SHAPEMOL: Modelling molecular line emission in planetary and protoplanetary nebulae with SHAPE

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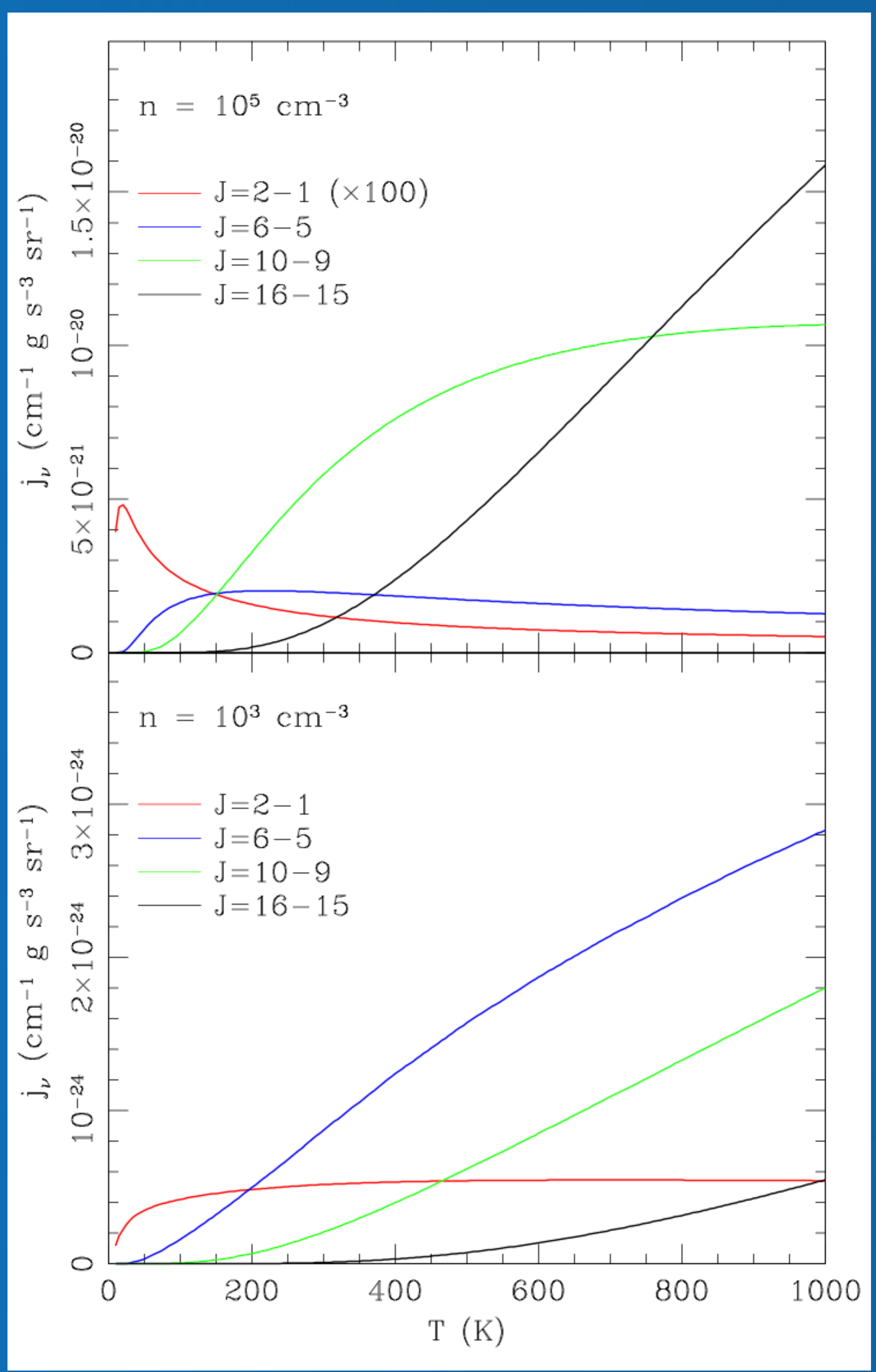
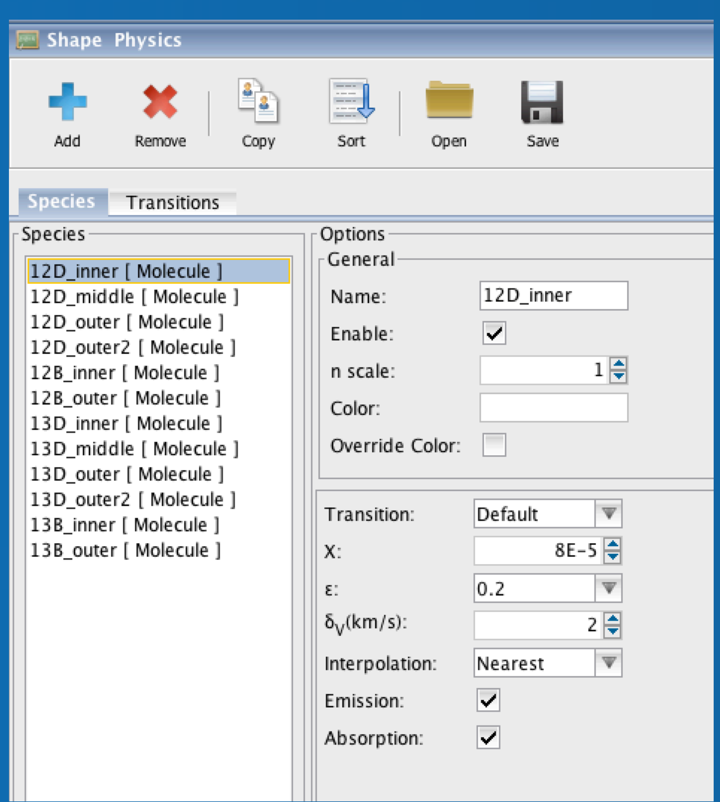
Introduction

