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# A geometric PIC Discretization of Vlasov–Maxwell Equations: Drift-Kinetic and Fully Kinetic Models in GEMPICX

IPP


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# Motivation

- Gyrokinetic modelling and beyond
- Plasma simulations require preserving conservation laws
- Edge/SOL regions in fusion devices need hybrid models
- Structure-preserving methods avoid numerical artifacts
- TSVV-4 D3 Investigating the limitations of gyrokinetics

# Overview: Field based gyrokinetics

We have proposed a new gyrokinetic model that includes the full electromagnetic fields and can be expressed as a macroscopic Vlasov-Maxwell system.

- gauge invariant. Can be expressed in terms of $\boldsymbol{E}_1$ and $\boldsymbol{B}_1$
- yields (compatible) macroscopic Maxwell's equations wherein the gyrokinetic model is a material property (with magnetization **M** and polarization **P**)
- possesses **equilibrium solutions** (field equations are satisfied if $\boldsymbol{E}_1 = \boldsymbol{B}_1 = 0$ )
- stems from a variational principle and is therefore energy conserving
- is suitable for **structure preserving** methods (i.e. gyrokinetic GEMPICX)

*Kraus et al. Journal of Plasma Physics 83.4 (2017): 905830401.*
*Kormann et al SIAM Journal on Scientific Computing 46.5 (2024): B621-B646*
***Guo Meng et al 2025 Plasma Phys. Control. Fusion 67 055007***

# Outline

1. **Physical Model**
2. Numerical Discretization: Mimetic Finite Differences
3. Numerical Results, Verification & Validation
4. Summary & Outlook

# A gauge-free DK model derived from an action principle

Hamiltonian of particle $H = q\phi + K$

$$K_0 = \frac{1}{2} m {v_\shortparallel}^2 + \mu |\boldsymbol{B}_{\text{ext}}|,$$

$$K_1 = \mu \boldsymbol{b}_{\text{ext}} \cdot \boldsymbol{B},$$

$$K_2 = \left(\mu |\boldsymbol{B}_{\text{ext}}| - m {v_\shortparallel}^2\right) \frac{|\boldsymbol{B}_\perp|^2}{2|\boldsymbol{B}_{\text{ext}}|^2} - \frac{m|\boldsymbol{E}_\perp|^2}{2|\boldsymbol{B}_{\text{ext}}|^2} - \frac{m v_\shortparallel \boldsymbol{E} \times \boldsymbol{b}_{\text{ext}} \cdot \boldsymbol{B}}{|\boldsymbol{B}_{\text{ext}}|^2},$$

$$\mathbf{P} = -\int \frac{\delta K}{\delta \boldsymbol{E}} f B_\shortparallel^* \mathrm{d}v_\shortparallel \mathrm{d}\mu,$$

$$\mathbf{M} = -\int \frac{\delta K}{\delta \boldsymbol{B}} f B_\shortparallel^* \mathrm{d}v_\shortparallel \mathrm{d}\mu.$$

$\boldsymbol{B}_{\text{ext}}$: external equilibrium magnetic field;

$\boldsymbol{E},\ \boldsymbol{B}$: perturbed fields, gauge-free.

*Burby J W and Brizard A J 2019 Phys. Lett. A 383 2172–5*

# Macroscopic Maxwell's equations in strong form for gyrocenters

- Ampère $\partial \mathbf{D}/\partial t - \nabla \times \mathbf{H} = -\mathbf{J}_{gc}$ (1)
- Faraday $\partial \mathbf{B}/\partial t + \nabla \times \mathbf{E} = 0$ (2)
- $\nabla \cdot \mathbf{D} = \rho_{gc}$ (3)
- $\nabla \cdot \mathbf{B} = 0$ (4)
- PIC $\boldsymbol{J}_{gc} = q\int \boldsymbol{v}_{gc} f B_{\shortparallel}^* \mathrm{d}v_{\shortparallel}\mathrm{d}\mu$

$$\boldsymbol{D} = \epsilon_0 \boldsymbol{E} + \mathbf{P},$$

$$\boldsymbol{H} = \frac{1}{\mu_0}(\boldsymbol{B}_{\text{ext}} + \boldsymbol{B}) - \mathbf{M}$$

