MPI-AMRVAC FOR SOLAR AND ASTROPHYSICS

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ABSTRACT

In this paper, we present an update to the open source MPI–AMRVAC simulation toolkit where we focus on solar and non-relativistic astrophysical magnetofluid dynamics. We highlight recent developments in terms of physics modules, such as hydrodynamics with dust coupling and the conservative implementation of Hall magnetohydrodynamics. A simple conservative high-order finite difference scheme that works in combination with all available physics modules is introduced and demonstrated with the example of monotonicity-preserving fifth-order reconstruction. Strong stability-preserving high-order Runge–Kutta time steppers are used to obtain stable evolutions in multi-dimensional applications, realizing up to fourth-order accuracy in space and time. With the new distinction between active and passive grid cells, MPI–AMRVAC is ideally suited to simulate evolutions where parts of the solution are controlled analytically or have a tendency to progress into or out of a stationary state. Typical test problems and representative applications are discussed with an outlook toward follow-up research. Finally, we discuss the parallel scaling of the code and demonstrate excellent weak scaling up to 30,000 processors, allowing us to exploit modern peta-scale infrastructure.

Key words: hydrodynamics – magnetohydrodynamics (MHD) – methods: numerical

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1. INTRODUCTION

Computational astrophysics witnessed an unprecedented growth in scope and diversity over the last few decades. While dedicated, problem-tailored software efforts continuously explore novel solution methods for challenging applications, a fair amount of progress has been realized through open source, community-driven software development. The study of astrophysical magnetofluid dynamics in particular, encompassing pure solar as well as general astrophysical research topics, has seen a flurry of codes generating new insights. Original codes like ZEUS (Stone & Norman 1992), Stagger (Galsgaard & Nordlund 1996), or the Versatile Advection Code (VAC; Tóth 1996; Tóth & Odstrčil 1996; Tóth 2000) exploited different discretizations applied to equivalent formulations of the governing partial differential equation (PDE) system for magnetohydrodynamics (MHD) and have already showed the benefit of having the option to select a discretization most suited for the problem at hand. The development of shock-capturing schemes, where in analogy with gas dynamics the hyperbolic structure of the ideal MHD system is exploited, has driven algorithmic improvements to solve especially shock-dominated problems (see, e.g., chapter 19 in Goedbloed et al. 2010). MPI–AMRVAC combines these algorithms with automated mesh refinement (AMR) for a fair selection of primarily hyperbolic PDE systems covering (multi-fluid) gas dynamics, non-ideal Newtonian, and ideal relativistic MHD.

A non-exhaustive list of software frameworks that are in active use and development to date includes Riemann (Balsara 2001), BATS-R-US (Powell et al. 1999; Tóth et al. 2012) (a key component of the Space Weather Modeling Framework (Tóth et al. 2005)), Nirvana (Ziegler 2008), Ramses (Fromang et al. 2006), AstroBear (Cunningham et al. 2009), Pluto (Mignone et al. 2007, 2012), HiFi (Lukin & Linton 2011), Enzo (Bryan et al. 2014), Echo (Del Zanna et al. 2007), FLASH (Fryxell et al. 2000), Raccoon (Dreher & Grauer 2006), COSBOLD (Freytag et al. 2012), Athena (Stone et al. 2008, Lare3D (Arber et al. 2001), Pencil (Brandenburg & Dobler 2002), A-MAZE (Walder & Folini 2000), Gmics (Gordeev et al. 2010), Pencil (Brandenburg & Dobler 2002), A-MAZE (Walder & Folini 2000), Gumics (Gordeev et al. 2010) have made significant progress on solar physics applications where MHD descriptions are combined with radiative transfer treatments. Other codes like WhiskyMHD or HARM concentrate on high-energy, general relativistic phenomena (Giacomazzo & Rezzolla 2007; Gammie et al. 2003). In this paper, we present an update to the open source software MPI–AMRVAC, which has evolved alongside the codes already mentioned, originally as a tool to study adaptive mesh refinement paradigms for hyperbolic PDE systems such as the ideal MHD set (Keppens et al. 2003; van der Holst & Keppens 2007), and currently evolved to a mature multi-physics software framework with the possibility to couple varying PDE models (Keppens & Porth 2014) across the block-adaptive AMR strategy. Using the LASY syntax (Tóth 1997) and with heritage in the solver part from VAC (Tóth & Odstrčil 1996), the software has kept its dimension-independent implementation while the AMR allows Cartesian, polar, cylindrical, or spherical coordinate systems (or generalizations thereof with simple Jacobians). Although the emphasis has lately been on handling special relativistic hydro to MHD applications (Meliani et al. 2007; van der Holst et al. 2008; Keppens et al. 2012), covering gamma-ray burst afterglow physics (Vlasis et al. 2011; Meliani & Keppens 2010), X-ray binary (Monceaux-Baroux et al. 2014) or active galactic nuclei relativistic jet modeling (Keppens et al. 2008; Walg et al. 2013; Porth 2013), and pulsar wind nebulae physics (Porth et al. 2014), the present version of the software incorporates many options for Newtonian applications inspired by astrophysical or solar phenomena. Since several of the most recent additions can be of generic interest to the astrophysical community, here we present an overview of both
algorithmic- and application-driven aspects that have not been documented elsewhere. The details of the parallel, block-adaptive implementation as in Keppens et al. (2012) remain irrespective of the precise discretization or physics module adopted and will not be repeated here. Instead, in Section 2, we explain how, in addition to the many flavors of shock-capturing schemes (e.g., TVDLF, HLL, HLLC, and Roe), we now incorporate higher than average, second-order accurate spatio-temporal discretizations as well. With respect to new physics applications, we chose to highlight the gas using a dust physics module where an arbitrary number of dust species can be dynamically followed in their size-dependent, drag-modulated evolution through a compressible gas. Recent applications of gas dynamics with relevant dust influences have looked at circumstellar bubble morphologies (van Marle et al. 2011b), Rossby Wave Instability development of vortices in accretion disks (Meheut et al. 2012), or Kelvin–Helmholtz developments in the context of molecular clouds (Hendrix & Keppens 2014b). Since the gas–dust physics module has not been described and tested in detail elsewhere, we here present a stringent suite of tests inspired by recent literature in Section 3. To make contact with modern efforts targeting plasma dynamics in solar conditions, Section 4 provides an update to the treatment of MHD and Hall-MHD applications and how we allow for background potential magnetic fields of significant complexity, based on data-driven extrapolations from actual magnetograms. An update of scaling on massively parallel computers is provided, while the appendices further report on the use of active and passive grid blocks, the means to generate slices or collapsed views on evolving three-dimensional (3D) dynamics during runtime, which are all of general interest to complementary coding efforts.

2. HIGH-ORDER METHODS

While a large share of spectacular astrophysical magnetofluids display shock-dominated dynamics, a number of interesting applications can be described as fairly “smooth.” These may involve the study of wave propagation in magnetically structured media, the in-depth study of magnetic reconnection processes when dissipative layers are resolved, and various other typical solar or stellar magnetoconvection problems. Beeck et al. (2012) recently compared high-order finite difference (FD; MURA-M, Stagger) with finite volume (FV) treatments (COSBOLD) for hydrodynamic convective layers with radiative transfer, with reasonable agreement but also subtle differences in turbulence properties. Simulations of magnetic reconnection in the regime of chaotic island formation (Keppens et al. 2013) also identified several pros and cons when different discretizations are used on the same problem. Having the option to choose a method depending on the application is obviously beneficial.

Discontinuous flows naturally call for an FD discretization which solves the fluid equations in their integral form. Like many open source software in active use today, MPI-AMRVAC offers a rather large option of FD schemes (Keppens et al. 2012) with total variation diminishing (TVD) type methods like TVDLF or full Riemann solver based solvers as originally described in Töth & Odstrčil (1996), extended with variants like HLL or HLLC. To varying degrees, these methods require adaptation to the set of governing PDEs at hand (Euler gas dynamics to MHD, Newtonian to relativistic). The pitfall of these methods, however, is that higher than second-order FV schemes must employ multi-dimensional stencils, which considerably increases the computational cost. In MPI-AMRVAC, all FV schemes can render up to second-order accuracy, while some reconstruction procedures with higher than second-order capabilities have been incorporated as well, typically to reduce the diffusion in these schemes. FD schemes, on the other hand, are well suited for smooth applications and can operate to high order with one-dimensional (1D) stencils. In this section, we describe the fairly general approach to conservative finite differencing of a hyperbolic conservation law as is now available in MPI-AMRVAC. The only requirement for implementation to a different physics module is knowledge of the fluxes and of the fastest characteristic velocity. Thus, the FD scheme can be applied to all physics modules from hydrodynamics over Hall-MHD to relativistic MHD, or any other PDE set which may be added as a new physics module.

2.1. Short Primer in Conservative Finite Differences

Given a set of (near-) conservation laws in Cartesian coordinates,
\[ \partial_t \mathbf{U} + \nabla \cdot \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U}); \quad \partial_t U_i + \sum_j \partial F_{ji}(\mathbf{U})/\partial x_j = S_i(\mathbf{U}), \]  

we seek the conservative FD discretization of the flux in the \( j \) direction \( \partial F_{ji}/\partial x_j \). Regarding only one component of the solution vector \( \mathbf{U} \) and dropping the index \( l \), the point-wise value at grid index \( i \) reads
\[ \frac{\partial F_j}{\partial x_j}_{|i} = \frac{1}{\Delta x_j} (\tilde{F}_j|i+1/2 - \tilde{F}_j|i-1/2); \quad F_j|i \]
\[ = \frac{1}{\Delta x_j} \int_{x_j|i-1/2}^{x_j|i+1/2} \tilde{F}_j(\chi) d\chi. \]  

We see that the point-wise value \( F_j|i \) is just the \( j \)-directional cell-average of the function \( \tilde{F}_j(\chi) \). For the discretized \( \partial F_{ji}/\partial x_j \), we require knowledge of the interface values of \( \tilde{F}_j(\chi) \) which is obtained by reconstruction of the cell-averages of \( \tilde{F}_j(\chi) \), and hence the known point-wise values of \( F_j|i \). This is simply the hallmark of FV reconstruction: obtain (point-wise) interface values of the solution vector from its cell-averages. Instead, in FDs, we can simply apply the FV reconstruction formula to the point-wise flux, to obtain
\[ \tilde{F}_j|i+1/2 = R_{i+1}(F_j). \]  

All directions are treated in analog fashion and we form the directionally unsplit time-update operator
\[ \mathcal{L}_i(\mathbf{U}) = - \sum_j \frac{\partial F_{ji}}{\partial x_j} + S_i(\mathbf{U}); \quad \frac{dU_i}{dt} = \mathcal{L}_i(\mathbf{U}), \]  

which represents an ordinary differential equation (ODE) in time for each spatial grid point.

2.2. Applied Flux Splitting

As in FD methods, for numerical stability, the flux needs to be upwinded. In FDs, this is achieved with flux vector splitting (FVS; see, e.g., the book of Toro 1999). Several approaches toward flux splitting exist and comprise the Roe flux split, the Marquina’s flux split (Fedkiw et al. 1998, and references

\footnote{The index \([i] \) in square brackets should remind us of the index-range given by the stencil of the reconstruction.}
In particular, we split the flux as

$$F_j^- = \frac{1}{2}(F_j - c_{\text{max}} U), \quad F_j^+ = \frac{1}{2}(F_j + c_{\text{max}} U),$$  \hspace{1cm} (5)

where $c_{\text{max}}$ is the grid-global maximal characteristic velocity of the hyperbolic system, and we reconstruct

$$\hat{F}_j^+_{i+1/2} = R(L)F_j^+; \quad \hat{F}_j^-_{i+1/2} = R(R)F_j^-.$$  \hspace{1cm} (6)

Finally, the interface flux is obtained as

$$\hat{F}_j_{i+1/2} = \hat{F}_j^+_{i+1/2} + \hat{F}_j^-_{i+1/2}.$$  \hspace{1cm} (7)

This is similar to MHD applications by Jiang & Wu (1999); Mignone et al. (2010) and to the relativistic hydrodynamic (HD) application by Radice & Rezzolla (2012). However, note that we omit the projection onto characteristic fields and instead apply two upwinded reconstructions per interface. The projection step is intended to reduce oscillations in the solution at the price of greatly increased computational cost. It has been observed (e.g., van Leer 1982; Toro 1999) that the Lax–Friedrichs FVS utilized here introduces excessive numerical diffusion at contact and tangential discontinuities.\(^4\) Thus, in problems where contacts and (viscous) boundary layers are of interest, one should resort to Riemann-based solvers provided by \texttt{MPI-AMRVAC}. This general flaw is less important in flows with few stagnant points and it can be alleviated substantially by adopting high-order reconstruction techniques. In the following sections, we demonstrate that the simplified scheme described here turns out to be quite capable in the treatment of “smooth” astrophysical flows. By the design of Equation (2), the scheme is fully conservative (save for the addition of geometric and physical source terms in step (4)) and can adopt a high spatial order by the choice of the reconstruction step 3. To this end, we provide compact stencil third-order reconstruction (\cite[C}ada & Torrilhon 2009, LIM03) and fifth-order, monotonicity-preserving reconstruction “MP5” by \cite{SuHu}.\(^5\)

### 2.3. Temporal Discretizations

Apart from the standard one-step, two-step predictor-corrector, and third-order Runge–Kutta (Gottlieb & Shu 1998, RK3), we have implemented two multistep, high-order, strong stability-preserving (SSP) schemes introduced by \cite{SpRu}. These yield an explicit numerical solution to the ODE given by Equation (4). Adopting a general $s$-step Runge–Kutta scheme in the notation of \cite{SpRu} (their Equation (2.1) a–c),

$$U^{(0)} = U^n, \hspace{1cm} (8)$$

$$U^{(i)} = \sum_{k=0}^{i-1} \alpha_{ik} U^{(k)} + \Delta t \beta_{ik} \mathcal{L}(U^{(k)}), \quad i = 1, 2, \ldots, s \hspace{1cm} (9)$$

$$U^{n+1} = U^{(s)}, \hspace{1cm} (10)$$

the available optimal $s$-step, $p$-order, SSP Runge–Kutta (SSPRK($s,p$)) schemes read.

