

Novel algorithms for the accurate and fast solution of the two-fluid plasma equations

X. Ke Lin, S.T. Millmore, N. Nikiforakis Laboratory for Scientific Computing, Department of Physics, University of Cambridge (xk215@cam.ac.uk)

Fusion HPC

Workshop



Introduction





≪ ≣⇒

æ

• is applicable in a regime between kinetic and MHD models





-> -< ≣ >

- is applicable in a regime between kinetic and MHD models
- valid in regimes with small length and time scales of the fundamental phenomena, such as those which occur over the Debye length, Larmor radius or plasma frequency scales

Fusion HPC

Workshop



- is applicable in a regime between kinetic and MHD models
- valid in regimes with small length and time scales of the fundamental phenomena, such as those which occur over the Debye length, Larmor radius or plasma frequency scales
- captures important physical phenomena: charge separation, Lorentz forces, self-generated electromagnetic fields, etc

Fusion HPC

Workshop



- is applicable in a regime between kinetic and MHD models
- valid in regimes with small length and time scales of the fundamental phenomena, such as those which occur over the Debye length, Larmor radius or plasma frequency scales
- captures important physical phenomena: charge separation, Lorentz forces, self-generated electromagnetic fields, etc

Fusion HPC

Workshop

3 / 46

• low-dimensionality compared to the Boltzmann equation





• Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models





< ∃ > < ∃ >





- Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models
- Reduce computational cost related to small timescales:





∃ ► < ∃ ►</p>



• Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models

Fusion HPC

Workshop

- Reduce computational cost related to small timescales:
 - Stiff source terms \rightarrow small CFL number





- Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models
- Reduce computational cost related to small timescales:
 - Stiff source terms \rightarrow small CFL number
 - \bullet Speed of light constraint \rightarrow higher than fluid speeds



A B F A B F



• Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models

∃ ► < ∃ ►</p>

4 / 46

Fusion HPC

Workshop

- Reduce computational cost related to small timescales:
 - Stiff source terms \rightarrow small CFL number
 - \bullet Speed of light constraint \rightarrow higher than fluid speeds
- Use divergence-free methods





- Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models
- Reduce computational cost related to small timescales:
 - Stiff source terms \rightarrow small CFL number
 - $\bullet~$ Speed of light constraint \rightarrow higher than fluid speeds
- Use divergence-free methods
 - Hyperbolic Divergence Cleaning (HDC) is frequently used

Fusion HPC

Workshop





- Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models
- Reduce computational cost related to small timescales:
 - Stiff source terms \rightarrow small CFL number
 - $\bullet~$ Speed of light constraint \rightarrow higher than fluid speeds
- Use divergence-free methods
 - Hyperbolic Divergence Cleaning (HDC) is frequently used

Fusion HPC

Workshop

4 / 46

• Divergence errors not completely removed





- Extending the validity of fluid models in the collisional regime and bridging the gap between fluid and kinetic models
- Reduce computational cost related to small timescales:
 - Stiff source terms \rightarrow small CFL number
 - $\bullet~$ Speed of light constraint \rightarrow higher than fluid speeds
- Use divergence-free methods
 - Hyperbolic Divergence Cleaning (HDC) is frequently used

Fusion HPC

Workshop

- Divergence errors not completely removed
- There are hyper-parameters



Governing Equations





- < 문 → < 문 →

Governing Equations

The ideal (five-moment) two-fluid plasma equations:

$$\frac{\partial \rho_{\alpha}}{\partial t} + \nabla \cdot \left(\rho_{\alpha} \boldsymbol{v}_{\alpha} \right) = 0 \tag{0.1}$$

$$\frac{\partial \rho_{\alpha} \boldsymbol{v}_{\alpha}}{\partial t} + \nabla \cdot \left[\rho_{\alpha} \boldsymbol{v}_{\alpha} \otimes \boldsymbol{v}_{\alpha} + p_{\alpha} \mathbb{I} \right] = \frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} + \boldsymbol{v}_{\alpha} \times \boldsymbol{B})$$
(0.2)

$$\frac{\partial \mathcal{E}_{\alpha}}{\partial t} + \nabla \cdot \left[\left(\mathcal{E}_{\alpha} + p_{\alpha} \right) \boldsymbol{v}_{\alpha} \right] = \frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} \cdot \boldsymbol{v}_{\alpha})$$
(0.3)

$$\frac{\partial \boldsymbol{B}}{\partial t} + \nabla \cdot \left(\mathbb{I} \times \boldsymbol{E} \right) = \boldsymbol{0} \tag{0.4}$$

$$\frac{\partial \boldsymbol{E}}{\partial t} + \nabla \cdot \left(-c^2 \mathbb{I} \times \boldsymbol{B} \right) = -\frac{1}{\lambda_D^2 r_{L_i}} (r_i \rho_i \boldsymbol{v}_i + r_e \rho_e \boldsymbol{v}_e)$$
(0.5)