Modern instrumentation in radioastronomy constitutes a valuable tool for studying the Universe: ALMA will reach unprecedented sensitivities and spatial resolution, while Herschel/HIFI has opened a new window (most of the sub-mm and far infrared ranges are only accessible from space) from where to probe molecular warm gas (~50-1000 K). On the other hand, the SHAPE software (*Steffen et al. 2010, IEEE Transactions on Visualization and Computer Graphics, April 2011 (vol. 17 no. 4),pp. 454-465*) has emerged in the last few years as the standard tool for determining the morphology and velocity field of different kinds of gaseous emission nebulae via spatio-kinematical modelling. Standard SHAPE implements radiative transfer solving, but it is only available for atomic species and not for molecules.

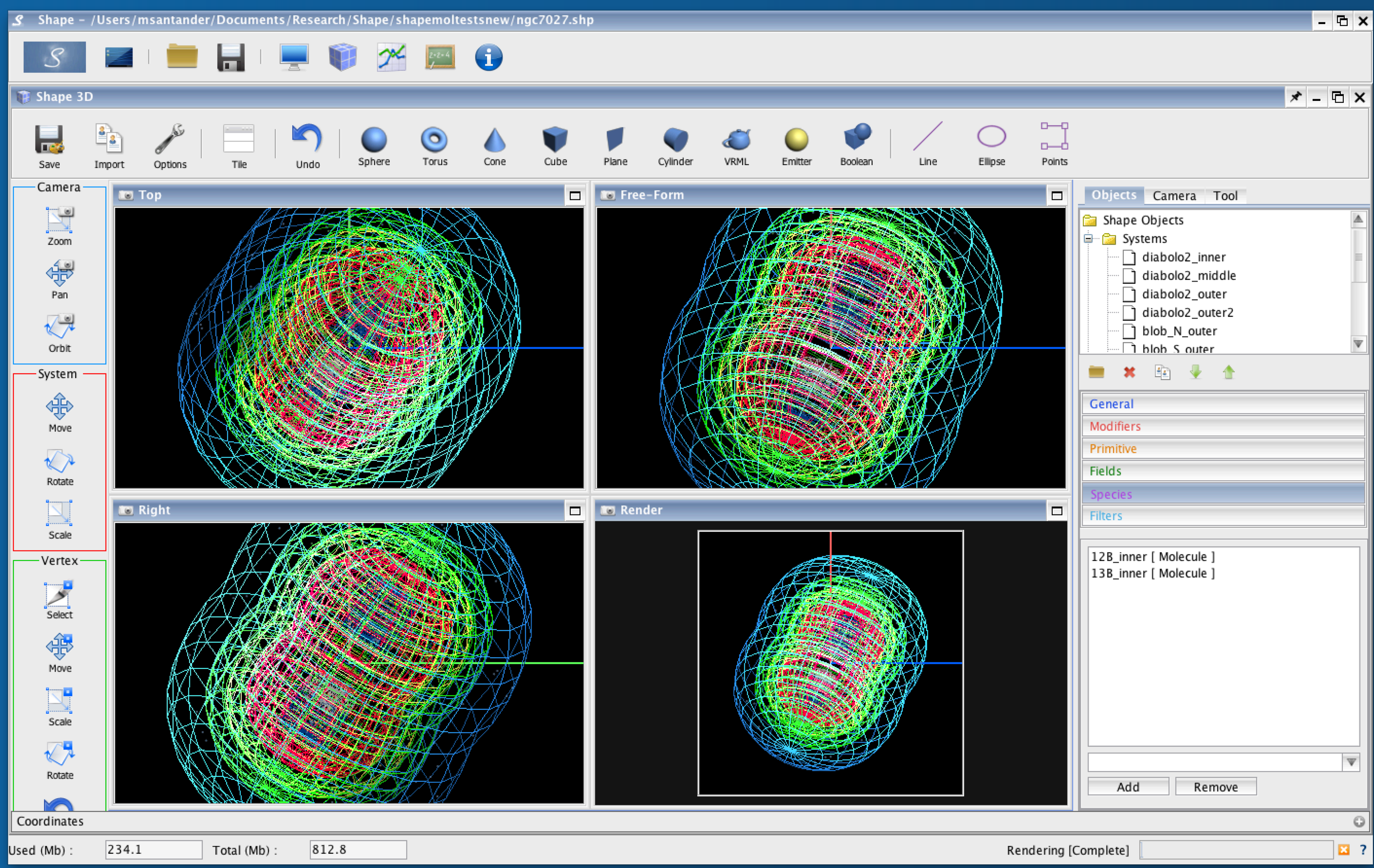
Being aware of the growing importance of the development of tools for easying the analyses of molecular data from new era observatories, we introduce a new version of the computer code *SHAPEMOL*, a plug-in completely integrated within *SHAPE* v5. *SHAPEMOL* enables spatio-kinematic modeling with accurate non-LTE calculations of line excitation and radiative transfer in molecular species. This code has been succesfully tested in the study of the excitation conditions of the molecular envelope of the young planetary nebula NGC 7027 using data from Herschel/HIFI and IRAM 30m *(Santander-García, Bujarrabal & Alcolea 2012, A&A, 545, 114)*. Currently, it allows for radiative transfer solving in the ^{12}CO and ^{13}CO J=1-0 to J=17-16 lines. *SHAPEMOL*, used along *SHAPE*, allows one to easily generate synthetic maps to test against interferometric observations, as well as synthetic line profiles to match single-dish observations.



In the molecular regime, the k absorption and j emission coefficients (the latter shown for some ^{12}CO transitions) depend on the density n and temperature T in a heavily non-trivial way. Hence the need for SHAPEMOL!