\(^4\) In fact, this is true for most schemes that are not based on complete Riemann solutions, with rare exceptions, e.g., pressure-split schemes (AUSM) in the tradition of Liou & Steffen (1993).

### 2.3.1. SSPRK(4,3)

$$(\alpha_{ik}) = \begin{pmatrix} 1 & - & - & - \\ 0 & 1 & - & - \\ 2/3 & 0 & 1/3 & - \\ 0 & 0 & 0 & 1 \end{pmatrix}; \hspace{1cm} (11)$$

$$(\beta_{ik}) = \begin{pmatrix} 1/2 & - & - & - \\ 0 & 1/2 & - & - \\ 0 & 0 & 1/6 & - \\ 0 & 0 & 0 & 1/2 \end{pmatrix}.$$  \hspace{1cm} (12)

This scheme requires storage of two intermediate steps and is SSP for a Courant number (CFL) of 2.

### 2.3.2. SSPRK(5,4)

$$(\alpha_{ik}) = \begin{pmatrix} 1 & - & - & - & - \\ 0.44437049406734 & 0.55562950593266 & - & - & - \\ 0.62010185138540 & 0 & 0.37989814861460 & - & - \\ 0.17807995410773 & 0 & 0 & - & - \\ 0.82192004589227 & 0 & 0 & 0 & - \\ 0.00683325884039 & 0 & 0 & 0 & 0.51723167208978 \end{pmatrix}.$$  \hspace{1cm} (13)

This scheme requires storage of four intermediate steps and is SSP for a CFL number of 1.50818004975927.

Combined with FDs and MP5 reconstruction, the latter scheme theoretically allows fourth-order accuracy in time and space. We validate the expected convergence behavior in Sections 4.5.1 and 4.5.3 on MHD problems, as realized by the plasma physics module in \texttt{MPI-AMRVAC}.

### 3. ASTROPHYSICAL GAS AND DUST DYNAMICS

Before describing the plasma physical module, we first discuss the recently added coupled gas–dust possibilities, which is of interest to a fair variety of astrophysical applications. We will use both FV implementations and the new FD schemes on a selection of test problems. In this dusty hydrodynamics module, \texttt{MPI-AMRVAC} handles the following set of governing equations.

#### 3.1. Continuity and Momentum Equations

The density $\rho$ and velocity vector field $\mathbf{v}$ combine in a conservation of mass, written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = S_\rho,$$  \hspace{1cm} (14)

where a user may prescribe the sink/source terms for mass loss/creation in $S_\rho$. The evolution for the velocity field incorporates inertial effects and pressure gradients, and can include external gravity, viscous forces, friction with multiple dust species, or any user-specified force written as

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \rho g - \nabla \cdot (\mu \mathbf{\hat{I}}) + \sum_{d=1}^{n_d} \mathbf{F}_d + \mathbf{S}_\nu.$$  \hspace{1cm} (15)
In this equation, the external gravitational field is quantified by the gravitational acceleration \( \mathbf{g}(x) \) and viscosity is quantified by the viscous force written with the aid of the traceless tensor \( \Pi = \frac{1}{2}(\nabla v + (\nabla v)^T) + (2/3)\hat{\nabla} \cdot v \) (with identity tensor entries \( \hat{\delta}_{ij} \)) and the coefficient of the dynamical viscosity \( \mu \). A set of \( n_d \) dust species is coupled to the gas with a drag force that has an essential dependence on \( \mathbf{f}_d(\rho, \rho_d, v_d, v) \), i.e., on the gas and dust densities and velocity differences. A user-defined force would enter through \( S_m \). In the MPI-AMRVAC code, the mass-conservation and velocity-evolution equations are actually combined into a momentum (with momentum density \( \mathbf{m} = \rho \mathbf{v} \)) conservation equation, written as

\[
\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot (\mathbf{m} + p \hat{\mathbf{1}}) = \rho \mathbf{g} - \nabla \cdot (\mu \hat{\nabla}) + \sum_{d=1}^{n_d} \mathbf{f}_d + \mathbf{S}_m + \mathbf{v} \mathbf{S}_p.
\]

The latter two terms then form the user-momentum source term \( \mathbf{S}_m = \mathbf{S}_d + \mathbf{v} \mathbf{S}_p \).

When dust species are present, each among the \( n_d \) dust species obeys a pressureless gas evolution, with dust density \( \rho_d \) and velocity \( v_d \), and hence momentum density \( \mathbf{m}_d = \rho_d v_d \), governed by

\[
\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d v_d) = 0,
\]

\[
\frac{\partial \mathbf{m}_d}{\partial t} + \nabla \cdot (\mathbf{v}_d \mathbf{m}_d) = - \mathbf{f}_d.
\]

In addition to the (user-controlled) addition of \( n_d \) dust species (when \( n_d = 0 \) no equations or variables are added), one may opt to add a number of \( n_{tr} \) tracer quantities \( \theta_{tr} \) (with \( tr = 1, \ldots, n_{tr} \)). Each tracer actually adds a simple equation of the form

\[
\frac{\partial D_{tr}}{\partial t} + \nabla \cdot (D_{tr} \mathbf{v}) = \theta_{tr} \mathbf{S}_p.
\]

This form ensures that while we can treat the quantity \( D_{tr} = \rho \theta_{tr} \) in a manner similar to the density evolution Equation (14), we can at each time use them to obtain the actual tracer values from \( D_{tr} / \rho \), which in turn obey the simple advection equation

\[
\frac{\partial \theta_{tr}}{\partial t} + \mathbf{v} \cdot \nabla \theta_{tr} = 0.
\]

### 3.2. Closure and Energy Equation

The above sets of equations need further closure, which can be obtained with one of the following options.

1. Prescribe the pressure-density relation, e.g., using a \( p = c_{ad} \rho^\gamma \) relation where one can adopt an isothermal (\( \gamma = 1 \)) or a polytropic relation. The constant \( c_{ad} \) is then either related to the squared isothermal sound speed or to constant entropy. Also, the case of a zero-temperature gas \( c_{ad} = 0 \) is contained in this closure. Under this setting for the equation of state, no further energy equation is needed.

2. Adopt an ideal gas with the internal energy density \( e = p / (\gamma - 1) \) itself governed by

\[
\frac{\partial e}{\partial t} + \nabla \cdot (ve) + p \nabla \cdot v = -(\mu \hat{\nabla} \cdot \mathbf{v}) \cdot \mathbf{v} + \nabla \cdot (\kappa \nabla T) - n_i n_e \Lambda(T) + S_e,
\]

where viscous heating represents the first term on the right hand side, isotropic thermal conduction introduces the temperature-dependent heat conduction coefficient \( \kappa(T) \), and an ideal gas law relates pressure, temperature, and density through \( p = (k_b / \mu m_p) \rho T \) (with mean molecular weight \( \mu_m \), Boltzmann constant \( k_b \), and proton mass \( m_p \)). Dimensionless, the latter is written as \( p = \rho T \). Optically thin radiative losses are represented by the term \(-n_i n_e \Lambda(T) \) which has a tabulated temperature-dependent loss function \( \Lambda(T) \) (several tables used in the solar to astrophysics literature are pre-implemented, while the ion-electron density product \( n_i n_e \) for a fully ionized hydrogen plasma is \( \rho^2 / m_p^2 \)). When optically thin radiative losses are incorporated (a module that is also relevant for Newtonian MHD), the need for AMR in combination with various (explicit, semi-implicit, and exact) local source evaluations was demonstrated in van Marle & Keppens (2011). A user can add an internal energy source/sink through \( S_e \).

In the latter case, instead of the internal energy Equation (20), the code evolves an evolution equation for the (conserved) total energy \( E \) consisting of internal and kinetic energy with \( E = p / (\gamma - 1) + \rho v^2 / 2 \). By combining Equation (20) and the velocity evolution Equation (15) (actually \( v \) operating on this equation), we obtain the total energy density evolution as

\[
\frac{\partial E}{\partial t} + \nabla \cdot (v(E + p)) = \rho \mathbf{v} \cdot \mathbf{g} + \nabla \cdot (\kappa \nabla T) - \nabla \cdot (\mathbf{v} \cdot \mu \hat{\nabla}) + \sum_{d=1}^{n_d} \mathbf{f}_d \cdot v - n_i n_e \Lambda(T) + S_e + \mathbf{v} \cdot \mathbf{S}_v.
\]

We have purposely written the governing equations in the form of Equation (1), indicating the terms treated as sources on the right-hand side, while fluxes as used in the different shock-capturing discretization schemes can be read on the left-hand side. The implemented equations thus consist of Equation (14), Equation (16), the optional equation sets of the form (17) for each dust species, or Equation (18) for each optional tracer, and when an energy equation is taken along, Equation (21) is evolved.

### 3.3. Dusty Gas Test Suite

As described earlier, the dust module is similar to the hydrodynamics module, with the addition of an arbitrary number of dust fluids which can be flexibly defined. Each dust fluid has several properties, such as the size of the represented particles, \( a_d \), and the internal density of the dust grains, \( \rho_p \). By having different values for \( a_d \) and \( \rho_p \), one can, for example, model the dynamical effect of a dust size distribution or the effect of...
having particles with different chemical compositions. A dust fluid typically interacts with the gas fluid through the combined Stokes/Epstein drag force $f_d$, defined as

$$f_d = -(1 - \alpha) \pi n_d \rho_d a_d^2 \Delta v_d \sqrt{\Delta u_d^2 + v_t^2}, \quad (22)$$

with $\alpha$ being a temperature-dependent sticking coefficient (Decin 2006), $T$ being the gas temperature, $n_d$ the dust particle density of the $d$th dust species, $\Delta v_d = v - v_d$ the difference between the gas and dust velocity, and $v_t$ the thermal speed of the gas. Other drag laws are available as well. No interaction between dust fluids is included. In the following, we present four tests performed with this dust module of the MPI-AMRVAC code. Due to the added complexity of having one or multiple dust species, it often becomes difficult or impossible to find analytical results for many test problems. To demonstrate the validity of the implementation, we have selected test problems with known solutions or problems for which the purely hydrodynamical variant has been studied in detail in other works. Note that three out of our four tests (the dustybox, dustywave, and the Sedov blast wave) have been presented in the test suite of the dust+gas smoothed particle hydrodynamics (SPH) simulations by Laibe & Price (2012). Additionally, a gas+dust variant of the Sod shock tube test (Sod 1978) performed with MPI-AMRVAC has been presented in Hendrix & Keppens (2014a). Furthermore, these tests highlight some typical dust features.

In all tests, we use the dust fluids to represent a dust mixture made of spherical silicates ($\rho_p = 3.3$ g cm$^{-3}$) with a dust grain size distribution $n(a_d)$, with sizes between $10^{-7}$ cm and $2.5 \times 10^{-5}$ cm. In the interstellar medium (ISM), this size range is typically observed to follow a distribution of $n(a_d) \propto a_d^{-3.5}$ (Draine & Lee 1984). We model this distribution by dividing the size range into bins with equal total mass, and representing each bin by a dust fluid with a specific dust particle size. This is explained in detail in Hendrix & Keppens (2014b). The local amount of dust in the system is often quantified by the dust-to-gas ratio $\delta$, which is the total mass density of the dust divided by the mass density of the gas.

### 3.3.1. Dustybox

In this test problem, one or multiple dust fluids start with an initial velocity difference with respect to a stationary gas fluid. Due to the drag force, the gas will be accelerated by the dust, and all dust species will decelerate at a rate imposed by the properties of the fluid. Laibe & Price (2011) presented analytical solutions for multiple drag laws in the presence of a single dust fluid and compared this with simulations in Laibe & Price (2012). To demonstrate the validity of our implementation, we compare a simulation with four dust species using the physical drag force described in Equation (22) with the semi-analytical solution of the problem. In the case of one dust species, the analytical solution of the change in velocities of the dust and gas fluid are given in Laibe & Price (2012). We expand this approach to provide a solution for an arbitrary number of dust fluids with the drag force in Equation (22), which leads to a set of $N$ coupled nonlinear ODEs for the time-dependent functions $f_i(t)$, $v_i(t)$, and $v_d(t)$, namely,

$$\frac{d\Delta v_d}{dt} = \frac{1}{\rho} \sum_{i=1}^{N} f_i + f_d,$$  \quad (24)

with $N$ being the number of dust fluids. Note that the terms $f_i$ are functions of $v_i$, as can be seen for the Epstein-Stokes drag in Equation (22). We can solve this set of differential equations using a Python script to find a semi-analytical solution. For the case of one dust fluid, we recover the analytical solution mentioned earlier.

We use a 1D setup, employing a uniform grid with 40 cells and periodic boundary conditions. Note, however, that the setup itself is resolution independent. We set uniform gas and dust densities with $\rho = 10^{-20}$ g cm$^{-3}$, and a 100 times lower ($\delta = 0.01$) total dust mass. Velocities are set to $v = 0$ and $v_d = 5 \times 10^3$ cm s$^{-1}$ for all dust species. The gas temperature is set to $T = 100$, giving a sticking coefficient $\alpha = 0.32$ in Equation (23). As our numerical scheme we use the TVD-LF solver (Tóth & Oströhl 1996) with a two-step time integration and a “Woodward”-type slope limiter (Colella & Woodward 1984). We use a CFL number of 0.2. The result of the simulation with four dust species, compared with the semi-analytical solution, is given in Figure 1. We see that we obtain a perfect fit between the simulation and the semi-analytical solution. The simulation demonstrates how the four dust fluids start with a velocity difference relative to the gas fluid. Due to the interaction with the gas, the dust fluids decelerate. Species 1 represents the smallest particles and can be seen to decelerate faster than the other dust fluids. Larger dust grains have a higher inertia and take longer before they come to an equilibrium velocity with the gas.

