SINGAPORE-MIT ALLIANCE
COMPUTATIONAL ENGINEERING PROGRAMME
CME5232: Cluster and Grid Computing Technologies for Scientific Computing
COMPUTATIONAL LAB No.1
3^{rd} July, 2009

INTRODUCTION TO HIGH PERFORMANCE COMPUTING RESOURCES

Objectives

To be familiar with the SMA Hydra Linux Cluster as the main High Performance Computing (HPC) platform for parallel computing tasks.

Background Knowledge

C/C++ programming languages, elementary knowledge of Unix/Linux commands.

CME5232 course information webpage

Some webpages containing useful course information (e.g. SMA Hydra Linux Cluster, etc) have been set up and its URL is as follows: **http//web.sma.nus.edu.sg/sma5232/**

Exercises (Due date: 9^{th} July, 2009)

You are required to submit only the report of your homework problem.

Please submit a short format report recording your observations based on the assigned exercises and programming assignments in a week's time. The report should be complete and clearly written to show what you have done and what you have observed and interpreted from these exercises. All equations, symbols etc. if any must be declared or explained clearly.

1. Getting to know the SMA Hydra Linux Cluster

You have been briefed on the HPC resources on the SMA Hydra Linux Cluster. By browsing through the hydra cluster website **http://hydra.sma.nus.edu.sg** (maintained by NovaGlobal Pte Ltd, http://www.noveglobal.com.sg), explore the cluster tools and language options to get a handle on the capabilities of the cluster.

2.The continuous integration problem

Given a function,

$$f(x) = \frac{x^2 + 2x + 3}{x^2 - 1} + 5sin^2(x), \tag{1}$$

continuous in range of $x \in [10, 20]$. The integration of the continuous line function $f(x)$ in range above can be approximated by trapezoidal rule as in equation (2);

$$\int_a^b f(x)dx = \Big(\frac{b-a}{n}\Big)\Big(\frac{f(a)+f(b)}{2} + \sum_{k=1}^{n-1} f\big(a + k\frac{b-a}{n})\Big), \tag{2}$$

and rectangular integration method as in equation (3);

$$\int_a^b f(x)dx = h\sum_{k=1}^{n-1} f\Big(k\frac{b-a}{n}\Big) \tag{3}$$

where n is number of regular element in the range of [a,b]=[10,20]. In these methods, the area under the function is divided into number of trapezoidal/rectangular of equal width, $(b-a)/n$. By adding up the areas of each trapezoid/rectangular, the integration of the function can be estimated. So, you are required

- To write serial codes to compute the integration of equation (1) using trapezoidal rule and rectangular integration method. (Write each method in a serial code).
- To Compile and run the both codes with difference number of element n with $n_t = 2n_{t-1}$ until n=167772160, where $n_0 = 10$. Plot the results and computational time. Discuss on the observations
- To compare the results of both methods with analytical solution. Plot the relative error, $\epsilon_{rel} = (Sol_{anal} - Sol_{num})/Sol_{anal}$, versus different number of element, n, in the range of [10,20], are $n_t = 2n_{t-1}$, until the relative error is smaller than $\epsilon = 10^{-6}$, where $n_0 = 10$. Discuss on the observations of the convergence rate. Where the function of analytical solution is

$$\int_a^b f(x)dx = x + \ln\Big|\frac{(x-1)^3}{(x+1)}\Big| + \frac{5}{2}(x - sin(x)cos(x)). \tag{4}$$

3. Monte Carlo method to compute the value of pi

In this method, we will use the probability and mathematical theory to estimate the value of PI. This method consists of inscribing a unit circle inside a square, and then throwing 'darts' at the square randomly. The ratio of darts that landed inside the circle (N) to the total of darts thrown (M) will be the areas of the circle to the square.

$$\frac{\pi r^2}{L^2} = \frac{N}{M}. \tag{5}$$

where $L = 2r$. Therefore, the value of PI is computed by

$$\pi = 4\frac{N}{M}. \tag{6}$$

In this Lab, you are expected to write out the sequential version of code to compute the value of PI. Then run the code with the varying the total number of the darts thrown, $N = 10^4, 10^5, 10^6, 10^7, 10^8, 10^9, 10^{10}$ and record the corresponding computational time and value of PI. Plot the convergence rate of your PI and PI25DT (PI25DT = 3.141592653589793238462643 is the true π value up to 25 digits of accuracy.), where the relative error is computed by

$$\epsilon_{rel} = \Big|\frac{\pi - PI25DT}{PI25DT}\Big|. \tag{7}$$