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Set 1 - Numerical Integration and Multithreading

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Question 1: Getting started on Brutus

Brutus is a computing cluster of ETH Zurich and consists of a variety of different CPU and GPU processors. The cluster works with a queueing system: you submit your program with its parameters (called job) to a queue and wait for it to be finished. Your first task consists of the following steps:

a) Visit `http://brutuswiki.ethz.ch/brutus/Brutus_wiki` (only accessible within the ETH Network[1]) and click on "Brutus account request" and then on "Get your account here" (you might be requested to enter your nethz username and password). Fill the form with your data, under shareholder select the option "STUDENT" at the end of the list, set Prof. Petros Koumoutsakos as supervisor, your department under "Address of institute" and HPCSE I under "Project description". This account will only be valid for the duration of the lecture and gives you access to up to 128 CPU cores.

Notes:

- You only need to complete this step if you don't already have an active account.
- If you need an account for uses unrelated to this class, please request a normal or a shareholder (if applicable) account.

b) Login from within the ETH network on Brutus via ssh:
`>ssh username@brutus.ethz.ch`
and insert your password when asked to.

Congratulations! You are now on a login node of the Brutus cluster. In this environment you can write code, compile and run small tests. Keep in mind that there are other people working on the same nodes, so be mindful on how you use them!

c) The Brutus environment is organized in modules, which are conceptually packages of settings that can be loaded and unloaded as needed. The basic commands to use the module system are:
`>module load <modulename>`: this command sets the environment variables related to the specified module.
`>module unload <modulename>`: this commands unsets the environment variables related to <modulename>.

[1] You may use VPN `http://www.vpn.ethz.ch` to connect to the ETH Network from home.

`>module list`: lists all the modules currently loaded.
`>module avail`: outputs a list of all the modules that can be loaded.

If, for example, we need to compile a program with the GNU compiler (gcc), we first load its module with
`>module load gcc`
and then proceed with the compilation of our program:
`>g++ -O2 main.cpp -o program_name`

d) Performance measurements and long computations should not be performed on the login nodes but rather they should be submitted to the queue. To submit a simple job to the queue, you can use the following command from the folder where your program is stored:
`>bsub -n 48 -W 08:00 -o output_file ./program_name program_args`
This command will submit a job for your executable `program_name` with arguments `program_args` by requesting 48 cores from a single node and a wall-clock time of 8 hours, after which, if the job is not already finished running, it will be terminated. The report of the job, along the information that would usually appear on the terminal, will be appended in the file `output_file`, in the folder from where the job started.

While your job is running you can always use the command:
`>bjobs`
to get the status of your jobs.

Additional information on the Brutus cluster, its instruments and on how to use it can be found at `www.brutuswiki.ethz.ch/brutus/Brutus_wiki`.

Question 2: Parallel Numerical Integration

The value of an integral of $\int_a^b f(x)dx$ can be approximated by computing its Riemann sum:

$$\mathrm{S} = \sum_{i=1}^{n} f(x_i^*)\Delta x$$

where $\Delta x = x_i - x_{i-1} = (b-a)/n$, x_i^* some point in the interval $[x_{i-1}, x_i]$, $x_0 = a$ and $x_n = b$. The *midpoint approximation* uses, in the Riemann sum, the middle point $\bar{x}_i = \frac{(x_{i-1}+x_i)}{2}$ of each interval $[x_{i-1}, x_i]$. In this question you will implement and parallelize this method.

a) Write a (serial) program that calculates the integral $\int_1^4 f(x)dx$, where $f(x) = \sqrt{x} \cdot ln(x)$, using Riemann sum with the midpoint approximation.

b) Parallelize your code by starting several threads to compute the Riemann sum. Make sure you do not introduce race conditions and verify your implementation by comparing the final result with that computed by the serial program. Note that each thread should handle a different interval of the integral.

c) Choose an appropriate number (n) of intervals and check how the wall-clock time for computing the integral reduces with respect to the number of threads. Plot the time versus the number of threads and report your observations.

   Notes:

   - You can optionally use the `timer` class, implemented in the `timer.hpp` file, for your time measurements.

- As your Brutus account may not be available, the time measurements can be performed on any computer system of your preference (e.g. personal laptop). In this case, you should report the hardware/software configuration of that system (i.e. number and type of cores, operating system and compiler).

Summary

Summarize your answers, results and plots into a PDF document. Furthermore, elucidate the main structure of the code and report possible code details that are relevant in terms of accuracy or performance. Send the PDF document and source code to your assigned teaching assistant.