where $r_{\alpha}=q_{\alpha}/m_{\alpha}$ and $\alpha=\{\text{ion,electron}\}$

UNIVERSITY OF

CAMBRIDGE

Fusion HPC Workshop

イロト イヨト イヨト イヨト

æ

Governing Equations: Fluid Equations

The ideal (five-moment) two-fluid plasma equations:

$$\frac{\partial \rho_{\alpha}}{\partial t} + \nabla \cdot \left(\rho_{\alpha} \boldsymbol{v}_{\alpha} \right) = 0$$

$$\frac{\partial \rho_{\alpha} \boldsymbol{v}_{\alpha}}{\partial t} + \nabla \cdot \left[\rho_{\alpha} \boldsymbol{v}_{\alpha} \otimes \boldsymbol{v}_{\alpha} + p_{\alpha} \mathbb{I} \right] = \frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} + \boldsymbol{v}_{\alpha} \times \boldsymbol{B})$$

$$\frac{\partial \mathcal{E}_{\alpha}}{\partial t} + \nabla \cdot \left[\left(\mathcal{E}_{\alpha} + p_{\alpha} \right) \boldsymbol{v}_{\alpha} \right] = \frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} \cdot \boldsymbol{v}_{\alpha})$$

$$\frac{\partial \boldsymbol{B}}{\partial t} + \nabla \cdot \left(\mathbb{I} \times \boldsymbol{E} \right) = \boldsymbol{0}$$
$$\frac{\partial \boldsymbol{E}}{\partial t} + \nabla \cdot \left(-c^2 \mathbb{I} \times \boldsymbol{B} \right) = -\frac{1}{\lambda_D^2 r_{L_i}} (r_i \rho_i \boldsymbol{v}_i + r_e \rho_e \boldsymbol{v}_e)$$

where $r_{\alpha} = q_{\alpha}/m_{\alpha}$ and $\alpha = \{\text{ion,electron}\}$



Fusion HPC Workshop

イロン イヨン イヨン -

7 / 46

э

Governing Equations: Maxwell Equations

The ideal (five-moment) two-fluid plasma equations:

$$\begin{aligned} \frac{\partial \rho_{\alpha}}{\partial t} + \nabla \cdot \left(\rho_{\alpha} \boldsymbol{v}_{\alpha}\right) &= 0\\ \frac{\partial \rho_{\alpha} \boldsymbol{v}_{\alpha}}{\partial t} + \nabla \cdot \left[\rho_{\alpha} \boldsymbol{v}_{\alpha} \otimes \boldsymbol{v}_{\alpha} + p_{\alpha} \mathbb{I}\right] &= \frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} + \boldsymbol{v}_{\alpha} \times \boldsymbol{B})\\ \frac{\partial \mathcal{E}_{\alpha}}{\partial t} + \nabla \cdot \left[\left(\mathcal{E}_{\alpha} + p_{\alpha}\right) \boldsymbol{v}_{\alpha} \right] &= \frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} \cdot \boldsymbol{v}_{\alpha})\\ \hline \frac{\partial \boldsymbol{B}}{\partial t} + \nabla \cdot \left(\mathbb{I} \times \boldsymbol{E}\right) &= \mathbf{0} \end{aligned}$$
$$\begin{aligned} \frac{\partial \boldsymbol{E}}{\partial t} + \nabla \cdot \left(-c^{2} \mathbb{I} \times \boldsymbol{B}\right) &= -\frac{1}{\lambda_{D}^{2} r_{L_{i}}} (r_{i} \rho_{i} \boldsymbol{v}_{i} + r_{e} \rho_{e} \boldsymbol{v}_{e}) \end{aligned}$$

where $r_{\alpha} = q_{\alpha}/m_{\alpha}$ and $\alpha = \{\text{ion,electron}\}$



Fusion HPC Workshop

8 / 46

ヘロト ヘロト ヘビト ヘビト

Governing Equations: Source Terms

The ideal (five-moment) two-fluid plasma equations:

