Parallel Performance Analysis Tools

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Reusing this material

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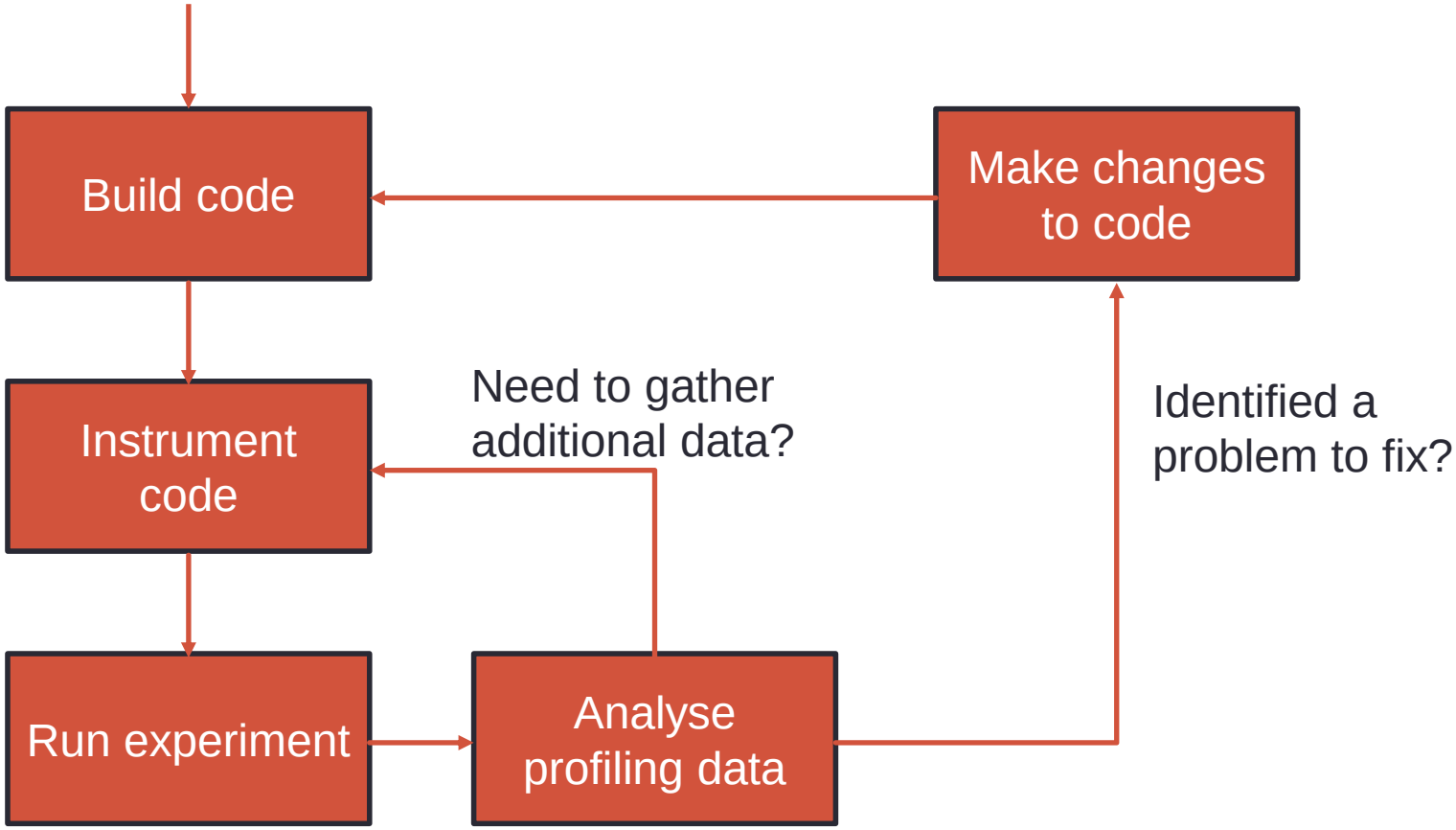
Outline

- Motivations
- Discussion of CrayPAT and Scalasca
- Outline example code
- CrayPAT Usage
- Scalasca Usage

Motivations – What is Profiling?

