**Objective:** Address algorithmic impasse on characterizing protein and peptide structural dynamics through a plug-and-play platform of open-source software elements.

**Premise:** Impasse can be addressed by integrating algorithmic efforts of AI researchers on search and optimization and modeling efforts of biophysics researchers on molecular mechanics.

Software elements integrate search and optimization algorithms inspired from robot motion planning with sophisticated molecular models grounded in the latest understanding of protein biophysics.

Work proceeds along three directions:

**Objective 1**
State-of-the-art Molecular Representations and Energetic Models

- Structure
- Molecular Tree
- Conformation
- Kinematic Representation
- Building Blocks
- Fine Energy
- Conformation
- Medium Energy
- Rosetta
- AMBER
- Head-Gordon
- Rosetta PDB
- Protrude
- Angle
- Building Blocks
- Fragment
- Rosetta
- AMBER

Several components completed: e.g., interface with AMBER and Rosetta
Pending work on representation switching
Work carried out by students in labs of PIs

**Objective 2**
Robotics-inspired Algorithms for Structure and Motion Computation

- Motion Planning
- Tree-based
- Roadmap-based
- Hybrid
- RRT
- EST
- Proj-based Variants
- SRT
- FeLTr
- PDST
- ...

RRT, FeLTr, PRM, and variants completed
Research and education interleaved: Robotics course work designed to include more students from courses taught by PIs

**Objective 3**
Standardized Performance and Data Analysis

- PCA
- MDS
- LLE
- Isomap
- SciMap

Several completed and evaluated
Stand-alone C++ module completed
Research and outreach interleaved: Python module designed by high-school student

Detailed H-Ras landscape and On-Off transitions

**Summary schematic of CaM**
Ca→Protein-bound Transitions

- Many apo-states are intermediates (PDB ids 2KOE, 1DMO)
- Reconciles: wet-lab findings, which suggest transitions from Ca-bound to protein-bound states depend on the target; in-silico findings which suggest transitions follow a general, common functioning scenario.

**Showcase of recent work:**

- Project Page: [http://cs.gmu.edu/~ashehu/?q=SI2-SSE15Project](http://cs.gmu.edu/~ashehu/?q=SI2-SSE15Project)
- Contact Info: amarda@gmu.edu
- Recent Work: