

Relativistic HPIC-LBM and its application in large temporal-spatial turbulent magnetic reconnection. Part I. model development and validation

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ABSTRACT

Magnetic energy release conversion, plasma heating and charged particle energization-acceleration in the magnetic fluctuation-induced self-generating-organization region and the plasma turbulence-induced self-feeding-sustaining region are key issues for large temporal-spatial scale turbulent magnetic reconnection (LTSTMR; observed current sheet thickness to characteristic electron length, electron *Larmor* radius for low- β and electron inertial length for high- β , ratios on the order of $10^{10} \sim 10^{11}$; observed evolution time to electron cyclotron time ratios on the order of $10^{10} \sim 10^{11}$) that ranges from Earth's magnetosphere to solar eruptions and other astrophysical phenomena. As the first part of a two-paper series, this paper introduces a relativistic hybrid particle-in-cell and lattice Boltzmann (RHPIC-LBM) model that describes the continuous kinetic-dynamic-hydro fully coupled LTSTMR evolution process. First, based on the governing equations of resistive relativistic magnetohydrodynamics (MHD), the relativistic discrete distribution functions for a magnetic field (D3Q7), electric field (D3Q13), electromagnetic field (D3Q13), charged particle (D3Q19) and neutral particle (D3Q27) of different plasma species are obtained for the RHPIC-LBM lattice grid. Then, the numerical process, algorithm, pseudocode, flowchart and GPU-CPU heterogeneous framework of the RHPIC-LBM are described. Finally, this model is tested and validated on *Tianhe-2* from the National Supercomputer Center in Guangzhou (NSCC-GZ) with 10,000 ~ 100,000 CPU cores and 50~120 hours per case. We investigate the solar atmosphere LTSTMR activities, including the picoscale (10^{-2} m ~ 10^5 m), nanoscale (10^5 m ~ 10^6 m), microscale (10^6 m ~ 10^7 m), macroscale (10^7 m ~ 10^8 m) and large hydroscale (10^8 m ~ 10^9 m). All the simulation results are consistent with observations and theories. The validated model is applied to explore the turbulence evolution

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³ Conceived the LBM model and verified its application in Geophysics.

of the interactions of the magnetic helical structures in the 3D LTSTMR self-generating-organization magnetic field region and self-feeding-sustaining plasma region in Part II.

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1. Introduction

Magnetic reconnection (MR) is believed to be the most important way to convert magnetic energy into thermal and kinetic energy in plasma [1–26]. The familiar two-dimensional (2D) cases and the more complicated three-dimensional (3D) scenarios [27–32] show that the development of 2D magnetic islands and 3D flux ropes plays a crucial role in particle acceleration in various MR events, from explosive astrophysical phenomena to laboratory plasma [3,18–26].

Despite the accumulation of considerable research results regarding MR [3,18–32], many uncertainties remain in the magnetic fluctuation-induced self-generating-organization region and in the plasma turbulence-induced self-feeding-sustaining region.

Quantitatively analyzing of the role of turbulence in these relativistic resistive magnetohydrodynamics (MHD) regions is important for understanding the mechanism of the magnetic energy release conversion, plasma heating and charged particle energization-acceleration in the continuous kinetic-dynamic-hydro fully coupled (microphysics, electron MHD [EMHD]; Hall physics, Hall MHD [HMHD]; macrophysics, ion MHD [IMHD]; large hydroscale physics) large temporal-spatial scale turbulent MR (LTSTMR).

Until now, the role of turbulence in these processes has been an open question that has been fiercely debated due to the lack of fine-scale 3D observations and experimental and numerical simulation data/evidence.

Solar atmosphere activities (e.g., limbs, flares, coronal mass ejections [CMEs], solar winds and so on), which are the most important phenomena in the solar and Sun-Earth space systems, are typical LTSTMRs [6–8,10,33–37] and possess the following characteristics:

- i) Multicomponent
There are several chemical compositions in the solar atmosphere (Table 1) that are dominated by hydrogen (73%) and helium (25%), but these components constitute only a small percent of the total mass.
In solar physics, we identify all the components as metals except hydrogen and helium, even though elements such as carbon and oxygen are included, which are not commonly considered to be metals [38,39].
- ii) Different degree of ionization
The plasma of the solar atmosphere activities includes partially and fully ionized plasma, and different layers have different thicknesses, temperatures and degrees of ionization [40–42].
The general description of the layers of the solar atmosphere is shown in Table 2. Typical LTSTMR occurs in the solar atmosphere activity.
- iii) Relativistic plasma
Observations show that the accelerated electron and ion particles reach relativistic energies in solar atmosphere LTSTMR activities [43–46].
- iv) Continuous kinetic-dynamic-hydro fully coupled physics process (EMHD, HMHD, IMHD, hydroscale physics).
Observations show that the solar atmosphere activities include many kinetic scale fractal and turbulence magnetic structures and are typical continuous kinetic-dynamic-hydro fully coupled LTSTMRs that cover the picoscale (10^{-2} m $\sim 10^5$ m), nanoscale (10^5 m $\sim 10^6$ m), microscale (10^6 m $\sim 10^7$ m), macroscale (10^7 m $\sim 10^8$ m) and large hydroscale (10^8 m $\sim 10^9$ m) [4,47–52].

Table 1
Chemical composition of the solar atmosphere [38,39].

Chemical composition	Percent of the overall mass	Type
Hydrogen	73%	Dominated
Helium	25%	Dominated
Oxygen	0.8%	Metals
Carbon	0.36%	Metals
Iron	0.16%	Metals
Neon	0.12%	Metals
Nitrogen	0.09%	Metals
Silicon	0.07%	Metals
Magnesium	0.05%	Metals
Sulphur	0.04%	Metals
Others combined	0.04%	Metals

Table 2
Layers of the Sun [40–42].

Layers	Thickness (km)	Temperature (K)	Type
Core	150,000	10,000,000	Inertial layer
Convection Zone	180,000	500,000	Inertial layer
Photosphere ^a	400	6400	Outer layer, un-magnetized, weakly ionized
Chromosphere	2100	4400 – 8000	Outer layer, magnetized, partly ionized ^b
Transition region	100	8000 – 500,000	Outer layer, magnetized, high ionized
Corona	5,000,000	1,000,000	Outer layer, magnetized, fully ionized

^a Neutral atoms (of H, He, etc.) and some ions (once-ionized Na, Mg, Fe) and free electrons e^- . there are only 10^{-8} H^- ions to every H atom.).

^b Lower chromosphere: $\sim$ degrees C $\sim$ with 200 km thickness. Top chromosphere: $\sim$ 8000 K degrees C with $\sim$ 800 km thick.

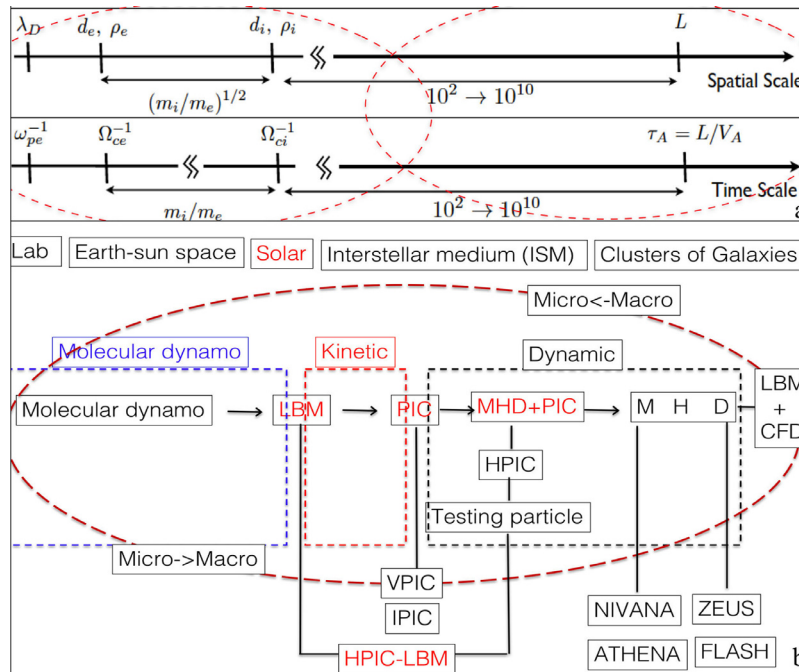


Fig. 1. Numerical methods/models for different temporal-spatial scale astrophysical magnetic reconnection problems.

The above introduction demonstrates that the LTSTMRs in solar atmosphere activities are very complicated, and many of the physical pictures are still unclear or controversial, especially in the 3D LTSTMR self-generating-organization magnetic field region and self-feeding-sustaining plasma region.

To date, to the best of the authors' knowledge, there are no continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale physical and mathematical models, algorithms, or codes for investigating solar atmosphere LTSTMR (Fig. 1).

In this paper, we develop a relativistic hybrid particle-in-cell and lattice Boltzmann (RHPIC-LBM) model that is applied in the second part of a two-paper series on *Tianhe-2* from National Supercomputer Center in Guang Zhou (NSCC-GZ) to investigate the role of turbulence in the interaction of flux ropes from the fully coupled kinetic-dynamic-hydro temporal-spatial 3D LTSTMR problem.

Section 2 depicts the physical and mathematical model, introduces the relativistic distribution function for real flow (neutral particle flow D3Q27 and charged particle flow D3Q19) RHPIC-LBM lattice grids of different species and virtual flow (magnetic field virtual flow D3Q7, electric field virtual flow D3Q13, and electromagnetic virtual flow D3Q13) RHPIC-LBM lattice grids.

The interactions between the fields (magnetic, electric and electromagnetic) and the particles (neutral and charged particles) are transformed into interactions between virtual particles in virtual flow (magnetic virtual flow and electric virtual flow) and real particles in real fluid flow (neutral fluid and charged particle fluid) in the RHPIC-LBM lattice grid mathematical model.

The numerical framework, flowchart and implementation of the RHPIC-LBM are introduced in Section 3. The testing and validation of the reliability, stability, and efficiency of the RHPIC-LBM algorithms are reported in Section 4.

Section 5 validates the solar atmosphere LTSTMR activities at various scales, including the picoscale (10^{-2} m $\sim 10^5$ m), nanoscale (10^5 m $\sim 10^6$ m), microscale (10^6 m $\sim 10^7$ m), macroscale (10^7 m $\sim 10^8$ m) and large hydroscale (10^8 m $\sim 10^9$ m); all the simulation results are consistent with observations [3–5,9,10,47,48,53–55] and theories [11,56–61].

2. Physical and mathematical model

2.1. Basic equation

For general LTSTMR phenomena, the state of the plasma can be specified by the distribution functions, $f_{i\xi}^{\zeta}(\mathbf{x}, \mathbf{p}, t)$, which characterize multicomponent particles in the finite number phase directions in $D_i^{\zeta}XQ\xi$ cubic lattice grid discretized temporal-spatial space, where $\mathbf{x}, \mathbf{p}, t$, and X represent the position coordinate, the momentum coordinate, the time coordinate and the dimension of the $D_i^{\zeta}XQ\xi$ cubic lattice grid, respectively.

These distribution functions describe the different physical properties ($\zeta = 1, 2, 3, \dots$ denotes density, momentum, velocity and so on) of different particles ($\zeta = 1, 2, 3, \dots$ denotes electrons, ions and neutrals) for different components ($i = 1, 2, 3, \dots$ denotes hydrogen, helium and other metal components) in different discretized spatial directions (ξ).

Then, the field variations (including magnetic, electric, electromagnetic, gravitational fields and so on), the motion of the plasma and the interaction between the fields and plasma motion in resistive relativistic MHD can be described by a system of Boltzmann equations that carries the distribution functions forward in time and can be written as,

$$\frac{\partial f_{i\xi}^{\zeta e}}{\partial t} + \frac{1}{\varepsilon_i^e} \mathbf{U}_i^e \cdot \nabla_{\mathbf{x}} f_{i\xi}^{\zeta e} + \mathbf{F}_i^e \cdot \frac{\partial f_{i\xi}^{\zeta e}}{\partial \mathbf{p}_i^e} = \frac{\theta_i^e}{(\varepsilon_i^e)^2} \nabla_{\mathbf{p}_i^e} \cdot \left(\nabla_{\mathbf{p}_i^e} f_{i\xi}^{\zeta e} + \mathbf{U}_i^e f_{i\xi}^{\zeta e} \right) \quad (1)$$

$$\frac{\partial f_{i\xi}^{\zeta i}}{\partial t} + \frac{1}{\varepsilon_i^i} \mathbf{U}_i^i \cdot \nabla_{\mathbf{x}} f_{i\xi}^{\zeta i} + \mathbf{F}_i^i \cdot \frac{\partial f_{i\xi}^{\zeta i}}{\partial \mathbf{p}_i^i} = \frac{\theta_i^i}{(\varepsilon_i^i)^2} \nabla_{\mathbf{p}_i^i} \cdot \left(\nabla_{\mathbf{p}_i^i} f_{i\xi}^{\zeta i} + \mathbf{U}_i^i f_{i\xi}^{\zeta i} \right) \quad (2)$$

$$\frac{\partial f_{i\xi}^{\zeta n}}{\partial t} + \mathbf{U}_i^n \cdot \nabla_{\mathbf{x}} f_{i\xi}^{\zeta n} + \mathbf{F}_i^n \cdot \frac{\partial f_{i\xi}^{\zeta n}}{\partial \mathbf{p}_i^n} = \nabla_{\mathbf{p}_i^n} \cdot \left(\nabla_{\mathbf{p}_i^n} f_{i\xi}^{\zeta n} + \mathbf{U}_i^n f_{i\xi}^{\zeta n} \right) \quad (3)$$

Eqs. (1)–(3) represent the governing equations of electron, ion and neutral particles, respectively. The terms on the left sides of Eqs. (1)–(3) represent the rates of change of the extended motion of the particles with respect to the extended position, momentum and time. In this paper, the left sides of these equations also refer to the extended free streaming of different extended particles in temporal-spatial space.

The terms on the right sides of Eqs. (1)–(3) represent the extended forces that induce the extended particle motion variations. In this paper, the right sides of these equations also refer to the extended interparticle interactions and collisions in temporal-spatial space.

The parameters $\mathbf{F}_i^e$, $\mathbf{F}_i^i$ and $\mathbf{F}_i^n$ in the third term of the left sides of Eqs. (1)–(3) are forces that are closely related to electron motion, ion motion and neutral particle motion, respectively.

$$\mathbf{F}_i^e = \frac{1}{\varepsilon_i^e} \mathbf{E} + (\delta_i^e)^2 \mathbf{U}_i^e \times \mathbf{B} \quad (4)$$

$$\mathbf{F}_i^i = \frac{1}{\varepsilon_i^i} \mathbf{E} + (\delta_i^i)^2 \mathbf{U}_i^i \times \mathbf{B} \quad (5)$$

$$\mathbf{F}_i^n = \mu' (\nabla \cdot \mathbf{U}_i^n) + \mu \nabla \cdot \left(\nabla \mathbf{U}_i^n + (\nabla \mathbf{U}_i^n)^T - \frac{2}{3} (\nabla \cdot \mathbf{U}_i^n) \mathbf{I} \right) - \nabla P_i^n + n_i^n \mathbf{g} \cdot \nabla \mathbf{U}_i^n \quad (6)$$

The dimensional parameters, ε_i^{ζ} , δ_i^{ζ} , and θ_i^{ζ} in Eqs. (4)–(6) can be expressed as,

$$\varepsilon_i^{\zeta} = q^2 c^{-1} \varepsilon_{0i}^{-1} n_i^{\zeta} \left(K T_{thi}^{\zeta} + 2 m_i^{\zeta} c^2 \right)^{1/2} \left(K T_{thi}^{\zeta} \right)^{-3/2} \quad (7)$$

$$\delta_i^{\zeta} = \left(1 + 2 m_i^{\zeta} c^2 / \left(K T_{thi}^{\zeta} \right) \right)^{-1/2} \quad (8)$$

$$\theta_i^{\zeta} = \chi_i^{\zeta} \varepsilon_i^{\zeta 2} \quad (9)$$

where q , m_i^{ζ} , $\mathbf{U}_i^{\zeta}$, $\mathbf{B}$, $\mathbf{E}$, $\mathbf{p}_i^{\zeta}$, t , c , ε_{0i} , $n_{\alpha i}^{\zeta}$, K , T_{thi}^{ζ} and χ_i^{ζ} represent the charge of the particles, rest mass of the particles, plasma relativistic velocity, strength of the magnetic field, strength of the electric field, relativistic momentum, time, speed of light, vacuum permittivity, number density of the particles, Boltzmann constant, temperature of the thermal bath and unit time-to-relaxation time ratio, respectively.

Analysis of the forces from the above equations shows that handling the interparticle interactions and/or collisions and the interactions of the fields and charged particles are of primary importance in the physical and mathematical model.

For interactions and/or collisions between real particles (charged particle-to-charged particle, charged particle-to-neutral particle, neutral particle-to-neutral particle), many achievements have been made with the original lattice Boltzmann model [62–65], and these interactions and collisions are accurately described by this model for fully ionized plasma ($v_{ei} > v_{en}$), partially ionized plasma ($v_{ei} \approx v_{en}$), and weakly ionized plasma ($v_{ei} < v_{en}$) cases Eqs. (4)–(6).

However, when referring to the interactions and/or collisions between real particles and virtual particles (charged particle-to-field), there is some controversy regarding whether the virtual flow validation of an algorithm can be considered to be a true validation of the interaction between a magnetic field and charged particles (Eqs. (4)–(5), even through many solid research achievements have been made in the past fifteen years in the solar astrophysics and astrophysics fields [66–71] using this type of method.

The role of turbulence in the interactions between flux ropes (magnetic fluctuation-induced self-generating-organization field), flux ropes and plasma bubbles (magnetic fluctuation-induced self-generating-organization field and plasma turbulence-induced self-feeding-sustaining motion), and plasma bubbles (plasma turbulence-induced self-feeding-sustaining motion) in the diffusion region is the key issue for exploring the magnetic energy conversion, plasma heating and particle acceleration in LTSTMR.

Thus, describing the interactions between real particles and virtual particles in the resistive relativistic MHD diffusion region is one of most important issue in the mathematical and numerical model.

2.2. Physical and mathematical model

In the physical and mathematical model of the RHPIC-LBM cubic lattice grid, the strength of the magnetic field ($\mathbf{B}$) and electric field ($\mathbf{E}$) in the diffusion region of the resistive relativistic LTSTMR are defined as virtual magnetic flow and virtual electric flow, respectively [66–75].

The RHPIC-LBM cubic lattice grids for magnetic virtual flow, electric virtual flow, ion & electron fluid flow and neutral particle fluid flow can be defined as D^B3Q7 , D^E3Q13 , D^e3Q19 , D^i3Q19 and D^n3Q27 [66,69,76–78] cubic lattice grids, respectively.

Previous LBM research demonstrates that the lattice Boltzmann equation can be considered as a special finite difference approximation of the Boltzmann equation, which provides a way to transfer a continuous Boltzmann equation (Eqs. (1)–(3)) into a discrete equation (discrete extended particle velocities, discrete geometry-topology of the fields, and discrete geometry of the simulation domain) in the mathematical model [79–82].

In the X -dimensional temporal-spatial space, the geometry space (geometry simulation domain) and physical space (motion turbulence, field fluctuation, and the interaction between them) can be classified into different types of regular cubic lattice grids.

Each lattice grid has ξ extended vectors $\mathbf{U}_{i\xi}^\zeta(\mathbf{x}, \mathbf{p}, t)$ that link the grid with its neighbors. Each extended vector is associated with a distribution function $f_{i\xi}^{\zeta\zeta}(\mathbf{x}, \mathbf{p}, t)$, which can be written as,

$$\mathbf{U}_{i\xi}^\zeta = \begin{cases} \mathbf{U}_{i\xi}^B & \xi = 1 \sim 7 \\ \mathbf{U}_{i\xi}^E & \xi = 1 \sim 13 \\ \mathbf{U}_{i\xi}^e & \xi = 1 \sim 19 \\ \mathbf{U}_{i\xi}^i & \xi = 1 \sim 19 \\ \mathbf{U}_{i\xi}^n & \xi = 1 \sim 27 \end{cases} \quad (10)$$

The distribution function evolves at temporal-spatial steps, $\delta\mathbf{x}$, δt , $\delta\mathbf{p}$, according to the following Lattice Boltzmann equation,

$$f_{i\xi}^{\zeta\zeta}(\mathbf{x} + \mathbf{U}_i^\zeta \delta t, \mathbf{p} + \delta\mathbf{p}_i^\zeta, t + \delta t) - f_{i\xi}^{\zeta\zeta}(\mathbf{x}, \mathbf{p}, t) = \frac{1}{\tau_i^\zeta \mathbf{U}_i^\zeta} \left(f_{i\xi}^{EM\zeta\zeta}(\mathbf{x}, \mathbf{p}, t) - f_{i\xi}^{EM\zeta\zeta eq}(\mathbf{x}, \mathbf{p}, t) \right) + \frac{c\delta t}{\tau_i^\zeta (K_B T_i^\zeta m_i^{\zeta-1})^{1/2}} \left(f_{i\xi}^{\zeta\zeta}(\mathbf{x}, \mathbf{p}, t) - f_{i\xi}^{\zeta\zeta eq}(\mathbf{x}, \mathbf{p}, t) \right) \quad (11)$$

where τ_i^ζ and $f_{i\xi}^{\zeta\zeta eq}$ represent the relaxation time and equilibrium function, respectively.

