A modern resistive magnetohydrodynamics solver using C++ and the Boost library.∗

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Abstract

In this paper we describe the implementation of our C++ resistive magnetohydrodynamics solver. The framework developed facilitates the separation of the code implementing the specific numerical method and the physical model, on the one hand, from the handling of boundary conditions and the management of the computational domain, on the other hand. In particular, this will allow us to use finite difference stencils which are only defined in the interior of the domain (the boundary conditions are handled automatically). We will discuss this and other design considerations and their impact on performance in some detail. In addition, we provide a documentation of the code developed and demonstrate that a performance comparable to Fortran can be achieved, while still maintaining a maximum of code readability and extensibility.

1. Introduction

The use of numerical simulations to study problems from the sciences is prevalent in both industry and academia. Due to the continuous increase in computing power more realistic (and thus more complex) physical models are considered in such simulations. This often requires the adaption of both the physical models as well as the numerical methods used to solve a given problem.

However, contrary to application development, many scientific codes are still written either in the Fortran or the C programming language (although there is a increasing tendency to use selected features from C++; see, for example, [3]). In our opinion, the reason for this is at least threefold. First, performance considerations are one of the (if not the) primary concern when developing scientific codes. This explains why interpreted languages (such as Python or Matlab)

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have generally only been employed for very specific applications. Second, object oriented programming has not been as successful as in other domains (even though, in principle, the value of this abstraction has been recognized; see, for example, [2]). Third, the need to interface with legacy code (which often has been extensively optimized) is an important consideration. Such code is almost exclusively written in either Fortran or C (many libraries provide interfaces for both languages).

Nevertheless, due to increasing code complexity, the need for suitable mechanisms of abstraction is a major concern if maintainable scientific codes are to be developed. However, due to performance considerations many programming paradigms present in the C++ language have either been dismissed or only used cautiously (such as abstract base classes) while other where often considered to be too cumbersome to use (such as templates). It has long been argued that Fortran gives superior performance to C since the impossibility of pointer aliasing provides the compiler with more opportunity to generate efficient code. This argument has to be considered in the context that the C++ standard library does not include a multidimensional array type. However, template based libraries have been developed that provide C++ with multidimensional arrays that rival the performance of Fortran (see e.g. [8]).

In this paper we will introduce a numerical solver for the equations of resistive magnetohydrodynamics (resistive MHD). This code employs a finite difference or finite volume discretization in space (basically the only assumption with respect to the space discretization made is that only a single value is stored per cell). For time integration the CVODE library (which is based on the backward differentiation formulas) is employed. We will explain the fundamental design principles of the code in section 3. These allow us to implement a given space or time discretization in a few lines without considering the specific boundary conditions and to implement the physical model in only a few lines of code that resembles the mathematical form of the equations. Nevertheless, binary compatibility with respect to the CVODE vector type (or any other C or Fortran vector type) is maintained.

This will be accomplished by the limited use of templates and by using the Boost library (where appropriate). Our general philosophy is that we limit ourselves to features of the C++ language for which there is no clear evidence that a significant performance penalty is incurred. In addition, we choose a more commonly employed class over a less well known one if the less well known implementation does not provide a clear performance advantage.

Let us also note that the framework we develop contains some template code. However, this code should be discernible for scientists even if they only have a passing familiarity with template techniques (in contrast to libraries such as Boost [1] or Blitz++ where significantly more involved template techniques are employed in order to provide a fast implementation as well as a convenient interface to the user). Furthermore, to implement a different numerical scheme or physical model no knowledge of templates techniques is necessary.

In section 4 we will consider two plasma physics problems. Numerical simulations and weak scaling tests will be conducted for the reconnection problem
and the Kelvin–Helmholtz instability. In addition, we also present the results of a strong scaling test. In section 5, we document the structure of the source code. Finally, we conclude in section 6.

It is our hope that the framework developed here can be used as a reference implementation and as a stepping stone if the effect of different numerical methods or physical models need to be evaluated.

2. Magnetohydrodynamics & numerical considerations

In this section we describe the equations of magnetohydrodynamics (MHD) which are often used to model a plasma system. These equations are justified if the assumption is made that the plasma under consideration is in thermodynamic equilibrium. The equations of MHD are described in terms of the density $\rho$, the fluid velocity $\mathbf{v}$, the magnetic field $\mathbf{B}$, the energy $e$, and the pressure $p$.

