in relation to both mesh-spacing and time-step refinement, the iterative approach avoids linearised formulations commonly used in matrix resolutions, and it is driven by upper limits of residuals (L ∞ norm) - Figure 1.

[1] C.S. Peskin, Acta Numerica,11,479-517(2002).
[2] G. Pereira, Conf. Multiscale Modelling in Medicine and Biology, Nottingham, UK(2012).
[3] R. Verzicco and P. Orlandi, J. Comput. Phys,123,402-414(1996).

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Steric PNP (Poisson-Nernst-Planck): Ions in Channels

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Ionic solutions are not ideal. Everything interacts with everything else, particularly in highly concentrated solutions (>10 M) in and near ion channels and active sites. A variational approach (J ChemPhys **133:**104104) is needed in interacting complex fluids. The first terms of a perturbation expansion below can produce current voltage curves in complex solutions and channels in a few hours on notebook computers. Equations are solved with multiblock Chebyshev pseudospectral methods using methods of lines (J Computational Physics 231:2498 and J Phys Chem B DOI 10.1021-jp305273n.

$$-\nabla\cdot(\varepsilon\nabla\phi)=\rho_0 e+\sum_{i=1}^{N} z_i e c_i,$$

$$\frac{\partial c_i}{\partial t}+\nabla\cdot\vec{J}_i=0,\qquad i=1,\cdots,N-1$$

$$\vec{J}_i=-D_i\nabla c_i-\frac{D_i c_i}{k_B T}z_i e\nabla\phi-\frac{D_i c_i}{k_B T}\sum_{j=1}^{N}\varepsilon_{ij}\delta^{-12+d}\left(a_i+a_j\right)^{12}\nabla c_j$$

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Dependence of Ions Transport by DNA Blockage in Alpha-Hemolysin and MspA Toxins Studied by Means of Gran-Canonical Monte-Carlo/ Brownian Dynamics with Effective Potentials

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A recent progress in the development of nanopore technology offers a unique chance for rapid and cost-effective DNA sequencing. Ion-transport dependent on DNA sequence as measured by electrophysiological setup allows relating ion current to a particular nucleotide blocking a narrow nanopore. However, numerous issues make unambiguous sequencing a challenging task. An understanding of molecular underpinning of pore-DNA interactions and relationship between DNA dynamics and resulting ion flow across the pore are among two most important targets for improving already existing nanopores. Several theoretical approaches have been formulated to assist experimental design of the pore ranging from very detailed all-atom MD simulations to models based on a random walk approach. The main challenge for application of all-atom techniques is a limiting time-scale of simulation, while field-based approximations are often lacking atomic-scale resolution. To fill the niche we have developed a novel scheme based on Grand-Canonical Monte-Carlo/Brownian Dynamics simulations and extended it to studies of ion current across two most used in sequencing nanopores, namely alpha-hemolysin and MspA. We also present a protocol for the development of nucleotide-ion effective interacting potentials based on the solution of reverse Monte-Carlo problem as formulated by Lubartzev and colleagues. We show that this inter-mediate resolution method is providing an excellent agreement with experimental results and data from previous studies utilizing computationally expensive Molecular Dynamics simulations.

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New Approaches for Dynamic Simulations of Implicit Solvent Coarse-Grained Models of Lipid Bilayer Membranes

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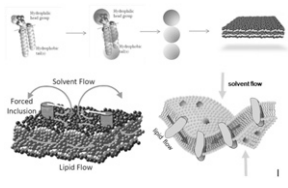
To access length and time scales relevant to biological systems, many coarse-grained models have been developed for lipid bilayer membranes by coarse-graining the lipid and protein degrees of freedom and by treating implicitly the solvent. These reduced descriptions have been successful in elucidating many equilibrium properties of lipid bilayers and protein inclusions, such implicit solvent models are of limited use for dynamical studies. To extend implicit solvent models, we present new approaches that introduce effective kinetic descriptions of the solvent through the use of fluctuating hydrodynamics. For dynamic coarse-grained molecular simulations, we present a new thermostat that uses exchange of energy and momentum with hydrodynamic degrees of freedom. We then present a dynamic coarse-grained model for lipid bilayer membranes parameterized to have bending elasticity, compression moduli, and shear viscosity comparable to experimentally studied bilayers. The importance of hydrodynamics is shown in dynamic studies of the dispersion relation of membrane undulations and the mobility of bilayer inclusions. We also discuss our package for LAMMPS.



