Benchmark solutions

An effective matrix-free implicit scheme for the magnetohydrodynamic solar wind simulations

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Abstract

The magnetohydrodynamics (MHD) modeling of the steady solar wind is an essential and important ingredient in numerical space weather study. Numerically solving the MHD equation system is not an easy work due to its complexity by combining the Euler equations of gas dynamics with the Maxwell's equations of electromagnetics and the solenoidal constraint. Moreover, the vast physical temporal and spatial scales of the solar wind simulation propose harsh requirements for computational efficiency and memory storage. Considering these factors, we develop an easily implemented finite volume (FV) scheme using the GMRES algorithm with an LU-SGS preconditioner for the three-dimensional (3D) MHD-based simulation. The steady-state solar wind from 1 R⊙ to 20 R⊙, during Carrington rotation (CR) 2051 is simulated for the validation of the proposed matrix-free implicit solver. Compared with the explicit solver, the implicit one can effectively enlarge the CFL number to 100 and achieve speedup ratios of 31.27 × and 28.05 ×, which reduces the computational time for the steady-state study from several days to only a few hours. The simulation captures main features of the solar corona and the mapped in-situ solar wind measurements. The scheme proposed here provides a promising choice to conduct the 3D MHD simulation of the solar wind background from the Sun to the Earth beyond.

1. Introduction

Numerical space weather modeling has been a promising tool used for space weather studies in recent decades, among which the study of steady solar wind is an essential and important ingredient. As the MHD equation system is the only self-consistent mathematical description currently used to model large-scale space weather phenomena, numerical MHD simulations are a powerful theoretical approach for retrieving the 3D structures and dynamics of the solar wind in solar-terrestrial space. Mathematically, the ideal MHD equations are a hyperbolic partial differential equation (PDE) system by combining the Euler equations of gas dynamics with the Maxwell’s equations of electromagnetics.

As solar-terrestrial physics phenomena involve vast physical temporal and spatial scales, efficiencies and computational costs in the numerical modeling of solar-terrestrial physics phenomena are important considerations in the numerical scheme. In an explicit time advance solver, the maximum allowable time step is always a much smaller value than that is needed to accurately resolve the transient behavior. The time step is set by the fast wave because the Courant–Friedrichs–Lewy (CFL) condition associated with the fast wave places much more restriction than that associated with the other waves. However, an implicit scheme can remove the numerically imposed time-step constraint, allowing much larger time steps. Generally at each time step or iteration, the implicit method need to solve a linear system of equations that is derived from the linearization of an implicit scheme. The most widely used methods to solve a linear system are iterative solution methods and approximate factorization methods. Some efficient iterative solution methods have been developed for computational fluid dynamics (CFD), such as the generalized minimum residual (GMRES) with an incomplete lower-upper (iLU) factorization preconditioner. But the requirement of large memory to store the Jacobian matrix may prohibit themselves for large-scale problems. The lower-upper symmetric Gauss–Seidel (LU-SGS) method was first proposed by Jameson and Yoon for the Euler equations. By making some approximations to the implicit operator, it can completely eliminate the storage of the matrix of the equation system in this approximate factorization method. Due to this attractive feature, LU-SGS has been successfully generalized and extended in many works. For example, Sitaraman et al. [6] applied this method to resistive MHD equations and developed a highly parallelizable matrix-free algo-
rithm on unstructured grids with an analytic form of the convective flux Jacobian. However, when compared with the most efficient iterative methods such as GMRES with an iLU preconditioner, this method still converges slowly and is less effective. Luo et al. [4] gave a fast, matrix-free implicit method, i.e. a GMRES algorithm with an LU-SGS preconditioner, to solve Navier-Stokes equations, which combines the efficiency of the iterative methods with low memory requirement of approximate factorization methods in an effort.

Inspired by the above considerations, we develop an easily implemented finite volume (FV) scheme using the GMRES algorithm with an LU-SGS preconditioner for the MHD-based 3D simulation, which is an effective and matrix-free implicit time advance solver, to study the ambient solar wind for CR 2051. This FV scheme is based on the six-component mesh grid system proposed by Feng et al. [7], which consists of six identical component meshes to envelope a spherical surface with partial overlap on their boundaries. The paper is organized as follows. Section 2 presents a brief description of the model, including both the governing equations and the grid system. An easily implemented finite volume scheme goes into details in Section 3. Then follows the implicit time integration of the GMRES with an LU-SGS preconditioner in Section 4. In Section 5 numerical results of CR2051 are analyzed and compared with the observational results. Finally, conclusions are made in Section 6.

2. Model description

2.1. Governing equations

The solar wind evolution is governed by a modified ideal MHD equations, which is characterized with a solar wind source term $Q_{\mathrm{solar}}$. The dominance of the magnetic energy density in the solar corona may incur negative pressure in the course of the simulation. To mitigate this problem effectively, the split of the magnetic field $B$ into a time-independent potential magnetic field $B_0$ and a time-dependent deviation $B_1$ (i.e. $B = B_0 + B_1$) is proposed in [7–9].

In numerical calculation, the solenoidal constraint $\nabla \cdot B = 0$ can only be satisfied up to a discretization error, which will produce a force parallel to the magnetic field in the conservative form of the momentum equation causing unphysical effects [10] and result in failure. To solve this problem, we adopt the eight-wave formulation approach [11] by adding the powell source term $S_{\text{powell}}$ to the right-hand-side of the governing equations to control $\nabla \cdot B_1$. It introduces a divergence wave to advect the $\nabla \cdot B_1$ errors away with the flow, which can control the $\nabla \cdot B_1$ errors to the order of truncation error and eliminate the unphysical effects.

