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VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

Dr. Benjamin T. Miller

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četrtek / Thursday, 4. 07. 2013, ob / at 13:00

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

Next generation tools for molecular modeling: Web interfaces and extreme parallelism

Recent, rapid growth of computing power has created substantial opportunities for advances in simulation research. However, programmers of simulation software often have difficulties taking advantage of large-scale parallel computing resources. Furthermore, many available programs are difficult and cumbersome to use, especially for new users. This talk addresses both of these issues. It describes how recent advances in sampling methods and multi-scale modelling can take advantage of the massive parallel computing resources that are becoming more widely available. It also shows how Web interfaces can be used to provide an introduction to simulation science to students and non-experts. Particular attention will be given to the CHARMMing web interface (www.charmming.org) and its use in education.

Vljudno vabljeni! / Kindly invited!

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