Simulating the chemical structure and emergent molecular line emission from protoplanetary disks

Dustbusters Summer School 2022

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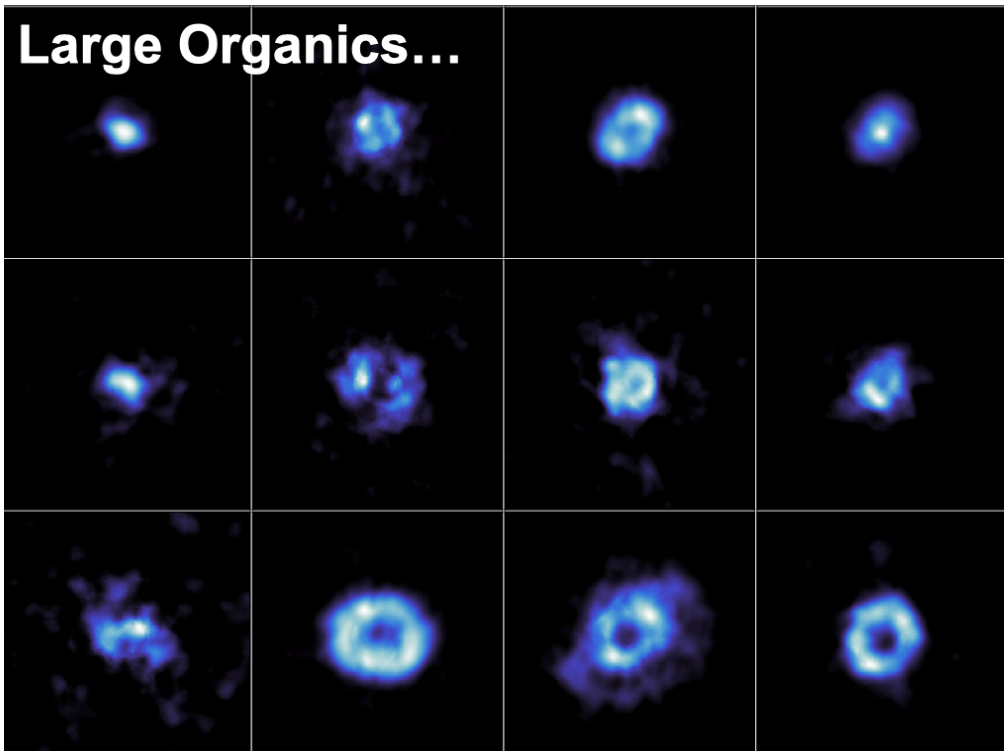

Moment 0 maps of rotational transitions from large organic molecules at a spatial resolution of 0.3" (Ilee & MAPS Team, 2022, ApJS, 257, 9).
www.alma-maps.info

The project will involve the setting up parametric chemical models of protoplanetary disks using already benchmarked physical models, and simulating the emergent molecular line emission using radiative transfer codes to compare directly with ALMA observations. We will guide you on how to extract quantitative information from your simulations such as line intensities and radial emission profiles, the comparison of which with observations will enable you to iterate the parametric chemical structure to better fit the data. You will gain skills in molecular line radiative transfer in protoplanetary disks, and an understanding of how simulations are used to extract information and understanding from observational data. *Software require: lime, Casa, python*

1. Download of software and tools

You will need a working installation of python 3.x and pip.

You will need the most recent version of CASA that works with your operating system
> CASA 6.x - https://casa.nrao.edu/casa_obtaining.shtml
> How to install - https://casa.nrao.edu/casadocs/casa-6.1.0/usingcasa/obtaining-and-installing

You will also need some additional analysis tools for imaging and analysis:
> GoFish - https://fishing.readthedocs.io/en/latest/ - > pip install gofish
> casatasks - https://pypi.org/project/casatasks/ -> pip install casatasks

Finally, you will need to install lime:
> https://github.com/lime-rt/lime

as well as the following dependences: qhull, cfitsio, and gsl
> https://github.com/lime-rt/lime/blob/master/README.md

If you are using a Mac, you can install these using macports or fink. We should have a working version available on the cluster during the summer school as well for those on other machines, or who are having difficulties.