Then the governing equations can be written in brief as:

$$
\partial_t \mathbf{U} + \nabla \cdot \mathbf{F} = S_{\text{powell}} + Q_{\text{solar}},
$$

with

$$
\mathbf{U} = (\rho, \rho \mathbf{v}, B_1, e_1)^T,
$$

$$
\mathbf{F} = \begin{pmatrix}
\rho \mathbf{v} \\
\rho \mathbf{vv} + (p + \frac{B_1^2}{2} + B_1 \cdot B_0) \mathbf{I} - B_1 B_0 - B_1 B_0 - B_0 B_0 \\
\mathbf{v} (e_1 + p + \frac{B_1^2}{2} + B_1 \cdot B_0) - B (\mathbf{v} \cdot B_1)
\end{pmatrix},
$$

$$
S_{\text{powell}} = -\nabla \cdot B_1 \begin{pmatrix} 0 \\ B \\ \mathbf{v} \\ \mathbf{v} \cdot B_1 \end{pmatrix}.
$$

Here, $U$ is the conservative variables containing the mass density $\rho$, the momentum density $\rho \mathbf{v}$, the deviation magnetic field $B_1$ and the modified total energy density $e_1 = \rho \frac{v^2}{2} + \frac{p}{\gamma} + \frac{B_1^2}{2}$. $F$ is the flux term.

As for the solar source term $Q_{\text{solar}}$, $r$ is the position vector originating at the center of the Sun, and $\mathbf{g} = -GM/r^2 \cdot r$ defines the solar gravitational force at $r$, $\rho$, $\mathbf{v}$, $\mathbf{B}$, $\rho$, $I$, $t$, and $\mathbf{g}$ are normalized by the characteristic values $\rho_0$, $v_0$, $B_0$, $\sqrt{\rho_0 v_0^2}$, $R_0$, $R_0$, and $a_0^2/R_0$, where $\rho_0$, $v_0$ and $R_0$ are the mass density, sound speed on the solar surface and solar radius. $\mathbf{Q}$ is the angular speed of the solar rotation, with $|Q| = 2\pi/25.38 \text{ radian day}^{-1}$ (here normalized by $a_0/R_0$) in the present study. $\gamma$ is the ratio of specific heats, and according to Feng et al. [7] we set $\gamma$ to vary from 1.05 to 1.5 along the heliocentric distance $r$, i.e. $\gamma = 1.05$ for $r/R_0 \leq 5$, $\gamma = 1.05 + 0.03(r/R_0 - 5)$ for $5 < r/R_0 \leq 20$, and $\gamma = 1.5$ for $r/R_0 > 20$. $E = \mathbf{v} \times \mathbf{B}$ and $J_0 = \nabla \times \mathbf{B}_0$, $S_0$ and $Q_0$ stand for the momentum source term and the volumetric heating function respectively, which are responsible for acceleration and heating of the solar wind. Taking into account the magnetic field topology effects [12], we prescribe them as

$$
S_m = M \left( \frac{r}{R_S} - 1 \right) \exp \left( -\frac{r}{L_M} \right) \cdot r/r,
$$

$$
Q_0 = Q_t \exp \left( -\frac{r}{L_{Q_0}} \right) + Q_s \left( \frac{r}{R_S} - 1 \right) \exp \left( -\frac{r}{L_{Q_s}} \right).
$$

Details about those parameters can be referred to Feng et al. [7].

2.2. Grid system

We inherit the six-component mesh grid system proposed by Feng et al. [7], that is composed of six identical component meshes to envelop a spherical surface with partial overlap on their boundaries. The sketch is shown in Fig. 1. This grid system provides a concise and balanced way to distribute computational domains to parallel computing system, and make it suitable to simulate large-scale heavy-calculation problems such as the solar wind evolution.

Each component grid is a low-latitude spherical mesh at $(\frac{\pi}{4} - \delta \leq \theta \leq \frac{\pi}{4} + \delta) \cap (\frac{\pi}{2} - \delta \leq \phi \leq \frac{\pi}{2} + \delta)$, where $\delta$ is proportionally dependent on the grid spacing entailed for the minimum overlapping area. Each component is divided in the spherical coordinates with the same procedure. In the $\theta$ and $\phi$ directions, the par-
The neighboring hexahedral cells $i$ and $j$ with the common face $A_{ij}$.

$$
\theta_j = \theta_{\text{min}} + j \Delta \theta, \quad j = 0, 1, \ldots, N_\theta + 1
$$
$$
\phi_i = \phi_{\text{min}} + i \Delta \phi, \quad i = 0, 1, \ldots, N_\phi + 1
$$

with $\Delta \theta = (\theta_{\text{max}} - \theta_{\text{min}})/(N_\theta - 1)$ and $\Delta \phi = (\phi_{\text{max}} - \phi_{\text{min}})/(N_\phi - 1)$. As for the mesh division in the radial direction, Feng et al. in [7] gave a suggestion for simulations of the solar wind as: for $1 - 25 R_\odot$ and $N_\phi = N_\theta = 2 \times 2^5 - 1$. $\Delta r(i) = 0.01 R_\odot$ if $r(i) < 11 R_\odot$, $\Delta r(i) = \min(A \times \log_{10}(r(i - 1)), \Delta \theta \times r(i - 1))$ with $A = 0.01/\log_{10}(1.09)$ if $r(i) < 3.5 R_\odot$; and $\Delta r(i) = \Delta \theta \times r(i - 1)$ if $r(i) \geq 3.5 R_\odot$. Parameters like 0.01, 1.09 etc. are chosen so as to make the cell as rectangular cube as possible, near the Sun. In this way, one mitigates this discrete or geometrical stiffness caused by disparate mesh cell widths. Field vectors on each component can be transformed to any other components in the Cartesian coordinate. This transformation can ensure data exchange between six components, especially when updating the boundary information after calculations at every time step. Details of vector transformation formulae are available in [7]. For the convenience of the later implicit treatment, we assign every cell in each component an identity number. For any cell $(i, j, \ell)$ which is the $i$th cell in $r$ direction, the $j$th cell in $\theta$ direction and the $\ell$th cell in $\phi$ direction, it specifies its identity number as $j \times (N_\theta + 2) \times (N_\phi + 2) + j \times (N_\phi + 2) + \ell$. In the following statements, we will use identity numbers to refer to cells. After the grid mesh partition in the spherical coordinates, we use their corresponding Cartesian ones to form the corresponding hexahedral cells as shown in Fig. 2.

In the following, a numerical implementation of the governing MHD equations on the hexahedral cells will be described in the Cartesian coordinate system, under the framework of MPI-parallel six-component mesh grid system.

### 3. Finite volume scheme

The finite volume form of Eq. (1) on the hexahedral cells in the six-component mesh grid system can be written as

$$
\frac{dU_i}{dt} + \sum_{face_{k}=1}^{6} \mathcal{R}^{-1}(n_{ij}) F_k \left( \mathcal{R}(n_{ij}) U_{il} - \mathcal{R}(n_{ij}) U_{jr} \right) A_{ij} = 0
$$

The conservative variable $U$ with subscript $i$ refers to the calculated cell, whose identity number is $i$. And the subscript $j$ stands for the identity number of cell j’s neighbor cell. As shown in Fig. 2, cell $i$ and cell $j$ share a common interface, and we number it as face$_j$. Obviously, every cell $i$ has six faces and six corresponding neighbor cells, and thus face$_j = 1, 2, \ldots, 6$. For the interface face$_j$ of cell $i$, its area is $A_j$ and its outward unit normal vector is $n_{ij}$ pointing from cell $i$ to cell $j$. $\Sigma_i$ is the volume of cell $i$.

$F_k$ stands for the numerical flux function in the $x$ direction. $U_{il}$ is the value at the centroid of the interface $ij$ extrapolated from cell $i$ by reconstruction, while $U_{jr}$ is that from cell $j$. $\mathcal{R}$ is the rotation matrix [13,14] that rotates the $x$-axis to the direction of $n_{ij}$ and $\mathcal{R}^{-1}$ rotates it back. By utilizing rotation matrix, we can consider flux calculations only in the $x$ direction about $F_k$ and solve the equations in a brief and easily implemented way. The flux term of $F_k$ at interface $ij$ is the approximate Riemann problem, of which a variety of solvers have been developed during the past decades. For simplicity, Lax-Friedrichs method is applied for the presentation

$$
F_k \left( \mathcal{R}(n_{ij}) U_{il} - \mathcal{R}(n_{ij}) U_{jr} \right) = \frac{1}{2} \left( F_k \left( \mathcal{R}(n_{ij}) U_{il} \right) + F_k \left( \mathcal{R}(n_{ij}) U_{jr} \right) \right)
$$

$$
- \frac{1}{2} \lambda_{ij} \left( \mathcal{R}(n_{ij}) U_{il} - \mathcal{R}(n_{ij}) U_{jr} \right).
$$

(3)

where $\lambda_{ij}$ is the largest eigenvalue of the Jacobian in the normal direction, taking its value at the interface of cell $i$ and cell $j$, i.e.

$$
\lambda_{ij} = \left| v_{ij} \cdot n_{ij} \right| + \frac{1}{2} \sqrt{\left( \frac{\gamma p_{ij} + B_{ij}^2}{\rho_{ij}} \right)^2 + 4 \left( \frac{\gamma p_{ij} + B_{ij}^2}{\rho_{ij}} \right)^2 - 4 \frac{\gamma p_{ij} B_{ij}^2}{\rho_{ij}^2}}
$$

(4)

The subscript $ij$ in Eq. (4) represents the corresponding arithmetic average values of $U_{il}$ and $U_{jr}$.

The volume-averaged value of source terms $S_{\text{power}}$ and $Q_{\text{Solar}}$ is considered as follows. For instance, the volume-averaged value of $S_{\text{power}}$ in cell $i$ can be expressed by

$$
S_{\text{power}} = -\left( \nabla \cdot B_{ij} \right) + \frac{1}{2 \Omega_i} \sum_{face_{k}=1}^{6} \left( B_{ij} \cdot n_{ij} \right) A_{ij} = \frac{\left( B_{ij} + B_{ij} \right)}{2}
$$

with

$$
\left( \nabla \cdot B_{ij} \right) = \frac{1}{\Omega_i} \sum_{face_{k}=1}^{6} \left( B_{ij} \cdot n_{ij} \right) A_{ij}
$$

(6)

Obviously, the volume-averaged value $S_{\text{power}}$ is still a function of $U_{il}$ and $U_{jr}$. For convenience, we denote it as $S_{\text{power}}(U_{il}, \left( \nabla \cdot B_{ij} \right))$.

### 3.1. Reconstruction

For the purpose of achieving second spatial accuracy, the limited linear least squares reconstruction is employed in this scheme, which has been successfully applied in many studies [11,15,16]. Denote $W_{(k)}$ the $k$th component of the primitive vector $W = (\rho, v, B_{ij})^T$ at $x_i$, and $\nabla W_{(k)}$ its gradient at $x_i$. The general formula for the limited reconstruction is applied on the primitive variables on cell $i$

$$
W_{(k)}(x_i) = W_{(k)} + \phi_{(k)}^{(i)} \nabla W_{(k)}(x_i) \cdot (x_i - x_i).
$$

(5)

where $x_i = (x_i, y_i, z_i)$ is the position of cell $i$’s centroid, and $W_{(k)}(x_i)$ is the value to be reconstructed at $x_i$. Here we take $x_i$ as the face centroid of cell $i$.

As usual, the gradient $\nabla W_{(k)}$ at $x_i$ is evaluated by the least-squares method [11]:

$$
[L_1 \quad L_2 \quad L_3] \cdot \nabla W_{(k)} = \mathcal{D}_w,
$$

with

$$
L_1 = \left( \begin{array}{c} \omega_{n1}(x_{n1} - x_i) \\ \vdots \\ \omega_{n1}(x_{n1} - x_i) \end{array} \right),
L_2 = \left( \begin{array}{c} \omega_{n1}(y_{n1} - y_i) \\ \vdots \\ \omega_{n1}(y_{n1} - y_i) \end{array} \right),
$$

$$
L_3 = \left( \begin{array}{c} \omega_{n1}(z_{n1} - z_i) \\ \vdots \\ \omega_{n1}(z_{n1} - z_i) \end{array} \right).
$$

(7)
\[ L_3 = \begin{pmatrix} \omega_{ng1} (Z_{ng1} - z_i) \\ \vdots \\ \omega_{ngN} (Z_{ngN} - z_i) \end{pmatrix}, \quad D_W = \begin{pmatrix} \omega_{ng1} (W_{ng1}^{(k)} - W_i^{(k)}) \\ \vdots \\ \omega_{ngN} (W_{ngN}^{(k)} - W_i^{(k)}) \end{pmatrix}. \]

The subscripts ng1\ldots ngN refer to the neighboring cells of cell \( i \)’s vertices, and \( N = 26 \) for our hexahedral cell. \( \omega_{ng} = \frac{1}{|x_{ng} - x_i|} \) is the weighting coefficient.

In Eq. (5), \( \phi_i^{(t)} \) is the slope limiter. In the present paper, we use Venkatakrishnan limiter [17], which is believed to not only produce monotonic solution without oscillation, but also keep the accuracy and convergence. As usual, Venkatakrishnan limiter \( \phi_i^{(t)} \) can be described as

\[
\phi_i^{(t)} = \begin{cases} 
\psi \left( \frac{W_i^{(k)} - (x_i - x) \cdot (x_i - x)}{\Delta h} \right) & \text{if } W_i^{(k)} \cdot (x_i - x) > 0 \\
\psi \left( \frac{W_i^{(k)} - (x_i - x) \cdot (x_i - x)}{\Delta h} \right) & \text{if } W_i^{(k)} \cdot (x_i - x) < 0 \\
1 & \text{if } W_i^{(k)} \cdot (x_i - x) = 0
\end{cases}
\]

where \( W_i^{(k)} = \max(W_i^{(k)}, -W_i^{(k)}) \) and \( W_i^{(k)} = \min(W_i^{(k)}, -W_i^{(k)}) \) are the maximum and minimum cell average values among cells ng1\ldots ngN and \( i \). \( \psi \left( \frac{\Delta h}{\Delta h} \right) \) is defined by the following function

\[
\psi \left( \frac{\Delta h}{\Delta h} \right) = \frac{1}{\Delta h} \left( \Delta h^2 + \epsilon^2 \Delta h + 2 \Delta h^2 \right),
\]

with \( \Delta h \) represents the denominator of the function variable, and \( \Delta h \), the numerator, \( \epsilon^2 = (K \Delta h)^2 \), in which \( \Delta h \) is the local grid size or characteristic length of the element \( V \), \( K \) is the tunable positive constant. In the present paper, according to [17], \( K = 0.3 \) and \( \Delta h \) is taken to be the diameter of the inscribed circle within the cell. To prevent division by a very small value, \( \Delta h \), in the term \( \frac{\Delta h}{\Delta h} \) is replaced by \( \text{sign}(\Delta h) \left( |\Delta h| + \omega \right) \) with \( \omega = 10^{-12} \) in practical implementation. Finally, Venkatakrishnan limiter \( \phi_i^{(t)} \) is defined by

\[
\phi_i^{(t)} = \min(\phi_i^{(t)}_1, \ldots, \phi_i^{(t)}_N).
\]

4. Implicit time integration

We rewrite Eq. (2) in a concise form as

\[
\Omega_i \frac{dU}{dt} = R_i,
\]

with

\[ R_i = F_x(U_i, U_j) + \Omega_i S_{\text{powell}}(U_i, (\nabla \cdot B_1) + \Omega_i S_{\text{eolar}}(U_j). \]

where

\[ F_x(U_i, U_j) = \left\{ \begin{array}{c}
- \sum_{r \in r} \mathcal{R}^{-1}(n_j) F_x(\mathcal{R}(n_j) U_{ik}) - \mathcal{R}(n_j) U_{jk} A_{ij}. \\
- \sum_{r \in r} \mathcal{R}^{-1}(n_j) F_x(\mathcal{R}(n_j) U_{ik}) - \mathcal{R}(n_j) U_{jk} A_{ij}. \\
\end{array} \right. \]

The braced part is denoted by the function \( F_x(U_i, U_j) \) for the convenience of the later statement.

In order to obtain a steady-state solution, Eq. (6) is integrated in time with backward Euler method as

\[
\Omega_i \frac{\Delta U_i}{\Delta t} = R_i^{n+1},
\]

with \( \Delta U_i = U_i^{n+1} - U_i^n \) is the difference of conserved variables between time levels \( n \) and \( n + 1 \). \( \Delta t \) is the time increment, and \( R_i \) is the right-hand side residual and is equal to zero for a steady-state solution. Linearizing the right-hand side of Eq. (8) in time we know that

\[
\Omega_i \frac{\Delta U_i}{\Delta t} = R_i^n + \frac{\partial R_i^n}{\partial U} \Delta U_i,
\]

which can be then written in the following compact matrix form

\[
A \Delta U^n = R^n,
\]

with \( A = \frac{\partial R_i^n}{\partial U} \). This linear algebraic equations need to be solved simultaneously at each time step. With respect to \( \frac{\partial R_i^n}{\partial U} \) in cell \( i \), from Eq. (7) we can get

\[
\frac{\partial R_i}{\partial U} = \frac{\partial F_x(U_i, U_j)}{\partial U} + \Omega_i \frac{\partial S_{\text{powell}}(U_i, (\nabla \cdot B_1)}{\partial U} + \Omega_i \frac{\partial S_{\text{eolar}}(U_i)}{\partial U},
\]

and

\[
\frac{\partial R_i}{\partial U} = \frac{\partial F_x(U_i, U_j)}{\partial U}.
\]

Here, the subscript \( j \) refers to cell \( j \)’s corresponding neighbor cell.

