TECHNISCHE UNIVERSITÄT DRESDEN

ZIH
Center for Information Services & High Performance Computing

OpenMP Booth Talk @ SC'18

STUDYING OPENMP WITH VAMPIR & SCORE-P

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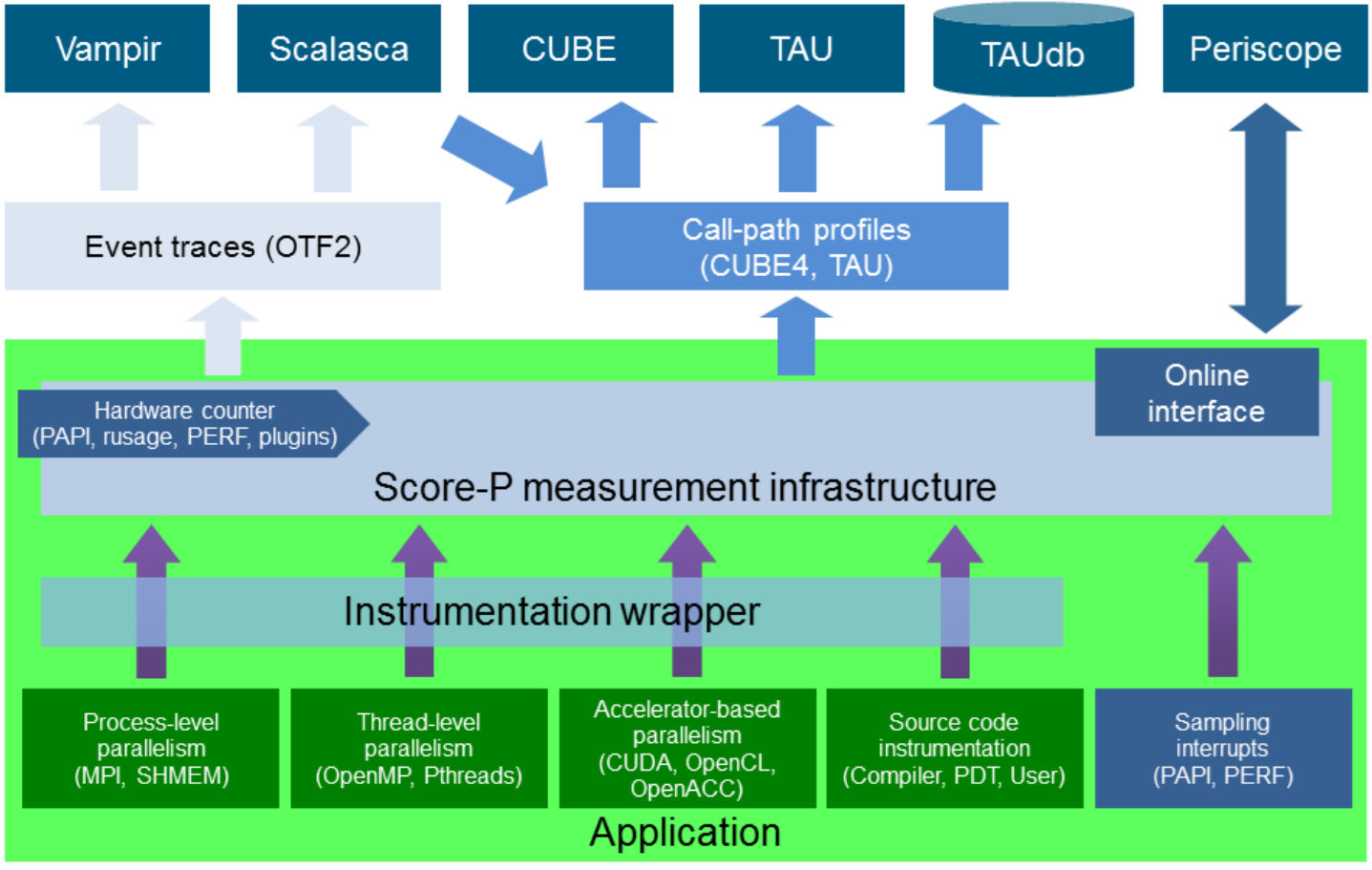
Score-P

