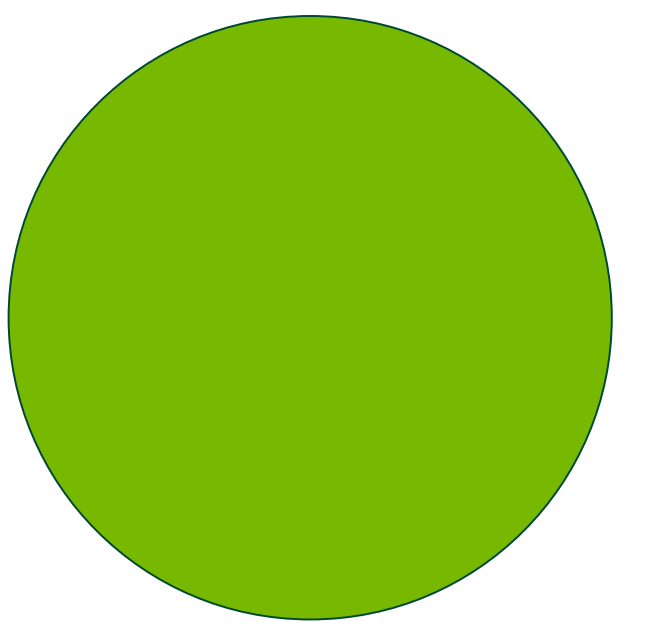


# Energy Evaluation of Rosetta Proteins Using CUDA



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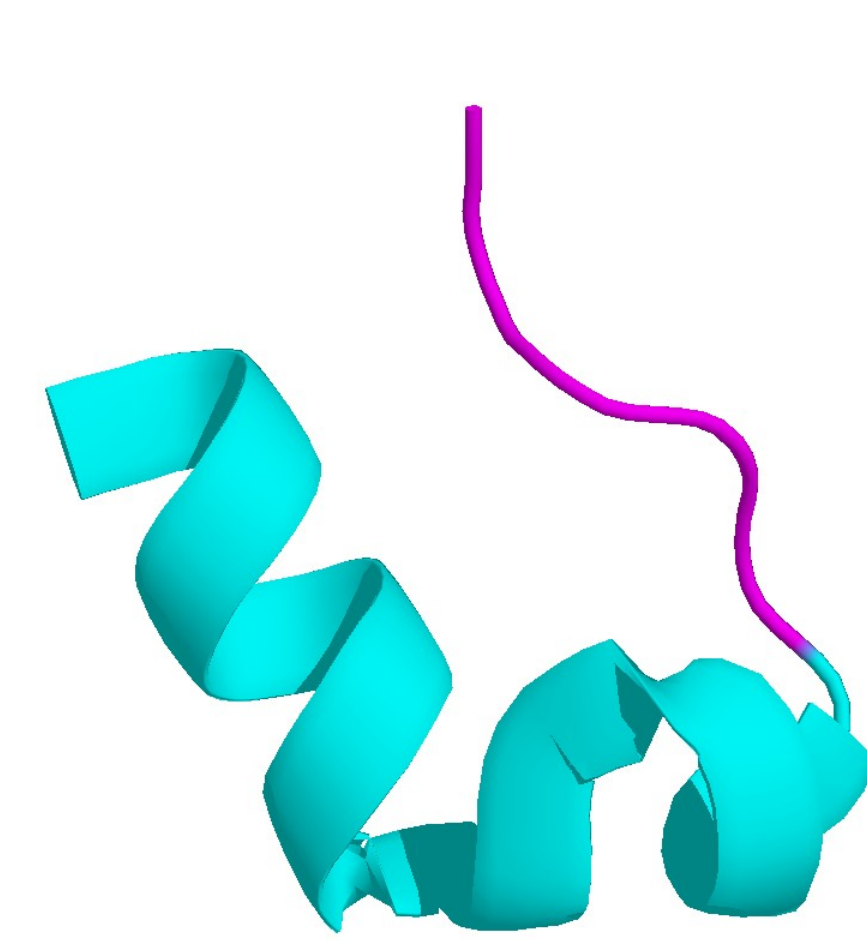
## Abstract

During the course of Rosetta's protein folding simulation, the energy of a protein's incrementally changing conformation is repeatedly evaluated as a way of measuring its stability. In general, if the folding trajectory results in a higher energy, the trajectory is disregarded in favor of a trajectory with lower energy. Energy evaluation is an N-body problem: every atom is paired with every other atom in its bounding sphere; then, each pair's energy is evaluated and summed. The Lennard-Jones potential forms the kernel of each pair evaluation and is of the form:  $V(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$ . Fortunately, each pair can be evaluated independently, leading to a large potential for parallel speedups.