### 3.3.2. Dustywave

The dustywave problem, presented in detail in Laibe & Price (2011), describes the propagation of a linear sound wave in a uniform, stationary medium with one or more embedded dust fluids. The coupling of the waves in the gas and dust fluids, as well as the dampening of the waves, are strongly dependent on the dust-to-gas ratio and the strength of the drag force.
Figure 2. Comparison between the simulation with 120 cells and the analytical solutions for different values of the drag coefficient $K$ at $t = 10$. The simulated values of the gas and dust velocities are represented by black filled and open circles, respectively, while the analytic velocities of the gas and dust are given by red solid and dashed lines. Note that the vertical scales for $K = 1$ and $K = 10$ differ from other simulations, as the velocities are damped more effectively in these cases.

Figure 3. Part of the domain in dustywave simulations with $K = 100$ at $t = 10$ (the whole domain is shown in Figure 2). Different spatial resolutions are compared with the analytic solution. The amplitude of the gas velocity at this time is correctly recovered, even for resolutions as low as 20 cells in the case of the high-order FD method. A lower accuracy is obtained for the lower-order solutions using a TVDLF scheme.

An analytic solution for a mixture with one dust fluid is known (Laibe & Price 2011), and is used here to demonstrate the accuracy of our simulations.

Following Laibe & Price (2011), we use $\rho = \rho_d = 1$, $v = v_g = 0$, and one dust species. Likewise, we use the isothermal equation of state $p = c_s^2 \rho$ and a speed of sound of $c_s = 1$. A sine-shaped perturbation in velocity and both gas and dust densities is added; in all cases, the amplitude of the perturbation is $10^{-4}$ and the wavelength is the same as the size of the domain. We simulate this setup in a 1D domain between $x = 0$ and $x = 1$ with several resolutions. For the purpose of testing and comparison, we now use a simplified drag force of $f_d = K \Delta v$ with a constant of $K$. We use the FD solver together with the fifth-order MP5 limiter and the SSPRK(5, 4) time integration using a CFL number of 0.5. In Figure 2, the simulation results at time $t = 10$ for simulations with weak ($K = 0.01$) up to strong drag ($K = 100$) are compared with the analytical solution. All simulations have the same resolution ($\Delta x = 8.33 \times 10^{-3}$, i.e., 120 cells with no AMR). For intermediate coupling ($K$ between 0.1 and 10), the solutions for the dust and gas velocity can be seen to be out of phase. This phase difference causes strong damping in the setups with $K = 1$ and $K = 10$. All cases are in good agreement with the analytic results and errors are typically below 0.5%. Importantly, in other approaches such as the SPH method in Laibe & Price (2012), overdamping of the velocity is seen for $K = 100$ due to the high drag force when the spatial resolution is low, leading them to propose a resolution criterion of $\Delta x \lesssim c_i t_s$ with $t_s$ representing the stopping time $t_s = \rho \rho_d / K (\rho + \rho_d)$, which in this test would mean about 200 cells. However, Figure 3 demonstrates that by using high-order schemes, we obtain results without overdamping with as little as 20 cells. In contrast, if we use a TVDLF scheme with a “Woodward”-type limiter (Colella & Woodward 1984) and a two-step time advance with a CFL number of 0.2, Figure 3 shows that stronger damping is observed for the case with 40 cells (≈4% at peak value, compared to only 0.2% for 40 cells with the high-order schemes). By lowering the resolution to 20 cells, a strongly dampened and shifted solution is found.

3.3.3. Sedov Blast Wave with Dust Species

The Sedov blast wave problem is a classical problem in which a high-energy perturbation is introduced in a static background, causing a shockwave to propagate through the external medium. It is often used to test codes, see for example Tasker et al. (2008), who compare the ability of several fluid and SPH codes to simulate the Sedov blast wave problem. A version with one
dust fluid is discussed in Laibe & Price (2012). In the gas-only case, an analytical solution for the location of the blast wave is known.

Our ambient medium has a uniform gas density \( \rho_0 = 6 \times 10^{-23} \text{ g cm}^{-3} \) and a dust-to-gas ratio of \( \delta = 0.01 \) using four dust species. The pressure is set to \( p = 1.44 \times 10^{-14} \text{ dyn cm}^{-2} \), except in the middle of the domain where we introduce high pressure \( (p = 7.49 \times 10^6 \text{ dyn cm}^{-2}) \) in a spherical region with a radius of 0.01 parsec. The gas fluid has an adiabatic index of 5/3. The simulations are performed in 3D with Cartesian coordinates, in a cubical domain with sides of one parsec. The boundaries have open outflow conditions. We use three levels of AMR, resulting in an effective resolution of 4003. With this resolution the middle region is covered in 280 cells, resulting in a total central energy of \( E_0 = 2.098 \times 10^{51} \text{ erg} \). We use the TVDLF solver with a three-step time integration and a “Woodward”-type slope limiter. We use a CFL number of 0.4. Figure 4 shows a two-dimensional (2D) output of the gas density in the 3D domain integrated along the line of sight using the collapse feature of MPI-AMRVAC, as described in Appendix B. The position of the shock front at time \( t \) has been calculated analytically in Sedov (1959) and Landau & Lifshitz (1959), and is found to be

\[
r(t) = \left( \frac{E_0}{\rho_0} \right)^{1/5} t^{2/5}
\]

with \( E_0 \) being the energy in the central region, \( \beta = 0.49 \) for an ideal gas with \( \gamma = 5/3 \) (Tasker et al. 2008), and an ambient density \( \rho_0 \). We simulate up to \( t = 3.16 \times 10^{15} \text{ s} \) (10 yr), at which time Equation (25) predicts a distance of 0.483 pc. Figure 4 demonstrates that the same radius is obtained in our simulations with the addition of dust with \( \delta = 0.01 \).

In Figure 5, a 1D cut is made clearly showing the distance which the gas and dust fluids have propagated. As the gas shock propagates through the ambient medium, dust is also accelerated. Small dust particles are more strongly coupled to the gas, resulting in a density peak close to the location of the shock. The density of dust species one is closely coupled to that of the gas. We see in Figure 4 how the dust separates into regions depending on the sizes of the particles. Figure 5 shows how dust species two, three, and four have two peaks. The one closest to the shock is due to the steady acceleration of ambient dust particles by the gas shock. The second peak is the result of the initially high velocity of the gas, which accelerates dust to a velocity that depends on the particle size as large dust particles take longer to accelerate. As this high-velocity dust moves outward, it sweeps up the dust in front of it, causing the second peak. Dust species one only has one peak as the initially accelerated dust moves along with the gas.

3.4. Cloud Shock in Gas–Dust settings

Our final gas–dust application models the interaction of a high-density structure with a shock wave. This test is clearly relevant in the ISM where dusty clouds are often seen to interact with supernova shocks. In the interstellar environment, the stability of high-density structures is of importance in estimating the rate of stellar formation. Numerically, the cloud is often modeled as a spherical high-density structure embedded in a lower-density ambient medium with a planar shock wave propagating through the domain (Patnaude & Fesen 2005; Nakamura et al. 2006; Agertz et al. 2007). The interaction between the shock wave and the cloud can cause several instabilities, which may lead to the disruption of the cloud. Here, we demonstrate the ability to add dust to the setup in both the cloud region and the ambient medium.

The cloud shock test is simulated in a 2D Cartesian domain with a size of \((3.34 \text{ pc})^2\). We use six levels of AMR to obtain an effective resolution of \((5120 \times 5120)\). The ambient medium and the cloud, which has a radius of 0.57 pc, are initially stationary. In the surrounding medium we have \( \rho_R = 10^{-21} \text{ g cm}^{-3} \), and in the cloud \( \rho = 10 \rho_R \). The pressure is set using

\[
p_R = \frac{\rho_R k_b T_R}{\mu_m m_p},
\]

where \( k_b \) is the Boltzmann constant, \( m_p \) is the hydrogen mass, and \( \mu_m = 2.3 \) is the molecular weight of the ISM at \( T_R = 200 \text{ K} \). On the left side of the simulation, we introduce a shocked region with values of \( \rho_L, \rho_L, \) and \( v_L \) calculated from the Rankine–Hugoniot conditions, that is,

\[
\rho_L = \frac{\rho_R \theta + \rho_{rat}}{1 + \theta \rho_{rat}},
\]

\[
v_L = c_R M \left( 1 - \frac{\theta + \rho_{rat}}{\theta + \rho_{rat}} \right)^2,
\]

\[
p_L = \frac{p_R}{\theta + \rho_{rat}},
\]

\[
\rho_{rat} = \frac{1}{1 + 2(M^2 - 1) \frac{\rho}{\rho_{rat}}}.
\]
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Figure 6. Left: density distribution at $t = 3.01 \times 10^5$ yr. The entire domain is shown. Typical features such as the bow shock, the disturbed cloud with Richtmyer–Meshkov features on the front side, and a low-density region Rayleigh–Taylor instability behind the cloud are shown. Right: a zoomed-in look at the dust density distribution of species two in the cloud region. The dust can be seen to be tightly coupled to the dynamics of the cloud.

(A color version of this figure is available in the online journal.)

\[
\theta = \frac{\gamma + 1}{\gamma - 1},
\]

\[(31)\]

\[
c_R = \sqrt{\frac{\gamma \rho_R}{\rho_R}},
\]

\[(32)\]

with a Mach number of $M = 10$ and $\gamma = 5/3$. This results in the initial values of $p_L = 1.25 \times 10^2 \rho_R$, $\rho_L = 3.88 \rho_R$, and $v_L = 7.42 c_R$ with $c_R$ representing the speed of sound in the ambient medium on the right-hand side. In this simulation, we use two dust species with $\delta = 0.01$ everywhere. We use the TVDLF solver (CFL number 0.1) with a “Koren”-type limiter (Koren1993) and a three-step time integrator. In this simulation, the gas can be seen to follow the typical evolution expected from the interaction of a supersonic shock, as shown on the left side of Figure 6. While the dust also interacts with the shock, in this case, the chosen size and density values of the cloud imply that the two dust species used in the simulation (like before, having sizes between 5 nm and 250 nm) are strongly coupled to the dynamics of the initial gas in the cloud. While the dust itself is not sensitive for the development of the Richtmyer–Meshkov or Rayleigh–Taylor instabilities, clear imprints in the dust distribution are visible. A more detailed discussion of the effect of dust on the latter instability can be found in Hendrix & Keppens (2014a).

4. MODULES FOR SOLAR APPLICATIONS

For solar physics applications, the MHD module of MPI-AMRVAC offers a fairly diverse choice of options to model typically magnetically dominated dynamics. By selecting the appropriate combination of settings for pre-compilation of this physics module, this choice encompasses zero-beta simulations, isothermal MHD at finite plasma beta, MHD in ideal to visco-resistive prescriptions, extensions to Hall-MHD, and many sources and sinks which play a role in the radiative plasma conditions of the solar corona. We first provide an overview of the implemented equations and then demonstrate their workings on selected applications.

4.1. Magnetohydrodynamics: Maxwell’s Equations and Ohm’s Law

We will give the complete set of equations tackled by the MHD module. Due to the possibility of background magnetic field splitting, the standard MHD equations take on a somewhat unusual guise which adds to the usefulness of this collection.

Starting with the homogeneous Maxwell’s equations,

\[
\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},
\]

\[
\nabla \cdot \mathbf{B} = 0,
\]

the MPI-AMRVAC MHD module allows the user to split off a time-invariant potential magnetic field, i.e., writing

\[
\mathbf{B} = \mathbf{B}_0 + \mathbf{B}_1; \quad \frac{\partial \mathbf{B}_0}{\partial t} = 0; \quad \nabla \times \mathbf{B}_0 = 0.
\]

(34)

Note then that $\mathbf{J} = \nabla \times \mathbf{B}_1$ and $\nabla \cdot \mathbf{B}_0 = 0 = \nabla \cdot \mathbf{B}_1$. The most general form for the electric field implemented in the code writes the generalized Ohm’s law as

\[
\mathbf{E} = -(\nabla \mathbf{B} + \frac{1}{en_e} \mathbf{J} \times \mathbf{B} + \eta \mathbf{J}).
\]

(35)

The first right-hand side term is applicable for an ideal MHD scenario in a perfectly conducting plasma. The last term is related to resistivity with the resistivity parameter $\eta$. The Hall (middle) term introduces a first ion-electron distinction within a single fluid plasma description, where $\rho = n_i m_i$ is related to the ions, and quasi-neutrality dictates $n_e = Z n_i$ for ion number density $n_i$ and a charge number $Z$, so we can write

\[
\mathbf{E} = -\left(\frac{\mathbf{v} - \eta \mathbf{J}}{\rho} \right) \times \mathbf{B} + \eta \mathbf{J}.
\]

(36)
where the Hall parameter \( \eta_h \propto m_i/eZ \) (dimensionalized\(^7\)) appears next to the resistivity parameter \( \eta \). Ideal MHD then sets \( \eta_h = 0 = \eta \), resistive MHD has \( \eta_h = 0 \) at finite resistivity, and Hall-MHD has finite values for both parameters.

If we insert the electric field expression (36) into the Maxwell Equations (33) and employ the splitting (34), then we obtain the following as the evolution equation for the magnetic field \( \mathbf{B}_1 \):

\[
\frac{\partial \mathbf{B}_1}{\partial t} + \nabla \cdot \left[ \mathbf{v} (\mathbf{B}_0 + \mathbf{B}_1) - (\mathbf{B}_0 + \mathbf{B}_1) \mathbf{v} \right] + \frac{\eta_h}{\rho} ((\mathbf{B}_0 + \mathbf{B}_1) \mathbf{J} - \mathbf{J} (\mathbf{B}_0 + \mathbf{B}_1)) = - \nabla \times \mathbf{J}. \tag{37}
\]

This directly corresponds to the numerical implementation where the terms in square brackets are treated as fluxes while the resistivity is added as a source.

The resistive source can be added in two ways. We note the equivalence of

\[
- \nabla \times \mathbf{J} = \eta \nabla^2 \mathbf{B}_1 + \mathbf{J} \times \nabla \eta, \tag{38}
\]

and the right-hand side lends itself to implementing an alternative evaluation using a compact stencil for the discretized Laplacian (compactres = T).

Note that since the Hall current enters directly into the flux, additional layers (and ghost zones) are required in the Hall-MHD case. For FV, this implies an additional reconstructed layer, while in an FD setting only the overall stencil is increased.

For the computation of the currents, we have implemented second- and fourth-order central differencing.