In the RHPIC-LBM, a regular cubic grid with lattice constant $\delta x = \sqrt{2}c\delta t$ is applied to the real particles (ion, electron and neutral particles), virtual particles (magnetic field, electric field, electromagnetic field, gravitational field and so on) and geometric lattice grid (geometric simulation domain).

For the D^B3Q7 lattice grid model, there are 7 vectors for the magnetic field, and the velocity vectors are denoted by $\mathbf{U}_{i\xi}^{\vartheta B}$, where $\vartheta = 0, 1, 2$, which indicates different location planes. The velocity vectors can be written as [63,66,69,76,83,84],

$$\mathbf{U}_{i\xi}^{\vartheta B} = c\sqrt{2} \left\{ \begin{aligned} & \left[\left(\cos \frac{(2\xi-1)\pi}{4} \vec{i} + \sin \frac{(2\xi-1)\pi}{4} \vec{j} \right) \sum_{w=2}^5 \delta_{\xi w} + (-1)^\xi \vec{i} \sum_{w=6}^7 \delta_{\xi w} \right] \delta_{(\vartheta+1)1} \\ & + \left[\left(\cos \frac{(2\xi-1)\pi}{4} \vec{i} + \sin \frac{(2\xi-1)\pi}{4} \vec{k} \right) \sum_{w=2}^5 \delta_{\xi w} + (-1)^\xi \vec{j} \sum_{w=6}^7 \delta_{\xi w} \right] \delta_{(\vartheta+1)2} \\ & + \left[\left(\cos \frac{(2\xi-1)\pi}{4} \vec{j} + \sin \frac{(2\xi-1)\pi}{4} \vec{k} \right) \sum_{w=2}^5 \delta_{\xi w} + (-1)^\xi \vec{k} \sum_{w=6}^7 \delta_{\xi w} \right] \delta_{(\vartheta+1)3} \end{aligned} \right\} \quad (12)$$

For the D^E3Q13 lattice grid model, there are 13 vectors for the electric field. The velocity vectors are denoted by $\mathbf{E}_{i\xi\xi}^{\vartheta e}$ and can be written as [63,66,69,76,83,84],

$$\mathbf{E}_{i\xi\xi}^{\vartheta E} = \frac{1}{2} \left(U_{i(\xi-1) \bmod 4}^{\vartheta B} \delta_{(\xi-1)1} + U_{i(\xi+1) \bmod 4}^{\vartheta B} \right) \quad (13)$$

Then, the 7 vectors for magnetic fields can be written as,

$$\mathbf{b}_{i\xi\xi}^{\vartheta B} = \frac{1}{2c^2} U_{i\xi}^{\vartheta B} \times \mathbf{E}_{i\xi\xi}^{\vartheta E} \quad (14)$$

The function δ_{ij} in Eqs. (12)~(14) is defined as Kronecker delta function. The function $\hat{\xi} = 0, 1, (\xi) \bmod 4$ is a function that gives the remainder of the division of ξ by 4.

The equilibrium distribution function for the electromagnetic field can be written as [63,66,69,76,83,84],

$$f_{i\xi}^{\vartheta EMeq}(x, \mathbf{p}, t) = \frac{1}{16} \mathbf{U}_{i\xi}^{\vartheta B} \cdot \mathbf{J} + \frac{1}{8c^2} \mathbf{E} \cdot \mathbf{E}_{i\xi\xi}^{\vartheta E} + \frac{1}{8} \mathbf{B} \cdot \mathbf{b}_{i\xi\xi}^{\vartheta B} \quad (15)$$

The discretized equilibrium distribution function for the magnetic virtual flow (D3Q7), electric virtual flow (D3Q13), and electron and ion flow (D3Q19) can be written as following equations, respectively [63,66,69,76,83,84],

$$f_{i\xi}^{\vartheta Beq}(x, \mathbf{p}, t) = \left(\frac{1}{6} \delta_{\xi 0} + \frac{1}{72} \delta_{\xi m} + \frac{1}{36} \delta_{\xi n} \right) \left[\frac{3}{c^2} \mathbf{E}_{i\xi\xi}^{\vartheta E} \cdot \mathbf{U}_{i\xi}^{\vartheta B} + \frac{9}{4c^4} \left(\mathbf{E}_{i\xi\xi}^{\vartheta E} \cdot \mathbf{U}_{i\xi}^{\vartheta B} \right)^2 - \frac{3}{2c^2} \mathbf{U}_{i\xi}^{\vartheta B} \cdot \mathbf{U}_{i\xi}^{\vartheta B} \right] \quad (16)$$

where $m = 1 \sim 4$, $n = 5 \sim 6$, and $\xi = 1 \sim 9$.

$$f_{i\xi}^{\vartheta Eeq}(x, \mathbf{p}, t) = \frac{1}{8} \delta_{\xi m} \left[\frac{3}{c^2} \mathbf{E}_{i\xi\xi}^{\vartheta E} \cdot \mathbf{U}_{i\xi\xi}^{\vartheta B} + \frac{9}{4c^4} \left(\mathbf{E}_{i\xi\xi}^{\vartheta E} \cdot \mathbf{U}_{i\xi\xi}^{\vartheta B} \right)^2 - \frac{3}{2c^2} \mathbf{U}_{i\xi\xi}^{\vartheta B} \cdot \mathbf{U}_{i\xi\xi}^{\vartheta B} \right] \quad (17)$$

where $m = 1 \sim 12$ and $\xi = 1 \sim 13$.

$$f_{i\xi}^{\vartheta jeq}(x, \mathbf{p}, t) = \frac{3c_{i0}^{j2}(\varepsilon_{i0}^j + p_i^j)\omega_\xi}{4c_{it}^j} \left\{ \begin{aligned} & 1 + \frac{3(\Gamma_i^j-1)(\varepsilon_i^j-n_i^j c^2)-\varepsilon_i^j}{(\Gamma_i^j-1)(\varepsilon_i^j-n_i^j c^2)+\varepsilon_i^j} - \frac{361(\Gamma_i^j-1)(\varepsilon_i^j-n_i^j c^2)-\varepsilon_i^j}{33(\Gamma_i^j-1)(\varepsilon_i^j-n_i^j c^2)-\varepsilon_i^j} \delta_{\xi 0} \\ & + c_{ia}^{jx} c_{ia}^{jy} \chi_{ia}^{jx} \chi_{ia}^{jy} + c_{ia}^{jx} c_{ia}^{jz} \chi_{ia}^{jx} \chi_{ia}^{jz} + c_{ia}^{jy} c_{ia}^{jz} \chi_{ia}^{jy} \chi_{ia}^{jz} + \left(\frac{c_{it}^j \chi_{it}^{j0}}{2c_{it}^{j2}} - \frac{\chi_{it}^{j0}}{v_i^j c_{it}^{j0}} \right) (c_{ia}^j \cdot \vec{\chi}_{it}^j) \\ & + \frac{4}{15} [(c_{ia}^{jx} \chi_{it}^{jx})^2 + (c_{ia}^{jy} \chi_{it}^{jy})^2 + (c_{ia}^{jz} \chi_{it}^{jz})^2 - \frac{4}{v_i^j} (\vec{\chi}_{it}^j \cdot \vec{\chi}_{it}^j)] \\ & + \frac{c_{i0}^{j2} \varepsilon_{i0}^j \omega_\xi}{c_{it}^{j2}} \left\{ \begin{aligned} & \frac{3(c_{ia}^{j2} B_{it}^j + E_{it}^{j2})}{2} + \frac{4(c_{ia}^{j2} B_{it}^j + E_{it}^j E_{it}^j)}{5} - \frac{v_i^j B_{it}^j \times E_{it}^j \cdot \vec{c}_{ia}}{\sqrt{3}} + \frac{v_i^2 [c_{ia}^2 (B_{it}^j \cdot \vec{c}_{ia})^2 + (E_{it}^j \cdot \vec{c}_{ia})^2]}{5} \\ & - \frac{v_i^2}{20} [c_{ia}^{jx} c_{ia}^{jy} E_{it}^{jx} E_{it}^{jy} + c_{ia}^{jx} c_{ia}^{jz} E_{it}^{jx} E_{it}^{jz} + c_{ia}^{jy} c_{ia}^{jz} E_{it}^{jy} E_{it}^{jz} + c_{ia}^{jx} c_{ia}^{jy} B_{it}^{jx} B_{it}^{jy} + c_{ia}^{jx} c_{ia}^{jz} B_{it}^{jx} B_{it}^{jz} + c_{ia}^{jy} c_{ia}^{jz} B_{it}^{jy} B_{it}^{jz}] \end{aligned} \right\} \end{aligned} \right\} \quad (18)$$

where $j = e, i$ denotes the electron and ions, respectively. c_0 , c_a and c_t are three constants related to the size of the lattice grid. ε_i^j and ε_{it}^{j0} denote the energy density including the rest mass energy and the permittivity of the free space with respect to the permeability of the free space, respectively. $v_i^j = \frac{c}{c_{is}^j} = c \sqrt{\frac{m_i^j}{k_B} T_i^j}$, $\chi_{it}^j = \frac{U_{it}^j}{c_{is}^j} = U_{it}^j \sqrt{\frac{m_i^j}{k_B} T_i^j}$ and $p_i^j = \frac{n_i^j}{v_i^2}$ are three variables closely related to the particle physical properties. $\Gamma_i^j = c_{ip}^j / c_{iv}^j$ is the adiabatic index and is $\frac{4}{3}$ for ultrarelativistic temperatures and $\frac{5}{3}$ for nonrelativistic temperatures. c_{ip}^j and c_{iv}^j represent specific heats at constant pressure and volume, respectively [63,66,69,76,83–87]. The discrete weight function w_ξ in Eq. (18) can be written as,

$$w_\xi = \left(1 + \frac{4c_{it}^{j2} v_{it}^{j2}}{361c_{i0}^{j2}} - \frac{c_{it}^{j2}}{c_{ia}^{j2} c_{i0}^{j2}} \right) \delta_{1\xi} + \frac{c_{it}^{j2}}{2166c_{i0}^{j2} c_{ia}^{j2}} (361 - 8c_{ia}^{j2} v_{it}^{j2}) \sum_{m=2}^7 \delta_{m\xi} + \frac{c_{it}^{j2}}{1083c_{i0}^{j2} c_{ia}^{j2}} \sum_{m=8}^{19} \delta_{m\xi} \quad (19)$$

Combined all the above distribution functions and the equilibrium distribution function for D3Q27 neutral particle flow [63,77,85–87], the interactions of the fields and particles will be transformed into the interactions of the virtual particles and real particles.

Then, the self-generating-organization fluctuation magnetic fields and self-feeding-sustaining turbulence plasmas in the resistive relativistic MHD can be translated into the interactions and/or collisions of the extended particles by following a numerical framework-flowchart and implementation.

3. Numerical framework, flowchart and implementation

In this section, we outline the major steps of the RHPIC-LBM lattice grid, flowchart and implementation applied to the RHPIC-LBM.

3.1. Discrete distribution function of a single charged particle (EMHD)

Plasma consists of a very large number of particles. Calculating the orbits of all the particles is extremely difficult, even for fully ionized particles with a single chemical composition and low β case (corona, hydrogen) for solar atmosphere LTSTMR activities (Tables 1 and 2).

To make the derivation of the RHPIC-LBM lattice grid easier to understand, in this section, we take $\varsigma = 1$ (density) and $\zeta = 1$ (electron).

We consider a single particle with orbit $(\mathbf{x}(t), \mathbf{U}_{i\xi}^{\rho e}(t))$ in 6-dimensional phase space whose *density* can be defined as the discrete distribution function of single particle, which is written as,

$$N_{i\xi}^{\rho e}(\mathbf{x}, \mathbf{U}, t) = \delta(x - x(t))\delta(y - y(t))\delta(z - z(t))\delta(U_{i\xi x}^{\rho e} - U_{i\xi x}^{\rho e}(t))\delta(U_{i\xi y}^{\rho e} - U_{i\xi y}^{\rho e}(t))\delta(U_{i\xi z}^{\rho e} - U_{i\xi z}^{\rho e}(t)) \quad (20)$$

3.2. Discrete distribution function of microscopic particles (HMHD and IMHD)

For charged particles in plasma, we sum all the microscopic discrete distribution functions, then the equation can be written as,

$$\begin{aligned} N_{i\xi}^{\rho e-micro}(\mathbf{x}, \mathbf{U}, t) &= \sum_i^N \delta(x - x_i(t))\delta(y - y_i(t))\delta(z - z_i(t))\delta(U_{i\xi x}^{\rho e} - U_{i\xi x}^{\rho e}(t))\delta(U_{i\xi y}^{\rho e} - U_{i\xi y}^{\rho e}(t))\delta(U_{i\xi z}^{\rho e} - U_{i\xi z}^{\rho e}(t)) \\ &= \sum_i^N \delta(\mathbf{x} - \mathbf{x}_i(t))\delta(\mathbf{U}_{i\xi}^{\rho e} - \mathbf{U}_{i\xi}^{\rho e}(t)) \end{aligned} \quad (21)$$

Here, $\mathbf{x}(t)$ and $\mathbf{U}_{i\xi}^{\rho e}(t)$ are the spatial and velocity trajectories as the particles move, which are determined by Eqs. (1~3).

All the particles ($i = 1 \sim N$) have time-dependent positions $\mathbf{x}(t)$ and $\mathbf{U}_{i\xi}^{\rho e}(t)$, and the particle paths at subsequent times are in a curve of temporal-spatial space.

3.3. Microscopic sources of RHPIC-LBM

The density of charge and current are defined as

$$\rho_{i\xi}^{\rho e-micro}(\mathbf{x}, \mathbf{U}, t) = \sum_{i=1}^s q_i \int N_{i\xi i}^{\rho e-micro}(\mathbf{x}, \mathbf{U}, t) dV \quad (22)$$

$$\mathbf{J}_{i\xi}^{\rho e-micro}(\mathbf{x}, \mathbf{U}, t) = \sum_{i=1}^s q_i \int \mathbf{U}_{i\xi i}^{\rho e-micro} N_{i\xi i}^{\rho e-micro}(\mathbf{x}, \mathbf{U}, t) dV \quad (23)$$

The three imperative steps above are used as a general guide to establish the RHPIC-LBM kinetic scale description, which involves all the information of the plasma turbulence motion, including self-feeding-sustaining with the magnetic fluctuation-induced self-generating-organization fields, and provides a basis for analyzing and examining the simulation behavior when designing the flowcharts.

In real solar atmosphere LTSTMR simulation (e.g., the corona number density $\sim 10^{15}/m^3$), a large number of particles has to be initialized in the numerical domain for good statistics (e.g., to remove and reduce the physical noise in the mathematical model, to determine the physical, numerical and system error limits in the RHPIC-LBM code and to avoid program interruptions and/or incorrect calculation results).

3.4. Discrete conservation of charged particles

$$\frac{\partial N_{i\xi}^{\rho e-micro}}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \frac{\partial N_{i\xi}^{\rho e-micro}}{\partial \mathbf{x}} + \mathbf{F}_i^e \cdot \frac{\partial N_{i\xi}^{\rho e-micro}}{\partial \mathbf{U}_{i\xi}^e} = \sum_{i=1}^3 \left(\frac{\partial N_{i\xi}^{\rho e-micro}}{\partial x_i \partial U_{i\xi x}^e} + i N_{i\xi}^{\rho e-micro} \right) \quad (24)$$

Eqs. (1)~(3) together with the charge and current density equation in step 3.3 provide an exact and complete description of the plasma properties (particle characteristics, flow characteristics, and particles held in place by magnetic fields) in the fully coupled kinetic-dynamic-hydro temporal-spatial scale.

This equation incorporates all the extended equations of particle motion into one equation for the characteristic profile in temporal-spatial space.

3.5. Conditions for the averaging procedure

The charged particle distribution in Eq. (24) in step 3.4 is a delta functions; this distribution requires the tracking of all the individual particles, which is not feasible on present supercomputer platforms, even **Tianhe-2**.

Thus, we need an averaging procedure to obtain a smooth function of the microscopic distribution to describe the motion of the charged particles.

In the RHPIC-LBM, we average over a small volume in phase space for the charged particles and average over an infinite number of realizations for the neutral particles.

For the charged particles, the following two conditions must be simultaneously satisfied:

- i) To ensure that each single lattice grid contains enough particles, the adjacent lattice grid distance should be much larger than the mean interparticle spacing, which brings small statistical fluctuations to the real simulation process.
- ii) The adjacent lattice grid distance should be shorter than or of the same order as the Debye length so the collective plasma response at the Debye length scale can be included in the physical and mathematical model (More details are shown in Appendix A).

The following equations provide the limitations of the distance for resistive relativistic IMHD (Eq. 25) and resistive relativistic EMHD (Eq. 26).

$$c\sqrt{\frac{m_i^i}{4\pi n_i^i z^2 e^2}} = \frac{c}{\omega_{pi}^i} < \Delta x < \lambda_{iD}^i = \sqrt{\frac{K_B T_i^i}{4\pi n_i^i e^2}} \quad (25)$$

$$c\sqrt{\frac{m_e^e}{4\pi n_e^e z^2 e^2}} = \frac{c}{\omega_{pe}^e} < \Delta x < \lambda_{eD}^e = \sqrt{\frac{K_B T_e^e}{4\pi n_e^e e^2}} \quad (26)$$

3.6. Averaging procedure

The average discrete distribution function of $N_{i\xi}^{\rho e-ave}$ can be defined as the number of particles in the small 6-dimensional phase space cubic lattice grid, which can be written as,

$$f_{i\xi}^{\rho e-ave}(\mathbf{x}, \mathbf{U}, t) \leq N_{i\xi}^{\rho e-ave}(\mathbf{x}, \mathbf{U}, t) \leq \lim_{c/\omega_{pe} < \Delta x < \lambda_D} \frac{\int_{\Delta V} d^3x \int_{\Delta V_{U_i^e}} d^3U_i^e N_{i\xi}^{\rho e-micro}}{\int_{\Delta V} d^3x \int_{\Delta V_{U_i^e}} d^3U_i^e} \quad (27)$$

where the average distribution $f_{i\xi}^{\rho e-ave}$ represents the smoothness of the charged particles (including different species and types). This equation satisfies the requirements of Δx in Eqs. (25~26) and mean field theory.

According to mean field theory, the relativistic plasma motion ($\mathbf{U}$), the strength of magnetic field ($\mathbf{B}$) and the electric field ($\mathbf{E}$) are decomposed into average components ($\bar{\mathbf{U}}, \bar{\mathbf{B}}, \bar{\mathbf{E}}$) and fluctuation components ($\tilde{\mathbf{U}}, \tilde{\mathbf{B}}, \tilde{\mathbf{E}}$).

In the RHPIC-LBM model, we use both the average and fluctuation components to describe the flow characteristics at the macrodynamics scale and the particle characteristics at the small-kinetic scale. In addition, we use the interaction of the fluctuation components ($\tilde{\mathbf{U}}$ -to- $\tilde{\mathbf{B}}$) to describe the characteristics of the particles held in place by the magnetic field (Step 3.4).

A more detailed introduction about magnetic mean field theory and its application in investigating the role of turbulence in flux ropes is given in the second part of this two-paper series.

3.7. Direct and indirect collisions in the RHPIC-LBM

Substituting Eq. (27) into Eq. (24), we obtain the discrete Boltzmann equation of a charged particle, which can be written as

$$\frac{\partial f_{i\xi}^{\rho e-ave}}{\partial t} + \tilde{\mathbf{U}}_t^e \frac{\partial f_{i\xi}^{\rho e-ave}}{\partial \mathbf{x}} + \frac{q}{m_i^e} \left(\bar{\mathbf{E}} + \frac{1}{c} \tilde{\mathbf{U}}_t^e \times \bar{\mathbf{B}} \right) \cdot \frac{\partial f_{i\xi}^{\rho e-ave}}{\partial \tilde{\mathbf{U}}_t^e} = \frac{q}{m_i^e} \left(\tilde{\mathbf{E}} + \frac{1}{c} \tilde{\mathbf{U}}_t^e \times \tilde{\mathbf{B}} \right) \frac{\partial N_{i\xi}^{\rho e-micro}}{\partial \tilde{\mathbf{U}}_t^e} \quad (28)$$

Then, we combine (Eqs. (1)–(3)) and Eq. (28), and the following features can be found:

- i) The left side of Eq. (28) describes the collective effects (1st term), the evolution of the smoothness, $f_{i\xi}^{\rho e-ave}$ (2nd term), and the response to the smooth-average magnetic fields and plasma motion (3rd term).
- ii) The right side of Eq. (28) represents the small two-particle correlations between discrete charged particles (e.g., electron-ion, electron-electron, and ion-ion interaction/collision effects on $N_{i\xi}^{\rho e-micro}$).
- iii) The third term on the left side of Eq. (28) represents the average component ($\bar{\mathbf{U}}, \bar{\mathbf{B}}, \bar{\mathbf{E}}$) simulations; we defined this term as an interaction in the RHPIC-LBM.
- iv) The term on the right side of the equation represents the fluctuation and turbulence component ($\tilde{\mathbf{U}}, \tilde{\mathbf{B}}, \tilde{\mathbf{E}}$) simulations. We defined this term as a collision in the RHPIC-LBM.

