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MIXKIP/RAPCAL: A Computational Package for Integrated Simulations of Large-Scale Atomic Kinetics and Radiation Transport in Non-Local Thermodynamic Equilibrium Plasmas

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Abstract. In many of the plasmas generated in many fields of the high energy density physics, the radiation can significantly alter the material response. A proper microscopic description of these plasmas entails integrated computer codes that self-consistently combines large-scale atomic kinetics and radiation transport. Due to the inherent complexity of this type of codes and its interest in the area of high energy density physics, new developments in this field are welcomed. In this work, we present MIXKIP/RAPCAL, an integrated computational package to perform 1D and 2D large-scale non-local thermodynamic equilibrium atomic kinetics and radiation transfer coupled simulations for high energy density plasmas. This package includes different modules that allow simulations of non-equilibrium plasmas under different degrees of detail and accuracy, depending on the requirements of the situations to analyze. Comparisons with experimental results of homogeneous optically thick plasmas of gold and xenon are presented in order to check its accuracy. The influence of different approaches of the spatial discretization of the plasma in the radiation dependent atomic kinetics simulations is also analyzed. Finally, this study is also made for a non-homogeneous optically thick aluminum plasma.

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Key words: Radiative transfer equation, large scale plasma kinetics simulations, self-consistent simulations.

1 Introduction

In many of the plasmas generated in many fields of the high energy density physics (HEDP), such as nuclear fusion, astrophysics or X-ray sources, the radiation plays a piv-

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otal role in their dynamics and energetics [1]. Therefore, in modeling these plasmas, it is essential to perform accurate and realistic simulations of the electronic states populations, radiative properties and radiation transport.

Most of these plasmas are in non-local thermodynamic equilibrium (NLTE) and, in this case, the atomic level populations must be determined using a set of coupled rate equations in the called collisional-radiative (CR) models [2], which include the transition rates among the atomic levels due to the collisions with electrons and photons. Therefore, all CR methods require atomic data to compute the level populations [3], being a crucial issue the selection of the atomic levels to be included. Since the achievement of the atomic state-space completeness is difficult or even impossible [4], the choice of the state space must be done carefully. Hence, for example, when the plasma is under the influence of high intense radiation fields, atomic configurations with inner shells open must be included. On the other hand, the number of double and single configurations could be limited for plasmas at intermediate densities, that are ruled by collisions with thermal electrons [4]. The number of levels to include can reach 10^6, which implies large-scale computational methods, and this fact conditions another important aspect in the CR models which is the degree of detail in the atomic description. For low- and intermediate-Z plasmas, detailed atomic descriptions such as detailed level or term accounting models can be used, including large degrees of configuration interaction. However, as the number of atomic levels increases exponentially with the complexity of the atom, for high-Z plasmas those detailed descriptions become sometimes intractable and, in this case, statistical approaches, such as the detailed configuration account (DCA) or superconfiguration account approaches (based on grouping detailed levels into configurations or superconfigurations, combined the unresolved transition array (UTA) [6] and supertransition arrays [7] formalisms, respectively, to group detailed transition lines), have been shown to be useful. However, for spectroscopic purposes, these statistical methods may lack the accuracy needed to describe isolated lines or transitions and, for this reason, hybrid methods that mix detailed and statistical descriptions have been developed [8,9]. In any case, the answers to the questions of which states and transitions should be included in an atomic model and what degree of averaging must be used are not obvious, even for a particular application in which the constrains are given [5].

The relevance of the NLTE kinetics and spectral calculations in the fields of astrophysics and HEDP has led to the development of many computational NLTE kinetics codes [1, 9–18]. The inherent complexity of the problem has led to the holding of a series of code comparison workshops for the purpose of validating and verifying these codes [19–26]. The problem becomes even more complex for optically thick plasmas. In this situation, radiation induced processes must be included in the CR model, being their rates calculated through integrals over the radiation field itself. On the other hand, the specific intensity in the plasma is commonly obtained from solving the radiative transfer equation (RTE), where the opacity and the emissivity are key quantities which, in turn, depend on the plasma level populations. Therefore, accurate modeling of optically thick plasmas entails a CR model coupled to the RTE, with photon escape an non-local zone-