$$\begin{aligned} \frac{\partial \rho_{\alpha}}{\partial t} + \nabla \cdot \left(\rho_{\alpha} \boldsymbol{v}_{\alpha}\right) &= 0\\ \frac{\partial \rho_{\alpha} \boldsymbol{v}_{\alpha}}{\partial t} + \nabla \cdot \left[\rho_{\alpha} \boldsymbol{v}_{\alpha} \otimes \boldsymbol{v}_{\alpha} + p_{\alpha} \mathbb{I}\right] &= \boxed{\frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} + \boldsymbol{v}_{\alpha} \times \boldsymbol{B})}\\ \frac{\partial \mathcal{E}_{\alpha}}{\partial t} + \nabla \cdot \left[(\mathcal{E}_{\alpha} + p_{\alpha}) \boldsymbol{v}_{\alpha} \right] &= \boxed{\frac{r_{\alpha}}{r_{L_{i}}} \rho_{\alpha} (\boldsymbol{E} \cdot \boldsymbol{v}_{\alpha})}\\ \frac{\partial \boldsymbol{B}}{\partial t} + \nabla \cdot \left(\mathbb{I} \times \boldsymbol{E} \right) &= \mathbf{0}\\ \frac{\partial \boldsymbol{E}}{\partial t} + \nabla \cdot \left(-c^{2} \mathbb{I} \times \boldsymbol{B} \right) &= \boxed{-\frac{1}{\lambda_{D}^{2} r_{L_{i}}} (r_{i} \rho_{i} \boldsymbol{v}_{i} + r_{e} \rho_{e} \boldsymbol{v}_{e})} \end{aligned}$$

where $r_{\alpha} = q_{\alpha}/m_{\alpha}$ and $\alpha = \{\text{ion,electron}\}$



Fusion HPC Workshop

9 / 46

イロン イヨン イヨン -

Governing Equations: Divergence Constraints

$$\nabla \cdot \boldsymbol{E} = \frac{\sigma}{\epsilon_0} \tag{0.6}$$
$$\nabla \cdot \boldsymbol{B} = 0 \tag{0.7}$$

Workshop

10 / 46

where $\sigma = q_i n_i + q_e n_e$ is the net charge density







★ 문 ► ★ 문 ►

11 / 46

æ

• Fluid equations:



- ▲日を ▲ 国を ▲ 国を 一国 うろのの

Fusion HPC Workshop

- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD

-> -< ≣ >

12 / 46

Fusion HPC

Workshop



• Fluid equations:

- Spatial reconstruction: 2nd-order TVD
- Hyperbolic solver: HLLC solver





-∢ ≣⇒

• Fluid equations:

- Spatial reconstruction: 2nd-order TVD
- Hyperbolic solver: HLLC solver
- Temporal discretization: explicit RK2





- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:

Fusion HPC

Workshop



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]

Fusion HPC

Workshop



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint

Fusion HPC

Workshop



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint

Fusion HPC

Workshop

12 / 46

• Finite-volume time-domain (FVTD) [6, 7, 8]



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint
 - Finite-volume time-domain (FVTD) [6, 7, 8]
 - Spatial reconstruction: 2nd-order TVD or 3rd-order WENO

Fusion HPC

Workshop



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint
 - Finite-volume time-domain (FVTD) [6, 7, 8]
 - Spatial reconstruction: 2nd-order TVD or 3rd-order WENO

G → A ≧ → A ≧ Fusion HPC

Workshop

12 / 46

• Hyperbolic solver: Multidimensional Riemann solver [6]



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint
 - Finite-volume time-domain (FVTD) [6, 7, 8]
 - Spatial reconstruction: 2nd-order TVD or 3rd-order WENO
 - Hyperbolic solver: Multidimensional Riemann solver [6]
 - $\bullet~$ Temporal discretization: explicit RK2 with ${\bf sub-cycling} \rightarrow c~{\rm constraint}$

✓ ② → < ≧ → < ≧ →</p>
Fusion HPC

Workshop



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint
 - Finite-volume time-domain (FVTD) [6, 7, 8]
 - Spatial reconstruction: 2nd-order TVD or 3rd-order WENO
 - Hyperbolic solver: Multidimensional Riemann solver [6]
 - $\bullet~$ Temporal discretization: explicit RK2 with ${\bf sub-cycling} \rightarrow c~{\rm constraint}$

✓ ② → < ≧ → < ≧ →</p>
Fusion HPC

Workshop

12 / 46

• Source terms:



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint
 - Finite-volume time-domain (FVTD) [6, 7, 8]
 - Spatial reconstruction: 2nd-order TVD or 3rd-order WENO
 - Hyperbolic solver: Multidimensional Riemann solver [6]
 - $\bullet~$ Temporal discretization: explicit RK2 with ${\bf sub-cycling} \rightarrow c~{\rm constraint}$

伺 と く ヨ と く ヨ と

12 / 46

Fusion HPC

Workshop

- Source terms:
 - Strang splitting



- Fluid equations:
 - Spatial reconstruction: 2nd-order TVD
 - Hyperbolic solver: HLLC solver
 - Temporal discretization: explicit RK2
- Maxwell equations \rightarrow divergence-free techniques:
 - Finite-difference time-domain (FDTD) [1, 2, 3]
 - implicit Crank-Nicolson [4, 5] $\rightarrow c$ constraint
 - Finite-volume time-domain (FVTD) [6, 7, 8]
 - Spatial reconstruction: 2nd-order TVD or 3rd-order WENO
 - Hyperbolic solver: Multidimensional Riemann solver [6]
 - $\bullet~$ Temporal discretization: explicit RK2 with ${\bf sub-cycling} \rightarrow c~{\rm constraint}$