### 4.2. \( \nabla \cdot \mathbf{B} \) Treatments

As has been thoroughly investigated by Tóth (2000), controlling solenoidality for magnetic fields in shock-capturing schemes can follow many approaches. Those handled by adding source terms (Powell et al. 1999) or additional equations which advect and diffuse monopoles (Dedner et al. 2002) are especially easily carried over to AMR settings, and several source term strategies have already been intercompared in Keppens et al. (2003). In order to control the numerical monopole errors introduced when large gradients arise and nonlinearities in the limited reconstructions exist, Equation (37) is replaced by one of the following options.

An error-related source term (Powell et al. 1999; Janhunen 2000) is added when writing

\[
\frac{\partial \mathbf{B}_1}{\partial t} + \nabla \cdot \left[ \mathbf{v} \mathbf{B}_0 - \mathbf{v} \mathbf{B} + \frac{\eta_h}{\rho} (\mathbf{BJ} - \mathbf{JB}) \right] = - \nabla \times \mathbf{J} - (\nabla \cdot \mathbf{B}_1) \mathbf{v}. \tag{39}
\]

The diffusive approach (Keppens et al. 2003) is

\[
\frac{\partial \mathbf{B}_1}{\partial t} + \nabla \cdot \left[ \mathbf{v} \mathbf{B}_0 - \mathbf{v} \mathbf{B} + \frac{\eta_h}{\rho} (\mathbf{BJ} - \mathbf{JB}) \right] = - \nabla \times \mathbf{J} + \nabla \left( C_d (\Delta x)^2 (\nabla \cdot \mathbf{B}_1) \right). \tag{40}
\]

\(^7\) When the dimensions are fixed through a reference density \( \rho_0 \), a reference length \( L_0 \), and a reference field strength \( B_0 \), we measure speeds with respect to the Alfvén speed \( V_{Ad} = B_0/\sqrt{\mu_0 \rho_0} \), and the unit of mass is \( L_0^2 \rho_0 \), while the time unit is \( t_0 = L_0/V_{Ad} \). Then, the dimensionalized parameters are actually \( \tilde{\eta} = \eta/(\mu_0 L_0 V_{Ad}) \), also referred to as the dimensionless Lundquist number, while \( \eta_h = V_{Ad}/(L_0 \Omega_{Ad}) \). The latter uses the reference ion gyrofrequency \( \Omega_{Ad} = eZ B_0/m_i \).

The generalized Lagrangian multiplier (GLM) \( \psi \) appears with an added extra equation in the GLM variants (Dedner et al. 2002), which we denote as glm1, being

\[
\frac{\partial \mathbf{B}_1}{\partial t} + \nabla \cdot \left[ \mathbf{v} \mathbf{B} - \mathbf{v} \mathbf{B}_0 + \frac{\eta_h}{\rho} (\mathbf{BJ} - \mathbf{JB}) + \psi \hat{I} \right] = - \nabla \times \mathbf{J}. \tag{41}
\]

The second variant glm2 is

\[
\frac{\partial \mathbf{B}_1}{\partial t} + \nabla \cdot \left[ \mathbf{v} \mathbf{B} - \mathbf{v} \mathbf{B}_0 + \frac{\eta_h}{\rho} (\mathbf{BJ} - \mathbf{JB}) + \psi \hat{I} \right] = - \nabla \times \mathbf{J} - (\nabla \cdot \mathbf{B}_1) \mathbf{v},
\]

\[
\frac{\partial \psi}{\partial t} + \nabla \cdot (c_b^2 \mathbf{B}_1) = - \frac{c_b^2}{c_p^2} \psi - \mathbf{v} \cdot \nabla \psi. \tag{42}
\]

A third variant glm3 based on Equation (41) omits all \((\nabla \cdot \mathbf{B}_1)\) and \(\psi\)-related source terms in the induction, energy, and momentum equations. This simpler scheme is often sufficient and naturally adopts the spatial order from the reconstruction procedure.

In all GLM treatments, the source term for the \( \psi \) variable can be handled in two ways, as originally described in Dedner et al. (2002). One can use the exact solution of \( (\partial \psi/\partial t) = -\left(c_b^2/c_p^2\right)\psi \)

to write

\[
\psi(t + \Delta t) = e^{-\left(\frac{\Delta t}{c_b/c_p}\right)} \psi(t)
\]

and prescribe the constant factor \( c_{ad} = e^{\left(\frac{\Delta t}{c_b/c_p}\right)} \). Another choice is to fix the ratio \( c_b^2/c_p = c_r \). It is also possible to perform the update implicitly by \( \psi^{n+1} = \psi^n/(1 + \Delta t(c_b^2/c_p)) \). In any case, we handle the source update of the \( \psi \) function in an operator split fashion.

### 4.3. Momentum Equation, Closure, and Energy Equation

The momentum equation in MHD has the Lorentz force \( \mathbf{J} \times \mathbf{B} \), which could be added as a source term for HD on the right-hand side of Equation (15) or Equation (16). Employing the identity \( (\nabla \times \mathbf{B}) \times \mathbf{B} = -\nabla \cdot ((\nabla B^2/2)\mathbf{I} - \mathbf{BB}) - \mathbf{B}(\nabla \cdot \mathbf{B}) \) and using the splitting of the field, we actually implement

\[
\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot \left( \mathbf{vm} + \left( p + \frac{B^2}{2} \right) \mathbf{I} - \mathbf{B} \mathbf{B} \right) = \rho \mathbf{g} - \nabla \cdot (\mu \mathbf{P}) + \mathbf{S}_m - \left( \mathbf{B}_0 + \mathbf{B}_1 \right) \nabla \cdot \mathbf{B}_1. \tag{43}
\]

The final term on the right-hand side is only present when the source term monopole approach (Powell et al. 1999) is adopted. To close the system, two options exist.

1. We can use an isothermal (e.g., used in the finite beta, stratified solar flux rope formation simulations by Xia et al. 2014) or isentropic closure as \( p = c_{ad} \rho \gamma \). Zero beta conditions prevail when \( c_{ad} = 0 \).
2. In the second option, we additionally solve an evolution equation for the partial energy (-density):

\[
E_1 = e + \frac{B^2}{2} + \rho v^2/2. \tag{44}
\]

This energy is the total energy when no splitting of the field is adopted. When splitting is adopted, the total energy...
is recovered as \( E = E_1 + B^2/2 - B_1^2/2 \). The governing equation for \( E_1 \) is obtained by combining the internal energy Equation (20) (which has an extra \( \eta J^2 \) right-hand side contribution from Ohmic heating), the velocity evolution equation (\( \mathbf{v} \) Equation (15) with the Lorentz force added), and the induction equation for the split-off field (in fact \( \mathbf{B}_1 \) Equation (37)).

Collecting all of these together yields

\[
\frac{\partial E_1}{\partial t} + \nabla \cdot \left( \mathbf{v} \left( E_1 + \frac{B^2}{2} + p \right) - (\mathbf{B}_1 \cdot \mathbf{v}) \mathbf{B}_1 \right) + \nabla \cdot \left[ \eta \left( \mathbf{B}_1 \right) \mathbf{v} \right] - (\mathbf{B}_1 \cdot \mathbf{v}) \mathbf{B}_1] + \nabla \cdot \left[ \eta \left( \mathbf{J} \cdot \mathbf{B}_1 \right) \mathbf{B}_1 - (\mathbf{B}_1 \cdot \mathbf{B}_1) \mathbf{J} \right] \\
= \nabla \cdot (\mathbf{B}_1 \times \eta \mathbf{J}) - \mathbf{B}_1 \cdot \nabla \psi + \rho \mathbf{v} \cdot \mathbf{g} + \nabla \cdot (\mathbf{k} \cdot \nabla T) \\
- \nabla \cdot (\mathbf{v} \cdot \mathbf{B}_1) - n_1 n_e \Lambda(T) + S_e + \mathbf{v} \cdot \mathbf{S}_e \\
- (\mathbf{v} \cdot \mathbf{B}_1) (\nabla \cdot \mathbf{B}_1). \tag{45}
\]

The heat conduction now contains only field-aligned heat transport, since we adopt \( \mathbf{k} = \kappa(T) \mathbf{B} \mathbf{B} / B^2 \) (note the total field here). The terms related to monopole control may not all be present (GLM introduces \(-\mathbf{B}_1 \cdot \nabla \psi\), and when source-based may use \(-\left(\mathbf{v} \cdot \mathbf{B}_1\right) (\nabla \cdot \mathbf{B}_1)\), depending on the importance of strict energy conservation). A compact stencil evaluation of the resistive source term (activated with compact res=0) may employ \( \nabla \cdot (\mathbf{B}_1 \times \eta \mathbf{J}) = \eta J^2 - \mathbf{B}_1 \cdot (\nabla \times \eta \mathbf{J}) = \eta J^2 + \mathbf{B}_1 \cdot (\eta \nabla \mathbf{B}_1 + \mathbf{J} \times \nabla \eta) \).

4.4. Conservative Hall-MHD

As the Hall-MHD module is a new addition to the code, we list here specifics of its implementation. Activation of Hall-MHD adds terms proportional to \( \eta \) to the fluxes in the induction Equation (37) and in the partial energy Equation (45). A straightforward implementation can be provided for conservative FDs and FVs using an HLL-type Riemann solver or a TVDFL-type scheme where no Riemann problem is solved (see, e.g., the review of Yee 1989). Recent implementations of Hall-MHD were also provided by Lesur et al. (2014) for the PLUTO code, by Bai (2012) for ATHENA, and Tóth et al. (2008) for BATSRUS. The crucial ingredient in Hall-MHD is that the current \( \mathbf{J} = \nabla \times \mathbf{B}_1 \) enters into the fluxes resulting in a non-hyperbolic set of PDEs.

1. For FV discretization, the strategy is to obtain \( \mathbf{J} \) from the interface values of the reconstructed magnetic field. In Cartesian coordinates, second- and fourth-order finite differencing for the \( l \)-component of the current vector yields

\[
J^l_{\mid j \pm 1/2} = \epsilon_{ijk} \frac{1}{2\Delta x_j} \left( B^l_{\mid j \pm 3/2} - B^l_{\mid j \pm 1/2} \right) \\
+ O(\Delta x_j^2) \tag{46}
\]

\[
J^l_{\mid j+1/2} = \epsilon_{ijk} \frac{1}{2\Delta x_j} \left( -B^l_{\mid j+5/2} + 8B^l_{\mid j+3/2} \\
- 8B^l_{\mid j-1/2} + B^l_{\mid j-3/2} \right) + O(\Delta x_j^3), \tag{47}
\]

where \( \mid j \pm 1/2 \) denotes the grid interface \( l + 1/2 \) in the \( j \) direction while the remaining directions remain with centered indices everywhere. The interface magnetic field in these equations is obtained either with a left-biased \( [L] \) or a right-biased stencil \( [R] \) yielding the currents \( \mathbf{J}^L \) and \( \mathbf{J}^R \), respectively. This interface current is then used along with the corresponding reconstructed variables to either compute fluxes according to Rusanov (1961) and update the state vector directly (yielding the TVDLF scheme) or to use with an HLL-type Riemann solver (see below).

2. In FDs, we merely need to obtain the cell-centered current prior to reconstruction of the fluxes as described in Section 2. We again use central differencing for the components of the current as in Equations (46) and (47) with the transformation \( l + 1/2 \rightarrow l \).

For upwinding \( (S^L) \) and the explicit time step criterion \( (c_w) \), the new local fastest wave speeds given by

\[
S^L(\mathbf{U}) = v_0 \pm \max \left( c_f, \eta \frac{|\mathbf{B}|}{\rho} \frac{k_{\max}}{\Lambda} \right),
\]

\[
c_w(\mathbf{U}) = |v| \pm \max \left( c_f, \eta \frac{|\mathbf{B}|}{\rho} \frac{k_{\max}}{\Lambda} \right) \tag{48}
\]

are used, where we take the maximum of the ordinary MHD fast velocity \( c_f \) and the fast-type whistler wave in the field direction with a wave number of \( k_{\max} \). The latter signifies the largest wave number allowed in the grid, \( k_{\max} = \max_{\varphi}(\pi/\Delta x_d) \), where the maximum is taken over all of the grid directions \( d \). We have found that the value of \( k_{\max} \) can often be reduced by a factor of two without seriously affecting the stability.

An HLL-type Riemann solver then follows naturally, giving the flux

\[
F_{\mid i+1/2} = \begin{cases} 
F^L_{\mid i+1/2} & ; S^L > 0 \\
F^R_{\mid i+1/2} & ; S^R < 0 \\
\end{cases} \quad \text{with}
\]

\[
S^L = \min(S^-(\mathbf{U}^L), S^- (\mathbf{U}^R)); \quad S^R = \max(S^+ (\mathbf{U}^L), S^+ (\mathbf{U}^R)). \tag{50}
\]

This parallels the implementation given by Lesur et al. (2014). The TVD FLF scheme follows with the setting

\[
S^R = \max(c_w(\mathbf{U}^L), c_w(\mathbf{U}^R)); \quad S^L = -S^R. \tag{51}
\]

Finally, numerical stability requires a time step satisfying

\[
\Delta t < \frac{\Delta x}{c_w}, \tag{52}
\]

which becomes \( \propto \Delta x^2 \) for small \( \Delta x \). As with explicit integration of diffusive terms, the time step will thus eventually become prohibitively small. Using high-order finite differencing to obtain high accuracy at moderate resolution can yield some mitigation to this problem.

