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SEMINAIRE

«High-resolution molecular dynamics simulations for biophysics with Tinker-HP»

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I will discuss our strategy for high-resolution molecular dynamics towards biophysical applications. As I detail the various protein targets that are currently under study, I will show how the newly developed multi-GPUs version of the Tinker-HP software [1, 2] can accelerate high-resolution molecular dynamics simulations. Indeed, thanks to adaptive sampling and new generation many-body polarizable force fields such as AMOEBA, long (μs) molecular dynamics simulations at enhanced accuracy become possible.[3] As I detail the currently available other enhanced sampling capabilities of the software, I will give some perspectives about the use of new hybrid physically-driven machine learning approaches [4] for condensed phase molecular dynamics.

References

1) Tinker-HP: a Massively Parallel Molecular Dynamics Package for Multiscale Simulations of Large Complex Systems with Advanced Polarizable Force Fields. L. Lagardère, L.-H. Jolly, F. Lipparini, F. Aviat, B. Stamm, Z. F. Jing, M. Harger, H. Torabifard, G. A. Cisneros,M. J. Schnieders, N. Gresh, Y. Maday, P. Ren, J. W. Ponder, J.-P. Piquemal, Chem. Sci.,2018, 9, 956-97 (Open Access), DOI: 10.1039/C7SC04531J

2) Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields using GPUs and Multi-GPUs systems. O. Adjoua, L. Lagardère, L.-H. Jolly, Arnaud Durocher, Z. Wang, T. Very, I. Dupays, T. Jaffrelot Inizan, F. Célerse, P. Ren, J. Ponder, J-P. Piquemal, J. Chem. Theory. Comput., 2021, 17, 4, 2034–2053 (Open Access), DOI: 10.1021/acs.jctc.0c01164

3) High-Resolution Mining of SARS-CoV-2 Main Protease Conformational Space: Supercomputer-Driven Unsupervised Adaptive Sampling. T. Jaffrelot Inizan, F. Célerse, O. Adjoua, D. El Ahdab, L.-H. Jolly, C. Liu, P. Ren, M. Montes, N. Lagarde, L. Lagardère, P. Monmarché, J.-P.Piquemal, Chem. Sci., 2021, 12, 4889-4907 (Open Access), DOI: 10.1039/D1SC00145K

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