Thus, the RHPIC-LBM covers the fully coupled kinetic-dynamic-hydro temporal-spatial scale for resistive relativistic MHD problems.

3.8. Finite-difference time-domain (FDTD) scheme & yee grid for boundary simulation domain

In Eq. (28), the distribution function changes with time in the electric field ($\frac{\partial f_i^{pe-ave}}{\partial t}$) and is dependent on the change in the magnetic field across space ($\frac{\partial f_i^{pe-ave}}{\partial x}$).

This relationship is the basic FDTD time-step relation. At any point in temporal-spatial space, the updated value of the electric field depends on the stored values of $\vec{U}_i^e \times \vec{B}$ and $\vec{U}_i^e \times \vec{B}$ [88–90].

When we use the discrete cubic lattice grid to solve Eq. (28), multiple dimensions must be considered, which makes the FDTD scheme very complicated.

In the RHPIC-LBM, we establish a lattice grid on the boundary domain (both the geometric and physical domains) by the following steps [63,77,85–88]:

- Set an electric field vector ($\vec{E}_n(.E_n|_x, .E_n|_y, .E_n|_z)$) in the middle of two magnetic fields ($\vec{B}_{n-1}(B_{n-1}|_x, B_{n-1}|_y, B_{n-1}|_z)$, $\vec{B}_{n+1}(B_{n+1}|_x, B_{n+1}|_y, B_{n+1}|_z)$) in the same lattice grid.
- Set all discrete field ($\vec{E}, \vec{B}, \vec{J}$) components on the top-bottom, front-rear, left-right planes of the lattice grid.
- Set all other parameters/variables related to the mass and motion in the center of the lattice grid.
- Set field vectors and mass-motion related vector components on the Lagrange coordinate system and Eulerian coordinate system, respectively.
- The FDTD & Yee grid are applied on the boundary domain, and the initial BC/IC of the fields are directly added to each cubic lattice grid plane.

3.9. Iteration of the RHPIC-LBM lattice grid in the $\delta t, \delta x, \delta p$ coordinate system [77,91–93]

Considering the number of particles involved in the numerical simulation, both the geometric domain discretization and physical domain discretization processes in the algorithms provide high degrees of available parallelism.

In the RHPIC-LBM code, the geometric lattice grid is independent of the physical lattice grid (total overlap, partial overlap, and no overlap).

The numerical implementation for the geometric domain is different from that for the physical domain.

In the $\delta t, \delta x, \delta p$ coordinate system, each center position (x) of lattice grid can be easily determined by time step δt , while the lattice grid moment (p) can be derived from the space step δx .

3.10. Algorithm, workflow and implementation of the RHPIC-LBM model

First, we frame some basic definitions of the lines, arrows, special symbols and texts used in the flowcharts and pseudocodes (Figs. 2–14).

The thickness of the black and blue solid lines indicates the main process and self-test process, respectively; the thickness of the red and blue dotted lines indicates the subordinate algorithm-block and inspection process, respectively; the black, blue, yellow-highlighted and pink-highlighted fonts indicate the normal program node, inspection program node, first order core program node, and second order core program node, respectively; the special shapes indicate different types of actions or steps in a process; and the lines and arrows indicate the sequence of the steps and the relationships among them.

A strong motivator for us to develop the RHPIC-LBM model has been that compared to the original 2D/2.5D/3D physical-mathematical-numerical models developed to solve magnetic reconnection problems in realistically turbulent plasma, LT-STMR has more obvious difficulties in physical, mathematical, numerical and computational modelling determined by its physical picture properties. More specifically, these difficulties manifest as follows:

i) Physical model

In the continuous kinetic-dynamic-hydro fully coupled LTSTMR simulation domain, the scales of x, y and z are in the order of $10^{10} \sim 10^{11}$, $10^8 \sim 10^9$ and $10^7 \sim 10^8$, respectively; in other words, the geometric simulation domain is a box in which the x -coordinate spans from 0.2 m to 1000,000 km, the y -coordinate spans from 0.2 m to 500,000 km, and the z -coordinate spans from 0.2 m to 100,000 km, respectively.

The evolution time-scale is of the order of $10^{10} \sim 10^{11}$, ranging from 10^{-5} s to 10^5 s; the temperature, density, ionization, magnetic strength, electron energy, and proton energy scales range from 3,000 K to 1000,000 K, $10^{27} m^{-3}$ to $10^{15} m^{-3}$, 10^{-6} to 1, 0 G to 1,000 G, KeV to MeV, and KeV to GeV (> 100 MeV, γ -ray emission), respectively.

The number of generalized hyper-singular terms in the distribution functions are larger and more complicated than the original 2D/2.5D/3D magnetic reconnection models in realistically turbulent plasma, and all the distribution functions must meet the self-consistent conditions in the evolution of the entire domain.

ii) Mathematical model

The explicit distribution functions must be derived from the RHPIC-LBM model in order to simultaneously ensure that the numerical sensitivity (reflection of a sensitive physical system with initial fluctuation components ($\vec{U}, \vec{B}, \vec{E}$))

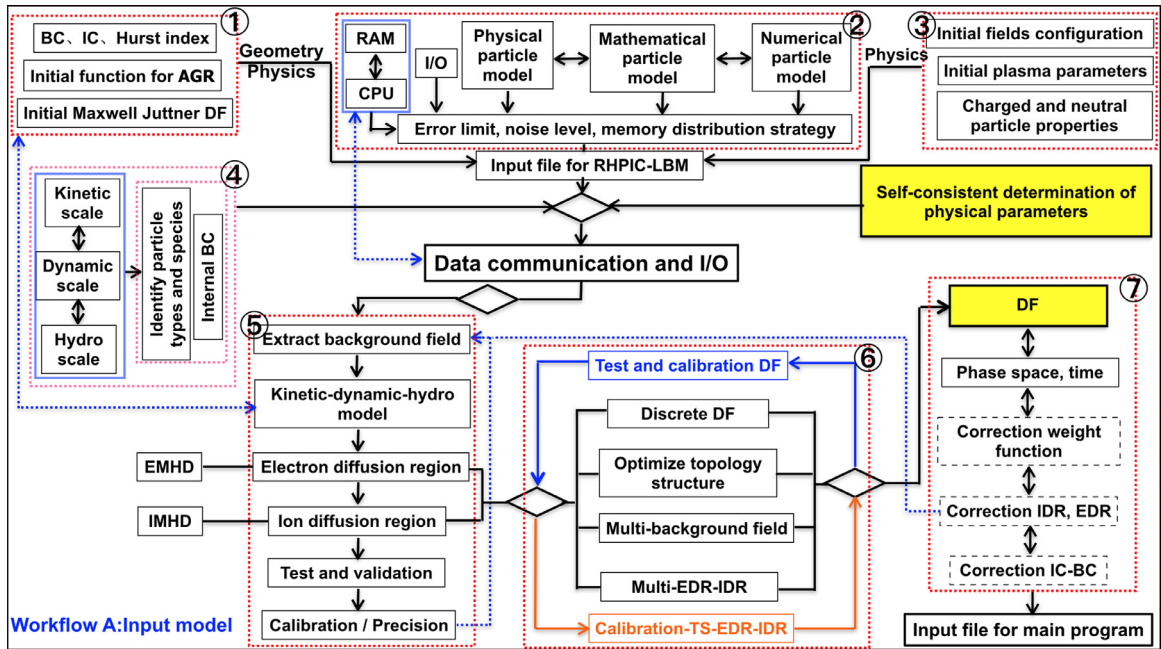


Fig. 2. Schematic of the flowchart and implementation for the input model.

Algorithm ① Geometry & physics input for RHPIC-LBM

Require:

DXQY: $D^B 3Q7 D^E 3Q13 D^F 3Q19 D^G 3Q19 D^H 3Q27$

DF: $f_{i\xi}^{B\text{eq}} f_{i\xi}^{E\text{eq}} f_{i\xi}^{F\text{Meq}} f_{i\xi}^{F\text{eeq}} f_{i\xi}^{G\text{jeq}} f_{i\xi}^{H\text{neq}}$

SCD: self-consistent determination. $\nabla \cdot B = 0$

H: Hurst index.

L: spatial scale.

N(H): particle number.

TI: temporal scale.

SD: simulation domain.

BL: simulation boundary.

SP: super particle.

FT1: fetch data from RAM or VRAM.

FT2: fetch data from Disk.

ST1: save data to RAM or VRAM.

ST2: save data to Disk.

1: FT2

2: for DXQY $\in$ SD do

3: FT1

4: DF $\rightarrow$ DXQY $\parallel$ IC

5: $\nabla \cdot B = 0$

6: for SP $\in$ L do

7: if $SP(L) < L_{kinetic}$ then

8: $SP(L) \rightarrow N(H)_{kinetic} \parallel$ IC for AGR

9: if $L_{kinetic} < SP(L) < L_{dynamic}$ then

10: $SP(L) \rightarrow N(H)_{dynamic} \parallel$ IC for AGR

11: if $L_{dynamic} < SP(L)$ then

12: $SP(L) \rightarrow N(H)_{hydro} \parallel$ IC for AGR

13: ST1

14: for DXQY $\in$ BL do

15: FT1

16: DF $\rightarrow$ DXQY $\parallel$ BC for BG

17: for SP $\in$ Inflow BL do

18: $\tilde{B}(TI) \rightarrow BL \parallel$ BC

19: $\nabla \cdot \tilde{B}(TI) = 0$

20: Plasma parameters $\rightarrow BL \parallel$ BC

21: for SP $\in$ SD do

22: $\tilde{B}(TI) \rightarrow SD \parallel$ IC for BG

23: $\nabla \cdot \tilde{B}(TI) = 0$

24: Plasma parameters $\rightarrow BL \parallel$ IC

25: ST1

26: ST2

Fig. 3. Pseudocode for the geometry & physics input algorithm.

Algorithm ② Error limit, noise level, memory distribution strategy for RHPIC-LBM

Require:
RHO: density.
CP: cores per CPU.
RAM: random access memory per node.
Nd: number of node.
Lm: memory load per node (RAM or VRAM).
Lc: CPU load per node.
EI: error limit of system.
P: P-order expansion of distribution function.
NL: noise level of system.
N(HP): particle number in physical particle system.
N(HM): particle number in mathematical particle system.
N(HS): particle number in numerical particle system.
I/O: data storage on hard disk.
PC: partition capacity of computing system.
II/O: I/O load per node.

1: Cat CPU, RAM on each computing node
2: FT2
3: FT1
4: Read L, TI, Nd
5: for $DXQY \in SD$ do
6: $RHO, SD, RAM_each\ node \rightarrow Nd$
7: if $Lm > 75\% \ \& \ Lc > 85\% \ \& \ Nd > 10,000$ then
8: $EI \rightarrow Low\ level \parallel INF, NAN$
9: $NL \rightarrow P \parallel INF, NAN$
10: if $Lm > 75\% \ \& \ Lc > 85\% \ \& \ 10,000 < Nd < 10,000$ then
11: $EI \rightarrow Middle\ level \parallel INF, NAN$
12: $NL \rightarrow P \parallel INF, NAN$
13: if $Lm > 75\% \ \& \ Lc > 85\% \ \& \ Nd < 10,000$ then
14: $EI \rightarrow High\ level \parallel INF, NAN$

15: $NL \rightarrow P \parallel INF, NAN$
16: ST1
17: Read $N, N(HP), N(HM), N(HS), RHO$
18: for $DXQY \in SD$ do
19: $RHO \rightarrow N(HP) \parallel IC\ for\ AGR$
21: if $NL > EI$ then
22: go to 6
23: if $NL < EI$ then
24: $\rho_{i,t} + \nabla \cdot (\rho U) = 0$
25: $N(HP) \rightarrow N(HM)$
26: if $NL > EI$ then
27: go to 6
28: if $NL < EI$ then
29: $N(HM) \rightarrow N(HS)$
30: if $NL > EI$ then
31: go to 6
32: if $NL < EI$ then
33: ST1
34: Read $L, TI, Nd, RHO, other\ plasma\ parameters$
35: for $Time \in TI$ do
36: for $space \in SD$ do
37: for $variable \in SD, DXQY$ do
38: if $data > PC$ then
39: go to 6
40: if $data < PC \ \& \ II/O > 85\%$ then
41: go to 6
42: if $data < PC \ \& \ II/O < 85\%$ then
43: ST1
44: ST2

Fig. 4. Pseudocode for the error limit, noise level and memory distribution strategy algorithm.

Algorithm ③ Normalization and self-consistent determination for RHPIC-LBM

Require:
Le: electron characteristic length.
Li: ion characteristic length.
Ln: Debye length.
Tle: electron characteristic time.
Tli: ion characteristic time.
Tln: neutral particle characteristic time.
L_MAW: ion MHD (IMHD) scale characteristic length.
L_KAW: electron MHD (EMHD) scale characteristic length.
TI_MAW: IMHD scale characteristic time.
TI_KAW: EMHD scale characteristic time.
Beta: ratio of plasma pressure to magnetic pressure.
Delta_L: DXQY characteristic length.
Delta_T: DXQY characteristic time.

1: FT2
2: Read all plasma parameters
3: Read $Le, Li, Ln, Tle, Tli, Tln, L_MAW, L_KAW, TI_MAW$
4: $TI_KAW, Beta, Delta_L, Delta_T$
5: for $DXQY \in SD$ do
6: FT1
7: Normalization all parameters and variables
8: if $SD \in EMHD\ temporal-spatial\ scale \ \& \ Beta < 0.1$ then
9: $Le \rightarrow electron\ cyclotron\ radius \parallel self-consistent$
10: $Le \rightarrow L_KAW \parallel self-consistent$
11: $Tle \rightarrow TI_KAW \parallel self-consistent$
12: if $SD \in EMHD\ temporal-spatial\ scale \ \& \ Beta > 0.1$ then
13: $Le \rightarrow electron\ inertia\ length \parallel self-consistent$
14: $Le \rightarrow L_KAW \parallel self-consistent$
15: $Tle \rightarrow TI_KAW \parallel self-consistent$

16: if $SD \in IMHD\ temporal-spatial\ scale \ \& \ Beta < 0.1$ then
17: $Li \rightarrow ion\ cyclotron\ radius \parallel self-consistent$
18: $Li \rightarrow L_MAW \parallel self-consistent$
19: $Tli \rightarrow TI_MAW \parallel self-consistent$
20: if $SD \in IMHD\ temporal-spatial\ scale \ \& \ Beta > 0.1$ then
21: $Li \rightarrow ion\ inertia\ length \parallel self-consistent$
22: $Li \rightarrow L_MAW \parallel self-consistent$
23: $Tli \rightarrow TI_MAW \parallel self-consistent$
24: ST1
25: for $DXQY \in SD$ do
26: FT1
27: for $SP \in L$ do
28: if $SP(L) < L_kinetic$ then
29: $Delta_L \rightarrow Le \parallel self-consistent\ AGR$
30: $Delta_T \rightarrow Tle \parallel self-consistent\ AGR$
31: if $L_kinetic < SP(L) < L_dynamic$ then
32: $Delta_L \rightarrow Li \parallel self-consistent\ AGR$
33: $Delta_T \rightarrow Tli \parallel self-consistent\ AGR$
34: if $L_dynamic < SP(L)$ then
35: $Delta_L \rightarrow Ln \parallel self-consistent\ AGR$
36: $Delta_T \rightarrow Tln \parallel self-consistent\ AGR$
37: ST1
38: ST2

Fig. 5. The pseudocode for the normalization and self-consistent determination algorithm.

Algorithm ④ Identify particle types & species and initial BC at the boundary of initial CS for RHPIC-LBM

```

Require:
Varsigman: different type of particles.
Zeta: different species components.
Xi: different discretized spatial directions.

1: FT2
2: Read all DXQY parameters
3: Read Varsigman, Zeta,  $X_i$ ,  $p_i$ ,  $X_i$ ,
4: for DXQY  $\in$  SD do
5: FT1
6:   Normalization all parameters and variables
7:   if Varsigman  $\rightarrow$  Hydrogen, helium and other metal components & Particle  $\in$ 
8:     Neutral fluid then
9:       DXQY  $\rightarrow$  D3Q27  $\parallel$  identify particle types & species
10:       $X_i \rightarrow$  Q28
11:     if Varsigman  $\rightarrow$  Hydrogen, helium and other metal components & Particle  $\in$ 
12:       Electron fluid then
13:         DXQY  $\rightarrow$  D3Q19  $\parallel$  identify particle types & species
14:          $X_i \rightarrow$  Q19
15:       if Varsigman  $\rightarrow$  Hydrogen, helium and other metal components & Particle  $\in$ 
16:         Ion fluid then
17:           DXQY  $\rightarrow$  D3Q19  $\parallel$  identify particle types & species
18:            $X_i \rightarrow$  Q19
19:            $\nu_{ei} > \nu_{en}$   $\parallel$  fully ionized plasma
20:            $\nu_{ei} \approx \nu_{en}$   $\parallel$  identify partially ionized plasma
21:            $\nu_{ei} < \nu_{en}$   $\parallel$  weakly ionized plasma
22:         ST1
23:         ST2  $\parallel$  identify real fluid
24:         =====
25:         FT2
26:       for DXQY  $\in$  SD do
27:         FT1
28:         if Pseudo fluid  $\rightarrow$  Electric filed & DXQY  $\in$  CS then
29:           DXQY  $\rightarrow$  D3Q13  $\parallel$  identify pseudo particles
30:            $X_i \rightarrow$  Q13
31:         if Pseudo fluid  $\rightarrow$  Magnetic filed & DXQY  $\in$  CS then
32:           DXQY  $\rightarrow$  D3Q7  $\parallel$  identify pseudo particles
33:            $X_i \rightarrow$  Q7
34:         if Pseudo fluid  $\rightarrow$  Electromagnetic filed & DXQY  $\in$ 
35:           BG then
36:             DXQY  $\rightarrow$  D3Q13  $\parallel$  identify pseudo particles
37:              $X_i \rightarrow$  Q13
38:           ST1
39:           ST2  $\parallel$  identify pseudo real fluid
40:           =====
41:           FT2
42:           for DXQY  $\in$  SD do
43:             FT1
44:             if SD  $\rightarrow$  Boundary on the BG then
45:               DF_BG  $\rightarrow$  DF_PIC  $\parallel$  identify initial BC near the
46:                 side of the BG
47:               DF_BG  $\rightarrow$  DF_LBM  $\parallel$  identify initial BC near the
48:                 side of the CS
49:             ST1
50:             ST2  $\parallel$  identify BC on BG and CS boundaries

```

Fig. 6. Pseudocode for the algorithm to identify particle types, species, and initial BC at the boundary of the initial CS.

is large enough in the whole simulation box, the high-order generalized hyper-singular terms are small enough, and the self-consistent conditions are tautologous in the continuous kinetic-dynamic-hydro fully coupled temporal-spatial evolution process.

To describe the particles' behavior inside the RHPIC-LBM model for each individual type of component ($\iota = 1, 2, 3 \dots$), a set of configuration variables and parameters need to be defined in the whole simulation domain (ideal MHD region, hydro scale), the ion diffusion region (non-ideal ion MHD (IMHD); dynamic scale), and the electron diffusion region (non-ideal electron MHD (EMHD); kinetic scale), respectively.

In RHIC-LBM, the ideal and non-ideal MHD (IMHD and EMHD) simulation domain are defined as the background (BG) and current sheet (CS) respectively; both simulation domains obey the same error limit, noise level and memory distribution strategy.

iii) Numerical model

Measurement, evaluation and control of the error limit, noise level and memory distribution strategy in the algorithm, especially in the self-consistent inspection during the streaming and collision (direct and indirect) processes between the particle and its neighboring particles throughout the particle system, are the most important indicators in the development and validation of the HPIC-LBM model.

To fully reflect both non-linear and continuous kinetic-dynamic-hydro fully coupled evolution in the physical picture, the sensitive physical system requires that enough hyper-singular terms exist in the distribution function. However, the hyper-singular terms greatly affect the stability of the numerical simulation system, which is one of the major causes of numerical instability in the algorithm.

As part of the basic principles of the algorithm design in RHPIC-LBM, we make the numerical sensitivity of the system higher than the physical sensitivity in the evolution of the entire domain.

iv) Computational platform

The 3D LTSTMR simulations, including their multiple different particles and components ($\zeta = 1, 2, 3 \dots$; $\iota = 1, 2, 3 \dots$), have high requirements for the memory (random access memory (RAM) and video random access memory (VRAM)), processing (central processing unit (CPU), graphics processing unit (GPU), node architecture and performance), data communication (within the CPU, RAM, and both within the GPU RAM and across the GPU and VRAM), and serial/parallel I/O controllers.

The performance of RHPIC-LBM will directly determine the system load (CPU load per node, GPU load per node, and memory load per node).

