SF2A 2019
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THE INTERSTELLAR MEDIUM IN SILICO

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Abstract.
I will review the contributions of numerical simulations to our understanding of the physics and chemistry of the interstellar medium.

1D simulations make justice to the rich microphysics of astrophysical gases. They can afford large chemical networks, detailed microscopic transport (viscosity, resistivity, ambipolar and chemical diffusion...), complex radiative transfer or can accommodate the multiple facets of dust grains physics. Although they remain in a constrained geometrical framework, they often are our primary link to observations.

Direct multi-dimensional simulations thrive on our national computing capabilities and trigger efforts for innovation in data analysis. They can be dedicated to isolated objects, or attempt to render statistical properties of the morphology or dynamics uncovered by observational surveys. Sometimes, statistical models themselves can be used to synthesise multidimensional observations: they help disentangle large scale structures from smaller scale turbulence and resolve observational biases.

These experiments "in Silico" help us to make the most of the interpretation of observational results and allow us to calibrate future instruments thanks to observational synthesis. I will brush some of the great challenges faced by these numerical experiments within the next few years: how to best extract dynamical information from the line shapes, how to master crucial dust physics ingredients (e.g. coagulation and rotation), and how we are going to need the help of engineers to go through the exascale transition.

Keywords: ISM, simulations, statistics

1 Introduction

The interstellar medium (ISM) is a *multi-phase* gaseous system where various phases have been obervationnally shown to coexist (hot ionised medium, warm ionised medium, warm neutral medium, cold neutral medium, diffuse and dense molecular media). These phases are in approximate pressure equilibrium, while their density and temperature span about six orders of magnitude. The characteristic scales of observed structures within these phases range from about 100pc (the galactic disc scale-height) down to shearing scales of a few mpc, and may range down to dissipative scales (viscous scales are on the order of 10^{-6} pc for diffuse gas): the ISM is a hugely *multi-scale* system. Finally, various forms of energy (thermal, internal, magnetic, gravitational, radiative, cosmic-rays) are observed to be in rough equipartition: the ISM is *multi-physics.*

The life of ISM modelers is hence as exciting as it is challenging... I am going to present here some of the tricks which numerical physicists of the ISM have resorted to in order to circumvent some of these difficulties. This review does not intend to be exhaustive, and I apologise to those who wished their work had been mentionned here. It is organised from the largest scales down to microphysics aspects, and illustrations ought to be found in the pdf presentation of my talk, so that the present text is going to be figure-less.

2 Global simulations of the ISM

Galactic scale simulations of the ISM include at least one pressure-scale height of the galaxy and attempt to resolve as much as they can the scales of the molecular clouds. The main physics ingredients are cooling, magnetic fields and gravitation (including both the galactic potential and self-gravitation).

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Hennebelle (2018) use the zoom technique to get the most of the adaptive mesh refinement of the code RAMSES (Fromang et al. 2006). The principle is to set a main regular "background" grid over the full extent of the computational domain (here a thousand pc), and decide on a choice region where the resolution needs to be pushed to the extreme (here a cubic region of 100 pc side-length, where the adaptive mesh capability of RAMSES is released to a maximum resolution of 4×10^{-3} pc). The focused region is embedded in several buffer zones with decreasing resolution to avoid sharp resolution jumps.

The resulting simulation allows to bridge the gap between galactic scales and a few mpc (a range of 260000 in scales !), thus providing access to small dense clumps in their natural environment for a relatively low cost compared to the resolution achieved (one such simulation is about 10 million CPU hours, and was awarded time by PRACE under the FRIGG project, PI P. Hennebelle). Statistical measurements reveal that resolution effects and sticky self-gravitating zones still remain to be better controlled, but the technique bears a huge potential for the future.

3 Local simulations of the ISM

On the contrary, one can focus on a local patch of the ISM, assuming statistically homogeneous properties (such as density, turbulent forcing, or r.m.s. velocity). The assumption of homogeneity requires to perform parameter studies, made possible by the lower computational cost compared to global simulations which are usually 'one shot'.

These simulations are more classic, less costly (about 100 000 CPU hours each), and allow to include more physics ingredients (such as radiative transfer González et al. (2015); Valdivia et al. (2016), minimal chemistry Valdivia et al. (2016), or dissipation physics Masson et al. (2016); Momferratos et al. (2014)).

For example, in the framework of the ERC MIST (PI E. Falgarone), we study dissipative structures and their observational signatures, in the hope of shedding light on the surprising molecular fertility of violent and dilute media. ERC funding allows a small team to own a machine with an available 2-3 million CPU hours per year which will later be incorporated in a meso-scale computational center (such as mesoPSL). These simulations have so far allowed us to show the unexpected weight of incompressible motions in the total dissipation budget. We show most of the dissipative structures have a sheet-like topology and we suspect these sheets project onto the plane of sky as sharp structures which can be identified as filaments by observers.