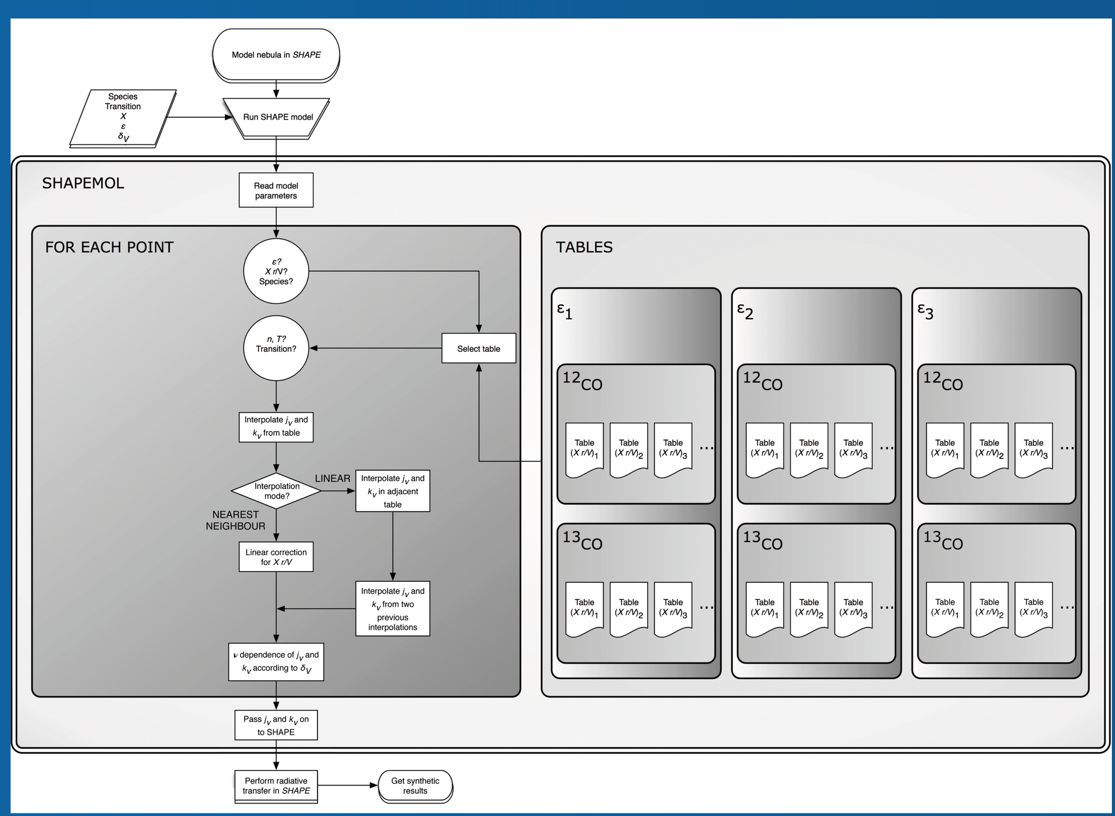
Detail of the Physics tab where molecular species and transitions are set up