- GC equation of motion

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = \frac{1}{B_{\shortparallel}^*}\left(\frac{1}{m}\frac{\partial K}{\partial V_{\shortparallel}}\boldsymbol{B}^* + \left(\boldsymbol{E} - \frac{1}{q}\frac{\mathrm{d}K}{\mathrm{d}\boldsymbol{X}}\right) \times \boldsymbol{b}_{\text{ext}}\right) = \boldsymbol{v}_{gc},$$

$$\frac{\mathrm{d}V_{\shortparallel}}{\mathrm{d}t} = \frac{1}{B_{\shortparallel}^*}\left(\frac{q}{m}\boldsymbol{E} - \frac{1}{m}\frac{\mathrm{d}K}{\mathrm{d}\boldsymbol{X}}\right)\cdot \boldsymbol{B}^* = a_{gc}.$$

$$\boldsymbol{A}^* = \boldsymbol{A} + \boldsymbol{A}_{\text{ext}} + \frac{m}{q}v_{\shortparallel}\boldsymbol{b}_{\text{ext}}, \quad \boldsymbol{B}^* = \nabla \times \boldsymbol{A}^*$$

$$= \boldsymbol{B} + \boldsymbol{B}_{\text{ext}} + \frac{m}{q}v_{\shortparallel}\nabla \times \boldsymbol{b}_{\text{ext}}, \quad B_{\shortparallel}^* = \boldsymbol{B}^* \cdot \boldsymbol{b}_{\text{ext}}$$

- magnetization **M** and polarization **P**

$$\mathbf{P}(t,\boldsymbol{x}) = -\int \frac{\delta K}{\delta \boldsymbol{E}} f B_{\shortparallel}^* \,\mathrm{d}v_{\shortparallel}\,\mathrm{d}\mu = \frac{m}{|\boldsymbol{B}_{\text{ext}}|^2}\int (\boldsymbol{E}_\perp + v_{\shortparallel}\boldsymbol{b}_{\text{ext}} \times \boldsymbol{B}) f B_{\shortparallel}^* \,\mathrm{d}v_{\shortparallel}\,\mathrm{d}\mu.$$

For a centered Maxwellian

$$\mathbf{P}(t,\boldsymbol{x}) = \frac{m n_M(\boldsymbol{x})\boldsymbol{E}_\perp(t,\boldsymbol{x})}{|\boldsymbol{B}_{\text{ext}}(\boldsymbol{x})|^2},$$

$$\mathbf{M}(t,\boldsymbol{x}) = -\boldsymbol{b}_{\text{ext}}\int \mu f B_{\shortparallel}^* \mathrm{d}v_{\shortparallel}\mathrm{d}\mu.$$

- polarization current $\boldsymbol{J}_{\text{pol}} = \partial \boldsymbol{P}/\partial t$

# Hybrid model--DK electrons & FK ions

$$\frac{\partial \boldsymbol{D}}{\partial t} - \nabla \times \boldsymbol{H} = -\boldsymbol{J},$$

$$\frac{\partial \boldsymbol{B}}{\partial t} + \nabla \times \boldsymbol{E} = 0,$$

$$\boldsymbol{D} = \epsilon_0 \boldsymbol{E} + \boldsymbol{P} = \epsilon_0 \left( \boldsymbol{E} + \frac{c^2}{v_{A,e}^2} (\boldsymbol{E}_\perp + u_{\shortparallel,e} \boldsymbol{b}_{\text{ext}} \times \boldsymbol{B}) \right),$$