Measurement Infrastructure


Vampir
Scalasca
CUBE
TAU
TAUdb
Periscope
Event traces (OTF2)
Call-path profiles
(CUBE4, TAU)
Online
interface
Hardware counter
(PAPI, rusage, PERF, plugins)
Score-P measurement infrastructure
Instrumentation wrapper
Process-level
parallelism
(MPI, SHMEM)
Thread-level
parallelism
(OpenMP, Pthreads)
Accelerator-based
parallelism
(CUDA, OpenCL,
OpenACC)
Source code
instrumentation
(Compiler, PDT, User)
Sampling
interrupts
(PAPI, PERF)
Application

OpenMP Instrumentation in Score-P

OPARI2

- Source-to-source instrumentation
- Annotation of OpenMP directives and runtime library calls
- Recompilation of code necessary

OMPT

- Standardized interface to obtain information from the OpenMP runtime system
- State information & event callbacks
- Support by OpenMP runtime implementations necessary (e.g., mandatory vs. optional event callbacks)

Case Studies

Sparse Matrix Vector Multiplication – Load Imbalances

Sparse Matrix Vector Multiplication

$$\begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix} = \begin{pmatrix} a_{11} & \cdots & a_{n1} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

- A sparse matrix is a matrix populated primarily with zeros
- Only non-zero elements of a_{ij} are saved efficiently in memory
- Algorithm

```
foreach row r in A
  y[r.x] = 0
  foreach non-zero element e in row
    y[r.x] += e.value * x[e.y]
```