For the purpose of performing the spatial discretization, these equations are often cast into the so-called divergence form. Then, the equations of motion read as (see e.g. [5])

$$\frac{\partial U}{\partial t} + \nabla \cdot F(U) = 0$$

with state vector

$$U = \begin{bmatrix} \rho \\ \mathbf{v} \\ \mathbf{B} \\ e \end{bmatrix}$$

and

$$F(U) = \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + (p + \frac{1}{2} B^2) I - \mathbf{B} \otimes \mathbf{B} \\ \mathbf{v} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{v} \\ (e + p + \frac{1}{2} B^2) \mathbf{v} - \mathbf{B} (\mathbf{B} \cdot \mathbf{v}) \end{bmatrix},$$

(1)

where we have denoted the tensor product by using the $\otimes$ symbol. The most common approach to close these equations (see e.g. [5]) is to supplement them with the following equation of state

$$e = \frac{p}{\gamma - 1} + \frac{\rho}{2} v^2 + B^2.$$

In this paper, as in [4] and [5], we will consider a slightly more general class of equations which, in addition to the dynamics discussed so far, includes dissipative effects (due to particle collisions in the plasma). To that end the hyperbolic flux vector $F(U)$ is extended in [4] by a diffusive part given by

$$F_d(U) = \begin{bmatrix} 0 \\ \mu \tau + \frac{\mu}{\gamma - 1} \nabla e + \eta \left( \frac{1}{2} \mathbf{B} \cdot \mathbf{B} \right) \\ \mu \tau \cdot \mathbf{v} + \frac{\mu}{\gamma - 1} \nabla e \end{bmatrix},$$

(2)
where
\[ \tau = \nabla v + (\nabla v)^T - \frac{2}{3}(\nabla \cdot \tau) I. \]

Note that \( F_d(U) \) as stated here is formulated in terms of the (dimensionless) viscosity \( \mu = Re^{-1} \), the (dimensionless) resistivity \( \eta = S^{-1} \), and the (dimensionless) thermal conductivity \( \kappa = Pr^{-1} \), where \( Re \) is the Reynolds number, \( S \) the Lundquist number, and \( Pr \) the Prandtl number. In all the simulations conducted, the heat capacity ratio \( \gamma \) is set to \( 5/3 \) which corresponds to a monoatomic ideal gas.

Thus, the form of the resistive MHD equations used for the spatial discretization is

\[ \frac{\partial U}{\partial t} + \nabla \cdot F(U) = \nabla \cdot F_d(U) \]

with \( F(U) \) given by equation (1) and where \( F_d(U) \) is given by equation (2).

For comparison and validation we have used the Fortran code developed in [4]. This code has been used to conduct plasma physics simulations (see e.g. [4], [5], and [6]) as well as to construct more efficient preconditioners in the context of implicit time integrators (see e.g. [5]).

Our implementation (as is the case for D. R. Reynolds’ Fortran code) assumes a finite difference or finite volume method where a single value is stored in each cell. Thus, in each cell we store the value of the density \( \rho \), the fluid velocity \( v \), the magnetic field \( B \), the energy \( e \) (but not the pressure \( p \)). In principle it is possible to implement any space discretization satisfying the constraints outlined above. For the numerical simulations conducted in section 4 we have implemented the 2.5-dimensional case (that is, the state variables do only depend on the \( x \)- and \( y \)-direction but both the velocity \( v(x,y) \) as well as the magnetic field \( B(x,y) \) are three-dimensional vectors) using a classic centered stencil for the divergence; that is, for each vector \( G \), corresponding to the flux of a given (scalar) state variable, we compute the following approximation of the divergence

\[ \nabla \cdot G(U) \approx \frac{G(U_{i+1,j}) - G(U_{i-1,j})}{2h} + \frac{G(U_{i,j+1}) - G(U_{i,j-1})}{2h}, \]

where \( i \) and \( j \) are the cell indices in the \( x \)- and \( y \)-directions, respectively and \( h \) is the cell size. To evaluate the spatial derivatives present in the diffusion vector \( F_d \) we employ the classic centered stencil in the interior of the domain and a one-sided stencil of order 2 near the boundary.

In order to integrate the resulting system of ordinary differential equations in time, we use the CVODE software package. The CVODE library employs a multistep scheme based on the backward differentiation formulas (BDF).