To be specific, \( \frac{\partial F_x(U_i, U_j)}{\partial U} \) in Eq. (10) is

\[
\frac{\partial F_x(U_i, U_j)}{\partial U} = \frac{1}{2} \left\{ \sum_{r \in r} \mathcal{R}^{-1}(n_j) F_x(\mathcal{R}(n_j) U_{ik}) - \mathcal{R}(n_j) U_{jk} A_{ij} \right\},
\]

and \( \frac{\partial F_x(U_i, U_j)}{\partial U} \) in Eq. (11) is

\[
\frac{\partial F_x(U_i, U_j)}{\partial U} = \frac{1}{2} \mathcal{R}^{-1}(n_j) F_x(\mathcal{R}(n_j) U_{ik}) - \mathcal{R}(n_j) U_{jk} A_{ij}.
\]

It should be noticed here that, \( \lambda_{ij} \) and \( (\nabla \cdot B_1) \) are functions of the conservative variables about cells \( i \) and \( j \), and should also be differentiated to obtain the Jacobian matrices of \( F_x(U_i, U_j) \) and \( S_{\text{powell}}(U_i, (\nabla \cdot B_1) \) respectively. However, taking true Jacobians is too complex and expensive. Barth in [18] analyzed the asymptotic convergence rates of both the true and the eigenvector transformed approximate Jacobian matrices. Test cases in his work showed that the spectral radius of the approximate Jacobian matrix was nearly identical with the true one at low CFL numbers, and was somewhat bigger at high CFL numbers. The performance of the approximate Jacobian matrix was mildly degraded at high CFL numbers but was still quite good overall, indicating that the use of eigenvector transformed approximate Jacobian is especially attractive to construct efficient, accurate implicit methods. And then, approximate Jacobians were widely adopted in many works [4,6,19]. Following previous experiments, we assume that \( \lambda_{ij} \) and \( (\nabla \cdot B_1) \) are locally constant. Even with general degradation in convergence, it will take less CPU time to compute the Jacobian matrix, and the conditioning of the simplified Jacobian matrix can be improved [4,18], resulting in the reduction of computational cost to solve the resulting linear system. Virtually, the mismatch and inconsistency between the right- and left-hand sides of Eq. (9), which is caused by these approximations, do not affect the solution accuracy, for the steady-state solution to \( R(U) = 0 \) in Eq. (9) is looked for. This approximation works reasonably well for the small change in solution. As pointed out formerly [18,19], alternative choice may be the finite difference perturbation for Jacobian calculation.

4.1. LU-SGS Preconditioner

The LU-SGS method proposed in [5] shows good stability and competitive computational cost in comparison to explicit methods. The matrix \( A \) is split into a strict lower matrix \( L \), a diagonal matrix \( D \), and a strict upper matrix \( U \). i.e. \( A = D + L + U. \) Then Eq. (9) can be written as

\[
(D + L)D^{-1}(D + U)\Delta U = R + (LD^{-1}U)\Delta U.
\]
The equations are approximately factored by neglecting the last term on the right-hand side of Eq. (12), and can be solved in the two steps that only involving simple block matrix inversions:

- Lower (forward) sweep:
  \[(D + \mathcal{L}) \Delta \mathbf{U}^* = \mathbf{R}.\]
- Upper (backward) sweep:
  \[(D + \mathcal{H}) \Delta \mathbf{U} = D \Delta \mathbf{U}^*.\]

Finally the system can be solved by:

\[
\begin{align*}
\Delta \mathbf{U}^* &= D^{-1} \left\{ \begin{array}{c}
\mathbf{R} - \sum_{j=1}^{m} \frac{1}{2} R_{ij}^{-1} (\mathbf{n}_j) \left[ \frac{\partial F_x (\mathbf{R}_j, \mathbf{U}_j) + \partial S_{\text{pow}} (\mathbf{U}_j, \mathbf{B}_j)}{\partial \mathbf{U}_j} - \frac{\partial Q_{\text{dial}} (\mathbf{U}_j)}{\partial \mathbf{U}_j} \right] - \frac{\partial \mathbf{U}_j}{\partial \mathbf{U}_j} \right|_{\lambda_j} A_{ij} \Delta \mathbf{U}_j^* \\
\mathbf{R} - \sum_{j=1}^{m} \frac{1}{2} R_{ij}^{-1} (\mathbf{n}_j) \left[ \frac{\partial F_x (\mathbf{R}_j, \mathbf{U}_j) + \partial S_{\text{pow}} (\mathbf{U}_j, \mathbf{B}_j)}{\partial \mathbf{U}_j} - \frac{\partial Q_{\text{dial}} (\mathbf{U}_j)}{\partial \mathbf{U}_j} \right] - \frac{\partial \mathbf{U}_j}{\partial \mathbf{U}_j} \right|_{\lambda_j} A_{ij} \Delta \mathbf{U}_j
\end{array} \right\},
\end{align*}
\]

4.2. GMRES algorithm

GMRES algorithm is the generalization of the conjugate gradient method proposed by Saad and Schultz [20] for solving a linear system where the coefficient matrix is not symmetric or positive definite. GMRES minimizes the norm of the computed residual vector over the subspace spanned by a certain number of orthogonal search directions, and the convergence speed of the iterative algorithm depends on the condition number of the coefficient matrix. So the preconditioner that attempts to cluster the eigenvalues at a single value is the easiest and most common way to improve the efficiency and robustness of GMRES [4]. GMRES with a LU-SGS preconditioner for Navier-Stokes equations developed by Luo et al. [4] not only converges effectively but also requires no additional memory storage by using the Jacobian matrix of the linearized scheme as a preconditioner matrix. By preconditioning Eq. (9) on the left, we have

\[
P^{-1} A \Delta \mathbf{U} = P^{-1} \mathbf{R},
\]

with the LU-SGS preconditioner defined by \( P = (D + \mathcal{L}) D^{-1} (D + \mathcal{H}) \). The preconditioned restarted GMRES(m) is described as Algorithm 1.

