Workflow Summary
– Getting your SHAPE models ready for pyCROSS

pyCross Quick start – To simply use an example SHAPE output file in pyCROSS see https://www.sciencedirect.com/science/article/pii/S2213133720300366 or https://arxiv.org/abs/2005.02749 for the open access version.

(I) Introduction

To effectively use the pyCROSS software package the reader is asked to first be familiar with the SHAPE, Cloudy & pyCloudy packages.

However, following the instructions here will allow for the generation of an example classical nova shell. The method of generating the SHAPE output file for pyCROSS input remains the same, i.e. independent of the shape and density structure of the axisymmetric nebula under study.

As this is not meant to be a tutorial in the use of SHAPE, only the features relevant to generating the input for pyCROSS are described here.
For a comprehensive introduction to the SHAPE software please see:
http://www.astrosen.unam.mx/shape/

(II) Observation considerations and preliminary simuation strategy

For reference to the user types of useful observational data that can inform the modelling strategy and a brief note on each follow.
(1) - *Narrow-band imaging*: helps inform the physical structure of the nebula. Can be simulated using SHAPE.
(2) - *High/medium-resolution spectroscopy* can be used for line profile modelling in SHAPE. In combination with (1) this is the most common method for determining the spatio-kinematic structure of a nebula.
(3) - *Broad wavelength coverage spectroscopy*. This data is used for line diagnostics that help inform the chemical and ionisation structure of the nebula. These diagnostics can be simulated in 1D with the use of Cloudy, pyCloudy (https://github.com/Morisset/pyCloudy/blob/master/pyCloudy/docs/Using_pyCloudy_2.ipynb), pyNeb (https://pypi.org/project/PyNeb/) or using a reference textbook such as Osterbrock and Ferland's Astrophysics of Gaseous Nebulae.
(4) - *Broad-band polarimetry*. This type of observation, both linear and circular, can give clues (provided the source is polarised) to the orientation of the structure in the plane of the sky. This type of observation is helpful, although not crucial, in the SHAPE modelling strategy. Polarimetric observations also inform the scattering properties of a nebula.
(5) - *Line polarisation*. Particularly useful with corresponding spectroscopic observations of similar spectral resolution for the same spectral lines. Informs scattering and extinction considerations.
(6) - *High-time resolution photometry/radial velocity measurements* of stellar component. A little more abstract, but nevertheless important. Axisymmetric nebulae, for which pyCROSS can be used, often have a binary stellar system at

their heart. Unsurprisingly, it can be shown that the orientation of the central binary is related to that of the nebula. Thus, for an eclipsing binary whose orientation can be understood it can help untangle the nebular component further.

