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Conditioning and variance reduction schemes for more accurate estimation of thermodynamic and transport properties of metal alloys - Manuel Athènes

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The Monte Carlo method is a stochastic simulation approach mainly used to estimate multi-dimensional integrals. This is traditionally done by generating a Markov chain of states and then implementing an estimator. In this context, conditioning is a trick consisting in doing part of the job in closed form, through numerical quadrature, so as to reduce the statistical variance associated with the estimator. In this talk, we present several applications of this variance reduction technique in Monte Carlo simulations of condensed-matter systems. In particular, we show how to sample multi-particle systems more ergodically with the help of adaptive biasing forces and how to estimate thermodynamic quantities more accurately through conditioning and the law of total variance. We then show that conditioning can also be used to improve the measurement of linear mass transport coefficients through a law of total diffusion and by solving the first-passage problems associated with the transport problem. Illustrative applications are chosen in the field of materials science: structural transitions in metallic clusters, phase diagram of FeCr alloy, migration barriers associated with point defects in α-Iron, thermo-elasticity of tungsten with data-driven force fields and elasto-diffusion in aluminium.

Classification de Session: Result Communication