3. Design principles

In this section we describe, in some detail, some of the design considerations outlined in the introduction. For the development of the program we have
used the clang C++ compiler as it provides more discernible error messages. However, in preliminary tests it was observed that the clang C++ compiler is, at least in some tests, significantly slower than both the gcc compiler and the Intel C++ compiler. Therefore, and because of the fact that the clang C++ compiler is usually not present on most supercomputers, in what follows, we provide only time measurements for the gcc compiler and the Intel C++ compiler.

3.1. The choice of an array class

Compared to Fortran (where usually the single and multi-dimensional arrays built into the syntax of the language are the best choice) there are a number of options available in the C++ programming language. The (traditional) C-style arrays have only limited support for multi-dimensional arrays and additional information (such as the length of the array) has to be stored separately. The latter (similar to the way arrays are handled in Fortran) increases code complexity while the former (contrary to how arrays are handled in Fortran) requires the user to develop a custom notation for array indexing.

In C++ two classes have been included in the standard library that can be used to replace dynamically allocated arrays (i.e. arrays where the number of elements is not known at compile time). The vector class and the valarray class. Both classes handle the allocation of memory, store the dimension of the array (which can be accessed by the size method), and allow access to elements by using the [] operator. Furthermore, both classes maintain compatibility to the standard C-style arrays in that all data are stored sequentially in memory.

The reason the valarray class has been introduced in C++ is to achieve performance comparable to Fortran. The idea is that since the valarray class will never hold any pointer type (thus the name value array) it can be implemented more efficiently than is the case for a generic container (such as the vector class). More detailed information can be found in [7].

In Table 1 the computation of the inviscid flux for a one-dimensional array of a given size is timed for the C-style array, the vector class, and the valarray class. We observe identical results (within measurement errors) with two exceptions. For the gcc compiler the valarray class is faster by about 50% as compared to all other implementations and for the Intel C++ compiler the Fortran implementation is faster as compared to all other implementations by approximately the same margin. In our implementation we have chosen to use the vector class as there is no clear speed advantage of the valarray class (in fact in one configuration the valarray class is faster and in another configuration the vector class is faster) and the vector class works better with the concept of iterators.

In the C++ standard libraries no class has been included to facilitate multi-dimensional arrays. However, the Boost library includes the multi_array class. It overloads the [ ] and the (,) operator to access elements and provides a

\[1\] In the C programming language macros are usually employed to accomplish this behavior.
mean to obtain lower-dimensional slices without copying any data (by returning
an iterator). Especially the latter does contribute to code simplicity as no
stride value has to be taken into account. Furthermore, the multi_array class
maintains memory compatibility with C-style arrays (the corresponding one-
dimensional array can be stored either in row-major or in column-major format).
Of course, performance is dependent on the order of iteration. An iteration with
stride 1 will, in general, result in better performance compared to an iteration
with stride \(N\) (where \(N\) is the size of the array in a single dimension). This has to
be taken into account; however, the same is true for any array implementation.

In Table 2 the computation of the inviscid flux for a two-dimensional array
of a given size is timed for the C-style array and the Boost multi_array class.
We observe that in this test the performance penalty for using the multi_array
class as compared to a C-style array is below 10\% if the gcc compiler is used. Let
us further note that the Intel C++ compiler is significantly slower than the gcc
compiler in all of these tests (although the Intel C++ compiler achieves similar
performance compared to the gcc compiler in case of the Fortran implementa-
tion). Let us further note that a convenient feature of the multi_array class is
that bound checking can be enabled while the application is being developed (in
the performance measurements conducted here these checks, as is usually the
case in a release build, have been disabled by defining \texttt{BOOST_DISABLE_ASSERTS})

3.2. Mapping state variables to physically relevant variables

In numerical simulations the phase space is usually represented as an array
of double precision floating point numbers. However, the physical variables
associated to this quantities are usually referred to by a well known designation
(such as \(\rho\) for the density or \(B\) for the magnetic field). From this consideration
two issues arise. First, it is not desirable to access physical quantities purely by
their array index. For example, code fragments similar to

\[
y(i,1)=x(i,1)\times x(i,3)
\]

are used in many Fortran, Matlab, and C implementations to compute the mass
flux with respect to the \(y\)-direction. Obviously code written in this fashion is
not easily discernible even if it is known that the first component represents the
density and that the third component represents the velocity in the \(y\)-direction.
Table 2: The inviscid flux for an array of size \( n = N^2 = 316 \cdot 316 \approx 10^5 \) is computed. The measured times are shown (the estimated standard deviations are computed using \( 10^4 \) repetitions and are shown in parenthesis). The simulations are conducted on the LEO III (Intel Xeon X5650 with gcc 4.4.6, icc 12.1, and Boost 1.51.0) and the VSC-2 supercomputer (AMD Opteron 6132 HE with gcc 4.4.7, icc 14.0.2, Boost 1.55.0). In both cases the -O3 compiler flag is used.

Second, some quantities can be considered as vector types (for example the magnetic field). Thus, some way to iterate over such variables has to be provided. A common way to implement this in C++ (or C) is to define an appropriate struct. In our case the state space would be represented by

```cpp
struct state {
    double rho;
    array<double,3> v;
    array<double,3> B;
    double e;
};
```

The issue with this implementation is that to implement collective operation on the entire state (such as component-wise addition and scalar multiplication) is either somewhat tedious as all the variables have been summed separately or does rely on techniques which are not type-safe (such as casting the struct to a double pointer).

Therefore, we have chosen to implement the state as a simple 8-dimensional array and to supply appropriate functions to access the physical variables.

```cpp
struct state {
    array<double, 8> data;
};

double& rho(state& s) {
    return s.data[0];
}
double& v(state& s, size_t dim) {
    return s.data[1+dim];
}
...
As can be seen from the code snippet, we employ a feature of C++ that allows us to return a value as a reference from a function. This in fact allows us to set as well as access (get) the desired values. The computation of the flux from the beginning of the section in this notation reads as

\[
\rho(y) = \rho(x) \ast v(x,1);
\]

We expect the compiler to inline this calls and thus no performance overhead should be incurred. We have conducted a number of numerical simulations which confirms this expectation.

The inviscid flux given in equation (1) can be implemented as follows

```cpp
#include <iostream>

using namespace std;

class state {
public:
    vector<double> rho, v, e;
}

double Bsq(state s) { return B(s) \cdot B(s); }

double pressure(state s) { return e(s) / rho(s) - 1; }

class state flux_inviscid(size_t dim, state s) {
    state r;
    rho(r) = -rho(s) \ast v(s, dim);
    double Bv = 0.0;
    for (int i = 0; i < 3; i++) {
        v(r, i) = -rho(s) \ast v(s, i) \ast v(s, dim)
                   - (pressure(s) + 0.5 \ast Bsq(s)) \ast (i == dim)
                   + B(s, i) \ast B(s, dim);
        B(r, i) = v(s, i) \ast B(s, dim) - B(s, i) \ast v(s, dim);
        Bv += B(s, i) \ast v(s, i);
    }
    e(r) = -(e(s) + pressure(s) + 0.5 \ast Bsq(s)) \ast v(s, dim)
           + Bv \ast B(s, dim);
    return r;
}
```

This form greatly increases readability and reflects the mathematical formulation of the MHD equation (the equation of state is implemented in the `pressure` function).

3.3. Boundary conditions

One aspect that frequently introduces mistakes in numerical code is the handling of boundary conditions. There are two commons ways to implement boundary conditions. First, they can be incorporated directly into the stencil. This approach, however, has the disadvantage that the stencil needs to be modified every time different boundary conditions are considered. In addition, a differentiation between different parts of the boundary is often necessary. The second approach employs so-called ghost cells, which are appended to the regular domain. This alleviates the issues discussed above but requires the extension of the domain. This in turn makes it often necessary to extract the physical domain in other parts of the code (for example in a parallel setting where the values in the interior of the domain have to be passed to a linear or nonlinear solver). Let us also note that these considerations are not only important at the physical boundary but also at the boundaries that exist between different nodes in a MPI parallelization, for example.

We have chosen to store the (inner) domain separately from the ghost cells (which form a halo region). An iterator is then defined which allows the developer implementing a stencil to only consider it in the interior of the domain. The boundary conditions are then automatically satisfied if the ghost cells are set.
Table 3: The first derivative for an array of size $n = 10^5$ is computed by using the classic centered stencil. The measured times are shown (the estimated standard deviations are computed using $10^4$ repetitions and are shown in parenthesis). The simulations are conducted on the LEO III (Intel Xeon X5650 with gcc 4.4.6, icc 12.1, and Boost 1.51.0) and the VSC-2 supercomputer (AMD Opteron 6132 HE with gcc 4.4.7, icc 14.0.2, Boost 1.55.0). In both cases the -O3 compiler flag is used.

|                | gcc (LEO III) | icc (LEO III) | gcc (VSC-2) | icc (VSC-2) |
|----------------|--------------|---------------|-------------|-------------|
| Direct impl.   | 1.086(80) ms | 1.282(73) ms  | 2.49(14) ms | 2.47(13) ms |
| Boundary iter. | 1.085(48) ms | 1.411(54) ms  | 2.234(73) ms| 2.637(23) ms|

appropriately. Also an implementation of additional boundary conditions would not require any modification of the stencil code. In Table 3 we have considered the impact on performance of this implementation for the classic centered difference stencil. For the gcc compiler no performance penalty can be observed while a small decrease in performance is observed for the Intel C++ compiler. Let us further note that the gcc compiler seems to perform consistently better than the Intel C++ compiler in this test.

3.4. std::transform

A common practice in scientific codes is to apply a function to each element in an array. In this instance one can use either one or multiple for loops to iterate over all the elements or use the `transform` function included in the C++ standard library. The latter conceivably has two advantages. First, it frees us from explicitly taken care of the array indices and we are thus able to write code that works independently of the dimension of the array under consideration. Second, the compiler can take advantage of the information that the operations for each element of the array are independent and possibly generate more efficient code.

In the numerical computations we have conducted (the result of which are shown in Table 3), we observe no clear advantage for using a for loop or the `transform` function. In fact, depending on the configuration either method can yield superior performance). As expected the `multi_array` class shows almost the same performance as the one-dimensional containers (as there is no difference in the manner the data are stored in memory). It is further interesting to note that the gcc compiler outperforms the Intel C++ compiler in all of these tests.

4. Numerical examples

To test and validate the code developed, we have run a number of simulations and compared them to the results produced by D. R. Reynolds’ Fortran code (as described in [4] and [5]). The first example we consider here is the so-called reconnection problem. This example models the reconnection of magnetic field lines. That is, as an initial value we impose an almost discontinuous magnetic field which points in opposite directions on different sides of the discontinuity. The dissipation included in the resistive MHD model then causes a reconnection of the field lines. The numerical results (shown in Figure 1) display the characteristic broadening/thinning of the density (see, for example, [4]).
Figure 1: The density $\rho$ is shown at times $t = 0$ (top), $t = 75$ (center), and $t = 150$ (bottom). In both space directions 256 grid points are employed. The dimensionless parameters are chosen as follows: $\mu = 10^{-3}$, $\eta = 10^{-3}$, and $\kappa = 10^{-2}$. 
Table 4: The inviscid flux for an array of size \( n = 10^5 \) is computed using the vector class (where \( F \) denotes that we are using a for loop and \( T \) denotes that we employ the transform function found in the C++ standard library). The measured times are shown (the estimated standard deviations are computed using \( 10^4 \) repetitions and are shown in parenthesis). The simulations are conducted on the LEO III (Intel Xeon X5650 with gcc 4.4.6, icc 12.1, and Boost 1.51.0) and the VSC-2 supercomputer (AMD Opteron 6132 HE with gcc 4.4.7, icc 14.0.2, Boost 1.55.0). In both cases the -O3 compiler flag is used.

| Cores | Time | RHS eval. | Nonlin. iter. | Linear iter. | Communication time |
|-------|------|-----------|---------------|--------------|--------------------|
| 1     | 0.8 s| 46        | 16            | 26           | 0.16 s             |
| 4     | 2.5 s| 90        | 34            | 52           | 0.75 s             |
| 16    | 10.5 s| 214       | 40            | 170          | 2.4 s              |
| 64    | 115 s| 474       | 40            | 430          | 15.9 s             |
| 256   | 495 s| 1317      | 44            | 1269         | 20.5 s             |

Table 5: Weak scaling test for the reconnection problem on the LEO3 HPC system at the University of Innsbruck [http://wwwuibk.ac.at/zid/systeme/hpc-systeme/leo3/]. The reconnection problem is integrated up to time \( t = 1 \). The dimensionless parameters are chosen as follows: \( \mu = 10^{-3} \), \( \eta = 10^{-2} \), and \( \kappa = 10^{-2} \). To each core we assign a slice of the domain with 128 grid points in both directions. The measured communication time includes both the time necessary to prepare the data as well as the transmission time.

The second example we consider is the so-called Kelvin–Helmholtz instability. That is, we consider a shear flow in a constant magnetic field in which the velocity field is perturbed. This leads to a time evolution with highly inhomogeneous magnetic fields. The results of the numerical simulation are shown in Figure 2.

We have chosen to use Boost.MPI to parallelize our code to multiple nodes of the cluster under consideration. Boost.MPI provides a convenient C++ interface to the Message Passing Interface. The only modification to the existing code that is required to use Boost.MPI is to add a serialization statement to the \texttt{state} class. This is necessary as Boost.MPI uses the serialization interface in order to convert custom data types to a bytestream that is send to different nodes.

In Table 5 a weak scaling test (that is, the size of the problem is proportional to the number of cores used) for the reconnection problem is performed. We observe that communication time necessary to evaluate the right-hand side is not a limiting factor up to at least 256 cores as most of the increase in the runtime is due to the increase in computational effort required by the iterative solver. To reduce this growth in computational effort (to some extent) a number of advanced preconditioning techniques have been developed (see, for example, [5]).

In Table 6 a weak scaling test for the Kelvin–Helmholtz instability is per-
Figure 2: The magnitude of the magnetic field in the z-direction at times $t = 1$, and $t = 2$ is shown. The initial value (i.e. the value at time $t = 0$) consists of a homogeneous field equal in strength to 10. In both space directions 256 grid points are employed. The dimensionless parameters are chosen as follows: $\mu = 10^{-3}$, $\eta = 10^{-3}$, and $\kappa = 10^{-2}$.
Table 6: Weak scaling test for the reconnection problem on the LEO3 HPC system at the University of Innsbruck (http://www.uibk.ac.at/zid/systeme/hpc-systeme/leo3/). The Kelvin–Helmholtz instability is integrated up to time $t = 0.05$. To each core we assign a slice of the domain with 128 grid points in both directions. The measured communication time includes both the time necessary to prepare the data as well as the transmission time.

| Cores | Time | RHS eval. | Nonlin. iter. | Linear iter. | Communication time |
|-------|------|-----------|--------------|--------------|--------------------|
| 1     | 7.5 s| 419       | 202          | 213          | 1.6 s              |
| 4     | 14 s | 506       | 167          | 335          | 4 s                |
| 16    | 39 s | 634       | 80           | 550          | 12 s               |
| 64    | 363 s| 1479      | 104          | 1371         | 55 s               |
| 256   | 1273 s| 3431      | 112          | 3315         | 55 s               |

Table 7: Strong scaling test for the reconnection problem on the LEO3 HPC system at the University of Innsbruck (http://www.uibk.ac.at/zid/systeme/hpc-systeme/leo3/). The reconnection problem is integrated up to time $t = 0.1$. The dimensionless parameters are chosen as follows: $\mu = 10^{-3}$, $\eta = 10^{-3}$, and $\kappa = 10^{-2}$. The domain consists of 1024 grid points in both directions. The measured communication time includes both the time necessary to prepare the data as well as the transmission time.

| Cores | Time (1024) | Speedup (1024) | Communication time |
|-------|-------------|----------------|--------------------|
| 1     | 126 s       | -              | -                  |
| 16    | 13 s        | 10             | 3.2 s              |
| 64    | 10 s        | 13             | 8.1 s              |

Table 6: Weak scaling test for the reconnection problem on the LEO3 HPC system at the University of Innsbruck (http://www.uibk.ac.at/zid/systeme/hpc-systeme/leo3/). The Kelvin–Helmholtz instability is integrated up to time $t = 0.05$. To each core we assign a slice of the domain with 128 grid points in both directions. The measured communication time includes both the time necessary to prepare the data as well as the transmission time.

formed. We draw the same conclusions as in the case of the reconnection problem.

However, what is more relevant with respect to the implementation considered here is how the communication cost increases as we increase the number of cores. In the weak scaling tests conducted above this behavior can not be easily observed as the total computational cost also increases as the problem size is increased. However, it is difficult to conduct a strong scaling test using the implicit time integrator as the memory available per core (on both HPC systems under consideration here) does not allow us to run a problem of significant size on a single node. Therefore, in Table 7 we show the results of a strong scaling test using the explicit Euler method as the time integrator.

Furthermore, we have compared the time it takes to compute the flux vector for D. R. Reynolds’ Fortran implementation and our code. For the Fortran implementation we measure approximately 12 ms (using the gcc Fortran compiler) and 10 ms (using the Intel Fortran compiler). For our C++ implementation we measure approximately 7.5 ms (using the gcc compiler) and 8.5 ms (using the Intel C++ compiler). These simulations have been conducted on the LEO3 HPC system and are consistent with the performance measurements presented in section 3. The results show a performance advantage of our C++ code of approximately 30%. Note, however, that caution is warranted in comparing these two implementations as there are small differences with respect to both the implementation and the numerical method that is implemented. However, what the comparison does show is that the performance achieved by the C++
code is certainly comparable to that of the Fortran code. Certainly there are a number of optimizations that, if carried out, could improve the performance of both codes. We should also emphasize at this point that the C++ implementation is certainly significantly shorter (measured in number of lines of code) compared to the Fortran implementation.

5. Documentation

The purpose of this section is to provide an overview of the C++ code discussed in this paper. All the routines which are not directly related to the MHD problem or the numerical scheme have been implemented in C++ header files (with the ending .hpp). These header files, as is necessary for template based programming, contain both the class and function declarations as well as their implementation. The files are

state.hpp  This file includes the state class and all the helper functions that are used to manipulate it. This includes the functions discussed in section 3.2.

boundary.hpp  This file includes the boundary2d class which stores the boundary conditions (both left/right and top/bottom). The boundary2d class includes methods to obtain iterators over the boundary elements.

domain.hpp  This file includes two classes. The interval class which is simply used to store the size of a given domain (in a single direction) and the domain class. The domain class stores a two-dimensional array with the values corresponding to the part of the domain residing on the corresponding processor. In addition, it includes a method to construct an initial approximation (from a function depending on both the x- and y-direction), a method to obtain a one-dimensional slice of the data, and a function to write the data to disk.

stencil_array.hpp  This file includes the stencil_array class which constructs a (virtual) array from an iterator to a slice of the interior domain and the appropriate boundary elements. The [] operator is overloaded in order to provide access to these (virtual) one-dimensional array.

stencil.hpp  This file includes the single function apply_stencil which applies a stencil (in the x-direction if the parameter dim is set to 0 or the y- direction if the parameter dim is set to 1) using the domain data dom and the boundary data bdr. The output is stored in out. The template parameter stencil (of type FUNC) is a function which computes the desired stencil giving a reference to an input and an output stencil array (these can be accessed as generic one-dimensional arrays as discussed above).

mpi.hpp  This file includes the parallel_mpi class which is responsible for mapping the MPI rank to the two-dimensional indices in the grid used for conducting the computation. Furthermore, it provides helper methods to check which physical boundaries the current core needs to handle.
cvode.hpp This file includes two classes: wrapper and cvode_wrapper. The former is a base class with a single virtual method. The second implements this method in order to conduct a time step using the CVODE library. All the code that interfaces with the CVODE library is included in this file.

timer.hpp This files includes the timer class which is used in order to time the code.

All of these files combined contain about 500 lines of source code. Their primary purpose is to separate the common tasks from the specific implementation of a given set of equations, the numerical scheme used, and the communication required. These remaining functions are all implemented in the mhd.cpp file which contains approximately 300 lines of code (of which about 100 lines of code are used to parse the command line arguments; the Boost.Program_options library is used for that purpose).

The program accepts a number of command line option. Using the command

```
./mhd --help
```

a list including a more detailed description can be obtained. For the two examples introduced in the previous section the commands

```
mpirun -np 4 ./mhd -m cvode -p recon -T 150 \
   --timestep 25 --nx 256 --ny 256
```

and

```
mpirun -np 4 ./mhd -m cvode -p kh -T 2 \
   --timestep 0.1 --nx 256 --ny 256
```

have been used. By default the workload is equally distributed among the two directions.

6. Conclusion & Outlook

We have outlined the design rationals upon which the implementation of our resistive magnetohydrodynamics solver is based. From our performance measurements it should be clear that this greatly improves code readability while it (at most) incurs a minimal performance penalty. In fact, the implementation compares very favorable to an existing Fortran implementation from the literature. Beyond the C++ standard library we only use the Boost library as well as CVODE (in order to conduct the time integration). It is quite surprising to us that (except for the Fortran benchmarks) the Intel C compiler was outperformed by the gcc compiler in almost every test. This behavior is consistent across at least two HPC systems.

The framework developed here can conceivably be used for problems different from MHD and additional time integration libraries can be included (an implementation that includes the, as of yet unpublished, EPIC exponential integrator library is currently in work).
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