G→ <≧> <≧> Fusion HPC

Workshop

- Source terms:
 - Strang splitting
 - locally implicit midpoint method [9] $\rightarrow CFL$ constraint



The conserved variables are grouped into three categories

$$U_1 = \{\rho_i, \rho_e, B\}^{\mathsf{T}}, \quad U_2 = \{\rho_i v_i, \rho_e v_e, E\}^{\mathsf{T}}, \quad U_3 = \{\mathcal{E}_i, \mathcal{E}_e\}^{\mathsf{T}}$$

then the (first-order [10]) update formula can be written as:

$$\boldsymbol{U}_1^{n+1} = \overline{\boldsymbol{U}}_1^n \tag{0.8}$$

Fusion HPC

Workshop

13 / 46

$$\boldsymbol{U}_{2}^{n+1} = \overline{\boldsymbol{U}}_{2}^{n} + \Delta t \, \boldsymbol{A}(\boldsymbol{U}_{1}^{n+1}) \boldsymbol{U}_{2}^{n+1}$$
(0.9)

$$U_{3}^{n+1} = \overline{U}_{3}^{n} + \Delta t \, S_{3}(U_{1}^{n+1}, U_{2}^{n+1})$$
(0.10)

The implicit step can be written as:

$$\boldsymbol{U}_{2}^{n+1} = (\mathbb{I} - \Delta t \, \boldsymbol{A}(\boldsymbol{U}_{1}^{n+1}))^{-1} \overline{\boldsymbol{U}}_{2}^{n}$$

$$(0.11)$$

Remark

This update allows a high CFL number. Second-order accuracy achieved by using the implicit midpoint method [9]



Innovations





< ∃⇒

æ

Innovations: FDTD (divergence-free technique)

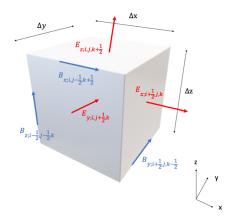


Figure: Collocation of the electromagnetic fields in FDTD. The magnetic field is defined at the edges and the electric field is defined at the faces, a = a = a = a



Fusion HPC Workshop

Innovations: FDTD

It is based on a second-order accurate Crank-Nicolson scheme and the semi-implicit discretization can be written as

$$\frac{\boldsymbol{E}^{n+1} - \boldsymbol{E}^n}{\Delta t} = c^2 \left(\frac{1}{2} \nabla \times \boldsymbol{B}^n + \frac{1}{2} \nabla \times \boldsymbol{B}^{n+1} \right)$$
(0.12)

$$\frac{\mathbf{B}^{n+1} - \mathbf{B}^n}{\Delta t} = -\left(\frac{1}{2}\nabla \times \mathbf{E}^n + \frac{1}{2}\nabla \times \mathbf{E}^{n+1}\right)$$
(0.13)

Fusion HPC

Workshop

16 / 46

which can be rearranged into the implicit equation

$$\left(1 - \frac{c^2 \Delta t^2}{4} \nabla^2\right) \left[\frac{\boldsymbol{B}^{n+1} - \boldsymbol{B}^n}{\Delta t}\right] = -\nabla \times \boldsymbol{E}^n + \frac{c^2 \Delta t}{2} \nabla^2 \boldsymbol{B}^n \qquad (0.14)$$

Remark

This implicit update relaxes the speed of light constraint.



Innovations: FVTD (divergence-free technique)

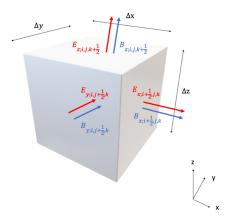


Figure: Collocation of the electromagnetic fields in FVTD. The magnetic field and the electric field are defined at the faces.



Fusion HPC Workshop

The explicit update for the x-components in 2D are

$$B_{x,i+\frac{1}{2},j}^{n+1} = B_{x,i+\frac{1}{2},j}^{n} - \frac{\Delta t}{\Delta y} \Big(E_{z,i+\frac{1}{2},j+\frac{1}{2}}^{*} - E_{z,i+\frac{1}{2},j-\frac{1}{2}}^{*} \Big)$$
(0.15)
$$E_{x,i+\frac{1}{2},j}^{n+1} = E_{x,i+\frac{1}{2},j}^{n} + c^{2} \frac{\Delta t}{\Delta y} \Big(B_{z,i+\frac{1}{2},j+\frac{1}{2}}^{*} - B_{z,i+\frac{1}{2},j-\frac{1}{2}}^{*} \Big)$$
(0.16)

< ロ > < 回 > < 回 > < 回 > < 回 >

Fusion HPC

Workshop

18 / 46

where B_z^* and E_z^* are states from the Multidimensional Riemann solver [6].

