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Modeling stellar atmospheres with PHOENIX

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ABSTRACT

We will present an overview of the general-purpose stellar and planetary atmosphere code PHOENIX. With PHOENIX one can calculate model atmospheres and spectra of stars all across the HR-diagram including main sequence stars, giants, white dwarfs, stars with winds, TTauri stars, novae, supernovae, brown dwarfs and extrasolar giant planets. To be able to compute models of such different types of astrophysical objects many different types of physical processes need to be included in model atmosphere codes like PHOENIX.

Most of the work with PHOENIX has been done by assuming the model atmospheres of the astrophysical objects to be one dimensional. Recent progress in computer science now allows for the development of a 3D stellar and planetary atmosphere code. We will present the recent achievements in the development of our 3D radiative transfer framework. We are able to solve the radiative transfer for given atmospheric structures of a stellar or planetary object in different geometries like Cartesian, spherical and cylindrical coordinate systems. We will also present the most recent extension of a time-dependent treatment of the radiative transfer equation in detail.

Keywords: computational physics and chemistry, radiative transfer, numerical methods.

1 INTRODUCTION

To understand and study observations of stars and other stellar like objects it is necessary to model the atmospheres of these objects and compare the calculated model spectra with observations. By changing the parameters of the model, the goal is to find the best fit to the observations to determine the detailed properties of the observed star. With this procedure it is possible to determine the effective temperatures, luminosities, masses and radii of the observed objects. Additionally, one might be able to determine the metallicity or even more exact abundances of different types of stellar-like objects.

To be able to obtain very good theoretical spectra it is absolutely necessary to include as much physical processes as possible into the stellar model atmosphere code. For different types of objects, the radiative transfer problem needs to be addressed always. The PHOENIX code solves the 1D radiative transfer equation including scattering. Further included is an equation of state and large lists of atomic and molecular lines. It is also possible to include certain species of elements for non-LTE computations. Many other physical processes have been implemented to address the special properties of the atmosphere of the many different types of objects PHOENIX can model. Recently, it is also possible to perform time-dependent computations with the PHOENIX code.

We will discuss in some detail all the important parts of the PHOENIX code and present some applications. In a further

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section, we present the newest implementation in our 3D radiative transfer framework of PHOENIX/3D. The extension of time dependence in the solution of the 3D radiative transfer equation is presented in a further section.

2 MODELING STELLAR ATMOSPHERES WITH PHOENIX

With now over 20 years of development of our stellar and planetary atmosphere code PHOENIX [1], today many different astrophysical objects with very different physical properties can be modeled with PHOENIX. However, for all these different model atmospheres, the radiative transfer problem needs to be solved for any type of stellar-like atmosphere. PHOENIX solves the 1D spherical symmetric radiative transfer equation for expanding atmospheres including the treatment of special relativity [3]. The opacities are sampled dynamically and include about 80 million atomic lines and billions of molecular lines. The atomic line list contains all lines from the Kurucz Database. Many different databases for molecular lines (e.g. HITRAN) are included in the molecular line list, and each one can be selected when needed for the computation. Since the opacities are calculated dynamically for each wavelength point when required, line blanketing is included by design. All important background opacities are also included. The atmosphere structures are iterated to obtain a stable atmosphere that is in radiative equilibrium [2].

The equation of state (EOS) includes a large number of atoms, ions, molecules and grains. It works in a large temperature range even down to low temperatures, which can be found in planetary atmospheres. PHOENIX allows for multilevel non-LTE calculations for atoms with a total of more than 10,000 levels and 100,000 primary lines [4]. To construct the model atoms, we take only lines with a $\log(gf) \leq 3$ from Kurucz Atomic Linelist and ignore all predicted lines. All the remaining levels and lines are considered for the full non-LTE calculations. It is posible to select only certain elements and ionization stages. Recently, a time-dependent treatment of the rate equation has been included and applied in the calculations of type II supernovae spectra [5]. The treatment of depth dependent Voigt profiles for Stark and van der Waals broadening is available. The treatment of special line profiles like the broad Na I D line, which are observed in cool atmospheres, are also included [6, 7]. The resulting theoretical spectra can be calculated for any desired high resolution.

