Computational Quantum Mechanics in Phase Space — An Attempt to Break the Curse of Dimensionality

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As a permanent goal and a tireless direction of computational mathematics, developing an accurate and stable high-dimensional solver has been attracting more and more attentions in recent years due to the urgent need in e.g., quantum science and high energy density physics. This talk represents our preliminary attempts to break the curse of dimensionality (CoD) which poses a fundamental obstacle to high-dimensional numerical simulations. More specifically, we will report some recent progress in both grid-based deterministic and particle-based stochastic methods for simulating high-dimensional Wigner quantum dynamics. A massively parallel solver, termed the characteristic-spectral-mixed scheme, is proposed to evolve the Wigner-Coulomb system in 6-D phase space. Within particle-based stochastic simulations, CoD, causing the unattainable exponential wall, reappears as the numerical sign problem. To this end, we propose a SPA (Stationary Phase Approximation) + SPADE (Sequential-clustering Particle Annihilation via Discrepancy Estimation) strategy is to overcome the numerical sign problem where it has been translated into a NP-hard problem that may have approximate solutions. Simulations of the proton-electron couplings in 6-D and 12-D phase space demonstrate the accuracy and the efficiency of our particle-based stochastic methods.

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