

Liquid argon

Supplementary material to paper by J. Kolafa and M. Lísal:

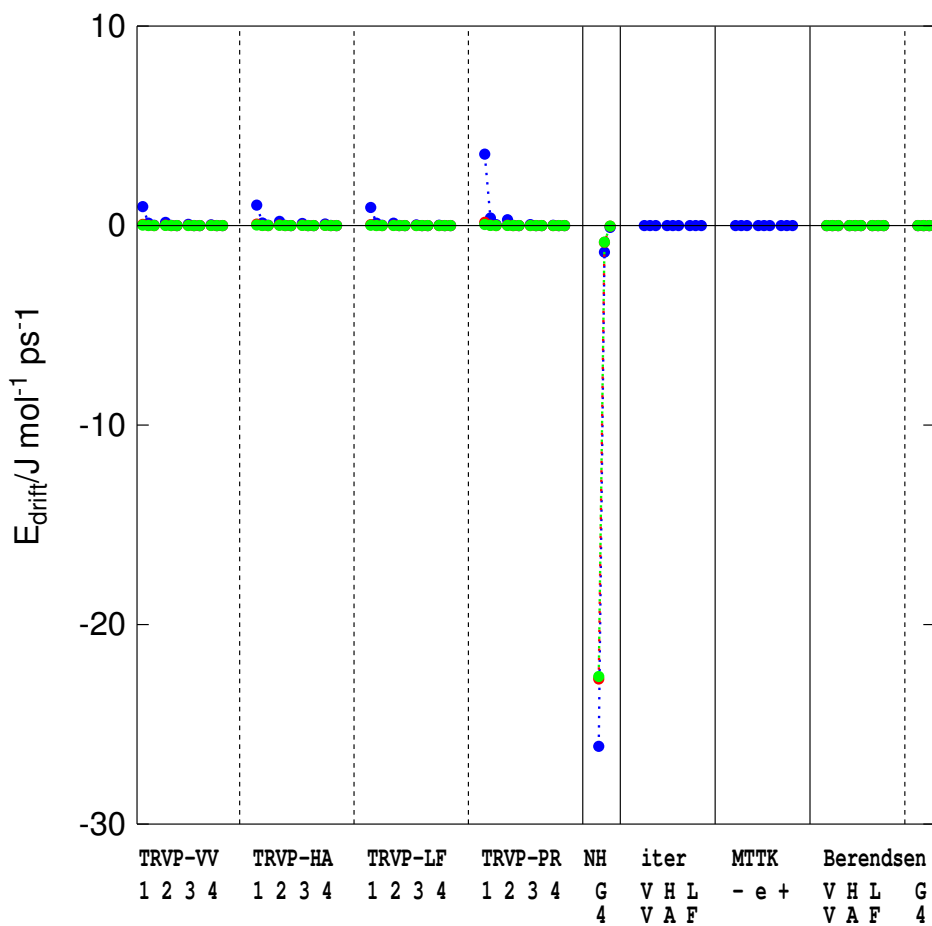
Time-reversible velocity predictor for Verlet integration with velocity-dependent right-hand side

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Drift of total energy

Drift in the total energy for liquid argon.