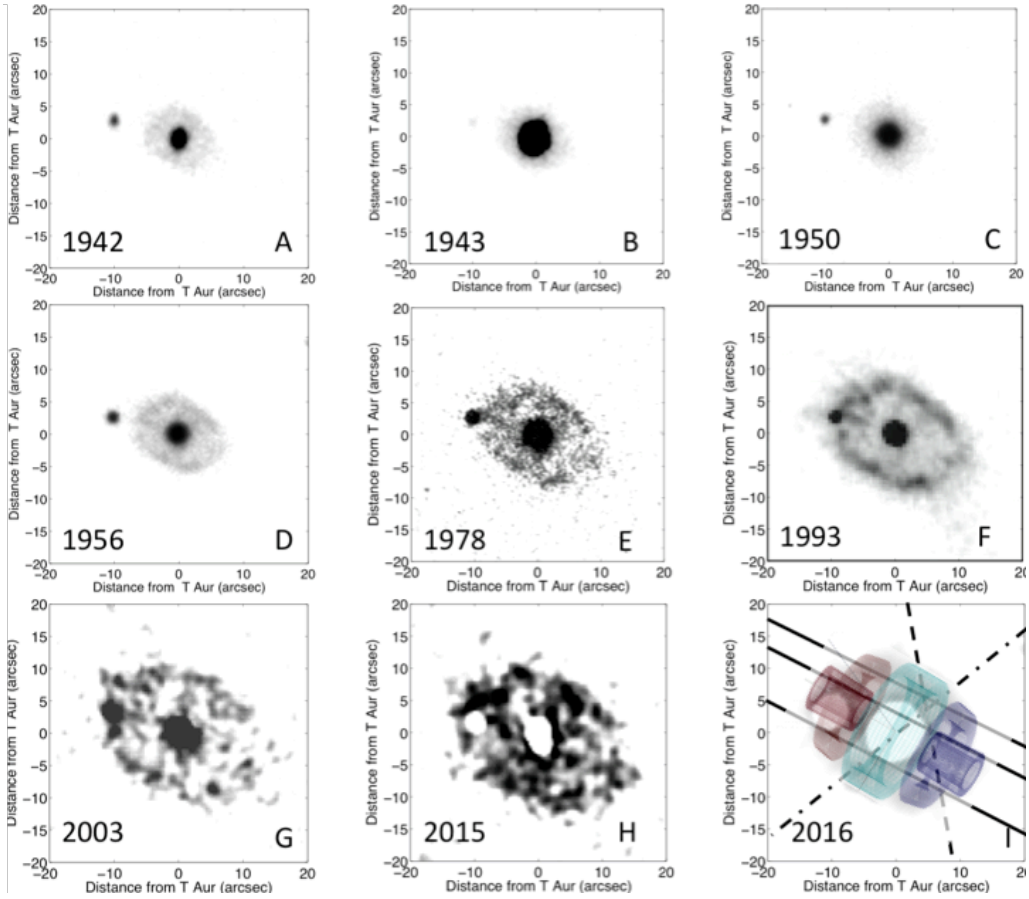

Fig. 1

This series of 9 panels below show imaging observations of the shell surrounding the nova progenitor T Aurigae, in Red and narrow-band (Hα +[NII]) filters. The corresponding year of each observation at the bootom-left of each panel. In the bottom-right panel the overlaid slits can be seen on top of the model matched to the 2016 image. Pairing high-resolution long-slit spectroscopy to imaging is an effective method in deriving the spatio-kinemtic structure of a nebula.