4.5. Selected Tests and Applications

In what follows, we present a fair variety of tests and applications which make use of the novel additions to the MHD physics module specifically, combined with the algorithmic improvements that are generic to all physics modules. We cover 3D ideal MHD wave tests to demonstrate observed accuracies, the possibilities for using high-order FD schemes on shock tube problems, and several novel tests for Hall-MHD scenarios. Solar physics applications illustrate the possibilities for splitting potential magnetic fields and a typical 3D magnetoconvection study.
Accordingly, the 3D domain is given by TVD time integration (RK3) by Gottlieb & Shu (1998). As reconstruction (ˇCada & Torrilhon 2009) with the third-order third- and fifth-order reconstructions. We combine the LIM03 problem reads

\[
(\rho, v_x, v_y, v_z, B_x, B_y, B_z)
\]

with the phase \( \phi = kx - \omega t \) and phase velocity given by the Alfvén speed \( v_A \equiv \omega/k = 1 \). The negative (positive) sign in the magnetic field components indicates a wave propagating in the positive (negative) \( x \) direction. For the amplitude, we set \( A = 0.1 \) and use the uniform background parameters \( \rho = 1 \) and \( \rho = 0.1 \). The wave-vector is given by \( k_x = 2\pi \) and \( k_y = k_z = 2k_x \), and we rotate the vectors given by Equation (53) accordingly. The 3D domain is given by \( x \in [0, 1] \), \( y \in [0, k_x/k_y] \), and \( z \in [0, k_x/k_z] \) and we run the setup (without AMR) over one period \( T = k_x/\sqrt{k_x^2 + k_y^2 + k_z^2} \).

The resulting convergence of the GLM-MHD state vector is shown in \( L_\infty \) and \( L_1 \) norms in the left panel of Figure 7 for the third- and fifth-order reconstructions. We combine the LIM03 reconstruction (ˇCada & Torrilhon 2009) with the third-order TVD time integration (RK3) by Gottlieb & Shu (1998). As expected, third-order convergence is achieved in both norms. Despite the formal fourth order of the SSPRK(5, 4) by Spiteri & Ruuth (2002), we obtain fifth-order convergence when using MP5 reconstruction. In the right panel of Figure 7, we show the divergence error of the magnetic field for both realizations. In both cases, we calculate the divergence using fourth-order central differences. As expected, the divergence of the magnetic field decreases with order given by the order of the spatial reconstruction minus one which demonstrates the effectiveness of the GLM approach.

### 4.5.2. Shocks, Discontinuities, and High-order FD Schemes

To investigate how the naive FD scheme handles discontinuous flows, we run a classical 1D MHD shock tube test from Brio & Wu (1988). This standard test was also adopted by Ryu & Jones (1995), Jiang & Wu (1999), and Mignone et al. (2010). In terms of the primitive variables, the initial Riemann problem reads

\[
(\rho, v_x, v_y, v_z, p, B_x, B_y, B_z)
\]

and we adopt a ratio of specific heats of \( \gamma = 5/3 \). The uniform grid is composed of 512 cells with \( x \in [-1, 1] \). In addition, a reference solution is obtained with a second-order TVD scheme at a ridiculously high resolution of 65 536 cells. Figure 8 collects our results with the schemes: RK3-LIM03-FD, SSPRK(5, 4)-MP5-FD, and SSPRK(5, 4)-MP5-FV. Due to their conservative nature, all schemes capture the general shock structure well. At the contact discontinuity, we obtain over- (under-) shooting in the density by \(-0.001\% \) for RK3-LIM03-FD, \( +2.7\% \) for SSPRK(5, 4)-MP5-FD, and \( +1.6\% \) for SSPRK(5, 4)-MP5-FV. The level of oscillations in the third-order scheme is encouraging despite the omission of characteristic reconstruction. With fifth-order reconstruction, the oscillations could be considered prohibitive for some applications. Note that the oscillations visible, for example, in the profiles of \( v_x \) are not a trademark of FD discretization alone, as our FV solution shows a similar behavior. The advantages of the simple FD scheme become apparent when one considers the speedup. Relative to RK3-LIM03-FD, the execution times become 1:2:2:3:5 for SSPRK(5, 4)-MP5-FD:SSPRK(5, 4)-MP5-FV. Thus, the FD scheme is faster than its (HLLC-based) FV counterpart by a factor of 1.6 as no Riemann problems are solved. Exploiting the SSP nature of the Runge–Kutta schemes, we also ran the shock tube at the maximal CFL yielding SSP. The results are shown in Figure 9. Here, the third-order scheme shows an excessive over- shoot while the level of oscillations in the fifth-order scheme is comparable to the case with a Courant number of 0.4. It is important to note that the amount of oscillations is damped with time, as illustrated in the right-hand panel of Figure 9.
moving contact, we adopt slab geometry and periodic boundary conditions and choose an advection velocity of $v_x = 1$. In this case, the domain spans $r \in [0, 2]$ discretized with 128 grid points. The density jumps at $x = 0.5$ and $x = 1.5$. In Figure 10, we compare the states obtained with the HLLC, HLL, and FD scheme at $t = 10$ (corresponding to several hundred sound crossing times). In all these cases, MP5 reconstruction and SSPRK(5, 4) time stepping is employed. As expected, HLLC preserves the stationary contact exactly, while HLL and FD are subject to numerical diffusion. The Lax–Friedrich split FD scheme is more diffusive than the HLL solver. For the advected discontinuity, HLLC loses its capacity to capture the contact exactly and we find that the results for HLLC and HLL almost coincide. Again, the FD scheme is the most diffusive of the three. In this setup, the level of diffusion for the FD scheme is comparable to a second-order HLLC scheme with Koren reconstruction. The latter is indicated as “HLLC, Koren” in the right panel of Figure 10. When run without high-order

Figure 8. 1D MHD compound wave shock tube test, case 5a of Ryu & Jones (1995) at $t = 0.2$. All solutions are obtained with a Courant number of 0.4. All conservative schemes reproduce the overall shock structure well. However, the amount of oscillations obtained with MP5 could be considered prohibitive in some applications. Note that the amplitude of these oscillations is comparable in FD and FV (using reconstruction of conserved variables and HLLC Riemann solver). The solutions obtained with MP5 are indeed more oscillatory than when characteristic fields are used for reconstruction, see Figure A.4 of Mignone et al. (2010).

Figure 9. Left and center: perpendicular velocity component in the 1D MHD compound wave at the maximal Courant number allowed by the time marching scheme. We show SSPRK(4, 3)-LIM03-FD at a Courant number of 2.0 (left panel) and SSPRK(5, 4)-MP5-FD (center panel) at a Courant number of 1.5. Right: long-term evolution of SSPRK(5, 4)-MP5-FD showing a decrease of the oscillation amplitude with time.
reconstruction, dissipation in the FD scheme is clearly excessive (see line labeled “FD, Koren”).

4.5.3. Circular Alfvén-Whistler Wave

In analogy to the MHD case, we can derive the equation for the circularly polarized Alfvén-Whistler wave. One can easily show that the wave is also a solution of the non-linear Hall-MHD system. The non-linear circularly polarized Alfvén-Whistler wave in the x direction reads

\[
\begin{pmatrix}
v_x \\ v_y \\ v_z \\
\end{pmatrix} = \begin{pmatrix}
0 \\ A \sin(\phi) v_A/v_{ph} k \ d f_e \\ A \cos(\phi)
\end{pmatrix};
\]

\[
\begin{pmatrix}
B_x \\ B_y \\ B_z
\end{pmatrix} = \begin{pmatrix}
-B_0 \\ -v_z (1/v_{ph} B_0 + B_0/v_A k \ sin(\phi)) \\ -v_z (1/v_{ph} B_0 + B_0/v_A k^2 d^2 f_e)
\end{pmatrix},
\] (55)

with

\[
f_e = \frac{1}{1 - (v_A/v_{ph})^2}
\] (56)

and the phase \( \phi = kx - \omega t \) and wave number \( k = 2 \pi m. A \) is the wave amplitude and is not necessarily small. The phase velocity follows from the Hall-MHD dispersion relation for propagation along the magnetic field

\[
(k^2 v_A^2 - \omega^2)^2 = d^2 k^4 v_A^2 \omega^2,
\] (57)

as

\[
v_{ph} \equiv \omega/k = v_A/2(d k + \sqrt{4 + d^2 k^2}),
\] (58)

which reduces to the Alfvén speed in the limit \( k \ d \to 0 \). In this limit, the solution is simply the circularly polarized Alfvén wave of ideal MHD. The parameter \( d \) corresponds to the Alfvén gyro radius as \( d = v_A/\Omega_i \) with the ion gyro frequency \( \Omega_i \). Note that the code-parameter \( \eta_h \) is connected to \( d \) via \( \eta_h = \sqrt{\rho d} \).

As the electron velocity depends on the current in the Hall approximation, the Alfvén-Whistler wave test is an inherently 3D problem. It can be used to test the realization of the dispersion relation (57) as well as the convergence order of the code in 3D.

The setup of the test case is as follows. We choose \( k_x = k_y = k_z = 2 \pi m \) with \( m = 2 \) and the state Equation (55) is rotated accordingly. The Alfvén ion-gyro-radius is set to \( d = 1 \) and we choose the plasma background parameters to satisfy \( v_A = 1 \). The wave amplitude is \( A = 1 \). A 3D Cartesian box with edge length \([1, 0.5, 0.5]\) is simulated with the finite differencing algorithm for one period,

\[
P = \frac{1}{\sqrt{3} m v_{ph}(k)},
\] (59)

using increasing resolution starting at \( N_x \times N_y \times N_z = 16 \times 8 \times 8 \) cells. The result of this test is presented in Figure 11. This result shows fourth-order convergence as expected based on the use of fourth-order central differencing of the current. In addition, the dispersion relation Equation (57) is realized by our code with increasing accuracy as the resolution is increased. The right-hand panel of Figure 11 demonstrates the low numerical diffusion obtained with the high-order scheme: already at a resolution of \( N_x = 32 \), by eye, it is hard to distinguish the profile of the propagated wave (gray) from the analytical expectation (black).

4.5.4. Group Diagram in Hall-MHD

A further test for the Hall-MHD module is the Friedrich diagram of the group velocity as known from the pure MHD case. This classical example of MHD wave propagation can be used to study the transition from the ideal to the Hall-MHD regime and provides a qualitative comparison for our Hall-MHD module. The Hall-MHD group diagram was first shown in Hameiri et al. (2005) and differs greatly from the ideal MHD case. In particular, the Alfvén-type ray surfaces—only the points in the ideal MHD case—change dramatically and develop an extended front as illustrated in the lower panel of Figure 12. Since the Hall-MHD system is not purely hyperbolic, the group diagram yields only an approximate “envelope” drawn by the fastest waves present.

Our numerical realization of the group diagram initializes a (small) point-perturbation of a homogeneous medium threaded by a constant magnetic field in the \( z \) direction (see also Keppens et al. 2012). The grid is adaptively refined to the sixth level, starting at a base resolution of \( 120^2 \) cells within a domain \( z, x \in [-1, 1] \). We again use the solver combination SSPRK(5, 4)-MP5-FD, formally yielding fourth-order accuracy in space and time. Information on the perturbed state is transported by slow, Alfvén, and fast wave packages forming the group diagram. We choose the background state \( v_A = 0.96824 \) and \( c_s = 1.29099 \), and adopt an Alfvén ion-gyro radius of \( d = 10^{-2} \).

Due to the dispersiveness of the modified Whistler waves, the group velocities in the Hall-MHD system depend on the wave-number \( k \), and thus our numerical realization consists of the interference of all \( k \) waves triggered by the initial perturbation.
Figure 11. Convergence for the 3D circularly polarized Alfvén-Whistler wave test using finite differencing in Hall-MHD. Reconstruction is performed using the MP5 algorithm, and currents are obtained by fourth-order central differences Equation (47) and time stepping with SSPRK(5, 4), yielding overall fourth-order accuracy (left panel). The right panel shows diagonal cuts in wave direction \( \hat{k} \) of \( B_z \) at \( t = 0 \) (black) and \( t = \rho \) (gray) for the two resolutions \( N_z = 32 \) (dashes) and \( N_z = 64 \) (dots).

Figure 12. Interference pattern resulting from the Friedrich wave diagram test with Hall-MHD. Top panel: out-of-plane velocity (left) and pressure (right). Bottom panel: analytic Hall-MHD group diagram for \( kd = 10 \) for Alfvén-type (solid) and fast-type (dashed) waves. One can clearly recognize the enveloping fast-type and Alfvén-type wave families.

Analytic envelope functions for fast- and Alfvén-type waves can be constructed for the highest \( k \) value present in the system, which in our explicit implementation depends on the numerical resolution. In Figure 12, we show realizations of the Friedrich diagram test in snapshots of out-of-plane velocity and pressure. An effective resolution of 3840^2 cells was used for this test, resulting in maximal wavenumbers of \( kd \sim 30 \). In contrast to the MHD case, the highly anisotropic (fast-type) Whistler waves propagate most rapidly in the direction of the magnetic field. Interference between the individual waves scrambles the signal, however, we can clearly make out two distinct types of waves. These are the fast-type and Alfvén-type waves as illustrated in the bottom panel of Figure 12.

4.5.5. Hall-MHD Reconnection

Magnetic reconnection plays a key role in plasma physics and many studies ranging from stationary resistive MHD (Parker 1957) over time-dependent MHD simulations up to full particle in cell simulations have been performed to date (see the discussion in Keppens et al. 2013). To test our code on a challenging problem, we employ the so-called double-GEM setup adopted from the well-known Geospace Environment Modelling (GEM) challenge. Ideal Hall-MHD reconnection was first employed to the GEM setup by Ma & Bhattacharjee (2001). The main difference in our setup to the classical GEM challenge is that the domain contains two alternating current sheets, which allows us to employ doubly periodic boundary conditions, facilitating inter-comparison between codes and checks on exact conservation properties (Keppens et al. 2013).

For completeness, the setup is described below. The domain is a 2D Cartesian square with dimensions \( (x, y) \in [-L/2, L/2] \) with \( L = 30 \), and the current sheets are located at \( y_{up} = 7.5 \) and \( y_{low} = -7.5 \). An ideal gas equation of state is adopted with a ratio of specific heats of \( \gamma = 1.66666667 \). We employ the
magnetic field

\[ B_x = B_0[-1 + \tanh(y - y_{\text{low}}) + \tanh(y_{\text{up}} - y)] + \delta B_x, \]
\[ B_y = \delta B_y, \]  

with perturbations

\[ \delta B_x = -2\pi L \cos \left(\frac{2\pi}{L}x\right) \left[ \sin \left(\frac{2\pi}{L}(y - y_{\text{low}})\right) + 2(y - y_{\text{up}}) \right] \times \exp \left(-\frac{2\pi}{L}x^2 - \frac{2\pi}{L}(y - y_{\text{low}})^2\right) + \frac{2\pi}{L} \right] \times \cos \left(\frac{2\pi}{L}y\right) \left[ \sin \left(\frac{2\pi}{L}(y - y_{\text{up}})\right) + 2(y - y_{\text{up}}) \right], \]
\[ \delta B_y = +2\pi L \cos \left(\frac{2\pi}{L}x\right) \left[ \sin \left(\frac{2\pi}{L}(y - y_{\text{up}})\right) + 2(y - y_{\text{up}}) \right] \times \exp \left(-\frac{2\pi}{L}x^2 - \frac{2\pi}{L}(y - y_{\text{up}})^2\right), \]

where the magnitude of the perturbation is set to \( \psi = 0.1 \), which is a factor of 10 lower than the background field amplitude \( B_0 = 1 \).