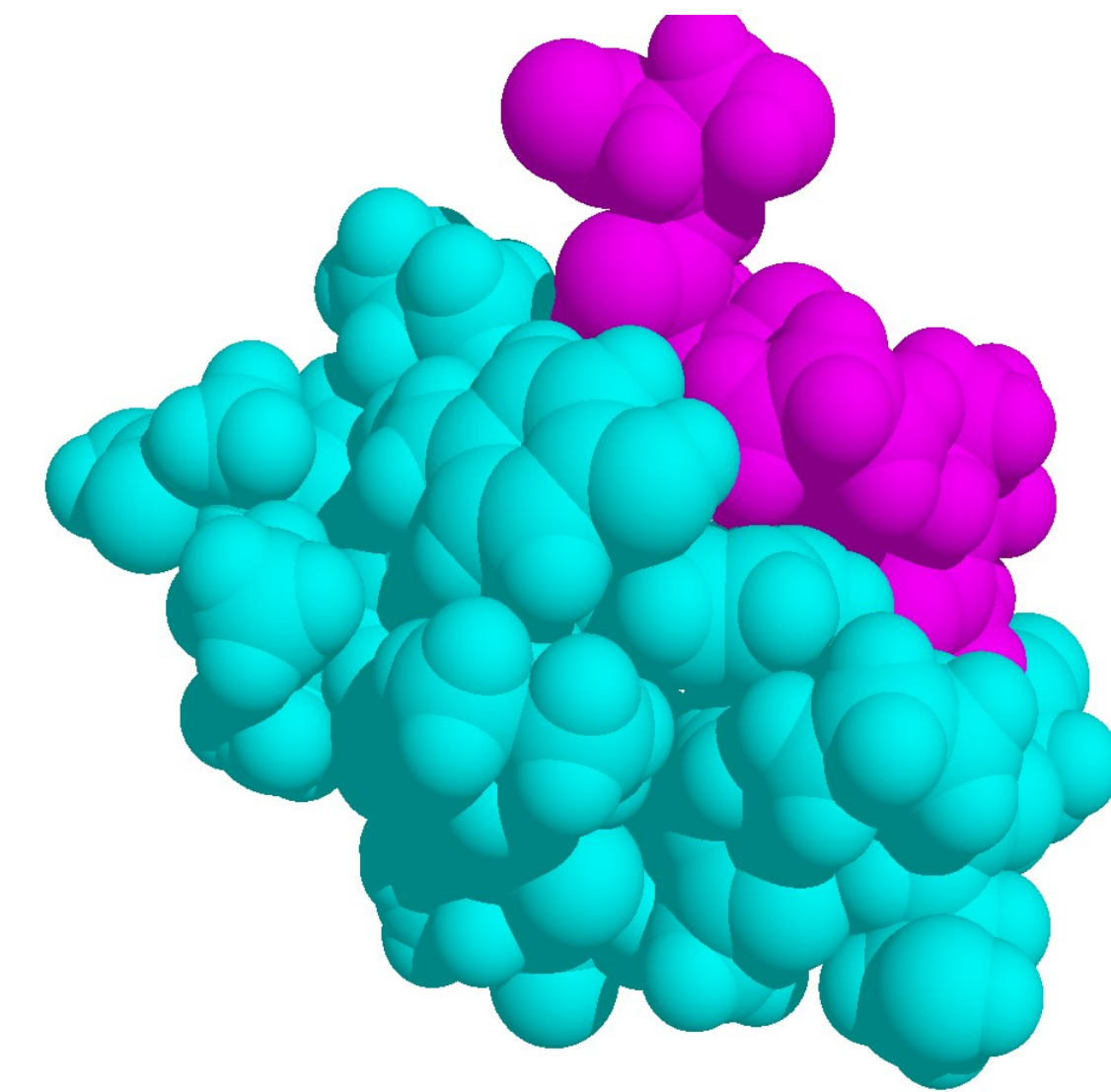
## Experiment Methodology

Our experimentation procedure is broken into three steps: 1) CPU-to-GPU transfer, 2) Energy evaluation, and 3) GPU-to-CPU transfer. While the first step requires transfer of the entire protein conformation, the return trip only requires transfer of three results: the summed attractive, repulsive, and solvation energies of the conformation. The GPU time to score a conformation is the summed time of the three steps above. Transfer times have been measured and GPU energy evaluation time is found by scaling average CPU time per pair evaluation by the number of pairs and GPU threads available. We then take the ratio of CPU-to-GPU time to find the speedup.

