrastructure such as OMPT and ThreadSanitizer to provide portability. As a result, Archer achieves very high accuracy and precision in the data race reports. Since 2019, the tool is developed within the LLVM project. Archer is distributed with all Clang-based compiler suites.

Typical questions Archer helps to answer

- My OpenMP program intermittently fails (e.g. hang, crash, incorrect results) or slows down, is this caused by a data race?
- At what point of execution (i.e., source line and stack trace), does this race occur exactly?
- What is the root cause (e.g., incorrect variable scoping and unsynchronized global variable access)?

Workflow

Compile the application with additional flags:

```
-fsanitize=thread -g -O3 -fno-omit-frame-pointer
```

Execute the application:

```
TSAN_OPTIONS='ignore_noninstrumented_modules=1' ./a.out
```

Platform support

Linux x86_64, IBM Power
Distributed with most Clang-based compilers (LLVM, Intel, AMD, HPE/Cray, ...)

License

Apache License 2.0 (LLVM)

Web page

`https://github.com/pruners/archer`

Contact

jenke@itc.rwth-aachen.de

Figure 2 gives detailed information for a data race detected by Archer in the source code displayed in Figure 1.

```
1  #include <stdio.h>
2  int main(int argc, char **argv) {
3    int a = 0;
4  #pragma omp parallel
5    {
6      // Unprotected read
7      if (a < 100) {
8  // Critical section
9  #pragma omp critical
10       {
11         // Shared memory access
12         a++;
13       }
14     }
15   }
16 }
```

Figure 1: OpenMP example with a data race.

```
WARNING: ThreadSanitizer: data race (pid=124)
  Write of size 4 at 0x7ffd6825da6c by main thread (mutexes: write M0):
    #0 main.omp_outlined_debug__ race.c:14:10 (race+0xeead8)
    #1 main.omp_outlined race.c:6:1 (race+0xeead8)
    #2 __kmp_invoke_microtask <null> (libomp.so+0xc3de8)
    #3 main race.c:6:1 (race+0xeea70)

  Previous read of size 4 at 0x7ffd6825da6c by thread T1:
    #0 main.omp_outlined_debug__ race.c:9:9 (race+0xeea9f)
    #1 main.omp_outlined race.c:6:1 (race+0xeea9f)
    #2 __kmp_invoke_microtask <null> (libomp.so+0xc3de8)
    #3 main race.c:6:1 (race+0xeea70)
```

Figure 2: Archer output identifying the data race. Mutex M0 represents the critical region.

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Caliper

Caliper is a performance analysis toolbox in a library. Caliper can be used for lightweight always-on profiling, such as printing performance reports for application logs. In addition, Caliper supports advanced MPI, tracing, call-stack sampling, I/O, memory, CUDA, and hardware counter analyses. Caliper region annotations can also be forwarded to third-party tools, such as Allinea MAP, TAU, Intel VTune, and NVidia Visual Profiler.

Typical questions Caliper helps to answer

- How much time does each program region take? How much time is spent in MPI or CUDA calls?
- How much memory and I/O bandwidth is used in each region?
- How does performance differ with different program inputs?

Workflow

Mark code regions of interest with Caliper's source-code annotation macros. Optionally, create a `ConfigManager` object at the start of the program, which provides access to Caliper's built-in measurement configurations through a short configuration string. This string can be hard-coded or provided by the user, for example as an application command-line argument. Alternatively, custom measurement configurations can be provided through environment variables or configuration files.

Caliper can aggregate measurement results on-the-fly, both within processes and across MPI ranks, and write out results in human-readable text form using a hierarchical or flat table layout. Alternatively, data can be written to disk in Caliper's native .cali format or various JSON formats for additional post-processing.

Caliper's annotation macros are designed to be permanently integrated in the target codes to enable lightweight, always-on performance profiling. Annotations are extremely flexible - in addition to source code regions, developers can add custom key:value attributes to describe domain-specific concepts. Moreover, Caliper can record run metadata, such as the system environment or program configuration, to simplify performance comparisons across multiple program runs.

Platform support

Any POSIX compatible OS. C, C++, and Fortran codes.

License

Modified BSD license.

Web page

`https://www.github.com/LLNL/Caliper`

Contact

`https://github.com/LLNL/Caliper/issues`

Figure 3 shows Caliper printing a performance report for a serial execution of a Caliper-enabled program with the inclusive and exclusive time as well as the memory high-water mark for each annotated region. This example uses Caliper's `ConfigManager` API and the configuration string given in the `-P` command-line option to control the performance measurement.

```
$ ./lulesh2.0 -q -i 10 -P runtime-report,mem.highwatermark,aggregate_across_ranks=false
Path                                      Inclusive time Exclusive time Time %    Max Alloc'd Mem
main                                            0.191317       0.009027  4.628020  8752390.000000
  lulesh.cycle                                  0.182290       0.000045  0.023071  8745749.000000
    LagrangeLeapFrog                            0.182153       0.000046  0.023584  8745749.000000
      CalcTimeConstraintsForElems               0.002079       0.002079  1.065875  8747829.000000
      LagrangeElements                          0.085915       0.000214  0.109715  8747829.000000
        ApplyMaterialPropertiesForElems         0.064767       0.000496  0.254292  8963829.000000
          EvalEOSForElems                       0.064271       0.018243  9.352938  9909669.000000
            CalcEnergyForElems                  0.046028       0.046028 23.597931  9977229.000000
        CalcQForElems                           0.009755       0.005823  2.985373 10173429.000000
          CalcMonotonicQForElems                0.003932       0.003932  2.015883 10173429.000000
        CalcLagrangeElements                    0.011179       0.000579  0.296845  9395829.000000
          CalcKinematicsForElems                0.010600       0.010600  5.434476  9395829.000000
      LagrangeNodal                             0.094113       0.001768  0.906430  8747829.000000
        CalcForceForNodes                       0.092345       0.000717  0.367596  8747829.000000
          CalcVolumeForceForElems               0.091628       0.000996  0.510636  9611829.000000
            CalcHourglassControlForElems        0.067312       0.037134 19.038098 19979829.000000
              CalcFBHourglassForceForElems      0.030178       0.030178 15.471851 25163829.000000
            IntegrateStressForElems             0.023320       0.023320 11.955847 14795829.000000
    TimeIncrement                               0.000092       0.000092  0.047167  8745757.000000
```

Figure 3: Printing a runtime report in a Caliper-enabled program.

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Callgrind

Callgrind is a profiling tool for multithreaded, compiled binary code using execution-driven cache simulation. It is able to build the dynamic call graph from execution on the fly. The results are best browsed with the KCachegrind GUI, which provides call graph and treemap visualizations as well as annotated source and assembler instruction views.

Simulating an easy-to-understand machine model, Callgrind allows for reproducible measurements which may not be available through hardware, such as sub-cacheline utilization.

Typical questions Callgrind helps to answer

- What is the dynamic call graph of a program?
- Is bad cache exploitation the reason for slow program execution?
- What are the call-paths suffering from bad cache behavior?
- Does a given cache optimization actually reduce misses?

Workflow

Callgrind does its observation of code execution by automatic runtime instrumentation using the open-source tool Valgrind. As such, the only preparation needed for detailed analysis is to add debug information to the optimized binary, typically via compiler options “-g -O2”. As simulation can induce a slowdown of up to factor 100, the program may be modified to execute only relevant parts. Further, for sections of code, cache simulation and/or call graph generation may be skipped for faster execution (with slowdown down to factor 3). The reproducibility of simulation allows for very detailed comparison of the effect of code modifications (especially cache optimization).

Platform support

Callgrind is part of Valgrind releases, and supports the same platforms (for Valgrind 3.14, this includes Linux on x86/x86_64, Power, ARM, MIPS).

License

GNU General Public License (GPL) v2

Web page

`http://www.valgrind.org`, `http://kcachegrind.sourceforge.net`

Contact

kcachegrind-callgrind@lists.sourceforge.net

Figure 4 shows the call graph of the inner workings of the Intel OpenMP runtime, calling tasks from a Jacobi solver which uses recursive blocking for cache optimization. Callgrind allows recursion levels of the same function to be shown as separate items.

While the GUI is comfortable, Callgrind also comes with standard terminal tools to show the results, such as annotated butterfly call relation lists. Further, it is possible to control running simulations (show current execution context, dump results, switch simulation on/off).

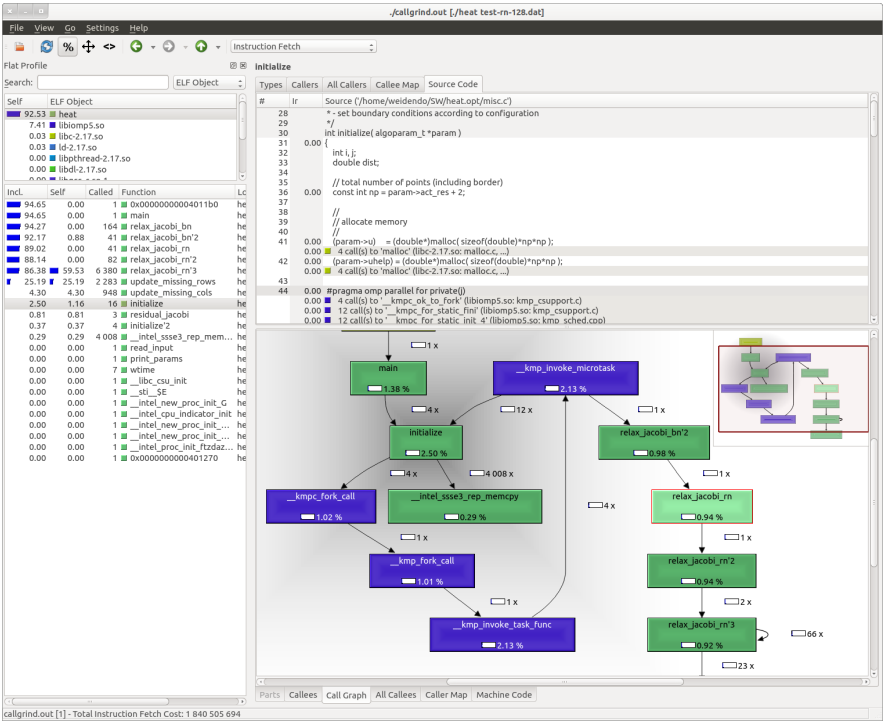

Figure 4: KCachegrind showing results from a Callgrind simulation run.

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CARM Tool

The CARM Tool performs the micro-benchmarking necessary to construct the Cache-Aware Roofline Model (CARM) for floating-point operations on CPUs. The CARM is an easy to use performance model that offers a high-level picture on the fundamental memory and compute performance limitations of a processor, while also providing intuitive analysis of the application execution bottlenecks. The CARM Tool provides as output a visualization of the model, as well as the measurements obtained for the different memory levels, types of FP instruction and SIMD capabilities. Application analysis can also be performed by using either performance counters (via PAPI) or dynamic binary instrumentation (via DynamoRIO or Intel SDE). All the information regarding the constructed CARM and profiled applications can be observed in the CARM tool GUI.

Typical questions the CARM Tool helps to answer

- How well does the program perform compared with the maximum possible performance of the architecture?
- What are the main optimization strategies to pursue for the best performance gains (memory-bound or compute-bound) based on the CARM?
- What is the maximum speed-up a program can achieve in a given architecture?
- What is the peak performance of a given architecture under different ISA/SIMD extensions and thread counts among other factors?

Workflow

To use the CARM Tool one should start by running the automatically generated tailored benchmarks to obtain the CARM plot for their target system. These allow for visualizing the peak performance of different memory levels, ISA extensions, threads, among other parameters. Then, to conduct application analysis in the scope of the CARM, users can rely on several performance tools the CARM Tool interfaces automatically with, i.e., PAPI, DynamoRIO, or Intel SDE. After application analysis is executed, the browser-based GUI of the CARM Tool is usually utilized to facilitate results visualization, to plot analyzed applications in the CARM and obtain the model's insight on the application performance for the target architecture.

Platform support

Linux: x86-64 (AVX512, AVX, SSE), ARM64 (Neon), RISC-V64 (RVV0.7/1.0)

License

GNU Lesser General Public License (LGPL) v2.1

Web page

`https://champ-hub.github.io/projects/The_CARM_Tool/`

Contact

carm@inesc-id.pt

Figure 5 illustrates the GUI of the CARM Tool, designed for the visualization of results. It highlights various features, including the capability to view various CARM plots tailored to specific configurations for comparative analysis. Additionally, the interface allows for the display of applications analyzed using the CARM Tool and includes annotations to important metrics, such as peak bandwidths of memory levels and peak GFLOP/s of the benchmarked system. The GUI is accessible through a Python script and is browser-based, ensuring compatibility across different computing environments. From the sidebar, users can also initiate CARM benchmarks and perform application analysis.