Recently, time dependence has been included into PHOENIX with the goal to compute the light curve of type Ia supernovae. PHOENIX can solve the time-dependent radiative transfer equation [8]. A simple hydrodynamical solver, which keeps track of the energy conservation, has been implemented to compute the evolution of the expanding envelope of a type Ia supernova explosion. We were able to compute light curves of type Ia supernovae in both the optical [9, 11] and near-infrared [10] wavelength range.

3 3D RT FRAMEWORK

On the way to a fully 3D model atmosphere code, we have developed a 3D radiative transfer framework [12, 13, 14, 15, 16, 17, 18, 19, 20]. In the 3D radiative transfer framework, the model atmosphere is divided into volume elements (voxels) which have constant properties as, for instance, temperatures, and opacities. The radiative transfer equation is then solved by following characteristics that are going through the whole voxel grid under different angles. The treatment of scattering is included as well as the treatment of line transfer [13]. The radiative transfer problem can be solved in different geometries like Cartesian, spherical and cylindrical coordinate systems and also with different boundary conditions [14, 15]. This allows to compute spherical stars, disks, or a detailed model of a part of a stellar surface in the appropriate coordinate systems. To treat rapidly expanding atmospheres like in supernovae, we extended the solution of the radiative transfer to include velocity fields like in homologous flows [16]. Additionally, the treatment of arbitrary velocity fields in the Eulerian frame has also recently been implemented [18]. This allows for a treatment of a slow velocity fields in stellar atmospheres like, for example, in stellar convection models. It is also important for the modeling of planetary atmospheres.

The 3D radiative transfer framework can so far only solve the radiative transfer problem for a given atmosphere structure. First applications of PHOENIX/3D have been calculated to solve the radiative transfer of given hydrodynamical structures of different types of stars or planets [17]. To have a full 3D model atmosphere code it is necessary to include time dependence into the 3D radiative framework to be able to iterate for atmospheres that are in radiative equilibrium. As a first step, the time dependence of the radiative transfer has already been included [20] and will be presented in detail in the following section.

4 TIME DEPENDENCE IN THE 3D RT FRAMEWORK

The newest development of the 3D radiative transfer framework is the introduction of time dependence into the radiative transfer equation [20]. We will briefly discuss the method used to solve the time-dependent radiative transfer equation and present some of the calculations that have been performed to test the extension. See [20] for a more detailed description and presentation of the time dependence implementation of our 3D radiative transfer framework.

To include the time dependence we use the radiative transfer equation in a flat space time in the comoving frame as described in [21]. In an earlier paper, the description of the $\partial I/\partial\lambda$-discretization for homologous velocity fields has already been presented [16]. We used this discretization method and extended it to include the $\partial I/\partial t$ time dependence in the solution of the radiative transfer. Along a characteristic the time dependent 3D radiative transfer equation is a modification of Eq. (15) in [16] and given by

$$\begin{aligned}\frac{\partial I_{\lambda,t}}{\partial s} + a(s)\frac{\partial}{\partial\lambda}(\lambda I_{\lambda,t}) + a(t)\frac{\partial}{\partial t}I_{\lambda,t} + 4a(s)I_{\lambda,t} \\ = -\chi_\lambda f(s)I_{\lambda,t} + \eta_\lambda f(s),\end{aligned} \tag{1}$$

where the new factor $a(t)$ is simply

$$a(t) = \frac{1}{c}. \tag{2}$$

The inclusion of time dependence leads to a modification of the effective optical depth length in [16] and is now defined by

$$\begin{aligned}d\tau = -\left(\chi_\lambda f(s) + 4a(s) + \frac{a(s)\lambda_l}{\lambda_l - \lambda_{l-1}} + \frac{a(t)}{\Delta t}\right) ds \\ \equiv -\hat{\chi}\, ds.\end{aligned} \tag{3}$$

