## 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.