

Title: Collaborative Research: NSCI Framework: Software: SCALE-MS - Scalable Adaptive Large Ensembles of Molecular Simulations

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PIs: Kristen Fichthorn (Penn State), Peter Kasson (Virginia), Michael Shirts (Colorado), Matteo Turrilli (Rutgers)

Sc Scalable: Weakly coupled algorithms to get near-linear scaling in time-to-solution with 10^4 to 10^6 copies, even with large (minutes) latency

A Adaptive: Simulations can communicate synchronously/asynchronously & make decisions altering the simulation ensemble

L Large: Effectively use leadership computing (and eventually cloud computing) for molecular problems

E Ensembles: Many accelerated simulation methods can be parallelized by running "infrequently" communicating copies

MS Molecular Simulations: Application domain is physics-based molecular models, but ideas are transferable