4 Link to observations

There are thousands of ways to look at a painting and convey what we've seen to another human being. One can simply take a high resolution picture of it, but the human eye can be stroke by colors, textures, contour shapes and their relative size or orientations, or more personal memories the painting brings back to us. Similarly, there are many statistical tools to assess an observational image: Fourier spectrum, filaments / clumps statistics, principal component analysis and variants (Gratier et al. 2017; Bron et al. 2018), intermittency statistics (increments statistics, structure functions or multi-fractal properties), and more recently wavelet scattering coefficients (Mallat 2012). A new version of the latter technique (Allys et al. 2019) which condenses the relative orientations between scales into a reduced set of coefficients has been recently shown to characterise very efficiently the non-linearities of the column-density maps of turbulent simulations.

The link to observations can also be realised by "painting" back observational properties on simplified simulations which are missing some of the necessary microphysics. For instance, Levrier et al. (2012) reproduced line-of-sights of a two-phase simulation of the ISM by using the Meudon PDR code (Le Petit et al. 2006) on the simulation density profiles to compute the column-density of observable tracers. Another approach can be to replay the thermodynamic history of lagrangian tracers with an extensive chemical network (Ruaud et al. 2018). This emphasises the need for sub-grid models in multi-dimensional simulations.

5 Low-dimensional models

Multi-dimensional simulations thus require calibration using 1D or 0D tools which allow to investigate an extensive range of the microphysics processes at play in the ISM (radiative transfer, detailed chemistry, grain physics using size by size bins etc..). These models (Meudon PDR code, Dustem, Paris-Durham shock code, TDR model...) capitalise on their simplified geometry to run very efficiently (a few CPU minutes on a laptop) and hence allow huge grids of parameters to be computed. These grids require new tools to be processed efficiently and the ISM database (ISMDB, see `http://ism.obspm.fr/`) provides efficient ways to inquire the huge variety of observables produced by these models and match them with actual observed data.

6 Microphysics rates

Finally, these low-dimensional models need refined collisional rates and atomic and molecular data to produce accurate predictions for the chemistry and line emission of observable tracers. Numerical computation for these rates span a huge range of computational needs depending on the degree of approximation used. The recent development of a versatile collection of computational platforms (from personal laptops, via meso-scale centers, to national computational capabilities) has allowed huge progress in the comparison between theory and experiments (Kashinski et al. 2017).

7 Prospects

To conclude, I will lay out three of the main ways of investigations which seem to be necessary for the near future in ISM computations.

7.1 Grain physics

Dust acts everywhere in the galactic matter cycle. It controls the amount of energy radiated away during protostellar collapse. It is the main catalyst for the formation of the most common molecule H_2. Icy grains surface chemistry is arguably one of the major paths towards molecular complexity. Feed back through AGB winds rely on the understanding of grains radiative properties. Grains often control the ionisation degree and the mass loading of magnetic fields. Polarisation measurements require dust polarisation models to test the interplay between magnetic fields and ISM dynamics. Anomalous emission from grains confirmed by Planck measurements hints at the importance of grains disruption by spinning (Hoang & Tram 2019; Tram et al. 2019). Many observational problems of the ISM seem to be linked to grain physics, which will likely be the focus of many ISM modelers in the next few years.

7.2 Line shapes

Until now, numerical simulations of the ISM have mainly focused on global emission properties (such as total line of sight column-densities or emission, or centroid velocities). But the advent of wide-field spectroscopy bears a wealth of dynamical information yet to be mined. Orkisz et al. (2017) have shown how to use statistically part of the velocity information by using its first and second moments. Tram et al. (2018) and Neufeld et al. (2019) have shown how detailed modeling of the line shape emission can lead to much refined diagnostics from shock emission, including the best proof of the existence of C-shocks to date. But I believe there is still a lot to be gained by understanding how chemistry, excitation and dynamics conspire to shape emission lines.

7.3 New hardwares

New generations of hardwares are motivated mainly by smart phones and video games, and are now more focused on the efficiency of energy consumption rather than sheer computational power. The future architectures are going to be more and more hybrid, extending the symbiosis between GPUs and CPUs which we have witnessed in the last two decades. This requires us to hire good computational engineers with a tight communication between them and the researchers. The development of DUMSES on GPUs by M. Joos is a nice example of the good practice which we should be aiming at.

This presentation was made in consulation with A. Faure, J. Pety, P. Hennebelle, B. Godard, F. Levrier, E. Falgarone, F. Le Petit, E. Allys and V. Wakelam, all of whom I thank for providing me material for my slides as well as comments.

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