The program skeletons of the numerical implementation are composed of five parts, including the input model (Figs. 2–8, discrete distribution function (DF) (Figs. 9 and 10, evolution, input/output (I/O) (Figs. 11 and 12, and data analysis (Figs. 13, 14).

Algorithm ⑤ Calibration on continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale for RHPIC-LBM	
Require: Delta_Xi_AGR: space step of DXQY. Delta_Ti_AGR: time step of DXQY. Delta_P_AGR: moment step of DXQY. 1: FT2 2: for DXQY ∈ SD do 3: FT1 4: if SD ∈ BG & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM. 5: Total-overlap.t(Delta_Xi,Delta_Ti,Delta_P) E & then 6: NO BOUNCE-BACK (D3Q13 EM,D3Q7 M) 7: if SD ∈ CS & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM. 8: Total-overlap.t(Delta_Xi,Delta_Ti,Delta_P) E & then 9: BOUNCE-BACK(D3Q13 EM,D3Q13 E) on all 13 direction 10: if SD ∈ BG & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM. 11: Partial-overlap.t(Delta_Xi,Delta_Ti,Delta_P) E & then 12: NO BOUNCE-BACK (D3Q13 EM,D3Q7 M) 13: if SD ∈ CS & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM. 14: Partial-overlap.t(Delta_Xi,Delta_Ti,Delta_P) E & then 15: BOUNCE-BACK(D3Q13 EM,D3Q13 E) on overlap direction 16: if TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM. 17: No-overlap.t(Delta_Xi,Delta_Ti,Delta_P) E & then 18: BOUNCE-BACK(D3Q13 EM,D3Q13 E) on all 13 direction 19: ST1 20: ST2 Normal collision step calibration for (EM, E) ===== 21: FT2 22: for DXQY ∈ SD do 23: FT1 24: if SD ∈ BG & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM.	25: Partial-overlap.t(Delta_Xi,Delta_Ti,Delta_P) M & then 26: NO BOUNCE-BACK (D3Q13 EM,D3Q7 M) 27: if SD ∈ CS & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM. 28: Partial-overlap.t(Delta_Xi,Delta_Ti,Delta_P) M & then 29: BOUNCE-BACK(D3Q13 EM,D3Q7 M) on overlap direction 30: if TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) EM. 31: No-overlap.t(Delta_Xi,Delta_Ti,Delta_P) E & then 32: BOUNCE-BACK(D3Q13 EM,D3Q7 E) on all direction 33: ST1 34: ST2 Normal collision step calibration for (EM, M) ===== 35: FT2 36: for DXQY ∈ SD do 37: FT1 38: if SD ∈ BG & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) E. 39: Partial-overlap.t(Delta_Xi,Delta_Ti,Delta_P) M & then 40: NO BOUNCE-BACK (D3Q13 E,D3Q7 M) 41: if SD ∈ CS & TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) E. 42: Partial-overlap.t(Delta_Xi,Delta_Ti,Delta_P) M & then 43: BOUNCE-BACK(D3Q13 E,D3Q7 M) on overlap direction 44: if TIME=0 & (Delta_Xi,Delta_Ti,Delta_P) E. 45: No-overlap.t(Delta_Xi,Delta_Ti,Delta_P) M & then 46: BOUNCE-BACK(D3Q13 E,D3Q7 M) on all direction 47: ST1 48: ST2 Normal collision step calibration for (E, M)

Fig. 7. Pseudocode for the algorithm to calibrate the continuous kinetic-dynamic-hydro fully coupled large temporal-spatial scale.

The preprocess, postprocess, and visualization are based on a GPU-CPU heterogeneous computing system, which has a significantly different architecture and program skeleton from a CPU isomorphic computing system.

3.10.1. Input model

In the input flow chart section of the RHPIC-LBM model, the workflow contains several algorithms; all the algorithm pseudocodes are shown in Figs. 3–8.

i) Geometry & physics input

In the pseudocode, the lattice models $D_i XQY$ (X and Y denotes the dimensionality and the number of discrete physical variables; $D^B 3Q7$, $D^E 3Q13$, $D^{EM} 3Q13$, $D^e 3Q19$, $D^i 3Q19$, $D^n 3Q27$), the distribution functions ($f_{i\xi}^{B eq}$, $f_{i\xi}^{E eq}$, $f_{i\xi}^{EM eq}$, $f_{i\xi}^{e eq}$, $f_{i\xi}^{ieq}$, $f_{i\xi}^{neq}$), and the super particles (SP, $\zeta = 1, 2, 3, \dots$, $\iota = 1, 2, 3, \dots$) in the continuous kinetic-dynamic-hydro fully coupled simulation domain are defined in the RHPIC-LBM model (Fig. 3).

ii) Error limit, noise level and memory distribution strategy

To maintain the load stability (CPU and RAM loads) in the entire particle system, we define different modes of the error limits and noise level on the different temporal-spatial scales.

In the RHPIC-LBM model development and validation process, we use 4000 identical computing nodes as the computational platform; each computing node is equipped with 64MB of RAM and 24 Intel(R) Xeon(R) CPU E5-4640 0 @ 2.40GHz CPU processors, with a cache size of 20480KB per CPU.

In this specific setup, a framework for predicting the computational resource consumption (CRC) of CPU ($.CRC|_{CPU}$) and memory ($.CRC|_{RAM}$) is designed in the algorithm. When the two predicted values ($.CRC|_{CPU}$, $.CRC|_{RAM}$) are inconsistent, the maximal value ($\max\{.CRC|_{CPU}, .CRC|_{RAM}\}$) is used as a parameter in the input file. Another method to reduce the CPU and RAM loads is to control the number of super particles in each DXQY model in the evolution of the entire domain (Fig. 4).

iii) Normalization and self-consistent determination

Normalization is an important step in the implementation of the algorithm, especially for the study of self-consistent determination in the relaxation of interaction between particles.

In the input setup section, all the input variables and parameters are transformed into dimensionless values based on the normalization method shown in the Appendix A.

The self-consistent determination for the initial fields and the plasma parameters in the ideal and non-ideal MHD (IMHD and EMHD) simulation domain is performed by applying the Gauss's law of magnetism and the continuity equation (Fig. 5).

iv) Identify particle types, species and initial BC at the boundary of the initial CS

Algorithm ⑥ Testing and calibration distribution functions for RHPIC-LBM

```

1: FT2
2: for DXQY ∈ SD do
3: FT1
4: if SD ∈ BG & TIME=0 then
5: NO BOUNCE-BACK (D3Q19|e,D3Q19|i)
6: || Collision calibration for electron and ion on BG
7: NO BOUNCE-BACK (D3Q19|e,D3Q27|n)
8: NO BOUNCE-BACK (D3Q19|i,D3Q27|n)
9: || Collision calibration for charged and neutral particle on BG
10: NO BOUNCE-BACK (D3Q7|M,D3Q13|E, D3Q13|EM,
11: D3Q19|e, D3Q19|i, D3Q27|n)
12: || Collision calibration for real and pseudo particles on BG
13: if SD ∈ BG & TIME=0 then
14: BOUNCE-BACK (D3Q19|e,D3Q19|i)
15: || Collision calibration for electron and ion on CS
16: BOUNCE-BACK (D3Q19|e,D3Q27|n)
17: BOUNCE-BACK (D3Q19|i,D3Q27|n)
18: || Collision calibration for charged and neutral particle on CS
19: BOUNCE-BACK (D3Q7|M,D3Q13|E, D3Q13|EM,
20: D3Q19|e, D3Q19|i, D3Q27|n)
21: BOUNCE-BACK (D3Q7|M,D3Q13|E, D3Q13|EM,
22: D3Q19|e, D3Q19|i)
23: || Collision calibration for charged and pseudo particles on CS
24: NO BOUNCE-BACK (D3Q7|M,D3Q13|E, D3Q13|EM, D3Q27|n)
25: || Collision calibration for neutral and pseudo particles on CS
26:  $\nabla \cdot \mathbf{B} = 0$ 
27:  $\rho_{,t} + \nabla \cdot (\rho \mathbf{U}) = 0$ 
28: ST1
29: ST2 || Collision calibration on BG and CS

```

Algorithm ⑦ Re-calibration distribution function for RHPIC-LBM

```

1: FT2
2: for DXQY ∈ SD do
3: for DF ∈ SD do
4: FT1
5: Algorithm ③ ④ ⑤ ⑥
6:  $\nabla \cdot \mathbf{B} = 0$ 
7:  $\rho_{,t} + \nabla \cdot (\rho \mathbf{U}) = 0$ 
8: Algorithm ① ④ ⑤ ⑥
9:  $\nabla \cdot \mathbf{B} = 0$ 
10:  $\nabla \cdot \mathbf{B} (TI) = 0$ 
11: ST1
12: ST2

```

Fig. 8. Pseudocode for the algorithm to test and calibrate the distribution function (left algorithm), re-calibrate the distribution function (right algorithm).

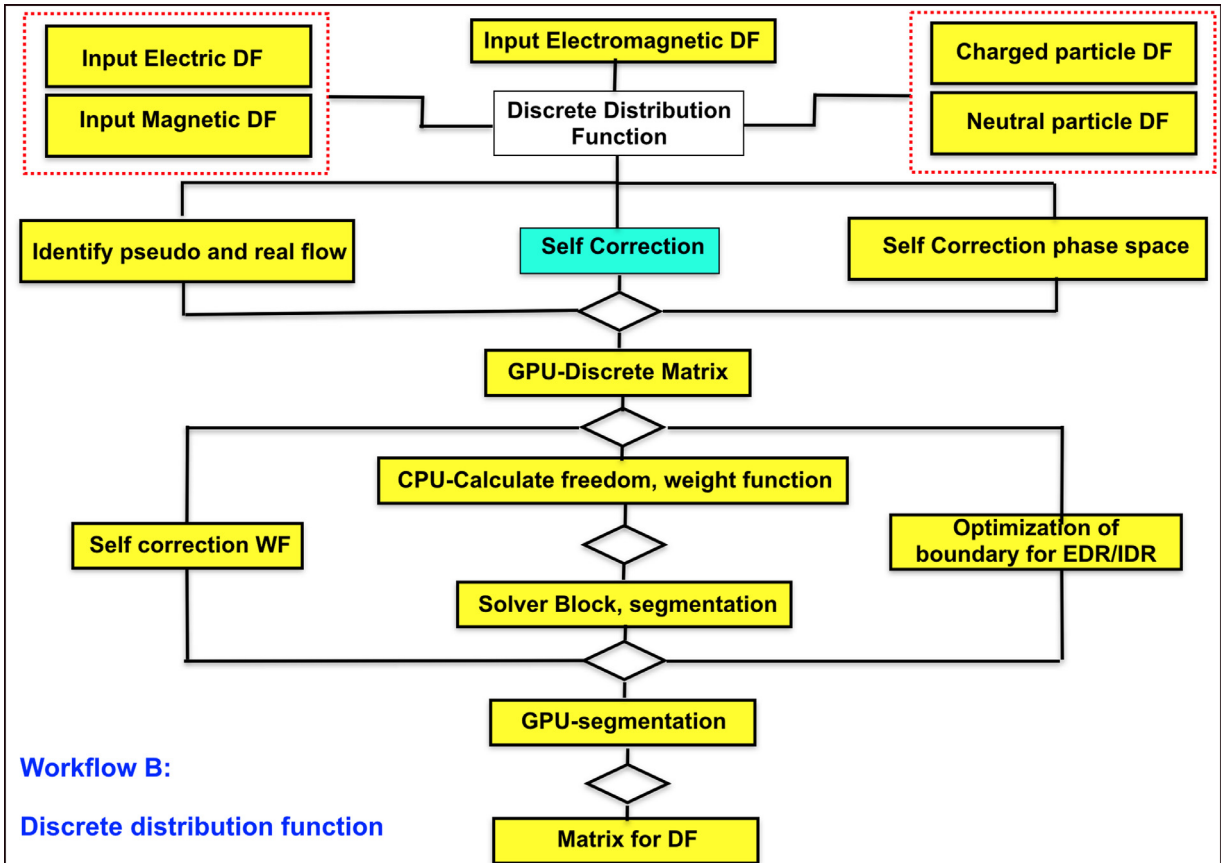


Fig. 9. Schematic of the flowchart and implementation of the discrete distribution function.

Algorithm: Discrete distribution functionS for RHPIC-LBM

GCP: cores per GPU.
DPRAM: random access memory per node.
GND: number of GPU node.
LGm: load of VRAM per node.
LGc: load of GPU per node.

```

24:  // Self Correction
25:  ST1
26:  ST2
=====
27:  Cat GPU, DPRAM at each computing node
28:  FT2
29:  for DXQY ∈ CS do
30:  FT1
31:  for Xi ∈ N_Xi do
32:  for Zeta ∈ N_Zeta do
33:    Input A_E, A_B, A_EM // Matrices for B,E,EM
34:    Input B_e|Zeta, B_i|Zeta // Matrices for Electron,Ion
35:    Input C|Zeta // Matrices for Neutral
36:    Input M_DF // General Outline Matrix
37:    if CS ∈ EMHD temporal-spatial scale then
38:      Define Matrix size (M_DF) > Max ( A_E, A_B,
39:        A_EM, B_e|Zeta, B_i|Zeta, M_DF)
40:      if CS ∈ IMHD temporal-spatial scale then
41:        Define Matrix size (M_DF) > Max ( A_E, A_B,
42:          A_EM, B_e|Zeta, M_DF)
43:      if LGm > 80% & LGc > 90% then
44:        EI → Low level // INF, NAN
45:        NL → P // INF, NAN
46:      if Lm > 70% & Lc > 80% then
47:        EI → Middle level // INF, NAN
48:        NL → P // INF, NAN
49:      if Lm > 60% & Lc > 70% then
50:        EI → High level // INF, NAN
51:  Save M_DF
52:  ST1
53:  ST2
=====
1:  FT2
2:  for DXQY ∈ SD do
3:  FT1
4:  for Xi ∈ N_Xi do
5:    for Zeta ∈ N_Zeta do
6:      Read fieBecq // B field
7:      Read fieBecq // E field
8:      Read fiemeq // EM field
9:      // Pseudo particle system
10:     Read fieBecq // Electron particle
11:     Read fieBecq // Ion particle
12:     // Charged particle system
13:     Read fiemeq // Neutral particle
14:     // Neutral particle system
15:     Read all plasma parameters
16:     { ∂tE(t,r) - ∇ × B(t,r) = - $\frac{j_i}{\epsilon_0}$  + J
17:       ∂tB(t,r) + ∇ × E(t,r) = 0
18:       ∇ · E(t,r) = ρi + D
19:     }
20:     { ∂tE(t,r) - ∇ × B(t,r) = - $\frac{j_e}{\epsilon_0}$  + J
21:       ∂tB(t,r) + ∇ × E(t,r) = 0
22:       ∇ · E(t,r) = -ρe + D
23:     }
  
```

Fig. 10. Pseudocode for the discrete distribution function algorithm.

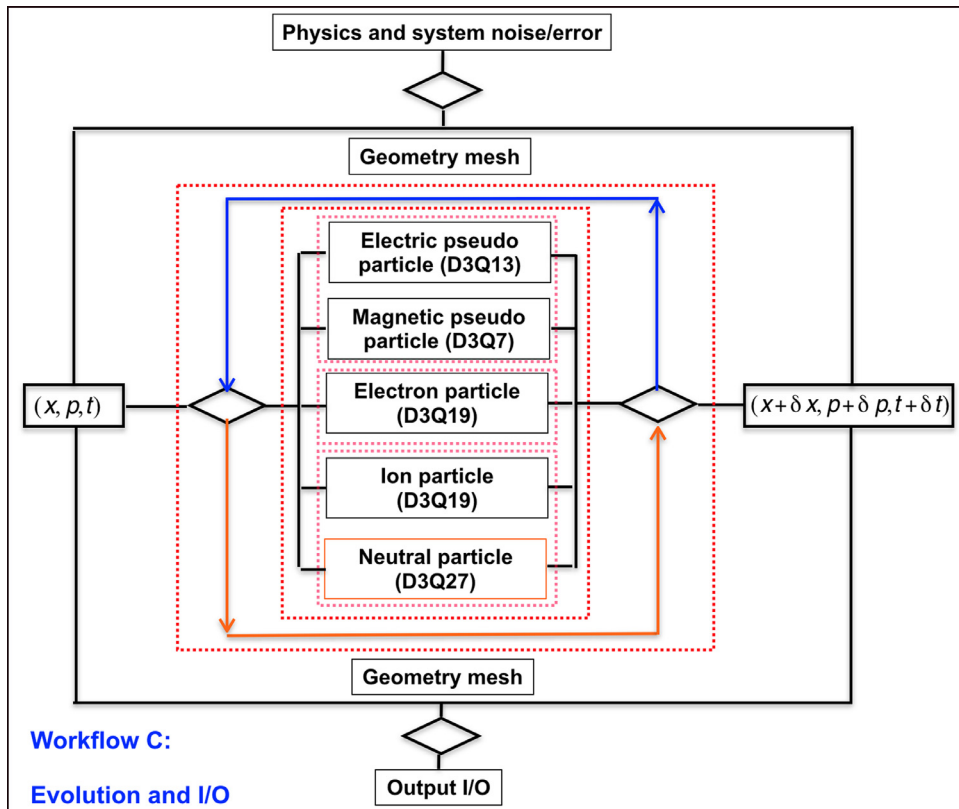


Fig. 11. Schematic of the flowchart and implementation of the evolution and I/O.

Algorithm: Evolution and I/O for RHPIC-LBM**Require:**

El_ps: error limit of pseudo particle system.
 El_cp: error limit of charged particle system.
 El_n: error limit of neutral particle system.
 El_f: error limit of E,B,EM fields.
 NI_ps: noise level of pseudo particle system.
 NI_cp: noise level of charged particle system.
 NI_n: noise level of neutral particle system.
 NI_f: noise level of E,B,EM fields.
 TI_mrt: multi relaxation time.

```

1: FT2
2: Define El_ps, El_cp, El_n, El_f, NI_ps, NI_cp, NI_n, NI_f
3: for DXQY ∈ SD do
4: FT1
5:   for Xi ∈ N_Xi do
6:     for Zeta ∈ N_Zeta do
7:       Read A_E, A_B, A_EM, B_e|Zeta, B_i|Zeta, C|Zeta, M_DF
8:       if CS ∈ EMHD temporal-spatial scale & Tle < TI_mrt then
9:         Bounce Back (D3Q13|EM, D3Q13|E, D3Q7|M, D3Q19|e)
10:        Bounce Back (D3Q13|EM, D3Q13|E, D3Q7|M, D3Q19|i)
11:        Bounce Back (D3Q19|e, D3Q19|i)
12:        Stream (D3Q13|EM, D3Q13|E, D3Q7|M, D3Q19|e, D3Q19|i)
13:        if El(El_ps, El_cp, El_n, El_f) > El or NI(NI_ps, NI_cp,
14:          NI_n, NI_f) > NL
15:          Stop
16:          Go to Algorithm ②
17:        if CS ∈ IMHD temporal-spatial scale & Tle < TI_mrt then
18:          Bounce Back (D3Q13|EM, D3Q13|E, D3Q7|M, D3Q19|i)
19:          Bounce Back (D3Q27|n, D3Q19|i)
20:          Stream (D3Q13|EM, D3Q13|E, D3Q7|M, D3Q19|i)
21:          if El(El_ps, El_cp, El_n, El_f) > El or NI(NI_ps,
22:            NI_cp, NI_n, NI_f) > NL
23:            Stop
24:            Go to Algorithm ②
25:          Write A_E, A_B, A_EM, B_e|Zeta, B_i|Zeta, C|Zeta, M_DF
26:          Write all parameters
27:          Save M_DF
28: ST1
29: ST2
  
```

Fig. 12. Pseudocode for the evolution and I/O algorithm.

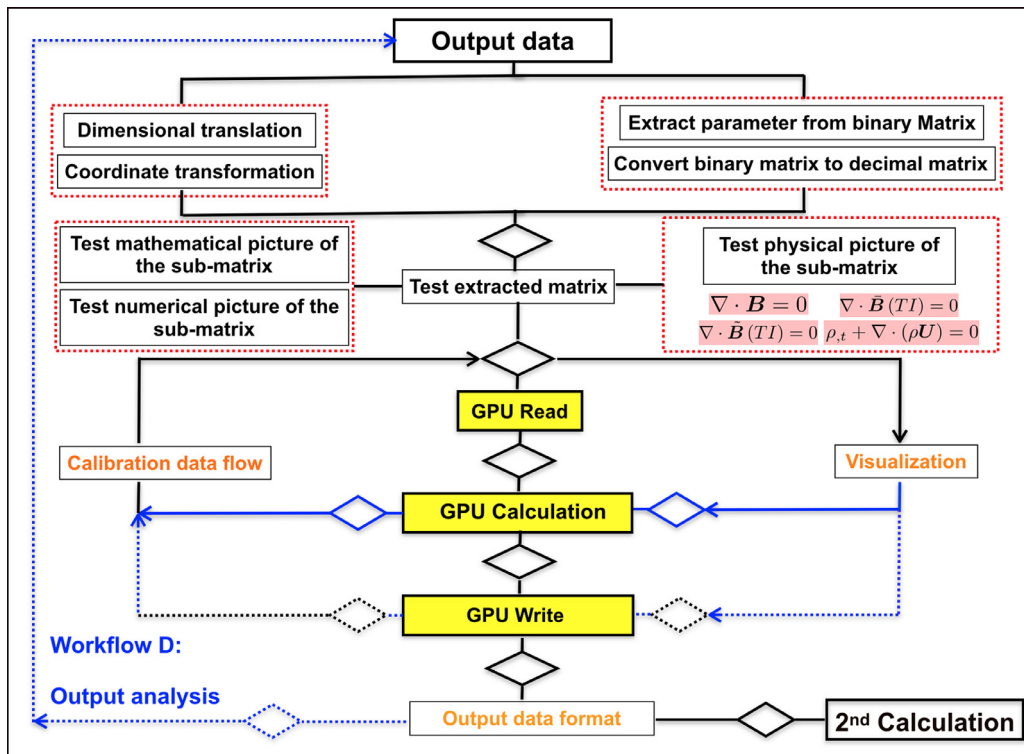


Fig. 13. Schematic of the flowchart and implementation of the output analysis.

Algorithm: Output analysis for RHPIC-LBM

```

Require:
M_M: output data of B field.
M_E: output data of E field.
M_J: output data of J.
M_Ue: output data of Ue.
M_Ui: output data of Ui.
M_Un: output data of Un.
M_Rho: output data of density.
M_T: output data of Temperature.
M_U: output data of U.
Phi_Ue: stream function of Ue.
Phi_Ui: stream function of Ui.
Phi_Un: stream function of Un.
Phi_U: stream function of U.
A: magnetic potential vector.

1: FT2
2: Read A_E, A_B, A_EM, B_e|Zeta, B_i|Zeta, C|Zeta, M_DF
3: Read All plasma parameters
4: Define M_M, M_E, M_J, M_Ue, M_Ui, M_Un, M_Rho, M_T, M_U
5: ST1
6: for L ∈ Spatial scale do
7:   for Time ∈ Temporal Scale do
8:     for Moment ∈ Temporal-spatial Scale do
9:       for Xi ∈ N_Xi do
10:        for Zeta ∈ N_Zeta do
11:          Extract (M_M, M_E, M_J, M_Ue, M_Ui, M_Un,
12:                M_Rho, M_T, M_U) from binary Matrix(A_E, A_B,
13:                A_EM, B_e|Zeta, B_i|Zeta, C|Zeta, M_DF)
14:          Binary Matrix to decimal Matrix(M_M, M_E, M_J,
15:            M_Ue, M_Ui, M_Un, M_Rho, M_T, M_U)
16:          Dimensional translation (M_M, M_E, M_J, M_Ue,
17:            M_Ui, M_Un, M_Rho, M_T, M_U)
18:          Coordinate translation (M_M, M_E, M_J, M_Ue,
19:            M_Ui, M_Un, M_Rho, M_T, M_U)
20:           $\nabla \cdot \mathbf{B} = 0$   $\nabla \cdot \mathbf{B}(TI) = 0$   $\nabla \cdot \mathbf{B}(TI) = 0$ 
21:           $\rho_{e,i} + \nabla \cdot (\rho \mathbf{U}) = 0$ 
22:          ST1
23:          ST2
24:          =====
25:          FT2
26:          Cat GPU, DPRAM at each computing node
27:          FT1
28:          for L ∈ Spatial scale do
29:            for Time ∈ Temporal Scale do
30:              for Moment ∈ Temporal-spatial Scale do
31:                for Xi ∈ N_Xi do
32:                  for Zeta ∈ N_Zeta do
33:                    Stream function (Phi_Ue, Phi_Ui, Phi_Un, Phi_U)
34:                    Potential function A
35:                     $\nabla \cdot \mathbf{B} = 0$   $\nabla \cdot \mathbf{B}(TI) = 0$   $\nabla \cdot \mathbf{B}(TI) = 0$ 
36:                     $\rho_{e,i} + \nabla \cdot (\rho \mathbf{U}) = 0$ 
37:                    ST1
38:                    ST2
39:                    =====

```

Fig. 14. Pseudocode for the output analysis algorithm.

There are several types ($\zeta = 1, 2, 3, \dots$) and species ($\iota = 1, 2, 3, \dots$) of particles throughout the simulation box; to make sure all the streaming and collisions mechanisms (direct and indirect) can be added to all the different particles of the system, the interactions between different particles on the BG, CS, and on the boundaries of the BG and CS have been defined in RHPIC-LBM (Fig. 6).

v) Calibration of the continuous kinetic-dynamic-hydro model

The purpose of the calibration is to identify the discrete DXQY and to eliminate the numerical error on the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale (Fig. 7).

vi) Test and calibration of distribution function

The calibration for collision on the BG is defined to achieve self-consistent interaction between different types and species of particles throughout the particle simulation system (Fig. 8).

vii) Re-calibration of distribution function

As the last step of the RHPIC-LBM input model, the discrete distribution functions are re-calibrated on the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale (Fig. 8).

3.10.2. Discrete distribution function

The most natural representation of the joint discrete distribution functions is as six ($\zeta = 1 \sim 3$, **B** field, **E** field, and **EM** field) 8×28 matrices of 8×28 independent components for each species ($\iota = 1, 2, 3, \dots$). The eight dimensions are based on the arrays labelled as $x_1, x_2, x_3, t, p_1, p_2, p_3$ and ζ .

The distribution functions discrete processing in RHPIC-LBM model can be outlined as seen in the flow chart in Figs. 9–10. The CPU matrices are responsible for storing the discrete distribution functions for subsequent calculations in the main program.

The GPU matrices, created according to the structures of the 8×28 matrices, are responsible for analyzing the output data in Section 4 (Figs. 13, and 14).

Here, an MHD plasma composed of mixed charged and neutral particles ($\iota = 1$, Hydrogen; $\nu \neq 0$, ionized plasma) is taken as an example for discretizing the distribution function, and the specific processes are introduced as follows (Figs. 9–10):

- Building the discrete distribution matrices ($[DF]_{8 \times 7}^B, [DF]_{8 \times 13}^E, [DF]_{8 \times 13}^{EM}, [DF]_{8 \times 19}^e, [DF]_{8 \times 19}^i$ and $[DF]_{8 \times 28}^n$) from GPU cores, where each component value of the given matrices is a function of eight independent variables ($x_1, x_2, x_3, t, p_1, p_2, p_3, \zeta$).
- Converting the six distribution function matrices into a general discrete distribution matrix ($[DF]_{8 \times (7+13+13+19+19+28)}^G$), identifying the pseudo and the real flow, and finishing the self-correction test in the phase space using Gauss's law of magnetism and the continuity equation.

- (iii) Decomposing the algebraic expression of the discrete distribution functions, determining the relationship between the $[DF]_{8 \times (7+13+13+19+19+28)}^G$ and the ionization parameter.
- (iv) Converting the $[DF]_{8 \times (7+13+13+19+19+28)}^G$ into a one-dimensional array $[DF]_{l=1}^{G_GPU}(w, v)$ in the GPU cores. The algorithm is able to utilize more resources on each GPU processor than on a CPU processor, which can store the discrete distribution function matrices ($l = 1$) on the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale.
- (v) Establishing a new array architecture based on the $[DF]_{l=1}^{G_GPU}(w, v)$, and then saving it to analyze output data created in Section 4.

3.10.3. Evolution and I/O

This part of the calculation consumes the most computational resources (CPU cores, memory and partition storage space), so we have established two parallel blocking systems (Figs. 11~12); a more detailed outline of the algorithm is shown as follows:

- i) The parallel geometric partitioning algorithm is applied to the background to keep all particles in a self-consistent status at time equals to zero.
- ii) The parallel particles (charged, neutral and pseudo-flow) partitioning algorithm is applied to the CS to realize the adaptive natural parameters (real particle density, pressure, temperature, current density, and other parameters) and field (**B** field, **E** field, and **EM** field) partitioning process in the evolution of the entire domain.
- iii) In order to ensure the evolution process of interactions between different particles, we create different arrays to save all the physical parameters, and then use these arrays to monitor the CPU, memory and communication loads at every simulation time step.

3.10.4. Output analysis

In RHPIC-LBM, the output data volume of each simulation case can range from 100TB to 150TB. When converting the output binary data to decimal data, the ASCII storage space (RSS) will exceed the space required to hold the binary data. Finding methods to analyze and visualize billions of rows of data from an HPC simulation is another important issue in RHPIC-LBM. We frame a general process as follows (Figs. 13~14):

- (i) Starting with the binary data, parameters from binary matrices are extracted, after which the binary sub-matrices are converted into decimal matrices.
- (ii) The dimensionless parameters and variables in the sub-matrices are then converted into real physical units. The specific processes are shown in the Appendix A (the dimensionless generalized Ohm's law).
- (iii) The integrity of all parameters in the process of conversion from the binary to decimal system is determined by calibrating the mathematical picture (data type of each parameter and its spatiotemporal distribution), the numerical picture (size, type, and properties of output data), and the physical picture (Gauss's law of magnetism and the continuity equation).
- (iv) These decimal sub-matrices are loaded and converted into a one-dimensional array by following the algorithm design established in Section 2 (Figs. 9~10).
- (v) The three-dimensional discrete magnetic potential vectors, discrete streaming functions, discrete charged particle energy distribution functions, and energy spectrum functions are then computed and reconstructed.

Essentially, the RHPIC-LBM program consists of three parts (input file preparation (Sections 1~2), computing (Section 3), and dummyTXdummy-(output data analysis (Section 4)), written in multiple languages (C, FORTRAN, PYTHON, IDL and TecPlot scripts). The preprocess, postprocess, and visualization are based on a GPU-CPU heterogeneous computing system, which has a significantly different architecture and program skeleton from the CPU isomorphic computing system.

A discrete CPU-GPU system provides high performance but has the disadvantage of slow communication between the GPU cores and CPU cores.

In the large-scale simulation, we divide computing and communication into two separate processes; the CPU handles the HPC computing tasks, while the GPU handles the I/O and communication processes.

The RHPIC-LBM is very expensive in terms of computational resources and memory; the major costs come from the following three factors:

- i) The self-consistency between the geometric adaptive lattice grid refinement (GALGR) and physical adaptive lattice grid refinement (PALGR, D^B3Q7 , D^E3Q13 , D^I3Q19 , D^J3Q19 and D^K3Q27) [66,69,76–78]. Improper setup causes physical, numerical and system errors that terminate the main program.
- ii) The self-consistency between the numerically implemented matrix size (collision and interaction between different size RHPIC-LBM lattice grids) and main memory. Improper setup results in reduced computational efficiency and leads to transient node overload.
- iii) The physical noise (error) due to the improper setup of initial conditions leads to simultaneous transient overload of all the computation nodes, which triggers system failure.

In the RHPIC-LBM, the pseudo-Larmor radius and pseudo-cyclotron time of the charged particles are defined by the fractal index and adaptive lattice grid refinement (GALGR and PALGR), which greatly improves the computational efficiency as compared to the traditional PIC and LBM algorithms.

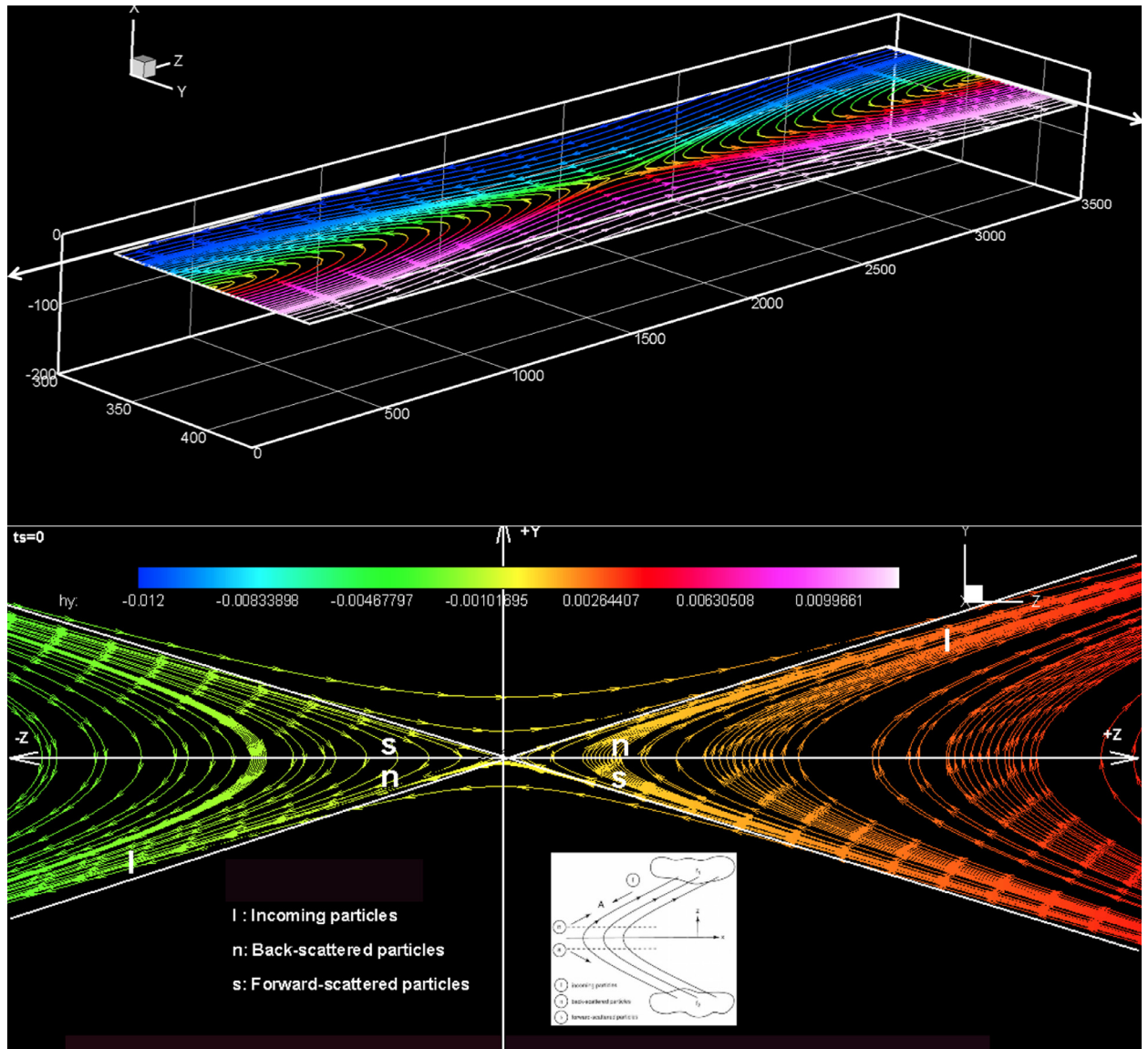


Fig. 15. Schematic drawing of the Harris-type initial magnetic field topology structure conditions.

4. Testing and validation of reliability, stability and efficiency of the RHPIC-LBM algorithms and code

4.1. Input parameters and BC/IC setup

As an initial condition of the RHPIC-LBM, the Harris-type magnetic field configuration is given over the entire physical simulation domain (Fig. 15).

For 2D/2.5D problems, the lattice grid is set as 64000×8000 , while the peak density equals $0.05 \times n_g$. n_g is the density of the background field, which is assumed to be 10^7 cm^{-3} .

The initial plasma temperature is assumed to be $T_{bk} = 10^6 \text{ K}$ for both electrons $T_{e|bk}$ and protons $T_{i|bk}$ in the background.

The total number of superparticles (SPs) is $64000 \times 8000 \times 2^{\hat{n}}$. $\hat{n} \geq 8$ represents a dimensionless parameter that establishes a bridge between the natural number density of the background and the number of particles in each simulation lattice grid.

The ion-to-electron temperature ratio is assumed to be $T_{i|cs}/T_{e|cs} = 5$ in the current sheet (CS). The background-to-CS temperature is assumed to be $T_{bk}/T_{e|cs} = 0.1$. The proton to electron mass ratio is assumed to be $m_i/m_e = 1836$.

The inertial depth is $c/\omega_{pe} = 10^{-3} \Delta$, the cyclotron time is $c/\omega_{ce} = 10^{-4} \Delta$, the time step is $dt = c\omega_{ce}^{-1}/2^{\hat{n}}$, and the magnetization parameter $(\omega_{ce}/\omega_{pe})^2 = 100$, where Δ represents the grid size.

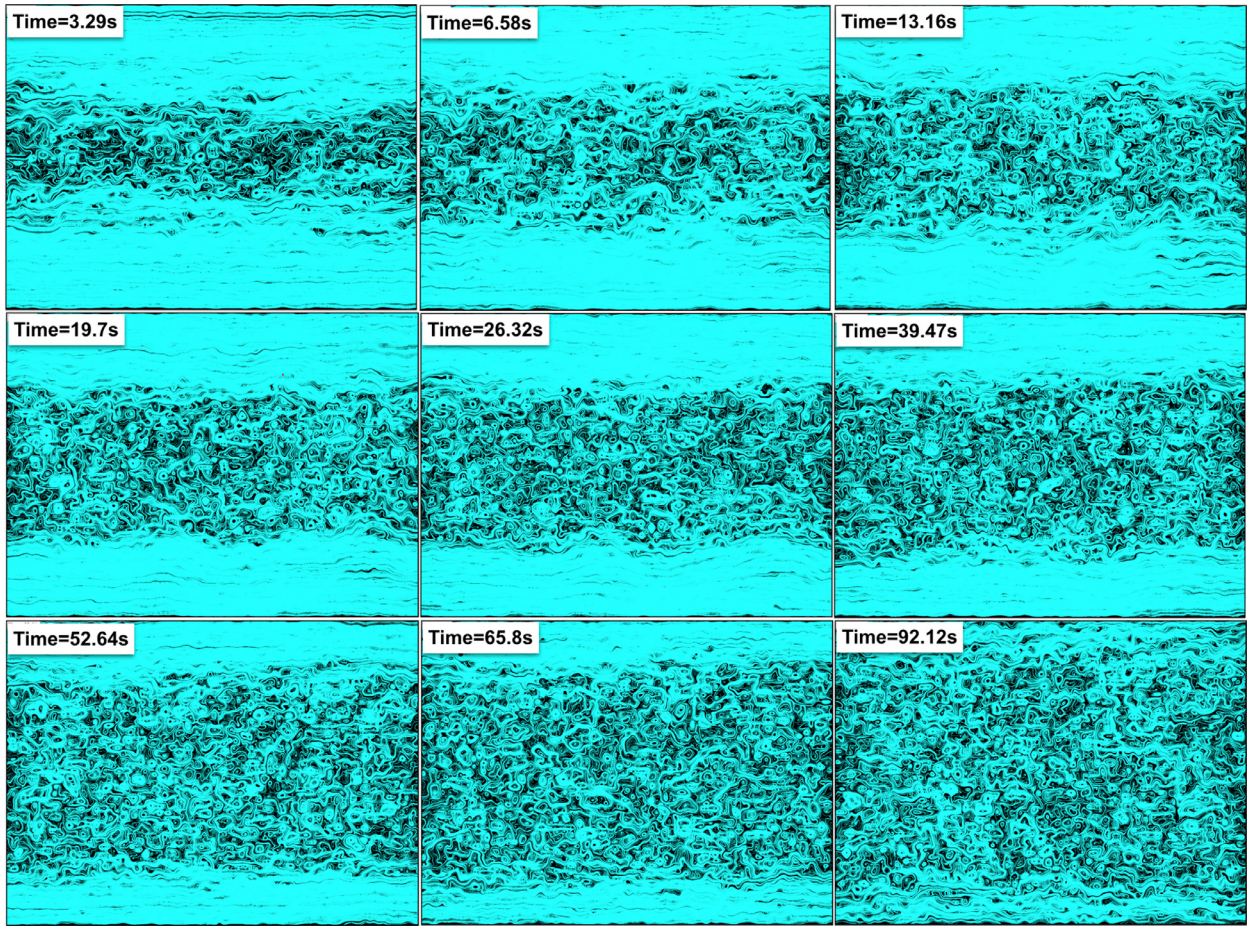


Fig. 16. Magnetic islands appear, grow and fully develop nonlinearly, testing the reliability, stability and efficiency of the RHPIC-LBM code (Supplementary video 1).

In this section, $\hat{n}$ equals 16 at the picoscale ($\sim 10\text{km}$, one SP contains $10^5 \sim 10^6$ real particles), 14 at the nanoscale ($\sim 500\text{km}$, one SP contains $10^5 \sim 10^6$ real particles), 12 at the microscale ($500\text{km} \sim 1000\text{km}$, one SP contains $10^6 \sim 10^7$ real particles), 10 at the macroscale ($\sim 10000\text{km}$, one SP contains $10^7 \sim 10^8$ real particles) and 8 at the large hydroscale ($\sim 10000\text{km}$, one SP contains $10^7 \sim 10^8$ real particles).

Open boundary and/or periodic boundary conditions are applied over the x and y directions. The length to the initial plasma CS thickness $\lambda = 10^{-4}\Delta$.

4.2. Testing and validation of magnetic island evolution

From the analysis of the physical mathematical model and the numerical framework-flowchart-implementation, we know that the collision and/or the interaction simulation is one of most expensive parts of the RHPIC-LBM.