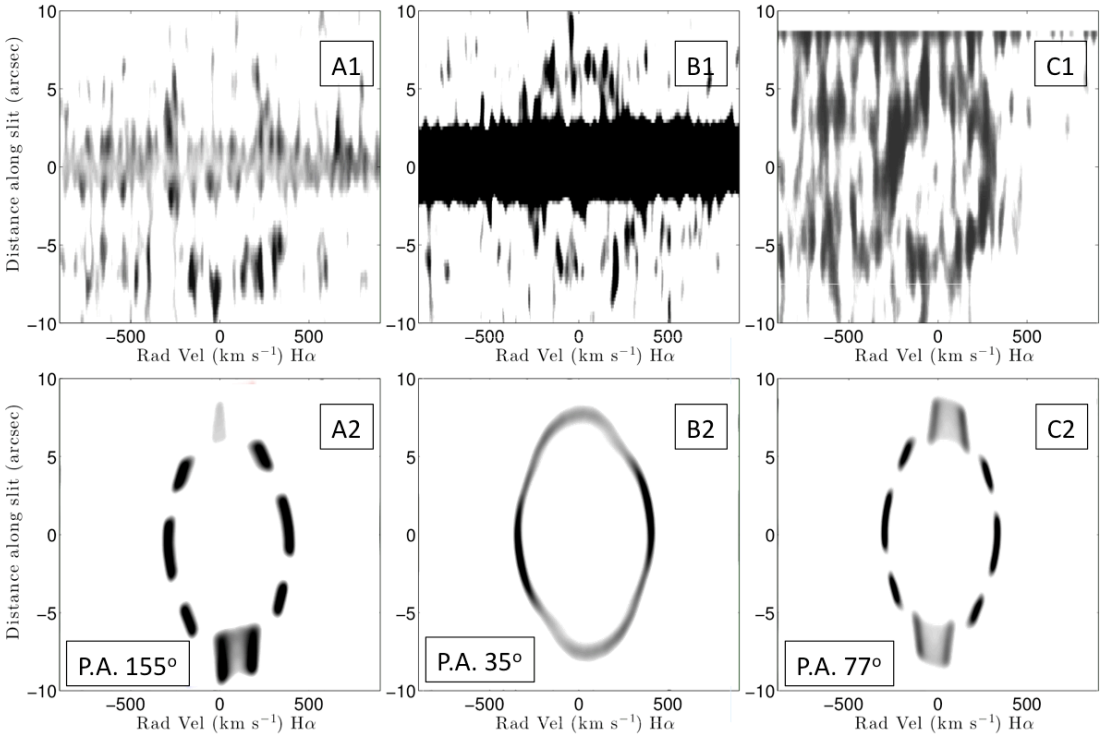

Fig. 2
This example demonstrates the technique of matching long-slit spectroscopy observations using the SHAPE software. The top row shows the long-slit spectroscopy observations of Fig. 1, whereas the bottom row shows their corresponding reproductions in SHAPE. The slits of the last panel of Fig. 1 match the 3 position angles stated in the bottom row of this figure.

(III) Output from SHAPE

To follow this section it is advisable to first be familiar with the SHAPE interface, especially the 'Render' and '3D module' tabs.

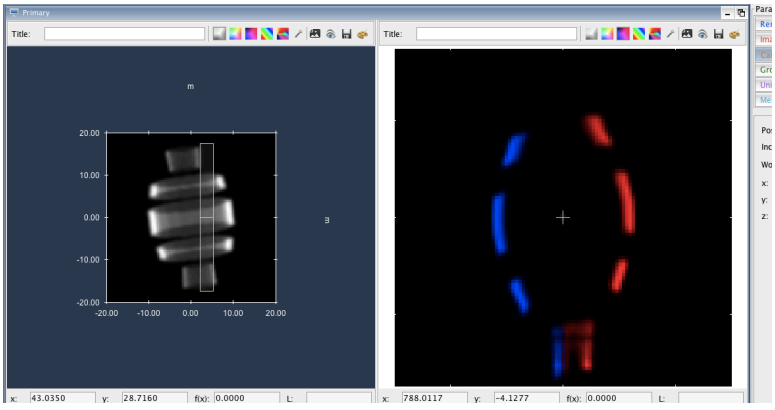

Fig. 3
In the image above we see the render window of the SHAPE interface. The left panel shows the simulated image at an arbitrary inclination and position angle. The rectangle overlayed is the simulated slit, of which the user has full control over. The panel on the right is the simulated position-velocity array corresponding to the slit in the panel on the left. The blue and red-shifted features are highlighted in their respective colours.

Once you are happy with your axisymmetric model set the position angle and inclination = 90 degrees. Arrange the positional arguments in the *Render tab* such that the upper right hand quarter of the structure occupies the entire Render panel. Then centre of the structure (0,0).
Position slit such that it falls square, covering the entirety of the Rendered Image panel, see Fig 4.
Go to the 3D window. Make invisible the components that do not feature in that quarter section. Go to the Primitive Tab, set phi min and phi max to -180 and -179 degrees respectively, see Fig 5.

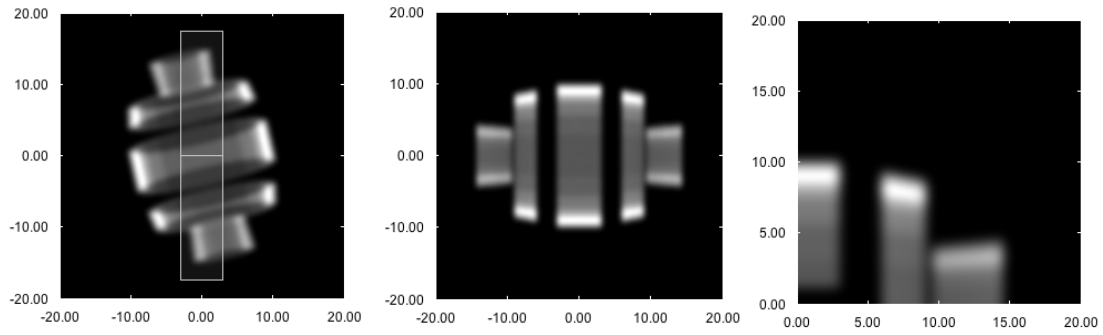

Fig. 4
Moving the slit and shell into place for use of the text output in pyCROSS. Remember the Slit should be placed to cover the entire square rendered image.

