**Blue Waters Petascale Semester Curriculum v1.0**

**Unit 1: Computation Across the Curriculum**

**Lesson 4: Scientific Examples on a Single Core**

**Exercise Instructions for Students**

*Developed by Beau Christ for the Shodor Education Foundation, Inc.*



*Except where otherwise noted, this work by The Shodor Education Foundation, Inc. is licensed under CC BY-NC 4.0. To view a copy of this license, visit*[*https://creativecommons.org/licenses/by-nc/4.0*](https://creativecommons.org/licenses/by-nc/4.0)

*Browse and search the full curriculum at*[*http://shodor.org/petascale/materials/semester-curriculum*](http://shodor.org/petascale/materials/semester-curriculum)

*We welcome your improvements! You can submit your proposed changes to this material and the rest of the curriculum in our GitHub repository at*[*https://github.com/shodor-education/petascale-semester-curriculum*](https://github.com/shodor-education/petascale-semester-curriculum)

*We want to hear from you! Please let us know your experiences using this material by sending email to* [*petascale@shodor.org*](mailto:petascale@shodor.org)

1. Compile and run the Drug Design code. Create a table that states a few different combinations of inputs (**max\_ligand** and **ligands**), as well as how long each combination of inputs took to run.
2. Compile and run the Pandemic code. Create a table that states a few different input combinations (there are a lot to try), as well as how long each combination of inputs took to run. Can you tell which input(s) cause the most trouble in terms of run-time as they get bigger?
3. Run the pandemic code with the default input values. What do you visually notice as the simulation runs?