For these cases, we add fluctuation of the magnetic field and turbulence of the plasma motion seeds to the initial CS diffusion region and test the RHPIC-LBM code's reliability, stability and efficiency in the linear, nonlinear and fully developed nonlinear turbulence evolution processes.

The complete evolution of multiple magnetic islands in the resistive CS of the LTSTMR is given in Fig. 16 and Supplementary video 1.

The simulation results cover the magnetic island evolution processes for the kinetic, dynamic and hydro temporal-spatial scales at the same time.

In addition, the simulation results show that the RHPIC-LBM code demonstrates the role of the extended forces from the fluctuations and turbulence components $\frac{q}{m_i^e}(\tilde{\mathbf{E}} + \frac{1}{c}\tilde{\mathbf{U}}_i^e \times \tilde{\mathbf{B}})$ on the left side of Eq. (28), and the role of extended force from average component part $\frac{q}{m_i^e}(\bar{\mathbf{E}} + \frac{1}{c}\bar{\mathbf{U}}_i^e \times \bar{\mathbf{B}})$ of the third item on the left side of Eq. (28), in both small and large size magnetic islands evolution, respectively.

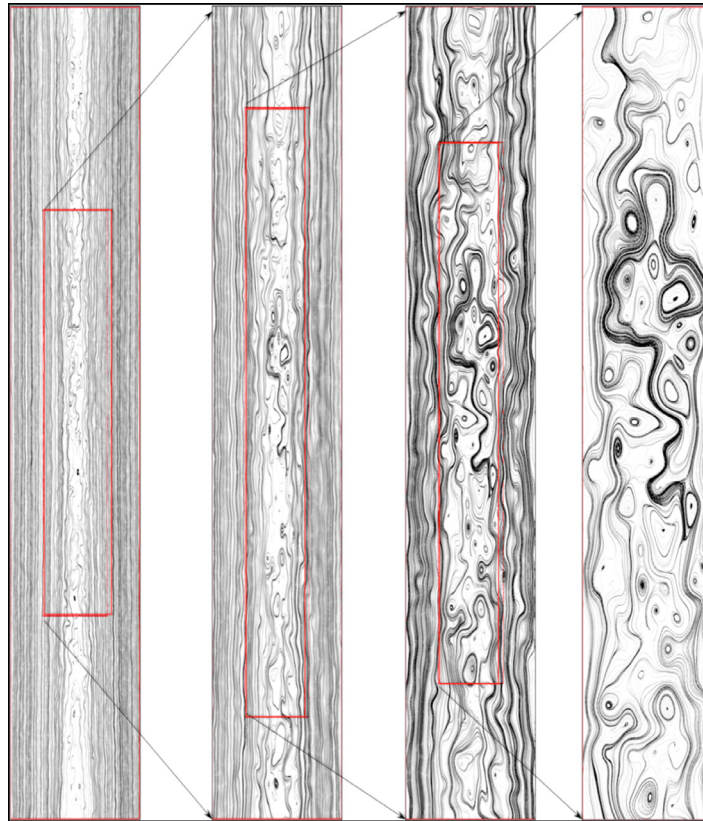


Fig. 17. Fractal nature of the cascade of the kinetic-dynamic-hydro temporal-spatial scale evolution with the double Harris-type initial magnetic configuration condition.

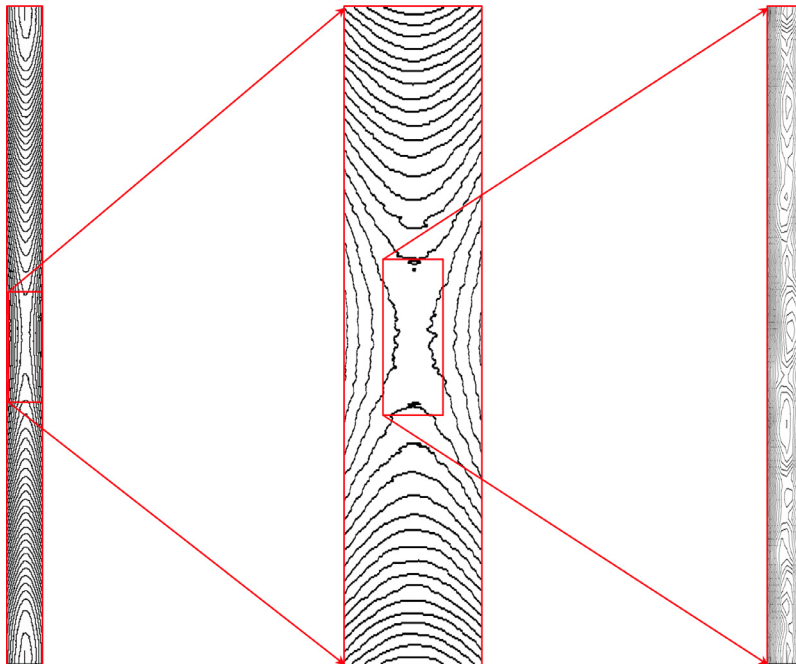


Fig. 18. Cascade of the kinetic-dynamic-hydro temporal-spatial scale evolution with the double Harris-type initial magnetic configuration condition. (Supplementary video 2 ~ 4).

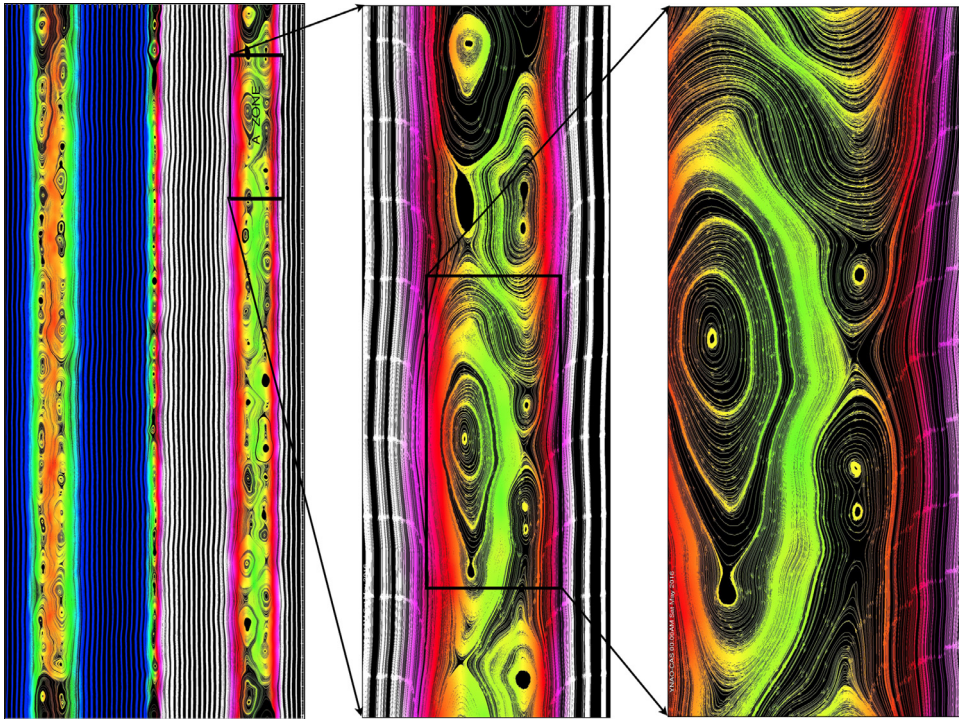


Fig. 19. Cascade of the kinetic-dynamic-hydro temporal-spatial scale evolution with the multi-Harris-type initial magnetic structure condition.

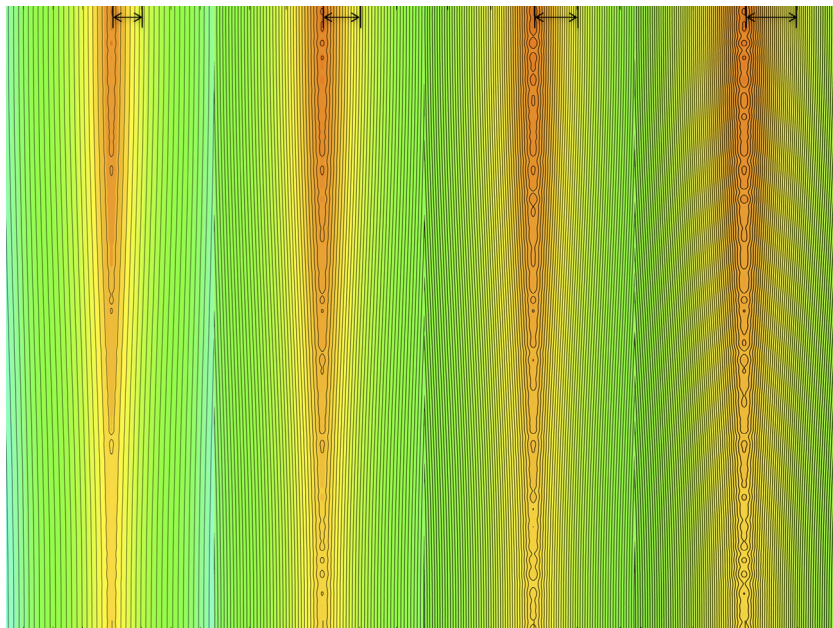


Fig. 20. Inverse cascade of the kinetic-dynamic temporal scale evolution with the single Harris-type initial magnetic structure condition.

This testing and validation provide prerequisites and necessary conditions for applying the RHPIC-LBM to explore the role of turbulence in flux ropes interaction that are given in second part of this two-paper series.

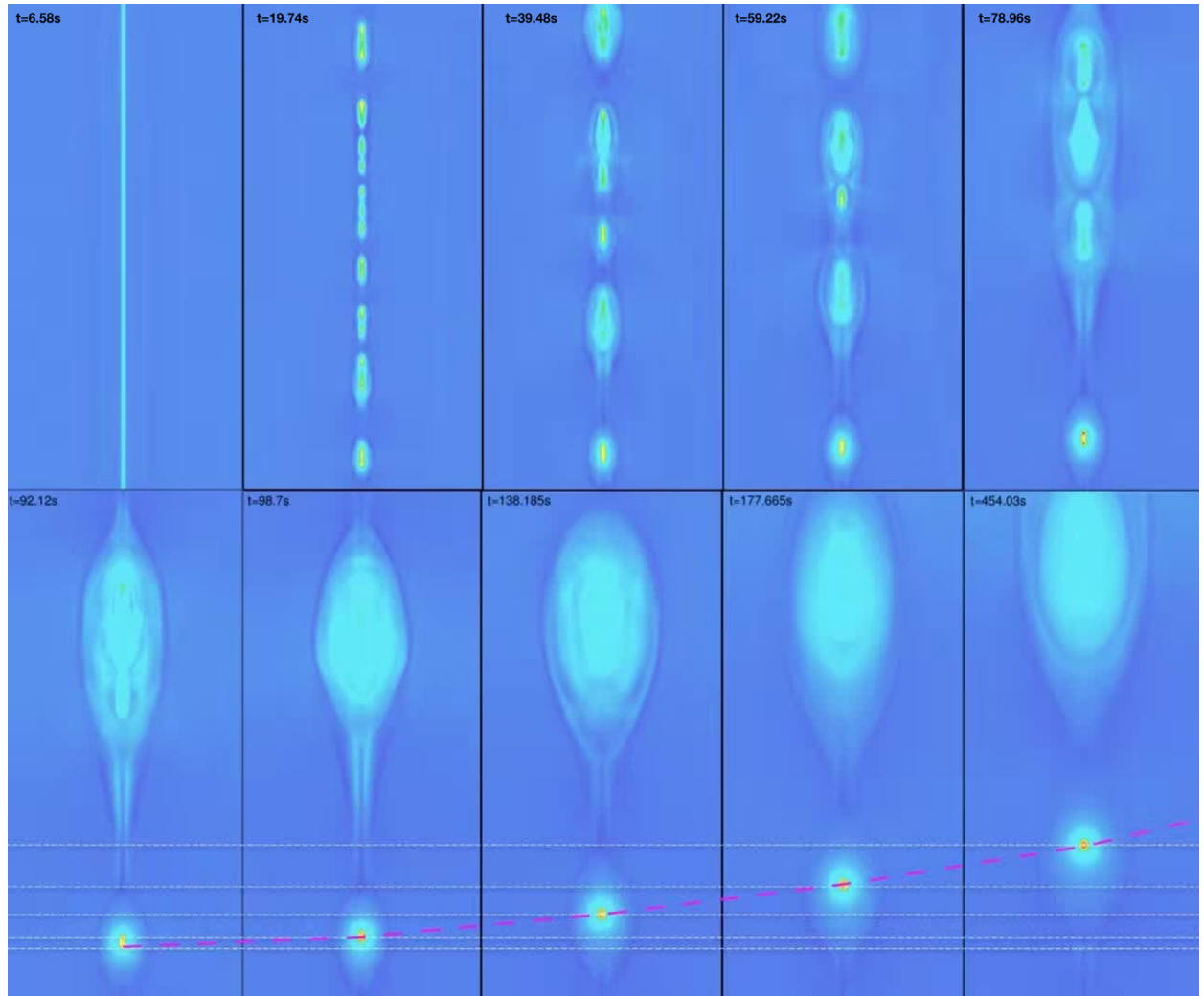


Fig. 21. Illustration of the reconnection during the formation, shrinking and breakup of the magnetic islands of the microkinetic stage ($0 \text{ s} \sim 9.87 \text{ s}$, $10^{-2} \text{ m} \sim 10^5 \text{ m}$), the reconnection during the merging/coalescence and growth of the magnetic islands of the cross-scale coupled microkinetic & macrodynamic stage ($9.87 \text{ s} \sim 78.96 \text{ s}$, $10^5 \text{ m} \sim 10^8 \text{ m}$), and the magnetic islands reaching constant sizes and eruptions with the *Alfvén* speed of the cross-scale coupled macrodynamic & large-hydro stage ($98.7 \text{ s} \sim 454.3 \text{ s}$, $10^8 \text{ m} \sim 10^9 \text{ m}$).

4.3. Testing and validation of cascade and fractal of magnetic structure at different temporal-spatial scales

To investigate the resistive diffusion region of LTSTMR over the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale, the GALGR and PALGR in the numerical framework-flowchart-implementation automatically vary from the large temporal-spatial scale to the small temporal-spatial scale in the RHPIC-LBM algorithm and code.

In the RHPIC-LBM, the initial scale of the LTSTMR system is defined by the initial CS thickness.

In this case, we define the initial distance d_{MFL} of the adjacent magnetic field lines (MFLs) in the simulation domain as equal to the length of the characteristic electron radius (EMHD MR) and 1/128 of the characteristic ion length (IMHD MR).

The lattice grid size (Δ) is equal to 1/16 of the distance between adjacent MFLs. At the kinetic scale (EMHD MR & HMHD MR), the geometric and physical scales vary by a magnitude of 3; in the dynamic scale (IMHD MR), the geometric and physical scales vary by a magnitude of 8.

It is an extremely small spatial scale in the solar atmosphere LTSTMR. For the fully ionized CME LTSTMR case, the values of λ_{iD}^e and λ_{iD}^i of (Eq. (25)–(26)) are equal to 0.02 m and 100 m , respectively.

With the evolution of the turbulence from a linear to a fully developed nonlinear process, the thickness of the simulation diffusion region increases and reaches an order of $\sim 10^7 \text{ m}$, which is consistent with observations (the thickness and length of the CS for a typical CME are at an order of $\sim 10^7 \text{ m}$ and $\sim 1.5\%$ of the solar radius, respectively).

The validation simulations of the cascades and the self-similar fractal properties of the magnetic structure with the scale down process are shown in Figs. 17–19 and Supplementary videos 2 ~ 4.

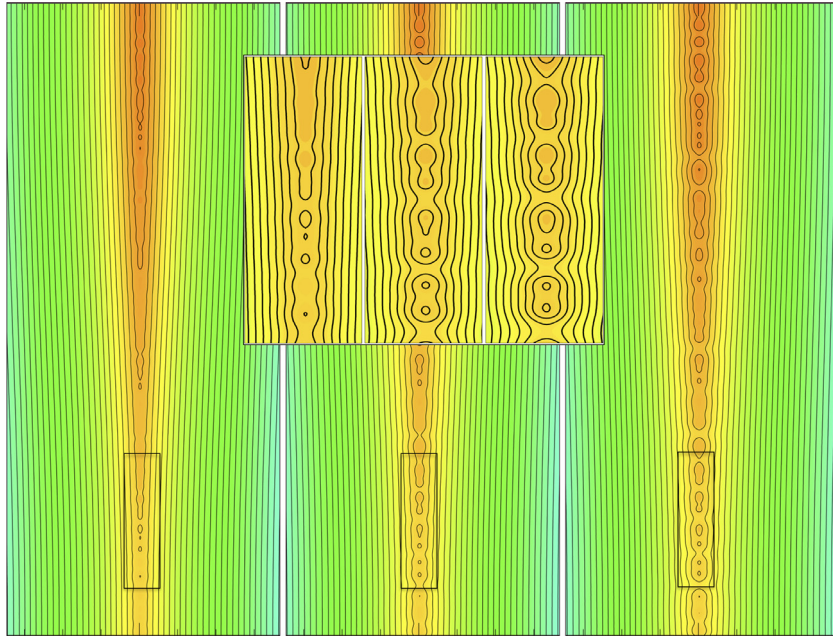


Fig. 22. Kinetic scale evolution stage: magnetic islands form, shrink and break into smaller sizes.

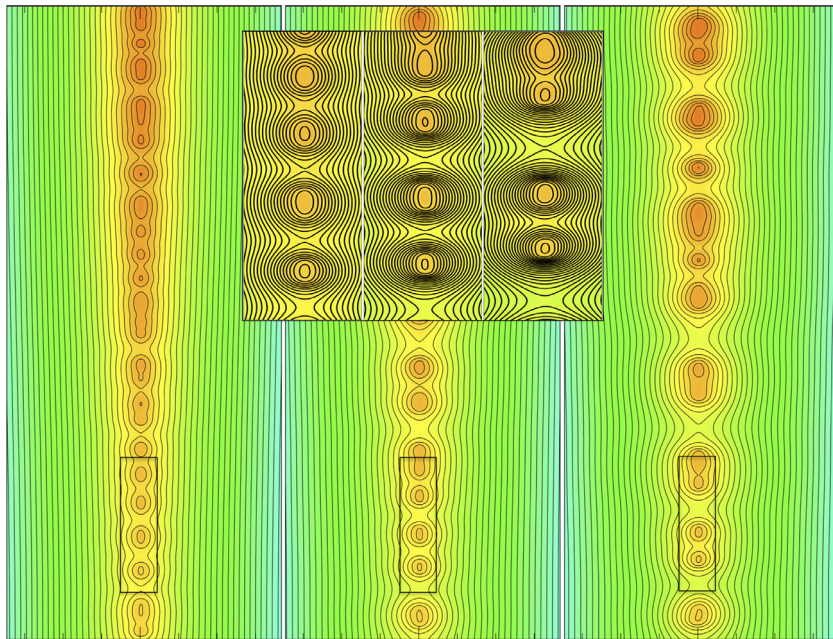


Fig. 23. Kinetic-dynamic stage: magnetic islands grow and merge into larger sizes.

The structure of the magnetic field at different temporal-spatial scales has cascades and self-similarities, which is consistent with observations and other 2D/2.5D simulations [94,95].

The self-similarity at different scales provides a way to calculate the Hurst index, and then, the fully developed turbulence evolution at the kinetic-dynamic-hydroscale can be quantitatively analyzed by the Hurst index within the above numerical framework-flowchart-implementation, which means that RHPIC-LBM provides way to simulate large scale LTSTMR.

A more detailed introduction for the cascade, self-similarity and fine structures (GALGR and PALGR) in LTSTMR is given for the solar atmosphere LTSTMR activity simulation in [Section 4.5](#).

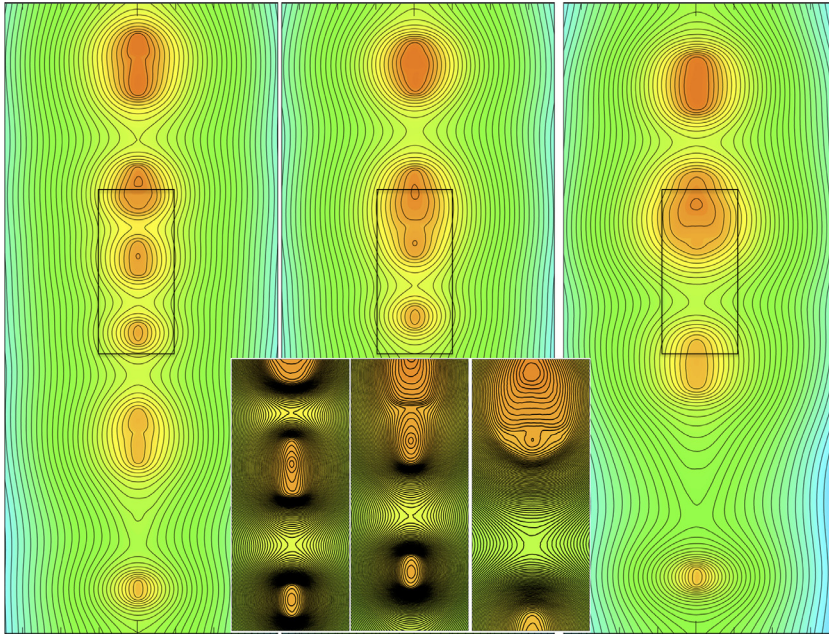


Fig. 24. Dynamic stage: magnetic islands grow, merge and increase in size.