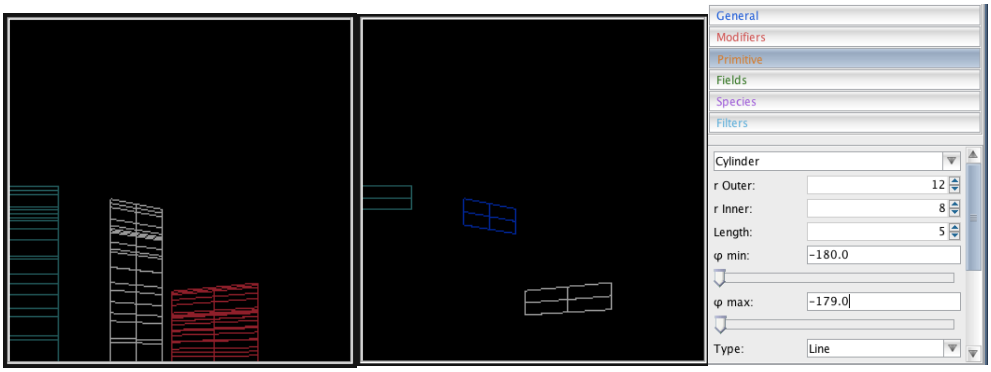

Fig. 5
Return to Render Tab. As your renderer type choose *Physical* and scoll down to *Output options*. A full description of the SHAPE render options can be found here: http://www.astrosen.unam.mx/shape/v4/manual/v4.0/Tutorials_Written/Rendering%20Interface/renderers.html

In summary the user must deselect the presets and click on File. Set a file path and the positional (Px, Py, Pz), velocity (Vx, Vy, Vz), density and temperature output arguments as shown in the below screenshot.

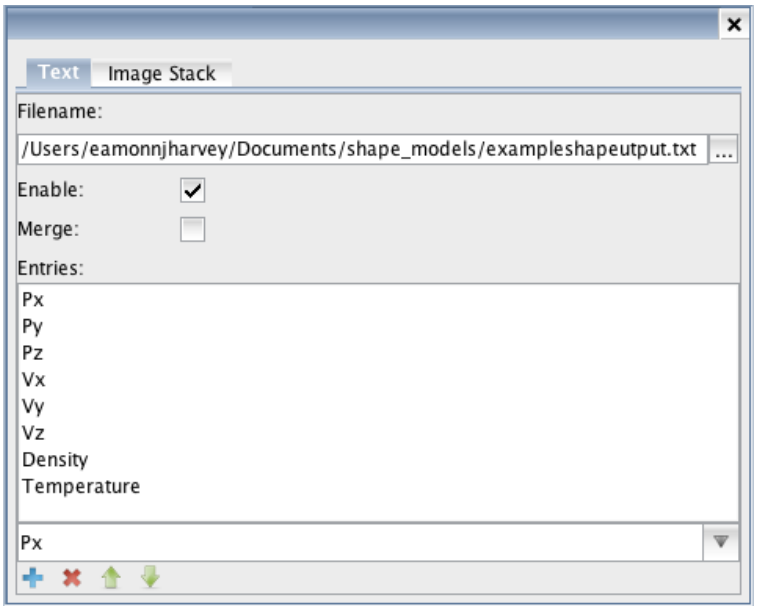

Fig. 6
Format of SHAPE output text file, as set in SHAPE.

