CSSI Element: **Element Software Enabling Millisecond-scale Biomolecular Dynamics**

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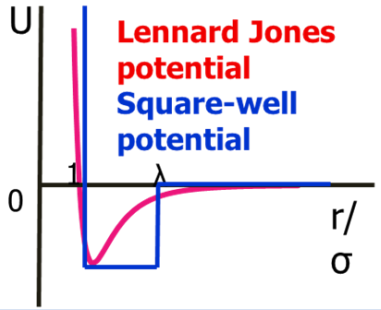
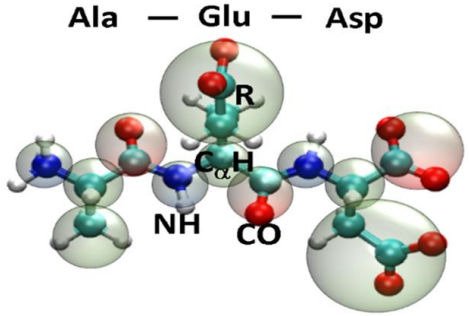
Award #: OAC-1835838

Background

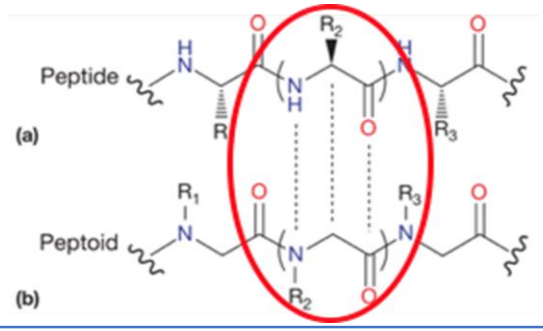
Discontinuous Molecular Dynamics



Coarse-grained (CG) Peptide Model

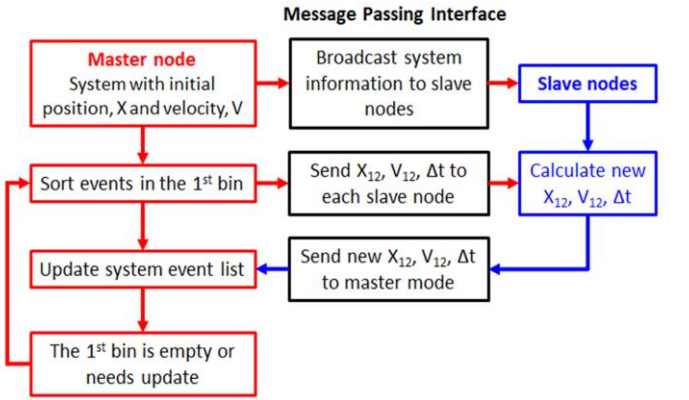


Peptoids vs Peptides



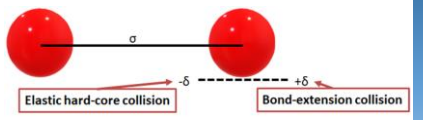
Goal 1
Develop parallel DMD package

Develop a parallel version of the existing serial DMD/PRIME20 code that will enable the leap from hundreds of microseconds to multiple milliseconds

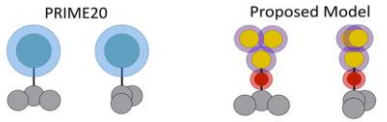


Goal 2
Improve PRIME20 model

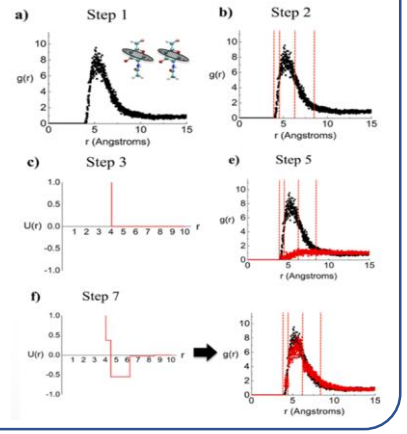
1. Improve efficiency



2. Improve geometry and energetics for better aromatic amino acid representation

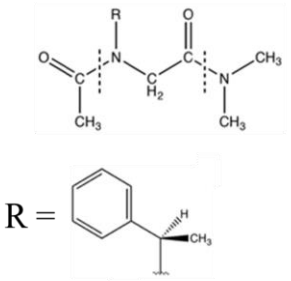


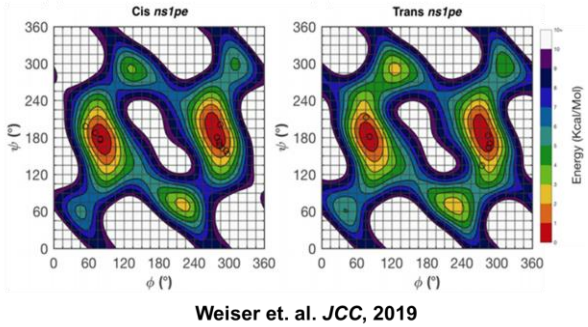
3. Develop a library of new coarse-grained parameters from atomistic simulations



Goal 3
Design CG forcefield for peptoids

Use top down (SAFT-VR) and bottom up (Relative Entropy) coarse graining to develop a DMD simulation forcefield for peptoids





Weiser et. al. *JCC*, 2019