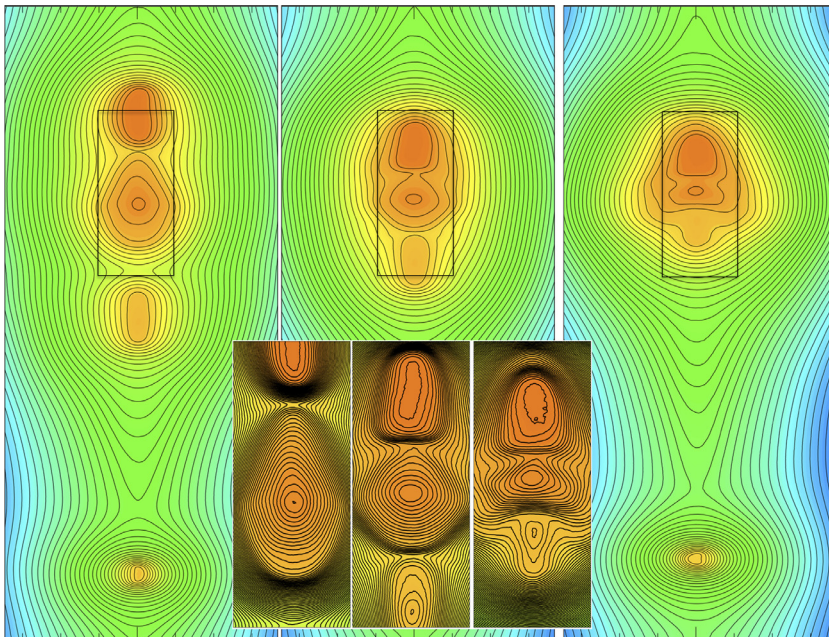


Fig. 25. Dynamic-hydro stage: magnetic islands merge and size remains quasi-constant.

4.4. Testing and validation of different initial magnetic configuration condition

There are many different kinds of LTSTMR in universal plasmas, such as Earth's ionosphere-magnetospheres, solar atmosphere activities, planetary magnetospheres, accretion disks, and pulsar magnetospheres. However, defining a reasonable initial magnetic configuration in the numerical framework-flowchart-implementation is another important step in studying LTSTMR phenomena with the RHPIC-LBM.

The RHPIC-LBM provides various initial magnetic structure conditions in the *input model* (workflow A in Fig. 2–8).

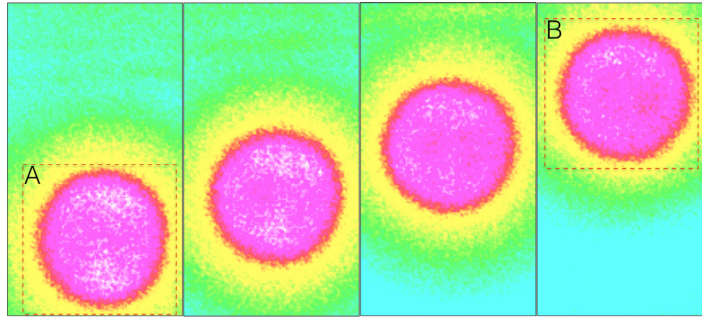


Fig. 26. Magnetic island fine structure evolution in the dynamic stage.

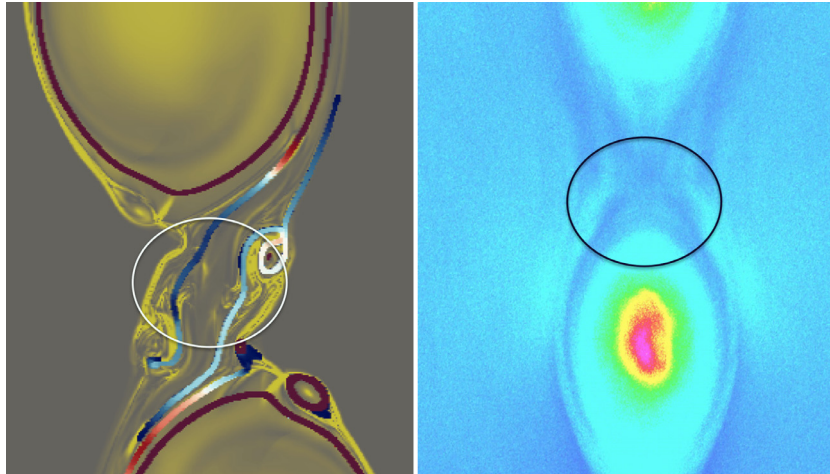


Fig. 27. Instabilities in adjacent macro-magnetic island coalescence. Left side, tilt-kink instabilities from MNPAS [56–58]. Right side, mixed tearing and oblique instabilities from the present RHPIC-LBM. (Supplementary videos 5–7).

In this section, the double Harris-type initial magnetic configuration (Figs. 16–18), the multi-Harris-type initial magnetic field configuration (Fig. 19), and the single Harris-type initial magnetic configuration (Fig. 20) are applied in the *input model* to test and validate the reliability, stability and efficiency of the RHPIC-LBM.

The results show that the numerical evolution of the MFLs agrees with theoretical prediction and observation and that the RHPIC-LBM program can execute good numerical simulation for different kinds of initial magnetic configurations.

Fig. 20 also provides numerical evidence of inverse kinetic-dynamic cascade phenomena in different temporal spaces in fixed spatial space, which also shows that the RHPIC-LBM can explore kinetic-dynamic-hydro fully coupled temporal-spatial LTSTMR problems.

4.5. Investigation and validation of solar atmosphere LTSTMR activities

To validate the RHPIC-LBM and to prove that it can be applied to solar atmosphere LTSTMR activities, a continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale LTSTMR evolution is simulated in this section. Fig. 21 shows that the simulation results cover the full scale of magnetic island evolution, including the picoscale (10^{-2} m $\sim 10^5$ m), nanoscale (10^5 m $\sim 10^6$ m), microscale (10^6 m $\sim 10^7$ m), macroscale (10^7 m $\sim 10^8$ m) and large hydroscale (10^8 m $\sim 10^9$ m).

In addition, the RHPIC-LBM can be applied to study the physical pictures of EMHD microphysics, Hall physics and IMHD macro physics in the diffusion region of continuous temporal-spatial scale MR.

4.5.1. Fine magnetic structure in the continuous kinetic-dynamic-hydro temporal-spatial scale

We present several specific evolution moments in Fig. 21 and show the geometry and topology structure of MFLs; the fine structure evolution results of the MFLs are obtained from different temporal-spatial scales (Figs. 22–26).

During the microkinetic evolution stage (Fig. 22), the tearing instabilities lead to combined 1st Fermi and betatron accelerations during the process of “head-on” separation (the adjacent magnetic islands are moving in opposite directions) of adjacent magnetic islands (10^{-2} m $\sim 10^6$ m). The magnetic islands ($\sim 10^5$ m) are squeezed before shrinking and then expand while breaking into sizes of 10^{-2} m $\sim 10^3$ m.

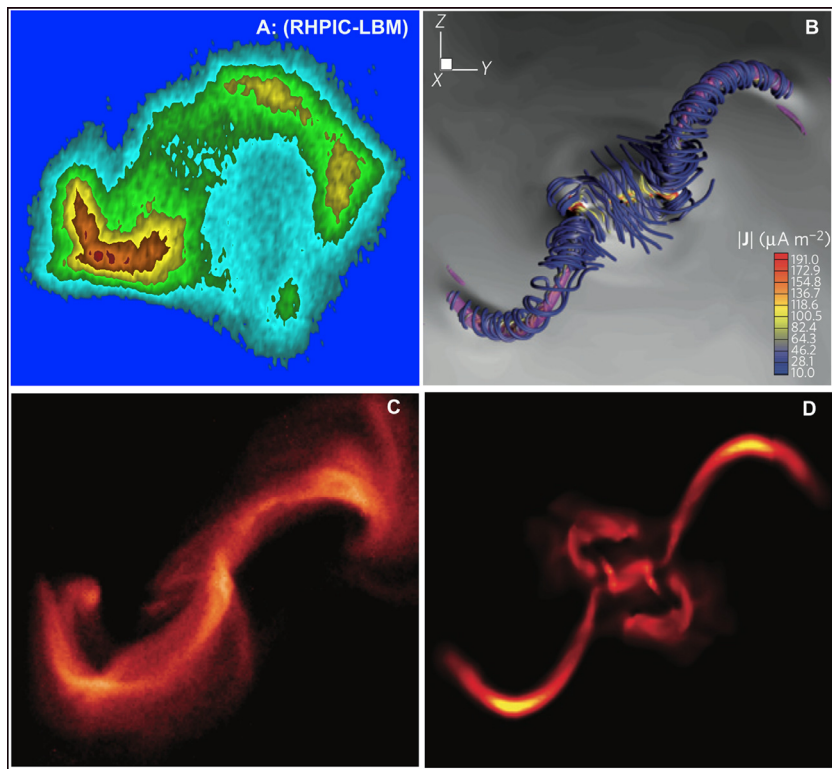


Fig. 28. Fine structure evolutions of adjacent magnetic islands coalescence with each other on the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale with RHPIC-LBM (Supplementary video 8).

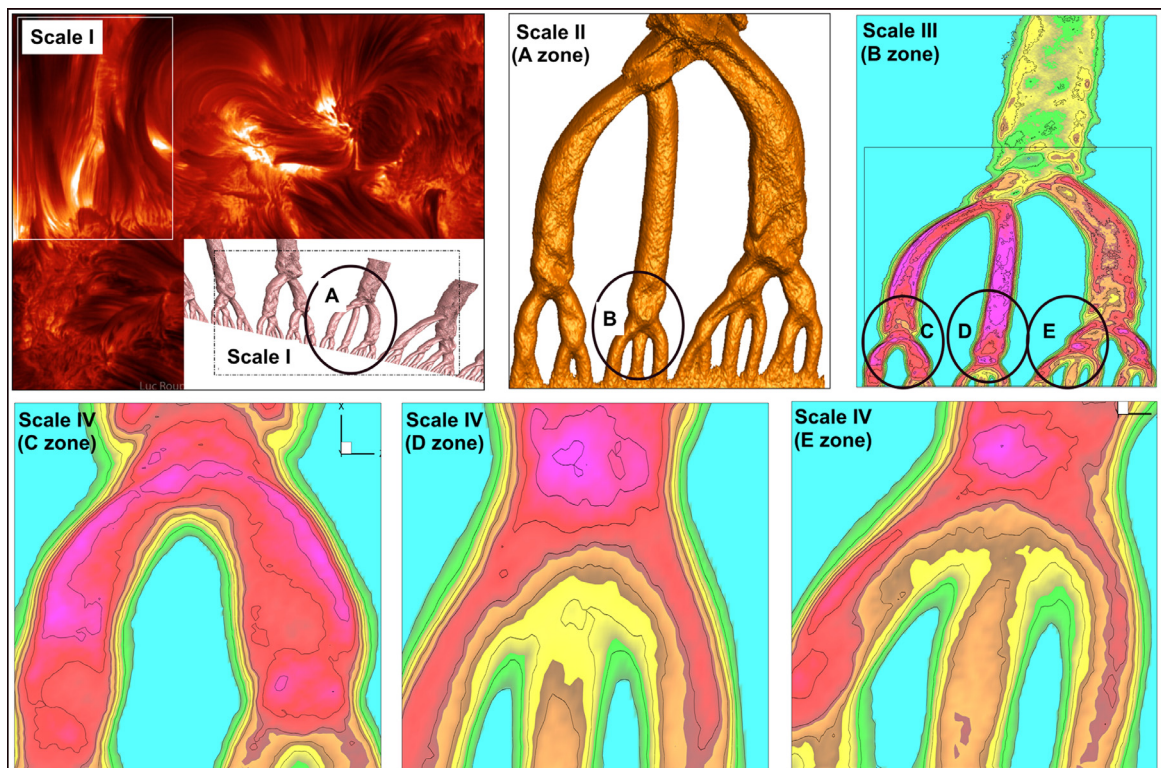


Fig. 29. Fine fractal structure of a solar flare on the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale with RHPIC-LBM.

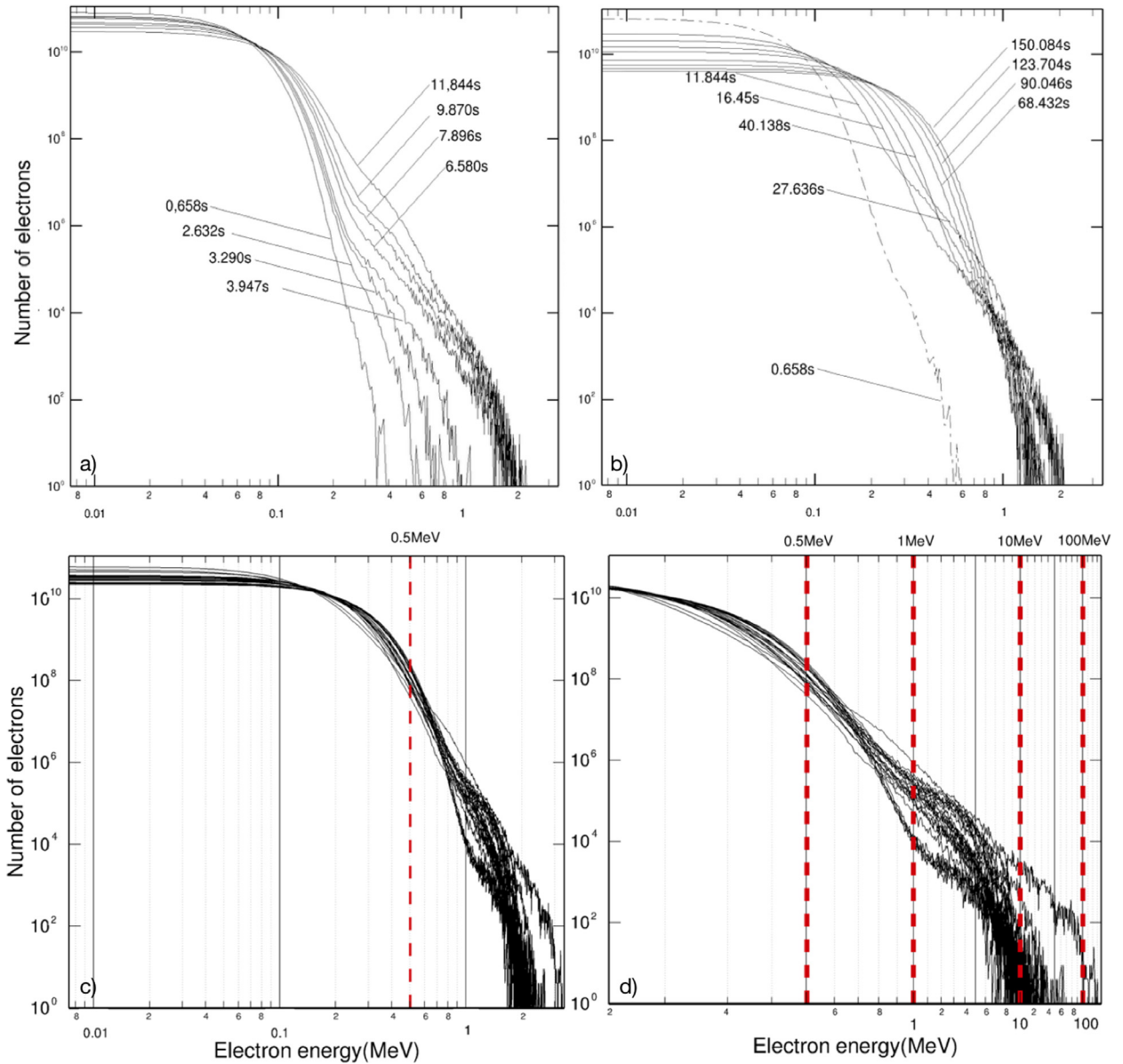


Fig. 30. Energy spectrum integrated over the entire simulation domain not considering relativistic effects (a ~ b) and that considering relativistic effects (c ~ d).

During the microkinetic and macrodynamic evolution stage (Fig. 23), the "head-on" and "head-on" collisions and "head-on" and "rear-end" collisions (the adjacent magnetic islands are moving in the same direction) lead to combined 1st and 2nd Fermi, betatron and turbulent accelerations during the growth of the magnetic islands (10^5 m $\sim$ 10^7 m).

During the macrodynamic and large-hydro evolution stage (Figs. 24–26), the "head on" and "rear-end" collision lead to combined 1st and 2nd Fermi and turbulent accelerations and, the size of a magnetic island remains constant (10^5 m $\sim$ 10^8 m) when the island reaches a size 0.3 times the macroscale CS thickness (117.665 s $\sim$ 454.03 s in Fig. 21).

4.5.2. Fine internal structure of the magnetic islands during coalescence and mergence process

GALGR and PALGR in the RHPIC-LBM allow us to understand what is happening inside magnetic islands during the process of coalescence and merging from the large scale to the small scale (Figs. 22–26), which provides direct evidence for the possible new physical picture of MR (e.g., slipping MR caused by continuous exchange between adjacent MFLs [96–104], mixed instabilities [tearing and kink instabilities combined] [56–58], and the mechanism of turbulence acceleration).

The refined structures of adjacent magnetic islands (Figs. 22–26 and Supplementary videos 5 ~ 6) show that the strength of magnetic field region greatly changes (external perturbations, kinetic Alfvén wave [KAW], slipping MR, quasiseparatrix

layers, or other physical pictures [5,54,59,105–108]) during the process of merging adjacent magnetic islands, which provides evidence for mixed tearing and oblique instabilities in 3D LTSTMR (Fig. 27) [56–58,109].

The fine structure evolutions of adjacent magnetic islands coalescence with each other on the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale, as shown in Fig. 28 and Supplementary video 8. The simulation result using RHPIC-LBM (Figure 28A) is consistent with observations and theories (Figs. 28B–28D) [11].

The fine fractal structure from RHPIC-LBM in Fig. 29 show that there are a lot of fractal structures within the giant arch (from feet to the arch in a solar flare loop) on the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale. It is confirmed for the first time that the magnetic field structure within the giant arch has multiple scale fractal properties, and because the fractal property is a parameter that does not depend on the temporal-spatial spatial scale, the fine fractal structure provides a novel method to investigate high-energy particle bursts in this area, such as X-rays from high-energy electrons and γ -rays from high-energy ions) [12–15].

A more detailed analysis about slipping MR, the mechanism of the mixed instabilities and turbulence acceleration in adjacent magnetic island (flux ropes in 3D) coalescence from the 3D model is given in part II of the paper.

4.5.3. Energy spectra with and without relativistic effects

Fig. 30 shows that the acceleration efficiency of the electron particles without relativistic effects (Fig. 30a–30b) is lower than that with relativistic effects (Figs. 30c–30d), which means that relativistic effects are vital in the electron acceleration process, especially when the particle energy reaches relativistic energy. This result is consistent with the solar energetic particle (SEP) events from observations [44–46,55].

5. Conclusions

As the first part of a two-paper series, we developed and validated the physical and mathematical model of RHPIC-LBM and the numerical framework-flowchart-implementation by investigating the resistive diffusion region of LTSTMR over the continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale. The main conclusions of this study are follows.

- i) The RHPIC-LBM, algorithm, CPU-GPU heterogenous frame, and performance are introduced in this paper.
- ii) The reliability, stability and efficiency of the four different benchmarks show that the RHPIC-LBM is an excellent model system for studying continuous kinetic-dynamic-hydro fully coupled temporal-spatial scale LTSTMR on a supercomputer platform (e.g., *Tianhe-2*).
- iii) The solar atmosphere LTSTMR activities at the picoscale (10^{-2} m $\sim 10^5$ m), nanoscale (10^5 m $\sim 10^6$ m), microscale (10^6 m $\sim 10^7$ m), macroscale (10^7 m $\sim 10^8$ m) and large hydroscale (10^8 m $\sim 10^9$ m) are explored with the RHPIC-LBM, and all the simulation results agree well with observations [3–5,9,10,47,48,53–55] and theories [11,56–61].
- iv) GALGR and PALGR in the RHPIC-LBM provide a numerical tool to explore the mechanisms of turbulence acceleration (magnetic KAWs-to-magnetic KAWs, magnetic KAWs-to-plasma KAWs, plasma KAWs-to-plasma KAWs, magnetic KAWs-to-charged particles, and plasma KAWs-to-charged particles [1,2,5–7,54,59,105–108]) and slipping MR-induced mixed tearing-oblique instabilities [5,54,56–59,105–109] during the process of merging adjacent magnetic islands. It is of great significance for investigating the role of turbulence in the magnetic energy release-conversion, plasma heating and charged particle energization-acceleration in LTSTMR.

