Instructor Guide

Two scientific applications are demonstrated to show the problem of why parallelization is eventually needed for large problems.

The codes are included and ready to compile/run. Encourage students to run both of these and to try varying the command-line arguments.

# Drug Design

To compile: g++ -o dd\_serial dd\_serial.cpp

To run: ./dd\_serial

Optional command line arguments (in this order):

1. maximum length of the randomly generated ligand strings
2. number of ligands generated
3. protein string to which ligands will be compared

Try a combination of small and large values to show that as the problem grows, the computational needs grow very quickly.

# Pandemic

To compile: make clean then make in the root directory

To run: ./pandemic\_serial

Optional command line arguments:

-n the number of people in the model

-i the number of initially infected people

-w the width of the environment

-h the height of the environment

-t the number of time days in the model

-T the duration of the disease (in days)

-c the contagiousness factor of the disease

-d the infection radius of the disease

-D the deadliness factor of the disease

-m the number of microseconds in between days in the model (used to speed  
 up or slow down the animation)

Try a combination of small and large values to show that as the problem grows, the computational needs grow very quickly.