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Real-Time Determination of Sarcomere Length of a Single Cardiomyocyte during Contraction

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Mean sarcomere length of a cardiomyocyte is an important control parameter for physiology studies on a single cell level. For instance, accurate determination of the mean sarcomere lenght in real-time is essential for performing single cardiomyocyte contraction experiments.

The aim of this work is to develop an accurate and efficient computational method for determining the mean sarcomere length from transmission images of a single contracting cardiomyocyte. This algorithm has to be robust to noise in input and exact for perfectly periodic input, that is, the best algorithm must have no systematic errors.

To accomplish the goal of this work we are (i) using unbiased measure of similarities to eliminate systematic errors from conventional autocorrelation function (ACF) based methods when applied to region of interest of an image, (ii) using a semi-analytical semi-numerical approach for evaluating the similarity measure to take into account spatial dependence of neighboring image pixels, (iii) and using a detrend algorithm to extract the sarcomere striation pattern content from the microscopy images.

The developed mean sarcomere length estimation procedure has superior computational efficiency and estimation accuracy compared to the conventional ACF and spectral analysis based methods using Fast Fourier Transform. As shown by analyzing synthetic images with the known periodicity, the estimates obtained by the developed method are more accurate at the sub-pixel level than ones obtained using ACF analysis. When applied in practice on rat cardiomyocytes, our method was found to be robust to the choice of the region of interest that may (i) include projections of carbon fibers and nucleus, (ii) have uneven background, and (iii) be slightly disoriented with respect to average direction of sarcomere striation pattern. The developed method is implemented in open-source software, see http://iocbio.googlecode.com.

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Using Raster Image Correlation Spectroscopy for the Detection of ADP/ ATP Diffusion Restrictions in Rat Cardiomyocytes

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A series of experiments show the existence of ADP/ATP diffusion restrictions in rat cardiomyocytes. At present, the nature of these restrictions is still unknown. In this work we hypothesize that the restrictions are in the form of membrane-like diffusion barries. We present a theoretical foundation for the use of raster image correlation spectroscopy (RICS) to determine the presence and the locations of such barriers. It is shown that in the proximity of the membrane, the diffusion pair correlation function (PCF) is not symmetric. For impermeable and semi-permeable membranes the difference between the PCF functions found for inhomogeneous and homogeneous media is an antisymmetric function with the membrane located exactly at the zero point. This property can be used to detect barriers. With a gaussian PSF, the PCF for an impermeable membrane can be calculated analytically, thus giving a convenient theoretical basis for the interpretation of microscope data. In the case of small permeability, the correlation function can be expressed in a form where only one convolution type integral is present, useful for both numeric calculation and theoretical understanding.

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Computational Analysis of Integrin Subunit Glycosylation: Investigations on its Role in Orienting Ligand-Receptor Interaction

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Integrins serve as the primary mediators of cellular adhesion to the extracellular matrix (ECM). Several cellular processes (e.g. apoptosis) are controlled through their interactions with ligands in the ECM. Integrins bind to their ECM ligands through their head domains. The crystal structure of an integrin heterodimer ($\alpha V\beta 3$) reveals the location of the ECM ligand binding site. Integrin function may be altered by the disruption of the ligand binding site either through changes in protein conformation or heterodimer binding orientation. Previous studies have suggested a link between disruptions of integrin function to changes in glycosylation. This study focuses on characterizing the effect of