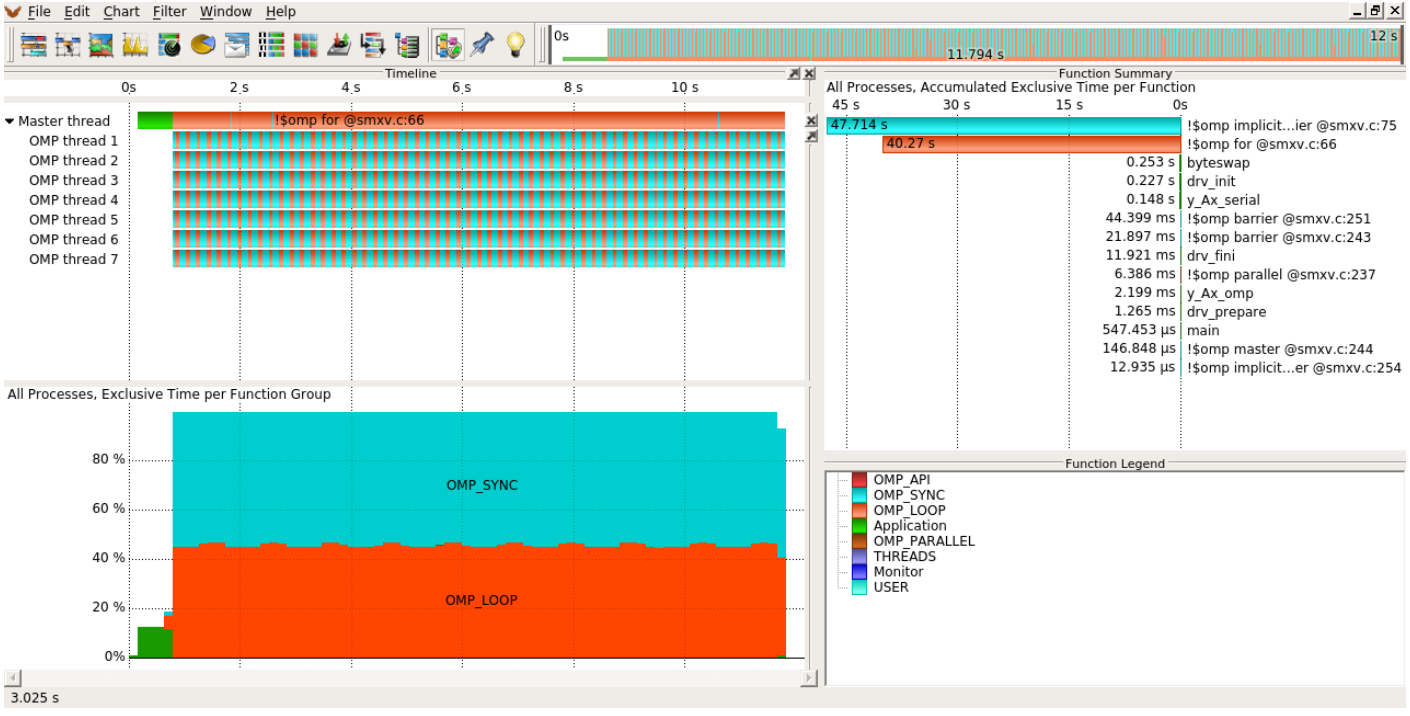
Sparse Matrix Vector Multiplication

- Naive OpenMP algorithm

```
#pragma omp parallel for
foreach row r in A
  y[r.x] = 0
  foreach non-zero element e in row
    y[r.x] += e.value * x[e.y]
```

- Distributes the rows of A evenly across the threads in the parallel region
- The distribution of the non-zero elements may influence the load balance in the parallel application

