Numerical Laboratory

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We are using *Mathematica* notebooks as a front end. Before beginning, make sure that you do *not* already have *Mathematica* running. (Quit out of it if you do.) To get started, from the command prompt in your home directory perform the following commands:

    $ mkdir -p tbss.work/numlab   *create a directory for the notebooks*
    $ cd tbss.work/numlab   *make it your current working directory*
    $ numlab   *copy over the notebooks and then open the first one*

(Note that "numlab" is really a symbolic link to the "tutorials/09-numerical-algorithms/run" script. If this symbolic link does not exist in your path, then you can create it locally by performing

    $ link -s /PATH/TO/tutorials/09-numerical-algorithms/run .

and then running the script as "./numlab".) Please be aware that you must always use this script to start the tutorial in order to configure environmental variables correctly (otherwise the lab exercises will not work as expected).

Once you begin the tutorial on the first notebook (1.nb), you later can open others by choosing "Open" from the "File" menu, or you can run "numlab 2.nb" to explicitly open the second notebook, *etc.* To evaluate a bracketed input "cell," click on it to highlight it (or click within it to place the cursor inside) and then press "shift–enter." Some input expressions merely define functions or variables. Others compute or plot a result. (There might be some delay while results are computed.) Generally, you should evaluate the input expressions sequentially. You may edit input in the usual way and reevaluate by again pressing "shift–enter." You may also cut and paste an expression into a new cell at the end of the notebook or in between two cells.

You may save your work back to the local notebook copies. To restore the original notebooks, perform:

    $ rm [1-6].nb   *remove all of the notebooks*
    $ numlab   *restore the original notebooks and then open the first one*

If there are any problems with *Mathematica* behaving unexpectedly on the notebooks, try quitting out of *Mathematica* and then restart with the "numlab" command.

Exercises 1, 4, and 5 use NAMD, and exercise 6 uses an experimental program MDX.

1. **Chaotic nature of MD trajectories.**

   System. Choice of waters or decalanine in vacuum.

   Input. Size of perturbation in initial positions of atoms.

   Output. Printing of time in fs and amplification factor for RMSD (root mean squared distance) between trajectories.

   Questions. For each system, what is the doubling time for the size of a perturbation?

       water _____

       decalanine _____

   Remark. Your answers will be much smaller than those obtained from the figures on page 398 of Schlick or page 77 of Allen & Tildesley because of the presence of unconstrained hydrogen atoms.

2. **Non-symplectic integration.** Standard Verlet is compared to the use of Verlet with velocity rescaling (non-symplectic), where at the end of each step the velocities are rescaled to conserve energy. If the potential energy exceeds the initial energy, the velocities are set to zero, and this attempt is counted as a failure. Rescaling will succeed in a future step.

System. Henon-Heiles Hamiltonian: $H = \frac{1}{2}(u^2 + v^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^2$. Space variables x, y and velocity variables u, v.

Input. Energy, step size, scaling off or on (an energy $> \frac{1}{12}$ gives a chaotic trajectory, an energy $> \frac{1}{6}$ gives a trajectory that goes to the abyss).

Output. Intersection of the energy surface with $x = 0$ projected onto the y-v plane (Poincaré section). If the original surface defined by the tail end of an (infinitely long) trajectory is N-dimensional, its intersection and projection will be of dimension $N - 1$. The points from the last half of the trajectory are shown in red color.

Questions. Is the "hypersurface" of constant energy of dimension 3, 2, 1, or 0?

energy $< \frac{1}{12}$ without rescaling _____   energy $< \frac{1}{12}$ with rescaling _____
energy $> \frac{1}{12}$ without rescaling _____   energy $> \frac{1}{12}$ with rescaling _____

Remark. There seems to be no clear conclusion in the case of velocity rescaling.

3. **Smoothness of potential.**

   System. 2 argon atoms with periodic BCs in 2D. Potential is multiplied by a switching function with continuity DC, C0, C1, or C2.

   Input. Choice of switching function (DC=0, C0=1, C1=2 and C2=3), switching distance (default=6), cutoff (default=8), step size (default=2).

   Output. Energy plot for 200,000 steps.

   Questions. For which switching functions do we get energy drift? _____
   For which switching functions do we get just fluctuations? _____

4. **Resonance.** If the step size is close to a simple fraction m/n of the numerically perturbed period of a significant high frequency normal mode, then this is manifested in the trajectory and energy. In particular, the total energy will seem to cycle through n different values.

   System. Flexible water.

   Input. Step size (start with the ones we provide). In a separate cell, guess the n in the resonance order $n : m$.

   Output. Energy for 250 steps. The guess for n joins every nth point, each set with a different color.

   Questions. For each step size below, what order of resonance (9:4, 7:3, 5:2, 8:3, 3:1, 10:3, 7:2, 4:1, 9:2, 5:1, 6:1, 7:1, 8:1, 9:1, 10:1) do you observe?

   2.78452 _____   2.51381 _____   1.8899 _____
   1.23044 _____   0.993579 _____

5. **Order of accuracy. I.** The order of accuracy is p if the error $\propto \Delta^p$ as $\Delta t \to 0$.

   System. Badly equilibrated alanine dipeptide.

   Input. Largest of 3 step sizes.

   Output. The end to end distance between two oxygens for 250 steps for a given step size, half of that step size, and a quarter of that step size — as a function of time.

   Questions. By what factor does error decrease if step size is halved? _____

6. **Order of accuracy. II.**

   System. Badly equilibrated decalanine and water.

   Input. The larger of 2 step sizes.

   Output. Error in energy and error in shadow energy for 250 steps for the given step size and half of that step size — as a function of time.

   Questions. By what factor does error decrease if step size is halved? _____