Abstract Submitted
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Mullti-scale Methods for Plasma Chemistry DAVIDE CURRELI, University of Illinois - Urbana Champaign — One of the key steps in modeling chemically-reactive plasmas is the construction of a reaction network and the determination of the reaction rates for each reaction participating to the network. This piece of information is in general difficult to construct or obtain, but is a fundamental link between the microscopic physics of atomic/molecular collisions, and the macroscopic transport of plasma species. In this talk we review some of the fundamental computational approaches for the construction of a reaction network and the determination of the corresponding reaction rates. We review different approaches and software for the determination of the thermo-chemistry and plasma-chemistry branches, including both commercial packages at a mature stage of development (eg: ChemKin, Quantemol, etc.) and open-source tools widely available to the community at several stages of development (eg: ZDPlasKin, Crane, etc.). We include in the talk mini-tutorials which can serve as training exercises. Examples include not only well-known systems such as noble gases and O2/N2, but also more complex reaction networks recently tackled, such as the uranium/oxygen system, and their inclusion into macroscopic transport solvers, such as COMSOL and the new MOOSE-based plasma application ZAPDOS-CRANE.

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