Sparse Matrix Vector Multiplication



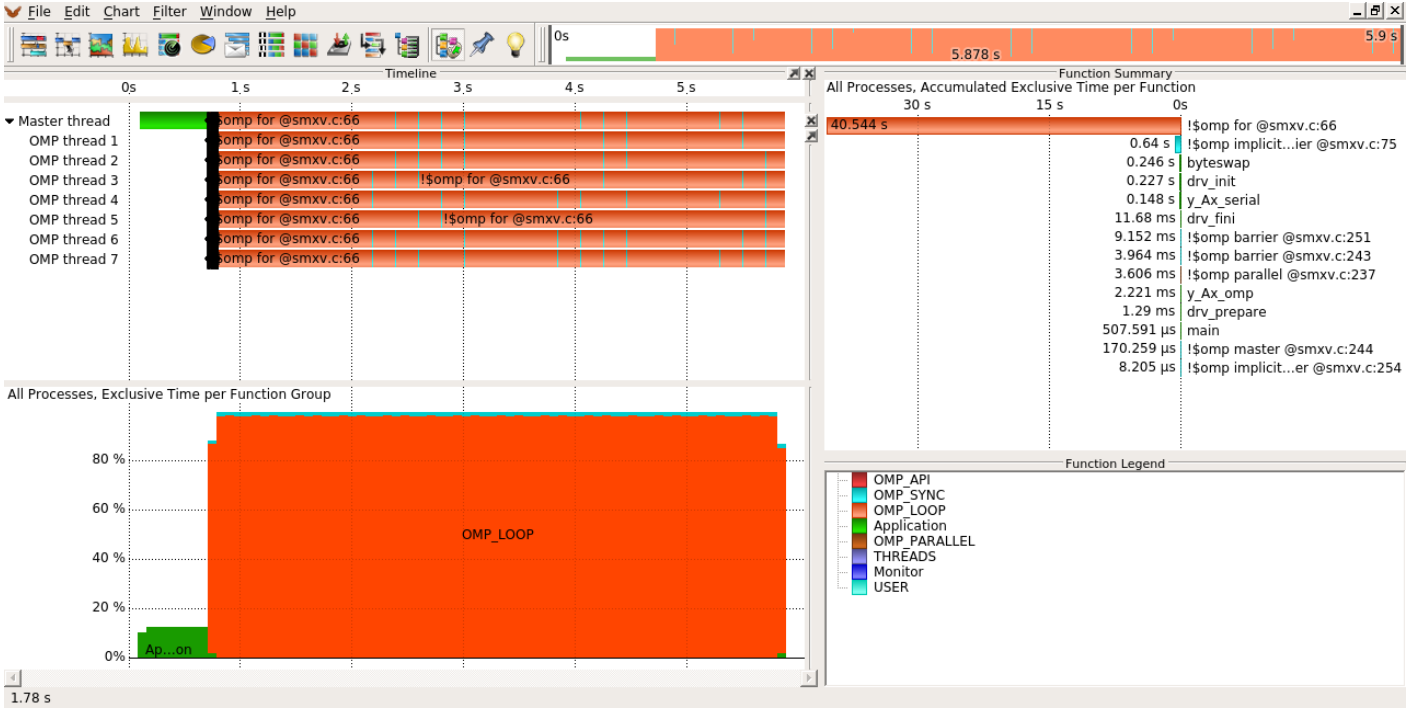
Sparse Matrix Vector Multiplication

- Improved OpenMP algorithm

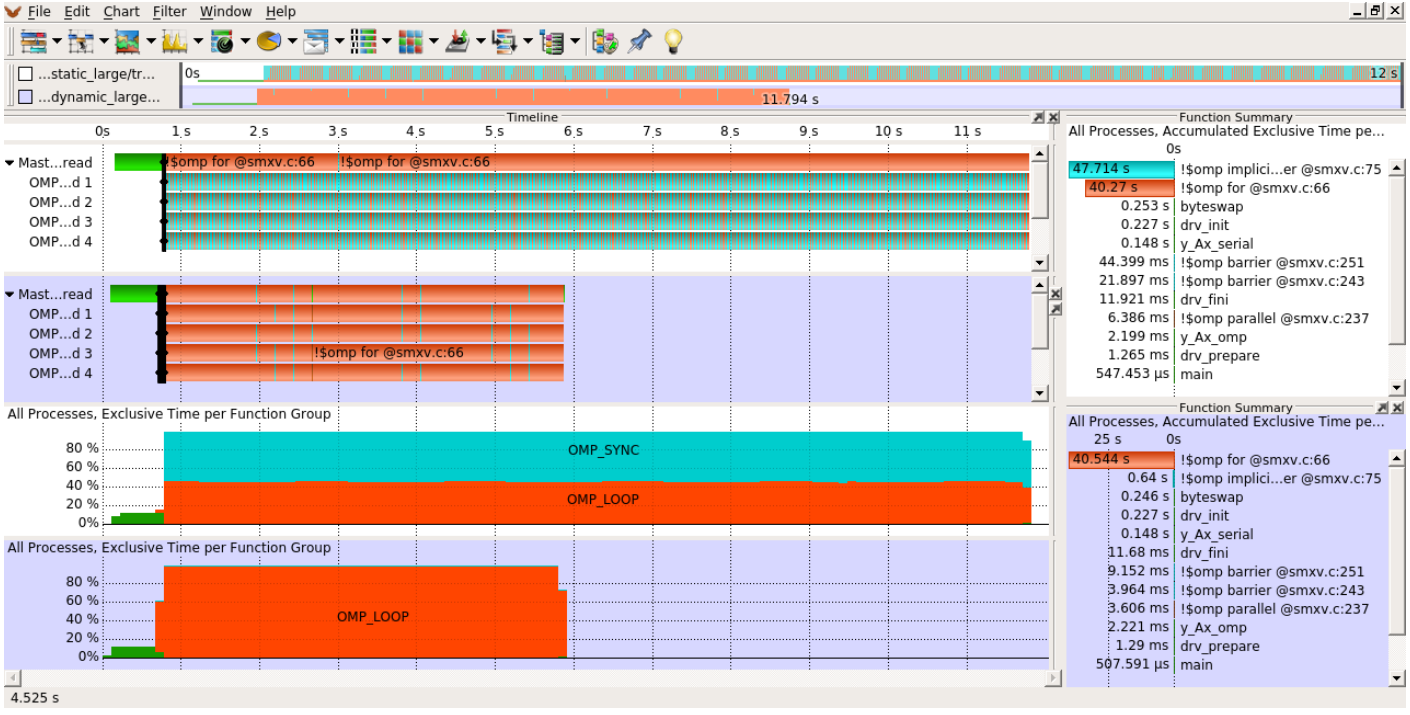
```
#pragma omp parallel for schedule(dynamic,1000)
foreach row r in A
  y[r.x] = 0
  foreach non-zero element e in row
    y[r.x] += e.value * x[e.y]
```