$$\boldsymbol{H} = \frac{1}{\mu_0} (\boldsymbol{B}_{\text{ext}} + \boldsymbol{B}) - \boldsymbol{M} = \frac{1}{\mu_0} \left( (1 + \frac{1}{2}\beta_e) \boldsymbol{B}_{\text{ext}} + \boldsymbol{B} - \frac{u_{\shortparallel,e}}{V_{A,e}(\boldsymbol{x})^2} \boldsymbol{E} \times \boldsymbol{b}_{\text{ext}} \right)$$

$$\boldsymbol{J} = q_e \int \boldsymbol{v}_{gc,e} f B_\shortparallel^* \, \mathrm{d}v_\shortparallel \, \mathrm{d}\mu + q_i \int f_i \boldsymbol{v} \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{v} = \boldsymbol{J}_{gc,e} + \boldsymbol{J}_i,$$

Drift kinetic — Fully kinetic

**GEMPICX**: C++
Based on the AMReX software framework

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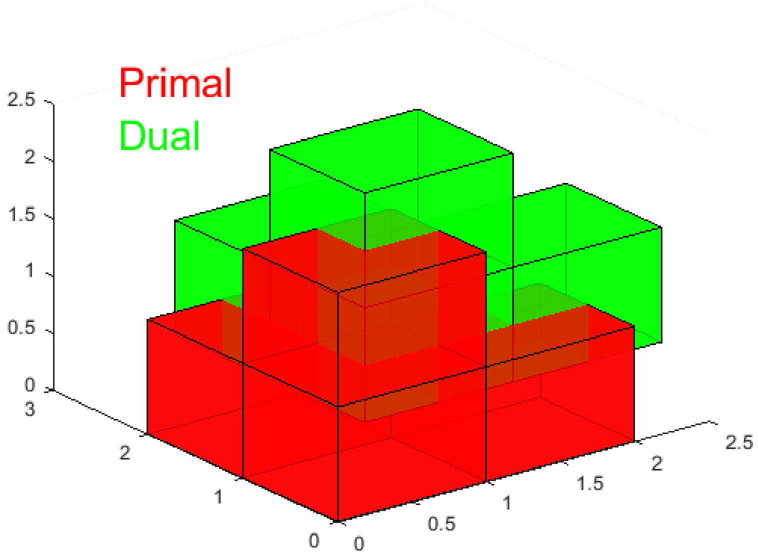
# Finite differences on dual staggered grids

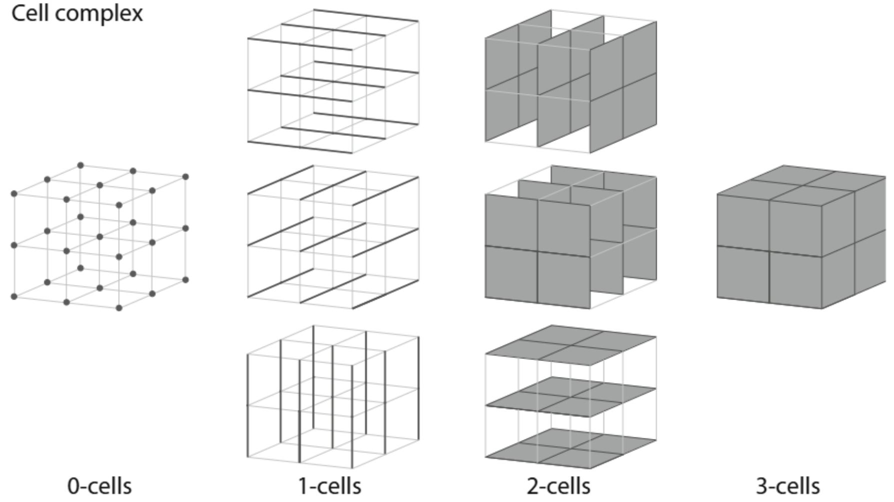
- Fields in GEMPICX are based on the 3D de Rham sequence [1], [2]




