Shellspec39 - a tool for modelling the spectra, light curves, and images of interacting binaries and exoplanets

Budaj Ján,\textsuperscript{1}
\textsuperscript{1}Astronomical Institute, Slovak Academy of Sciences, Tatranská Lomnica,
Slovak Republic; budaj@ta3.sk

Abstract. Program SHELLSPEC is designed to calculate light curves, spectra, and images of interacting binaries and extra-solar planets immersed in a moving gaseous or dusty circumstellar matter. It solves simple radiative transfer along the line of sight in 3D moving media. The Roche model and synthetic spectra from the stellar atmosphere models such as TLUSTY from Ivan Hubeny can be used as a boundary condition for the radiative transfer. The latest publicly available version is Shellspec39. The code has been combined with other methods such as Doppler tomography and interferometry and used to analyze spectroscopic, photometric, and interferometric observations of binary stars and transiting exoplanets. A few examples are briefly mentioned.

1. Introduction

A significant fraction of stars are single and have the spherical shape. The light we detect originates from their atmospheres. There are sophisticated computer codes which calculate models of the atmospheres such as TLUSTY (Hubeny 1988; Hubeny & Lanz 1995) and spectra emerging from such models such as SYNSPEC (Hubeny & Lanz 2017). However, many stars are in binary systems and many of them form close systems which triggers a mutual interaction between the components. As a result the shape of the objects departs from the sphere and acquires the Roche shape. Impinging irradiation heats the adjacent faces of the stars (planets) as well as is scattered or reflected off the surfaces. Mass can be transferred between the components or can escape from the system forming plethora of accretion structures (streams, discs, jets, shells,...). These may give rise to various emission and absorption lines with complicated profiles. These lines carry the information about the velocity field and state quantities such as temperatures and densities. To analyze such information 3D radiative transfer codes are being developed (Ibgui et al. 2013). Such modelling is very complicated and demanding on the computer time and memory. A certain simplification may be very useful, especially when one wants to solve the inverse problem of finding some optimal properties of the model. That usually requires fitting of large volumes of observed data involving frequent on-fly recalculation of the models.

With this in mind we developed a program called SHELLSPEC. It might be used to calculate light curves, spectra, and images of interacting binaries and extra-solar planets immersed in a moving gaseous or dusty circumstellar matter (CM). It solves simple radiative transfer along the line of sight in 3D moving media. The Roche model and synthetic spectra from the stellar atmosphere models such as TLUSTY can be used
as a boundary condition for the radiative transfer. The scattered light from the two stars can be taken into account assuming that CM is optically thin. Scattering is non-isotropic and described by the proper phase function which may be crucial especially in the case of Mie scattering on large dust grains. The other assumptions include LTE and optional known state quantities and velocity fields in 3D. These can be taken e.g. from the 3D hydrodynamic simulations. Alternatively, a 3D model can be composed of a number of predefined (non)transparent objects such as: a central star, companion star, envelope, spot, stream, ring, disc, nebula, flow, jet, ufo, or a shell which are described below.

At present, still a limited number of opacities in CM are taken into account: line opacity with the natural, Stark, and Van der Waals broadening, an additional extra true absorption opacity in the form of a table or an opacity distribution function as a function of frequency and temperature, HI bound-free and free-free opacity, H$^-$ bound-free and free-free, Thomson scattering on free electrons, Rayleigh scattering on neutral hydrogen, and Mie scattering and absorption on dust. There is a ’quick and dirty’ way how to include opacity of some molecular species using those extra opacity distribution functions. Corresponding thermal and scattering emissivities are included. Model is defined in a 3D Cartesian grid and spectra are calculated by ray tracing in another grid aligned with the observer’s line of sight. The code was written from scratch but we adopted a few subroutines from other sources. Mainly partition functions from the UCLSYN code (Smith & Dworetsky 1988) and a few subroutines from the SYNSPEC code (Hubeny & Lanz 2017). A brief description of the version No.39 follows below.

2. Input

Depending on the problem to be solved the user has to supply a proper input. Here is the list of most important input files.

- `shellspec.in` - is the main input file where you define the 3D model. It can be composed of a number of predefined structures briefly described in the next section or loaded from a separate file called `shellspec.mod`.