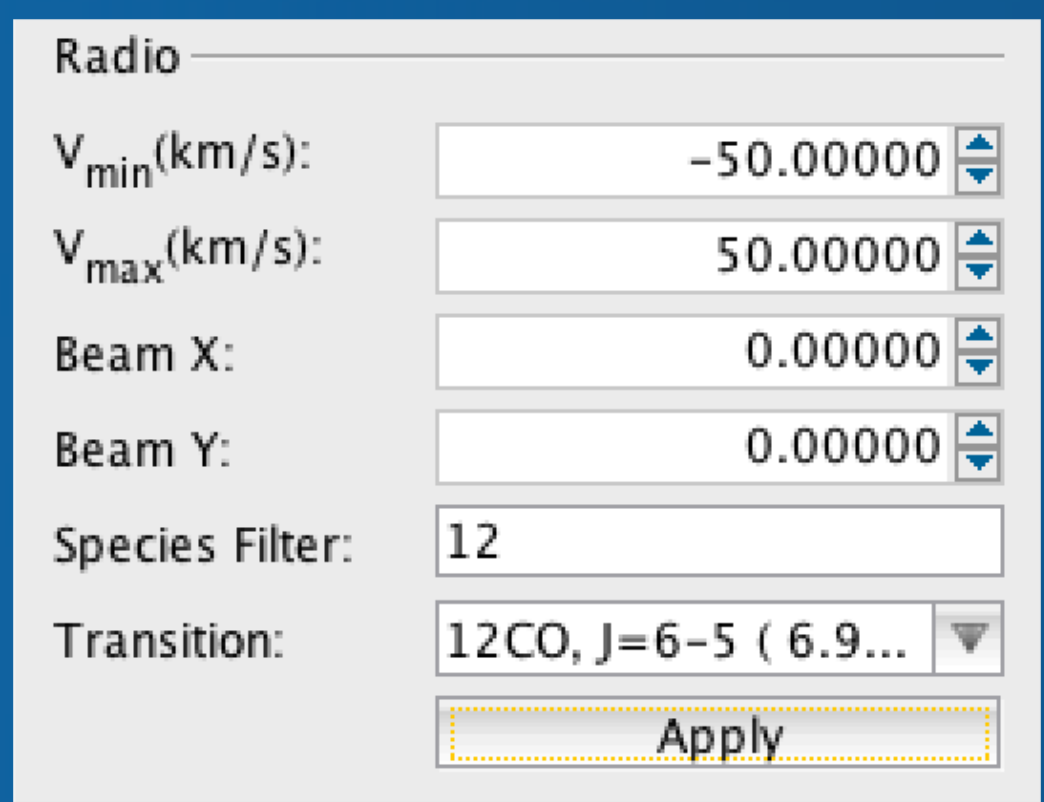
Modelling process: *SHAPE* and *SHAPEMOL*

Shapemol is now fully integrated within SHAPE. The process is as simple as follows:

1. Model the nebula in *SHAPE* as usual and provide it with velocity, density (10^8-10^{13} m^{-3}) and temperature (10-1000 K) modifiers.
2. Define the desired species (^{12}CO or ^{13}CO) in the physics tab, one per system in the nebula, and assign them to the corresponding system in the 3D module.
3. Define the desired transitions (J=1-0 to 17-16) together with the beam size of the telescope at that frequency.
4. Select the desired species and transition in the Render Module and clic on the Shape button to perform the radiative transfer and render the model!



