Variational-Based Data Assimilation of Initial Value Problems for Ideal Magnetohydrodynamic Equations Subject to Solenoidal Constraint

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Abstract—Recently, the authors have proposed an adjoint-based data assimilation strategy that optimizes initial conditions from the discrepancy of numerical solutions and observed data in computations of canonical, one-dimensional (1D), MHD problems. However, despite the success of the aforementioned study, all available information associated with the magnetic field data could not be ingested due to issues with the solenoidal property associated with the magnetic field ($\nabla \cdot \mathbf{B} = 0$). Therefore, this study proposes an adjoint-based data assimilation procedure that ensures the solenoidal constraint on the magnetic field is satisfied. This new data assimilation scheme involves two novel components: (1) the initial magnetic field is expressed with a divergence-free parametrization; and (2) the ideal MHD equations are augmented with either the Powell source term or a generalized Lagrange multiplier (GLM) formulation. In the case of the former, instead of correcting the initial magnetic field directly, optimal parameters are sought so as to best match the observed data while maintaining the solenoidal property by construction. In the latter, the Powell and GLM approaches are used to remove via transport any non-zero $\nabla \cdot \mathbf{B}$ errors generated within the simulation. The adjoint terms corresponding to the Powell and GLM strategies are derived and added directly to the adjoint equations of the original equation system. The proposed data assimilation schemes are assessed for 1D MHD initial value problems, and the ability to correct all components of the magnetic field is demonstrated. In addition, the extension of the data assimilation strategy to 3D simulations is discussed.

Keywords—Magnetohydrodynamics; Data Assimilation; Computation Fluid Dynamics; Inverse Problems.

I. INTRODUCTION

Over the last several decades, significant effort has been devoted to the development of efficient computational fluid dynamics (CFD) algorithms for a variety of physically-complex flows, including the simulation of space-physics phenomena [1]–[3]. The latter are very often based on the equations of ideal magnetohydrodynamics (MHD), an extension of conventional fluid dynamic descriptions to electrically conducting fluids. Although sophisticated, CFD models are limited in their ability to provide accurate predictions when model input parameters are poorly known. Such is the case in space-weather forecasts where the specification of appropriate initial and boundary data can be a formidable challenge. The true initial and boundary conditions are not known and must therefore be estimated.

Presently, state-of-the-art space-weather models rely on magnetic field measurements of the solar surface, known as magnetograms, to infer their inner boundary conditions [4]. These magnetograms are extrapolated from the solar surface to the model’s inner boundary, generally located at around 25 solar radii, using a variety of techniques [5], [6]. Moreover, the extrapolated magnetic field is related to the remaining plasma properties via empirical relations [7]. Despite these efforts, the inferred estimates may deviate significantly from the true plasma properties [8]. The use of data assimilation techniques is therefore an attractive step towards further constraining space-weather models.

Data assimilation (DA) is a field of study that seeks to optimally combine the outputs of numerical models with real measurements of a system. In moving towards the application of DA in space-weather forecasting, the authors have recently proposed an adjoint-based DA strategy that optimizes initial conditions from the discrepancy of numerical solutions and observed data in computations of canonical, one-dimensional (1D), MHD problems [9]. Prior to considering more realistic simulations, one unaddressed challenge remains: the
solennoidal property of the magnetic field ($\nabla \cdot B = 0$). The aforementioned DA strategy does not take into account this constraint, leading to unphysical magnetic fields. Therefore, in the 1D setting, the $x$ component of the magnetic field cannot be assimilated. In three-dimensional (3D) computations the problem is aggravated — the magnetic field in whole cannot be corrected. Much of the MHD literature is focused on the preservation of divergence-free magnetic fields throughout the flow evolution. For example, Powell’s 8-wave formulation [10] and Dedner’s Generalized Lagrange Multiplier (GLM) approach [11] transport $\nabla \cdot B$ errors out of the domain. The so-called constraint-transport method [12] and its variants maintain $\nabla \cdot B = 0$ to machine precision in a specific discretization of the magnetic field. Nevertheless, these techniques are unsuitable for addressing the DA problem since they necessitate an initially solennoidal magnetic field. Therefore, this study proposes a novel adjoint-based data assimilation procedure that ensures the solennoidal constraint is initially satisfied. The divergence cleaning methods of Powell or Dedner are then used to remove via transport any non-zero $\nabla \cdot B$ errors generated within the simulation.

