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The ODALISC Project:
Accurate atomic data for complex radiation-hydrodynamics simulations.

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1. Introduction

Complex simulations are central in a growing number of scientific fields such as astrophysics, laboratory astrophysics or inertial fusion science. Simulation codes incorporate sophisticated physical models (including hydrodynamics, radiative transfert, conduction, etc..). These codes need to be fed with atomic data in order to make predictions realistic as compared to experiments or observations. The reliabilty of these predictions is strongly correlated to the quality/completeness of the atomic data used. In order to fully understand many physical phenomena such as the solar evolution, supernovae explosions, radiative shocks or the interpretation of laser experiments, accurate atomic data, and in particular opacities, are required. However, providing these data is not enough. It is necessary to be able to qualify them, quantify the uncertainties attached so one can propagate them into the simulations. It is also necessary to develop diagnostic tools to allow users/producers to choose/analyze the data they need/provide.

To try and fullfil this task, the SINERGHY project (P.I. E. Audit) is developing a database (ODALISC) of spectral and mean opacities for a large range of physical conditions, covering a broad ensemble of elements of astrophysical and experimental interest. Several groups of atomic physicists are involved in providing the data using different methods. This will allow us to compare them, define some relative uncertainties associated to the data and determine the ρ-T regimes that best suit each method. Specialists of simulations are involved in estimating the influence of atomic data uncertainties on the models and to define the need of the users. Experimentalists are developing critical experiments to estimate the precision of the theoretical results. In order to allow the data to be tested and validated by a large part of the scientific community and to optimize the effort of atomic physicists, all the results will be made freely available on the ODALISC database (http://irfu.cea.fr/Projets/COAST/odalisc.htm)

2. Atomic data and opacities

The calculation of opacities depends on two principal steps. The description of the state of the medium and the definition of the atomic processes between the photons and the atoms/ions/electrons present in the medium. The first step determines the populations, and the second step, the extinction coefficients of the different processes involved. Detailed comparaisons will allow to test both of these steps.

In this preliminary work we have used opacity tables generated by two different codes. Both are based on the average atom model. The first one, GOMME [1] is a screened-hydrogenic average atom model without l-splitting [2,3]. It is simple and allows quick calculations. The second, POTREC [4], is based on the average atom model including the splitting in l allowing $\Delta n=0$ transitions to be accounted for. In figure 1 we have represented the results for the two model (black curves for GOMME and red for POTREC). We clearly see the effect of the different levels of sophistication of the two models on the spectral and mean opacities shown in figure 1. The details of the comparison will be presented elsewhere (ODALISC collaboration, in preparation).

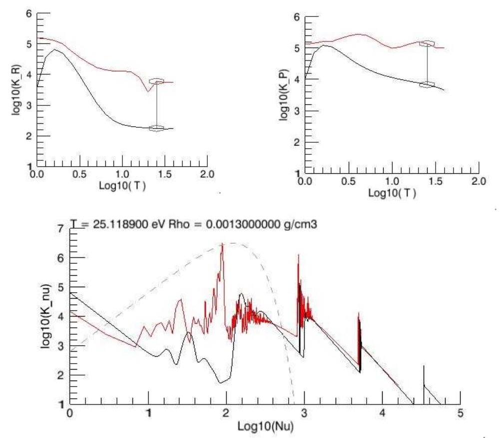

Figure 1: Rosseland (top left) and Planck (top right) mean opacities as a function of T for ρ=1.3 10^{-3} obtained with the codes GOMME (black) and POTREC (red). On the bottom panel the spectral opacities for a given ρ-T corresponding to the point shown on the top panels curves are represented.