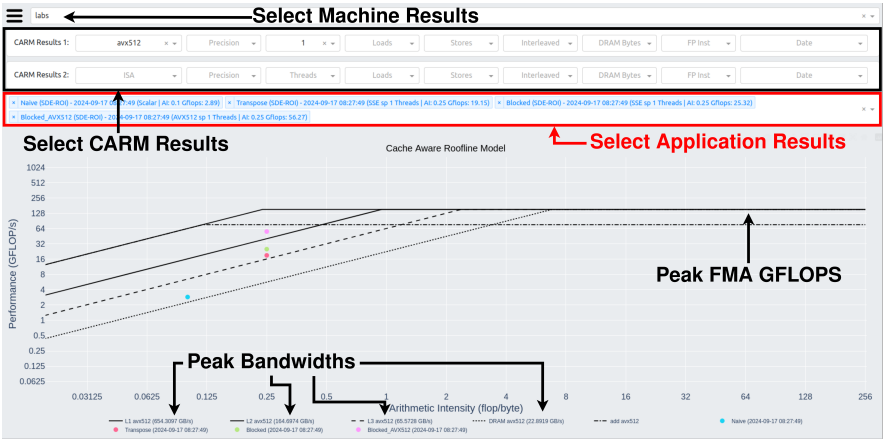

Figure 5: CARM Tool GUI Overview

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Cube

Cube is a generic tool for manipulating and displaying a multi-dimensional performance space consisting of the dimensions (i) performance metric, (ii) call path, and (iii) system resource. Each dimension can be represented as a tree, where non-leaf nodes of the tree can be collapsed or expanded to achieve the desired level of granularity and present inclusive or exclusive metric values. In addition, Cube can display multi-dimensional Cartesian process topologies, highlight a region from a source file, and present descriptions of metrics.

Typical questions Cube helps to answer

- Which metrics have values indicating performance problems?
- Which call-paths in the program have these values?
- Which processes and threads are most affected?
- How are metric values distributed across processes/threads?
- How do two analysis reports differ?

Workflow

Scalasca, Score-P and other tools use the provided libraries to write analysis reports in Cube format for subsequent interactive exploration in the Cube GUI. Additional utilities are provided for processing analysis reports.

Platform support

GUI: Linux (x86/x86_64/IA64/PPC/Power), macOS (x86_64), Windows 10;

Libraries & utilities: IBM Blue Gene/P/Q, Cray XT/XE/XK/XC, SGI Altix (incl. ICE + UV), Fujitsu FX-10/100 & K Computer, Tianhe-1A, IBM SP & Blade clusters (incl. AIX), Intel Xeon Phi, Linux clusters (x86/x86_64)

License

BSD 3-Clause License

Web page

`https://www.scalasca.org`

Contact

scalasca@fz-juelich.de

Figure 6 shows a screenshot of a Scalasca trace analysis of the Zeus/MP2 application in the Cube analysis report explorer. The left panel shows that about 10% of the execution time is spent in the “Late Sender” wait state, where a blocking receive operation is waiting for data to arrive. The middle panel identifies how this wait state is distributed across the call tree of the application. For the selected `MPI_Waitall` call, which accumulates 12.8% of the Late Sender time, the distribution across the system is presented in the right panel, here in the form of a 3D process topology which reflects the domain decomposition used by Zeus/MP2.

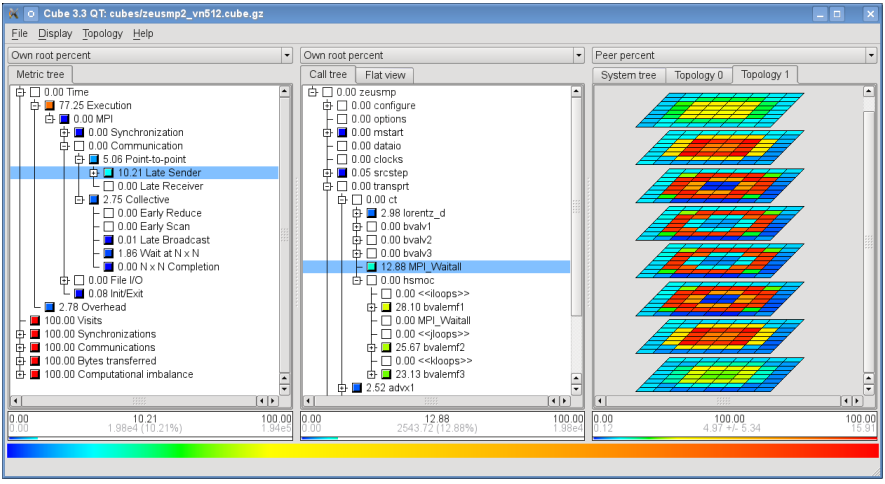

Figure 6: Scalasca trace analysis result displayed by Cube for exploration.

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Dimemas

Dimemas is a performance analysis tool for message-passing programs. The Dimemas simulator reconstructs the temporal behavior of a parallel application using a recorded event trace and allows simulating the parallel behavior of that application on a different system. The Dimemas architecture model is a network of parallel clusters. Dimemas supports two main types of analyses: what-if studies to simulate how an application would perform in a given scenario (e.g. reducing to half the network latency, moving to a CPU three times faster...), and parametric studies to analyze the sensitivity of the code to system parameters (e.g. the execution time for varying network bandwidths..). The target system is modeled by a set of key performance factors including linear components like the MPI point to point transfer time, as well as non-linear factors like resources contention. By using a simple model Dimemas allows executing parametric studies in a very short time frame. Dimemas can generate a Paraver trace file, enabling the user to conveniently examine and compare the simulated run and understand the application behavior.

Typical questions Dimemas helps to answer

- How would my application perform in a future system?
- Increasing the network bandwidth would improve the performance?
- Would my application benefit from asynchronous communications?
- Is my application limited by the network or the serializations and dependency chains within my code?
- What would be the impact of accelerating specific regions of my code?

Workflow

The first step is to translate a Paraver trace file to Dimemas format. Thereby, it is recommended to focus on a representative region with a reduced number of iterations. Second, the user specifies via a configuration file the architectural parameters of the target machine and the mapping of the tasks on to the different nodes. Third, the output Paraver trace file allows then to analyze and compare the simulated scenario with the original run using the Paraver tool.

Platform support

Linux (x86/x86_64, ARM, Power), SGI Altix, Fujitsu FX10/100, Cray XT, IBM Blue Gene, Intel Xeon Phi

License

GNU Lesser General Public License (LGPL) v2.1

Web page

`http://tools.bsc.es/dimemas`

Contact

tools@bsc.es

Figure 7 shows the results of an analysis of sensitivity to network bandwidth reductions for two versions of WRF code, NMM and ARW, and with different number of MPI ranks. We can see that the NMM version demands less bandwidth (256MB/s) than the ARW version.

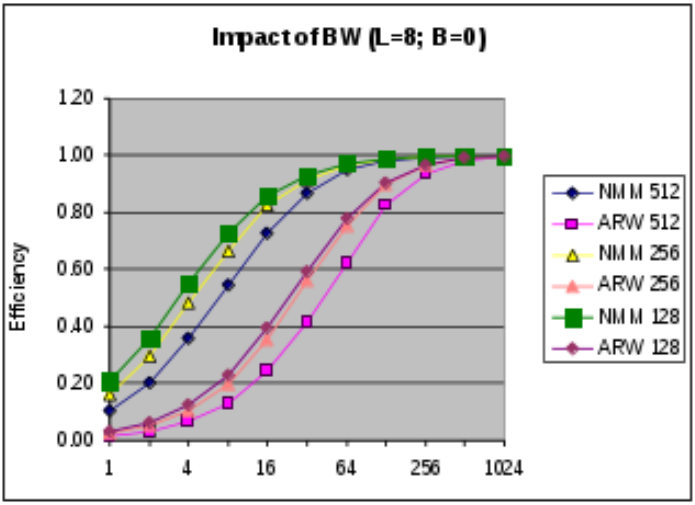

Figure 7: Dimemas sensitivity analysis to network bandwidth.

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DiscoPoP

DiscoPoP is a tool that helps software developers parallelize their programs with threads. It discovers potential parallelism in a sequential program and makes recommendations on how to exploit it using OpenMP. Because a compiler does not know the precise value of pointers and array indices computed at runtime, it may assume parallelism-preventing data dependences in places where they would never occur in practice. As a result, automatic parallelization becomes too conservative.

With our parallelism discovery tool DiscoPoP, we aim to circumvent this problem. We abandon the idea of fully automatic parallelization and instead, point the programmer to likely parallelization opportunities that we identify via a combination of static and dynamic dependence analysis. In this way, we consider only data dependences that actually occur. From these dynamic dependences, we derive possible parallel design patterns, which we propose to the programmers to parallelize their programs.

Typical questions DiscoPoP helps to answer

- Is there potential parallelism in my program?
- If yes, which parts of my program can I parallelize?
- How can I parallelize them?

Workflow

Figure 8 shows a high-level overview of DiscoPoP and how it finds parallelization opportunities.

DiscoPoP is built on top of LLVM and achieves its goals in four steps: the decomposition of the program into parts with negligible internal parallelism, called computational units, the identification of data dependences among those units, the selection of parallel design patterns, and finally the suggestion of suitable OpenMP parallelization constructs and data-sharing clauses to the programmer. To find data dependences, the tool instruments all memory accesses and control regions. The instrumented application is then

Figure 8: The workflow of DiscoPoP.

executed on actual hardware, and profiling data generated by the instrumented code is analyzed on-the-fly to find data dependences among the computational units. Based on the resulting dependence graph, DiscoPoP discovers parallelism in terms of parallel design patterns, including pipeline, doall, geometric decomposition, reduction, and task parallelism. Finally, it issues recommendations on how to parallelize the program using OpenMP. Figure 9 shows the parallelization of an example program using DiscoPoP. The recommendations can be created, browsed, managed, and applied with the help of an openly available extension to Visual Studio Code.

Platform support

Linux x86_64, depends on LLVM/Clang

License

BSD 3-Clause License

Web page

`https://www.discopop.tu-darmstadt.de/`
`https://github.com/discopop-project/discopop`

Contact

discopop-support@lists.parallel.informatik.tu-darmstadt.de

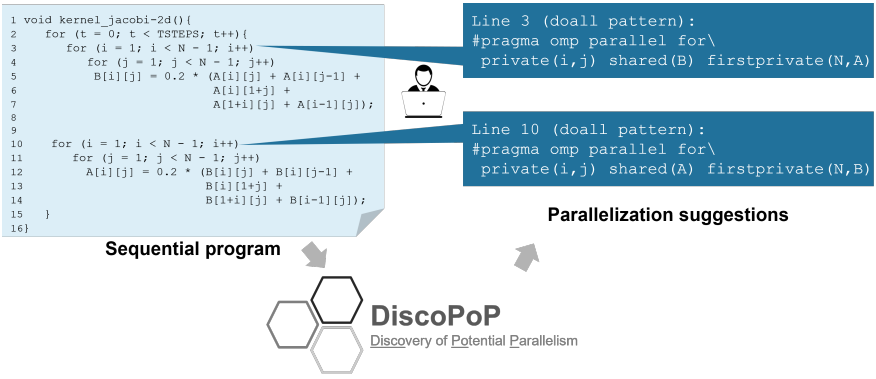

Figure 9: The automation of the parallelization process with DiscoPoP.

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Extrae

The Extrae measurement infrastructure is an easy-to-use tool for event tracing and online analysis. It uses different interposition mechanisms to inject probes into the target application gathering information regarding the application performance. Most of these mechanisms work directly with the production binary, not requiring any special compilation or linking.

Extrae is the instrumentation tool for Paraver and Dimemas and supports a wide range of HPC platforms and programming models and languages.

Typical questions Extrae helps to answer

- How much time is spent in the parallel runtimes?
- What is the average IPC achieved?
- What is the location in the source code of a given MPI call?

Workflow

Instrumenting with Extrae the production binary only requires to modify few lines of the execution script. The execution command of the program to analyze has to be preceded by a *launcher* script (namely *trace.sh*). This script contains just a few definitions to load and configure the Extrae tool. Users only need to specify:

1. where is Extrae installed (EXTRAE_HOME);
2. which information will be captured (EXTRAE_CONFIG_FILE); and
3. the Extrae tracing library (LD_PRELOAD). Please select the proper library depending on the type of parallel application (MPI, OpenMP, OmpSs, Pthreads, CUDA, OpenACC, OpenCL, GASPI, or hybrid combinations).

Once the trace is collected, it is ready to be analysed with Paraver.

Platform support

Linux (x86/x86_64, ARM, RISC-V, Power), SGI Altix, Fujitsu FX10/100, Cray XT, IBM Blue Gene, Intel Xeon Phi, GPU (CUDA, OpenCL)

License

Web page

`http://tools.bsc.es/extrae`

Contact

tools@bsc.es

Figure 10 illustrates two basic examples of how to use the Extrae instrumentation package to generate a Paraver trace for MPI (10(a)) and OpenMP (10(b)) applications. For further reference, please refer to the Extrae's user guide:
`https://tools.bsc.es/doc/pdf/extrae.pdf`

trace.sh

```
#!/usr/bin/env sh

export EXTRAE_HOME=/extrae/installation/root
export EXTRAE_CONFIG_FILE=extrae-config.xml
source ${EXTRAE_HOME}/etc/extrae.sh
export LD_PRELOAD=${EXTRAE_HOME}/lib/libmpitrace.so

$*
```

```
> mpirun ./trace.sh <mpi_binary> <args>
```

(a) MPI applications

trace.sh

```
#!/usr/bin/env sh

export EXTRAE_HOME=/extrae/installation/root
export EXTRAE_CONFIG_FILE=extrae-config.xml
source ${EXTRAE_HOME}/etc/extrae.sh
export LD_PRELOAD=${EXTRAE_HOME}/lib/libomptrace.so

$*
```

```
> ./trace.sh <omp_binary> <args>
```

(b) OpenMP applications

Figure 10: Basic examples to activate Extrae

Focus

single

parallel

perform

debug

correct

workflow

Prog. model

MPI

OpenMP

Pthreads

OmpSs

CUDA

HIP

OpenCL

OpenACC

UPC

SHMEM

GASPI

Language

C

C++

Fortran

Python

Processor

x86

Power

ARM

GPU

Extra-P

Extra-P is an automatic performance-modeling tool that supports the user in the identification of *scalability bugs*. A scalability bug is a part of the program whose scaling behavior is unintentionally poor, that is, much worse than expected.

Extra-P uses measurements of various performance metrics at different processor configurations as input to represent the performance of code regions (including their calling context) as a function of the number of processes. All it takes to search for scalability issues even in full-blown codes is to run a manageable number of small-scale performance experiments, launch Extra-P, and compare the asymptotic or extrapolated performance of the worst instances to the expectations. Besides the number of processes, it is also possible to consider other parameters such as the input problem size, as well as combinations of multiple parameters.

Extra-P generates not only a list of potential scalability bugs but also human-readable models for all performance metrics available such as floating-point operations or bytes sent by MPI calls that can be further analyzed and compared to identify the root causes of scalability issues.

Typical questions Extra-P helps to answer

- Which regions of the code scale poorly?
- Which metrics cause the run-time to scale poorly?
- What are the best candidates for optimization?
- How will my application behave on a larger machine?

Workflow

Extra-P accepts input files in the Cube format and generates performance models for each metric and call path rather than individual measured values. Tools such as Scalasca, Score-P, and others are provided with libraries that produce analysis reports in the Cube format. The Extra-P GUI provides the means to visualize, browse, and manipulate the resulting models. Detailed textual results are also generated by Extra-P for the in-depth analysis of sensitive code regions.

Platform support

Extra-P is platform independent. It requires only a working Python installation ($\geq$3.7) as it is installed via pip.

License

BSD 3-Clause License

Web page

`https://github.com/extra-p/extrap`

Contact

extra-p-support@lists.parallel.informatik.tu-darmstadt.de

Figure 11 shows performance models as generated for different call paths in Kripke, an open-source 3D Sn deterministic particle transport code. The performance models are functions of number of processes p, the number of direction-sets d, and the number of energy groups g. The call tree on the left allows the selection of models to be plotted on the right. The color of the squares in front of each call path highlights the complexity class.

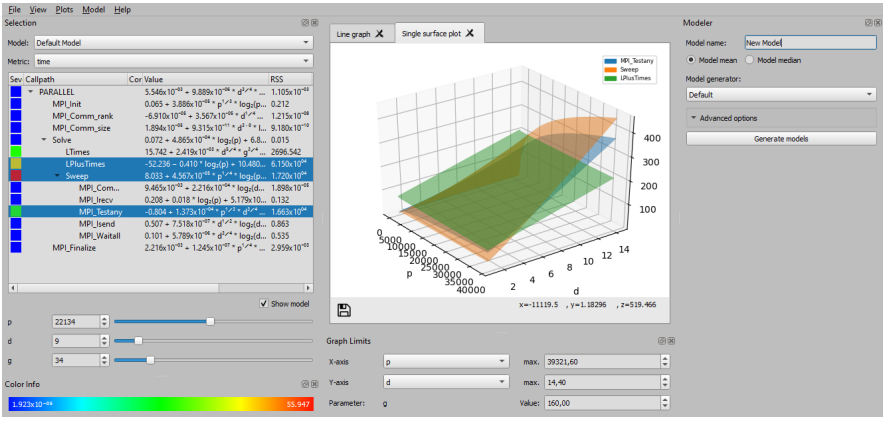

Figure 11: Interactive exploration of performance models in Extra-P.

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GASPI

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C++

Fortran

Python

Processor

x86

Power

ARM

GPU

JUBE

The JUBE environment provides a script-based application and platform independent framework, which allows the creation and parametrisation of an automatic workflow execution to be used in benchmark, test or production scenarios.

Typical questions JUBE helps to answer

- How to run my application in a reproducible way?
- How to easily create a parameter study for my application?
- How to parametrise the different parts of my application from a single point?

Workflow

JUBE is a Python-based tool which is configured using XML files. Within these input files an application workflow is based on different steps, where dependencies and related files can be configured. For program execution JUBE uses normal Linux shell commands, which allows developers to keep their existing mechanism to start or manage applications.

In addition JUBE allows a flexible way to specify parameters, which can be used to control the compilation of the application, its runtime arguments and behaviour, or the job execution environment.

After program execution, JUBE can also run post-processing tools or scan any ASCII-based program output to extract useful information like timing information or performance data. This information is gathered and displayed in a combined output form together with the selected parametrisation.

Platform support

Linux x86_64, (Python2.6, Python2.7, Python3.2 or any newer version)

License

GPLv3

Web page

`http://www.fz-juelich.de/jsc/jube`

Contact

jube.jsc@fz-juelich.de

Figure 12 shows an example of the command-line interface used to control the JUBE execution. Each individual run is stored separately, with a unique identifier, in the filesystem to allow reproducibility and easier data exchange.

```
> jube continue benchmarks/ -r
################################################################
# benchmark: ior
#
#
################################################################

Running workpackages (#=done, 0=wait, E=error):
############################################################ (  6/  6)

  stepname | all | open | wait | error | done
  ---------+-----+------+------+-------+-----
   compile |   1 |    0 |    0 |     0 |    1
   execute |   5 |    0 |    0 |     0 |    5

>>>> Benchmark information and further useful commands:
>>>>       id: 33
>>>>   handle: benchmarks
>>>>      dir: benchmarks/000033
>>>>  analyse: jube analyse benchmarks --id 33
>>>>   result: jube result benchmarks --id 33
>>>>     info: jube info benchmarks --id 33
>>>>      log: jube log benchmarks --id 33
################################################################
>>> Start analyse
>>> Analyse finished
result:
nodes | tasks |   api | filePerProc | collective | Aggregatesize | blockSize | transferSize | segmentCount | RDbwmax | RDbwmean | RDbwmin |
------+-------+-------+-------------+------------+---------------+-----------+--------------+--------------+---------+----------+---------+
    1 |    24 | POSIX |           0 |          0 |        48 GiB | 268435456 |      4194304 |            8 |  5589.3 |   5547.9 |  5478.0 |
    1 |    24 | POSIX |           1 |          0 |        48 GiB | 268435456 |      4194304 |            8 |  6147.9 |   6128.6 |  6116.6 |
    1 |    24 | MPIIO |           0 |          0 |        48 GiB | 268435456 |      4194304 |            8 |  5714.0 |   5690.7 |  5659.7 |
    1 |    24 |  HDF5 |           0 |          0 |        48 GiB | 268435456 |      4194304 |            8 |  5678.5 |   5653.1 |  5604.7 |
    1 |    24 | NCMPI |           0 |          0 |        48 GiB | 268435456 |      4194304 |            8 |  5665.9 |   5639.1 |  5621.2 |
```

Figure 12: Command-line view of a JUBE-based benchmark execution.

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Python

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ARM

GPU

LIKWID

LIKWID is a tool suite for performance-oriented programmers offering command line tools for system topology, CPU/task affinity, hardware performance monitoring, micro-benchmarking and more. Besides the command line tools tools, almost all functionality is provided as a C library to be integrable in other tools.

Typical questions LIKWID helps to answer

- How does my system look like? How many threads are available?
- How well does my code exploit the provided hardware features?
- How to measure typical performance metrics (like floating-point operations, memory bandwidth or performance per watt) for my application
- How to reduce performance variation and control the placement of my software threads?
- How can I benchmark my code with different CPU frequencies?
- How does my code behave when hardware prefetcher X is disabled?
- How to run my application on X nodes and measure the metric Y for all processes?

Workflow

When freshly accessing a new machine, you want to get the system topology (likwid-topology) to determine the number of threads and the hardware threads (CPU cores) the application should run on (likwid-pin). If you have an MPI application, determine the affinity strategy once and run your MPI+X application (likwid-mpirun). What is the metric X for my whole application run or how does it evolve over time (likwid-perfctr)? If you want to measure loop(s) or routine(s) running on CPUs or GPUs, add MarkerAPI instrumentation to your code once and control the measurement from the command line.

You want to get an impression how well a feature improves your performance? Write a small benchmark in assembly (to avoid compiler "optimizations") and run it in a controlled environment.

Platform support

x86/x86_64 (Intel & AMD), ARM8 (Marvell Thunder X2, Fujitsu A64FX, AWS Graviton2), POWER (POWER8 and POWER9) and Nvidia/AMD GPUs under the Linux OS.

License

GPLv3

Web page

`https://hpc.fau.de/research/tools/likwid/`
`https://github.com/RRZE-HPC/likwid/wiki`
Python interface: `https://github.com/RRZE-HPC/pylikwid`
Julia interface: `https://github.com/JuliaPerf/LIKWID.jl`

Contact

rrze-likwid@fau.de or matrix.org chat

```
+----------------------+-----------+-----------+-----------+-----------+
|        Metric        |   Core 0  |   Core 1  |   Core 2  |   Core 3  |
+----------------------+-----------+-----------+-----------+-----------+
|  Runtime (RDTSC) [s] |    2.4796 |    2.4796 |    2.4796 |    2.4796 |
| Runtime unhalted [s] |    2.2949 |    2.2932 |    2.2868 |    2.2935 |
|      Clock [MHz]     | 3392.1738 | 3392.1734 | 3392.1724 | 3392.1754 |
|          CPI         |    5.1572 |    5.0843 |    5.1161 |    5.1234 |
|  Load to store ratio |    1.8224 |    1.8419 |    1.8332 |    1.8309 |
|      Load ratio      |    0.2352 |    0.2313 |    0.2329 |    0.2335 |
|      Store ratio     |    0.1291 |    0.1256 |    0.1270 |    0.1275 |
+----------------------+-----------+-----------+-----------+-----------+

+--------------------------+------------+-----------+-----------+-----------+
|          Metric          |     Sum    |    Min    |    Max    |    Avg    |
+--------------------------+------------+-----------+-----------+-----------+
|  Runtime (RDTSC) [s] STAT |     9.9184 |    2.4796 |    2.4796 |    2.4796 |
| Runtime unhalted [s] STAT |     9.1684 |    2.2868 |    2.2949 |    2.2921 |
|      Clock [MHz] STAT     | 13568.6950 | 3392.1724 | 3392.1754 | 3392.1737 |
|          CPI STAT         |    20.4810 |    5.0843 |    5.1572 |    5.1202 |
|  Load to store ratio STAT |     7.3284 |    1.8224 |    1.8419 |    1.8321 |
|      Load ratio STAT      |     0.9329 |    0.2313 |    0.2352 |    0.2332 |
|      Store ratio STAT     |     0.5092 |    0.1256 |    0.1291 |    0.1273 |
+--------------------------+------------+-----------+-----------+-----------+
```

Figure 13: Measurement of the load-store-ratio (DATA performance group) of an application running on four CPU cores ($0-3$). The first table lists metrics for each CPU core while the second table contains statistics of the per-core measurements.