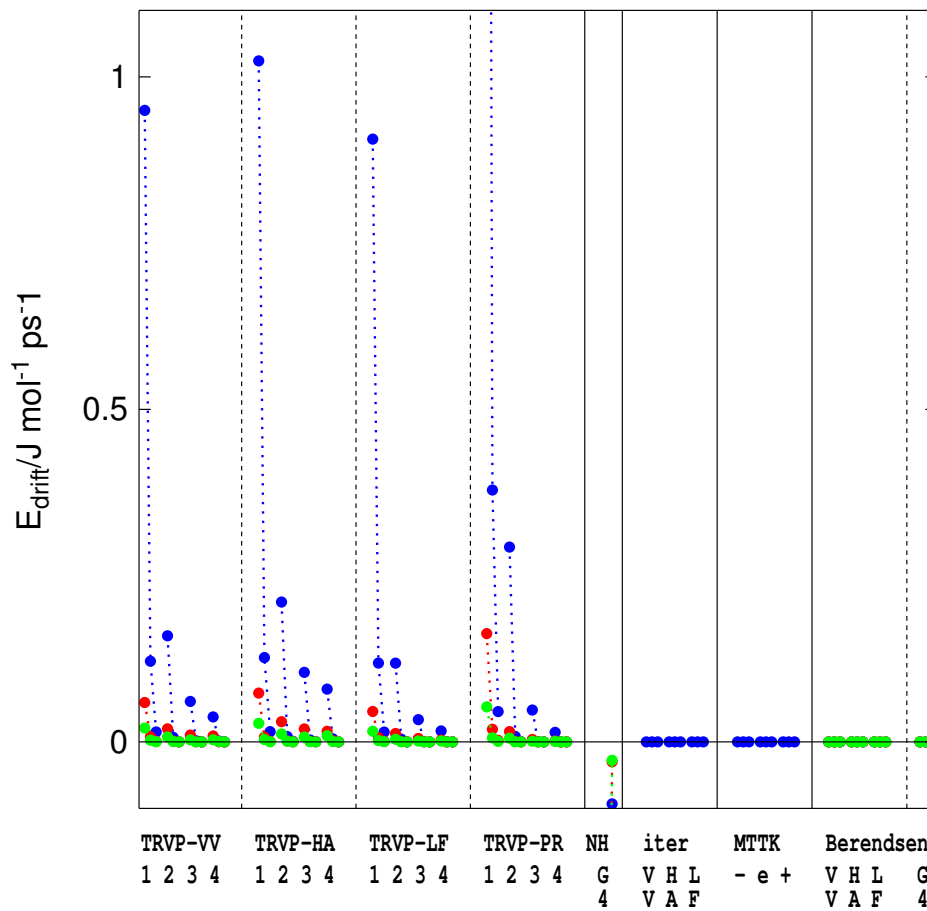
The triplets connected by dotted lines correspond (from left) to timesteps 20 fs, 10 fs, and 5 fs. Colors are: blue $\tau = 0.1$ ps, red $\tau = 0.3$ ps, green $\tau = 0.5$ ps. Label ‘TRVP’ denotes the proposed Nosé-Hoover integration with velocity predictor, the numbers below denote the value of k . Label ‘iter’ denotes the iteration method (Version 2) with the number of iterations controlled by precision. Symbols ‘VV’, ‘HA’, ‘LF’, and ‘PR’ refer to the kinetic temperature version. MTTK is the Martyna et al.¹ method and the symbol below defines function $\text{sym}()$, eqs 22–24. Label ‘G’ denotes the Gear method ($m = 4$), either with Nosé-Hoover (NH) or Berendsen thermostat.



¹G. Martyna, M. E. Tuckerman, D. J. Tobias, M. L. Klein: Explicit reversible integrators for extended systems dynamics, *Mol. Phys.* **87**

