A Plug-and-Play Software Platform of Robotics-Inspired Algorithms for Modeling Biomolecular Structures and Motions

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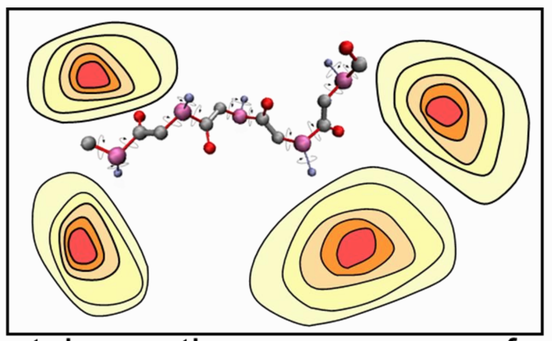
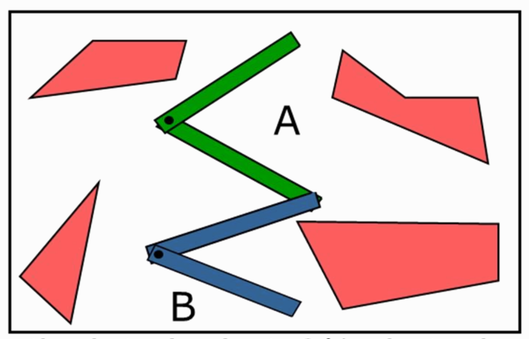
Project Page: http://cs.gmu.edu/~ashehu/?q=SI2-SSE15Project

- **Objective:** Address algorithmic impasse on characterizing *protein and peptide structural dynamics* through a *plug-and-play platform of open-source software elements*.
- **Premise:** Address by integrating algorithmic efforts of AI researchers on *search and optimization* and modeling efforts of biophysics researchers on molecular mechanics and energetics.

Application Setting:
Protein and peptide structure and dynamics.

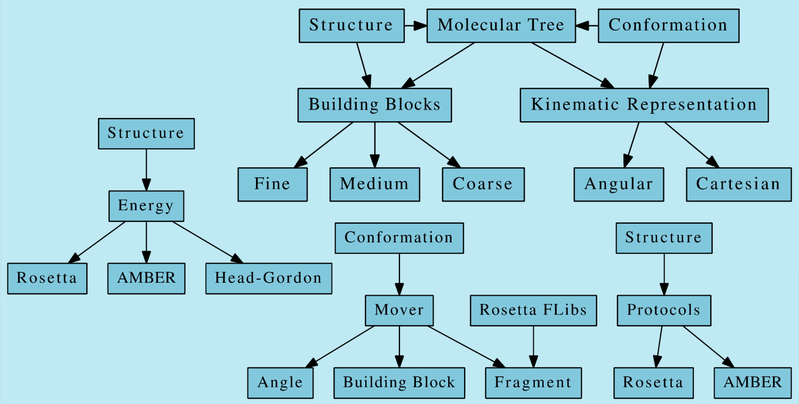
Software elements integrate search and optimization algorithms inspired from robot motion planning with sophisticated molecular models grounded in the latest understanding of protein biophysics.


protein: continuous energy surface

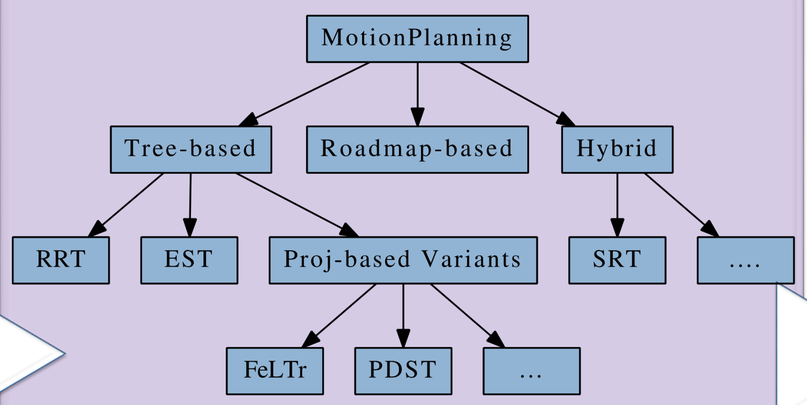


articulated robot: 0/1 obstacles

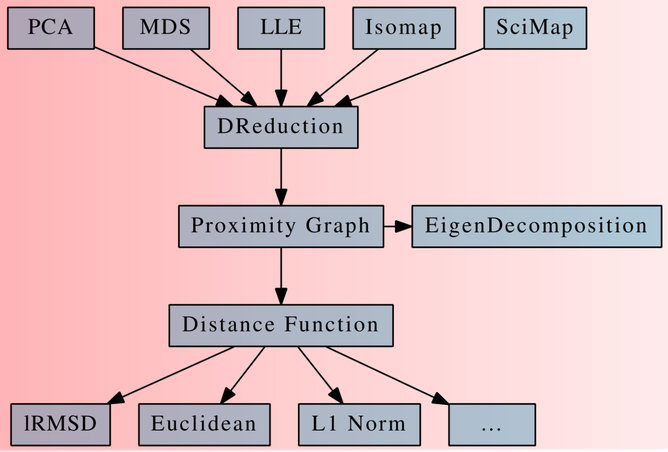
State-of-the-art Molecular Representations and Energetic Models



Robotics-inspired Algorithms for Structure and Motion Computation



Standardized Performance and Data Analysis



Dissemination:

- Open-source software (ROMEO) on gitlab.
- Workshops at ACM BCB 2018-2016, IEEE BIBM 2015, ACM GECCO 2017-2015.
- Tutorials on ROMEO at ACM BCB 2018, 2017.
- Testing labs of research collaborators (Ruth Nussinov/NCI, John Choy/Catholic Univ. of America, Carla Mattos/Northeastern Univ., Christopher McDermott-Roe/University of Pennsylvania).
- Educational partners (Nurit Haspel/Univ Mass Boston, Jing He/Old Dominion Univ., Brian Chen/Lehigh Univ, Lydia Tapia/Univ New Mexico, and others).
- Research articles (BMC Genomics 2018, JCB 2017, IEEE BIBM 2017, IEEE ICCABS 2017, JAIR 2016, ACM BCB 2016, IEEE/ACM TCBB 2016, Robotica 2016, IEEE NanoBioScience 2016, IEEE BIBM 2016, BICoB 2015).

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Showcase of Select Findings: