**Science and Publications with Tinker-HP**

Jean-Philip Piquemal

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1) Scalable evaluation of the polarization energy and associated forces in polarizable molecular dynamics: I. towards massively parallel direct space computations.F. Lipparini, L. Lagardere, B. Stamm, E. Cances, M. Schnieders, P. Y. Ren, Y. Maday, J.-P. Piquemal, J. Chem. Theory. Comput., **2014**, 10, 1638-1651.
   DOI: 10.1021/ct401096t
2) Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. F. Lipparini, L. Lagardere, C. Raynaud, B. Stamm, E. Cances, M. Schnieders, P. Y. Ren, B. Mennucci, Y. Maday, J.-P. Piquemal, J. Chem. Theory. Comput., **2015**, 11, 623-634.
   DOI: 10.1021/ct500998q
3) Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II.Towards Massively Parallel Computations using Smooth Particle Mesh Ewald. L. Lagardere, F. Lipparini, E. Polack, B. Stamm, E. Cances, M. Schnieders, P. Y. Ren, Y. Maday, J.-P. Piquemal, J.Chem. Theory. Comput., **2015**, 11, 2589-2599.
   DOI: 10.1021/acs.jctc.5b00171
4) Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles.Christophe Narth, Louis Lagardere, Etienne Polack, Nohad Gresh, Qintao Wang, R. Bell, David, Joshua . Rackers, Jay W. Ponder, Pengyu Y. Ren, Jean-Philip Piquemal ,J. Comput. Chem., **2016**, 37(5), 494-506(COVER)
   DOI: 10.1002/jcc.24257
5) LICHEM: A QM/MM Program for Simulations with Multipolar and Polarizable Force Fields. E. G. Kratz, A. R. Walker, L. Lagardere, F. Lipparini, J.-P. Piquemal and G. A. Cisneros, J. Comput. Chem., **2016**, 37(11), 1019-1029 (COVER).
   DOI: 10.1002/jcc.24295
6) Truncated Conjugate Gradient (TCG): an optimal strategy for the analytical evaluation of the many-body polarization energy and forces in molecular simulations. F. Aviat, A. Levitt, Y. Maday, B. Stamm, P. Y. Ren, J. W. Ponder, L. Lagardère, J.-P.Piquemal, J. Chem. Theory. Comput., **2017**, 13, 180-190.
   DOI: 10.1021/acs.jctc.6b00981
7) Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. Daniele Loco, Louis Lagardere, Stefano Caprasecca, Filippo Lipparini, Benedetta Mennucci, Jean-Philip Piquemal, J. Chem. Theory. Comput, **2017**, 13, 4025-4033.
   DOI: 10.1021/acs.jctc.7b00572
8) Towards Scalable and Accurate Molecular dynamics using the SIBFA polarizable force field. L. Lagardère, L. El-Khoury, S. Nassem-Kahn, F. Aviat, N. Gresh, J.P. Piquemal, AIP Conf. Proc., **2017**, 1906, 030018 (Proceedings of the ICCMSE 2017 conference).
   DOI:10.1063/1.50122972018

9) The Truncated Conjugate Gradient (TCG), a Non-iterative/Fixed-cost Strategy for Computing Polarization in Molecular Dynamics: Fast Evaluation of Analytical Forces. F. Aviat, L. Lagardere, J.P. Piquemal, J. Chem. Phys., **2017**, 147, 161724(special issue: from Quantum Mechanics to Force fields)
DOI: 10.1063/1.4985911
10) Unusual Influence of the Fluorinated Anions on the Stretching Vibrations of Liquid Water. Maciej SmiechowskiThe Journal of Physical Chemistry B, **2018**, 122(12), 3141-3152
DOI: 10.1021/acs.jpcb.7b11334
11) 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, 956-972
DOI: 10.1039/C7SC04531J
12) AMOEBA Polarizable Force Field Parameters of the Heme Cofactor in its Ferrous and Ferric Forms. X. Wu, C. Clavaguera , L. Lagardère , J-P. Piquemal, A. de la Lande, J. Chem. Theory. Comput., **2018**, 14 (5), pp 2705–2720
DOI: 10.1021/acs.jctc.7b01128
13) Massively Parallel Implementation of Divide-and-Conquer Jacobi Iterations Using Particle-Mesh Ewald for Force Field Polarization. Dominique Nocito, Gregory J. Beran, **2018**, online.
DOI: 10.1021/acs.jctc.8b00328
14) How to make continuum solvation incredibly fast in a few simple steps: a practicle guide to the domain decomposition paradigm for the Conductor-like Screening Model. B. Stamm, L. Lagardère, G. Scalmani, P. Gatto, E. Cancès, J.-P. Piquemal, Y. Maday, B. Mennucci, F. Lipparini, Int. J. Quant. Chem., **2018**, in press.
DOI: 10.1002/qua.25669
15) A rigorous derivation of the Ewald summation for arbitrary orders of multipoles: The self-terms. B. Stamm,L. Lagardère, É. Polack, Yvon Maday, J.-P. Piquemal, **2018**, to appear in J. Chem. Phys.
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16) Tinker 8: Software Tools for Molecular Design. J. A. Rackers, Z. Wang, C. Lu, M. L. Laury, L. Lagardère, M. J. Schnieders, J.-P. Piquemal, P Ren, J. W. Ponder, **2018**, to appear in J. Chem. Theory Comput.
DOI: 10.10
17) Performance of the Tinker-HP Massively Parallel Molecular Dynamics Package on Intel architectures: a living review. L. H. Jolly, A. Duran, D. Guibert, J. W. Ponder, P. Y. Ren, L. Lagardère, J.-P. Piquemal, **2018,** to appear in LiveCoMS.
DOI: 10.10