- `line.dat` - atomic data for the spectral lines formed in the CM (Kurucz format, optional)

- `shellspec.mod` - 3D model that contains for each point in space: temperature and density of the gas and dust, electron number density is optional (it can be calculated in LTE), velocity vector, and micro-turbulence. This can be e.g. an output of a 3D hydrodynamic simulation (optional).

- `abundances` - abundances of the CM (optional).

- `starspec1`, `starspec2`, `starspec3` - specify the grid of spectra of up to three non-transparent objects. This is the boundary condition for the radiative transfer in the CM. Default format is the output of the model atmosphere codes TLUSTY and SYNSPEC (optional).

- `albedo1`, `albedo2` - albedo of the primary and secondary stars as a function of the wavelength. Necessary for the reflection effect between the objects (optional).
• dust_opac, mie_phase - these are tables with the dust opacities and phase functions and are required only if there is a dust. We pre-calculated such tables to be used within TLUSTY but they can be used also here (Budaj et al. 2015) (optional).

• gas_opac - this is a table with molecular cross-sections as a function of wavelength. Default format is as in EXOMOL database (Tennyson & Yurchenko 2012) (optional).

• chem_eq_tab - this is a table with molecular population for a particular molecule as a function of gas temperature, density, and chemical composition. It was calculated with the code ÆSOPUS by Marigo & Aringer (2009) (optional).

3. Predefined structures

As a simple alternative to a more sophisticated 3D model there are a few simple pre-defined structures available which can be used to compose the 3D model. In case the structures happen to overlap in space a particular point will bear the properties of the higher priority object. Objects/structures ranked according to their priority are listed and briefly described below.

STAR: a central nontransparent object which can rotate as a solid body or possess a differential rotation with an optional inclination of the rotational axis and have a net space velocity. Can be treated as a black body or have its own spectrum. May be of the spherical or Roche shape. Limb and gravity darkening can be applied to it. Spherical star may have a circular spot on the surface of different temperature at a fixed location. Irradiation effect on its surface (from the COMPANION) can be considered. The light scattered in the circumstellar medium which originates from this object can be taken into account (neglecting its rotation, irradiation effect and assuming spherical shape). Differential rotation applies only to the spherical shape and does not affect the location of the spot. Designed to model mainly hotter or more luminous stellar components as well as extra solar planets.

COMPANION: similar to the STAR. Designed to model mainly a secondary (cooler or fainter component of a binary system).

ENVELOPE: is an object enclosing the central STAR (or STAR and COMPANION). It is subject to the Roche shape and can be detached or contact. It rotates as a solid body, does not have limb nor gravity darkening, has constant temperature and densities. It is possible to constrain this structure within a certain height above and below the orbital plane.Designed to model envelopes and common envelopes of e.g. W UMa type stars.

SPOT: a spherical object which can rotate as a solid body with an optional inclination of the rotational axis and have a net space velocity. Designed to model a third body, spots on accretion discs, direct impact regions, rotating circum-stellar shells.

STREAM: has the shape of a cylinder or cone with velocity varying linearly along the cone. Stream may rotate or be a subject of some rotational drag. It may also have a net space velocity so that it can e.g. follow the movement of some associated star. Density of the stream changes along the stream to satisfy the continuity equation with some modification to allow for modelling of additional phenomena. Designed to model the mass transfer streams, outflows, or shadows.
RING: is a circular ring or part of the ring (arc) with optional inclination and location. Mass in the center determines its Keplerian velocity. However, the velocity is uniform throughout the cross-section. The cross-section of the ring, $C$, has shape of a rectangle and may vary along the arc. Density, dust density and electron number density may change along the arc to satisfy the continuity equation and/or additional phenomena e.g. dust destruction etc. Designed to model rings around objects, arcs, comets.

DISC: has either the shape of a rotating wedge (space complement to two opposite cones) or of a slab, or of a rotational ellipsoid surrounding the central object with some mass. It is farther constrained by two surfaces: its inner spherical surface with radius $r_{\text{in}}$ and outer spherical or ellipsoidal surface with radius $r_{\text{out}}$. This structure may have optional location and inclination. The velocity field of the disc depends on the mass of the central object, and is Keplerian within the disc plane. Densities may vary in the radial direction as a power law. Temperature may be either constant, or have a radial power law dependence, or obey a radial accretion disk structure of Pringle (1981).

