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VABILO NA PREDAVANJE
INVITATION TO THE LECTURE

Dr. Bernard R Brooks

Laboratory of Computational Biology, NHLBI/NIH, Bethesda, Maryland, USA

Torek / Tuesday, 14. 9. 2010 ob / at 13:00

Velika predavalnica Kemijskega inštituta /
Lecture Hall at the National Institute of Chemistry
Hajdrihova 19, Ljubljana

Improved Self Guided Langevin Dynamics (SGLD): Enhanced sampling that preserves the ensemble and Multiscale modeling efforts involving CHARMM

Rapid exploration of local conformational space using simple integration techniques is critically important for calculating free energies or any thermodynamic properties that depend on a reasonable estimate of the partition function. Most enhanced sampling methods focus on enhancing a few pre-determined reaction coordinates, but Self Guided Langevin Dynamics (SGLD) and Self Guided Molecular Dynamics (SGMD), are approaches that improve sampling for all degrees of freedom. A major drawbacks of the original version (Wu X, Brooks BR. Self-guided langevin dynamics simulation method. Chemical Physics Letters. 2003;381(3-4):512-8) is that stronger coupling resulted in a serious distortion of the ensemble. Recent enhancement to SGLD and SGMD will be presented that demonstrate how the ensemble can be preserved without sacrificing rapid sampling efficiency. These techniques can be combined with other enhanced sampling techniques, such as replica exchange, with good effect.

This presentation also focuses on our recent efforts to develop general multi-scale macromolecular modeling methods and to apply them to problems of examining protein dynamics and function. One objective in developing multi-scale modeling techniques is to be able to include multiple scale representations within a single study. By combining scales within a single calculation, one can examine properties that would be difficult or too costly to examine with a single model. Examples of modeling scales that can be connected and combined with the "multiscale" command within CHARMM and experiences and examples of newer methods building and expanding upon the multiscale command will be briefly presented and discussed.

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