5. Numerical results

To validate the capability of the scheme proposed above, we employ it to numerically study the ambient solar wind of CR 2051, which lasted from December 12, in 2006 to January 7, in 2007 in the descending phase during the solar minimum. The computational domain of the solar wind evolution ranges from the solar surface to 20 Rₖ. In the computational domain, the time-independent \( B_0 \) is a 3D global magnetic field produced by utilizing the potential field (PF) model based on the radial photospheric magnetic data from the Global Oscillation Network Group
Algorithm 1 GMRES with LU-SGS preconditioner.

Input: $\Delta U_0, A, R, P$
Output: $\Delta U_0$

1: $L_2^{last} = +\infty$
2: for itr=1, itr$_{\text{max}}$ do
3: $v_0 := R - A\Delta U_0$
4: $r_0 := P^{-1}v_0$
5: ExchangeBoundary($r_0$)
6: $\beta := \| r_0 \|_2$  \hspace{1cm} \text{LU-SGS as the preconditioner}
7: $v_1 := r_0/\beta$
8: for $j=1, m$ do
9: $v_0 := \text{LU-SGS}$
10: $v_{j+1} := P^{-1}v_0$
11: ExchangeBoundary($v_{j+1}$) \hspace{1cm} Through the six-component grid system
12: for $i=1, j$ do
13: \hspace{1cm} $h_{i,j} := (v_{j+1}, v_i)$
14: \hspace{1cm} $v_{j+1} := v_{j+1} - h_{i,j}v_i$
15: $\Delta U_0 := \Delta U_0 + \sum_{i=1}^{m} v_{j+1}$ \hspace{1cm} Gram-Schmidt step
16: $L_2^{last} \leftarrow L_2$
17: $z := \min_j \| \beta e_1 - Hz \|_2$
18: if $L_2 < \epsilon$ or $L_2 > L_2^{last}$ then exit \hspace{1cm} Stopping Criterion
19: $L_2 = \| \beta e_1 - Hz \|_2$
20: $L_2^{last} = L_2$
21: return $\Delta U_0$

(GONG) program, and the time-dependent magnetic field $B_t$ is initially set as zero. The initial distributions of plasma mass density $\rho$, pressure $p$ and velocity $v$ are given by Parker’s solar wind flow [21]. The temperature and number density on the solar surface are $T_S = 1.3 \times 10^5$K and $n_S = 1.5 \times 10^8 \text{cm}^{-3}$, respectively.

We take the $L_2$ norm of the residual as a criterion to check convergence, and the solution tolerance $\epsilon$ is set to $1.0 \times 10^{-4}$. The maximum allowable number of iterations $\text{itr}_{\text{max}}$ is set to 20. However, this criteria is often not reached within the allowable number of iterations. We found in practice that, the $L_2$ norm of the residual declines during the first several iterations, and then it hovers around some extent. For the purpose of not wasting efforts and time in extra iterations, we set another stopping criterion for iterations, i.e. when the $L_2$ norm of the residual is larger than that in the last iteration.

Our computing environment is offered by TH-1A supercomputer from National Supercomputing Center in Tianjin, China. Each node on TH-1A is equipped with two Intel Xeon X5670@2.93GHz high-performance processors. Every program employs 120 processes and runs on 10 nodes parallelly by utilizing message passing interface (MPI) for communication. In this section, time cost and memory storage for the implicit and explicit scheme are compared, and then the simulated results of steady solar wind for CR 2051 are presented and compared with observational data. It should be noticed here that, in the following we present the simulated pictures from the implicit scheme by default, unless otherwise specified.

5.1. Time cost and memory storage

To testify the efficiency of our implicit solver, we make a comparison between the implicit and explicit solvers that adopt the same FV scheme. As the simulation of the ambient solar wind is a steady problem, we measure the time cost of reaching a basically steady state, of which the termination criterion of the simulation is set as $\left| p_{n+1} - p_n \right| p_n^0 \leq 3.9 \times 10^{-7}$. As usual, the CFL number in the explicit solver is set as 0.5, while the CFL number is enlarged to 100 in the implicit solver. Table 1 presents the time spent for two sampled mesh divisions, i.e. $115 \times 42 \times 42$ and $150 \times 62 \times 62$ meshes in $(r, \theta, \phi)$ per component. The averages of the time costs are used for comparison after each program runs 5 times. With the mesh division of $115 \times 42 \times 42$, the explicit solver takes $33.77$ h of wall time, while the implicit solver costs only about $1.08$ hours, with a speedup ratio of $31.27 \times$. As for the mesh division of $156 \times 62 \times 62$ in $(r, \theta, \phi)$, the implicit solver only takes an average of $3.29$ hours of wall time, which is $28.05\times$ times faster than the explicit one. The speedup ratio of the $156 \times 62 \times 62$ mesh division is somewhat smaller than that of the $115 \times 42 \times 42$ mesh division. This is because that with more meshes, the implicit solver costs nonlinearly more calculation and time to converge a steady state. Even so, the speedup with denser mesh is very impressive, by reducing the time cost from several days to only a few hours.

The utilization of the GMRES with an LU-SGS preconditioner in the implicit solver not only significantly speeds up the convergence, but releases us from storing the large matrix of the equation system, which is also crucial to large-scale studies. Especially in our parallel and distributed computation, it is almost impracticable. By using the Jacobian matrix of the linearized scheme as the preconditioner matrix, LU-SGS preconditioner can be directly derived from the available flux term without storing the large matrix of the equations.

