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Molecular Dynamics of Hot Dense Plasmas: New Horizons[1]

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We describe the status of a new time-dependent simulation capability for hot dense plasmas. The backbone of this multi-institutional computational and experimental effort—the Cimarron Project—is the massively parallel molecular dynamics (MD) code "ddcMD". The project's focus is material conditions such as exist in inertial confinement fusion experiments, and in many stellar interiors: high temperatures, high densities, significant electromagnetic fields, mixtures of high- and low-Z elements, and non-Maxwellian particle distributions. Of particular importance is our ability to incorporate into this classical MD code key atomic, radiative, and nuclear processes, so that their interacting effects under non-ideal plasma conditions can be investigated. This talk summarizes progress in computational methodology, discusses strengths and weaknesses of quantum statistical potentials as effective interactions for MD, explains the model used for quantum events possibly occurring in a collision and highlights some significant results obtained to date. We will also discuss a new idea called kinetic theory MD which now being explored to deal more efficiently with the very disparate dynamical timescales that arise in fusion plasmas. We discuss how this approach can be derived rigorously from the n-body quantum Wigner equation and illustrate the approach with an example.

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