Focus

single

parallel

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workflow

Prog. model

MPI

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Pthreads

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SHMEM

GASPI

Language

C

C++

Fortran

Python

Processor

x86

Power

ARM

GPU

Linaro DDT

Linaro DDT is a modern and easy to use parallel debugger widely used by software developers and computational scientists in industry, academia and government research. Its interface simplifies concurrency and is highly responsive even at extreme scale.

The tool is part of Linaro Forge, a development solution that includes both debugging and profiling capabilities.

Typical questions Linaro DDT helps to answer

- Where is my application crashing?
- Why is my application crashing?
- Why is my application hanging?
- What is corrupting my calculation?

Workflow

Linaro DDT can be used on any supported platform to debug problems in application behaviour. The first step should be to compile the errant application with the “-g” compiler flag to ensure debugging information is provided to the debugger.

Thanks to its "reverse connect" capability, Linaro DDT can be very easily attached to an application submitted via the batch scheduler. Where an application has hung, the debugger can attach to existing processes. A native remote client allows users to debug graphically from remote locations.

Users interact with the debugged processes - being able to step or “play” processes, and examine where all processes are, and their variable values and array data across processes. Memory debugging can be enabled to detect common errors such as reading beyond array bounds automatically.

Platform support

Any Linux running on aarch64, x86_64, and Nvidia GPUs.

License

Commercial

Web page

`https://www.linaroforge.com`

Contact

`https://www.linaro.org/support#for-linaro-forge4`

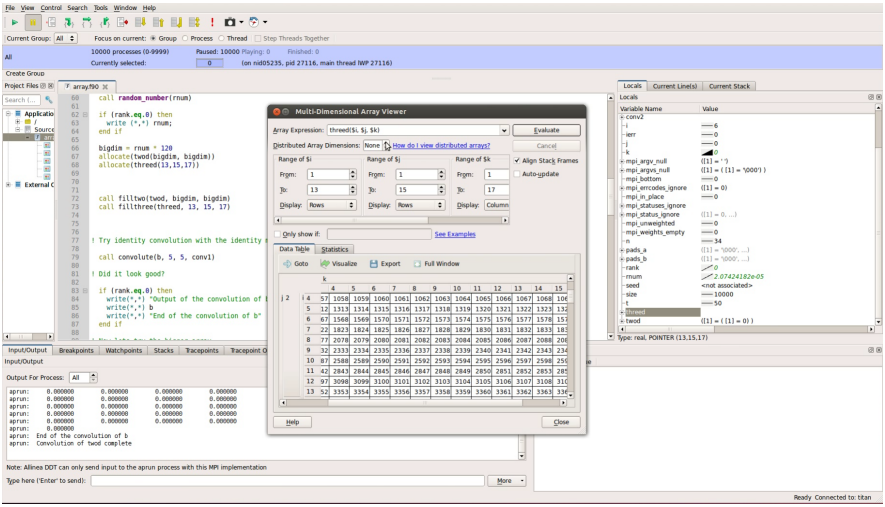

Figure 14: Linaro DDT parallel debugging session showing multi-dimensional array viewer.

Focus

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workflow

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SHMEM

GASPI

Language

C

C++

Fortran

Python

Processor

x86

Power

ARM

GPU

Linaro MAP

Linaro MAP is a modern and easy to use profiling tool that is designed to help users visually identify performance issues in their application. It integrates profiling information alongside source code and can show metrics such as vectorization, communication and I/O.

The tool is part of Linaro Forge, a development solution that includes both debugging and profiling capabilities.

Typical questions Linaro MAP helps to answer

- Where is my code slow - what line and why?
- Am I achieving good vectorization?
- Is memory usage killing my performance?

Workflow

Applications can be launched via Linaro MAP and the performance data will be recorded automatically. There is no need to recompile, although a “-g” flag will ensure accuracy of source line information. The “.map” files are analysed inside the tool and are sufficiently compact to be easily shared.

Platform support

Any Linux running on aarch64, x86_64 and Nvidia GPUs.

License

Commercial

Web page

`https://www.linaroforge.com`

Contact

`https://www.linaro.org/support#for-linaro-forge4`

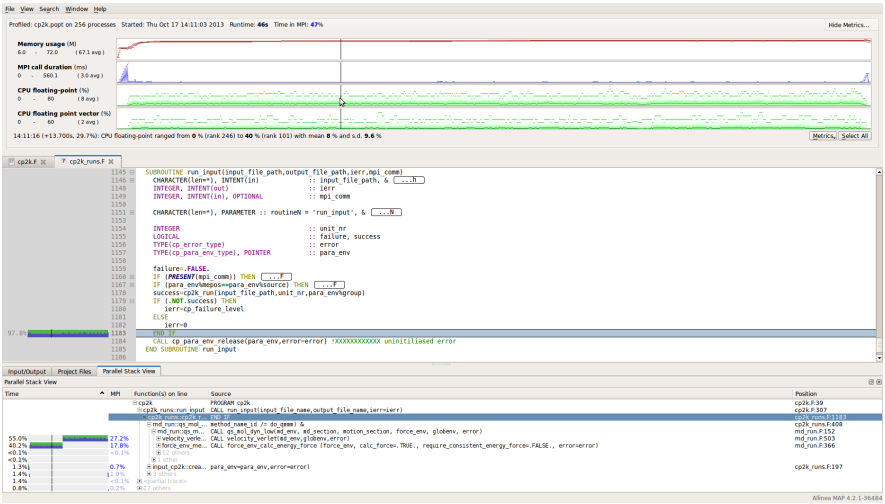

Figure 15: Linaro MAP parallel profiling session showing execution hotspots and evolution charts.

Focus

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workflow

Prog. model

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Pthreads

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GASPI

Language

C

C++

Fortran

Python

Processor

x86

Power

ARM

GPU

Linaro Performance Reports

Linaro Performance Reports is a performance tool that aims to provide information for anyone involved in HPC, not just software developers. It does not require configuration or any change to the profiled application.

The output provided from a run is a single one-page report on application performance - containing information such as vectorization, communication, energy usage and I/O - with advice about what can be explored to improve the performance.

The tool is part of Linaro Forge, a development solution that includes both debugging and profiling capabilities.

Typical questions Linaro Performance helps to answer

- What can I do to improve the efficiency of my application?
- What system or usage changes could I make to improve performance?
- How does the underlying hardware impact the performance of my applications?

Workflow

Applications are launched with a simple prefix-command (“perf-report”) to the existing MPI launch line. There is no need to recompile or relink on most platforms. The “.html” report file created is then viewable in any standard browser.

Platform support

Any Linux running on aarch64, x86_64, and Nvidia GPUs.

License

Commercial

Web page

`https://www.linaroforge.com`

Contact

`https://www.linaro.org/support#for-linaro-forge4`

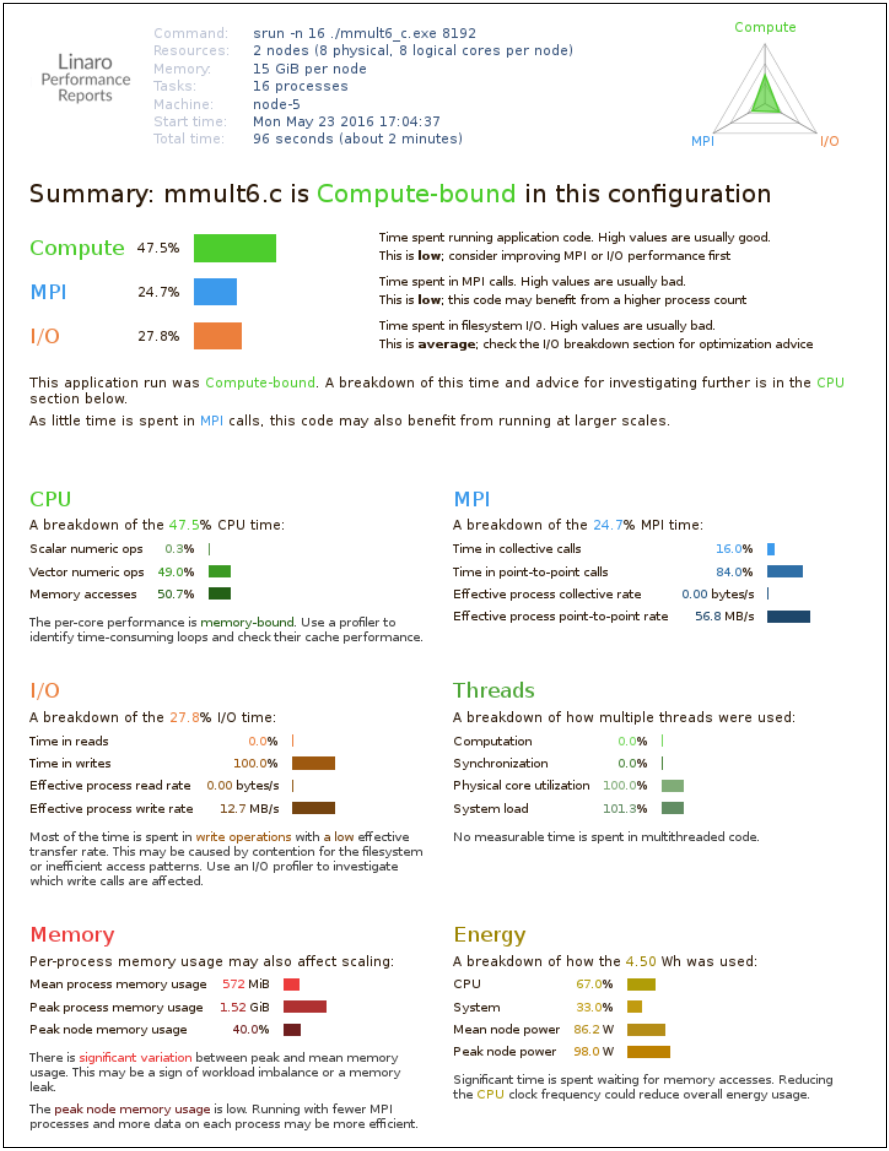
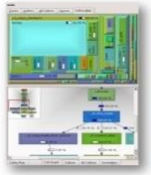


Figure 16: Linaro Performance Reports single page report of an application's CPU, MPI, I/O and Memory usage.

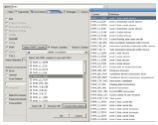
VI-HPS Tools Overview

CALIPER / LIKWID /
MAP/PR / MPIP /
O|SS / MAQAO

KCACHEGRIND



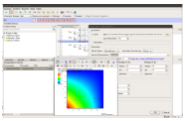
PAPI



Hardware
monitoring

MUST /
ARCHER

DDT



Debugging,
error & anomaly
detection

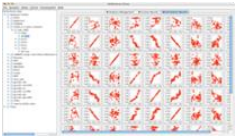
JUBE

STAT

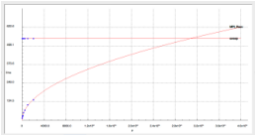
Execution

LIKWID /
MEMCHECKER /
SPINDLE / SIONLIB

TAU

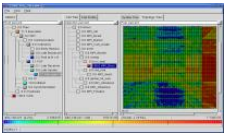


EXTRA-P



Automatic profile & trace analysis

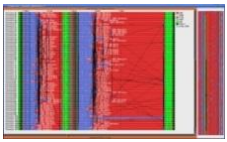
SCALASCA / CUBE



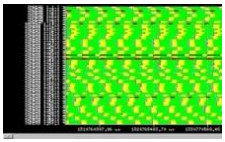
SCORE-P / EXTRAE

Visual trace analysis

VAMPIR



PARAVER



Optimization

MAQAO

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Prog. model

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OpenCL

OpenACC

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Language

C

C++

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Processor

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Power

ARM

GPU

MAQAO

MAQAO (**M**odular **A**ssembly **Q**uality **A**nalyzer and **O**ptimizer) is a core performance centric binary analysis and optimization framework operating on executable binary applications (no recompilation necessary). The tool applies dynamic and static analyses on extracted/reconstructed high level structures - loops and functions - to guide application developers through optimization by providing synthetic and human-friendly reports and hints.

