process, but our theory is based on stochastic energetics, which is thermodynamics in fluctuating small world.
Here, I will show energetics of single active diffusion trajectories, where the instantaneous diffusion coefficient (IDC) as a new diffusion analysis quantity is derived. Considering decomposition of energy dissipation in a non-equilibrium steady state, we can make implication of the IDC clear. An advantage of our theory is to be able to discuss the meso scale energetics from only single-particle tracking data without measuring response.

2379-Pos Board B516
Analysis of Amino Acid Properties in Interaction Surfaces of Decoys Generated by Re-Docking Scheme
Nobuyuki Uchikoga[1], Yuri Matsuzaki[2], Masahito Ohue[3,4], Takatsugu Hirokawa[5], Yutaka Akiyama[2,4].
[1]Department of Physics, Chuo University, Tokyo, Japan, [2]ACLS, Tokyo Inst. Tech., Tokyo, Japan, [3]JSPS Research Fellow, Tokyo, Japan, [4]Grad. Sch. Inform. Sci. and Eng., Tokyo Inst. Tech., Tokyo, Japan, [5]MolProf, AIST, Tokyo, Japan.
Rigid-body docking processes generate many protein complexes (decoys) for searching near-native decoys (NN-decoys) in post-docking processes with analyzing various pairs of surfaces on two input proteins, using properties of electrostatics and desolvations between two molecules or proteins. Many powerful docking computer softwares were developed and were used for resolving various categories of problems, for example, analysis of protein interaction networks or drug design. Rigid-body docking process is popular and useful in such works. However, there are some unfortunate cases, which could not obtain NN-decoys. Then, we developed Re-docking scheme using interaction fingerprints (IFPs). Re-docking scheme is the process of iterating rigid-body docking for generating more NN-decoys. After initial-docking, we classify decoys into several interaction surfaces. Thereafter, other docking processes are performed with more fine searching limited in every interaction surfaces classified. We could obtain NN-decoys even if no NN-decoys in initial-docking process [Uchikoga et. al. (2013) PLOS ONE 8:e69365]. Then, we approach a problem of prediction of protein-protein interactions by using IFPs, which gives us properties of physico-chemical interactions because IFPs are composed of interacting amino acid pairs [Uchikoga & Hirokawa (2010) BMC Bioinform. 11:236]. By using IFPs, we can obtain these properties easily and trace interaction surfaces in docking processes. In this work, docking search spaces become to be seen by using amino acid properties involved in molecular surfaces of many decoys, generating by Re-docking scheme. Then, we would like to discuss about understanding interaction mechanisms.

2380-Pos Board B517
Inferencemap: Mapping of Single-Molecule Dynamics using Bayesian Inference
Mohamed El Beheiry[1], Maxime Dahan[1], Jean-Baptiste Masson[2,3].
[1]Physical Chemistry, Institut Curie, Paris, France, [2]Physics of Biological Systems, Institut Pasteur, Paris, France, [3]Janelia Farm Research Campus, Ashburn, VA, USA.
Single-molecule imaging has become ubiquitous in biophysics, biology, biochemistry and biotechnology, covering a large range of in vitro and in vivo applications. This ever-growing field now requires new and reliable statistical tools for data analysis. This is especially true for high-density single-molecule tracking methods that yield massive amounts of data and invite the use of statistics-based methods for analysis. Of particular importance is the extraction of dynamic properties (such as diffusion and transport parameters) and the ability to map these properties at different spatial scales (up to the full extent of the cell).
Bayesian analysis is a powerful method that has recently garnered interest in the treatment of single-molecule trajectories. Previously, we have shown that it provides an efficient means for estimating the relevant physical parameters that characterize the motion of individual molecules. Of particular importance, we have shown that interaction fields (which are systematically neglected in most approaches) play a paramount role in the long-term dynamics of biomolecules.
With this motivation, we present InferenceMAP, an interactive software tool that uses a powerful Bayesian technique to extract the parameters that describe the motion of individual molecules from single-molecule trajectories. The main features of our tool include:
•A versatile calculation platform for estimating dynamic parameters, including the ability to specify relevant prior probabilities.
•Adaptive meshing methods to conform to different temporal and spatial scales
•The ability to generate vast three-dimensional landscapes of single-molecule dynamics
We present relevant applications inside lipid rafts, glycine receptors, and HIV assembly platforms.