- Distributes the rows of A dynamically across the threads in the parallel region

Sparse Matrix Vector Multiplication



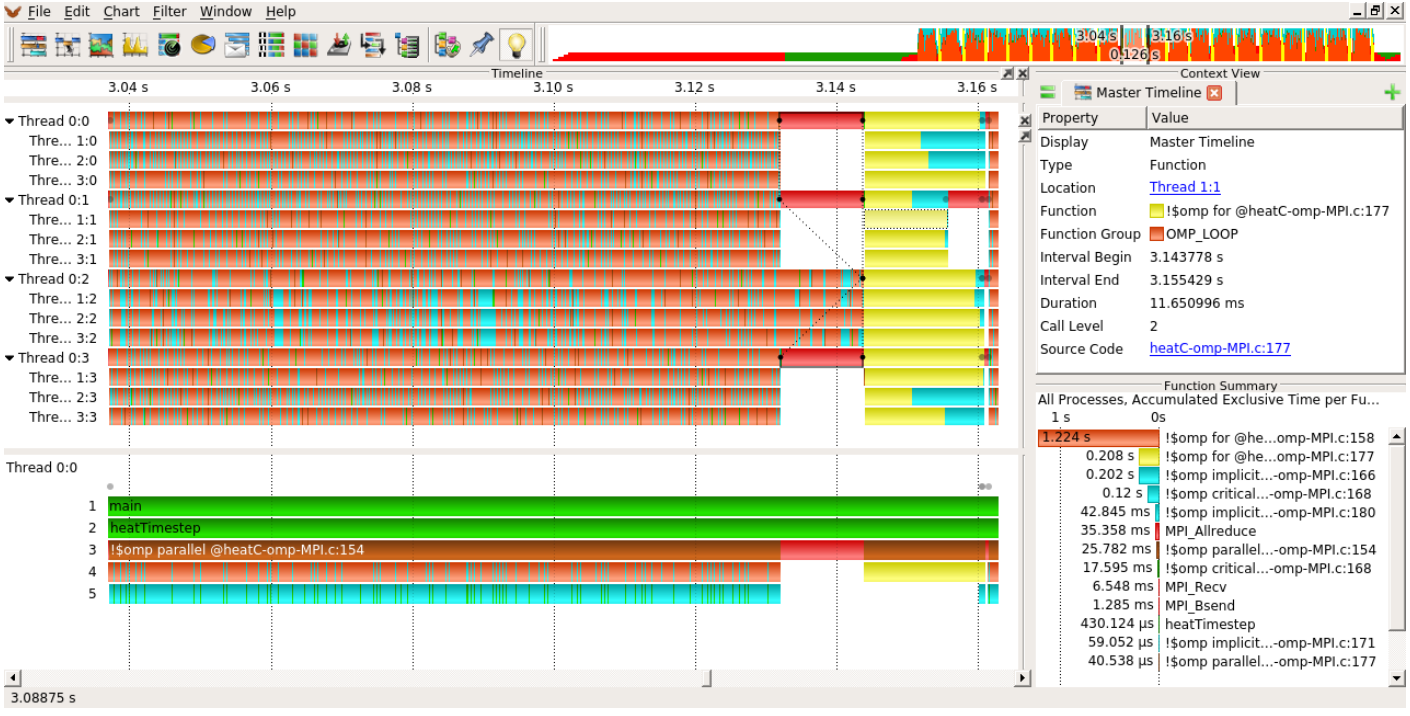
Sparse Matrix Vector Multiplication



Case Studies

Heat Conduction – Propagation of Load Imbalances

Heat Conduction

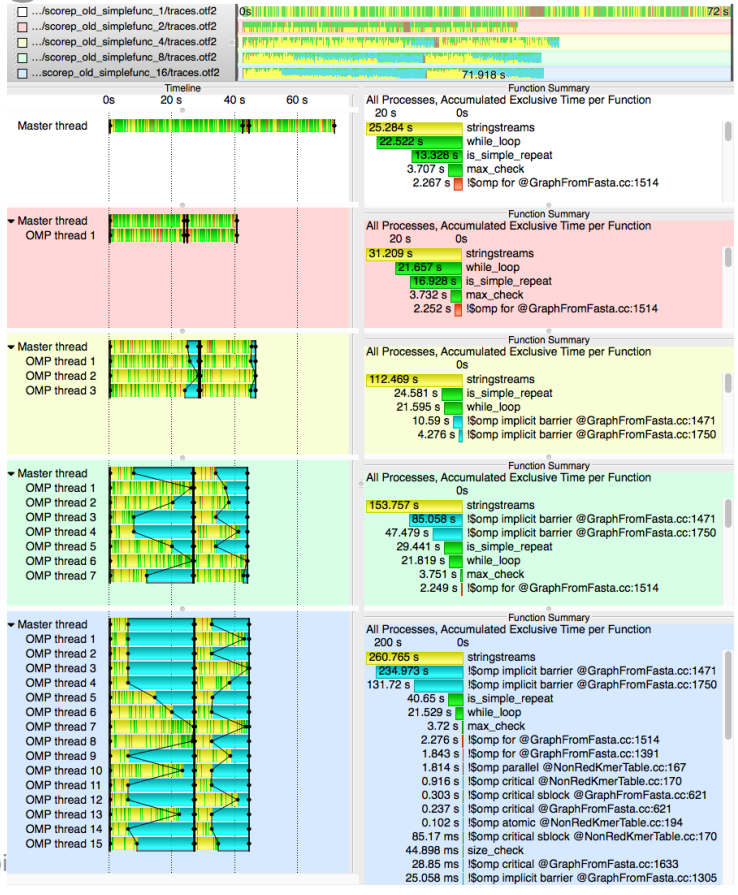


Case Studies

Trinity RNA-Seq Assembler – Comparing Performance between Different Process Numbers

Trinity RNA-Seq Assembler – Comparing Performance between Different Process Numbers