MAQAO was designed as an extensible framework allowing users to easily develop analysis and instrumentation modules using a Lua API, and it comes with three ready-to-use modules: LProf (Lightweight Profiler), a sampling-based profiler that provides a list of hot spots (loops and functions) collected during program execution; CQA (Code Quality Analyzer), a static analyzer that uses a machine model to evaluate the assembly code quality of target loops and functions by using key metrics such as arithmetic units usage and vector length usage; ONE View, a module that invokes LProf and CQA and aggregates their results in order to build a human-friendly report that spans a large set of key performance elements.

Typical questions MAQAO helps to answer

- Which functions and loops are the most profitable to optimize?
- What optimizations will be beneficial to a loop and how much gain can be expected?
- Is a specific loop or function compute-bound or memory-bound?
- How much gain improved parallelization can provide?

Workflow

The analysis process is driven by ONE View, using a configuration file containing the parameters necessary to launch the target application and run the analysis modules. Once the analysis is complete, ONE View generates a human-friendly synthetic HTML report.

This report includes a list of hot spots categorized by their origin: parallel runtime, I/O, memory, main code, etc. For each hot spot, the report provides a description of potential issues, an estimation of the impact on overall application performance, and hints on how to improve performance through compiler directives or implementation tweaks. MAQAO can also generate comparison reports between multiple runs of an application with different datasets or parallel execution parameters.

Platform support

Linux clusters (x86_64 and aarch64)

License

GNU Lesser General Public License (LGPL) v3

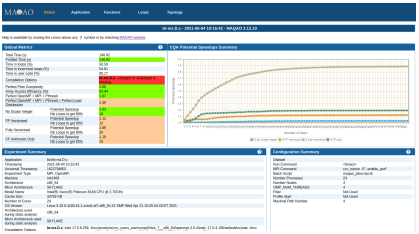
Web page

`http://www.maqao.org`

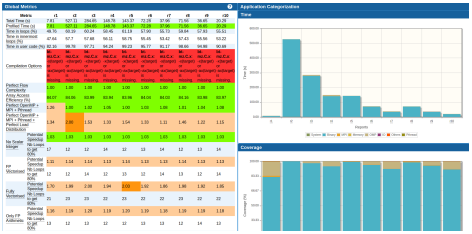
Contact

contact@maqao.org

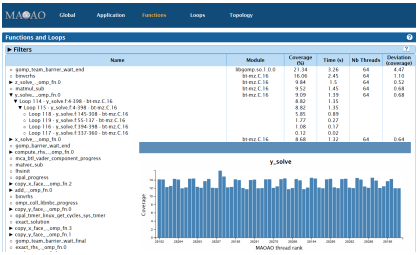
Figure 17 presents views from the HTML output generated by ONE View: (17(a)) an overview of the application performance and estimated achievable speedups, (17(b)) a comparison between multiple runs with different parallel execution parameters, (17(c)) the list of functions and loops hot spots, (17(d)) code quality hints and associated relative potential gains.



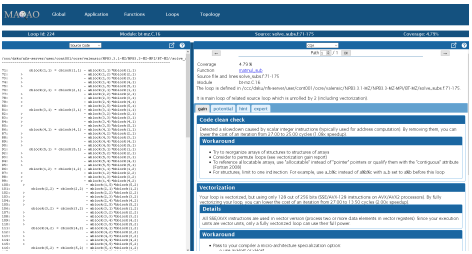
(a) Global view



(b) Multi-runs comparison (scalability mode)



(c) Functions profile



(d) Code quality report

Figure 17: Some of MAQAO ONE View HTML outputs.

Focus

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GPU

MERIC runtime system

The MERIC runtime system from the MERIC energy efficiency HPC software suite is a tool for energy efficiency analysis of scientific applications. The runtime system (library) and its utilities provide information about the hardware and its usage by the application execution. Besides the power management related metrics measurement, the MERIC library allows to control hardware power management knobs (if rights elevated by system administrators) and to identify optimal parameter configurations for each instrumented region.

MERIC is designed as a runtime system, which automatically identifies an optimal configuration of available hardware power management knobs to save energy with no or user-defined execution time penalty limit. However, it can also be used as a user tool, which only measures the hardware resource usage.

Typical questions MERIC runtime system helps to answer

- How much energy does an application execution consume?
- Is my application using the CPU / GPU energy efficiently?
- Which hardware platform to use for my application to be energy efficient?
- How much energy can be saved using dynamic tuning of power management knobs with no (or limited) performance penalty?

Workflow

Energy consumption measurement of an application execution can be done using a command-line utility, which requires being executed three times: to start, stop, and evaluate a measurement. For additional power management-related metrics (i.e., FLOPs, vectorization ratio, CPU frequencies, power capping activity ratio), it is necessary to link the application to be evaluated with the MERIC library. The library must be initialized, closed, and regions of interest should be identified using the library API. The application is executed as usual, while MERIC usage is configured using environment variables.

MERIC stores output to ".CSV" files, which can be analysed using the RADAR visualizer – a PyQt6 graphical tool designed to present metrics not only from a single application execution, but also to compare a region's resource usage in various configurations.

Platform support

Linux x86_64, ARM64, IBM POWER8/9/10, NVIDIA GPUs, AMD GPUs

Supported power monitoring systems

Intel/AMD RAPL, NVML, ROCm, A64FX, ATOS HDEEM, OCC, DiG

License

BSD 3-Clause license

Web page

`https://code.it4i.cz/energy-efficiency/meric-suite/meric`

Contact

meric@it4i.cz

Figure 18 presents a window from the RADAR visualizer showing how the power consumption of the compute blade, CPUs, and DDR memories varies in time in reaction to changes in the boundedness of the executed workload.

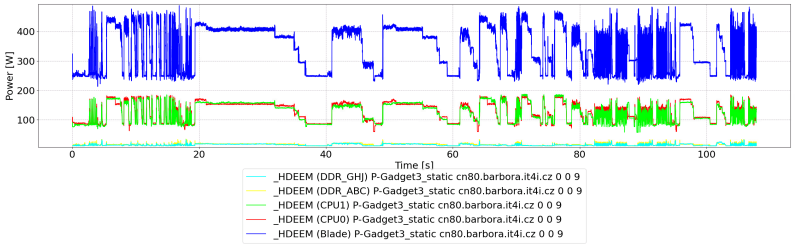

Figure 18: Power consumption timeline of an executed application.

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Python

Processor

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MUST

MUST detects whether an application conforms to the MPI standard and is intended to scale with the application (O(10,000) processes). At runtime it transparently intercepts all MPI calls and applies a wide range of correctness checks (including type matching checks and deadlock detection) to their arguments. This allows developers to identify manifest errors (ones you already noticed), portability errors (manifest on other platforms), and even unnoticed errors (e.g., silently corrupted results). When an application run with the tool finishes it provides its results in a correctness report for investigation.

Typical questions MUST helps to answer

- Has my application potential deadlocks?
- Am I doing type matching right?
- Does my application leak MPI resources?
- Other hidden errors?

Workflow

Replace mpiexec/mpirun/runjob/.. by mustrun:
`mpiexec -np 1024 executable` → `mustrun -np 1024 executable`
After the run inspect the outputfile `MUST_Output.html` with a browser (w3m, firefox, . . .).

For Batchjobs: Note that the run uses extra MPI processes to execute checks, use "--must:info" to retrieve resource allocation information.

Platform support

Linux x86_64, IBM Blue Gene/Q, Cray XE (early support), SGI Altix4700
Tested with various MPI implementations:
Open MPI, Intel MPI, MPICH, MVAPICH2, SGI MPT, . . .

License

BSD 3-Clause License

Web page

`https://www.itc.rwth-aachen.de/must`

Contact

must-feedback@lists.rwth-aachen.de

Figure 19 gives detailed information for a deadlock situation detected by MUST (caused by mismatching *tags*):

Rank 0 reached `MPI_Finalize`.

Rank 1 is at `MPI_Recv(`*`src`*`=MPI_ANY_SOURCE, `*`tag`*`=42)`.

Rank 2 did `MPI_Ssend(`*`dest`*`=1, `*`tag`*`=43)`.

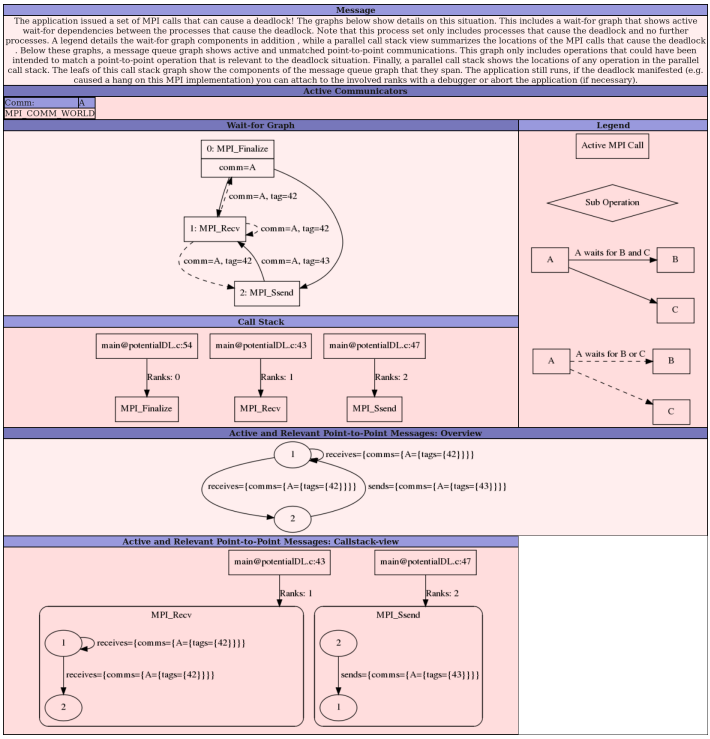

Figure 19: Visualization of a deadlock situation.

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OSACA

The **O**pen-**S**ource **A**rchitecture **C**ode **A**nalyzer (OSACA) is a Python-based static analysis tool for in-core performance prediction of inner-most assembly loops. It is available both as command line application and as tool within the Compiler Explorer and provides the user with a throughput prediction of their code in steady state, a critical path analysis and an across-loops-dependency analysis. Besides its provided machine models for several x86 and ARM micro-architectures, it is designed in a way so that the user can easily add its own machine models for architectural exploration and integrate it in their own workflow via a Python API.

Typical questions OSACA helps to answer

- How fast can my code possibly run (when all data is in L1 cache)?
- What optimizations will be beneficial for my code?
- What is a more realistic roofline for my target code region?
- What are the bottlenecks of my code?
- Why does the code of compiler A perform better than the code of compiler B?

Workflow

Having the assembly code of your target high-level code, identify the region of interest and mark it with specific OSACA comment markers (either manually or with the built-in `-insert-marker` feature) or reduce the code to the specific section with the `-lines` option. Start the analysis by running OSACA and specify your target hardware with `-arch`. You will receive a light-speed throughput prediction showing a perfect scheduling based on the machine model, the critical path (CP) of your code, and all loop-carried dependencies (LCD). As a rule of thumb for steady-state loop kernels, the runtime prediction is the maximum of the most-occupied port and the LCD. Furthermore, you can generate a `.dot` graph file to visualize your dependencies in your assembly loop.

Platform support

The CLI runs under any platform with a Python 3 installation. OSACA currently comes with support for various micro-architectures, including

Intel x86_64 (Sandy Bridge, Ivy Bridge, Haswell, Broadwell, Skylake X, Cascade Lake X, Ice Lake, Sapphire Rapids), AMD x86_x86 (Zen 1, Zen 2, Zen 3, Zen 4), and ARM AArch64 (Marvell ThunderX2, ARM Neoverse N1, ARM Cortex A72, Fujitsu A64FX, HiSilicon TaiShan v110, Apple M1, Neoverse V2/NVIDIA Grace CPU).

License

GNU Affero General Public License v3.0 (AGPL-3.0)

Web page

`https://github.com/RRZE-HPC/OSACA`
`https://github.com/RRZE-HPC/OSACA/wiki`
Python ReadTheDocs: `https://osaca.readthedocs.io/en/latest/`
`https://godbolt.org/`

Contact

nhr-osaca@fau.de or OSACA Github Issues

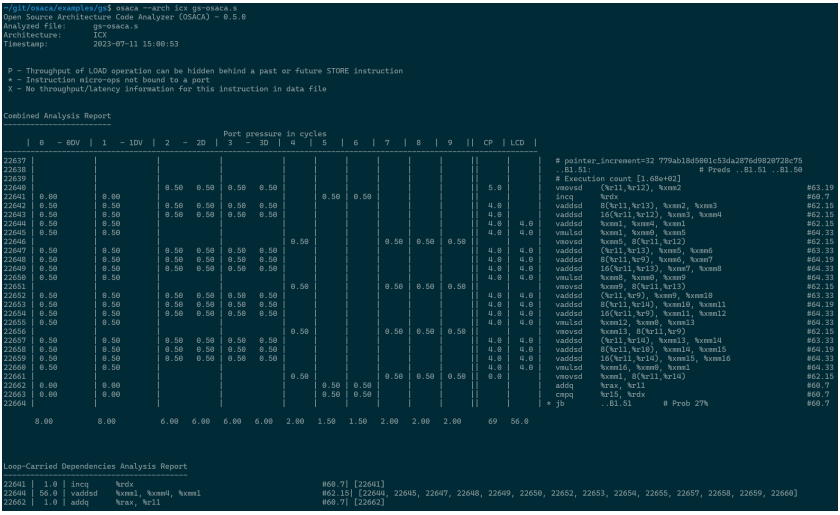

Figure 20: OSACA analysis of the Gauss-Seidel method, compiled on and analyzed for an Intel Ice Lake Server system. The predicted runtime would be 56 cy per assembly loop.

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Open|SpeedShop

Open|SpeedShop is an open source multi platform performance tool that is targeted to support performance analysis of applications running on both single nodes and large scale platforms. Open|SpeedShop is explicitly designed with usability in mind and provides both a comprehensive GUI as well as a command line interface (CLI). The base functionality includes sampling experiments, support for callstack analysis, access to hardware performance counters, tracing and profiling functionality for both MPI and I/O operations, as well floating point exception analysis. Each of these functionalities is available as an *Experiment* that a user can select and execute on a given target application. Several other experiments, such as memory analysis and CUDA support, are available in experimental versions.

Typical questions this tool helps to answer

- In which module, function, loop or statement is my code spending most of its time (Experiment name: pcsamp)?
- On which call paths were my hotspots reached (Experiment name: usertime)?
- Which hardware resources cause bottlenecks for my execution (Experiment name: hwcsamp)?
- How do hardware performance counter results, like TLB misses, map to my source (Experiment name: hwc/hwctime)?
- How much time am I spending in I/O or MPI operations (Experiment name: io/iot and mpi/mpit)?

Workflow

Open|SpeedShop can be applied to any sequential or parallel target application in binary form. To get finer grained attribution of performance to individual statements, it is recommended to apply the tool to codes compiled with -g, although this is not a requirement. The user picks an experiment (starting with the simple sampling experiment pcsamp is typically a good idea) and prepends the execution of the code (incl. MPI job launcher) with an Open|SpeedShop launch script for that experiment.

For example, if the target application is typically launched with:

```
mpirun -np 128 a.out
```

launching it with the pcsamp experiment would be:

```
osspcsamp "mpirun -np 128 a.out"
```

At the end of the execution, the tool provides a first overview of the observed performance and then creates a database with all performance data included, which can viewed in the Open|SpeedShop GUI:

```
openss -f <database-filename.openss>
```

Platform support

Linux x86_64 workstations and clusters, IBM Blue Gene, and Cray.

License

Open|SpeedShop is available under LGPL (main tool routine: GPL).

Web page

`http://www.openspeedshop.org/`

Contact

oss-questions@krellinst.org

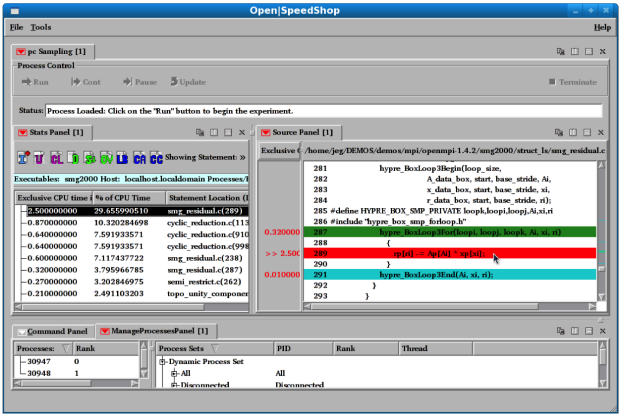

Figure 21: GUI showing the results of a sampling experiment (left: time per statement, right: information mapped to source)

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Language

- C
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- Fortran
- Python

Processor

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- GPU

OTF-CPT

OTF-CPT collects an application's critical path and various metrics during execution (on the fly). Upon completion, it generates a performance report in the form of model factors, also known as fundamental performance factors. OTF-CPT supports MPI, OpenMP, and hybrid MPI+OpenMP parallel programming paradigms. After conducting a series of scaling experiments, the tool can offer new insights into the scaling behavior of the parallel application.

Typical questions OTF-CPT helps to answer

- My hybrid MPI + OpenMP application spends 80% of the time in OpenMP barriers. Is this cased by inefficient use of OpenMP or caused by MPI communication?
- According to Amdahl's law, my parallel efficiency is only 30%. What is the cause of this inefficency?

Workflow

Execute the application with OTF-CPT:

```
mpirun -np 4 env OMP_NUM_THREADS=4 LD_PRELOAD=libOTFCPT.so \
  OMP_TOOL_LIBRARIES=libOTFCPT.so ./app
```

Platform support

Depends on OMPT support, so no gcc

License

Apache License 2.0 (LLVM)

Web page

https://github.com/RWTH-HPC/OTF-CPT

Contact

jenke@itc.rwth-aachen.de

#ranks x #threads	64x12	128x12	256x12	512x12	1024x12
Parallel Efficiency	81.4	68.3	52.6	30.7	15.9
Load Balance	97.6	95.9	94.6	91.9	88.3
Communication Efficiency	83.3	71.2	55.6	33.4	18.0
Serialisation Efficiency	84.6	76.0	65.5	54.1	43.8
Transfer Efficiency	98.4	93.8	84.8	61.7	41.2
MPI Parallel Efficiency	83.5	69.7	53.4	32.4	17.3
MPI Load Balance	98.7	96.9	95.3	93.0	90.3
MPI Communication Efficiency	84.6	72.0	56.1	34.9	19.1
MPI Serialisation Efficiency	85.9	76.7	66.1	56.5	46.4
MPI Transfer Efficiency	98.5	93.8	84.9	61.8	41.2
OMP Parallel Efficiency	97.5	97.9	98.4	94.7	92.1
OMP Load Balance	98.9	98.9	99.3	98.9	97.7
OMP Communication Efficiency	98.5	99.0	99.1	95.7	94.3
OMP Serialisation Efficiency	98.6	99.0	99.2	95.8	94.3
OMP Transfer Efficiency	100.0	100.0	99.9	99.9	100.0

Figure 22: Breakdown of performance model factors for a hybrid MPI + OpenMP application.

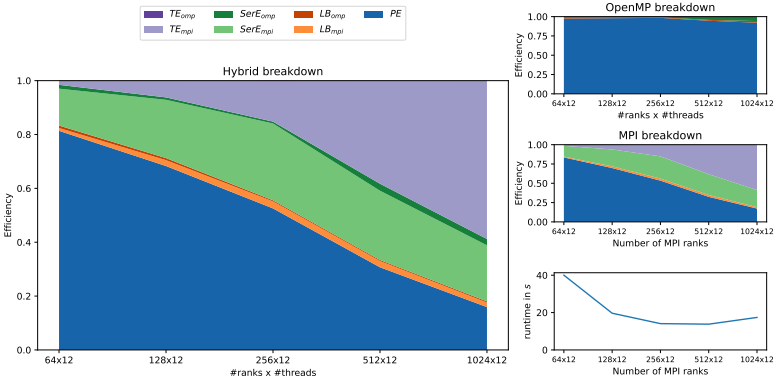

Figure 23: Plot of the data shown in Figure 22

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PAPI

Parallel application performance analysis tools on large scale computing systems typically rely on hardware counters to gather performance data. The PAPI performance monitoring library provides tool designers and application engineers with a common and coherent interface to the hardware performance counters (available on all modern CPUs) and other hardware components of interest (e.g., GPUs, network, and I/O systems). PAPI offers its features through an API that can be integrated into C/C++/Fortran applications, a Python API, and a set of command line utilities.

Typical questions PAPI helps to answer

- What is the relation between software performance and hardware events?
- What are the number of cache misses, floating-point operations, executed cycles, etc. of the routines, loops in my application?
- How much data is sent over the network? How much data originates from a node and how much is passed through a node?
- What is the system's power usage and energy consumption when my application is executed?
- How can the internal behavior of my software be exported to third party developers?
- What type of hardware is available on my platform?

Workflow

While PAPI can be used as a stand-alone tool, it is more commonly applied as a middleware by third-party profiling, tracing as well as sampling tools (e.g., CrayPat, HPCToolkit, Scalasca, Score-P, TAU, Vampir), making it a de facto standard for hardware counter analysis.

The events that can be monitored involve a wide range of performance-relevant architectural features: cache misses, floating point operations, retired instructions, executed cycles, and many others. By tightly coupling PAPI with the tool infrastructure, pervasive performance measurement capability - including accessing hardware counters, power and energy measurements, and data transfers, at either the hardware or software library level - can be made available.

Platform support

- AMD up to Zen5 and power
- AMD GPUs up to MI250x (beta support for MI300), power, temperature, fan
- ARM Cortex, ARM64, uncore support
- Cray Slingshot, Gemini, and Aries interconnects, power/energy
- Fujitsu K Computer
- IBM Blue Gene Series (5D-Torus, I/O system, CNK, EMON power)
- IBM Power Series, Nest-events through PCP, power monitoring and capping
- Intel up to Sapphire Rapids, AlderLake, RaptorLake, RAPL (power/energy), power capping
- Intel GPUs
- Nvidia up to Ampere, Hopper, multi-GPU, NVLink, NVML (power/energy), power capping

License

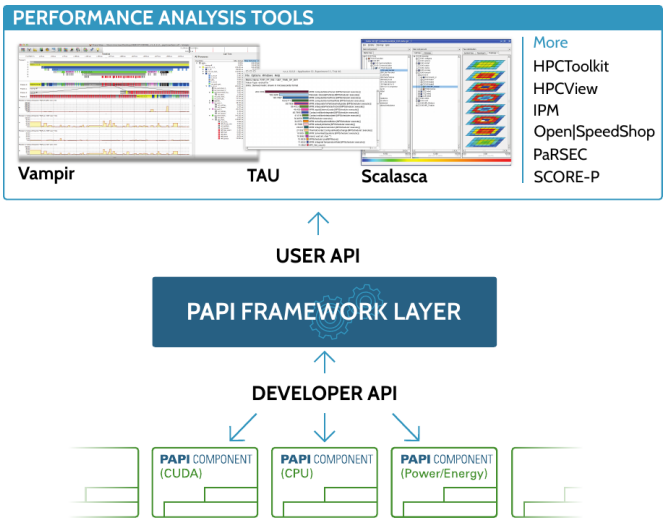
BSD 3-Clause License

Web page

`https://icl.utk.edu/papi`
`https://github.com/icl-utk-edu/papi`

Contact

ptools-perfapi@icl.utk.edu



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Paraver

Paraver is a performance analyzer based on event traces with a great flexibility to explore the collected data, supporting a detailed analysis of the variability and distribution of multiple metrics with the objective of understanding the application's behavior. Paraver has two main views: The timeline view displays the application behavior over time, while the statistics view (histograms, profiles) complements the analysis with distribution of metrics. To facilitate extracting insight from detailed performance data, during the last years new modules introduce additional performance analytics techniques: clustering, tracking and folding allow the performance analyst to identify the program structure, study its evolution and look at the internal structure of the computation phases. The tool has been demonstrated to be very useful for performance analysis studies, with unique features that reveal profound details about an application's behavior and performance.

Typical questions Paraver helps to answer

- How well does the parallel program perform and how does the behavior change over time?
- What is the parallelization efficiency and the effect of communication?
- What differences can be observed between two executions?
- Are performance or workload variations the cause of load imbalances in computation?
- Which performance issues are reflected by hardware counters?

