Contribution ID: **62** Type: **Poster**

Enhancing Accuracy in Molecular Dynamics Simulations: Web service for Metal ions Force Field generation

Tuesday, 1 October 2024 18:00 (1 hour)

Molecular Dynamics (MD) simulations provide unique insight into the structural and dynamics of biological macromolecules, contingent upon their accuracy. Two primary determinants of accuracy include the precision of the MD model, particularly the molecular mechanics force field, and the depth of the sampling performed for the simulated system.

The purpose of the conventional force fields is to approximate the energetics of interatomic interactions in MD with relatively simple mathematical formulas. Such force fields are predominantly tailored for biomolecules due to their composition from recurring building blocks, namely amino acids and nucleotides. However, their accuracy diminishes notably for molecules that incorporate metal ions. In particular, metal ions typically form coordination bonds at catalytic sites and are crucial for recapitulating accurately the biological behavior of proteins.

In this contribution, we propose a service that provides a web user interface for the development of force fields for proteins containing metals. Within this service, we have implemented the automatic generation of generalised force field for proteins that contain zinc(II) ions [1]. The service takes a pdb file as input and searches for the amino acids that bind these ions. As output, the user receives a zip file containing the input files necessary to initiate a Molecular Dynamics simulation using the Amber or Gromacs suite. Furthermore, we are actively working to implement additional metals as generalized force fields, such as Cu and Fe.

[1] A Comparison of Bonded and Nonbonded Zinc(II) Force Fields with NMR Data. Bazayeva M, Giachetti A, Pagliai M, Rosato A. Int J Mol Sci. 2023. doi: 10.3390/ijms24065440.

Topic

Needs and solutions in scientific computing: Platforms and gateway

Primary author: GIACHETTI, Andrea (CIRMMP)

Co-author: Prof. ROSATO, Antonio (University of Florence)

Presenter: GIACHETTI, Andrea (CIRMMP)

Session Classification: Demonstrations & Posters