Improving the scaling of new generation molecular dynamics classical simulations: a dialog between Mathematics and Theoretical Chemistry

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In this talk, recent developments concerning the optimization of new generation polarizable forces fields dedicated to large scale molecular dynamics simulations on massively parallel supercomputers are presented. As we focus on the strategies required to solve the polarization energy equations [1], the importance of mathematics in the design of future methods and its links with physics and chemistry will be highlighted.
[1
Texte de la communication avec ses références bibliographiques éventuelles [1][**?**].

Références

[1] F. Lipparini, L. Lagardere, B. Stamm, E. Cances, M. Schnieders, P. Y. Ren, Y. Maday, J.-P. Piquemal, *Scalable evaluation of the polarization energy and associated forces in polarizable molecular dynamics: I. towards massively parallel direct space computations.*, J. Chem. Theory. Comput, 2014.

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