

# CS4414. Supercomputing Allocation Panel Mock Review

The following is a request for computational time on BlueWaters supercomputer. Analyze and give your recommendations: Grant/reject. If "reject", give further recommendations on improving the request. Assume that the "science" part is OK, that is the algorithm can fold the protein with the amount of computation they are thinking about. So you only want to critique the computational part of the request

## **Fold small protein via simulated annealing. Proposal**

Time is requested to predict, via simulated annealing, the 3D structure of a 30 residue protein. Based on the experimental folding times for this protein, and previous published studies of very similar proteins, we estimate that we would need 1000 independent runs, each of  $10^7$  cycles of annealing to make a reliable prediction. Preliminary testing on a single core of 3.0 GHz in-house machine shows code (NAMD) performance of  $0.3 * 10^5$  cycles per day. Assuming a reasonable project duration of one month, we therefore request  $10^4$  cores on BlueWaters – best available machine – for 1 month.