The remainder of this paper is structured as follows: Sections II and III describe the equations of ideal MHD and a finite-volume solution procedure respectively. Section IV presents the proposed DA strategy which is numerically tested in Section V. Finally, concluding remarks are provided in Section VI.

II. GOVERNING EQUATIONS OF IDEAL MAGNETOHYDRODYNAMICS

As previously discussed, computational models of space plasmas generally invoke an MHD approximation for the solar atmosphere, solar wind, and the Earth’s magnetosphere. In so doing, viscosity and resistivity are neglected, ions and electrons are treated as a single fluid, and particle distributions are assumed to be Maxwellian. While these restrictive assumptions cannot strictly be expected in actual space plasmas, the equations of ideal MHD provide a self-consistent mathematical description that span the enormous spatial and temporal scales of SW phenomena and are widely used.

The Ideal MHD equations, in non-dimensional, strong-conservation form may be written as

$$\frac{\partial U}{\partial t} + \nabla \cdot F = S,$$  \hspace{1cm} (1)

where,

$$U = \begin{bmatrix} \rho \\ \rho u \\ E \\ B \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u u - B B + p_T I \\ (E + p_T)u - (u \cdot B) B \\ B u - u B \end{bmatrix}.$$  \hspace{1cm} (2)

Here $\rho$, $u$, $E$, $B$, $p_T$, and $I$ are the plasma density, velocity, specific total energy, magnetic field, total pressure, and the identity dyad, respectively. The total pressure and specific total energy (with the assumption of a calorically perfect gas) are given by

$$p_T = p + \frac{|B|^2}{2}, \quad E = \frac{\rho|u|^2}{2} + \frac{p}{\gamma - 1} + \frac{|B|^2}{2},$$  \hspace{1cm} (3)

where $p$ is the thermal pressure, and $\gamma$ is the ratio of specific heats.

Eq. (1) may not look to be in strong-conservation form due to the presence of $S$. However, at the PDE level, $S$ vanishes as it is depends on $\nabla \cdot B$, which is zero by Gauss’ law. Nevertheless, $S$ is retained to control errors in $\nabla \cdot B$ that arise from discretizing the magnetic field and to ensure the Galilean invariance of the equations. Using the original formulation given by Powell and Godunov, or the modifications made with the GLM approach, $S$ reads

$$S_p = - \begin{bmatrix} 0 \\ B \\ u \cdot B \\ u \end{bmatrix}, \quad S_{GLM} = - \begin{bmatrix} (\nabla \cdot B)B \\ \nabla \cdot B \\ 0 \end{bmatrix}$$  \hspace{1cm} (4)

respectively. Furthermore, the GLM approach adds an additional equation for the evolution of the Lagrange multiplier, $\psi$, which reads

$$\frac{\partial \psi}{\partial t} + c_h^2 \nabla \cdot B = -c_h^2/c_p \psi,$$  \hspace{1cm} (5)

where $c_h$ and $c_p$ are tunable parameters that control the advection speed and damping rate of $\nabla \cdot B$ errors.

III. FINITE-VOLUME METHOD FOR IDEAL MHD

The hyperbolic system of Eq. (1) is numerically solved using a second-order MUSCL-type finite-volume scheme [13] on a uniform 1D mesh. The semi-discrete form of the finite-volume formulation applied to the $\text{i}^{\text{th}}$ computational cell can be expressed as

$$\frac{dU_i}{dt} = -\frac{1}{\Delta x} [\mathcal{F}_{i+1/2} - \mathcal{F}_{i-1/2}] + S_i$$  \hspace{1cm} (6)

where $\mathcal{F}_{i+1/2}$ is the upwind value of the numerical flux evaluated at the $i + 1/2$ cell boundary; $U_i$ and $S_i$ are the cell-averaged values of the conserved solution vector and source term of cell $i$ respectively. The numerical flux, $\mathcal{F}_{i+1/2}$, is determined from the solution of a Riemann problem given the left and right primitive interface solution values, $W_l$ and $W_r$ respectively. The approximate Riemann solver of Powell [10] is used herein. Second-order spatial accuracy is achieved via piece-wise limited linear reconstruction of the primitive solution vector, $W = [\rho, u, p, B]^T$. Second order temporal accuracy is achieved via a strong stability preserving second-order Runge-Kutta [14], [15] time-marching scheme.