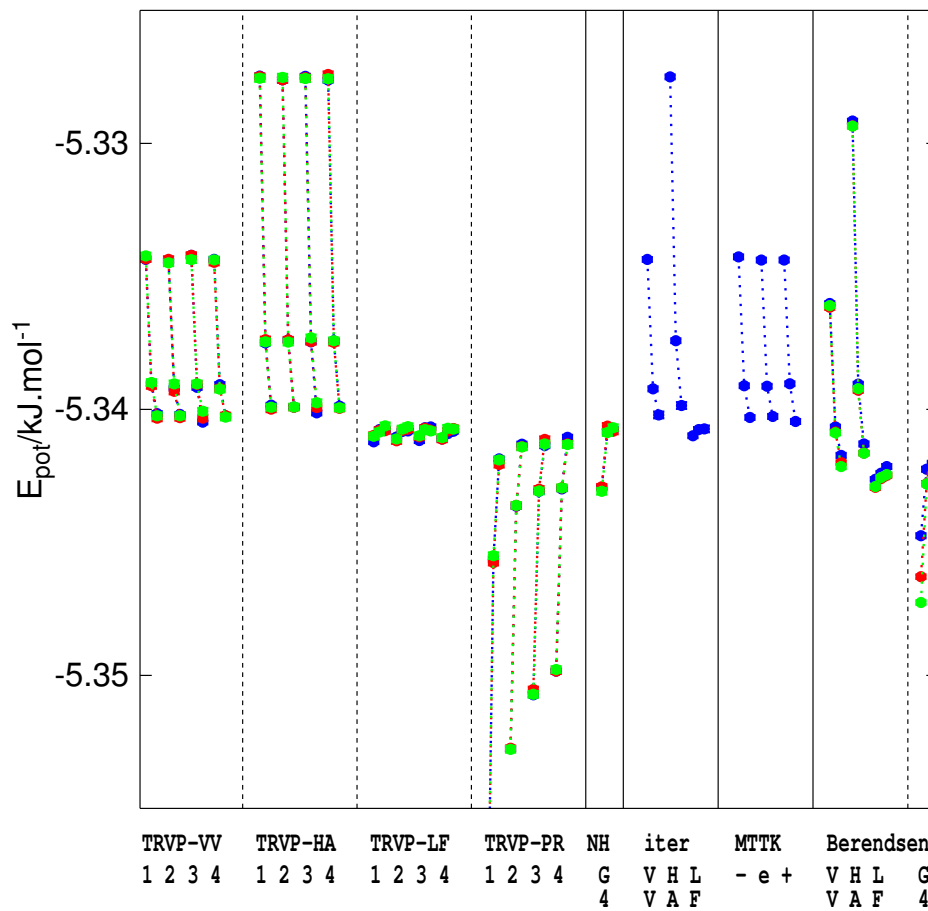
Drift of total energy

As above, enlarged.



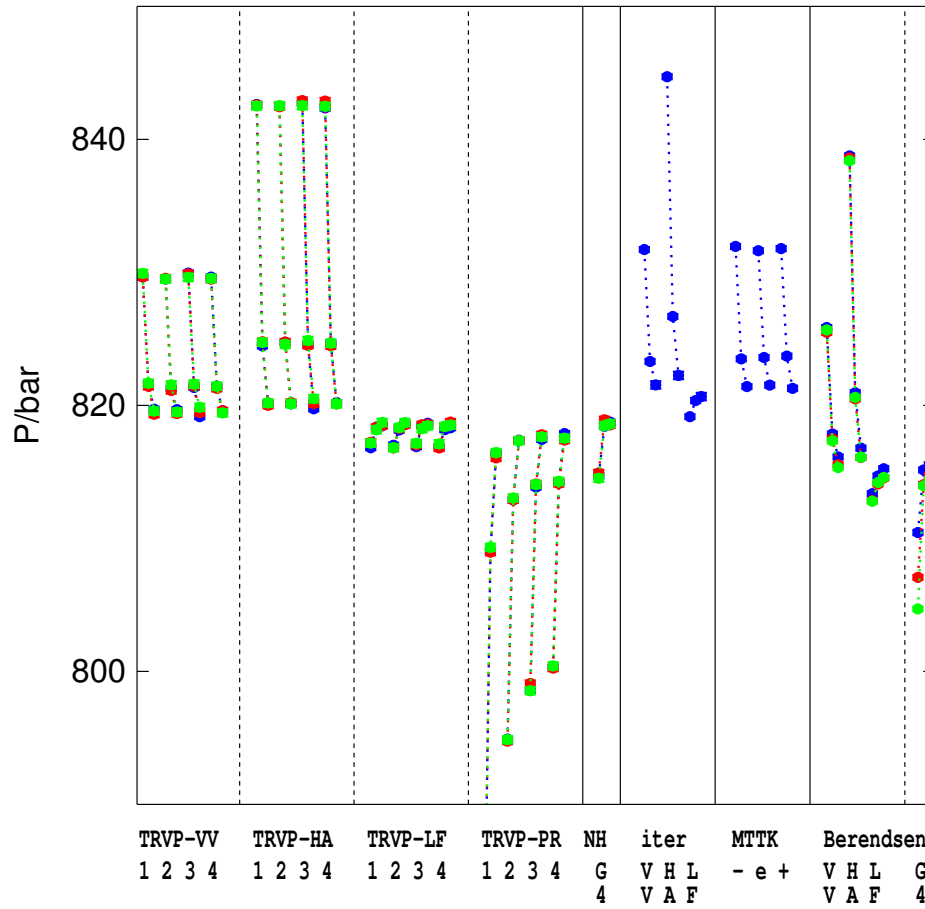
Potential energy

Averaged potential energy of liquid argon. See the first figure for symbol explanation.