Additionally, the source function is modified and now defined by

$$\begin{aligned}\frac{dI_\lambda}{d\tau} = I_\lambda \\ +\frac{\chi_\lambda}{\hat{\chi}_\lambda}\left(S_\lambda f(s) + \frac{a(s)}{\chi_\lambda}\frac{\lambda_{l-1}I_{\lambda_{l-1}}}{\lambda_l - \lambda_{l-1}} + \frac{a(t)}{\chi_\lambda}\frac{1}{\Delta t}I_{t-1}\right)\end{aligned} \tag{4}$$

$$\equiv I_\lambda - \hat{S}_\lambda. \tag{5}$$

The discretization of the $\partial I/\partial t$ term modifies the generalized optical depth and adds an additional term to the generalized source function. This approach to include time dependence in the 3D RT framework is similar to the first discretization method for the 1D case as described in [8].

To test the new extension, we first performed a test calculation with an atmosphere that is constant in time. All test calculations have been performed with the spherical coordinate system of our 3D RT framework. Since there are no time-dependent variations in the atmosphere, the mean intensities in every voxel should be constant in time. This test showed that we needed to introduce a new method of saving the intensities of the last time step and also a more accurate way of including these old intensities in the computations of the solution of the next time step. Using this new subvoxel method, we obtained an atmosphere where the intensities are as expected constant in time. We also showed that it is important to have a very high resolution in the radial direction to minimize the error in the mean intensities of the outer layers. In this spherical symmetric test case, a high resolution in θ and ϕ is not important.

Another test was to compare the results of our new extension with an atmosphere in spherical symmetry with our well tested 1D time-dependent spherically symmetric code [8]. For this test, we placed a light bulb at the center of our test atmosphere. This light bulb represents an additional inner boundary condition. This light bulb is then switched on to cause a change of the inner boundary condition, meaning that radiation is now entering at the inner boundary. This perturbation then moves through the atmosphere and reaches after a certain time the outermost voxels. This light bulb is a good way of introducing time dependence into a constant atmosphere. It also allows to follow these time-dependent perturbations on the way through the atmosphere.

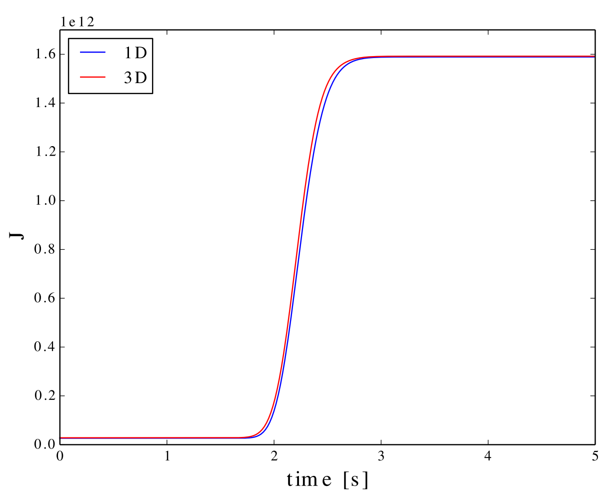

Figure 1 – The mean intensity of the outermost radius versus time computed with 3D and 1D time dependent radiative transfer.

The mean intensities of one outermost voxel versus time are shown in Figure 1. It takes about 2 s until the perturbation of the inner boundary reaches the outermost voxels. For this test we put a 1D spherically symmetric atmosphere structure into the 3D radiative transfer framework. We solved the same atmosphere also with our well test 1D code. It can be clearly seen that there are only very small differences between the 1D and 3D RT time-dependent calculations. This indicates that the 3D implementation works as expected.

To further test the extension of time-dependence, we performed some tests with a time-dependent inner boundary condition. We let the light bulb, which we had placed at the center of the test atmosphere, vary sinusoidally in time. This leads to an atmosphere where the mean intensity should vary sinusoidally everywhere.