3. Simulations – radiative shock in Xe gas

To illustrate the strong influence of opacities on dynamical processes, we have studied the propagation of a radiative shock in xenon using two sets of opacities. We present in figure 2, the density, temperature and opacity profiles for a shock travelling at 30 km/s in low density

Xe (ρ=1.1 10^{-3} g/cm^3). The profiles are obtained 5 ns after the shock was launched. Similar shocks have been obtained experimentally by different teams [5,6,7]. Several quantities such

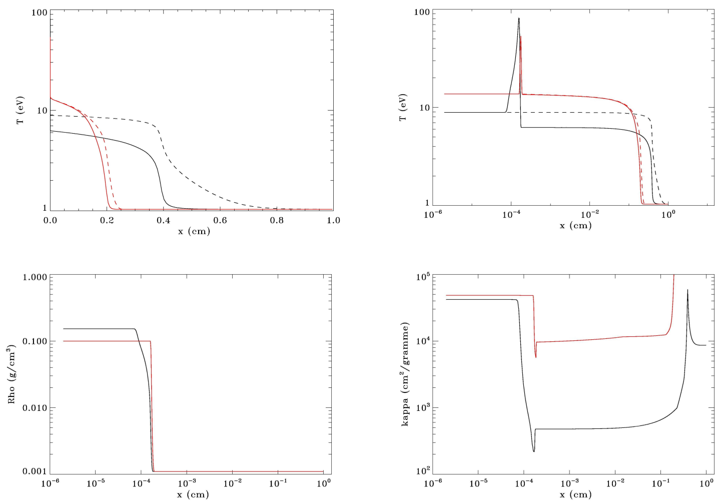

Figure 2: ρ, T, κ profiles for a shock in low density Xenon gas. In black are the results for opacities obtained with a simple model (code: GOMME) and in red are the results for more sophisticated opacities (code: POTREC)

as the velocity of the shock and of the radiative precursor, the temperature or the electronic density have been measured in these experiments. The black curves in figure 2 were obtained using opacities calculated with GOMME while for the red curve using opacities generated with POTREC. The shock velocity depends mainly on our boundary condition (or on the driving in real experiments) and therefore is not very sensitive to the opacity. But, as can be seen on figure 2, the precursor extension (and velocity) is greatly affected by the opacity. The precursor velocity obtained using GOMME opacities is almost twice the value obtained with POTREC. The temperature and shock compression also show some significant differences. Even for this simple comparaison using only two opacity models, the differences we observe are larger than the experimental uncertainties.

4. Conclusion and perspectives.

We have shown how the differences in the opacities influence simulations in the case of a shock in xenon. Other tests of the impact of uncertainties in opacities on other applications (stellar modelling) have been published [8,9]. It is becoming crucial to define precisely the uncertainties attached to atomic data and opacities in order to properly propagate them into applications and estimate the errors they are producing in simulation predictions. To quantify the uncertainties in the opacity data, we have organized a team of atomic physicists dedicated to the production and comparison of the atomic data using different methods. At every steps, we compare and interpret the differences in the results. We are analysing the reasons as well as the effects of the differences in the ionic fractions, in the configurations expansion and interaction, of the coupling schemes (LS versus LSJ) on the opacity results.

We are presently working on detailed opacity calculations of Xe at two ρ-T points. They will be also compared to the results from GOMME and POTREC as well as the different detailed methods. From these comparisons an estimate of the relative differences will be determined. We are also producing tables on a ρ-T grid typical of radiative shocks to extend the present work and derive more precisely the effect of the propagation of uncertainties.

We are planning studies of other elements (O, Ar, Fe, Kr) to probe the behavior of the different methods through the periodic table. This will allow us to determine the domain of validity of the different methods and the necessity of an intermediate one for the transition from light to heavy species. An experimental program on several large laser facilities (LULI, PALS, LIL,...) is in progress for the coming years. This will provide a powerful diagnostic for the different theoretical results and the determination of an "absolute" scale for uncertainties on the opacity data.

The strength of the ODALISC project, is in the close collaboration between atomic physicists, expermentalists and specialists of simulations. This will allow us to provide a large set of data and to strongly constrain their quality to answer the request of an important part of the scientific community.

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