Remark

These updates are constrained by the speed of light. Sub-cycling can be used to relax the constraint.



Innovations: Projection methods [11, 12]

Remark

Projection methods are used to reduce divergence errors from averaging electric fields from cell centers to cell faces.

One can express the electric field (with divergence errors) E^* in terms of a constraint-preserving part E^c and a scalar ϕ as

$$\boldsymbol{E}^* = \boldsymbol{E}^c + \nabla \phi \tag{0.17}$$

so that one can solve for the potential ϕ as

$$\nabla^2 \phi = \nabla \cdot \boldsymbol{E}^* - \frac{\sigma}{\epsilon_0} \tag{0.18}$$

and the constraint-preserving electric field can be recovered as

$$E^{c} = E^{*} - \nabla \phi \qquad (0.19)$$
Fusion HPC
$$19 / 46$$
Workshop



- () update the source terms at cell centers for $\Delta t_{fluid}/2$
- obtain face-averaged electric field
- O advance the fluid variables for Δt_{fluid} using spatial reconstructions and RK time stepping
- (a) use FDTD with an implicit update for Δt_{fluid} or use FVTD with sub-cycling with Δt_c

・ 同 ト ・ ヨ ト ・ ヨ ト

20 / 46

Fusion HPC

Workshop

- obtain cell-averaged electromagnetic fields
- ${\small \small \bigcirc}$ update the source terms at cell centers for $\Delta t_{fluid}/2$
- ø obtain face-averaged electric field
- use projection methods to reduce electric divergence errors



Results





≪ ≣⇒

21 / 46

æ

• Computational Framework: AMReX



Fusion HPC Workshop

< ロ > < 回 > < 回 > < 回 > < 回 >



æ

- Computational Framework: AMReX
- Parallelization using MPI





< 日 ▶



- Computational Framework: AMReX
- Parallelization using MPI
- Run on a desktop with 16 cores unless otherwise specified

Workshop



- Computational Framework: AMReX
- Parallelization using MPI
- Run on a desktop with 16 cores unless otherwise specified
- Aim will be to compare implicit FDTD and explicit FVTD with sub-cycling

22 / 46

Fusion HPC

Workshop



- Computational Framework: AMReX
- Parallelization using MPI
- Run on a desktop with 16 cores unless otherwise specified
- Aim will be to compare implicit FDTD and explicit FVTD with sub-cycling
- FVTD results used 2nd-order TVD unless otherwise specified

Fusion HPC

Workshop



- Computational Framework: AMReX
- Parallelization using MPI
- Run on a desktop with 16 cores unless otherwise specified
- Aim will be to compare implicit FDTD and explicit FVTD with sub-cycling
- FVTD results used 2nd-order TVD unless otherwise specified
- As a reference, results using HDC and FVTD without sub-cycling are also shown

Fusion HPC

Workshop



Computational domain: [0,1]								
Transmissive boundaries								
	$ ho_i$	$ ho_e$	$oldsymbol{v}_lpha$	p_{lpha}	B_x	B_y	B_x	E
Left	1.0	1.0/m	0.0	0.5	0.75	1.0	0.0	0.0
Right	0.125	0.125/m	0.0	0.05	0.75	-1.0	0.0	0.0

Table: Initial data for the two-fluid Brio and Wu test.

▶ < E >

23 / 46

17 ▶ **Fusion HPC**

Workshop

$$\gamma=5/3$$
 , $r_{L_i}=\{1,0.1\}$, $\lambda_D=0.01$, $m=m_i/m_e=1836$ and $c=100$



Results: Brio and Wu Test

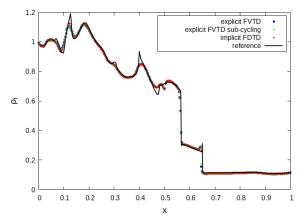


Figure: Ion density for the two-fluid Brio and Wu test for $r_{L_i} = 0.1$ using 1024 cells at t = 0.1. Reference from Abgrall and Kumar [10] using 10016 cells.



Fusion HPC Workshop

Results: Brio and Wu Test

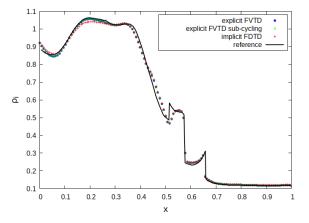


Figure: Ion density for the two-fluid Brio and Wu test for $r_{L_i} = 1$ using 1024 cells at t = 0.1. Reference from Abgrall and Kumar [10] using 10016 cells. FVTD solutions were slightly more accurate.



Fusion HPC Workshop

Maxwell	Time stepping	Steps	CPU time (s)	CPU time/step (s)	
FVTD	explicit	25600	250.46	$9.78 \cdot 10^{-3}$	
FVTD	explicit sub-cycling	13115	147.51	$1.12\cdot 10^{-2}$	
FDTD	implicit	13281	174.14	$1.31 \cdot 10^{-2}$	

Table: CPU timings for the Brio and Wu test for $r_{L_i} = 1$.