In Figure 2, the resulting mean intensities for different radii are plotted versus time. It again takes about 2 s before the perturbation has moved outwards to affect the outermost layers. The sinusoidally varying mean intensity is then observed in every layer. The phase shift between the inner and outer radii is approximately π, which is about 2 s in time.

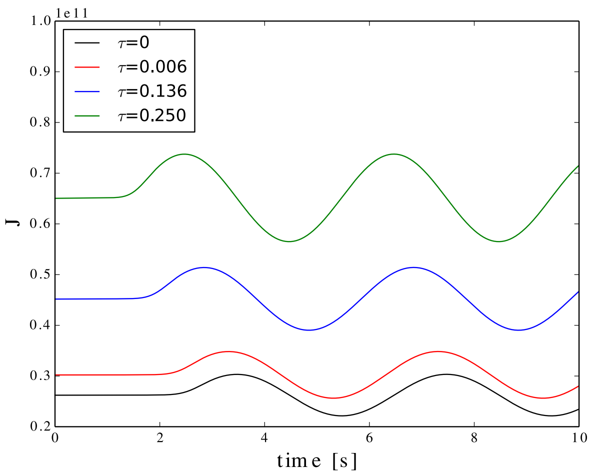

Figure 2 – The mean intensity at different optical depths, τ, with a sinusoidally varying light bulb at the center of the sphere.

All comparisons with our well-tested 1D spherically symmetric code show that the results of the test models for our implemented time-dependent 3D radiative transfer framework are in good agreement. We now want to verify that our 3D time dependent extension also works for test cases of a fully 3D test model atmosphere. To check that, we placed a Gaussian perturbation of the temperature and, therefore, the local source function at an off-center position in the sphere. For the first time step, the time-independent model without the perturbation is solved. After the first time step, the perturbation is introduced and remains constant for the rest of the calculation. Unfortunately, we cannot compare these results to our 1D code, but we can discuss whether the results are reasonable.

Figure 3 shows a plot of the intensity J at a ring of outermost voxels. As expected, the voxels closer to the perturbation have a higher mean intensity J. It is also clear that it takes more time for the radiation to reach voxels that are farther away from the perturbation. All these performed test calculations indicate that the extension is working correctly.

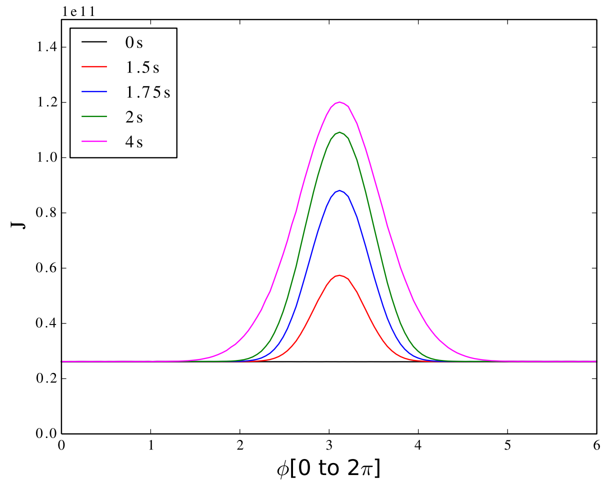

Figure 3 – The mean intensity, J, at a ring of outermost voxels ($\theta = 0$) at different times for a test case with an off-center perturbation.

5 CONCLUSIONS

We presented a brief description of the state-of-the-art stellar and planetary atmosphere code PHOENIX. It is possible to model many different types of stellar and stellar-like atmospheres with PHOENIX. The resulting theoretical spectra can be used to determine properties of stars by comparing them to observations. We further presented the recent progress in developing a 3D radiative transfer framework. We implemented time dependence into the radiative transfer equation and tested the extension with some test calculations. All tests indicate that the new implementations work as intended. For the future, further work needs to be done to achieve a full 3D model atmosphere code.

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