**Nucleation of Protein Crystals and Strong Scaling on Summit**Jens Glaser, Peter Schwendeman, Joshua A Anderson, and Sharon C Glotzer  
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**Abstract**

We discuss results for protein crystallization obtained from large-scale parameter sweeps and free energy calculations on Titan. Protein crystallization is a ubiquitously applied technique for elucidating molecular structure but predicting experimental crystallization conditions and structure from molecular sequence and shape remains a challenge. Here we explore an anisotropic, patchy shape simulation model of rubredoxin, which is experimentally known to crystallize into an orthorhombic P2\_1 2\_1 2\_1 symmetry, the most frequently observed space group among proteins. Using rigid-body molecular dynamics, our model reproduces crystallization into this structure. We show how a two-step nucleation process emerges and can be understood in terms of the free energy surface.

As a second part of this poster, we present our ongoing efforts to port HOOMD-blue, an open-source GPU-accelerated particle simulation library, to efficiently run on the Summit dense multi-GPU architecture. We show how the use of CUDA unified memory allows strong scaling on a single node of Summit, and when combined with MPI, across many nodes.