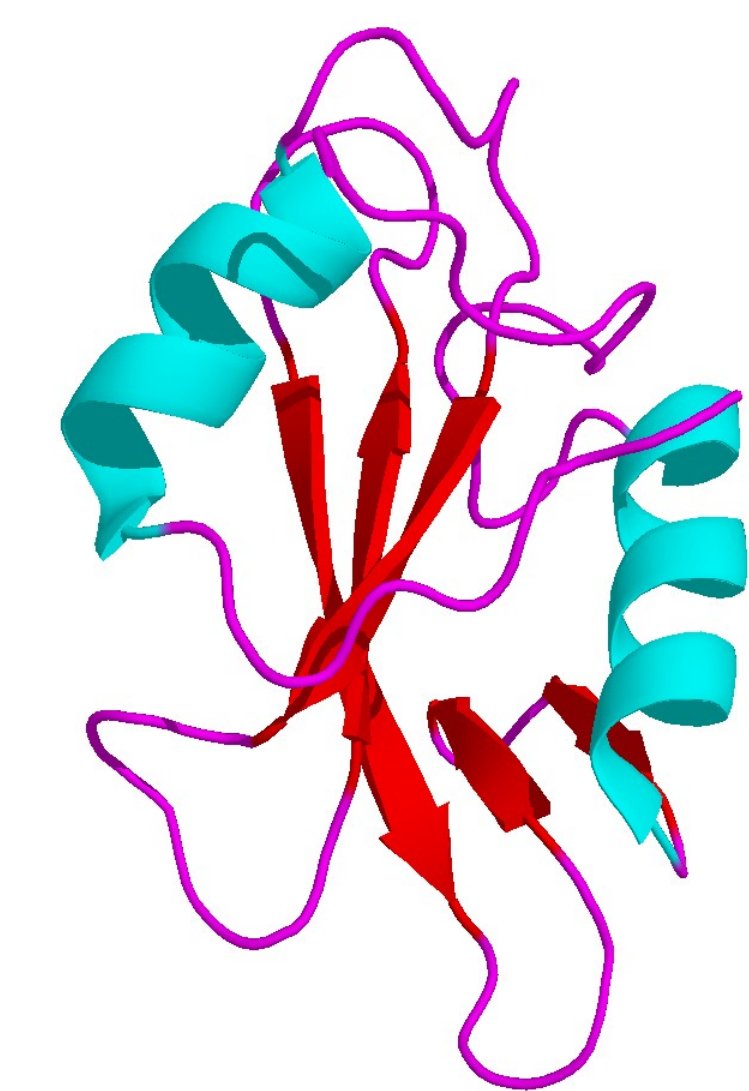
## Preliminary Results



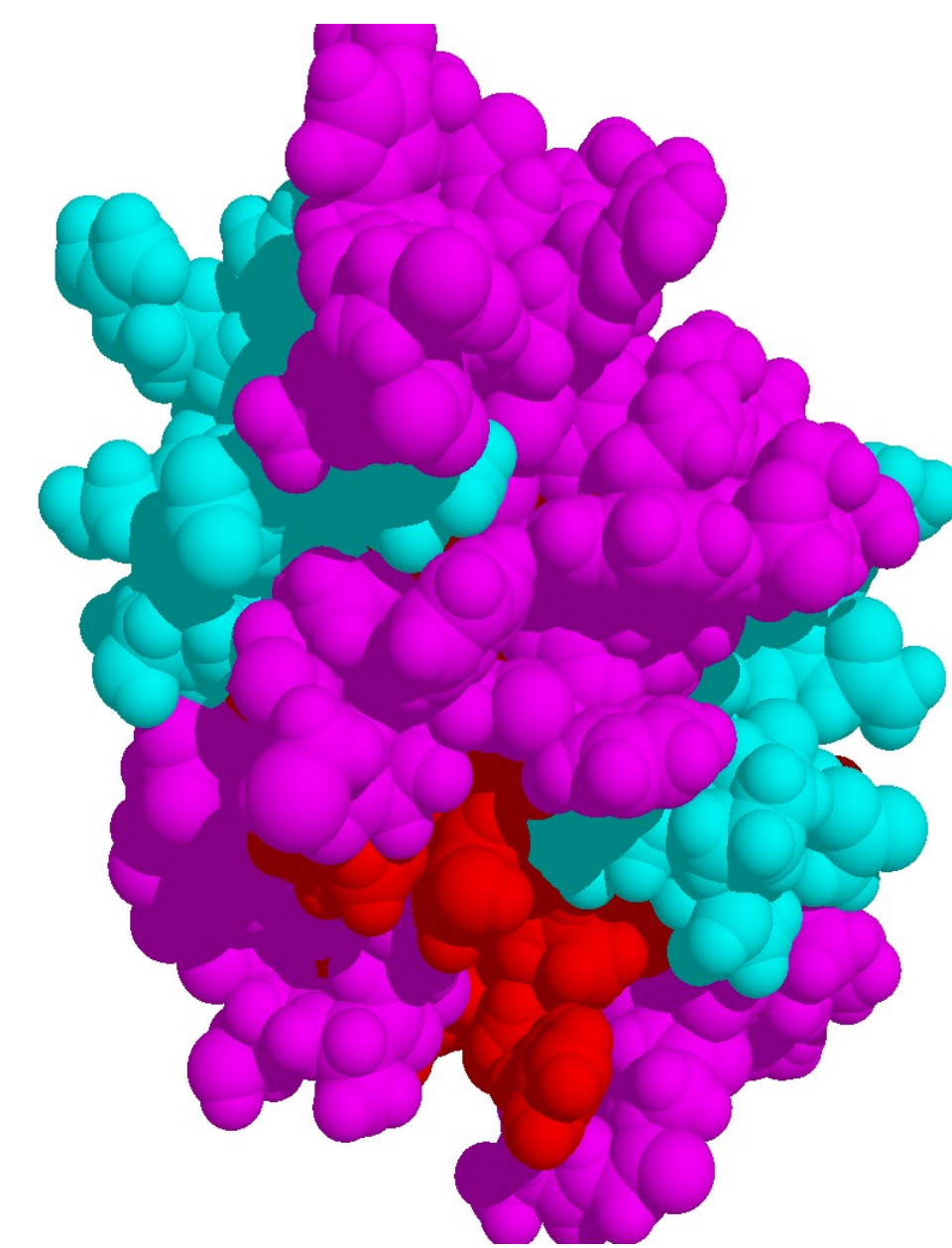
1L2Y Cartoon Representation



1L2Y Space-Filling Representation



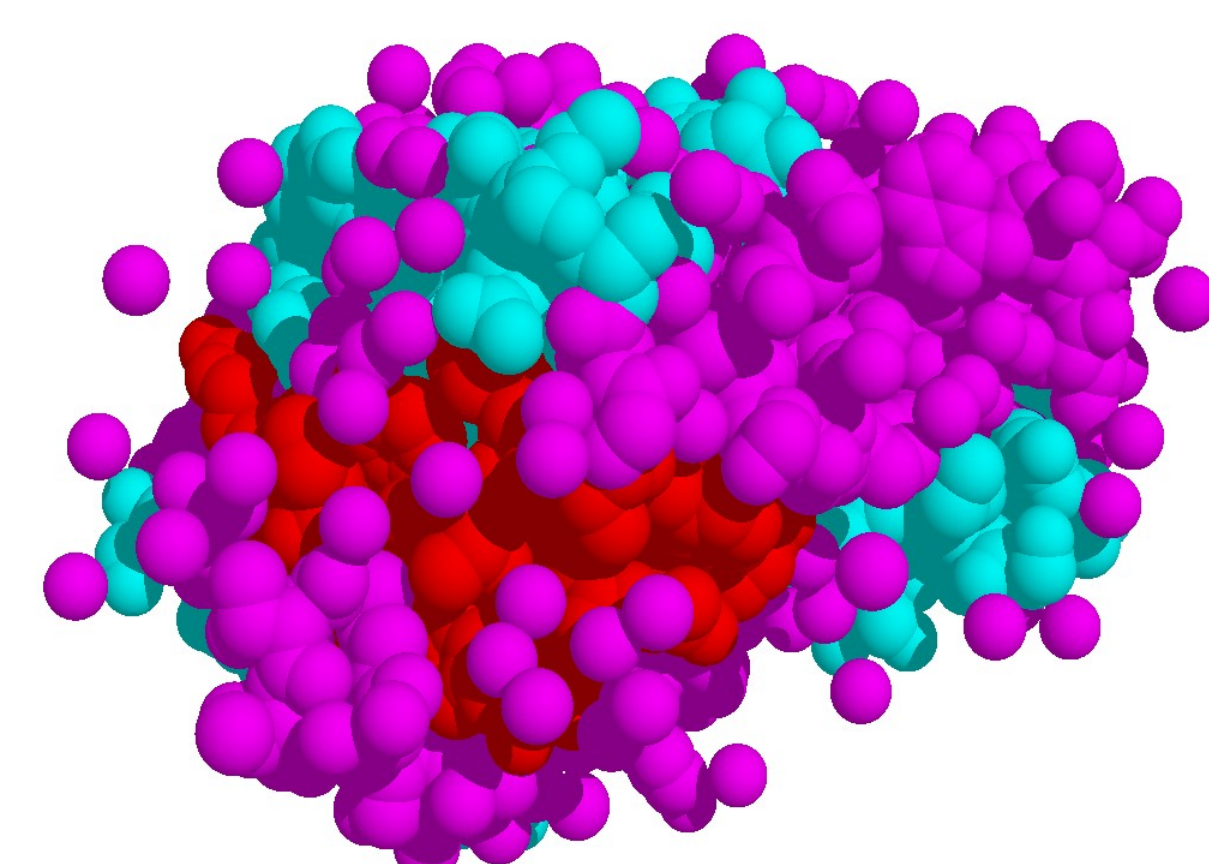
1RJA Cartoon Representation



1RJA Space-Filling Representation



1IAC Cartoon Representation



1IAC Space-Filling Representation



### Small Protein (1L2Y)

20 residues

CPU-to-GPU Transfer: 169 us

Energy Evaluation: 0.18 us =  $\text{ceil}(7,500 \text{ pairs} / 30,720 \text{ threads}) * 180 \text{ CPU ns} / \text{pair}$

GPU-to-CPU Transfer: 12 us  
181 GPU us

1,350 CPU us (180 ns \* 7,500 pairs) / 181 GPU us = **7x speedup**

### Medium Protein (1RJA)

100 residues

CPU-to-GPU Transfer: 877 us

Energy Evaluation: 0.36 us =  $\text{ceil}(50,000 \text{ pairs} / 30,720 \text{ threads}) * 180 \text{ CPU ns} / \text{pair}$

GPU-to-CPU Transfer: 12 us  
889 GPU us

9,000 CPU us (180 ns \* 50,000 pairs) / 889 GPU us = **10x speedup**

### Large Protein (1IAC)

200 residues

CPU-to-GPU Transfer: 2,209 us

Energy Evaluation: 0.72 us =  $\text{ceil}(100,000 \text{ pairs} / 30,720 \text{ threads}) * 180 \text{ CPU ns} / \text{pair}$

GPU-to-CPU Transfer: 12 us  
2,222 GPU us

18,000 CPU us (180 ns \* 100,000 pairs) / 2,222 GPU us = **8x speedup**