The density profile is taken as

\[ \rho = [\rho_{\text{at}} + \cosh^{-2}(y - y_{\text{low}}) + \cosh^{-2}(y - y_{\text{up}})], \]

and an MHD equilibrium configuration is obtained via the pressure profile

\[ p = \frac{B_0^2 \rho}{2}. \]

Thus far, the setup differs from Keppens et al. (2013) only in the higher atmospheric density (outside the current sheets) with a value of \( \rho_{\text{at}} = 0.2 \) in Equation (62), compared to \( \rho_{\text{at}} = 0.1 \) in the original study. As the Hall-MHD evolution involves low plasma beta regions, the latter proved necessary to assure numerical stability. This choice of parameters results in plasma \( \beta = 0.2 \), atmospheric Alfvén velocity \( v_A = B_0/\sqrt{\rho_{\text{at}}} \approx 2.23 \), and sound speed \( c_s = \sqrt{\gamma p_{\text{at}}/\rho_{\text{at}}} \approx 0.91 \). We choose an Alfvén ion-gyro radius of \( d = 1 \) with the setting \( \eta_b = 1/\sqrt{B_0} \). Resistivity is chosen as \( \eta = 10^{-3} \) and we adopt a dynamic viscosity of \( \mu = 10^{-3} \). In these runs, we employ a base resolution of \( 10^2 \) cells and add adaptive refinement based on variations in density (following the prescription of Lohner 1987) to a total of three (low-resolution case) and four levels (high-resolution case).

The evolution of the high-resolution run is portrayed in Figure 13. We observe the rapid development into an X point through which reconnection of the magnetic field proceeds. In contrast, the visco-resistive MHD case shown in the right panel of Figure 13 develops a near-stationary current sheet with a well-defined aspect ratio.

The energetics of the reconnection process is shown in Figure 14. In the Hall-MHD case, the initial magnetically dominated equilibrium reaches equipartition between internal and magnetic energy at \( t \approx 80 \). This is also where the dissipation rate peaks. Afterward, the thermal energy increases more gradually and we observe fluctuations in the energetics that stem from compressive waves permeating the system. On the other hand, in the resistive MHD case, the dynamics is dominated by Ohmic heating and the dissipation rate is nearly constant up to \( t = 200 \). Conservation of total energy is granted with a relative error of \( \Delta E/E = -1.46 \times 10^{-5} \) in the Hall case and with \( \Delta E/E = 4.1 \times 10^{-5} \) in the purely resistive case. This small energy error stems from the fact that resistive terms are currently not added in a conservative fashion. As noted previously (e.g., Shay et al. 2001; Birn & Hesse 2001), inclusion of the Hall term is vital to obtain reconnection rates comparable to full kinetic descriptions. Indeed, the reconnection rate of the in-plane flux \( R(t) \) (see, e.g., Fitzpatrick (2004) for a definition of this rate of reconnected flux) shown in Figure 15 (right panel) increases over the resistive MHD case by more than a factor of 100. In Hall-MHD, electrons and ions decouple on the scale of the ion-gyroradius. Ideal Hall-MHD retains the frozen-in condition of ordinary MHD, however, field-lines are advected only with the electron flow. The stream-lines in our reconnection setup are drawn in the vicinity of the X point in the left panel.
of Figure 15. It shows the decoupling on the scale of the Alfvén ion-gyroradius $d = 1$ with momentary electron streamlines (black) and ion streamlines (white) on a background of the parallel electric field component $E_{||} = \mathbf{E} \cdot \hat{\mathbf{B}}$. Upon entering the reconnection region, electron and ion flows are well aligned. In regions of strong $E_{||}$ at the “wings” of the X point, the incoming electron flow is deflected sharply toward the O point. Eventually, the ion flow is deflected as well, however, owing to its higher inertia with a larger radius of curvature.

4.5.6. Options for Splitting Magnetic Fields: Field Line Extrapolations

As indicated when describing the MHD equations as implemented, it is possible to split off a potential field solution $\mathbf{B}_0$ and reformulate the evolution equations in terms of the deviation $\mathbf{B}_1$ from this steady background field. This is particularly useful when one wishes to follow both gradual and more violent plasma dynamics in a realistically structured, solar coronal field topology. To that end, here we demonstrate the available options for generating exact potential field solutions from actual magnetogram data. In the context of this paper, we demonstrate the availability (as additional open source modules) of frequently used models for global spherical (potential field source surface, PFSS) models, as well as for local Cartesian box models (Green function based) and make some observations concerning their accuracy.

4.5.7. Global Spherical PFSS Model

The fundamental assumption made in the PFSS model (Altschuler & Newkirk 1969; Schatten et al. 1969; Hoeksema 1984; Wang & Sheeley 1992; Schrijver & De Rosa 2003) is that the magnetic field $\mathbf{B}_0$ is potential within the coronal volume, allowing a magnetic potential $\Phi$ to be defined such that $\mathbf{B}_0 = -\nabla \Phi$. Since $\nabla \cdot \mathbf{B}_0 = 0$ everywhere, the potential $\Phi$ satisfies a Laplace equation, $\nabla^2 \Phi = 0$. The solution in spherical coordinates is

$$\Phi(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[ A^m_l r^l + B^m_l r^{-(l+1)} \right] Y^m_l(\theta, \phi),$$

where the $Y^m_l$ indicate spherical harmonic functions of degree $l$ and order $m$, and the coefficients $A^m_l$ and $B^m_l$ are determined by the imposed radial boundary conditions. By definition, $Y^m_l(\theta, \phi) = C^m_l P^m_l(\cos \theta)e^{im\phi}$, where $P^m_l$ are the associated Legendre functions and the constants $C^m_l$ are determined as

$$C^m_l = (-1)^m \frac{2l + 1 \ (l - m)!}{4\pi \ (l + m)!} \frac{1}{2}.$$

The photospheric boundary condition for $\Phi$ is

$$\frac{\partial \Phi}{\partial r} = -B^m_l(1, \theta, \phi),$$
where $B_{r}^{0}(1, \theta, \phi)$ denotes the radial magnetic field as measured at the photosphere (quantified from a line-of-sight magnetogram). If we denote the spherical harmonic coefficients of $B_{r}^{0}(1, \theta, \phi)$ as $F_{l}^{m}$, such that $B_{r}^{0}(1, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{l}^{m} F_{l}^{m}$, then applying the boundary condition on $r = 1$ for $\Phi$ leaves us with

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{l}^{m} \left[ A_{l}^{m} r^{l} - B_{l}^{m} (l + 1) r^{-(l+1)} \right] = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{l}^{m} F_{l}^{m}. \tag{66}$$

In principle, the coefficients $F_{l}^{m}$ are determined by the equation

$$F_{l}^{m} = \int_{0}^{2\pi} \int_{0}^{\pi} d\phi \sin \theta Y_{l}^{m}(\theta, \phi) B_{r}^{0}(1, \theta, \phi) = \int_{0}^{\pi} d\theta \sin \theta C_{l}^{m}(\cos \theta) F_{m}(\theta), \tag{67}$$

where $Y_{l}^{m}(\theta, \phi)$ is the complex conjugate of the spherical harmonic functions and $F_{m}(\theta)$ is the continuous spherical harmonic transform on the photospheric magnetic field. Instead of knowing the continuous function $B_{r}^{0}(1, \theta, \phi)$, we only know the values of the photospheric magnetic field at $N_{\theta} \times N_{\phi}$ points $(\theta_{i} \text{ and } \phi_{j})$ with $i = 1, 2, \ldots, N_{\theta}$ and $j = 1, 2, \ldots, N_{\phi}$ obtained by observations. The discrete spherical harmonic transform is then given by

$$F_{l}^{m} = \sum_{i=1}^{N_{\theta}} \left[ w_{i} C_{l}^{m}(\cos \theta_{i}) \sum_{j=1}^{N_{\phi}} e^{-i m \phi_{j}} B_{r}^{0}(1, \theta_{i}, \phi_{j}) \right]$$

$$= \sum_{i=1}^{N_{\theta}} \left[ w_{i} C_{l}^{m}(\cos \theta_{i}) F_{m}(\theta_{i}) \right], \tag{68}$$

where the weights $w_{i}$ are obtained with the help of Legendre functions of the first kind.

The outer radial boundary condition is obtained by the “source surface” assumption. As source surface, we define the sphere $r_{ss} = 2.5 r_{s}$ which is threaded by a purely radial field, giving the von Neumann boundary condition $\partial_{r} \Phi(r_{ss}, \theta, \phi) = \delta_{r} \Phi(r_{ss}, \theta, \phi) = 0$. This is satisfied if $\Phi$ is constant on this sphere and we can choose $\Phi(r_{ss}) = 0$. Thus, we obtain the relation between the expansion coefficients

$$A_{l}^{m} r_{ss}^{l} + B_{l}^{m} r_{ss}^{-(l+1)} = 0. \tag{69}$$

Once the coefficients $F_{l}^{m}$ are determined from the magnetogram using relation (68), the coefficients for $A_{l}^{m}$ and $B_{l}^{m}$ follow from Equation (66) using the orthogonality of the spherical harmonics. We can then determine the magnetic field from the equation $B_{r} = -\nabla \Phi$, or written out per component we obtain

$$B_{l} = \text{Re} \left( \sum_{l,m} Y_{l}^{m} \left[ A_{l}^{m} r^{l-1} - B_{l}^{m} (l + 1) r^{-(l+2)} \right] \right), \tag{70}$$

$$B_{\theta} = \text{Re} \left( \frac{1}{r \sin \theta} \sum_{l,m} Y_{l}^{m} \left[ R_{l}^{m} (l - 1) \left[ A_{l-1}^{m} r^{l-1} + B_{l-1}^{m} r^{-l} \right] - R_{l+1}^{m} (l + 2) \left[ A_{l+1}^{m} r^{l+1} + B_{l+1}^{m} r^{-(l+2)} \right] \right] \right), \tag{71}$$

where the factor $R_{m}^{m}$ is defined as $R_{m}^{m} \equiv \sqrt{(l^{2} - m^{2})/l(l+1)}$. Note that the field components are real, while $Y_{l}^{m}$, $A_{l}^{m}$, $B_{l}^{m}$, and $F_{l}^{m}$ are actually all complex numbers.

### 4.5.8. PFSS Extrapolation for Carrington Rotation CR2029

Synoptic magnetograms with resolution $N_{\theta} \times N_{\phi}$ can be used as input to estimate the solar coronal magnetic field. We can routinely use inputs from GONG observations at a resolution of $180 \times 360$ and from MDI at a resolution of $1080 \times 3600$. MDI is an instrument onboard the Solar and Heliospheric Observatory (SOHO). We make use of these magnetograms after performing a magnetogram remeshing technique using the Chebyshev collocation method (e.g., Carpenter & Gottlieb 1995). The latter interpolates the original grid where the grid points are spaced equally in $\cos(\theta)$ onto a uniform $\theta$ grid. Here, we present a study for the solar Carrington rotation number CR2029 in 2005 using observations from the space telescope instrument MDI. We pay particular attention to two active regions within CR2029: one located in the north hemisphere AR10759 and one in the south hemisphere AR10756. These two dominant active regions on each hemisphere will be used to (1) compare the global PFSS spherical extrapolation approach and a local potential field Cartesian approach, and (2) to understand the influence of raising the number of spherical harmonics. For the latter, we will take active region AR10756 as the photospheric region for which we examine the radial magnetic field variation over a line crossing the active region’s opposite polarities, as influenced by the number of spherical harmonics taken.

In Figure 16, we first present an impression of the global magnetic field topology obtained from the full MDI magnetogram, used to generate a PFSS model up to $l_{\max} = 720$ and exploiting a three level block-AMR grid with an effective resolution of $240 \times 360 \times 720$. In order to investigate the effect of the number of spherical harmonics which we include in our computations on the accuracy of our results, we construct several PFSS models and compare them to a reference case. For this comparison, all of these models exploit a fixed uniform resolution of $150 \times 180 \times 360$, but we vary $l_{\max} = 90, 135, 270, 540, 720$, where $l_{\max}$ is the maximum degree of the spherical harmonic functions used in each case for the magnetic field calculation. The case with $l_{\max} = 720$ determines our reference case since it is the maximum degree which we can use for MDI magnetograms according to alias-free conditions as mentioned by Suda & Takami (2002): $l_{\max} \leq \min((2N_{\theta}/3), (N_{\phi}/3)) \Rightarrow l_{\max} \leq 720$. In order to compare the different runs, we examine the radial component of the magnetic field on the photosphere as it varies along a line that crosses active region AR10756, as demonstrated in Figure 17. As the number of spherical harmonics increases, the magnetic field maximal amplitude grows and gradually approaches the reference case variation. At the same time, the intensity of the ringing effect (Tóth et al. 2011) affecting the magnetic field

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8 The Global Oscillation Network Group (GONG) is a community-based program intended to conduct a detailed study of solar internal structure and dynamics using helioseismology, see http://gong.nso.edu/.

9 See http://sohowww.nascom.nasa.gov/, a project of international collaboration between ESA and NASA to study the Sun from its deep core to the outer corona and the solar wind.
value around the active region diminishes and the curve becomes smoother.