5.2. Comparisons between the modeled and observational results

In this part, we make comparisons of the simulated results with the available coronal observations and mapped interplanetary measurements from different perspectives, such as coronal holes,
bipolar and unipolar coronal streamers, the HCS and high- and low-speed streams.

Solar coronal holes where the magnetic field lines extend to the heliosphere are the most easily-recognized signatures that appear as dark regions in X-ray and EUV images due to reduced emission from solar plasma localized at open magnetic field footpoints [22–25]. Fig. 3 displays the longitude-latitude maps of the coronal holes near the solar surface simulated by the MHD model (left) and observed by the 195 A observations (right) from the Extreme ultraviolet Imaging Telescope (EIT) on board the SOlar and Heliospheric Observatory (SOHO). In the left panel, open-field regions are shaded black while the closed-field regions white. The open- and closed-field regions are determined by tracing the magnetic field lines from 6 Rs back to the photosphere. As for the observed map, coronal holes are represented by dark color. From both maps, we can find that the equatorward boundaries of both polar coronal holes (PCHs) in the simulation almost coincide the observation. What is more, the shapes and locations of the extending holes from the southern PCH are well captured by the model. It is also characterized for the observation of CR 2051 that a band-shaped isolated coronal hole appears in low-latitude region at the Longitude of around 100°, which is reproduced in the simulated map as well. De Toma [26] and Yang [27] discovered that a significant portion of the solar surface was covered with the middle- and low-latitude coronal holes in the 2006–2009 solar minimum, and point out that their presence resulted from the relatively weak polar magnetic fields in this solar minimum.

Corresponding to the pattern of open- and closed-field regions near the solar surface, the coronal plasma exhibits non-uniform distribution that can well be qualitatively represented by the coronal white-light polarized brightness (pB) images produced by Thomson scattering from free electrons in the coronal plasma [28–30]. In Fig. 4, we compare the numerical results and the observational at the meridian planes to demonstrate that our solver can achieve the synthesized coronal white-light pB images basically consistent with the observation. The first row are the pB images synthesized from the simulated result from 2.3 to 6 Rs at the planes of φ = 180° − 0° (left column) and φ = 270° − 90° (right column) and the second row are those observed by the Large Angle and Spectrometric Coronagraph C2 (LASCO-C2) on board SOHO with the same radius range as before. The left coronal picture is taken at the seventh day of the CR, corresponding to the observation at the φ = 180° − 0° plane while the right one is taken at the fourteenth day, corresponding to the numerical φ = 270° − 90° plane. Both these observational and numerical pictures show streamers ranging from 2.3 to 6 Rs. From the modeled and observed pB images, we observe that the streamer-like structures do not extend radially outward from their foot points, but cover relatively larger latitudes near the Sun [27]. Furthermore, we can find that two bright structures extend outward at the east limb and a few diffuse bright structures covers the west limb for the pB image on the plane of φ = 180° − 0°. For the observed and synthesized pB images of the meridian plane of φ = 270° − 90°, two bright structures are captured at the east limb and one brightest and sharpest structure is reproduced at the latitude of 30°N at the west limb. Comparing the pB images with the modeled magnetic field topologies in the third row, we can easily deduce that northeast structure at the plane of φ = 180° − 0° corresponds to the emission from the unipolar streamer at the latitude of 25°N and the other bright structures result from bipolar streamers. It should be
noted that the faint structure at the northwest limb of the plane of \( \phi = 180^\circ - 0^\circ \) comes from the low emission from an isolated coronal hole, which can be inferred from Figs. 5 and 6.

It is instructive to validate the capability of the model developed in the previous sections by comparing the simulated results from the proposed implicit and explicit solvers. In Fig. 5, we present longitude-latitude maps for the proton number density from the implicit solver (top panels) and the explicit one (middle panels) and the relative difference between them at 2.5 \( R_e \) (bottom left panel) and 20 \( R_e \) (bottom right panel). The corresponding maps for the radial velocity of plasma flows are displayed in Fig. 6. Here the relative differences of the proton density and the radial velocity are defined as \( \frac{\rho_{\text{im}} - \rho_{\text{ex}}}{\rho_{\text{im}}} \) and \( \frac{V_{\parallel \text{im}} - V_{\parallel \text{ex}}}{V_{\parallel \text{im}}} \), respectively, with subscripts “im” and “ex” referring to the implicit and the explicit solvers. The black line in each panel of the top and middle rows denotes the magnetic neutral line (MNL), the extension of which shapes the HCS. The HCS is one of the most important interplanetary structures because it separates oppositely directed magnetic field lines, and various solar wind parameters vary with the distance from the HCS. From Figs. 5 and 6, the simulated results from both the implicit and the explicit solvers show that the coronal plasma moves faster at a larger heliocentric distance. Both figures also reveal that the HCS can be described as a two-hump and two-trough wavy structure, and the high-density low-speed plasma flow dominates the area in the vicinity of the HCS. Meanwhile, the low-density and high-speed plasma flow pervades the polar or high-latitude regions. Additionally, we find that there are very small relative differences between the densities and between the radial speeds achieved from the implicit and the explicit solvers. For most regions, the relative differences between the modeled densities are below 0.04 and the relative differences between the modeled radial speeds are less than 0.05.

The white-light polarized brightness at the east limb from SOHO/LASCO C2 at 2.5 \( R_e \) for CR 2051 are presented in Fig. 7. By comparing the longitude-latitude map at 2.5 \( R_e \) with the synoptic map of p8 observation, we find that the area near the magnetic neutral is characteristic of the bright structures. Roughly speaking, the HCS at 20 \( R_e \) is similar to the magnetic neutral line at 2.5 \( R_e \), while the magnetic neutral line at 2.5 \( R_e \) extends a little higher latitude than the HCS at 20 \( R_e \). There are subtle differences between them by examining carefully. In addition, the first rising slope and the last falling gradient at 20 \( R_e \) become more gentle than those at 2.5 \( R_e \).