- Examine the behaviour of the code
- Pick out any subroutines/functions that cause slowdown or have unusual behaviour
- Two types:
  1. Sampling (periodically queries running code to determine what function the code is in)
  2. Tracing (adds instructions into the code that report when entering/leaving functions, and various statistics)

Motivations – What is Profiling?



Picking an Example to Analyse

- Profiling generates a lot of extra data, and can cause your code to run more slowly
  - Need to choose a reasonably short example, but:
    - Program execution must be representative of a production run
    - Must be long enough to hide start-up and finalisation costs
    - Should include all the I/O of a normal job

- A good choice is something like a benchmark problem that takes a few minutes to run on a node/handful of nodes

Motivations - Why Profile?

- For developers:
  - Understand what the most time-consuming parts of the program are
  - Understand communication patterns and problems
    - E.g. load imbalance, synchronisation costs
  - Tool to help direct development efforts to give maximum benefits
- For users?
  - Understand why your program performs in a certain way
  - Help with choice of appropriate parameters, MPI processes…

Profilers: CrayPAT and Scalasca

- In this course we will consider two parallel performance analysis tools; CrayPAT and Scalasca

- With each tool you
  1. Instrument your code (typically during building)
  2. Run your code
  3. Analyse results

CrayPAT

+ Various levels of detail
+ Extreme customisibility for expert users

- Only available on Cray Platforms
- GUI is not particularly useful

Scalasca

+ Open source
+ Portable
+ Allows you to determine early/late senders etc…
+ Useful GUI (Cube)

- Unable to trace CUDA, SHMEM events or OpenMP nested parallelism

Example Test Code - CFD

- In this tutorial we will use a simple MPI code to demonstrate parallel performance analysis

- A computational fluid dynamics (CFD) code is employed, which calculates the flow of fluid within a cavity with an inlet in one side, and an outlet on another.

- The code can calculate the inviscid or viscid fluid flow.

Example Test Code - CFD

- Solves Poisson's Equation for the streamfunction:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\zeta$$

$$u_x = \frac{\partial \psi}{\partial y};\ u_y = -\frac{\partial \psi}{\partial x};\ \zeta = \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y}$$