In order to quantify this better, we compute the errors $\mathcal{E}$ of the magnetic field magnitude for each of the above models with respect to the reference case with maximal $l_{\text{max}} = 720$. In Figure 18, the error calculation is demonstrated with two norms, the $L_1$ (lowest curves) and $L_\infty$ norms (upper data). The solid line indicates a power-law fitting curve given by $\mathcal{E} = 836.3152 l_{\text{max}}^{-2.32912}$, and the dashed line has $\mathcal{E} = 0.05634 e^{-0.0087419 l_{\text{max}}}$ as an exponential fit for the $L_1$ norm. For the $L_\infty$ norm, the dotted line is the power-law fitting curve $\mathcal{E} = 25.7 \times 10^6 l_{\text{max}}^{-2.30698}$, and the dot-dashed line $\mathcal{E} = 1.3 \times 10^3 e^{-0.00918513 l_{\text{max}}}$ is the exponential fit. The two norms differ by about four orders of magnitude for all PFSS models reported in the plot, which indicates that our main errors originate from specific localized regions. This conclusion is realistic, as we would expect that the main errors are introduced by the existence of regions where the magnetic field is noted to show a sudden increase of orders of magnitude, i.e., the active regions.

4.5.9. Global versus Local Cartesian Extrapolation

Besides the global PFSS model using full-sun synoptic maps, we also implemented a local potential field extrapolation method, which is useful when we are interested in simulating specific local active region behavior. This local Cartesian approach uses exact closed-form solutions of the force-free magnetic field boundary-value problem with the help of Green’s function method (Chiu & Hilton 1977). When the photospheric surface corresponds to the $z = 0$ plane, the problem still reduces to solving the Laplace equation for the magnetic potential $B_p(z)$ given by the magnetograms. When we take as the second boundary condition $B_0 \to 0$ as $z \to \infty$, the Cartesian components of the magnetic field in Green’s function forms are given by

$$
\overline{B}_i = \frac{1}{2\pi} \int_{y_a}^{y_b} \int_{x_a}^{x_b} dx' dy' \mathcal{G}_i(x, y, z; x', y') B_0^p(x', y')
$$

for $i = x, y, z$.
where \( [x_a, y_b] \) and \( [y_a, y_b] \) are the boundaries of the extracted magnetogram and the integrals contain

\[
\bar{G}_x = \frac{x - x'}{R} \frac{\partial \Gamma}{\partial z} + \alpha \frac{y - y'}{R},
\]

(74)

\[
\bar{G}_y = \frac{y - y'}{R} \frac{\partial \Gamma}{\partial z} + \alpha \frac{x - x'}{R},
\]

(75)

\[
\bar{G}_z = \frac{z}{r^3} \cos(\alpha r) + \frac{\alpha z}{r^2} \sin(\alpha r),
\]

(76)

\[
\bar{\Gamma} = \frac{z}{Rr} \cos(\alpha r) - \frac{1}{R} \cos(\alpha z),
\]

(77)

\[
\frac{\partial \Gamma}{\partial z} = \left( \frac{1}{Rr} - \frac{z^2}{Rr^3} \right) \cos(\alpha r) - \frac{\alpha z^2}{R r^2} \sin(\alpha r) + \frac{\alpha}{R} \sin(\alpha z),
\]

(78)

where \( R^2 = (x - x')^2 + (y - y')^2 \) and \( r^2 = R^2 + z^2 \) are the position vector squared. The above formulae allow for a constant nonzero value of \( \alpha \), generating a linear force-free field, while for \( \alpha = 0 \) we get the potential magnetic field solution which can be split off. This exact solution does not suffer from the need to truncate at a specific angular degree \( l_{\text{max}} \) encountered when using spherical harmonics. For the integral evaluations, a simple midpoint rule is adopted.

To qualitatively compare this local extrapolation method with the PFSS model in global spherical geometry, we can do the following, which are all shown in Figure 19. We can start from a synoptic magnetogram of a full Carrington rotation so that the observational input is in the form of a 2D matrix of size \( N_\theta \times N_\phi \); for MDI, this is \( 1080 \times 3600 \). The above mentioned Chebyshev remeshing technique is first used to transform the whole magnetogram into a uniform \((\theta, \phi)\) grid, similar to the global case. This uniform \((\theta, \phi)\) grid can be transformed into a Cartesian grid with each angular degree corresponding to a length equal to \( \pi r_s / 180 \). Finally, an area of interest is extracted in Cartesian coordinates \( \Delta y \times \Delta x \) in the form of a 2D submatrix corresponding to a user-selected \( \Delta \theta \times \Delta \phi \) angular portion of the magnetogram. Here, we take a \( 30^\circ \times 30^\circ \) portion containing AR10759, which counts \( 181 \times 301 \) grid points, covering a region of \( 364.8 \times 364.8 \text{Mm}^2 \). We use this as a bottom magnetogram for a local extrapolation using the above method, where we use a four level AMR grid with an effective resolution of \( 384 \times 384 \times 384 \) with a maximal resolving power in each direction, where \( \Delta x = \Delta y = \Delta z = 0.95 \text{ Mm} \). We also take the full MDI magnetogram as the bottom boundary for a global PFSS extrapolation, this time using a uniform \( 180 \times 270 \times 540 \) grid in spherical coordinates \((\rho, \theta, \phi)\), where the radial range goes up to the source surface. This latter spherical grid ensures an effective resolving power of about \( 8 \times 8 \text{Mm}^2 \) on the solar surface.

The field lines for both kinds of extrapolation are drawn in Figure 19 where we show a zoomed view on the active region from the global PFSS model and the local Cartesian result. We selected 20 specific points to start drawing the field lines. In the same figure, there is also an observational EIT\(^{10}\) image of active region AR10759 at 195 Å, which corresponds to Fe XII and a temperature of \( 1.6 \times 10^6 \text{ K} \). The two approaches show similar structure, as expected. We underline that for the local simulation, there is no source surface (the top boundary differs for the exploited Green function), a fact that explains why we have more dominant open field line topology in the right panel of Figure 19. The remaining differences are due to finite curvature effects not present in the Cartesian approach. The extrapolations agree only qualitatively with the observational data in the extreme ultraviolet. The (magnetically structured) plasma morphology visible at this wavelength shows similarities with the open and closed field lines of both the global and local simulations, but may well deviate significantly from potential field conditions. For example, at the center of the active region in the EIT view, a region with negative polarity differs most from the bottom magnetogram structure, as this filter shows the plasma to be higher inside the low corona than the photosphere itself. By inspection, the potential field extrapolation misses the implied magnetic connectivity in those regions.

4.5.10. Magnetocovection

As a representative, time-dependent, solar application where non-ideal MHD processes are incorporated, we simulate compressible magnetoconvection in a strongly stratified layer, following Rucklidge et al. (2000). Their parametric survey focused on a prescribed polytropic atmosphere, initially modified with a uniform vertical magnetic field, and varied the field strength, the relative importance of magnetic diffusion, (isotropic) thermal conduction, and viscosity, as well as geometric parameters like the box aspect ratio. Augmented with simple boundary prescriptions fixing the top to bottom temperature contrast and fields, these authors conducted a systematic parameter study, identifying transitions from essentially 2D to 3D behavior, from kinematic to more magnetically influenced cases, and from ordered to chaotic regimes. A detailed analysis of the (loss of) symmetry in the convecting endstates could benefit from group

\(^{10}\) Extreme ultraviolet Imaging Telescope (EIT) is an instrument on the SOHO spacecraft, sensitive to four different wavelengths 171, 195, 284, and 304 Å with a 17 minute cadence and a spacial resolution of \((1800 \text{ km})^2\).
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PORTH ET AL.

Figure 19. Local potential field extrapolation in Cartesian coordinates (left) vs. a zoomed view taken from a global PFSS model in spherical coordinates (right) for CR2029 zoomed in to AR10759. The effective resolution for the local simulation is 384 × 384 with a cell size of 0.95 Mm, while for the global simulation we exploit 180 × 270 × 540 with on-disk 8 Mm per cell. We visualize and compare the magnetic field topology for the two approaches of the same model. The middle panel is an extreme ultraviolet observation from EIT 195 Å for AR10759.

A color version of this figure is available in the online journal.

Theoretical classifications using the linear eigenfunction behaviours. This allowed us to obtain bifurcation diagrams, serving to classify the large variety of steady to unsteady magnetoconvection patterns. Here, we will adopt two realizations: one in the steady regime and one in the unsteady, chaotic parameter regime.

In a 3D Cartesian box \([0, \lambda] \times [0, 1] \times [0, \lambda]\) with gravity along the negative \(y\) direction and periodic horizontal \(x\) and \(z\) directions, we initialize the density and pressure as

\[
\rho(y) = [1 + \theta (1 - y)],
\]

\[
\rho(y) = [1 + \theta (1 - y)]^2,
\]

such that the dimensionless temperatures at the top \(T(1) = 1\) and bottom \(T(0) = 1 + \theta\) are fixed when \(\theta = 10\). This dimensionalization uses the top layer temperature \(T_0\) and density \(\rho_0\), together with the layer depth \(d_0\), to set dimensionless profiles and parameter values. Specifically, the atmosphere obeys hydrostatic equilibrium with a dimensionless gravity parameter of \(\tilde{g} = g d_0/R_c T_0 = 2\theta\) for the gas constant \(R_c\). Similarly, non-ideal parameters enter for viscosity \(\mu = \mu/\rho_0 d_0 \sqrt{R_c T_0}\), thermal conduction \(\tilde{k} = \kappa/\rho_0 d_0 R_c \sqrt{R_c T_0}\), and resistivity \(\tilde{\eta} = \eta/\rho_0 \sqrt{R_c T_0}\). The original study fixed the Prandtl parameter as \(\sigma = (\mu/\kappa)(\gamma/\gamma - 1) = 1\) (with the ratio of specific heats \(\gamma = c_p/c_v = 5/3\), where \(R_e = c_p/c_v\)), and then varied the initial settings through a Chandrasekhar number \(Q\) and a Rayleigh number \(R\). The ratio of magnetic to thermal diffusivities is dimensionally fixed by \(\zeta = (\eta \rho_0 c_p/\kappa) = (\tilde{\eta}/\tilde{k})\gamma/\gamma - 1\), and we will focus on cases where the related mid-layer value \(\zeta_m = \zeta(1 + \theta/2)\) is set to 1.2 (the ‘astrophysically relevant situation’, as stated in Rucklidge et al. (2000)). The Chandrasekhar number was always computed from \(Q = 1200/\zeta_m = 1000\), and our dimensionalization yields the initial dimensionless magnetic field strength as \(B_0(t = 0) = \sqrt{Q/\tilde{\eta}}\). All parameters then become fixed by the value of the Rayleigh number \(R\), whose value at the mid-layer in essence determines thermal conduction through the relation

\[
R = 2 \left[ 1 - 2 \frac{\gamma - 1}{\gamma} \right] (1 + \theta/2) \frac{\theta^2 \gamma}{\bar{\sigma}} \frac{\tilde{k}^2 (\gamma - 1)}{2},
\]

Note that here we employ isotropic thermal conduction (in analogy with the original study, although MPT+ARMAVAC allows for anisotropic heat conduction physics as exploited in Xia et al. (2012) and Fang et al. (2013)), together with uniform resistivity and full tensorial viscosity. We used a deterministic incompressible velocity perturbation found from

\[
v = \nabla \times \Psi,
\]

\[
\Psi_x(x, y) = \sum_{j=1}^{N_x} \frac{0.05}{j} \cos \left( \frac{2\pi j x}{\lambda} + \phi_j \right) \exp \left( -\frac{(y - 0.5)^2}{0.2} \right),
\]

\[
\Psi_y(x, z) = \sum_{j=1}^{N_x} \frac{0.05}{j} \cos \left( \frac{2\pi j z}{\lambda} + \phi_j \right) \exp \left( -\frac{(y - 0.5)^2}{0.2} \right),
\]

where \(N_x = N_z = 6\) modes with the specific phases \(\phi_{j,x}^{z}\) were used. Boundary conditions are double-periodic sideways, while both the top and bottom use symmetric conditions for the density, \(\rho\), and velocity components, \(v_x\) and \(v_z\), with asymmetry for \(v_y\) and \(B_y\) and \(B_z\). The pressure is set in the ghost cells to \(p = \rho T\) with the fixed top \(T(1) = 1\) and bottom \(T(0) = 1 + \theta\) values. A second-order central differencing formula on the solenoidal constraint is used to extrapolate \(B_y\), while the GLM scalar \(\psi = 0\) in the ghost cells.

We use a multi-stage (ssprk54), FD scheme with MPS reconstruction. Two cases are shown below, one (top part of Figure 20) is at an aspect ratio of \(\lambda = 8/3\) and \(R = 45.000\), a case known to allow steady-state solutions with irregular hexagons consisting of a fixed number of uprising plumes. While both 8 and 9 plume solutions were reported in Rucklidge et al. (2000), we found a 7 plume pattern which can be safely quantified as a true steady-state solution in a domain decomposition run with an overall resolution of \(160 \times 60 \times 160\).
Figure 20. Magnetoconvection simulations in a parameter regime allowing for steady (top) vs. unsteady (bottom) behavior. See the text for a discussion.

(A color version of this figure is available in the online journal.)

Figure 20 shows the magnetic pressure $B^2/2$ pattern in the endstate (with flow field vectors on the sidepanels), and the temporal evolution of the residual, reaching a value of $2 \times 10^{-8}$ after time $t = 150$. The slightly erratic oscillations between this value and $4 \times 10^{-7}$ are thereafter influenced by IO operations, which have, e.g., switched conservative to primitive variables in place at selected save times.

Another case is shown in the lower panel of Figure 20 for the parameters $\lambda = 8$ and $R = 100,000$ at a resolution of $240 \times 60 \times 240$. In this parameter regime with a very wide box, one witnesses a flux separation where narrow strong field lanes surround patches that are almost field-free with vigorous convective motions. The field-free regions merge and split in a continuously evolving fashion. We show a snapshot taken at time $t = 50$, where the bottom and top planes are colored by magnetic pressure, the two sidepanels quantify the instantaneous temperature difference $T(t) - T(t = 0)$, and the velocity field is shown as arrows in the midplane colored by this latter quantity. It shows the close relation between up flows versus down flows and the local temperature variations.

5. SCALING EXPERIMENTS

Here, we report on the results of scaling experiments for MPI-AMRVAC performed on various supercomputing platforms.