Fig. 8 shows the magnetic filed lines at the meridian plane of \( \phi = 180^\circ - 0^\circ \) (top row) and \( \phi = 270^\circ - 90^\circ \) (bottom row). The radial speed \( V_r \) on the left column and the number density \( N \) on
the right column are also superposed in color contours, while the arrowheads on the black lines represent the directions of the magnetic fields. The figure shows the same pattern of the high- and low-speed solar wind as Fig. 6 and a helmet streamer stretched by the solar wind. Between different magnetic polarities forms a thin current sheet.

To further demonstrate the radial variations of the solar wind parameters in coronal holes and near the HCS region, we shows the number density and radial velocity profiles along two radial lines ranging from 1 Rs to 20 Rs in Fig. 9. The solid lines represent the profiles in the HCS region along the radial line of $(\theta, \phi) = (-29^\circ, 1^\circ)$, while the dashed lines denote the profiles in the coronal hole along the radial line of $(\theta, \phi) = (5^\circ, 8^\circ)$. The proton number densities in the HCS region and in coronal hole are almost the same near the solar surface. With the heliocentric distance increasing from 1 Rs to 20 Rs, the density in the HCS region keeps higher than that in coronal hole, and the gap between them becomes more significant. What’s more, this trend will maintain in interplanetary space. The figure demonstrates that the solar wind speed rises from about 340 km s$^{-1}$ at 5 Rs to about 720 km s$^{-1}$ at 20 Rs, which is compatible with the previous study on coronal observations [31]. Meanwhile, the solar wind speed near the MNL increases from about 140 km s$^{-1}$ to about 360 km s$^{-1}$, which agrees with the conclusion inferred from time-lapse sequences of white-light images [32].

In order to fill the observational gap near the outer boundary in our simulation, we map the in-situ measurements at 1 AU back to 20 Rs by using a ballistic approximation [e.g., 27], which assumes a plasma parcel travels from 20 Rs to the spacecraft with at a speed measured at 1 AU. The temporal profiles of the radial solar wind speed and the radial magnetic field polarities at 20 Rs are shown in Fig. 10 with the simulated results denoted by red lines and the mapped observational results of the OMNI data by black lines. We can easily find that the profiles of the solar wind from both the simulation and the in-situ observation go with the same trend in general. In the profile of the radial velocity, it is characterized of
three high-speed peaks centered at Longitudes 25°, 100° and 260° and three low-speed streams centered at Longitudes 60°, 180° and 340° in the OMNI data. All of these streamers are captured at precisely same longitudes by the simulated result. As for the speed maxima, the high-speed peaks in simulation range between 640 km s\(^{-1}\) and 680 km s\(^{-1}\), while the low-speed streams flows at a speed of 350 km s\(^{-1}\). We also note that the speed of the simulated stream at Longitude 100° is a little lower than the OMNI data. The polarities of the radial magnetic field is on the right of the top panel in Fig. 10. Though there are a few deviations, sectors of different polarity of the numerical result are generally in agreement with that of the observation. The hit ratio of the simulated radial magnetic field polarities to the observed ones for CR 2051 is 84.53%. This possibly results from both the error of the simulated results and the effect of the waves and perturbations in the solar wind that can lead to the opposite polarity to be measured rather than the true field polarity [27,33]. To sum up, high- and low-speed streams are captured by our MHD model, and the observed polarities of the radial magnetic field are mostly reproduced by our simulation with reasonable accuracy. In the bottom panel of Fig. 10, we also present the longitudinal variations of the radial magnetic fields at 20 Rs achieved from the simulation and the mapped in-situ measurements without considering the factor of \(r^{-2}\). If we take this factor into account, the modeled radial magnetic fields are only one-third of the corresponding measurements, which is also present in previous studies [34−37]. Linker [37] attributed the deficiency of the open magnetic flux to either the underestimation of the Sun's magnetic flux by typical observatory maps, or other sources of open magnetic flux other than the regions that are obviously dark in EUV and X-ray emission.

6. Conclusions

In this paper, we develop an easily implemented FV scheme with the GMRES algorithm and an LU-SGS preconditioner on the six-component mesh grid system to solve the MHD equations governing the solar wind plasma. The implicit and the explicit solvers of the same FV scheme are implemented and run on the same computing cluster by evoking 120 processes. The comparisons show that the implicit solver can effectively shorten the time cost from several days to only a few hours and aquire speedup ratios of 31.27 \(\times\) and 28.05 \(\times\), with two sampled mesh divisions. Besides the significant computational efficiency, the LU-SGS preconditioner does not require any additional memory storage and is easy to implement on the parallely distributed cluster. We further employ the proposed MHD scheme to simulate the 3D large-scale structures of the steady-state solar wind from 1 Rs to 20 Rs during CR 2051. The simulated results capture many features of the solar corona. The simulation and the observation achieve similar isolated low-latitude coronal holes and almost the same shapes and sizes of the PCHs. The white-light p8 images synthesized from the simulated results and observed by LASCO/SOHO show basically consistent distributions of bright structures. In addition, the radial profiles of the solar wind radial bulk speed from 2.6 Rs to 20 Rs are consistent with previous observational studies [31,32]. The simulated results at 20 Rs capture the mapped in-situ observations with reasonable accuracy. Therefore the simulation exhibits the potential capability of numerically modeling the space weather event from the Sun to interplanetary space.

Generally speaking, it is formidable to conduct the real-time 3D MHD simulation for a specified space weather events from the Sun.
to the Earth beyond because the simulation is too time-consuming and needs too much computational resources. The significant computational efficiency of the FV scheme with a GMRES algorithm and an LU-SGS preconditioner will be a promising choice to complete the tough task after improvements, which will be our future consideration in further studies http://omniweb.gsfc.nasa.gov.

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