IV. A SOLENOIDAL PRESERVING VARIATIONAL DATA ASSIMILATION STRATEGY

As mentioned earlier, the field of data assimilation aims at optimizing the estimation of a real system by combining observational data, $d$, with a numerical model. In the present study, the goal is to combine measurements of plasma flows with the output of an MHD model, $U$. To achieve this, we
first assume that the error in both the data and the model’s initial condition is Gaussian distributed. Mathematically, this assumption can be expressed as
\[ d^n = \mathcal{H}(U^n_{\text{truth}}) + e^n, \quad \text{with} \quad e^n \sim N(0, \Sigma_d), \]  
(7)
\[ U^0 = U^n_{\text{truth}} + \xi^0, \quad \text{with} \quad \xi^n \sim N(0, \Sigma_U). \]  
(8)
Here, \( \mathcal{H} \) is the so-called observation operator that maps the true state of the plasma flow, \( U^n_{\text{truth}} \) to the corresponding measurements. \( e^n \) denotes the error in the data at time-step \( n \). This error is assumed to be normally distributed with zero mean and known covariance, \( \Sigma_d \). Similarly, the error in the initial condition, \( \xi^0 \), is assumed to be normally distributed with zero mean and known covariance, \( \Sigma_U \). With these assumptions, it may be shown that an optimal initial condition may be found by solving the following optimization problem
\[ \min_{U^0} J = ||U^0 - U^b||^2_{\Sigma_U^{-1}} + \sum_{n=1}^{N} ||\mathcal{H}(U^n) - d^n||^2_{\Sigma_d}, \]  
subject to \( \frac{dU_i}{dt} + \frac{1}{\Delta x}[F_{i+1/2} - F_{i-1/2}] - S_i = 0. \)  
(9)
Here, the vector \( U^b \) denotes the first estimate of \( U^0 \), known as the ‘background’. The cost function, \( J \), measures two competing quantities. The first term measures the difference between the background and optimal \( U^0 \), weighted by the precision of the model error. The second term measures the difference between the model and the data, weighted by the precision of the data.

Using the Adjoint state method, the gradient of \( J \) can be efficiently calculated. Though not presented here, the authors have previously formulated a discrete adjoint model for the ideal MHD equations. This adjoint model did not previously include the divergence cleaning source terms of Powell or Dedner (Eq. (4)). As such, the Jacobians of these terms are provided in Appendices A and B.

With the gradient information, the optimization problem of Eq. (9) can be iteratively solved using a plethora of gradient-based minimization algorithms. The Limited-memory BFGS algorithm is a common choice for example. However, with this approach, the \( \nabla \cdot B \) problem becomes immediately clear. Any solution of Eq. (9) will almost always violate \( \nabla \cdot B = 0 \) as this constraint is not enforced. One may attempt to add \( \nabla \cdot B = 0 \) directly to Eq. (9), but it is then not clear how one can efficiently solve the optimization problem. Instead, the main idea of this study is to use the \( \nabla \cdot B = 0 \) constraint to parametrize the control vector \( U^0 \). In the 1D setting, the solution is almost obvious. \( \nabla \cdot B = 0 \) implies that \( B_x \) is a constant. Therefore, the initial condition, \( U^0 \), is parametrized in terms of the constant \( \overline{B}_x \), i.e.,
\[ B^0_x(x) = \overline{B}_x \quad \forall x. \]  
(10)
In 3D, a little more effort is needed. Helmholtz decomposition of the magnetic field, together with the solenoidal property, implies that the magnetic field may be written as the curl of a vector field, i.e.,
\[ B^0 = \nabla \times A. \]  
(11)
The vector field, \( A \), is known as the magnetic vector potential and is characterized by the fact that it is not unique. One may add any scalar potential, \( \nabla f \), to \( A \) without changing the magnetic field, \( B \). This fact follows from the vector identity \( \nabla \times (\nabla f) = 0 \). This property, known as gauge freedom, grants us the liberty to ‘pick’ a gauge. To simplify the parametrization, the so-called axial gauge is employed which fixes \( f \) such that \( A_x = 0 \).

With Eqs. (10) and (11) in mind, the new control vector \( U^0 \) is defined according to
\[ U^0_{1D} = [\rho^b, \rho u^0, E_0, \overline{B}_x, B_y^b, B_z^b]^\top, \]  
(12)
\[ U^0_{3D} = [\rho^b, \rho u^0, E_0, A_y, A_z]^\top. \]  
(13)
The minimization problem of Eq. (9) is thus replaced with
\[ \min_{U^b} J = ||U^b - U^0||^2_{\Sigma_U} + \sum_{n=1}^{N} ||\mathcal{H}(U^n) - d^n||^2_{\Sigma_d}, \]  
subject to \( \frac{dU_i}{dt} + \frac{1}{\Delta x}[F_{i+1/2} - F_{i-1/2}] - S_i = 0, \)  
(14)
where \( U^b \) is the initial estimate of \( U^0 \), and \( \Sigma_U \) is the error covariance of \( U^0 \). With this new parametrization, the optimal initial condition can now be sought while preserving the solenoidal property. Additionally, the number of design parameters is reduced. For example, if a computational mesh contains \( M \) cells, the number of design parameters is reduced from \( 8M \) to \( 7M + 1 \) in 1D and \( 7M \) in 3D.

V. NUMERICAL RESULTS

To assess the efficacy of the proposed DA strategy outlined in Section IV for the ideal MHD equations, a set of numerical experiments are conducted. The canonical initial-value problem (IVP) of Brio and Wu [16] is studied in the context of DA. The Brio-Wu IVP is an ideal MHD shock-tube problem consisting of a high density, high pressure plasma that is initially separated from a low density, low pressure plasma of opposite polarity by a thin membrane. When the membrane is removed, a series of MHD waves – including a shock-, rarefaction-, and compound-wave – propagate throughout the domain. The initial value of the primitive variables is given by
\[ W = \begin{cases} [1, 0, 0, 0, 1, 3/4, 1, 0]^\top & x \leq 0 \\ [1/8, 0, 0, 0, 1/10, 3, 4, -1, 0]^\top & x > 0, \end{cases} \]  
(15)
which represents the true parameters that we hope to recover. The background initial condition is formed by adding a random perturbation to the true initial condition. Figure 1 compares the background and true initial condition of the density field. Not shown is the component of the magnetic field which has a background value of 0.848. Synthetic observations are generated by sparsely sampling the true model evolution with added Gaussian noise. The sampling takes place along the trajectory of a fictitious spacecraft that orbits the domain 5 times as shown in Figure 2. With this observation system, only a few observations are available at any given time step.
Figure. 1. Comparison of the true and background initial conditions.

Figure. 2. Observation locations of the fictitious observer. Locations are coloured by the true value of density.

The standard deviations of the measurement noise is reported in Table I.

The present evaluation consists of two assimilations. In the first, the synthetic data and the evolution of the background state are combined without applying the proposed divergence-free parametrization. As such, the $x$ component of the magnetic field cannot be assimilated. In the second, the divergence-free parametrization is applied, allowing for the assimilation of the whole magnetic field. For these two cases, the types of observations assimilated are also varied. At each observation location, observations of just $\rho u$ and $B$, or $\rho$ and $\rho u$, or all $\rho$, $\rho u$, $E$ and $B$ are available.

The density field and its error are compared for the background (i.e. no DA), the assimilation without $B_x$, and the assimilation with $B_x$ in Figures 3 and 4 respectively. As can be seen, both the assimilation with and without $B_x$ are able to use the observed data to significantly reduce the error in the simulation. However, the assimilation with the solenoidal parametrization achieves better performance. To quantitatively assess the total error in the assimilations, the root mean square error (RMSE) is plotted with time in Figure 5. Furthermore, measures of the RMS error as a percentage of the background RMS error are reported in Table II. It is evident that in all cases, the assimilations that include $B_x$ match the true model evolution much more closely. This is expected, as the $x$ component of the magnetic field plays an important role in the dynamics of the shock-tube. Interestingly, similar performance was achieved when observations included all conserved quantities vs when only density and momentum were included. In contrast, significantly less error reduction was achieved when observations contained only momentum and magnetic field.