5.1. Weak Scaling

We start with a weak scaling experiment of the MPI-AMRVAC code on the BGQ Fermi computer, as quantified in Figure 21. The setup actually realizes a 3D, compressible MHD setup inspired by the discussion in Longcope–Strauss (Longcope & Strauss 1994) where the authors argue for
near-singular current sheets developing from coalescence instability. Our setup has four “magnetic islands”, which have purely planar \( (B_z = 0) \) magnetic fields from \( B_x = B_0 \sin(2\pi x) \cos(2\pi y) \) and \( B_y = -B_0 \cos(2\pi x) \sin(2\pi y) \) initially, in a 3D unit-sized triple periodic box. The pressure varies with \((x, y)\) to realize an equilibrium and the temperature is initially uniform. The velocity perturbation takes a small amplitude incompressible planar \( v_x \propto \sin(2\pi y), \ v_y \propto \sin(2\pi x) \), with an extra perturbation for a velocity component \( v_z \propto \sin(z) \) in the \( z \) dimension. We use resistive MHD on a uniform grid in this domain decomposition parallel scaling experiment. We use the HLLC scheme for the spatial discretization and a third-order \( \tilde{\text{C}} \text{ada limiter} \) \( \tilde{\text{C}} \text{ada} \) 

\& Torrilhon (2009b) for the time advance. To perform the weak scaling, we set up the problem with a fixed number of grid blocks per CPU (i.e., 4 blocks, each having \( 32^3 \) cells, excluding ghost cells). When we increase the number of CPUs, the resolution of the simulation is increased as well, keeping the number of blocks per CPU fixed. For the smallest number of processors available on Fermi, which is 1024, the resolution is thus \( 512^3 \). At the highest number of CPUs, 31,250 (almost 1 rack at Fermi), the resolution is 1600^3. For each setup, we calculate 100 iterations. For all numbers of processors, this takes about 1074 s IN wall clock time, proving excellent weak scaling in the domain decomposition case. The obtained efficiency is plotted in the figure and the snapshot shows a visualization of the density and current sheet structure. The four flux tubes, with initial predominant poloidal magnetic field, are susceptible to kink instability, while the central current sheet formation happens as before. An ongoing study will further investigate its fully nonlinear evolution.

5.2. Strong Scaling with AMR

Strong scaling of MPI–AMRVAC using adaptive mesh refinement has been investigated using the Jade supercomputer\(^{11} \) with the relativistic jet-formation scenario discussed in Porth (2013).

\(^{11}\) Centre Informatique National de l’ Enseignement Supérieur: http://www.cines.fr

For this test, we simulate one physical time unit starting from a snapshot roughly at the midpoint of the total simulation time, giving a reasonable estimate of the average workload of the simulation. The AMR blocksize for this test is \( 12^3 \) cells and two ghost cells are used on each side of the blocks. The efficiency quantification of a \( 160 \times 10^6 \) cell, five-level production setup (case 160M), as well as a small domain case with \( 40 \times 10^6 \) cells and four levels (case 40M), is shown in Figure 22. We normalize the efficiency to the lowest processor number used, corresponding to 128 processors for case 160M and 64 processors for case 40M.\(^{12}\) At the lowest processor number, the simulations

\(^{12}\) Here, “processor” is synonymous with “core,” and thus denotes the atomic computing unit.
perform 29,437 (160M) and 30,964 (40M) cell updates per second per core.

For case 40M, we quantified the AMR speedup by restarting from a corresponding snapshot where all of the cells were refined to the highest level. This yields a total of 65,536 blocks, to be compared to 21,216 blocks on the highest level of case 40M. We would thus expect a speedup due to more efficient space-filling by a factor of 3.1. The observed run time comparison at 256 processors agrees roughly with this estimate and yields a speedup by a factor of 2.8 when AMR is used, resulting from an AMR overhead of approximately 10%.

5.3. Strong Scaling without AMR

A strong scaling test on a uniform grid version of the cloud shock test with one dust species (discussed in Section 3.4) was performed on the SuperMUC cluster.13 We now adopt Cartesian coordinates in 3D and use a uniform grid size of 4803 cells (110M cells) divided into 83 blocks (totaling 216k blocks) with two ghostcell layers on each block face. The result of the scaling test for one “island” of SuperMuc is shown in Figure 23. For this setup, we find that the efficiency actually increases with processor number up to 2048 processors. At 2048 processors, we obtain a peak performance of ~150 k cell updates per processor per second. We suspect that this super-linear scaling is a result of the network configuration of the SuperMUC cluster: the tree topology allows direct communication between each individual computational nodes within one island. This causes the total communication bandwidth to increase when more nodes are used. Consequently, the time spent in the routine which communicates the boundary conditions between the blocks on different nodes (see Figure 23) is decreased dramatically. When more than 2048 cores are used, the efficiency drops again, as the communication time is becoming predominantly latency limited. Note that at 8192 cores, the efficiency is still 96% as compared to 1024 cores.

6. SUMMARY AND OUTLOOK

We provided an update on the MPI-AMRVAC development, with a focus on the latest additions to our open-source repository (see http://gitorious.org/amrvac). The block AMR, fully parallel software has many possibilities for gas dynamical and plasma physical applications, inspired by concrete astrophysical or solar physical observations. The presentation here emphasized the newest additions to the non-relativistic physics modules, although the high-order FD schemes and time steppers are directly available to all physics modules, including the relativistic HD and MHD ones. In the appendices, we present details on how we produce sliced or collapsed views which fully account for the AMR structure during runtime, as well as the added benefits of being able to distinguish between active and passive grid blocks. These can be of generic interest to all complementary coding efforts on open source, grid adaptive, parallel software for astrophysical applications.

In the future, we plan to extend recent works (van Marle et al. 2011b; van Marle & Keppens 2012) on prominence formation in realistic flux rope configurations, based on the steps already taken in 2.5D MHD or in 3D isothermal MHD (Xia et al. 2012, 2014). Global as well as local solar modeling will use the potential field extrapolation possibilities in ultimately data-driven scenarios to complement state-of-the-art simulations such as those presented by Riley et al. (2011); van der Holst et al. (2014). These can also aid ongoing efforts on global magnetospheric modeling with MPI-AMRVAC, such as those for the Jovian case, as performed by Chané et al. (2013).

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APPENDIX A

SLICING A MORTON-ORDER AMR GRID

Simulations in 2D and 3D frequently lead to large data sets which are not easily visualized. For a quick look into the N-dimensional data, however, it is often sufficient to examine sub-dimensional slices. MPI-AMRVAC is capable of slicing any of its grids along the coordinate directions and of producing the N−1 dimensional data during runtime. The algorithm takes advantage of the tree-based grid structure and is described below.

13 Leibniz-Rechenzentrum, Garching: http://www.lrz.de
1. Given the direction perpendicular to the resulting slice \( d \) and the coordinate value along \( d, x_d^i \), for each level we calculate the grid index indicated by the slice:

\[
g^d(l) = \text{int}(\frac{(x_d^i - x_d^{\min})}{\Delta g^d(l)}) + 1,
\]

where \( \Delta g^d(l) \) is the extent of a grid block (in direction \( d \) on level \( l \)) and \( x_d^{\min} \) is given by the minimal domain boundary. An exemplary 2D grid is shown in Figure 24.

2. For every base grid at \( g^d(l) \), \( l = 1 \):

(a) For every child in a direction other than \( d \), we descend (recursively) into the child:

\[
c^d = g^d(l + 1) - 2g^d(l) + 2,
\]

where the child index is defined as \( c^d = 1 \) for the left child and \( c^d = 2 \) for the right child.

i. Upon encountering a leaf, we take the corresponding block and fill a sub-dimensional solution block given the cells closest to \( x_d^i \).

3. Output sub-dimensional solution block in order of their encounter.

The resulting sub-dimensional grid is again in tree form and reflects the original adaptive, mesh which can be valuable for data inspection. Due to the recursion, the new sub-dimensional, space-filling curve (SFC) is Morton ordered. This strong correspondence between the data structures even allows us to restart an AMR run in \( N - 1 \) dimensions without further modifications, implying \( \hat{g}_d = 0 \). The presented algorithm can be applied to any dimensionality \( N \) and optimally takes advantage of the grid structure since grids relevant for the slice are known a priori (from step 1.). The outer loop thus scales as \( O(N - 1) \), while the complexity added by the recursive inner loop depends on the number of dimensions and levels.

**APPENDIX B**

**COLLAPSING A MORTON-ORDER AMR GRID**

The dimensionality of the grid can also be reduced by integration along coordinate directions, thus “collapsing” the data onto a plane. This yields surface densities, etc. The following algorithm can collapse data onto any level \( l \) during runtime while taking advantage of the underlying data structure.

1. Given the direction of integration \( d \) and the target level of the resulting data \( l_t \), we first sum the quantity \( q \) for each block,

\[
Q(i^P, l) = \Delta x^d(l) \sum_{i^d} q(i),
\]

where \( i^P = P^d(i) \) is the orthogonal projection of a (index) vector along \( d \). The projection simply removes the \( d \) direction in the arrays, leaving the order of the remaining directions unaffected. After this elemental collapse operation, we drop the superscript \( P \) and work only in the reduced index space.

2. Each processor \( j \) allocates the global array for collapsed data \( C_j(P^d(N(l_i))) \), where the number of cells in each direction follows from the number of grid blocks in the target level \( N_g(l_i) \) and the number of cells within each block \( N_i(l_i) = N_g(l_i) N_i^c \).

3. We add up all of the collapsed blocks \( Q \) in the \( C \)-array, using block index and level to fill the correct bins:

\[
i^i(i^d, l) = \text{int}(\frac{i^d - i_B + N_i^c(g^d(l) - 1)}{\Delta^d(l)} + 1).
\]

where \( i^d \) is the local index in the block, \( i_B \) is the number of ghost cells, and the term \( N_i^c(g^d(l) - 1) \) is added to translate from the local block cell index to the corresponding global cell index on level \( l \). Thus, for all blocks on the processor \( j \), we perform

\[
C_j(i_k) = \sum_{i_{l_i}=0}^{\text{last}(l_i)} Q(i, l) \delta S(N, l, l_i);
\]

\[
\delta S(N, l, l_i) = \begin{cases} 
2^{N-l-1} & ; l > l_i \\
1 & ; l \leq l_i
\end{cases}
\]

where the term \( \delta S(N, l, l_i) \) (with \( N \) being the original dimensionality) results in an averaging of the data on levels higher than the target level. Each process now holds a version of the \( C_j(i_k) \) array, and hence the final step is as follows.

4. We use the MPI reduce operation to obtain

\[
C(i_k) = \sum_j C_j(i_k)
\]
on the head node. The final array $C(i)$ is then written out either as a comma-separated value ascii data-file or in binary .vti format.

APPENDIX C
DYNAMIC GRID ACTIVATION

In many applications, parts of the simulation domain can be well described by stationarity or as analytic (e.g., self-similar) solutions, while other parts require for direct numerical simulation. Examples for the “passive” regions are injected supersonic stellar winds, jets that have settled to a stationary state (starting near the injection boundary), or simply the static initial configuration that is still unaffected by the dynamical evolution. Especially for problems that involve a large separation of scales, as in the case of space weather, the computation can be significantly sped up if these passive regions are taken out of the integration loop.

We have implemented a scheme that can dynamically (de-) activate grid blocks in an AMR setting, depending on the solution itself or on temporal/spatial properties. Since the implementation acts only on the grid structure, it can be directly used with all available physics modules. In the following, we describe the strategy and give an example application from recent special relativistic magnetohydrodynamic simulations (Porth et al. 2014).

1. Loop over all grid blocks and flag grids to be deactivated based on a user-defined criterion.
2. Loop over the candidate passive blocks and reactivate the block if an active neighbor is detected.
3. Create final lists of the active and passive blocks.

The second step can be repeated to increase the number of safety blocks. Note that this procedure works seamlessly across level changes. For the ensuing time-integration, only the list of active blocks is advanced. In principle, a separate loop can then also advance the passive blocks, following, for example, a self-similar analytic evolution or employing a completely different physics module.

With active and passive zones present, the parallel load balancing of the code needs some attention. While normally a balanced load is achieved by cutting off the SFC such that the number of blocks per processor is balanced for all processors, it is clear that the introduction of passive blocks violates the identity of block and computational load. Hence, we introduce different weights for active and passive blocks. This allows us to better balance the true computational load and at the same time sets a limit for the permitted memory imbalance. In practice, 

\[
\mathcal{L}(i_B) = \begin{cases} w_a; & \text{Block } i_B \text{ is active} \\ w_p; & \text{Block } i_B \text{ is passive,} \end{cases}
\]

which is balanced by suitably cutting the SFC. The imbalance of load $X_{load}$ and memory $X_{mem}$ considering all processors $N_{pe}$ is

\[
X_{load} = \frac{\max_{i_p=1...N_{pe}}[N_{active}(i_p)]}{\min_{i_p=1...N_{pe}}[N_{active}(i_p)]};
\]

\[
X_{mem} = \frac{\max_{i_p=1...N_{pe}}[N_{active}(i_p) + N_{passive}(i_p)]}{\min_{i_p=1...N_{pe}}[N_{active}(i_p) + N_{passive}(i_p)]}.
\]

Choosing $w_p = 0$ balances the active blocks exactly but could lead to significant memory imbalance. Given the weights, the maximum permitted memory imbalance defined above is 

\[
\hat{X}_{mem} = w_a/w_p.
\]

We typically adopt $\hat{X}_{mem} = 2 \ldots 3$, which gives the best results for the problems and hardware considered so far.

In Figure 25, we illustrate dynamic grid activation for the example of a relativistic pulsar wind simulation from Porth et al. (2013). Cells marked yellow in the left panel of the figure are not advanced in the time loop but hold the stationary solution of the unshocked wind. Note that in this particular application, the origin was refined up to level 20 to properly resolve the
inner regions (the shock is situated on level 9). For the case where the shock is squeezed back to the pulsar, these grids can be automatically activated. In this case, the main speedup is not due to the reduced number of active grids to be advanced but to the larger resulting global CFL-limited time step.

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