- Available in both C and Fortran

Example Test Code - CFD

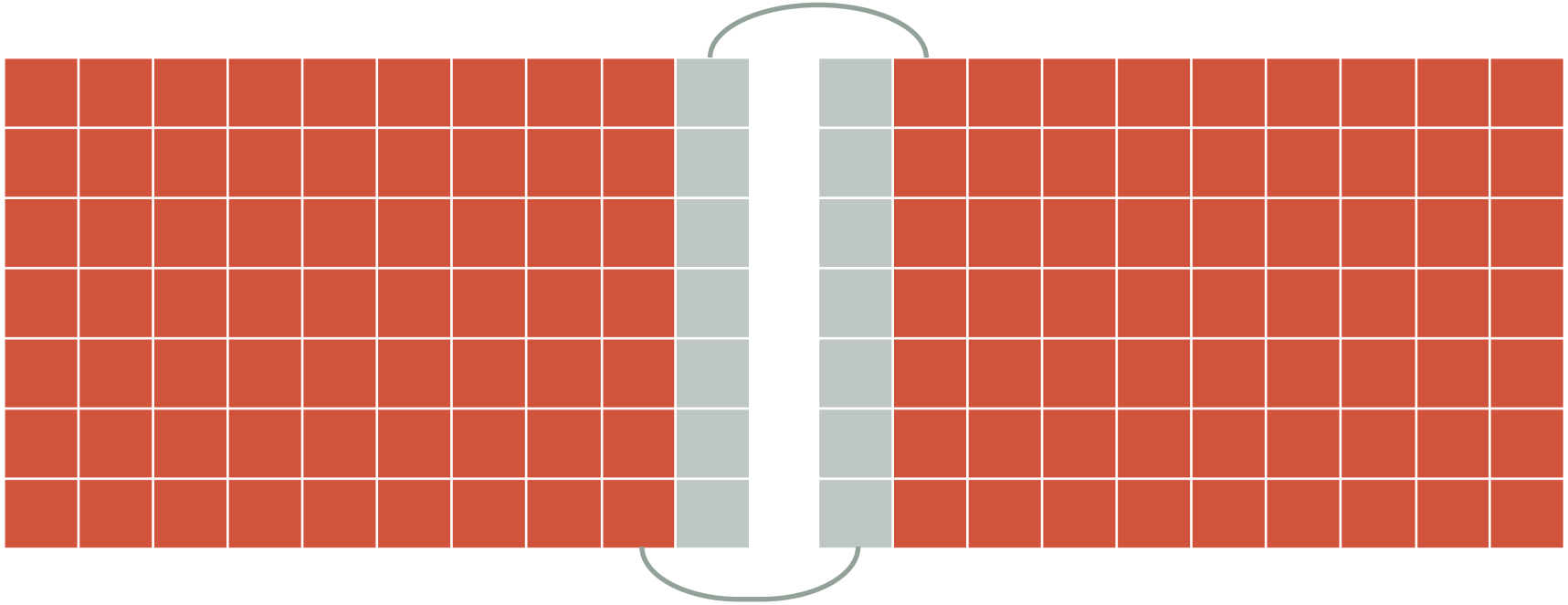
- Iterate until convergence

$$\psi_{i,j}^{\text{new}} = \frac{1}{4}\left(\psi_{i-1,j}^{\text{old}} + \psi_{i+1,j}^{\text{old}} + \psi_{i,j-1}^{\text{old}} + \psi_{i,j+1}^{\text{old}}\right) - \zeta_{i,j}^{\text{old}}$$

$$\begin{aligned}\zeta_{i,j}^{\text{new}} = &\frac{1}{4}\left(\zeta_{i-1,j}^{\text{old}} + \zeta_{i+1,j}^{\text{old}} + \zeta_{i,j-1}^{\text{old}} + \zeta_{i,j+1}^{\text{old}}\right) \\ &- \frac{R_e}{16}\Big[\left(\psi_{i,j+1}^{\text{old}} - \psi_{i,j-1}^{\text{old}}\right)\left(\zeta_{i+1,j}^{\text{old}} - \zeta_{i-1,j}^{\text{old}}\right) \\ &- \left(\psi_{i+1,j}^{\text{old}} - \psi_{i-1,j}^{\text{old}}\right)\left(\zeta_{i,j+1}^{\text{old}} - \zeta_{i,j-1}^{\text{old}}\right)\Big]\end{aligned}$$

