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Chemical complexity in simulations of circumstellar discs formation

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Accurately modelling complex chemistry in numerical simulation is challenging, and is often avoided by relying instead on post-processing techniques. This implies computing the evolution of chemistry over the dynamic history of particles within the raw data. Our aim is to study complex chemistry over existing smoothed particle hydrodynamics (SPH) simulations of star cluster formation by employing this technique over the simulation data.

The base simulation employed in this study is the solar metallicity case of the four radiation hydrodynamical simulations presented in Bate (2019), which evolves a low mass clump of 500 $M_{\odot}$, performed using the smoothed particle hydrodynamics code SPHNG. Each calculation uses about 3.5×10^7 SPH particles to model the cloud.

To perform this study we apply a slightly modified version of the post-processing routines presented in Ferrada-Chamorro et al. (2021) to a small fraction of the entire particle set, by employing the chemistry package KROME (Grassi et al., 2014) to analyze and recover the abundances of different chemical species over the simulation data.

We first extract a small subset at the end of the simulation enclosing a small rectangular region with side $\sim$ 0.01 pc nearly at the center of the cloud resulting in a $\sim$ 330000 SPH particle subset. This data is extracted in GIZMO compatible files in order to correctly apply the post-processing routines presented above. To correctly model chemistry over the data we need to extract some important local properties on which chemical reactions depend (i.e., temperature, density, visual extinction A_v). We also need to specify a chemical network, which includes the tracers we want to study under the given conditions. In our case we employ a basic H-C-O network including molecules like CO and H2O.

The output of the post-processing are new snapshots including information for the chemical species indicated in the chemical network, allowing us to study them over the data without the need to recreate the simulations with on-the-fly (OTF) chemistry.

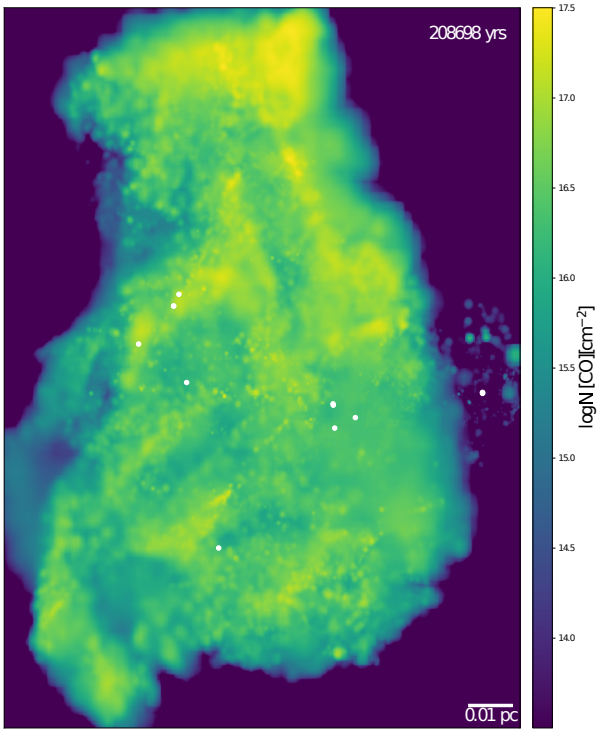

Figure 1. CO column density map for the sub-region at time $t \approx 1.1\ t_{\rm ff}$. Stars are plotted using white dots.

The purpose of using this method instead of just OTF chemistry is the large reduction of computational cost and the accuracy achieved when performing these post-processing routines, as already pointed out in Ferrada-Chamorro et al. (2021).

In Fig. 1 we report a CO column density map for the sub-region at an advanced stage by performing the post-processing routines over the data.

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