Then by clicking the SHAPE icon the textfile is generated in the folder set by the user. This text file can then be imported directly from the pyCross GUI.

```
# Name  Px      Py      Pz      Vx      Vy      Vz      Density Temperature
#
Barrel, Default [ Default ]     0.109375        7.984375        0.546875        -57.03125       399.21875       27.34375        6.4     500.0
Barrel, Default [ Default ]     0.109375        7.984375        0.765625        -57.03125       399.21875       38.28125        6.4     500.0
Barrel, Default [ Default ]     0.109375        7.984375        0.984375        -57.03125       399.21875       49.21875        6.4     500.0
Barrel, Default [ Default ]     0.109375        7.984375        1.203125        -57.03125       399.21875       60.15625        6.4     500.0
Barrel, Default [ Default ]     0.109375        7.984375        1.421875        -57.03125       399.21875       71.09375        6.4     500.0
Barrel, Default [ Default ]     0.328125        7.984375        0.546875        -46.09375       399.21875       27.34375        6.4     500.0
Barrel, Default [ Default ]     0.328125        7.984375        0.765625        -46.09375       399.21875       38.28125        6.4     500.0
Barrel, Default [ Default ]     0.328125        7.984375        0.984375        -46.09375       399.21875       49.21875        6.4     500.0
Barrel, Default [ Default ]     0.328125        7.984375        1.203125        -46.09375       399.21875       60.15625        6.4     500.0
Barrel, Default [ Default ]     0.328125        7.984375        1.421875        -46.09375       399.21875       71.09375        6.4     500.0
Barrel, Default [ Default ]     0.546875        7.984375        0.546875        -35.15625       399.21875       27.34375        6.4     500.0
Barrel, Default [ Default ]     0.546875        7.984375        0.765625        -35.15625       399.21875       38.28125        6.4     500.0
Barrel, Default [ Default ]     0.546875        7.984375        0.984375        -35.15625       399.21875       49.21875        6.4     500.0
Barrel, Default [ Default ]     0.546875        7.984375        1.203125        -35.15625       399.21875       60.15625        6.4     500.0
Barrel, Default [ Default ]     0.546875        7.984375        1.421875        -35.15625       399.21875       71.09375        6.4     500.0
Barrel, Default [ Default ]     0.765625        7.984375        0.546875        -24.21875       399.21875       27.34375        6.4     500.0
Barrel, Default [ Default ]     0.765625        7.984375        0.765625        -24.21875       399.21875       38.28125        6.4     500.0
Barrel, Default [ Default ]     0.765625        7.984375        0.984375        -24.21875       399.21875       49.21875        6.4     500.0
Barrel, Default [ Default ]     0.765625        7.984375        1.203125        -24.21875       399.21875       60.15625        6.4     500.0
Barrel, Default [ Default ]     0.765625        7.984375        1.421875        -24.21875       399.21875       71.09375        6.4     500.0
Barrel, Default [ Default ]     0.984375        7.984375        0.546875        -13.28125       399.21875       27.34375        6.4     500.0
Barrel, Default [ Default ]     0.984375        7.984375        0.765625        -13.28125       399.21875       38.28125        6.4     500.0
Barrel, Default [ Default ]     0.984375        7.984375        0.984375        -13.28125       399.21875       49.21875        6.4     500.0
Barrel, Default [ Default ]     0.984375        7.984375        1.203125        -13.28125       399.21875       60.15625        6.4     500.0
Barrel, Default [ Default ]     0.984375        7.984375        1.421875        -13.28125       399.21875       71.09375        6.4     500.0
Barrel, Default [ Default ]     1.203125        7.984375        0.546875        -2.34375        399.21875       27.34375        6.4     500.0
Barrel, Default [ Default ]     1.203125        7.984375        0.765625        -2.34375        399.21875       38.28125        6.4     500.0
Barrel, Default [ Default ]     1.203125        7.984375        0.984375        -2.34375        399.21875       49.21875        6.4     500.0
Barrel, Default [ Default ]     1.203125        7.984375        1.203125        -2.34375        399.21875       60.15625        6.4     500.0
Barrel, Default [ Default ]     1.203125        7.984375        1.421875        -2.34375        399.21875       71.09375        6.4     500.0
```

Fig. 7
The beginning of an example SHAPE output text file can be seen below. The density arguments must be given in dex, as that is what Cloudy uses. Note in the first column the name of the component of the modelled nebula is named. The scale of which you generate your SHAPE model is not critical, as this is set in the pyCROSS interface when loading the SHAPE file. However, it is critical to match the thickness/extension ratio between the SHAPE and pyCROSS models as otherwise the axial ratio of the structure is modified.

