A new 3D transport and radiation code for galactic cosmic rays

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Abstract: We show the necessity for a new approach towards comprehensive and consistent simulations of the propagation of galactic cosmic rays. Our developments are optimised for addressing the spatially 3-dimensional inhomogeneous diffusion problem and utilise contemporary numerical methods. We aim to address the transport problem in a full 3-dimensional environment. For that, we test the transition from 2D to 3D simulation results within an existing propagation code. We present sub-kpc scale simulations that allow the investigation of small-scale structures regarding different model conditions such as variety regarding non-axisymmetric cosmic ray source distributions. These results are discussed critically and motivate our development of a new transport code for galactic cosmic rays. The capabilities of this code are outlined.

Keywords: cosmic rays, propagation,

1 Introduction

The challenge in modelling the propagation of cosmic rays (CRs) in our Galaxy is at least twofold: Implementing a realistic and accordingly complex physics model of CR propagation in our Galaxy and devising a numerical scheme that can solve the underlying transport equations accurately but efficiently. These two conflicting aspects are often consolidated by making several more or less justified simplifications in the underlying CR propagation physics and/or the input parameter space (i.e. galactic magnetic field, gas distribution, radiation fields, isotropic diffusion). Consequently, current available transport codes feature CR propagation models of varying complexity [1], from single species fluid models to codes that account for a nuclear reaction network of multiple CR species. DRAGON [2] and GALPROP [3] are considered the most capable of the currently publicly available codes. Both compute the CR distribution in our Galaxy by solving the CR transport equation for each CR species using a mostly second-order Crank-Nicolson discretisation. The most prominent CR interactions with the radiation fields and matter distributions in our Galaxy are taken into account, furthermore both allow the computation of secondary particles, e.g. γ-rays. Gamma-rays are of particular interest as they offer a testing ground for the validity of CR particle transport modelling results via comparison to measurements of the galactic diffuse γ-ray emission.

Despite their capabilities current propagation scenarios are still relying on simplifications that have been rendered obsolete by tighter constraint on the input parameters as provided by new experimental results, i.e. matter distributions, magnetic field models, radiation fields, CR source distributions, and perhaps more importantly by the increase in computational power that allows a more realistic 3-dimensional non-isotropic treatment of CR propagation. Only recently steps have been made to overcome the 2D-paradigm that clearly demonstrate that new insights on current topics in astroparticle physics can be gained [4].

We show if and how 3-dimensional sub-kpc scale propagations scenarios can be treated using GALPROP and test the validity by comparing these results to 2-dimensional simulations. We demonstrate the capabili-
cuss current limitations of GALPROP thereby motivating the necessity of new code developments.

2 Beyond the 2D-paradigm

2.1 2D to 3D comparison

We test consistency of the solution for a 3D-propagation scenario obtained by GALPROP with that obtained in the 2D case by formulating a 2D \((z,r)-\)coordinates scenario using an axisymmetric source distribution (source model=1) and an equivalent 3D propagation scenario that should in principle result in the same CR distribution. We use a spatial resolution of 0.1 kpc for the \(z\)-direction and 0.15 kpc for the \(r,x,y\)-directions. In these scenarios our Galaxy is confined within a box ranging from \(x,y = \pm 15\) kpc (\(r = 15\) kpc in the 2D scenario) and a height ranging from \(z = \pm 4\) kpc. Here we discuss protons and electrons only, although tests with nuclei up to \(Z = 8\) have been performed. The energy grid uses 23 logarithmically equidistant energy points ranging from 100 MeV to about 1 TeV. The size of the time steps used by the solver ranges from \(10^8\) yrs to \(10^2\) yrs. We find that the 2D and 3D proton distributions match and that any deviations are on the percent level. This is exemplary shown for \(E_{\text{kin}} = 100\) MeV protons in Figure 1. Up to a certain degree of accuracy, GALPROP provides a consistent solution. We use the CR proton spectrum at Earth to quantify the remaining discrepancies between the 2D and 3D solutions and investigate their dependence on parameters that govern the numerical solver. This is shown exemplary for the parameter \(\text{timestep\_repeat}\) (the number of iterations in each time step) in Figure 2.

We performed a similar analysis for electrons. As an example we show the spatial electron distribution at an energy of \(E_{\text{kin}} = 1.2\) TeV in Figure 3 where deviations are considerably larger. In Figure 4 we show that the solutions of the 2D and 3D scenarios for energies above 200 GeV do not match as well as for CR protons. We use the electron spectra at Earth to quantify the deviations and find that the deviations increase with increasing energy. We do not find any dependence on the number of iterations in each time step nor the size of the smallest time step. If this discrepancy hints at an error in the numerics, e.g., that the high energy boundary conditions are handled incorrectly, or that the time scales associated with energy loss are simply too small, is still under investigation.

2.2 3D modelling

3D-simulations allow us to model propagation scenarios that do not feature \(\phi\)-symmetry. To demonstrate this we implemented a source distribution following a logarithmic spiral arm pattern derived from COBE observations of FIR cooling lines [5]. Figure 5 shows the resulting distribution of CR protons at an energy of \(E_{\text{kin}} = 444\) MeV. This allows

Figure 2: Comparison of CR proton spectra obtained from 2D and 3D scenarios: for \(\text{timestep\_repeat} = 20\) (red crosses) and 200 (blue crosses). Deviations of 2D solutions: for \(\text{timestep\_repeat} = 20\) to = 200 (magenta crosses), 200 to 2000 (light green crosses) and 2000 to 20000 (dark green crosses) as well as for 3D solution using \(\text{timestep\_repeat} = 20\) compared to = 200 (black crosses).

