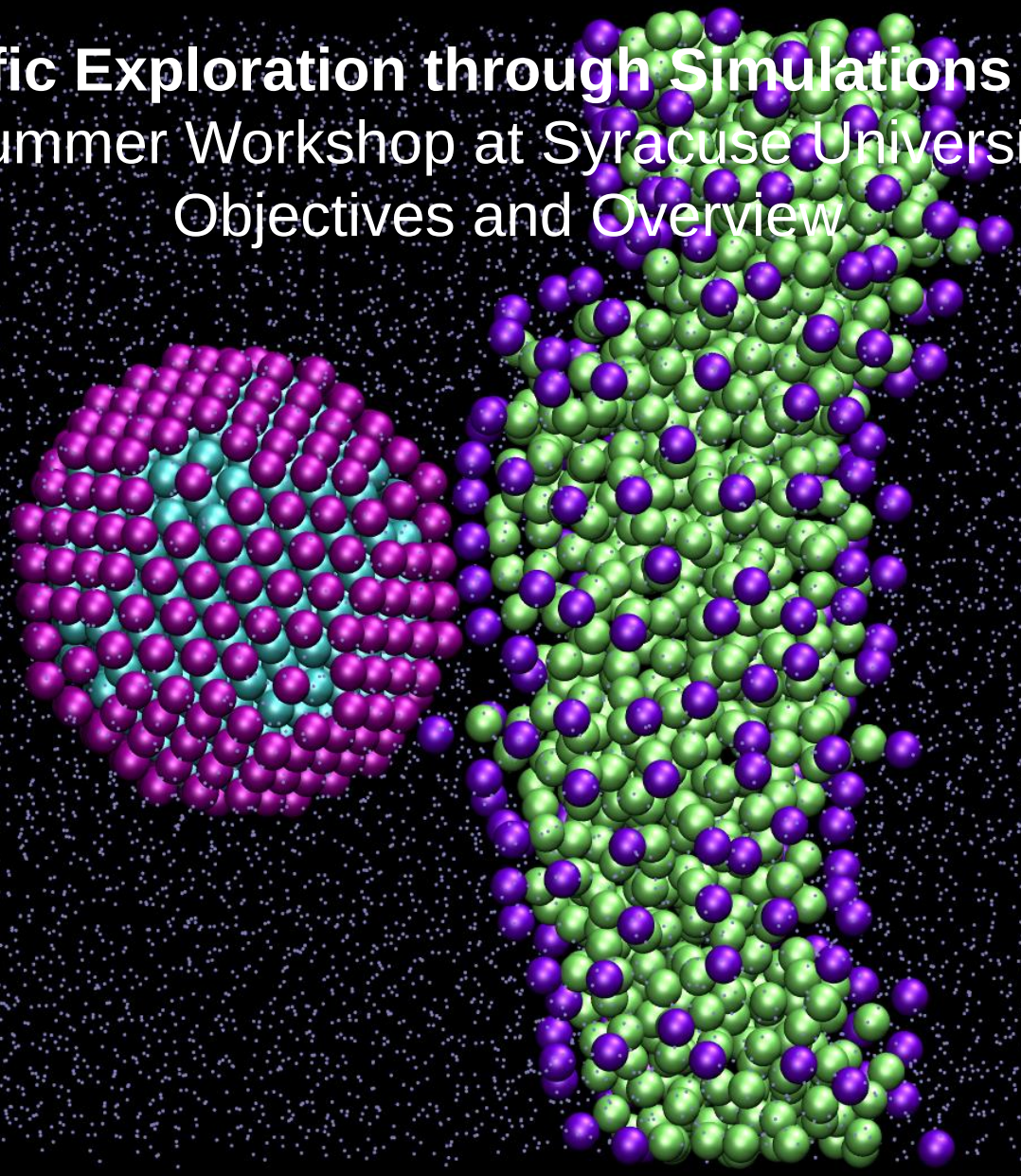
Scientific Exploration through Simulations (SETS)

Summer Workshop at Syracuse University

Objectives and Overview



OBJECTIVES

- ❑ Gain appreciation of computer simulations and their applications to various fields of science and technology

- ❑ Introduce and provide hands on training to K-12 teachers and students in state-of-the-art, open source computer simulations that help understand molecular structure/dynamics and molecular-scale phenomena in physical, chemical and biological systems
  - ❑ AVOGADRO
  - ❑ VMD
  - ❑ MOLECULAR DYNAMICS (GROMACS)

- ❑ Work collaboratively to test/evaluate the software components and develop mechanisms (e.g. home works, projects) to help integrate the computer simulations into the school curricula.

- ❑ Identify means by which students can continue to be engaged in hypothesis-driven research beyond the workshop

OVERVIEW OF KEY ACTIVITIES

Refer to workshop program for details

- ❑ Setup, Orientation, Discussion of Workshop Objectives
- ❑ Introduction to Computer Simulations
- ❑ Building and Analyzing Molecular Structures (AVOGADRO)
- ❑ Visual Molecular Dynamics (VMD)
- ❑ Performing Molecular Dynamics Simulation
  - ❑ Introduction, Demonstration and Hands-on Training
  - ❑ Testing Hypothesis using MD (Team-based Activity)
- ❑ Integration of Software Components into Curricula
  - ❑ Lectures, Homeworks, After-school Activities etc.
- ❑ Enabling Continued Student Engagement in Research