(IV) Starting with pyCROSS

Equipped with a SHAPE output textfile, or indeed more broadly any output in the format matching that of **Fig. 7** above, the user is now ready to proceed. A full

description of pyCROSS use and functionality can be found in
https://www.sciencedirect.com/science/article/pii/S2213133720300366

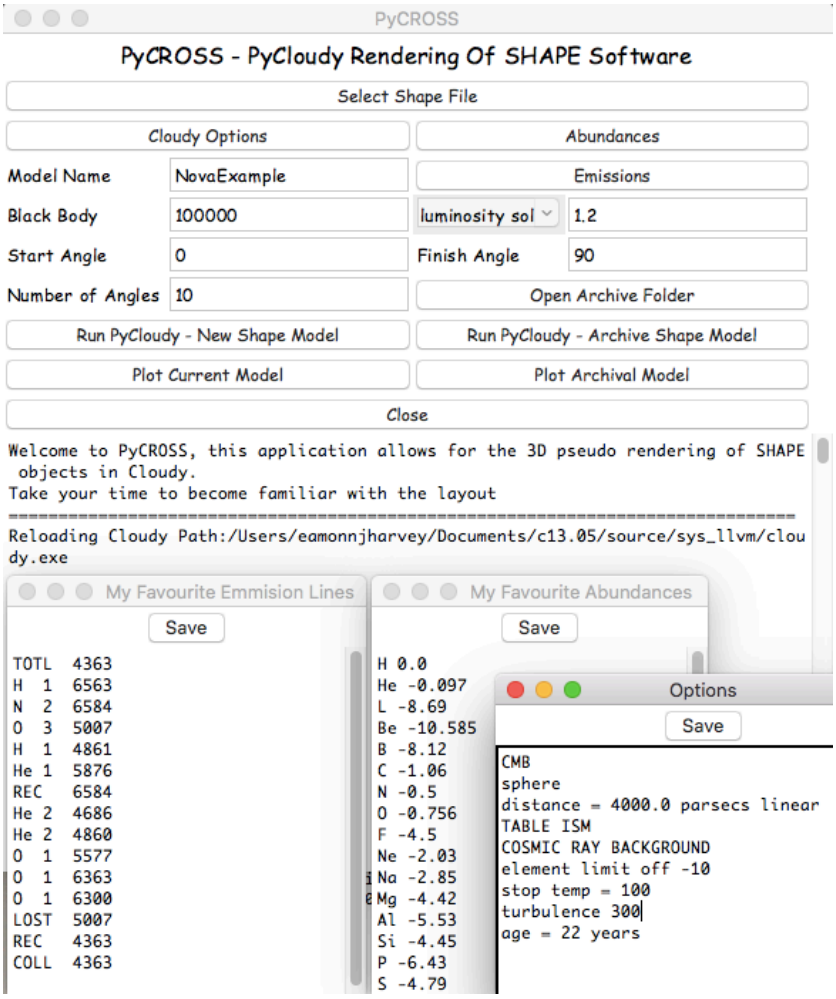

Fig. 8
Example input to pyCROSS interface. The inner shell and outer shell radii are set when the user clicks “Select Shape file”. After the radii are set in the pop-up boxes the Shape output text file is selected. Then all the user must do is click “Run PyCloudy”. When the simulation has finished running you may then select “Plot current model” and you will be taken to a new window.

If this is your first time opening up pyCROSS then you need to set the path to your Cloudy executable. Then, once you set your input parameters and load your SHAPE output text file into the pyCROSS interface, you are ready to go!