Before proceeding with the next steps, make sure that you can open casa and casaviewer from the command prompt and that you have a working version of lime.

2. Download of project materials

For the simulation step of the project, we will be working directly with the already benchmarked physical models generated by the ALMA Large Program, MAPS (Molecules with ALMA on Planet Forming Scales; www.alma-maps.info). We will be directly comparing your simulated spectral cubes with the data, which will be generated by another project team. We encourage you to work together to share progress and outputs and regularly compare results with each other.

Once the group members are assigned, Catherine will e-mail you a link to download all the project materials.

3. *Project steps*

3.1 Data simulation step

Download the benchmarked models for either HD 163296 or MWC 480 . The original data can be obtained from https://alma-maps.info/data.html but we provide the data all in one place for convenience:

> HD_163296_disk_structure.npz
> MWC_480_disk_structure.npz

We will first simulate the emission maps for the HC_3N 11-10 and 29-28 transitions using the radiative transfer code, lime. Lime produces a simulated spectral cube of molecular line emission and requires a density, temperature, and abundance structure, as well as the molecular data.

We provide the needed data files, c code, and also a wrapper script for python which will create new models for you:

> create_model.py
> HC3N_model.c
> HC3N_mol.dat

Rerunning the “create_model.py” code will generate a new header file “HC3N_model.h” which is used by the “HC3N_model.c” code.

To run lime in the terminal:
> lime HC3N_model.c

The python script contains all instructions on how to set-up the parametric model. The code, “HC3N_model.c” is also fully commented and it should be clear how to set up a new model and how to adapt the requested output.

When you have generated your first simulated spectral cubes, you can move to the data comparison step, where we will smooth the data to the required ALMA beam, and where we will generate some derived products to be directly compared with the observations.

Note that this project is set up to be iterative. You will be repeating steps 3.1 to 3.3 to work towards producing an image and radial profile that reproduces the observations within the error bars (or as close as is possible in the time available).

3.2 Data comparison step

The observational side of the project is being conducted by another team. We encourage you to liaise with them on the progress of their analysis, to which you will be directly comparing your model results.

There are several steps needed to compare your simulations with real data.

For each transition, we will:
> smooth the simulations to the beam size of the observations
> produce moment 0 (integrated intensity), 1 (intensity-weighted velocity), and 8 (peak intensity) maps
> extract the disk-integrated line profile and line flux
> produce a radial profile of the emission

We provide a bespoke outline script to conduct these analyses:
> analysis_script.py

3.3 Rotation diagram

Once the disk-integrated line fluxes are measured for both transitions from the simulations, we will perform a rotational diagram analysis to empirically determine the disk-averaged rotational temperature and column density of HC_3N in the disk. This should help you determine in which direction to move the parametric model to better reproduce the data (i.e. whether to not to change the abundance, or to move the location of the molecule to a different temperature regime).

We will use the methodology outlined in:

> Loomis et al. 2018, ApJ, 859, 131
> Ilee et al. 2021, ApJS, 257, 9

Once again we provide an outline script:
> rotation_diagram_script.py

You only need to modify the information at the bottom of this script before running. You will need the disk-integrated fluxes from the two transitions from your simulations. Use the errors for both transitions as measured from the observations.

Compare your disk-averaged column densities and rotational temperatures with those from Ilee et al. (2021) and the other team.

4. *Further work*

If you and your team get through the above well ahead of the time allocated for project work during the summer school, there are several additional steps you can take:

> you can perform a similar analysis on another MAPS dataset: https://alma-maps.info/data.html
> for example, you could do the same analysis on brighter lines, e.g., HCN
> you can download some data products from the ALMA archive for a different disk/line transition

As an alternative, for those that are interested:

> you can have a go at some astrochemical modelling of HC3N in protoplanetary disks

If you would like to do the latter, make contact with Catherine who will supply you with some codes and template disk models to compute the chemistry.