Flow chart describing the process performed by SHAPEMOL



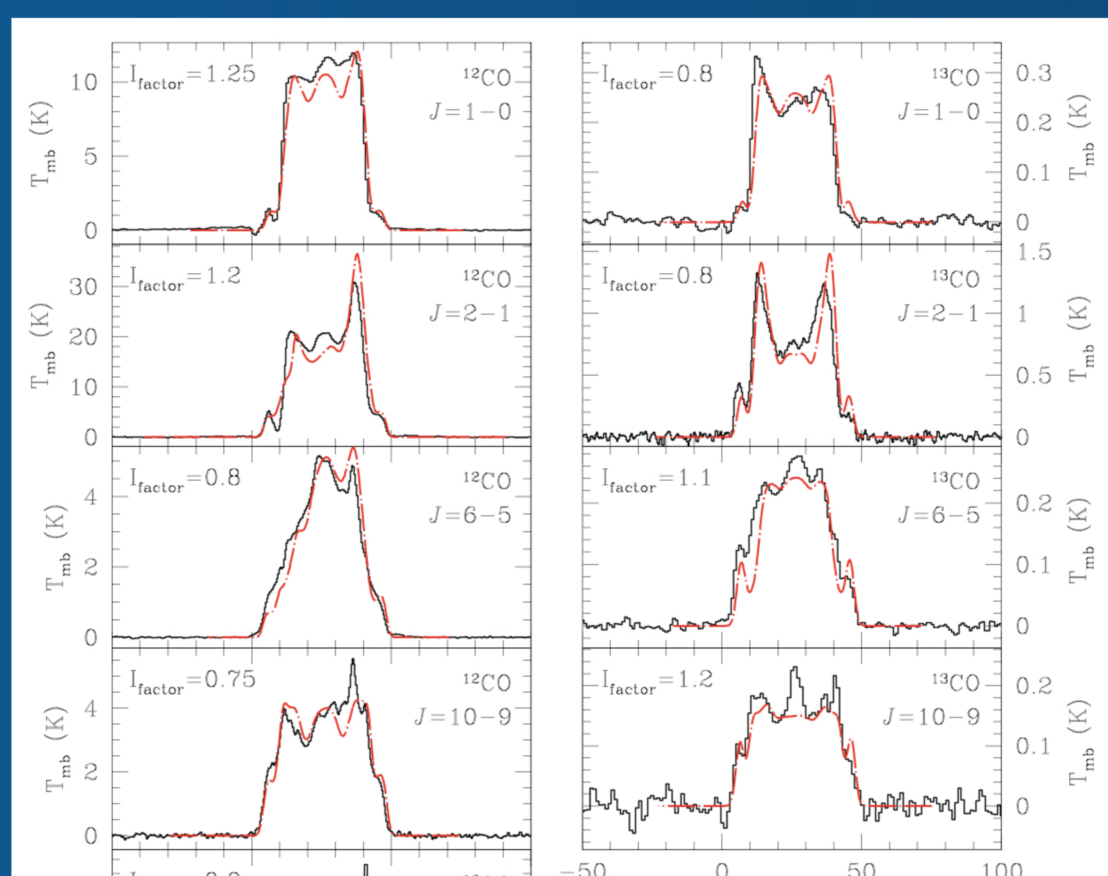
Detail of the Radio tab in the Render Module

NGC 7027, a test case

We have built a relatively simple model of the molecular gas of NGC 7027. It consists of four nested, mildly bipolar shells with different conditions (thickness, CO abundance, constant density and temperature), and a pair of high-velocity polar blobs. Since our data lack any information on the geometry of the nebula, we have imposed similar distance, morphology and orientation to those found in other studies in low-excitation CO or H_2 (e.g. *Cox et al. 2002, A&A, 384, 603, Nakashima et al. 2010, AJ, 140, 490*). For each shell, we have assumed a velocity field composed of (a) a radial, constant component plus (b) a constant axial component which is triggered for distances to the nebular equator greater than 1 arcsec.

The resulting synthetic spectra of our model in the light of ^{12}CO J=1-0, 2-1, 6-5, 10-9 and 16-15 and ^{12}CO J=1-0, 2-1, 6-5 and 10-9 are shown here along with the observations.

The inner shell, located just beyond the photodissociation region (PDR), is rather different from the other three: its low-abundance, high-density, hot temperature (T~400K), and, furthermore, the fact that its velocity is 25% greater than the velocity of the middle and outer shells, are indicative of a front shock traveling outwards through the nebula, in a similar way as the low-velocity shock front found in CRL 618 (*Sánchez Contreras et al. 2004, ApJ, 617, 1142*, later confirmed by *Bujarrabal et al. 2010, A&A, 521, L3*), in which a bipolar cavity is expanding against the nebular halo. This shock front, along with the high-velocity blobs, is likely to have major implications on the shaping of the nebula, which is currently at work (see *Santander-García, Bujarrabal & Alcolea 2012, A&A, 545, 114*).



Resulting synthetic spectra (red) and observations (black) for 9 different ^{12}CO and ^{13}CO transitions in NGC 7027.