Observations

Sub-cycling and implicit time stepping reduced the number of steps and the CPU times. In this problem, $\Delta t_{fluid} \approx 2\Delta t_c$ and sub-cycling is more efficient.

< ロ > < 回 > < 回 > < 回 > < 回 >

Fusion HPC

Workshop



Computational domain: $[0, 2\pi] \times [0, 2\pi]$						
Periodic boundaries						
ρ_{α}	$oldsymbol{v}_lpha$	p_{lpha}	B	E		
γ^2	$\begin{pmatrix} -\sin(y)\\ \sin(x)\\ 0.0 \end{pmatrix}$	γ	$\begin{pmatrix} -\sin(y)\\\sin(2x)\\0.0 \end{pmatrix}$	$-oldsymbol{v}_lpha imesoldsymbol{B}$		

Table: Initial data for the ideal MHD Orszag-Tang vortex.

$$\gamma=5/3,\,r_{L_i}=0.01,\,\lambda_D=0.1,\,r_i=-r_e=1$$
 and $c=10$

Remark

UNIVERSITY OF

CAMBRIDGE

Small Larmor radius r_{L_i} models the MHD regime.

Fusion HPC Workshop

・ロト ・日ト ・モト・モート



э

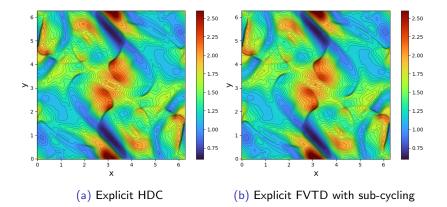


Figure: Ion density for the Orszag-Tang vortex using 256^2 cells at t = 5. Very similar solutions but HDC required some parameter tuning. HDC was also more expensive than FVTD.



Fusion HPC Workshop

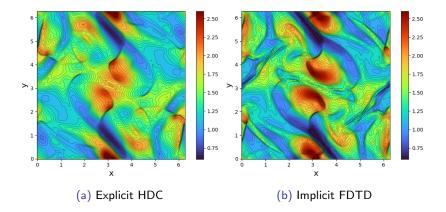
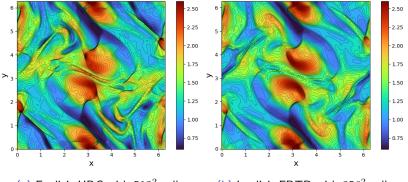


Figure: Ion density for the Orszag-Tang vortex using 256^2 cells at t = 5. FDTD captured better the features.

Fusion H<u>PC</u>

Workshop





(a) Explicit HDC with 512^2 cells (b) Implicit FDTD with 256^2 cells

.⊒ ▶ ∢

30 / 46

Fusion HPC

Workshop

Figure: Ion density for the Orszag-Tang vortex at t = 5. FDTD solution was close to a high resolution solution.



Maxwell	Time stepping	Steps	CPU time (s)	CPU time/step (s)	
HDC	explicit	5093	911.64	0.18	
FVTD	explicit sub-cycling	1147	235.41	0.21	
FDTD	implicit	1205	203.84	0.17	

Table: CPU timings for the ideal MHD Orszag-Tang vortex using 256^2 cells.

The high resolution (512^2 cells) fully explicit HDC method took 7514.98s (about 35 times more than the low resolution implicit FDTD method).

Observations

In this problem $\Delta t_{fluid} \approx 4\Delta t_c$. When the speed of light is much higher than the fluid speeds, sub-cycling loop becomes more expensive and less efficient than implicit time stepping.

Fusion HPC

Workshop



 $\label{eq:computational domain: } \begin{array}{|c|c|} \hline Computational domain: \ [-L_x/2, L_x/2] \times [-L_y/2, L_y/2] \\ \hline Periodic in the x-direction and conducting wall in the y-axis \\ \hline n & v_{z,e} & \mathsf{p} & B_x \\ \hline n_0(sech^2(\frac{y}{\lambda}) + \frac{1}{5}) & j_z/n_eq_e & B_0^2/2\,(sech^2(\frac{y}{\lambda}) + \frac{1}{5}) & B_0tanh(\frac{y}{\lambda}) \end{array}$

Table: Initial data for the unperturbed Harris sheet configuration.

