CPP 28: Poster: Computational Physics of Soft Matter

Time: Tuesday 18:15–21:00 Location: Poster B2

CPP 28.1 Tue 18:15 Poster B2

Dimensionality aware method for the domain decomposition of homogeneous and inhomogeneous molecular dynamics simulations — •Horacio V. Guzman, Torsten Stuehn, and Kurt Kremer — Ackermannweg 10, 55128 Mainz

Molecular simulations are a scientific tool that has enabled theoretical and computational methods to tackle soft matter research. This is reflected in the permanent development and enhancement of new methodologies within scientific codes[1,2,3]. One of the challenges in molecular dynamics simulations is to improve efficiency in the parallelization of domain decomposition schemes. Here, we present a new iterative method to optimize the decomposition of the simulation box which combines the dimensionality of the system and the level of parallelization to be used. In addition the proposed method also includes a shifting domain walls feature for an adpatative load balancing of inhomogeneous systems[4]. We have implemented the method in ESPResSo++[1] which allowed us to benchmark both homogeneous[5] and inhomogeneous systems. By comparing the existing domain decomposition scheme[1] with the new dimensionality aware method, we prove that the latter enables a computationally more efficient domain decomposition for both homogeneous and inhomogeneous systems, and hence a speedup increase, as well as, a higher upper bound scaling. [1] J. D. Halverson et al., Compt. Phys. Comm. 184 (2013) [2] W. M. Brown et al., Comput. Phys. Comm. 195 (2015) [3] B. Hess et al., J. Chem. Theory Comput. 4 (2008) [4] M. Praprotnik et al., Phys. Rev. E 73 (2006) [5] L. Moreira et al., Macromol. Theory Simul. 24(2015)

CPP 28.2 Tue 18:15 Poster B2

SAMC simulation of single peptides in the PRIME20 model — •Arne Böker and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg

A number of current problems in medical science can be attributed to misfolding of proteins when these reach non-native free energy minima stabilized by aggregation. Describing these aggregation phenomena for relevant protein sizes requires the use of coarse-grained models. However, strongly coarse-grained computational models tend to simplify the free energy surface in such a way that these local minima are suppressed. To circumvent this problem, the level of coarse graining needs to be chosen appropriately.

PRIME20[1] is an intermediate-resolution model for proteins. It provides reasonable detail by mapping each amino acid to four beads, but keeps parameter space relatively simple with the set of interactions reduced to 19 parameters. We perform thermodynamic simulations of single PRIME20 chains using the "SAMC"[2] variation of Wang-Landau Monte Carlo samplng which provides insight in different statistical ensembles at the expense of dynamic information.

[1] M. Cheon, , I. Chang, C. K. Hall, Proteins **78**(2010):2950

[2] B. Werlich, T. Shakirov, M. P. Taylor, W. Paul, Comp. Phys. Comm. **186**(2015):65

CPP 28.3 Tue 18:15 Poster B2

Stiffness of Homopolymer Chains — •Benno Werlich[1], Timur Shakirov[1], Mark P. Taylor[2], and Wolfgang Paul[1] — [1]Institut für Physik, Martin-Luther Univerität Halle-Wittenberg, Halle (Saale) — [2]Department of Physics, Hiram College, Ohio, USA

For studying structure formation of homopolymer chains we use an off-lattice hard-sphere coarse grained model with square-well interactions. The indication of first and second order like pseudophase-transitions has been done with the help of microcanonical and canonical analysis. Therefore, a stiffness dependent state-diagram is shown for 40-mers. An example of various chain lengths for fixed stiffness shows an evolution of pseudophase-transitions. Beside nonspecific square-well interactions we introduced additional specific square-well interactions and study its effects. The simulations have been performed with the help of the Stochastic Approximation Monte Carlo Method (SAMC). SAMC is a type of Wang-Landau Monte Carlo.

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Differences in the structural flexibility of the sulfur and oxygen mustards molecules from Car-Parrinello molecular dynamics simulations — •Joanna Lach[1], Pawel Rodziewicz[2], Mariana Kozlowska[2], and Maciej Baradyn[2] — [1]Faculty of Physics, Vilnius University, Lithuania — [2]Institute of Chemistry, University of Bialystok, Poland

Sulfur mustard (SM) is an organic blister chemical warfare agent (CWA). It was thought that huge amounts of water can neutralize CWAs, thus after II World War large amounts of CWA were dumped into the Baltic Sea. Due to the high toxicity, SM, was often replaced with its structural analogue, namely, oxygen mustard (OM).

The conformational analysis of the SM and OM molecules was performed utilizing ab initio calculations. The dynamics of the system and all structural rearrangements between the local and global minima were studied at finite temperature by Car-Parrinello molecular dynamics (CP-MD) simulations. Post-processing population analysis of the relative low energy conformations was carried out. The existence of the most probable rearrangements was investigated. Crucial differences between structures of global and local minima for both SM and OM molecules were reported.

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FT-IR matrix isolation and theoretical study of tetrahydrofuran pseudorotation — •Joanna Lach[1], Justinas Ceponkus[1], Valdas Sablinskas[1], and Pawel Rodziewicz[2] — [1]Faculty of Physics, Vilnius University, Lithuania — [2]Institute of Chemistry, University of Bialystok, Poland

Tetrahydrofuran (THF) is an organic heterocyclic compound, used as an efficient solvent in multifunctional carbon-based nanomaterials e. g. carbon nanotubes. To investigate the interplay between nanomaterial and THF the exact conformation of the solvent should be analyzed in detail. The conformational diversity of the THF molecule is determined by two conformations (C_s envelope, C_2 twisted) with the energy barrier of 1.77 kJ/mol.

In this work matrix isolation infrared absorption spectroscopy was used to study the conformational diversity of the THF molecule at low temperatures. The recorded FT-IR spectra show that at 9 K only one THF conformer is trapped in N_2 matrix, so the pseudorotation is not observed. After heating of the matrix to 25 K additional bands in the IR spectra were observed, what indicates the presence of the second conformer. The *dynamics* of the model THF/N_2 system and the structural rearrangements between its local and global minima have been studied at finite temperature by Car-Parrinello molecular dynamics (CP-MD) simulations.

CPP 28.6 Tue 18:15 Poster B2

Assessment of coarse-grained models of conjugated polymers: Poly(3-hexylthiophene) (P3HT) — •Christoph Scherer and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

P3HT is the 'fruit fly' of polymeric organic semiconductors. Its self-assembly into lamellar structures and phase-separation in P3HT:PCBM blends has recently been studied using various computer simulation techniques [1,2,3]. The accuracy of coarse-grained (CG) models was, however, never assessed. Here, (iterative) Boltzmann inversion and force-matching schemes are used to derive interaction potentials for the CG representation of the molecule. The resulting potentials are compared to the ones reported in Refs. [2,3] and are benchmarked against the stability of the crystalline molecular arrangements and the persistence length of a single chain in solvent. The perspective is to include many-body terms into the description of the non-bonded interactions and to implement them into the VOTCA package [4]. The extension of the non-bonded interactions to at least 3-body terms should improve the prediction of the alignment of the polymers as 2-body terms cannot capture the directionality of the Pi-Pi interactions between the thiophene rings of the polymer backbones.

[1] C. Poelking, et al., Adv. Polym. Sci.,265, 139-180, 2014

[2] K. N. Schwarz, et al., Nanoscale, 5, 2017-2027, 2013

[3] E. Jankowski, et al., Macromolecules, 46, 5775-5785, 2013

[4] V. Rühle, et al., J. Chem. Theory Comput., 5, 3211-3223, 2009