Example Test Code - CFD

- Parallelised in the x (C) or y (Fortran) directions



- Halos transferred via MPI_Sendrecv

Example Test Code - CFD

- The code can be found on the course web pages

- To run it, use

  aprun –n [nprocs] ./cfd <scale> <numiter> <Re>

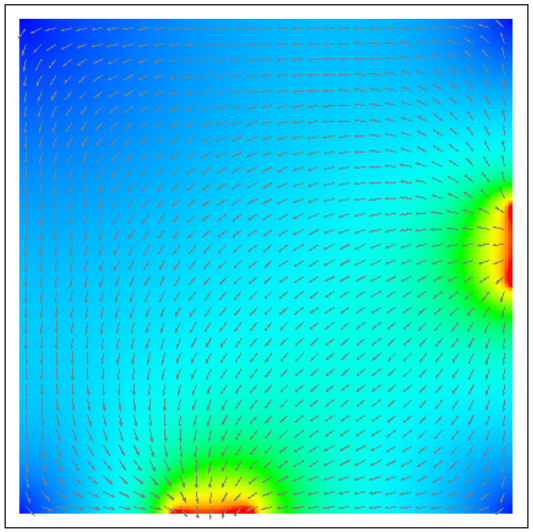
Where

- nprocs is the number of MPI processes
- scale scales the size of the box (32 x scale cells)
- numiter is the number of iterations
- Re (optional) is the Reynolds number ($0 \leq Re < 3.7$)

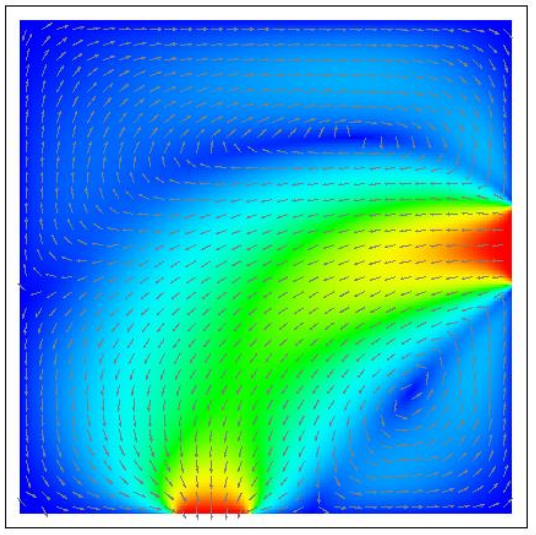
Example Test Code - CFD

- The output can be visualised using:

  $ gnuplot –persist cfd.plt



$R_e = 0$



$R_e = 3.0$

Examples of Performance Tools

- I will now go onto demonstrate CrayPAT and Scalasca on ARCHER using the CFD code.

- Afterwards you will get an opportunity to try using CrayPAT/Scalasca yourselves

- For best results, it is recommended that you to login to ARCHER with an X-windows connection, e.g.

  $ ssh –X [username]@login.archer.ac.uk

Using CrayPAT - Sampling

- Load the CrayPAT modules:

  $ module load perftools-base

  $ module load perftools

- Build executable as normal

  $ make clean; make

- Instrument the binary using pat_build

  $ pat_build ./cfd

Using CrayPAT - Sampling

- Instrumentation creates a new binary cfd+pat
- Modify the job submission script to run this new binary, then submit the job

  $ qsub submit.pbs

- This will run the cfd code with sampling

Using CrayPAT - Sampling

- Once the job has completed, it will have created an additional file: cfd+pat+<number>.xf

- Generate a human-readable report using pat_report

  $ pat_report cfd+pat+<number>.xf

(You can put this information into a file by using the argument '–o <file>')

Using CrayPAT - Sampling

Table 1: Profile by Function

```
  Samp% |    Samp | Imb. |  Imb. |Group
        |         | Samp | Samp% | Function
        |         |      |       |  PE=HIDE

 100.0% | 1,906.5 |   -- |    -- |Total
|-----------------------------------------
|  96.6% | 1,842.0 |   -- |    -- |USER
||----------------------------------------
||  74.9% | 1,427.2 | 15.8 |  1.5% |jacobistepvort
||  21.0% |   401.0 |  8.0 |  2.6% |main
||========================================
|   3.3% |    62.5 |   -- |    -- |MPI
||----------------------------------------
||   3.1% |    58.5 | 25.5 | 40.5% |MPI_Sendrecv
|=========================================
```