Workflow

The basis of an analysis with Paraver is a measurement of the application execution with its performance monitor Extrae. After opening the resulting trace file in Paraver the user can select from a subset of introductory analysis views that are hinted by the tool based on the recorded metrics. These basic views allow an easy overview of the application behavior. Next to that, Paraver includes a multitude of predefined views enabling a deeper analysis. Furthermore, Paraver offers a very flexible way to combine multiple views, so as to generate new representations of the data and more complex derived metrics. Once a desired view is obtained, it can be stored in a configuration file to apply it again to the same trace or to a different one.

Platform support

Linux (x86/x86_64, ARM, Power), SGI Altix, Fujitsu FX10/100, Cray XT, IBM Blue Gene, Intel Xeon Phi, Windows, macOS

License

GNU Lesser General Public License (LGPL) v2.1

Web page

`http://tools.bsc.es/paraver`

Contact

tools@bsc.es

Figure 24 shows a histogram of the computation phases colored by the clustering tool. Small durations are located in the left of the picture, and large durations on the right. The variability between the cells that have the same color indicate variance on the duration that would be paid as waiting time within MPI. We can see that the larger computing region (light green on the right) is the one with larger imbalance.

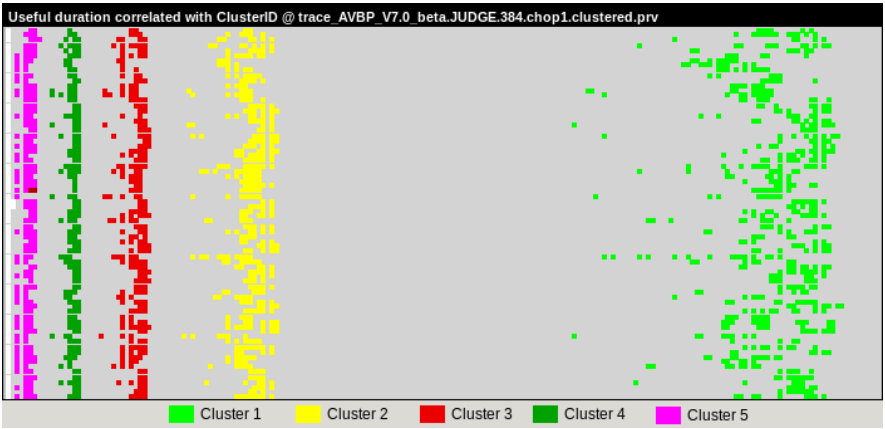

Figure 24: Paraver histogram of the computation phases colored with the cluster ID.

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Language

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- Python

Processor

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Scalasca Trace Tools

The Scalasca Trace Tools support performance optimization of parallel programs with a collection of highly scalable trace-based tools for in-depth analyses of concurrent behavior. The Scalasca tools have been specifically designed for use on large-scale systems such as the IBM Blue Gene series and Cray XT and successors, but is also well suited for small- and medium-scale HPC platforms. The automatic analysis identifies potential performance bottlenecks – in particular those concerning communication and synchronization – and offers guidance in exploring their causes.

Typical questions the Scalasca Trace Tools help to answer

- Which call-paths in my program consume most of the time?
- Why is the time spent in communication or synchronization higher than expected?
- For which program activities will optimization prove worthwhile?
- Does my program suffer from load imbalance and why?

Workflow

Before any Scalasca analysis can be carried out, an execution trace of the target application needs to be collected. For this task, Scalasca leverages the community-driven instrumentation and measurement infrastructure Score-P. After an optimized measurement configuration has been prepared based on initial profiles, a targeted event trace in OTF2 format can be generated, and subsequently analyzed by Scalasca's automatic event trace analyzer after measurement is complete. This scalable analysis searches for inefficiency patterns and wait states, identifies their root causes (i.e., delays) also along far-reaching cause-effect chains, collects statistics about the detected wait-state instances, and determines a profile of the application's critical path. The result can then be examined using the interactive analysis report explorer Cube.

Platform support

Continoulsy tested on: HPE Cray XC and EX, various Linux (Intel, AMD, IBM, ARM) clusters with GNU, Intel, NVIDIA, IBM, and AMD compilers.
Previously tested on: Intel Xeon Phi (KNL), IBM Blue Gene/Q, Cray XT/XE/XK, Fujitsu FX systems

License

BSD 3-Clause License

Web page

`https://www.scalasca.org`

Contact

scalasca@fz-juelich.de

Figure 25 shows part of a time-line of events from three processes, exemplifying results of the Scalasca trace analyzer. First, wait states in communications and synchronizations are detected, such as the "Late Sender" wait states in both message transfers (C→A and A→B) due to receive operations blocked waiting for messages to arrive. Second, the analysis identifies that the wait state on process A is caused directly by the excess computation in `foo` on process C. Besides the extra receive operation on process A, this imbalance is also identified as a cause for the wait state on process B through propagation: by inducing the wait state on process A it is also delaying the following send operation further. Finally, the analysis determines the critical path of execution (outlined), whose profile highlights call paths that are good candidates for optimization.

The analyzer quantifies metric severities for each process/thread and call path, and stores them in an analysis report for examination with Cube. Additional wait-state instance statistics can be used to direct Paraver or Vampir trace visualization tools to show and examine the severest instances.

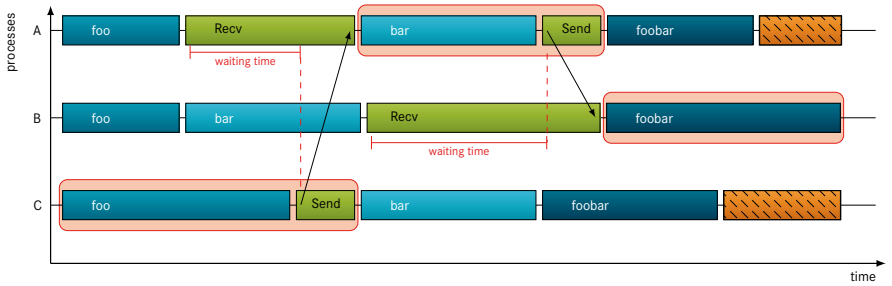

Figure 25: Scalasca automatic trace analysis identification of time in message-passing wait states and on the critical path.

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Score-P

The Score-P measurement infrastructure is a highly scalable and easy-to-use tool suite for profiling and event tracing. It supports a wide range of HPC platforms and programming models. Score-P provides core measurement services for a range of specialized analysis tools, such as Vampir, Scalasca, TAU, or Extra-P.

Typical questions Score-P helps to answer

- Which call-paths in my program consume most of the time?
- How much time is spent in communication or synchronization?

Further analysis tools can also be employed on Score-P measurements.

Workflow

1. Preparation. To create measurements, the target program must be instrumented. Score-P offers various instrumentation options, including automatic compiler instrumentation or manual source-code instrumentation. As an alternative to automatic compiler instrumentation, events can be generated using a sampling approach.

2. Measurement. The instrumented program can be configured to record an event trace or produce a call-path profile. Optionally, PAPI, rusage, and perf hardware metrics can be recorded. Filtering techniques allow precise control over the amount of data to be collected.

3. Analysis. Call-path profiles can be examined in TAU or the Cube profile browser and serve as Extra-P input. Event traces can be examined in Vampir or used for automatic bottleneck analysis with Scalasca.

Platform support

Continoulsy tested on HPE Cray EX, various Linux (Intel, AMD, ARM) clusters with GNU, Intel, NVIDIA, IBM, AMD, and Clang compilers. Successful RISC-V QEMU build with GNU compilers. Previously tested on Intel Xeon Phi, IBM Blue Gene/Q, Cray XT/XE/XK/XC, and Fujitsu FX systems.

License

Web page

`https://score-p.org`
Python bindings: `https://github.com/score-p/scorep_binding_python`

Contact

support@score-p.org

Figure 26 is an overview of the Score-P instrumentation and measurement infrastructure and the analysing tools from the VI-HPS ecosystem. Supported programming models and other event sources are modularized at the lowest level. Score-P instruments the application at build time with the necessary code to perform the measurement. Measurement mode and any external sources such as PAPI are specified at runtime. The performance data is stored for postmortem analysis in the open data formats CUBE4 for call-path profiles and OTF2 for event traces. Multiple analysis tools can then work on the same data from a single measurement run.

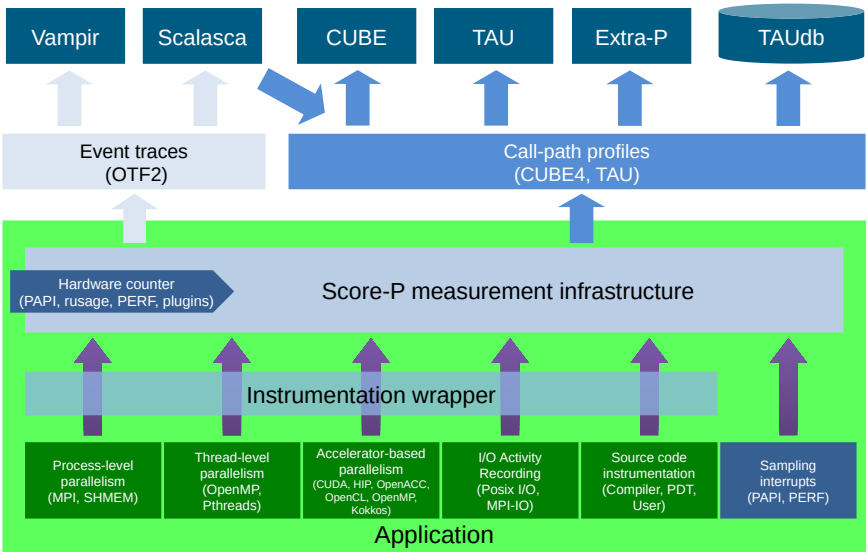

Figure 26: Overview of Score-P, produced dataformats, and analysing tools.

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GPU

STAT — The Stack Trace Analysis Tool

The Stack Trace Analysis Tool gathers and merges stack traces from all processes of a parallel application. The tool produces call graphs: 2D spatial and 3D spatial-temporal; the graphs encode calling behavior of the application processes in the form of a prefix tree. The 2D spatial call prefix tree represents a single snapshot of the entire application. The 3D spatial-temporal call prefix tree represents a series of snapshots from the application taken over time (see Figure 27). In these graphs, the nodes are labeled by function names. The directed edges, showing the calling sequence from caller to callee, are labeled by the set of tasks that follow that call path. Nodes that are visited by the same set of tasks are assigned the same color, giving a visual reference to the various equivalence classes.

Typical questions STAT helps to answer

- Where is my code stuck?
- Which processes have similar behavior?
- Where do I need to start debugging?

Workflow

STAT comes with its own GUI, invoked with the `stat-gui` command. Once launched, this GUI can be used to select the application to debug (in the context of MPI applications typically the job launch process, i.e., mpirun or equivalent). STAT will then attach to the target application processes, gather the stack traces and display them within the GUI for analysis.

Platform support

Linux x86_64 workstations and clusters, IBM Blue Gene, and Cray XT/XE/XK.

License

BSD

Web page

`http://www.paradyn.org/STAT/STAT.html`

Contact

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Figure 27 shows a call prefix tree generated by STAT from a sample MPI application which is stalled. At a high-level (before MPI internals), the code has three groups of processes: rank 1 in `do_SendOrStall`, rank 2 in `MPI_Waitall`, and the other 4094 processes in `MPI_Barrier`. Using this information it is sufficient to apply a debugger only to one representative process from each group in order to be able to investigate this problem.

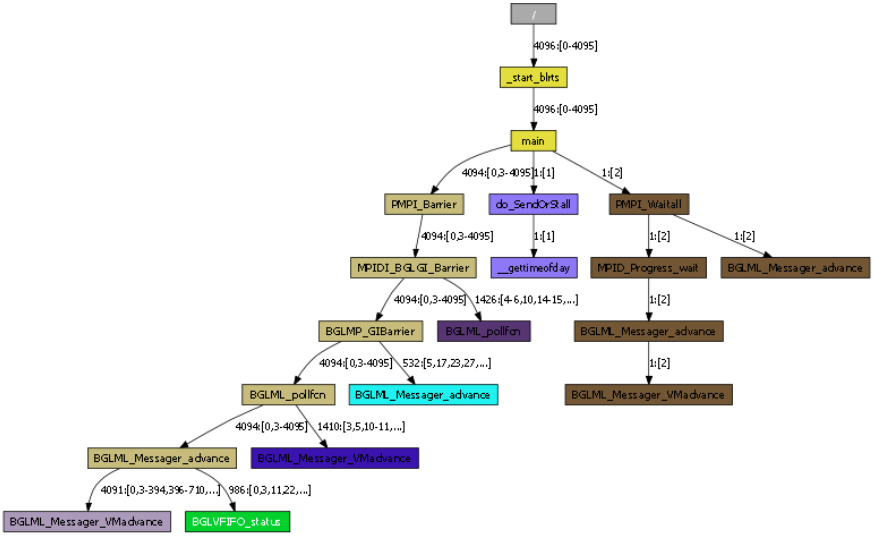

Figure 27: STAT 3D spatial-temporal call prefix tree of stalled execution.