In general, this paper only shows certain numerical evidence of 2D/2.5D LTSTMR; a more detailed analysis of the role of turbulence in self-generating-organization magnetic fields and self-feeding-sustaining plasma motion during the interaction of magnetic strength fluctuation and plasma turbulence is introduced in the 3D RHPIC-LBM application section.

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Appendix A. The dimensionless generalized Ohm's Law

The momentum equation for two-species fully ionized plasma of electrons and ions ($j=e$ or i) can be written as [110,111],

$$m_j n_j \left(\frac{\partial \mathbf{U}_j}{\partial t} + (\mathbf{U}_j \cdot \nabla) \mathbf{U}_j \right) = -\nabla \cdot (\mathbf{P}_j \mathbf{I} + \boldsymbol{\pi}_j) + q_j n_j (\mathbf{E} + \mathbf{U}_j \times \mathbf{B}) + n_j \frac{m_i m_e \nu_{ei}}{m_i + m_e} (\mathbf{U}_i - \mathbf{U}_e) \quad (\text{A.1})$$

Substitute above equation into electric current density equation $\mathbf{J} = n_e q_e \mathbf{U}_e + n_e q_e \mathbf{U}_e$ and neglects the gradients of small perturbations ($\mathbf{U} \cdot \nabla \mathbf{U} \approx 0$), we can get,

$$\begin{aligned} \frac{\partial \mathbf{J}}{\partial t} = & -\frac{q_e}{m_e} \nabla \cdot (P_e \mathbf{I} + \boldsymbol{\pi}_e) - \frac{q_i}{m_i} \nabla \cdot (P_i \mathbf{I} + \boldsymbol{\pi}_i) + \left(\frac{n_e q_e^2}{m_e} + \frac{n_e q_e^2}{m_e} \right) \mathbf{E} + \left(\frac{n_e q_e^2}{m_e} \mathbf{U}_e + \frac{n_e q_e^2}{m_e} \mathbf{U}_i \right) \times \mathbf{B} \\ & + \frac{q_e m_i \nu_{ei}}{m_i + m_e} (\mathbf{U}_i - \mathbf{U}_e) + \frac{q_i m_e \nu_{ei}}{m_i + m_e} (\mathbf{U}_i - \mathbf{U}_e) \end{aligned} \quad (\text{A.2})$$

For an electrically neutral plasma, put $\mathbf{U} = \frac{n_e m_e \mathbf{U}_e + n_e m_e \mathbf{U}_e}{n_e m_e + n_i m_i}$ into above equation, the Eq. (A.2) can be rewritten as,

$$\frac{\partial \mathbf{J}}{\partial t} = -\frac{q_e}{m_e} \nabla \cdot (P_e \mathbf{I} + \boldsymbol{\pi}_e) - \frac{q_i}{m_i} \nabla \cdot (P_i \mathbf{I} + \boldsymbol{\pi}_i) + \left(\frac{n_e q_e^2}{m_e} + \frac{n_i q_i^2}{m_i} \right) (\mathbf{E} + \mathbf{U} \times \mathbf{B}) + \frac{\nu_{ei}}{m_i + m_e} (q_e m_i - q_i m_e) (\mathbf{U}_i - \mathbf{U}_e) \quad (\text{A.3})$$

For fully ionized plasma ($q_i = -q_e$, $n_i = n_e$), the current density can be rewritten as $\mathbf{J} = n_e q_e (\mathbf{U}_e - \mathbf{U}_i)$, the above equation can be simplified to,

$$\frac{\partial \mathbf{J}}{\partial t} = -\frac{q_e}{m_e} \nabla \cdot (P_e \mathbf{I} + \boldsymbol{\pi}_e) + \frac{q_e}{m_i} \nabla \cdot (P_i \mathbf{I} + \boldsymbol{\pi}_i) + n_e q_e^2 \left(\frac{1}{m_e} + \frac{1}{m_i} \right) (\mathbf{E} + \mathbf{U} \times \mathbf{B}) + q_e \left(\frac{1}{m_e} + \frac{1}{m_i} \right) (\mathbf{J} \times \mathbf{B}) - \frac{\nu_{ei}}{n_e} \mathbf{J} \quad (\text{A.4})$$

Introducing the Spitzer resistivity η to describe the interactional/collisional term from charged particles (ions-to-ions, ions-to-electrons, electrons-to-electrons) instead of interaction/collision frequency ν_e , the $\frac{\nu_{ei}}{n_e} \mathbf{J}$ can be approximation with $n_e q_e^2 \left(\frac{1}{m_e} + \frac{1}{m_i} \right) \eta \mathbf{J}$ [112–116]. The generalized resistive Ohm's law can be written as [110,111],

$$\begin{aligned} \frac{\partial \mathbf{J}}{\partial t} = & -\frac{q_e}{m_e} \nabla \cdot (\mathbf{P}_e \mathbf{I} + \boldsymbol{\pi}_e) + \frac{q_e}{m_i} \nabla \cdot (\mathbf{P}_i \mathbf{I} + \boldsymbol{\pi}_i) \\ & + n_e q_e^2 \left(\frac{1}{m_e} + \frac{1}{m_i} \right) (\mathbf{E} + \mathbf{U} \times \mathbf{B}) + q_e \left(\frac{1}{m_e} - \frac{1}{m_i} \right) (\mathbf{J} \times \mathbf{B}) - n_e q_e^2 \left(\frac{1}{m_e} + \frac{1}{m_i} \right) \eta \mathbf{J} \end{aligned} \quad (\text{A.5})$$

Then, the electric field $\mathbf{E}$ can be written as,

$$\begin{aligned} \mathbf{E} = & -\mathbf{U} \times \mathbf{B} + \frac{m_i}{q_e (m_i + m_e)} \nabla \cdot (\mathbf{P}_e \mathbf{I} + \boldsymbol{\pi}_e) \\ & - \frac{m_e}{q_e (m_i + m_e)} \nabla \cdot (\mathbf{P}_i \mathbf{I} + \boldsymbol{\pi}_i) - \frac{m_i}{q_e (m_i + m_e)} (\mathbf{J} \times \mathbf{B}) + \eta \mathbf{J} \end{aligned} \quad (\text{A.6})$$

The induction equation for resistive MHD can be written as,

$$\begin{aligned} \frac{\partial \mathbf{B}}{\partial t} = & -\nabla \times \mathbf{E} \\ = & -\nabla \times \left[-\mathbf{U} \times \mathbf{B} + \frac{m_i (\nabla P_e + \nabla \cdot \boldsymbol{\pi}_e)}{q_e (m_i + m_e)} + \eta \mathbf{J} - \frac{m_e (\nabla P_i + \nabla \cdot \boldsymbol{\pi}_i)}{q_e (m_i + m_e)} - \frac{m_i}{q_e (m_i + m_e)} (\mathbf{J} \times \mathbf{B}) \right] \\ = & -\nabla \times \left\{ -\mathbf{U} \times \mathbf{B} + \frac{m_i \nabla P_e - m_e \nabla P_i}{q_e (m_i + m_e)} + \frac{m_e \nabla \cdot \boldsymbol{\pi}_e + m_i \nabla \cdot \boldsymbol{\pi}_i}{q_e (m_i + m_e)} \right. \\ & \left. - \frac{m_i}{q_e (m_i + m_e)} \left[\left(\frac{\nabla \times \mathbf{B}}{\mu} \right) \times \mathbf{B} \right] + \frac{\eta \nabla \times \mathbf{B}}{\mu} \right\} \\ = & \nabla \times (\mathbf{U} \times \mathbf{B}) - \frac{\eta}{\mu} \nabla^2 \mathbf{B} + \frac{\nabla \eta}{\mu} \times (\nabla \times \mathbf{B}) + \frac{m_i \nabla \times (\nabla \times \mathbf{B}) \times \mathbf{B} - m_i \nabla \times (\nabla P_e) + m_e \nabla \times (\nabla P_i)}{q_e \mu (m_i + m_e)} \end{aligned} \quad (\text{A.7})$$

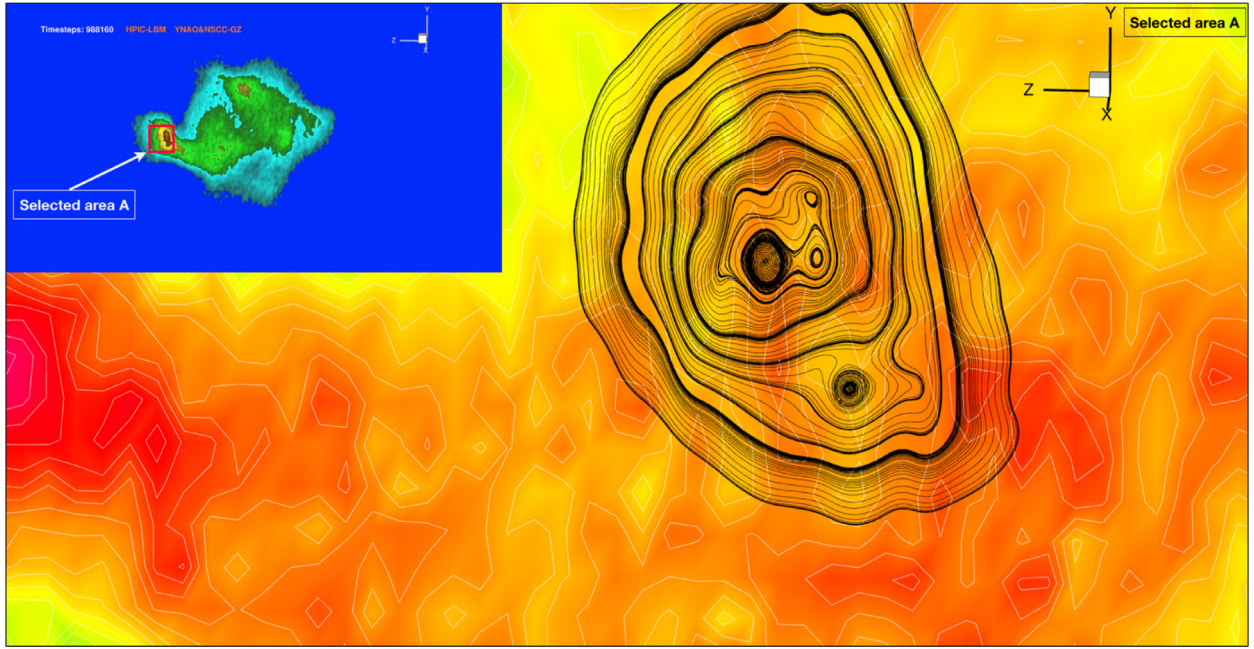


Fig. A.1. Plasma streamlines (white solid) and magnetic field lines (black solid) on the moment of 988,160 time step.

Define $\hat{t} \equiv tU_A L^{-1}$, where U_A and L is a characteristic velocity (e.g., the Alfvén velocity) and characteristic length, respectively. $\hat{\nabla} = L\nabla$, $\hat{U} = UU_A^{-1}$, the dimensionless equation can be written as,

$$\frac{\partial B}{\partial \hat{t}} = \hat{\nabla} \times (\hat{U} \times B) - \frac{\hat{\nabla}^2 B}{R_m} + \frac{\hat{\nabla} \eta}{\mu L V_A} \times (\hat{\nabla} \times B) + \frac{\beta \hat{\nabla} \times (\hat{\nabla} \times B) \times B - \beta \hat{\nabla} \times (\hat{\nabla} P_e) + \hat{\nabla} \times (\hat{\nabla} P_i)}{q_e (1 + \beta) L^2 V_A \mu} \quad (A.8)$$

Appendix B. Fine structure at different time on the same site in beyond ideal MHD region

The frozen-in condition (FIC) for ions and electrons is broken inside the dissipative region around the magnetic reconnection null points, and this beyond ideal MHD creates algorithmic challenges for LTSTMR. To verify that the RHPIC-LBM can distinguish the different evolution between the plasma motion and the magnetic field in the dissipative region, we selected a special site from the Fig. 28A and the Supplementary video 8, and show the results of fine structure at different time ($t_s = 988160, 1,018,880$ and $1,029,120$) on the same site (selected area A) in the Figs. A.1–A.3.

List of Symbols

$f_{i\xi}^{\zeta\zeta}(\mathbf{x}, \mathbf{p}, t)$	The distribution function
$\mathbf{x}$	The space coordinates
$\mathbf{p}$	The momentum
t	The time coordinates
$\mathbf{U}$	The plasma relativistic velocity
$\mathbf{F}$	The force
X	The dimension, the indices $x = 2, 3$ denote 2D model and 3D model, respectively.
q	The charge of particles
m	The rest mass of particle
B	The strength of magnetic fields
E	The strength of electric fields strength
$\mathbf{p}$	The relativistic momentum

(continued on next page)

c	Speed of light
n_α	The number density of particles
K	Boltzmann constant
T_{th}	The temperature of the thermal bath
ν_{ei}	The electron-ion collision frequency
ν_{en}	The electron-neutral collision frequency
c_0, c_a, c_t	The constants related to the size of the lattice grid
ε_i^j	The energy density including the rest mass energy
ε_i^0	The permittivity of free space with relates to the permeability of the free space
v_i^j, χ_i^j, p_i^j	Three variables closely linked to the charged particles physical properties.
χ_i^j	The adiabatic index and is $\frac{4}{3}$ for ultrarelativistic temperatures and $\frac{5}{3}$ for nonrelativistic temperatures.
c_{ip}^j	Specific heats at constant pressure
c_{iv}^j	Specific heats at constant volume
$N_{i\xi}^{\varsigma}(x, \mathbf{p}, t)$	The discrete distribution function of single particle
$(\mathbf{x}(t); \mathbf{U}_{i\xi}^{\rho e}(t))$	A single particle with orbit
$N_{i\xi}^{\rho e-ave}$	The average discrete distribution function
Δx	The adjacent lattice grid distance
n_0	The peak density in the simulation domain
n_b	The background density in the simulation domain
T_{bk}	The initial plasma temperature of background
$T_{e bk}$	The initial electron temperature of background
$T_{i bk}$	The initial ion temperature of background
$T_{e cs}$	The electron temperature of CS
$T_{i cs}$	The ion temperature of CS
$\hat{n}$	The dimensionless parameter
$\mathbf{V}$	The velocity of charged particle
n_h	The parameters closely linked to hydrogen
w	The weight function for distribution function
Greek	
ε_i^ς	The dimensional parameter
δ_i^ς	The dimensional parameter
θ_i^ς	The dimensional parameter
ε_0	Vacuum permittivity
χ	The unit time-to-relaxation time ratio
τ_i^ς	The relaxation time
ϑ	The different plane of location in D3Q7 cubic lattice grid
δ_{ij}	The Kronecker delta function
Δ	The lattice grid size
Superscripts	
ς	Refer to the physical properties of different species, $\varsigma = 1, 2, 3, \dots$ denote density, momentum and so on, respectively.
ζ	Refer to the different particles in one species, $\zeta = 1, 2, 3$ denote electron, ion and neutral, respectively.
e	Refer to the electron
i	Refer to the ion
n	Refer to the neutral particle/flow
Subscripts	
ι	Species of different compositions, $\iota = 1, 2, 3, \dots, n$ denote hydrogen, helium, oxygen, carbon, iron, neon, nitrogen and so on, respectively.
ξ	Different discretized phase space direction in $D_i^\xi X Q \xi$ cubic lattice grid discretized phase space
$\parallel$	Refer to components parallel to B
$\perp$	Refer to components perpendicular to B
e	Refer to the electron particle
i	Refer to the ion particle
n	Refer to the neutral particle
$-$	Refer to the average component of a vector
$\sim$	Refer to the fluctuation (magnetic field) or turbulence (plasma motion) component of a vector

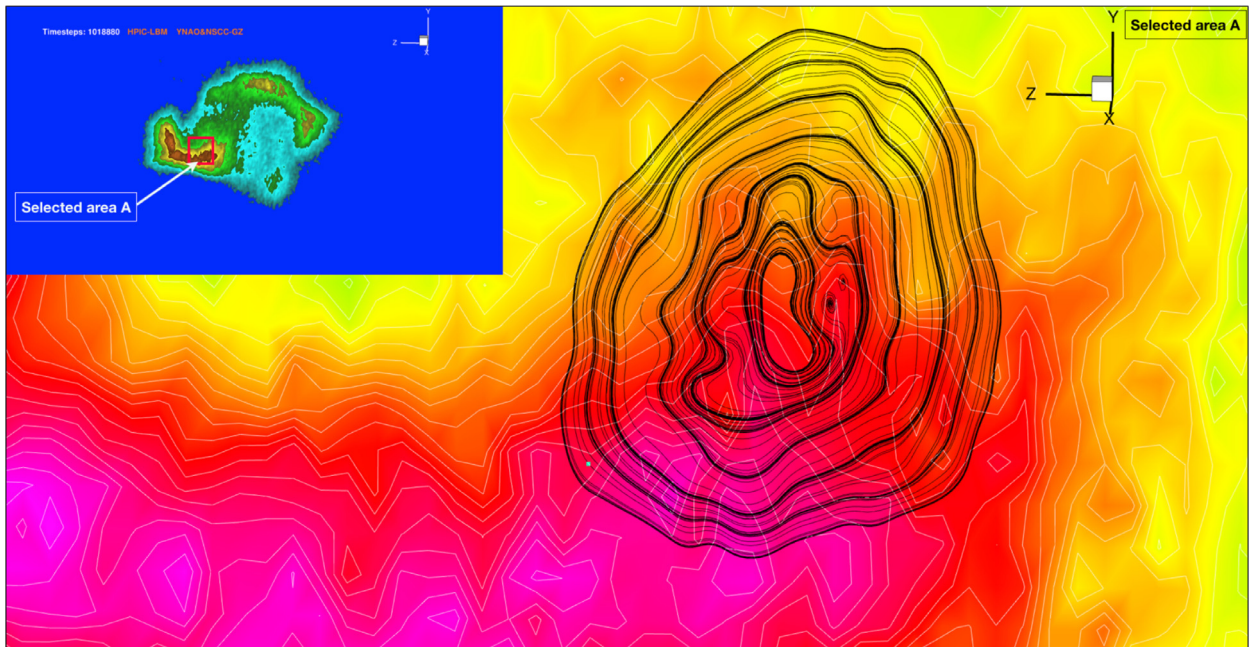


Fig. A.2. Plasma streamlines (white solid) and magnetic field lines (black solid) on the moment of 1,018,880 time step.

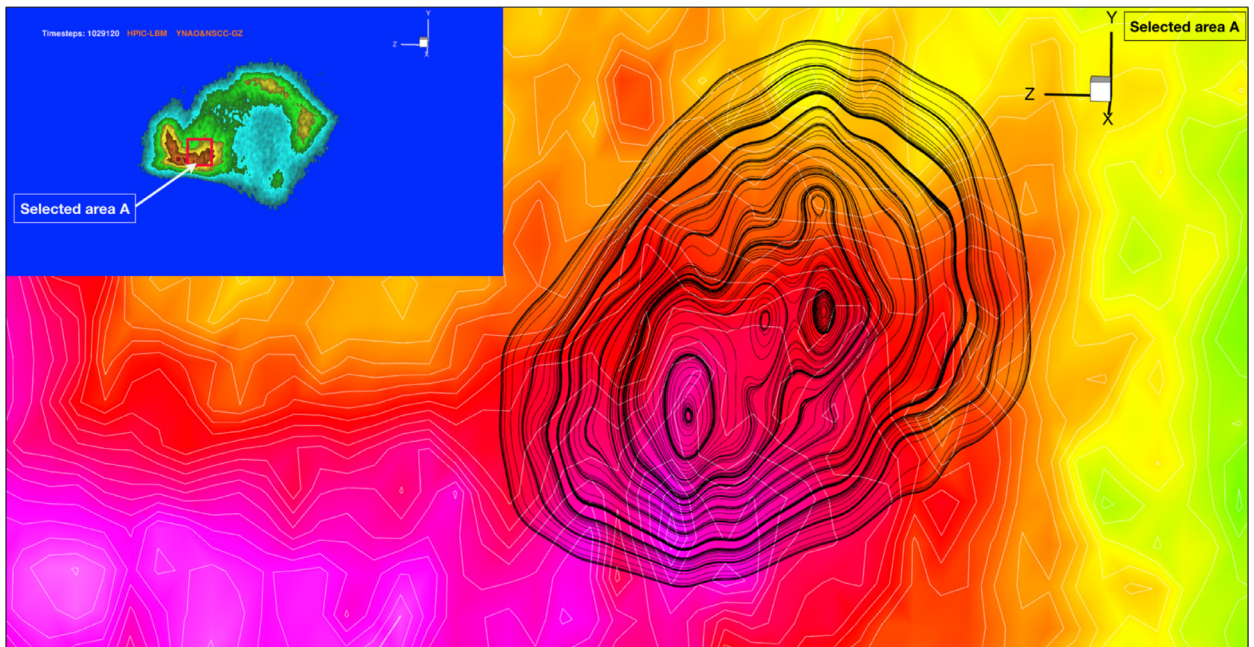


Fig. A.3. Plasma streamline (white solid) and magnetic field line (black solid) on the moment of 1,029,120 time step.

Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:[10.1016/j.apm.2019.09.043](https://doi.org/10.1016/j.apm.2019.09.043).

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