CS 677 High-performance Computing
Programming Assignment #1

Calculating Minimum-Energy Reaction Pathways

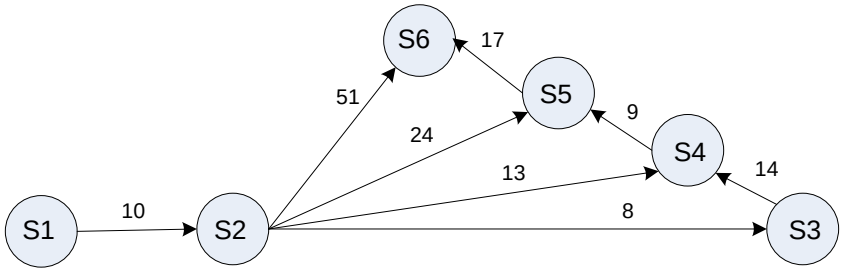
Overview

This is a simple "Warm-up" exercise. The main purpose of this assignment is to demonstrate your problem-solving ability and coding skills.

Specifications

Consider a simple biochemical reaction system containing several molecular species (compounds). The system contains multiple, different reaction channels or enzyme-powered pathways that can be followed (think of substrates and their various possible metabolites). Typically, different reaction pathways are followed depending upon the nature of the enzymes introduced into the system.

In the diagram below, the nodes represent six molecular compounds. The directed edges define the allowable biochemical reactions (e.g. compound S_1 is always metabolized to compound S_2). The weights on each edge represent the amount of energy required to effect the molecular transformation (i.e. its "cost").



The goal of this assignment is to calculate and print the "minimum-energy" reaction cost sufficient to metabolize the original compound (in this case, S_1) into its final form (in this case, compound S_6).

Notes:

- You may use the programming language of your choice.
- Be sure to use "good" programming style and practices.
- Generalize your solution as much as possible.
- Try to optimize your solution for efficiency (running time, memory usage).
- Consider any enhancements you can make to your solution (e.g. user-defined parameters, a graphical display…).

Deliverables

- Submit a hard-copy of your source-code, output file, and design document.
  - What data structures did you implement/employ? How did you implement/represent the graph?
  - What algorithm(s) did you use, and why?
- Be prepared to present and discuss your solution in class.
  - What language/libraries did you use?
  - What interesting problems (and solutions) did you discover?

Addenda

Here are two more sample pathways on which to test the correctness of your program, and to demonstrate the generality of your solution: