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Magritte: a new Multidimensional Accelerated General-purpose Radiative Transfer code

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ABSTRACT

The In this paper we present the basis for a new multidimensional accelerated general-purpose radiative transfer code, called Magritte.

Key words: radiative transfer, astrochemistry, methods: numerical

1 INTRODUCTION

The Radiative Transfer problem is one of the oldest and

New C++ code based on 3D-PDR Bisbas et al. (2012) improved performance. separate modules for chemistry, radiative transfer and thermal balance.

The paper is organized as follows. In section 2 we present the new computational scheme and the different modules of Magritte. Section 3 describes the different benchmarks that were done to test the code and to compare its performance with 3D-PDR. In Section 4 we present the new applications that have become feasible through the nove Finally our conclusions are discussed in Section 5.

2 COMPUTATIONAL SCHEME

Although Magritte is based on 3D-PDR, the whole code has been rewritten from scratch.

2.1 Data structures and memory layout

Magritte assumes an unstructured grid of cells

Much better memory scaling and impoved overall performance.

Plot of memory use as function of the number of grid cells, Magritte vs. 3D-PDR.

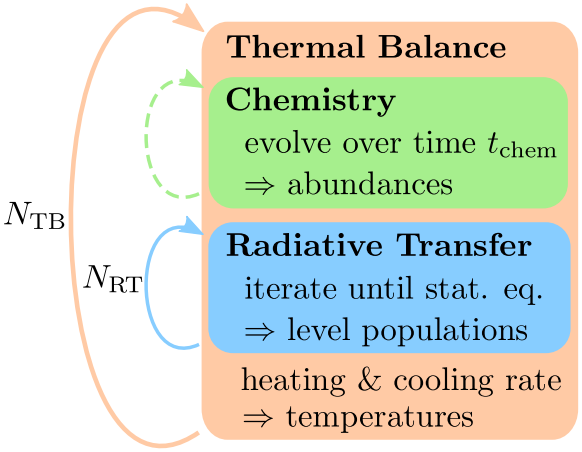

Figure 1. Iteration schemes of the Magritte workflow, different boxes represent the different modules.

2.2 Modules

To facilitate the incorporation of Magritte in other codes, the code is structerd into separate dedicated modules each handling a specific part of the calculaltion.

2.2.1 Ray-tracing

On the length and time scales considered in Magritte simulations, light travels on straight lines. The first step in

The direction of a ray is determined by the HEALPix[1] discretization of the sphere Górski et al. (2005)

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[1] healpix.sourceforge.net

2.2.2 Chemistry

Magritte determines the relative abundances of a limited number of atomic and molecular species at each cell. This is done by solving the time-dependent chemistry of a self-contained network of formation and destruction reactions. The chemical network is a subset of the most recent UMIST data base of reaction rates Woodall et al. (2007), consisting of 320 reactions between 33 species (including electrons), and includes photoionization and photodissociation reactions in addition to the standard gas-phase chemistry.

2.2.3 Radiative transfer

Lines plus continuum.

The line data were taken from the Leiden Atomic and Molecular Database (LAMDA, Schöier et al. 2005).

Acceleration methods Ng-acceleration Ng (1974) and Rybicki-Hummer acceleration scheme Rybicki & Hummer (1991). The combination of both acceleration schemes yield a significant speed up in the convergence of the level populations. The approximated lambda operator for the Sobolev case is simply given by

$$\Lambda^* = 1 - \beta \tag{1}$$

Later versions will be able to treat multiple dust scattering

2.2.4 Thermal balance

Magritte can self-consitently determine the temperature assuming local thermal balance, i.e. equal heating and cooling rates for each cell. (Argument on time scales?)

2.3 Parallelization strategy

3 BENCHMARKS

4 APPLICATIONS

The modular character of Magritte allows it to be easily used in various astrophysical simulations.

5 CONCLUSIONS

We have presented Magritte: a new multidimensional accelerated general-purpose radiative transfer code.

Once all modules are finished and extensively tested, the source code for Magritte and its separate modules will be made freely available on github.com/Magritte-code.

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REFERENCES

Bisbas T. G., Bell T. A., Viti S., Yates J., Barlow M. J., 2012, Mon. Not. R. Astron. Soc., 427, 2100
Górski K. M., Hivon E., Banday A. J., Wandelt B. D., Hansen F. K., Reinecke M., Bartelmann M., 2005, ApJ, 622, 759
Ng K.-C., 1974, J. Chem. Phys., 61, 2680
Rybicki G. B., Hummer D. G., 1991, Astron. Astrophys., 245, 171
Schöier F. L., van der Tak F. F. S., van Dishoeck E. F., Black J. H., 2005, A&A, 432, 369
Woodall J., Agúndez M., Markwick-Kemper A. J., Millar T. J., 2007, A&A, 466, 1197

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