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Towards multiscale modeling of non-LTE conditions: validation of microscopic models

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Multiscale modeling of matter away from local thermodynamic equilibrium (i.e., non-LTE conditions) requires the tabulation of material properties over not just temperature, pressure, and density - but the state of the ambient radiation field, as well. This compounds the typical computational demands of using multi-atom first principles models to create such tables by introducing yet another (high-dimensional) independent state variable and imposing conditions that test the limits of the attendant theories. To confront the problem of multiscale non-LTE simulation, it is thus essential to validate average-atom models with moderate fidelity and high computational efficiency against high-fidelity multi-atom models with vastly less computational efficiency. I will describe work that we have been doing to validate and improve average atom models against multi-atom models based on real-time time-dependent density functional theory, in this context. I will primarily focus on comparisons made between the two in the context of stopping power and dynamic structure factor calculations, but I will give secondary focus to ongoing work aimed at understanding more fundamental quantities (namely collision rates) that might be a better point of comparison. This work was supported by SNL's LDRD program, project number 222396. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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