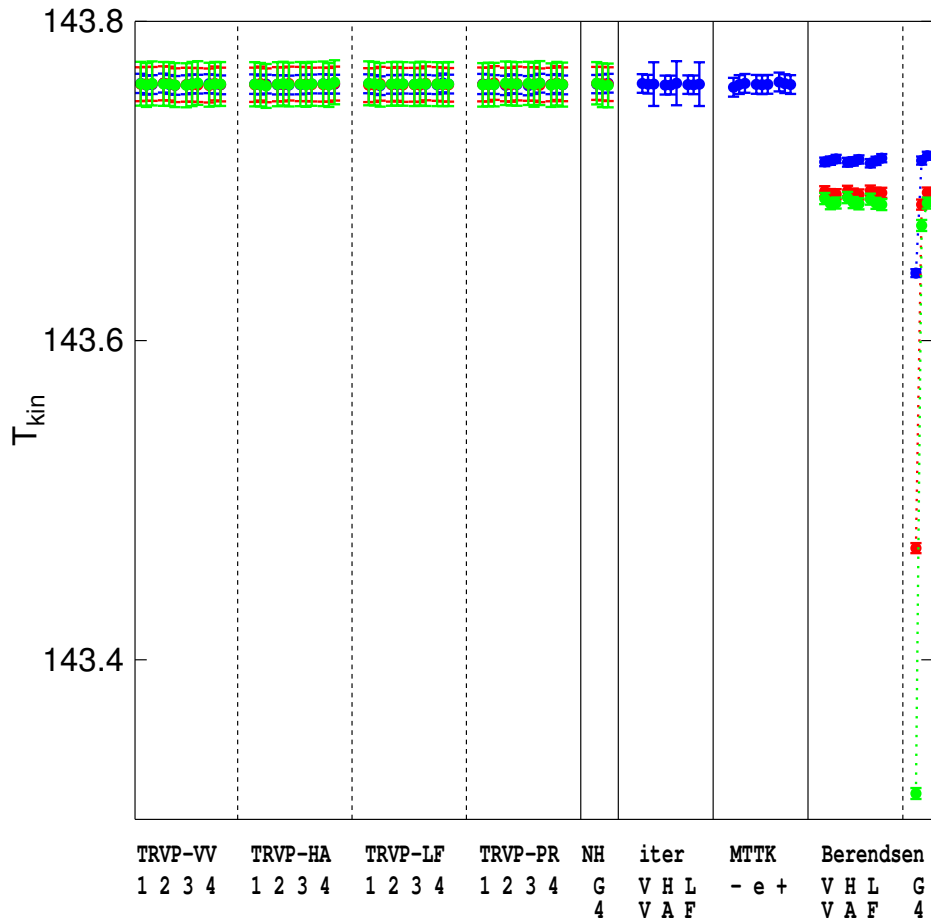
Pressure

Pressure of liquid argon. See the first figure for symbol explanation.