Staggered grids

$\mathbf{E} \in \mathcal{C}_1, \quad \mathbf{B} \in \mathcal{C}_2,$

$\tilde{\mathbf{H}} \in \tilde{\mathcal{C}}_1, \quad \tilde{\mathbf{D}} \in \tilde{\mathcal{C}}_2 \quad \tilde{\mathbf{J}} \in \tilde{\mathcal{C}}_2,$




Discrete unknowns on a Cartesian grid

```
node 0form, edge 1form
face 2form, cell 3form
```

| | |
|---|---|
| B | p2 |
| E | p1 |
| D | d2 |
| H | d1 |
| J | d2 |
| phi | p0 |
| $\rho$ | d3 |
| divD | d3 |

*[1] Kraus et al. Journal of Plasma Physics 83.4 (2017): 905830401.*
*[2] Kormann et al SIAM Journal on Scientific Computing 46.5 (2024): B621-B646*

# Time loop: Low Storage Runge Kutta

Time loop: Williamson (2N) [1] LSRK method

$$u' = F(t, u) \quad u(0) = u_0,$$

$s$-stage method

$$
\begin{aligned}
&S_1 := u^n \\
&\text{for } i = 1 : s \text{ do} \\
&\quad S_2 := A_i S_2 + \Delta t F(S_1) \\
&\quad S_1 := S_1 + B_i S_2 \\
&\text{end} \\
&u^{n+1} = S_1.
\end{aligned}
$$

Coefficients:

$$
\begin{array}{c|c}
A_1 & B_1 \\
\vdots & \vdots \\
A_s & B_s
\end{array}
$$

Note $A_1 = 0$

*[1] J.H. Williamson, Low-storage Runge–Kutta schemes, Journal of Computational Physics 35 (1980) 48–56.*

# For each RK stage, 5 steps update the electromagnetic fields and particle quantities:

1. **Ampere's Law**: Update the electric displacement field $\tilde{\mathbf{D}}_{\text{new}}$ using $\tilde{\mathbf{H}}_{\text{old}}$, $\tilde{\mathbf{J}}_{\text{old}}$, $\tilde{\mathbf{D}}_{\text{old}}$
2. **Push Particles and Deposit Current**:
   - Initialize the current density: Set $\tilde{\mathbf{J}} = 0$
   - Push particles: Update particle positions and velocities $(\mathbf{X}_{\text{new}}, \mathbf{V}_{\text{new}})$ using $\mathbf{E}_{\text{old}}$ and $\boldsymbol{B}_{\text{old}}$
   - Deposit the current: Deposit the current $\tilde{\mathbf{J}}_{\text{new}}$ based on particle updates $(\mathbf{X}_{\text{new}}, \mathbf{V}_{\text{new}})$
   - Synchronize current through a post-particle loop synchronization
3. **Faraday's Law**: Update the magnetic field $\mathbf{B}_{\text{new}}$ using $\mathbf{E}_{\text{old}}$, $\mathbf{B}_{\text{old}}$
4. **Hodge for $\mathbf{B}$ and $\tilde{\mathbf{H}}$**: Update the magnetic field intensity $\tilde{\mathbf{H}}_{\text{new}}$ using $\mathbf{B}_{\text{new}}$
5. **Hodge for $\tilde{\mathbf{D}}$ and $\mathbf{E}$**: Update the electric field $\mathbf{E}_{\text{new}}$ using $\tilde{\mathbf{D}}_{\text{new}}$

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# Dispersion relation for DK electron