NEBULA: is another disk-like structure. It is located around the central object with a certain mass, has a Keplerian rotation, and may have also a net space velocity. It is defined in the cylindrical coordinates $(r, \theta)$. Surface density, $\Sigma$, varies as a power law with the distance from the center. Mid-plane density, $\rho_0$, is then determined as a function of distance from the surface density and vertical scale height, $H$. Vertical scale height is a function of Keplerian velocity, $v$, and sound speed, $c_s$. Vertical density behaviour is Gaussian with some modification to allow for modelling of additional phenomena (e.g. wind). Temperature structure in the radial direction is similar to DISC. There is an option of a simple vertical gas temperature dependence (e.g. inversion). This is another option to model flared accretion or protoplanetary disks.

FLOW: is identical to the STREAM but has a lower priority. Designed to model the mass transfer streams, outflows, or structures symmetric to the STREAM.

JET: has the shape of one or two opposite cones emerging from the center. It allows optional inclination and is farther limited by its inner, $r_{\text{in}}$, and outer, $r_{\text{out}}$, radii. It has constant temperature and velocity along the beam. However, it may have a net space velocity so that it can move e.g. with the STAR. Densities vary along the jet to satisfy the continuity equation. Designed to model mainly jets or, e.g., ‘shadows’ cast by a cool, extended secondary from a more compact hot primary.

UFO: is identical to the DISC but has lower priority. Intended to model an extension or atmosphere of the DISC or a second disc.

SHELL: has the shape of a shell surrounding the central object. A few different velocity fields are built in. The temperature is kept fixed and densities are either constant or satisfy the continuity equation. It may have a net space velocity.

4. Output

Here is a list of all output files.

- shellspectrum - spectra of the model from different view points.
- lightcurve - light curve at different wavelengths obtained by combining a sequence of spectra from different view points.
- fort.xx - are 2D images at some frequency from different view points.
• shellspec.out - a more detailed output of opacities, emissivities, optical depths, ... along some selected rays.

5. Applications

Possible application of this code include interacting binaries (Budaj et al. 2005; Ghoreyshi et al. 2011; Gorlova et al. 2012; Bozic et al. 2013; Richards et al. 2014) and some exoplanets. For example, Tkachenko et al. (2009, 2010) converted an earlier version70 into Fortran90 an wrote an inverse program which was used to analyze oscillating Algol type binaries. Chadima et al. (2011) used it for post-processing of the 3D hydrodynamic simulations to study variability in the Hα emission caused by a discontinuous mass transfer in binaries. Atwood-Stone et al. (2012) combined the spectroscopic observations with the synthetic spectra and the Doppler tomography to analyze an Algol type binary AU Mon. Lehmann et al. (2013) analyzed the properties of the eclipsing δ Scuti star KIC 10661783. Bakış et al. (2016) modelled the circumstellar material around the active binary R Arae. Šejnová et al. (2016) studied a dynamical evolution of the disk of the Be star 60 Cygni. Garai (2018) used the code to analyze the Kepler light curve of a peculiar extra-solar planet KOI 2700b featuring variable asymmetric transits of its comet-like dusty tail. Most recently Mirek Brož and Janka Nemravová wrote a package of codes in python that calculate interferometric observables from the Shellspec images and fit them simultaneously with the light curves. The method was used to determine the properties of a bright binary star β Lyr (Mourard et al. 2018). The reflection effect which is included in the Shellspec code (Budaj 2011) was now generalized and included in the PHOEBE 2 package for modelling eclipsing binaries and exoplanets (Horvat et al. 2018).

6. Summary

The latest publicly available version No.39 can be found here with the complete documentation, and example runs:
http://www.ta3.sk/~budaj/shellspec
A more detailed description is in Budaj & Richards (2004) and in the updated user manuals. Dust phase functions and opacities can be found here with the description and references to the refractive index measurements adopted:
http://www.ta3.sk/~budaj/dust
Any comments, suggestions, or bug reports will be appreciated. Thank you.

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