Using CrayPAT - Sampling

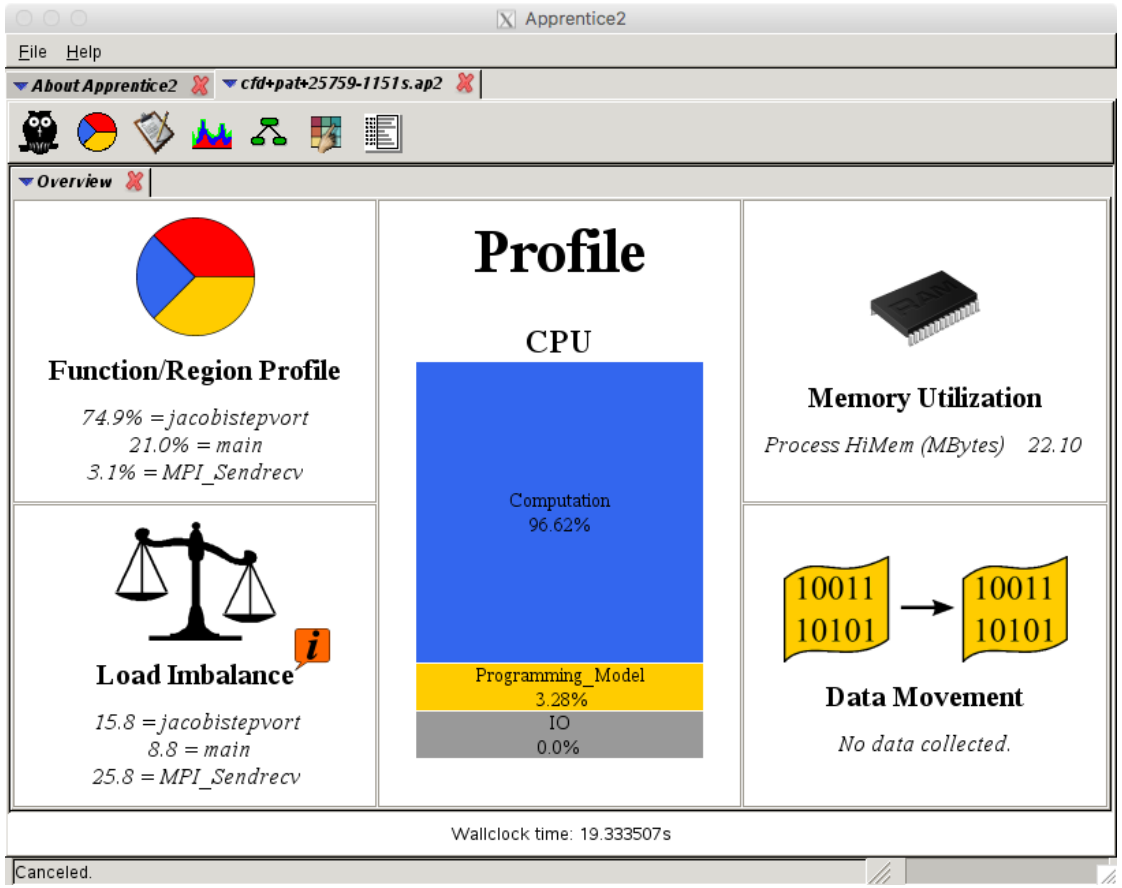
Pat_report also produces two other files; an .ap2 file, and an .apa file:

- The ap2 file acts as an input to the Apprentice2 graphical interface for viewing performance statistics

  $ app2 <file>.ap2

- The apa file contains suggested configuration options for a traced experiment

Using CrayPAT – Apprentice2



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Using CrayPAT - Tracing

- Instrument the binary for tracing using the .apa file as an input to pat_build

  $ pat_build -O cfd+pat+<number>.apa

- Modify the job submission script to use the new binary then submit the job

  $ qsub submit.pbs

- View the results data using pat_report as before

  $ pat_report cfd+apa+<number>.xf

- Then use Apprentice2 if desired

  $ app2 cfd+apa+<number>.ap2

Using CrayPAT

- This process can be continued as necessary until the information you need has been obtained/you have gained the desired understanding of your code's performance