Focus

single

parallel

perform

debug

correct

workflow

Prog. model

MPI

OpenMP

Pthreads

OmpSs

CUDA

HIP

OpenCL

OpenACC

UPC

SHMEM

GASPI

Language

C

C++

Fortran

Python

Processor

x86

Power

ARM

GPU

TAU

TAU is a comprehensive profiling and tracing toolkit that supports performance evaluation of programs written in C++, C, UPC, Fortran, Python, and Java. It is a robust, flexible, portable, and integrated framework and toolset for performance instrumentation, measurement, debugging, analysis, and visualization of large-scale parallel computer systems and applications. TAU supports both direct measurement as well as sampling modes of instrumentation and interfaces with external packages such as Score-P, PAPI, Scalasca, and Vampir.

Typical questions TAU helps to answer

- Which routines, loops, and statements in my program consume most of the time?
- Where are the memory leaks in my code and where does my program violate array bounds at runtime?
- What is the extent of I/O and what is the bandwidth of I/O operations?
- What is the performance of kernels that execute on accelerators such as GPUs and Intel Xeon co-processors (MIC).
- What is the extent of variation of the power and heap memory usage in my code? When and where does it show extremes?

Workflow

TAU allows the user to instrument the program in a variety of ways including rewriting the binary using *tau_rewrite* or runtime pre-loading of shared objects using *tau_exec*. Source level instrumentation typically involves substituting a compiler in the build process with a TAU compiler wrapper. This wrapper uses a given TAU configuration to link in the TAU library. At runtime, a user may specify different TAU environment variables to control the measurement options chosen for the performance experiment. This allows the user to generate callpath profiles, specify hardware performance counters, turn on event based sampling, generate traces, or specify memory instrumentation options.

Performance-analysis results may be stored in TAUdb, a database for cross-experiment analysis and advanced performance data mining operations using TAU's PerfExplorer tool. It may be visualized using ParaProf, TAU's 3D profile browser that can show the extent of performance variation and compare executions.

Supported platforms

IBM Blue Gene P/Q, NVIDIA and AMD GPUs and Intel MIC systems, Cray XE/XK/XC30, SGI Altix, Fujitsu K Computer (FX10), NEC SX-9, Solaris & Linux clusters (x86/x86_64,MIPS,ARM), Windows, macOS.

Supported Runtime Layers

MPI, OpenMP (using GOMP, OMPT, and Opari instrumentation), Pthread, MPC Threads, Java Threads, Windows Threads, SHMEM, CUDA, OpenCL, OpenACC, ROCm.

License

BSD style license

Web page

`http://tau.uoregon.edu`

Contact

tau-bugs@cs.uoregon.edu

Figure 28 below shows a 3D profile of the IRMHD application that shows the extent of variation of the execution time over 2048 ranks. Notice the shape of the *MPI_Barrier* profile.

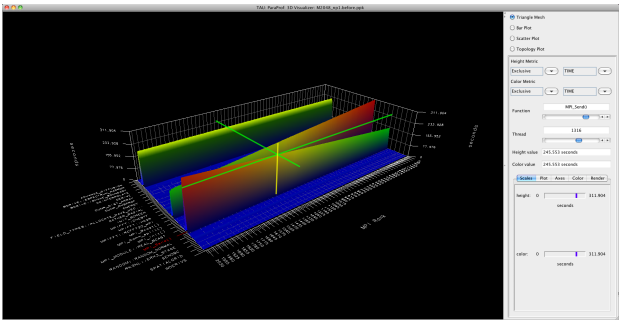

Figure 28: TAU's ParaProf 3D profile browser shows the exclusive time spent (height, color) over ranks for all routines in a code.

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Vampir

The Vampir performance visualizer allows to quickly study a program's runtime behavior at a fine level of detail. This includes the display of detailed performance event recordings over time in timelines and aggregated profiles. Interactive navigation and zooming are the key features of the tool, which help to quickly identify inefficient or faulty parts of a program. Vampir is language independent. It supports 4 input formats, allowing it to work with many measurement systems. Vampir works closely with Score-P, part of the VI-HPS ecosystem, which generates *Open Trace Format Version 2* (OTF2) traces. The older *OTF* format is also supported for backwards compatibility. Vampir also supports the JSON-based *Chrome Trace Event* format, which is produced by many tools both inside and outside the HPC community for application tracing, and the *WfCommons* format for workflow execution traces.

Typical questions Vampir helps to answer

- How well does my program make progress over time?
- When/where does my program suffer from load imbalances and why?
- Why is the time spent in communication or synchronization higher than expected?
- Are I/O operations delaying my program?
- Does my hybrid program interplay well with the given accelerator?

Workflow

Before using Vampir, an application program needs to be instrumented and executed with Score-P. Running the instrumented program produces a bundle of trace files in OTF2-format with an anchor file called `traces.otf2`. When opening the anchor file with Vampir, a timeline thumbnail of the data is presented. This thumbnail allows to select a subset or the total data volume for a detailed inspection. The program behavior over time is presented to the user in an interactive chart called Master Timeline. Further charts with different analysis focus can be added.

Platform support

Linux (x86/x86_64, ARM, Power), Windows, Apple macOS.

License

Commercial

Web page

`https://vampir.eu`

Contact

service@vampir.eu

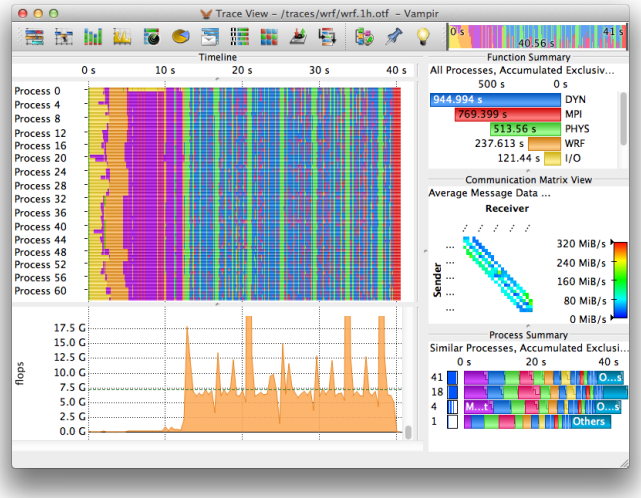


Figure 29: A trace file in the Vampir performance browser.

After a trace file has been loaded by Vampir, the Trace View window opens with a default set of charts as depicted in Figure 29. The charts can be divided into timeline charts and statistical charts. Timeline charts (left) show detailed event based information for arbitrary time intervals while statistical charts (right) reveal accumulated measures which were computed from the corresponding event data. An overview of the phases of the entire program run is given in the Zoom Toolbar (top right), which can also be used to zoom and shift to the program phases of interest.

VI-HPS training

Next to the development of state-of-the-art productivity tools for high-performance computing, the VI-HPS also provides training in the effective application of these tools. Workshops and tutorials are orchestrated in close collaboration of the host organization to fit the particular need of the audience.

Training events can be a tuning workshop, a custom workshop or course, or a tutorial conducted in collaboration with an HPC-related conference. Sign up to the VI-HPS news mailing list via our website to receive announcements of upcoming training events.

Tuning workshop series VI-HPS Tuning Workshops are the major training vehicle where up to 30 participants receive instruction and guidance applying VI-HPS tools to their own parallel application codes, along with advice for potential corrections and optimizations. Feedback to tools developers also helps direct tools development to user needs, as well as improve tool documentation and ease of use. These workshops of three to five days at HPC centres occur several times per year, and feature a variety of VI-HPS tools.

Other training events VI-HPS Tuning Workshops are complemented by additional courses and tutorials at conferences, seasonal schools and other invited training events which have taken place on four continents. Training events of individual VI-HPS partners can also be found on their own websites.

Course material Coordinated tools training material is available with emphasis on hands-on exercises using VI-HPS tools individually and interoperably. Exercises with example MPI+OpenMP parallel applications can be configured to run on dedicated HPC compute resources or within the virtual environment provided by a free Linux Live ISO that can be booted and run on an x86_64 notebook or desktop computer.

Linux Live-ISO The downloadable VI-HPS Linux Live-ISO image provides a typical HPC development environment for MPI and OpenMP containing the VI-HPS tools. Once booted, the running system provides the GNU Compiler Collection (including support for OpenMP multithreading) and OpenMPI message-passing library, along with a variety of parallel debugging, correctness checking and performance analysis tools.

The latest ISO/OVA files are currently only available as 64-bit versions, requiring a 64-bit x86-based processor and a 64-bit OS if running a virtual machine. Depending on available memory, it should be possible to apply the provided tools and run small-scale parallel programs (e.g., 16 MPI processes or OpenMP threads). When the available processors are over-subscribed, however, measured execution performance will not be representative of dedicated HPC compute resources. Sample measurements and analyses of example and real applications from a variety of HPC systems (many at large scale) are therefore provided for examination and investigation of actual execution performance issues.

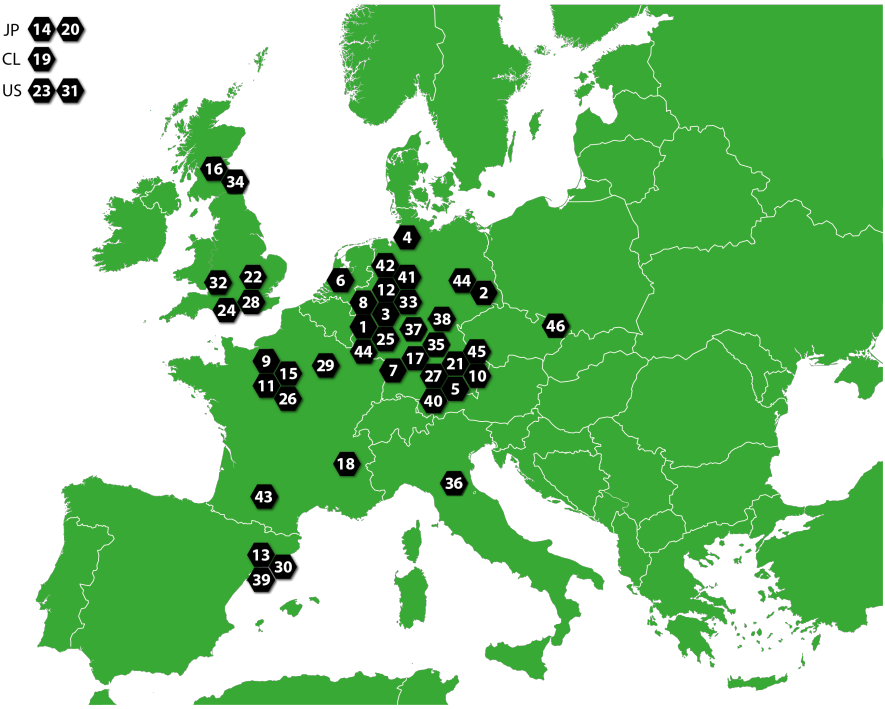
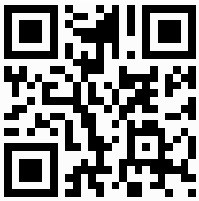


Figure 30: VI-HPS Tuning Workshop locations (2008–2024).

VI-HPS Tools Guide

The Virtual Institute – High Productivity Supercomputing (VI-HPS) aims at improving the quality and accelerating the development process of complex simulation codes in science and engineering that are being designed to run on highly-parallel HPC computer systems. For this purpose, the partners of VI-HPS are developing integrated state-of-the-art programming tools for high-performance computing that assist programmers in diagnosing programming errors and optimizing the performance of their applications.

This VI-HPS Tools Guide provides a brief overview of the technologies and tools developed by the 17 partner institutions of the VI-HPS. It is intended to assist developers of simulation codes in deciding which of the tools of the VI-HPS portfolio is best suited to address their needs with respect to debugging, correctness checking, and performance analysis.



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