

Software Developed in CTBP

CTBP researchers are constantly developing new tools for the study of biological physics. Here is a listing of some of the resources that are available.

Actively Supported Software Packages

Proteins and Macromolecules

SMOG - The Structure-Based Model ("SMOG") software has been collaboratively developed and maintained by the [Whitford](#) and [Onuchic](#) groups for the last 10 years. This software has a web-based interface (SMOG 1), which is based on old Fortran code, as well as a more versatile downloadable version (SMOG 2). This software allows one to define and share new variants of structure-based force fields, which can be used with most major MD software packages (Gromacs, NAMD, openMM and LAMMPS). The lead developers are Jeff Noel and Paul Whitford.

OpenSMOG - This is an OpenMM library that provides integrated support for SMOG models, and it is part of the SMOG set of tools supported by the Whitford and Onuchic Groups. With the design structure of OpenMM, OpenSMOG allows one to use SMOG2 to construct more creative versions of SMOG models. The lead developers are Antonio Oliveira and Vinicius Contessoto.

RADtool - The Ribosome Analysis Database is driven by RADtool. This is a Tcl-based plugin for VMD that can be used to retrieve and analyze ribosome structures. The plugin can identify subunits, align them to a common references, identify structurally-conserved regions, calculate rotation angles, and more. The software may be used via the command line, or one may use the GUI (recommended in most cases). This tool provides a systematic framework for the analysis and comparison of ribosome structures. RADtool was developed by the Whitford Group.

openAWSEM - An implementation of the AWSEM coarse-grained protein folding forcefield in OpenMM. openAWSEM is the last iteration of the AWSEM forcefield family, which is being developed by the Wolynes group. There is a iteration in LAMMPS that is still being used <http://awsem-md.org/>. The lead developers are Wei Lu and Nick Schafer with collaboration of other members of the Wolynes group.

open3SPN2 - A Implementation of the 3SPN.2 and 3SPN.2C coarse-grained molecular model of DNA in OpenMM. 3SPN.2 and 3SPN.2C are DNA coarse-grained forcefields developed by the de Pablo group. Each DNA nucleotide is modelled by 3 beads: one bead for the phosphate, a second one for the sugar and a third one nucleobase. These forcefields were adapted by the Wolynes group to model protein-DNA interactions as a complement for the openAWSEM coarse-grained protein forcefield. The lead developers are Carlos Bueno, Wei Lu and Shikai Jin, with feedback from the de Pablo group.

Genome Organization and Chromatin Dynamics

OpenMiChroM - OpenMiChroM is a versatile Python library designed for executing chromatin dynamics simulations. By utilizing the OpenMM Python API and implementing the MiChroM (Minimal Chromatin Model) energy function, OpenMiChroM generates an ensemble of 3D chromosomal structures that align with experimental Hi-C maps. The lead developers are Antonio Oliveira and Vinicius Contessoto.

PyMEGABASE - A a highly accurate, maximum-entropy-based neural network model that predicts (sub)compartment annotations of a locus based solely on the 1D local epigenome tracks, such as ChIP-Seq of histone post-translational modifications. The lead developer is Esteban Dodero-Rojas.

Software provided without active support

Here are some tools that have been developed previously, but are not actively maintained. Links to the software are provided as a courtesy.

CoarseGrainedActin - A coarse grained model of actin filaments with 4 particles per bead based in the Voth model. This project is still on the early stages of development. The lead developer is Carlos Bueno.