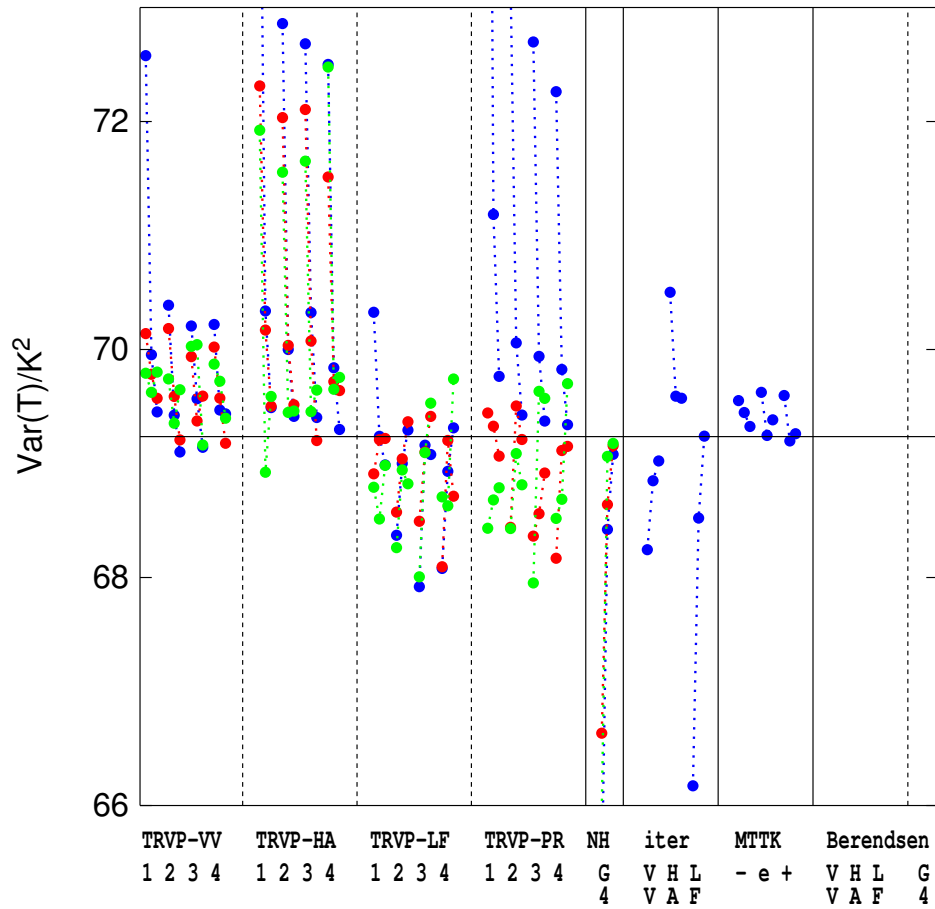
Averaged kinetic temperature

kinetic temperature of liquid argon. See the first figure for symbol explanation.



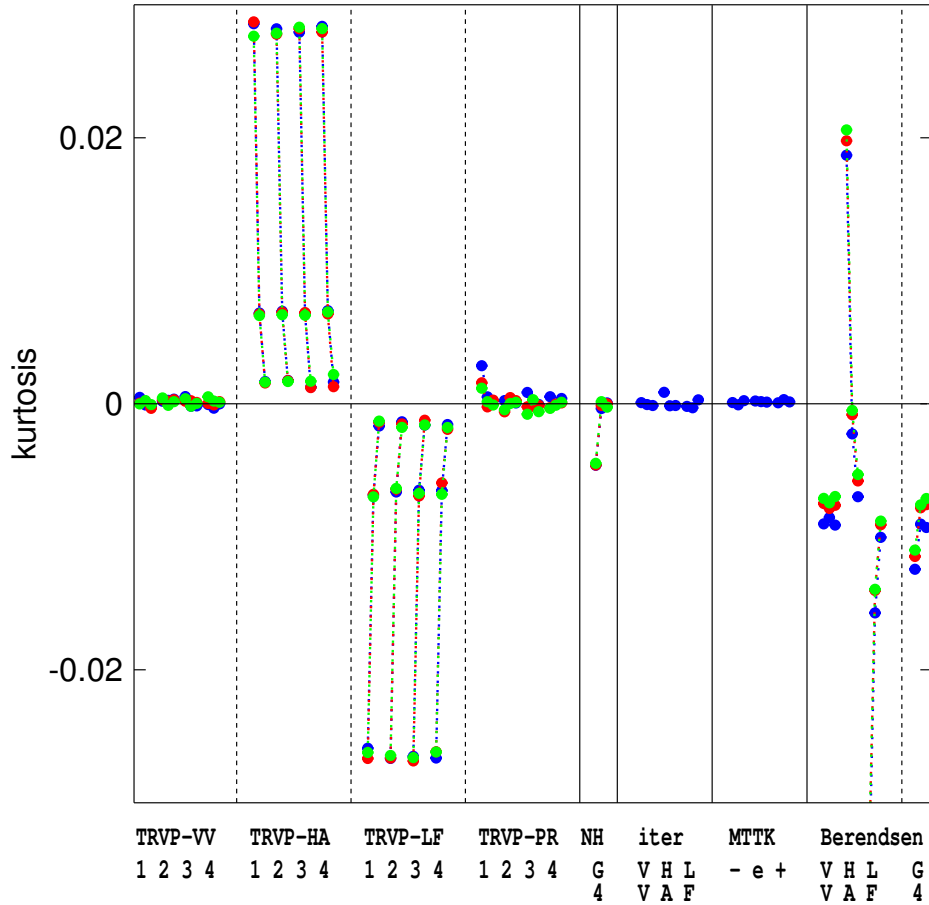
Temperature variance

Variance of the kinetic temperature of liquid argon. The horizontal line is the theoretical value. See the first figure for symbol explanation.



Kurtosis of velocity distribution

Kurtosis of the velocity distribution of liquid argon. Note that the kurtosis for the TRVP method is calculated from the “natural” velocity definition (i.e., used for the kinetic temperature) while for the iteration method and MTTK it is calculated from the VV formula $\dot{r} = [r(t+h) - r(t-h)]/(2h)$. See the first figure for symbol explanation.



Diffusivity

Diffusion coefficient of liquid argon. See the first figure for symbol explanation.