A slab with a constant and uniform magnetic field $\boldsymbol{B}_{\text{ext}}$ in $z$ direction

$$\overleftrightarrow{D}(\boldsymbol{k},\omega)\boldsymbol{E} = (1+\boldsymbol{\chi})\boldsymbol{E} + \frac{c^2}{\omega^2}\boldsymbol{k}\times\boldsymbol{k}\times\boldsymbol{E} = 0.$$

$$D_{xx} = \left(1+\frac{c^2}{V_{A,e}^2}\right) - \frac{c^2}{\omega^2}k_\parallel^2$$

$$D_{xy} = -D_{yx} = i\frac{q_e n_M}{\epsilon_0 B_{ext}\omega} = i\frac{c^2\omega_{ce}}{V_{A,e}^2\omega}$$

$$D_{xz} = D_{zx} = \frac{c^2}{\omega^2}k_\parallel k_\perp$$

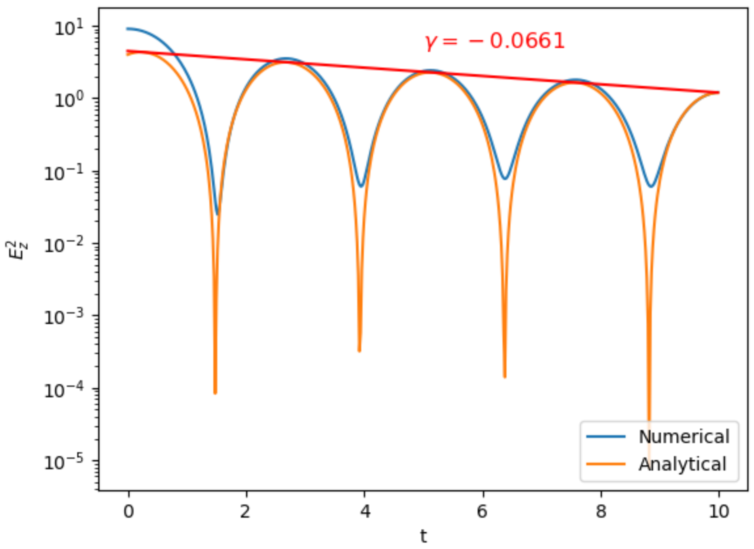
$$D_{yy} = \left(1+\frac{c^2}{V_{A,e}^2}\right) - \frac{c^2}{\omega^2}(k_\parallel^2 + k_\perp^2)$$

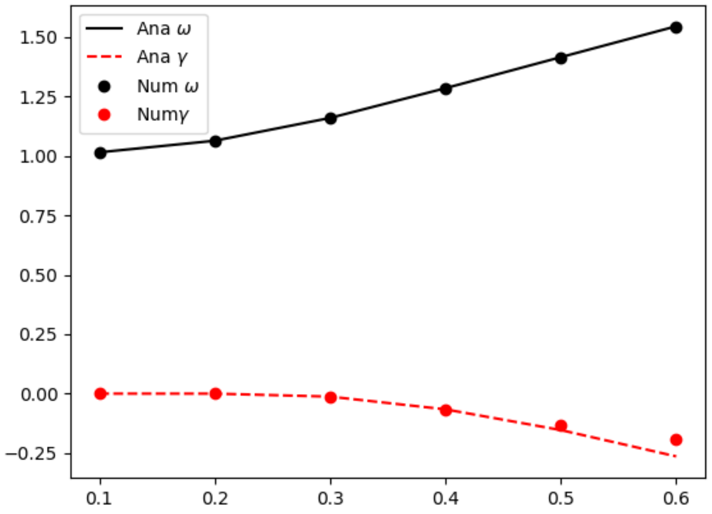
$$D_{yz} = -D_{zy} = 0$$

$$D_{zz} = 1 + \frac{\omega_{pe}^2}{k_\parallel^2 v_{th,e}^2}\left[1+\zeta_e Z(\zeta_e)\right] - \frac{c^2}{\omega^2}k_\perp^2 \qquad \zeta_e = \frac{\omega}{\sqrt{2}k_\parallel v_{th,e}}$$