Figure 3: Above: \(E_{\text{kin}} = 1.2\) TeV electron density distribution as obtained by a 2D propagation scenario. Middle: \(x,z\)-slice of the \(E_{\text{kin}} = 1.2\) TeV electron density distribution obtained by a 3D propagation scenario. Below: Residual \((|2D - 3D|)\) of the two electron distributions shown above. Colour scale of CR density in arbitrary units.

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The corresponding GALDEF files are available upon request.
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Figure 4: Comparison of CR electron spectra at Earth for: Spectra derived from 2D scenario divided by spectra obtained from 3D simulations for timestep_repeat = 20 (blue crosses), = 200 (red circle and end_timestep = 10 yrs (purple star)). Comparison of 2D spectra obtained with end_timestep = 100 yrs to = 10 yrs (magenta crosses) and analogously for 3D (black arrows) and using end_timestep = 10 yrs (black circle)

us to study a range of new aspects inaccessible by 2D scenarios, for instance the significant change of the CR flux at Earth with Earth’s position relative to the spiral arms. This is shown in Figure 6.

For all its capabilities and its long history of development heritage GALPROP has several shortcomings which demand improvement of the existing or the development of a new CR transport code. Higher resolutions require the code to perform well on parallel high performance computer architectures. GALPROP is capable of running on multiple cores on shared memory systems using the OpenMP API but, as we show in Figure 7, the speed-up gained by using additional computing cores is far from optimal. We note that in most cases the limiting factor is the available memory. Currently, GALPROP cannot take advantage of distributed memory machines, thus, high spatial resolution simulations are impossible on such computing infrastructures. GALPROP also does not allow a quantification of the numerical error and convergence towards a solution has to be determined by trial and error [3]. GALPROP relies on the assumption that CR diffusion is isotropic and uses a scalar for the diffusion coefficient rather than a tensor. A recent study has shown that abandoning isotropic diffusion has a substantial effect on the CR spectrum at Earth [6]. A further limitation is that GALPROP calculates the nuclear reaction network after it obtains a propagation solution and is therefore unable to include time-dependent effects of the nuclear reaction network correctly.

3 A new CR transport code

In the previous section we identified the lack of control over convergence in the GALPROP code as a fundamental problem for the numerical solver. While we showed that it is actually possible to find a meaningful quantification of the convergence of the code, the less experienced user of such a code, is hardly interested in repeatedly conducting convergence studies between any major change in the physical setup.

This problem is actually connected to the way the transport equation is solved within GALPROP: the transport equation is integrated in time until the user-specified total propagation time is reached. In this case the user has to make sure that the overall time integrated by the solver is sufficiently long for a steady state solution to be achieved. An obvious alternative to this scheme would be to compute a steady-state solution directly without any time-integration. This, however, forbids a time-splitting approach as utilised within GALPROP: a first order operator splitting method is applied in a way that all dimensions are alternately solved for, while keeping the remaining coordinate dimensions fixed.

Therefore, we are deploying an alternative solver which no longer uses the dimensional operator splitting. This of course has the drawback that for a Crank-Nicolson dis-
cretisation of the diffusion problem the resulting matrix-equation no longer has tri-diagonal form. While the tri-diagonal form has the advantage that a solution can be computed directly and efficiently, modern numerical methods can handle sparse matrix problems very efficiently, too. We are currently testing the implementation of such a method. In particular the solution of the steady state problem is very efficient as it does not invoke any time-integration steps. Here we are using two different approaches in parallel. On the one hand we implemented a method, which solves the steady state problem only. This has the advantage that there is no longer a decrease in accuracy due to the order of the time discretisation. On the other hand we also implemented a time-dependent solver, where we can follow the time-dependent evolution of the Cosmic Ray distribution within the Galaxy. This is, e.g., used in cases where temporally variable sources are needed to be considered. For the latter we use the result from the steady state solver as an initial condition that is to be modified by temporal effects. The new solver uses operator splitting for the time-dependent problem. We use adapted solvers for each physically distinct term in the transport equation instead of simple dimensional operator splitting as used within GALPROP. That is we apply different solvers for spatial convection, spatial diffusion and diffusion and energy losses in momentum space. Within the solution of the transport problem we allow for a full spatial variation of the diagonal components of the diffusion tensor. Corresponding analytical tests show satisfactory results.

A specific description of these new solvers will be given in an upcoming publication where we will show the convergence properties and the numerical error by comparison to analytical tests. In particular, the final result will no longer rely on convergence criteria to be selected by the user. This allows the user to concentrate on the physical problem at hand and facilitate consistent comparisons within the community. Our new CR transport code is capable of utilizing modern parallel computing architecture by using the Message Passing Interface (MPI) standard.

4 Summary and Discussion

New observational constraints on the input parameters of CR transport models as well as the increase in available computing power necessitate a transitions from 2D modelling towards 3D simulations of CR propagation in our Galaxy. We study this transition from 2D to 3D simulations using an existing code (GALPROP), and find significant deviations for electrons with energies higher than 200 GeV. For protons we find a general agreement except for discrepancies on the percent level. Our comparison shows the need for practical and universal convergence criteria. Using sub-kpc scale 3D simulations we investigate a non-axisymmetric CR source distributions following a spiral arm pattern that allows us to address scientific questions inaccessible to 2D simulations. We demonstrate the need for an efficient CR transport code that makes use of parallel computing architectures.

Motivated by our findings we present a brief overview of our new CR transport code. This code uses contemporary numerical methods in a way that the user no longer unknowingly faces convergence issues. The new code will rely on a number of solvers, each optimized for different physical sub-processes in the CR propagation equation, and is capable of treating anisotropic diffusion. Our CR transport code utilises modern parallel computing architectures.

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