University of Saskatchewan
Department of Computer Science

Numerical Software
(CMPT 898 (02))
Instructor: Dr. Raymond J. Spiteri

MILESTONE 04
Closes: 2:30 p.m., Tuesday, April 09, 2013

1. **[50 marks]** Go to

   `http://software-carpentry.org/4_0/index.html`

   Watch the set of videos associated with your assigned topic (see below).

Student	Video Series
Frost	Counting Things
Haghgoo	Handling Configuration Files
Mirshekari	Provenance
Preuss	Saving and Loading Data
Qian	Data

   Prepare a brief presentation (5–10 mins.) on your assigned topic. The presentations should provide a summary of the three most important points made in the videos. Emphasis is to be placed on identifying what your learned or found particularly interesting or useful. The presentations will take place Tuesday, April 02, 2013 during class, with the order of the presenters to be determined. Slides are to be e-mailed in PDF format to the instructor by noon of the presentation day.

   Everyone is encouraged to watch all the assigned videos so they can ask questions or add insight to the presentations.

2. **[50 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.