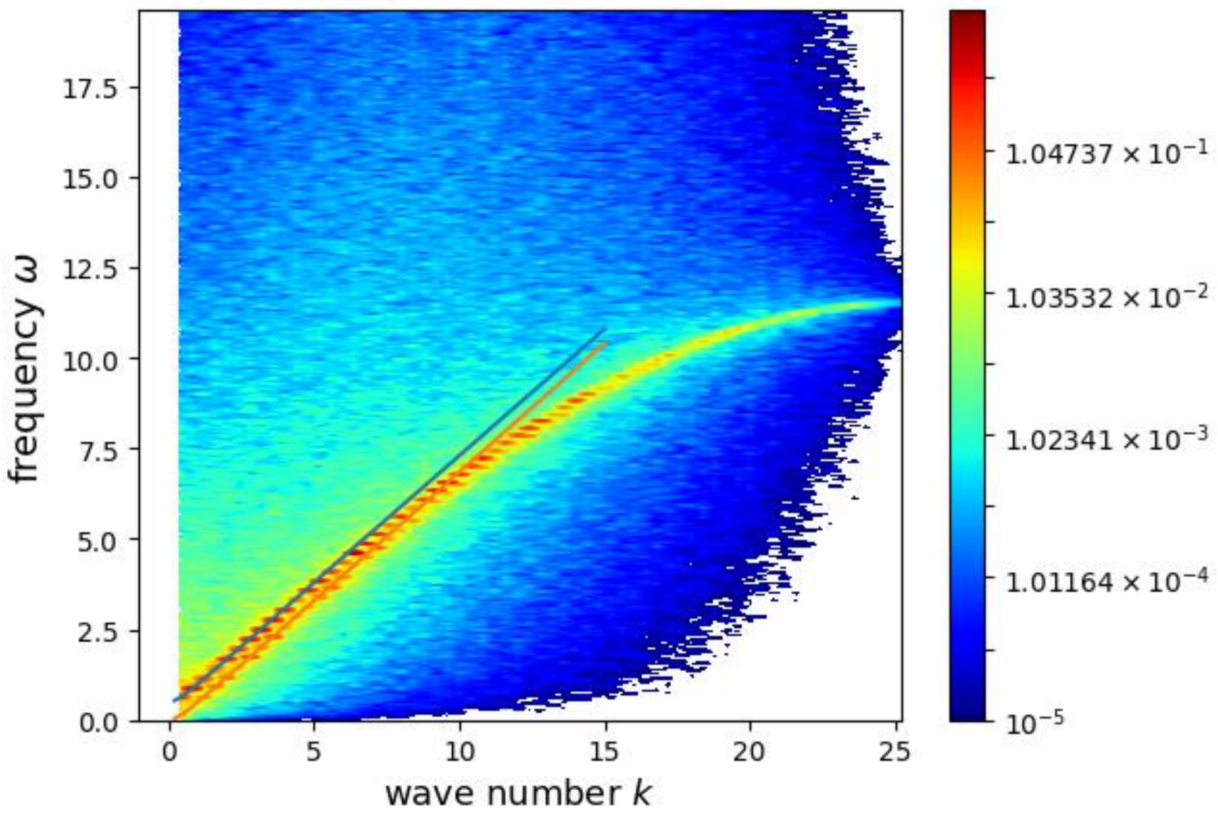
# 1sp simulations: DK electrons

Landau damping of Langmuir waves



# Electric Magnetic perturbation



# 2 Species simulations: to compare FK, hybrid, DK models

2SP Cold Plasma Dispersion Relation

$$\overleftrightarrow{\mathbf{D}}(\boldsymbol{k},\omega) = \begin{bmatrix} S - n^2\cos^2\theta & -iD & n^2\sin\theta\cos\theta \\ iD & S - n^2 & 0 \\ n^2\sin\theta\cos\theta & 0 & P - n^2\sin^2\theta \end{bmatrix}$$

