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Strongly-correlated quantum-plasma simulations via classical maps and density-functional theory - going beyond big codes CHANDRE DHARMA-WARDANA, National Research Council of Canada, Ottawa, Canada — A nominally "high-temperature" plasma may be a "cold quantum system" if the ratio $T/E_F < 1$, where T is the temperature (energy units), and E_F is the Fermi energy. The electron spin and possible ionization states Z^{i+} require multi-component simulations versatile enough for quantum, classical and thermal effects, bound states, etc., when e-e, e-ion and ion-ion interactions are not weak. In *ab initio* calculations, the densities and T (or several subsytem temperatures) are inputs. The outputs are the equation of state, transport and optical properties. Density-functional-theory (DFT) and molecular-dynamics (MD) based simulations via codes like VASP (Vienna ab-initio simulation package) treat a small number of particles in a box. These methods do not accurately implement e-e pair correlations. The particle statistics are poor for multi-component systems. The computational effort is very large and demanding. We present simpler methods using liquid structure theory, classical maps of quantum systems, and DFT to establish simple, accurate computational procedures for highly correlated multi-component systems. Such quantum calculations for jellium at $T = 0$, finite-T high density H-plasmas and Al-plasmas, are contrasted with equivalent calculations from Quantum Monte-Carlo, or VASP-based simulations.

Chandre Dharma-wardana
National Research Council of Canada, Ottawa, Canada

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