- More information on CrayPAT can be found using the commands

  $ pat_help

  $ man intro_pat

  $ man pat_build

  $ man pat_report

Using Scalasca - Sampling

- Load the Scalasca module

  $ module load scalasca

- Instrumentation must be carried out during compilation by prepending scorep to the compiler. For example

  $ scorep cc -c foo.c or $ scorep ftn –c foo.f90

- Modify the compiler line in Makefile to include scorep:

  CC = scorep cc

  FC = scorep ftn

Using Scalasca - Sampling

- It is important to ensure that scorep is used during the linking of the object files.

- Functions/subroutines/files that you do not need/want to instrument do not need to be compiled with scorep

- Build the executable

  make clean; make

Using Scalasca - Sampling

- Modify the submission script to launch the parallel job with scalasca –analyze, e.g.

  scalasca –analyze aprun –np 4 ./cfd <options>

- Submit the job

  $ qsub submit.pbs

- A measurement directory scorep_cfd_4_sum is created during the job's execution which contains all the log files

Using Scalasca - Sampling

- To analyse the output data, first run

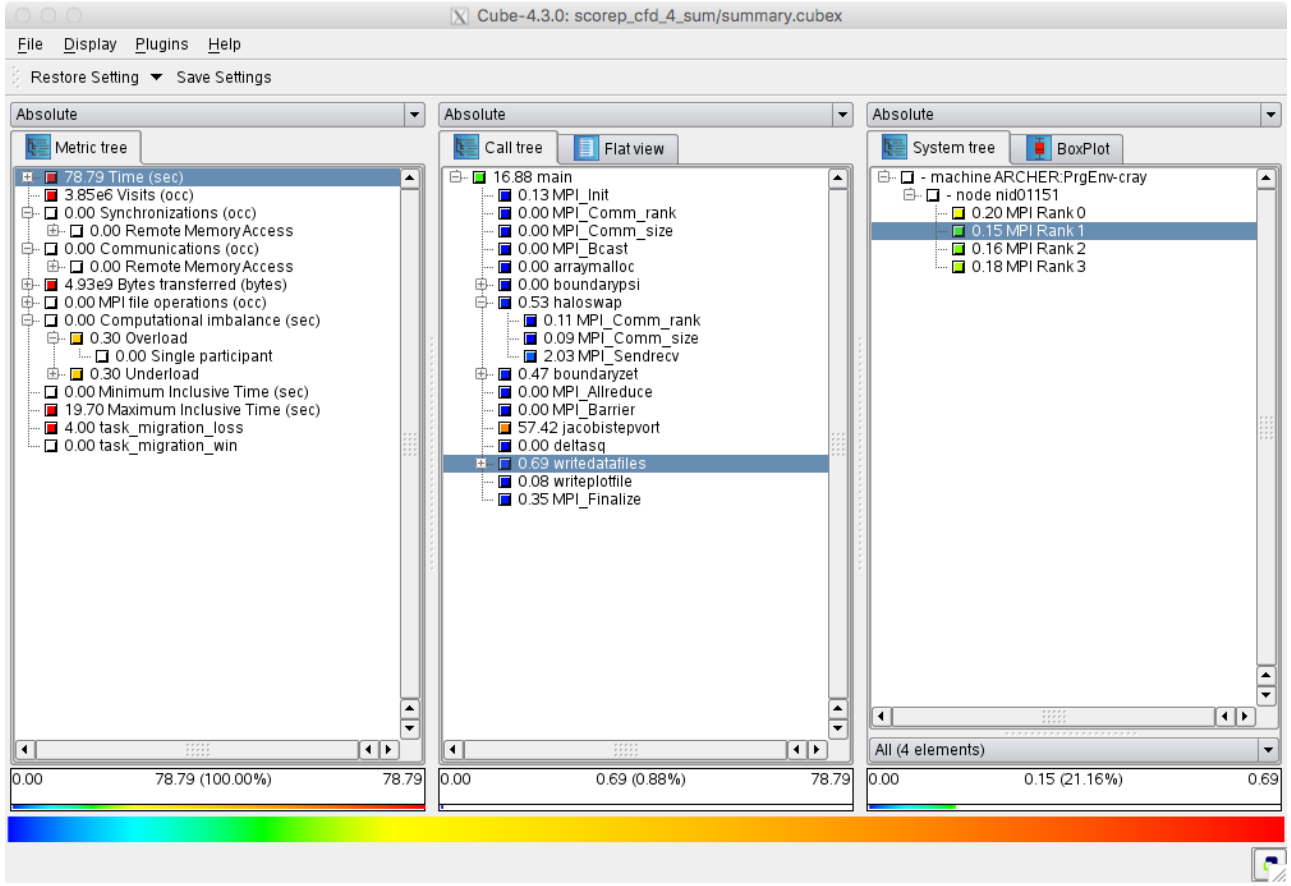
  $ scalasca –examine scorep_cfd_4_sum

- This will open the cube browser, which allows you to examine the code's timings

- Using the –s option produces a file (scorep.score) that can be used to advise you about setting up a tracing experiment

  $scalasca –examine –s scorep_cfd_4_sum

Using Scalasca - Cube



Using Scalasca - Tracing

Examining the scorep.score file in the measurement directory reveals information on the estimated final disk usage and memory usage of a trace

Estimated aggregate size of event trace: 128MB
Estimated requirements for largest trace buffer (max_buf): 32MB
Estimated memory requirements (SCOREP_TOTAL_MEMORY): 34MB
(hint: When tracing set SCOREP_TOTAL_MEMORY=34MB to avoid intermediate flushes or reduce requirements using USR regions filters.)