Stix's notation

$$\boldsymbol{k} = (k\sin\theta, 0, k\cos\theta)$$

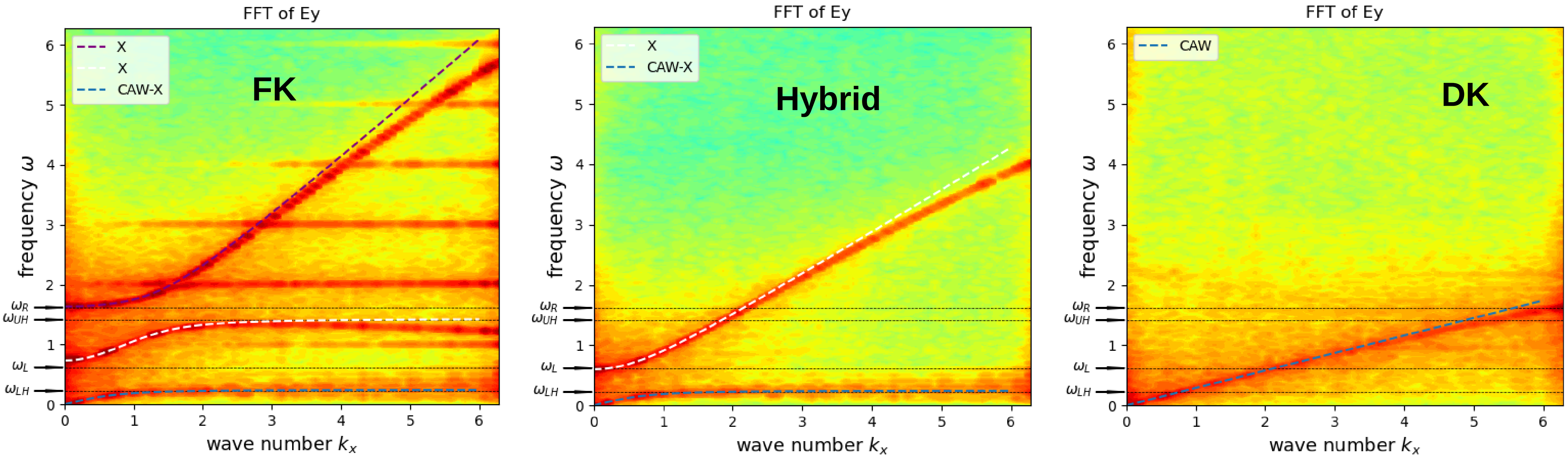
FK
$$S = 1 - \sum_s \frac{\omega_{ps}^2}{\omega^2 - \omega_{cs}^2}, \quad D = \sum_s \frac{\omega_{cs}\omega_{ps}^2}{\omega(\omega^2 - \omega_{cs}^2)}, \quad P = 1 - \sum_s \frac{\omega_{ps}^2}{\omega^2}$$

hybrid
$$S = 1 + \frac{\omega_{pe}^2}{\omega_{ce}^2} - \frac{\omega_{pi}^2}{\omega^2 - \omega_{ci}^2}, \quad D = -\frac{\omega_{pe}^2}{\omega\omega_{ce}} + \frac{\omega_{ci}\omega_{pi}^2}{\omega(\omega^2 - \omega_{ci}^2)}, \quad P = 1 - \frac{\omega_p^2}{\omega^2}$$