Table I

<table>
<thead>
<tr>
<th>SD</th>
<th>$\rho$</th>
<th>$\rho u_x$</th>
<th>$\rho u_y$</th>
<th>$\rho u_z$</th>
<th>$B_y$</th>
<th>$B_z$</th>
<th>$E$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.017</td>
<td>0.007</td>
<td>0.018</td>
<td>0.007</td>
<td>0.017</td>
<td>0.017</td>
<td>0.022</td>
</tr>
</tbody>
</table>

The density field and its error are compared for the background (i.e. no DA), the assimilation without $B_x$, and the assimilation with $B_x$ at the end of the assimilation phase. At each observation location, all conserved quantities are assimilated.
measurements. This reduction in performance can be attributed to the regions of the flow where the velocity is zero. Here, momentum observations cannot in principle be used to infer density data.

VI. CONCLUSIONS AND FUTURE EFFORTS

An important challenge in MHD data assimilation is the treatment of the solenoidal property of the magnetic field. If unaccounted for, data assimilation algorithms produce magnetic field estimates which are unphysical. The presence of large $\nabla \cdot \mathbf{B}$ errors in the solution is not only undesirable from a physical perspective, but it can also lead to unstable simulations. One common approach to this issue is to simply prohibit the correction of the magnetic field. While effective, this solution is not optimal. Therefore, this paper develops a methodology for performing variational data assimilation on ideal MHD flows while accounting for the solenoidal nature of the magnetic field. The main idea is to parametrize the magnetic field in a divergence-free fashion. Instead of correct-ing the magnetic field directly, the parameters are optimized instead. By doing so, one can assimilate the magnetic field while maintaining the solenoidal property by construction. In addition, it was shown that the parametrization also reduces the number of design variables.

The proposed methodology was evaluated in the context of a canonical 1D ideal MHD shock-tube problem. The solenoidal parametrization allowed for the assimilation of all components of the magnetic field. The errors in the assimilated solution were an order of magnitude lower than those achieved without

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
Observations & $\frac{\text{RMSE}_{\text{end}=0.4}}{\text{RMSE}_{\text{end}=0.4}^{\text{background}}}$ & $\frac{\sum_{t=0.4}^{t=0.8} \text{RMSE}}{\sum_{t=0.4}^{t=0.8} \text{RMSE}_{\text{background}}}$ & \\ 
\hline
$[\rho, \mathbf{u}]$ & 46.10\% & 15.73\% & 56.90\% & 14.41\% & \\
$[\rho, \mathbf{u}, \mathbf{B}]$ & 41.22\% & 2.58\% & 45.25\% & 2.55\% & \\
$[\rho, \mathbf{u}, \mathbf{B}, \mathbf{E}]$ & 36.54\% & 2.22\% & 48.47\% & 2.52\% & \\
\hline
\end{tabular}
\caption{Error reduction measured as the RMS error at the end of the assimilation (2nd column) and sum of the RMS error in the forecast phase (3rd column). Both measures of error reduction are given as a percentage of the error in the background solution.}
\end{table}
the parametrization.

Though the novel methodology is developed for both the 1D and 3D setting, it was only assessed for the 1D case. The application of the solenoidal parametrization to 3D problems is thus the focus of future studies. While not relevant in the 1D setting, the specification of boundary conditions of the magnetic vector potential must be addressed. Additionally, a general procedure for specifying the background magnetic vector potential from the background magnetic field should be developed. With these additions, the assimilation of in situ heliospheric data with an MHD-based solar-wind model can be pursued in future follow-up studies.

APPENDIX

A. Jacobian of Powell Source Term

The derivatives of the Powell source term with respect to the conserved solution can be described by a block tridiagonal Jacobian matrix. The diagonal terms are given by,

$$\frac{\partial S_i}{\partial U_i} = - (\nabla \cdot B)_i \times I,$$

and the off diagonal terms are given by

$$\frac{\partial S_i}{\partial U_{i+1}} = \frac{1}{2\Delta x} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

where \((\nabla \cdot B)_i\) is evaluated as

$$\langle \nabla \cdot B \rangle_i = \frac{B_{z,i+1} - B_{z,i-1}}{2\Delta x}.$$ 

B. Jacobian of GLM Source Term

The derivatives of the GLM source term with respect to the conserved solution can also be described by a block tridiagonal Jacobian matrix. The diagonal terms are given by,

$$\frac{\partial S_i}{\partial U_i} = - \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

and the off diagonal terms are given by

$$\frac{\partial S_i}{\partial U_{i+1}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

where \(g = \gamma - 1\).

REFERENCES