type	max_buf[B]	visits	time[s]	time[%]	time/visit[us]	region
ALL	33,493,662	3,848,767	78.79	100.0	20.47	ALL
MPI	22,401,846	2,000,134	2.95	3.7	1.47	MPI
USR	7,491,672	1,248,609	57.90	73.5	46.37	USR
COM	3,600,144	600,024	17.95	22.8	29.91	COM

Using Scalasca - Tracing

- To trace the code, alter your job submission script to contain:

  scalasca –analyze –q –t aprun –np 4 ./cfd <options>

- Don’t forget to also set SCOREP_TOTAL_MEMORY in the script as suggested in the .score file:

  export SCOREP_TOTAL_MEMORY=34MB

Using Scalasca - Tracing

- A new directory scorep_cfd_4_trace is created, and the results can be examined using

  $ scalasca -examine scorep_cfd_4_trace

- This time, more information is present, such as that on late senders/receivers.

Using Scalasca - Tracing

- If the estimated disk/memory usage for tracing is too high, you may need to consider to avoid tracing certain functions by using a filter file:

```
SCOREP_REGION_NAMES_BEGIN
  EXCLUDE
    jacobistepvort
    MPI_Sendrecv
SCOREP_REGION_NAMES_END
```

- Usage:

  scalasca –examine –f filter.txt aprun ...

  scalasca –analyze –q –t –f filter.txt aprun ...

Using Scalsca

- More information can be found on the Scalasca website
  http://www.scalasca.org

- In particular their user's guide:
  http://apps.fz-juelich.de/scalasca/releases/scalasca/2.3/docs/UserGuide.pdf

Practical: CFD

- Try out using CrayPAT and/or Scalasca to investigate the performance of the CFD code

- Options:
  - Try using different values for scale, and investigate turning viscosity on and off
  - How does the profile change when running on large numbers of processes?
  - Terminate calculation based on a tolerance value (see comments in code), investigate only computing this infrequently
  - Investigate using serialised Send / Receive functions (see alternative boundary source files) instead of Sendrecv