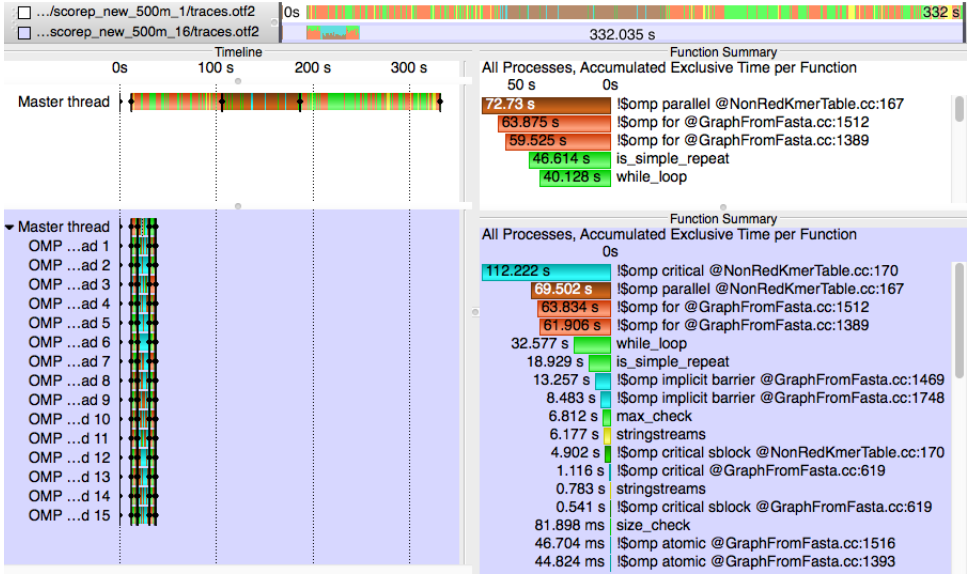
- Analyzes and optimization of the RNA-Seq assembler Trinity [1]
- Trinity is a pipeline of up to 27 individual components invoked by a main perl script
- One main performance issue was the poor intra-node scaling of the GraphFromFasta module
- Intra-node parallelism (OpenMP) achieved a speed up of only 2.27 with a full 16-core node, the figure shows traces in comparison for 1, 2, 4, 8, and 16 threads
- The first part of GraphFromFasta increases nearly linearly with the number of OpenMP threads; there is practically no parallel speed up with more than two threads
- Time spent **stringstreams** increases from about 25s with one thread to 260s with 16 threads



1. Wagner, M., Fulton, B., Henschel, R.: Performance Optimization for the Trinity RNA-Seq Assembler, pp. 29-40. Springer (2016)

Trinity RNA-Seq Assembler – Comparing Performance between Different Process Numbers

- Root cause was the frequent creation and destruction of string stream objects within an inner loop
- The creation was internally locked by a mutex, which produced excessive wait times
- Solution was to move the string stream object creation before the loop and only clear the string streams in the inner loop
- This resulted in better scaling (parallel speed up increased from 2.3 to 8.9) and reduced serial runtime (for the test data set from 72s to 45s)
- The introduced modifications resulted in a 22% improvement in overall run time

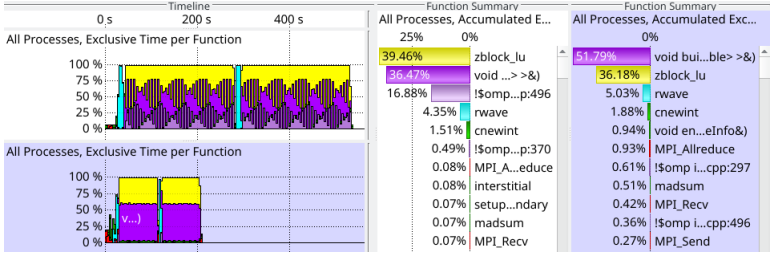


Case Studies

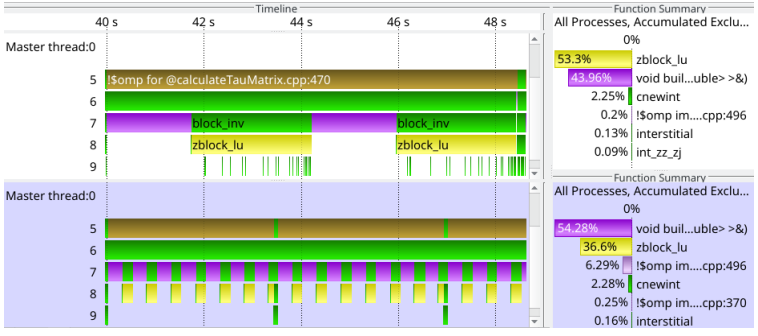
LSMS – Comparing Performance between Different Hardware