2381-Pos Board B518
Neuroimage: A Novel Highly Efficient Tool for Image Processing of in vivo Neural Networks
Christian Heusinger, André Drews, Aune Koitmäe, Robert Blick.
Physics, University of Hamburg, Hamburg, Germany.
Simulation of biological neural networks has been of great interest in the last years with well-established simulation tools like NEURON being constantly developed on, while tools for image processing of experimental neuron data are still lacking.
We present an image processing tool that takes confocal fluorescence microscopic 2D data of a neural network and converts it into a NeuroML file containing the network morphology. Thereby the network data is ready to be imported into neuroConstruct or any NeuroML compliant tool, where the network then can be visualised, manipulated and simulated using a broad range of already available simulators and cell models.
We investigate a neural network of in-vivo neuron cells extracted from mouse brain tissue and grown on a semiconductor substrate. Besides obtaining the positions of somae and axons together with their network topology we identify so-called micro tubes which are built for future experiments seeking to measure the action potentials of axons going through them. Our image processing is used here to analyse the preparation process, in particular the positioning of cells on the substrate and success rate of axons growing through micro tubes. Furthermore the tool offers the interface for subsequent simulation in neuroConstruct and NEURON.
Simulation of a simple electrophysiological input and output will be presented and will allow comparison with future experimental data.

2382-Pos Board B519
Integrative Modeling Approaches to Interpret High-Resolution cryo-EM Reconstructions
Alejandro Jesús Canosa-Valls, Erney Ramírez-Aportela, Pablo Chacón, **José R. López-Blanco**.
Biological Physical Chemistry, Institute of Physical Chemistry, Madrid, Spain.
Modeling 3D-EM reconstructions with computational tools currently enables the interpretation at near-atomic resolution of different functional states of macromolecules, thereby deciphering the functional mechanism of biologically relevant complexes. Recent advances in cryo-EM, such as direct electron detectors, specimen preparation, image processing, and data automation, are increasing the number of determined structures, particularly at high (<5 Å) resolutions. Here, several new integrative approaches are presented to retrieve structural information from these accurate reconstructions by incorporating modeling constraints from complementary biophysical techniques (crystallography, SAXS, FRET, etc.) or any other source of structural information (cross-linking, mutagenesis, prediction data, etc.). First, a two-step integrative approach was developed to unravel the topology of helical bundles using cryo-EM maps, distance restraints, and secondary structure predictions. This method unambiguously localized all helices of a key unassigned proteasome helical bundle and provided a topologically correct model that was later confirmed by crystallography. Second, our normal mode based flexible fitting algorithm, iMODFIT, was accelerated and adapted to deal with high resolution cryo-EM maps and other experimental constraints. Third, a fast loop-closure algorithm (RCD) was combined with integrative fitting strategies for modeling loops into unfilled densities. We strongly believe that these tools will facilitate the interpretation of the incoming high-resolution maps.

2383-Pos Board B520
Energy Tabulation Strategies for Accelerated Monte Carlo Simulation at Multiple Length Scales
Justin M. Spiriti, Daniel M. Zuckerman.
Computational and Systems Biology, University of Pittsburgh, Pittsburgh, PA, USA.
We have constructed novel coarse-grained models based on dividing biomolecular systems into rigid fragments and constructing six-dimensional tables of the interaction energy between them as a function of their relative displacement and orientation. The approach can be used for simulations on two length scales: conformational sampling within a macromolecule (e.g., protein) and interactions between elements of a multi-molecular complex (e.g., viral capsid). For conformational sampling of proteins, we tabulate interaction and solvation energies for small rigid fragments, obtained from an underlying atomistic force field. By applying potential energy smoothing techniques to these tables, we are able to improve sampling of these proteins, while maintaining secondary structure without added restraints. We use a similar tabulation strategy, based