Fusion HPC

Workshop

Perturbation:
$$-\hat{e}_z \times \nabla \left(\frac{1}{10} \cos \left(\frac{2\pi x}{L_x} \right) \cos \left(\frac{\pi y}{L_y} \right) \right)$$

 $n_0 = 1.0, B_0 = 1.0 \ \lambda = 0.5, L_x = 25.6, L_y = 12.8$
 $\gamma = 5/3, r_{L_i} = 1, \lambda_D = 0.1, m_i/m_e = 25 \text{ and } c = 10$



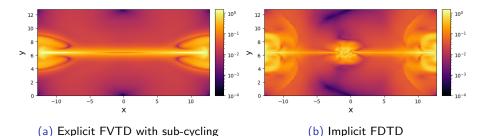
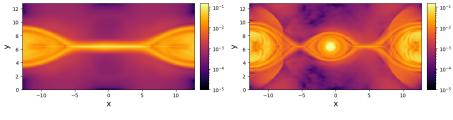


Figure: Ion momentum for the GEM reconnection challenge with using 512×256 cells at t = 25 (log-scale). The central magnetic island could be captured by the FDTD method.

Fusion HPC

Workshop





(a) Explicit FVTD with sub-cycling

(b) Implicit FDTD

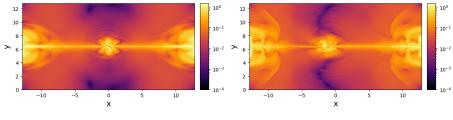
Fusion HPC

Workshop

34 / 46

Figure: Electron momentum for the GEM reconnection challenge with using 512×256 cells at t = 25 (log-scale). The central magnetic island could be captured by the FDTD method.





(a) Explicit FVTD with sub-cycling

(b) Implicit FDTD

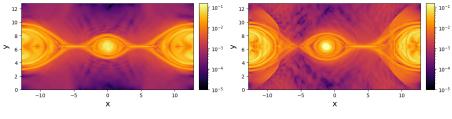
Fusion HPC

Workshop

35 / 46

Figure: Ion momentum for the GEM reconnection challenge using 1024×512 cells at t = 25 (log-scale). FVTD method needed high resolution to capture the magnetic island.





(a) Explicit FVTD with sub-cycling

(b) Implicit FDTD

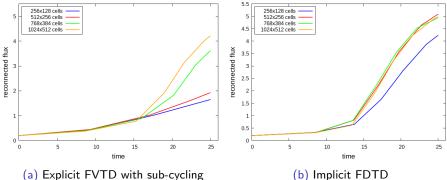
Fusion HPC

Workshop

36 / 46

Figure: Electron momentum for the GEM reconnection challenge using 1024×512 cells at t = 25 (log-scale). FVTD method needed high resolution to capture the magnetic island.





(b) Implicit FDTD

イロト イヨト イヨト イヨ

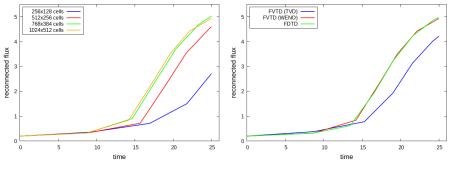
Fusion HPC

Workshop

37 / 46

Figure: Reconnected fluxes for the GEM reconnection challenge. The FDTD method reached convergence faster.





(a) FVTD (WENO) with sub-cycling

(b) Comparison using 1024×512 cells

Fusion HPC

Workshop

38 / 46

Figure: Reconnected fluxes for the GEM reconnection challenge. FVTD with 3rd-order WENO is also shown (all previous FVTD results used 2nd-order TVD). FVTD with WENO and FDTD solutions had the same reconnected fluxes.



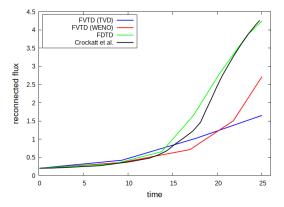


Figure: Reconnected fluxes for the GEM reconnection challenge using 256×128 cells. Reference solutions from Crockatt et al. [13] using 960×480 cells. The low resolution implicit FDTD method produced a similar reconnected flux to the high resolution reference case.



Fusion HPC Workshop

Conclusion





< ∃⇒

40 / 46

æ

• The speed of light constraint was relaxed and divergence-free methods were used





- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems





41 / 46

< 回 > < 回 > < 回 >

- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)

✓ ② → < ≧ → < ≧ →</p>
Fusion HPC

Workshop



- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)

Fusion HPC

Workshop

41 / 46

• FVTD method with 3rd-order WENO



- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)
- FVTD method with 3rd-order WENO
 - More efficient (at achieving given accuracy) than FVTD with 2nd-order TVD

✓ ② → < ≧ → < ≧ →</p>
Fusion HPC

Workshop



- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)
- FVTD method with 3rd-order WENO
 - More efficient (at achieving given accuracy) than FVTD with 2nd-order TVD

✓ ② → < ≧ → < ≧ →</p>
Fusion HPC

Workshop

41 / 46

• More expensive than FDTD method



- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)
- FVTD method with 3rd-order WENO
 - More efficient (at achieving given accuracy) than FVTD with 2nd-order TVD

Fusion HPC

Workshop

- More expensive than FDTD method
- Higher-order WENO might become more efficient



- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)
- FVTD method with 3rd-order WENO
 - More efficient (at achieving given accuracy) than FVTD with 2nd-order TVD

Fusion HPC

Workshop

- More expensive than FDTD method
- Higher-order WENO might become more efficient
- Next steps: 10-moment two-fluid model (and higher moments)



- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)
- FVTD method with 3rd-order WENO
 - More efficient (at achieving given accuracy) than FVTD with 2nd-order TVD

・ロト ・回ト ・ヨト ・ヨト

Fusion HPC

Workshop

- More expensive than FDTD method
- Higher-order WENO might become more efficient
- Next steps: 10-moment two-fluid model (and higher moments)
 - 5-moment model assumes local thermal equilibrium



- The speed of light constraint was relaxed and divergence-free methods were used
- Implicit FDTD method was more efficient in most problems
- FVTD method was better for problems with very strong initial discontinuities (e.g. Brio and Wu test)
- FVTD method with 3rd-order WENO
 - More efficient (at achieving given accuracy) than FVTD with 2nd-order TVD
 - More expensive than FDTD method
 - Higher-order WENO might become more efficient
- Next steps: 10-moment two-fluid model (and higher moments)
 - 5-moment model assumes local thermal equilibrium
 - $\bullet\,$ Higher-moment models describe the deviation from the local thermal equilibrium $\to\,$ transition from high to low collisionality plasmas



Fusion HPC Workshop Special thanks to S.T. Millmore and N. Nikiforakis for invaluable guidance and mentorship. Appreciation to the Laboratory for Scientific Computing team members who contributed to various aspects of this work.

This work was supported by the University of Cambridge Harding Distinguished Postgraduate Scholars Programme and the Centre for Scientific Computing.



Thank you!





★ 문 ► ★ 문 ►

43 / 46

æ

- K. Yee. "Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media". In: *IEEE Transactions on antennas and propagation* 14.3 (1966), pp. 302–307.
- [2] A. Taflove and M. E. Brodwin. "Numerical solution of steady-state electromagnetic scattering problems using the time-dependent Maxwell's equations". In: *IEEE transactions on microwave theory and techniques* 23.8 (1975), pp. 623–630.
- [3] A. Taflove. "Review of the formulation and applications of the finite-difference time-domain method for numerical modeling of electromagnetic wave interactions with arbitrary structures". In: *Wave Motion* 10.6 (1988), pp. 547–582.
- C Sun and C. Trueman. "Unconditionally stable Crank-Nicolson scheme for solving two-dimensional Maxwell's equations". In: *Electronics letters* 39.7 (2003), pp. 595–597.

Fusion HPC

Workshop



References II

- [5] Y Yang, R. Chen, and E. K. Yung. "The unconditionally stable Crank Nicolson FDTD method for three-dimensional Maxwell's equations". In: *Microwave and Optical Technology Letters* 48.8 (2006), pp. 1619–1622.
- [6] D. S. Balsara et al. "A high-order relativistic two-fluid electrodynamic scheme with consistent reconstruction of electromagnetic fields and a multidimensional Riemann solver for electromagnetism". In: *Journal of Computational Physics* 318 (2016), pp. 169–200.
- [7] D. S. Balsara et al. "Computational electrodynamics in material media with constraint-preservation, multidimensional Riemann solvers and sub-cell resolution-Part I, second-order FVTD schemes". In: *Journal of Computational Physics* 349.C (2017).
- [8] D. S. Balsara et al. "Computational electrodynamics in material media with constraint-preservation, multidimensional Riemann solvers and sub-cell resolution-Part II, higher order FVTD schemes". In: *Journal of Computational Physics* 354 (2018), pp. 613–645.

イロト イヨト イヨト イヨト

Fusion HPC

Workshop



References III

- [9] L. Wang et al. "Exact and locally implicit source term solvers for multifluid-Maxwell systems". In: *Journal of Computational Physics* 415 (2020), p. 109510.
- [10] R. Abgrall and H. Kumar. "Robust finite volume schemes for two-fluid plasma equations". In: *Journal of Scientific Computing* 60 (2014), pp. 584–611.
- [11] J. Bell, L. Howell, and P. Colella. "An efficient second-order projection method for viscous incompressible flow". In: 10th Computational Fluid Dynamics Conference. 1991, p. 1560.
- [12] J. U. Brackbill and D. C. Barnes. "The effect of nonzero ∇ · B on the numerical solution of the magnetohydrodynamic equations". In: *Journal of Computational Physics* 35.3 (1980), pp. 426–430.
- [13] M. M. Crockatt et al. "An implicit monolithic AFC stabilization method for the CG finite element discretization of the fully-ionized ideal multifluid electromagnetic plasma system". In: *Journal of Computational Physics* 464 (2022), p. 111228.

<ロ> (日) (日) (日) (日) (日)

Fusion HPC

Workshop

