University of Saskatchewan
Department of Computer Science

**Parallel Programming for Scientific Computing**
(CMPT 851)
Instructor: Dr. Raymond J. Spiteri

ASSIGNMENT 04
**Due: 1:00 p.m. Monday, April 28, 2014**

1. **[20 marks]** Prepare a referee's report as per the instructions on the course webpage.

2. **[20 marks]** In this question, we (finally) find the true global minimum of the function

$$f(x,y) = e^{\sin(50x)} + \sin(60e^y) + \sin(70\sin x) + \sin(\sin(80y)) - \sin(10(x+y)) + \frac{x^2+y^2}{4}.$$

This was Problem 4 of the SIAM 100-digit challenge. The goal was to compute the answer correct to 10 significant digits. A bit of straightforward analysis yields that the global minimum must lie not too far from the origin, so we restrict our attention to the domain $\{(x,y) \in [-1,1] \times [-1,1]\}$.

Use the Matlab Global Optimization Toolbox on `socrates` to find the global minimum to 10 significant digits.

Compare the execution times when running with 1, 2, 4, and 8 workers on one node and with one worker per node.

Comment on the scalability of the timings.

3. **[75 marks]** In this question, we will use the `SNES` library of PETSc to solve the following "tridiagonal" system of nonlinear algebraic equations

$$\mathbf{F}(\mathbf{x}) = \mathbf{0}, \tag{1}$$

where

$$\begin{aligned} F_1(\mathbf{x}) &= 4(x_1 - x_2^2), \\ F_i(\mathbf{x}) &= 8x_i(x_i^2 - x_{i-1}) - 2(1 - x_i) + 4(x_i - x_{i+1}^2), \quad i = 2, 3, \ldots, m-1, \\ F_m(\mathbf{x}) &= 8x_m(x_m^2 - x_{m-1}) - 2(1 - x_m), \end{aligned}$$

and $m = 6000$. The solution we desire to (1) is $\mathbf{x}^* = (1, 1, \ldots, 1)^T$.

There are several factors to consider when solving nonlinear systems of algebraic equations, including the initial guess, the choice of linear solver, how to compute the Jacobian, and any parallelization.

(a) With the initial guess $\mathbf{x}^{(0)} = 2\mathbf{x}^*$, write a serial program that uses PETSc to solve (1) using the exact Jacobian and `GMRES` and `BiCGStab` as the linear system solver with no preconditioner. Report the infinity norm of the error in the computed solution and the number of iterations required.

(b) Repeat part (a) with $\mathbf{x}^{(0)} = 3\mathbf{x}^*$.

(c) Repeat part (a) with $\mathbf{x}^{(0)} = 4\mathbf{x}^*$.

(d) With the initial guess $\mathbf{x}^{(0)} = 2\mathbf{x}^*$, write a parallel program that uses PETSc to solve (1) using the exact Jacobian and `GMRES` as the linear system solver with no preconditioner. Record execution times with `np`$= 1, 2, 4, 8$ processes on `socrates` first on only one node then with only one process per node.

(e) Repeat part (d) with $m = 6000$`np`, i.e., the problem size scales with the number of processes.

(f) Comment on your results from parts (d) and (e).

Defaults can be used for (the many) quantities not mentioned, e.g., tolerances, maximum iterations and function evaluations, etc.