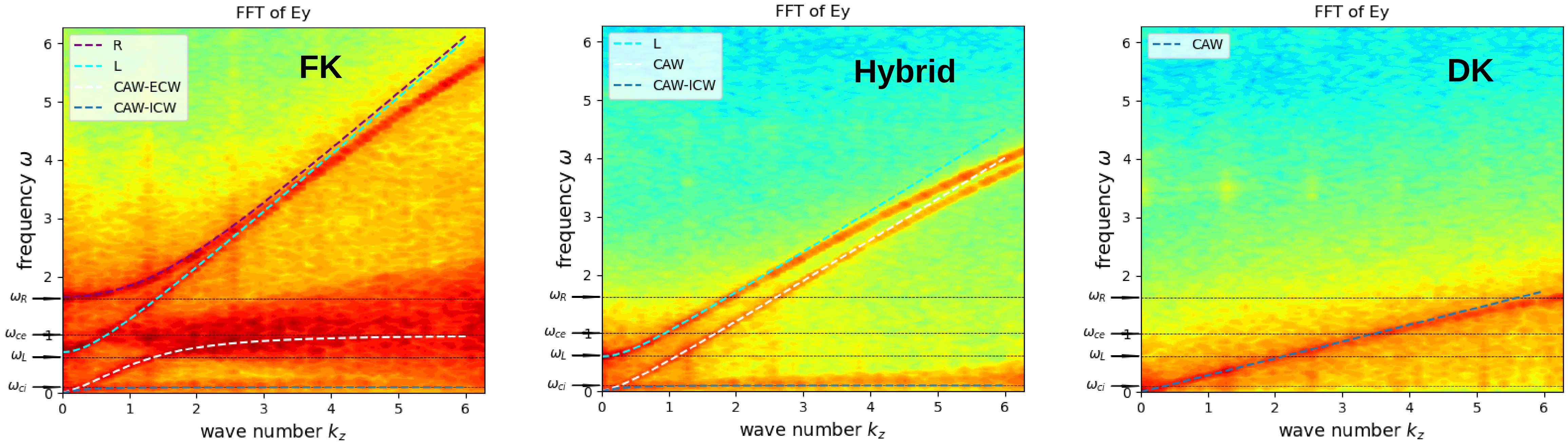
DK
$$S = 1 + \sum_s \frac{\omega_{ps}^2}{\omega_{cs}^2}, \quad D = -\sum_s \frac{\omega_{ps}^2}{\omega\omega_{cs}}, \quad P = 1 - \frac{\omega_p^2}{\omega^2}.$$

# Uniform magnetized plasma $\boldsymbol{k} \perp \boldsymbol{B}_{ext}$

Waves in Uniform magnetized plasma: 2-SPecies, mass ratio $m_i/m_e = 10$, $q_i = e$, $v_{th,e} = 0.05c$, $T_e = T_i$, Cartesian grid with periodic boundary conditions, constant $B_{ext}$ along the $z$-axis, $\omega_{p,e}/\omega_{c,e} = 1$.



# Uniform magnetized plasma $\boldsymbol{k} \parallel \boldsymbol{B}_{ext}$



# Summary and outlook

- ICRF (Ion Cyclotron Radio Frequency) physics
- Better conservation property→ transport time scale GK simulations (1s)
- Gauge-free, hybrid model developed
- Geometric discretization ensures conservation
- Outlook:
- Quasi-neutrality approximation ($\epsilon_0 \to 0$) removes light waves and Langmuir wave.
- Comparison with hybrid codes (ssV), more involved in the TSVV4 project
- edge physics, collision

# More approximations needed for low frequency simulations

- Gyrokinetic approximation of Vlasov equations removes Bernstein waves, but other high frequency waves remain.
- Assuming polarization and magnetization linearized around centered Maxwellian, gyrokinetic Maxwell equations read

$$\epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} + \frac{(m_i + m_e) n_0}{B_0^2} \frac{\partial \boldsymbol{E}_\perp}{\partial t} - \nabla \times \boldsymbol{B} = -\boldsymbol{J}$$

- Quasi-neutrality approximation ($\epsilon_0 \to 0$) removes light waves and Langmuir wave.
- No time stepping for $\boldsymbol{E}_\parallel$.
- For fully kinetic ion and drift-kinetic electrons, only electron polarization term remains, which should also be neglected (same magnitude as $\epsilon_0$ in typical tokamak). No time stepping for $\boldsymbol{E}$

- *from Eric's talk at IPP Programme day 2025*