Abstract Submitted
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Developing Chemistry and Kinetic Modeling Tools for Low-Temperature Plasma Simulations[1] THOMAS JENKINS, KRIS BECKWITH, BRADLEY DAVIDSON, SCOTT KRUGER, ALEXEI PANKIN, CHRISTINE ROARK, PETER STOLTZ, Tech-X Corporation — We discuss the use of proper orthogonal decomposition (POD) methods [del-Castillo-Negrete et al., PoP **15**, 092308 (2008)] in VSim, a FDTD plasma simulation code capable of both PIC/MCC and fluid modeling. POD methods efficiently generate smooth representations of noisy self-consistent or test-particle PIC data, and are thus advantageous in computing macroscopic fluid quantities from large PIC datasets (e.g. for particle-based closure computations) and in constructing optimal visual representations of the underlying physics. They may also confer performance advantages for massively parallel simulations, due to the significant reduction in dataset sizes conferred by truncated singular-value decompositions of the PIC data. We also demonstrate how complex LTP chemistry scenarios can be modeled in VSim via an interface with MUNCHKIN, a developing standalone python/C++/SQL code that identifies reaction paths for given input species, solves 1D rate equations for the time-dependent chemical evolution of the system, and generates corresponding VSim input blocks with appropriate cross-sections/reaction rates. MUNCHKIN also computes reaction rates from user-specified distribution functions, and conducts principal path analyses to reduce the number of simulated chemical reactions.

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