LSMS – Comparing Performance between Different Hardware

- OLCF ports applications from Titan to Summit (early development system called Summitdev)
- Summitdev contains NVIDIA P100 GPUs providing 4x the theoretical DPFLOPS peak performance than the Tesla K20X in Titan
- One Summitdev node (20 cores) has four GPUs instead of one for Titan (16 cores). The system supports CUDA MPS, which allows sharing of GPUs between multiple processes
- This case study explores how these differences affect the performance of the CORAL benchmark code LSMS
- The faster GPU and better GPU/CPU pairing factor of 5 (20 cores/4 GPUs) cause the GPU-accelerated function **zblock_lu** to speed up on Summitdev, while the non-GPU-enabled function **buildKKRMatrix** gains in relative execution time



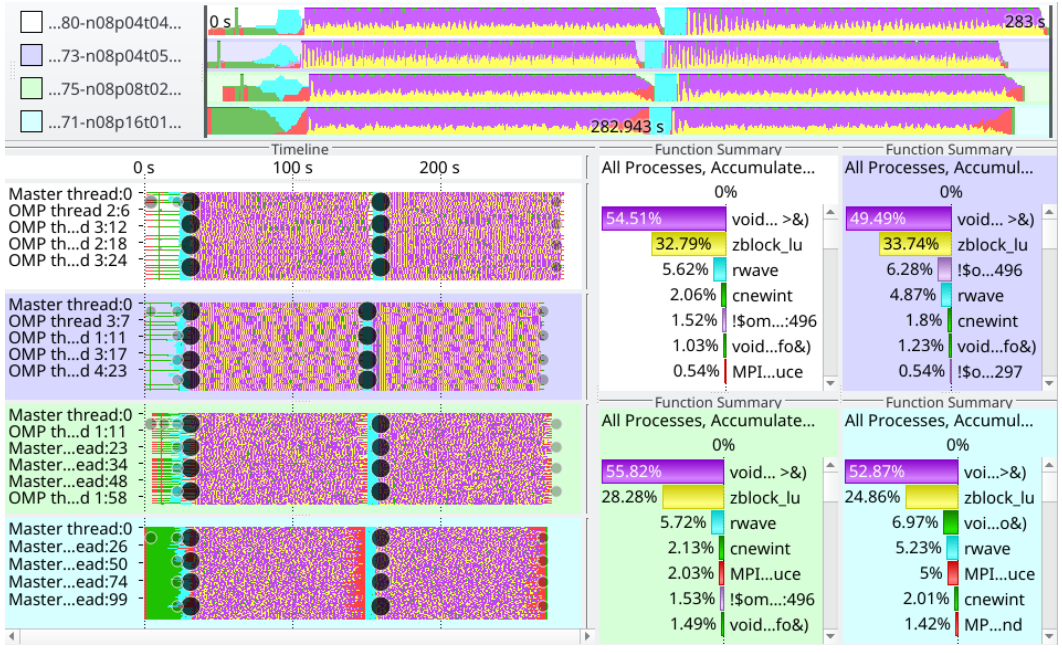
Overview of a 80-GPU LSMS run on Titan (80 nodes, white background) and Summitdev (20 nodes, blue background)



Detailed comparison of one iteration on Titan vs. roughly 2.5 on Summitdev

LSMS – Comparing Performance between Different Hardware

- To evaluate if CUDA MPS can speed up LSMS, we run it with varying numbers of threads and processes per node
- LSMS is most resource efficient if the total number of threads and processes divides the number of simulated atoms evenly
- Using all 20 cores is faster than the other variants, although it adds occasional waiting time on the "left-over" threads
- The increase in MPI waiting time (more red in the green and cyan timelines) is negated by better GPU utilization
- GPU MPS uses the GPU more efficiently. But not using four cores per node negates this advantage



Exploratory comparison of different process vs. thread setups.
- White: 4 processes times 4 threads per node (16 total) (1 process per GPU)
- Blue: 4 processes times 5 threads per node (20 total) (1 process per GPU)
- Green: 8 processes times 2 threads per node (16 total) (2 processes per GPU)
- Cyan: 16 processes times 1 thread per node (16 total) (4 processes per GPU)