PETSc in the Ionosphere

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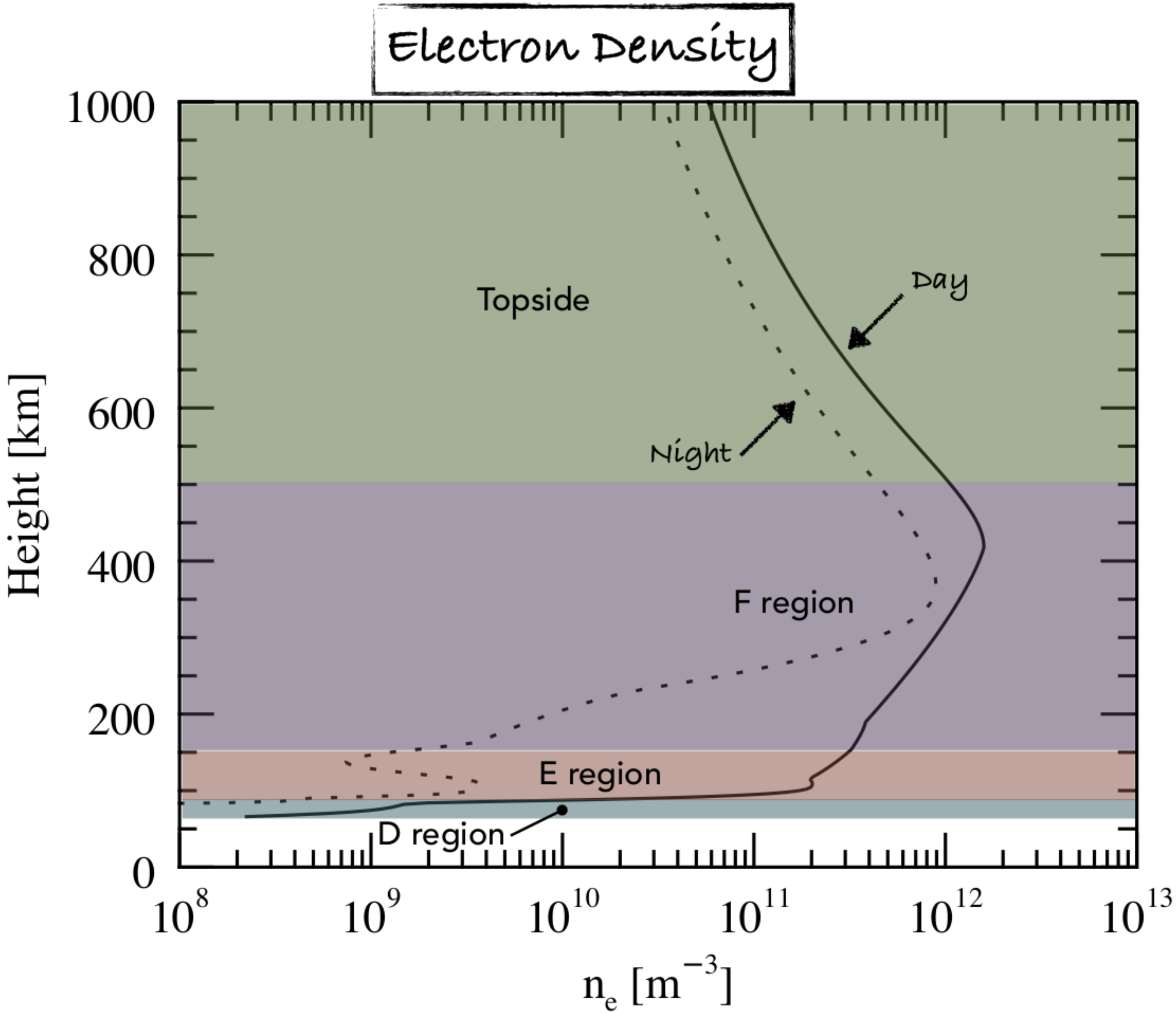
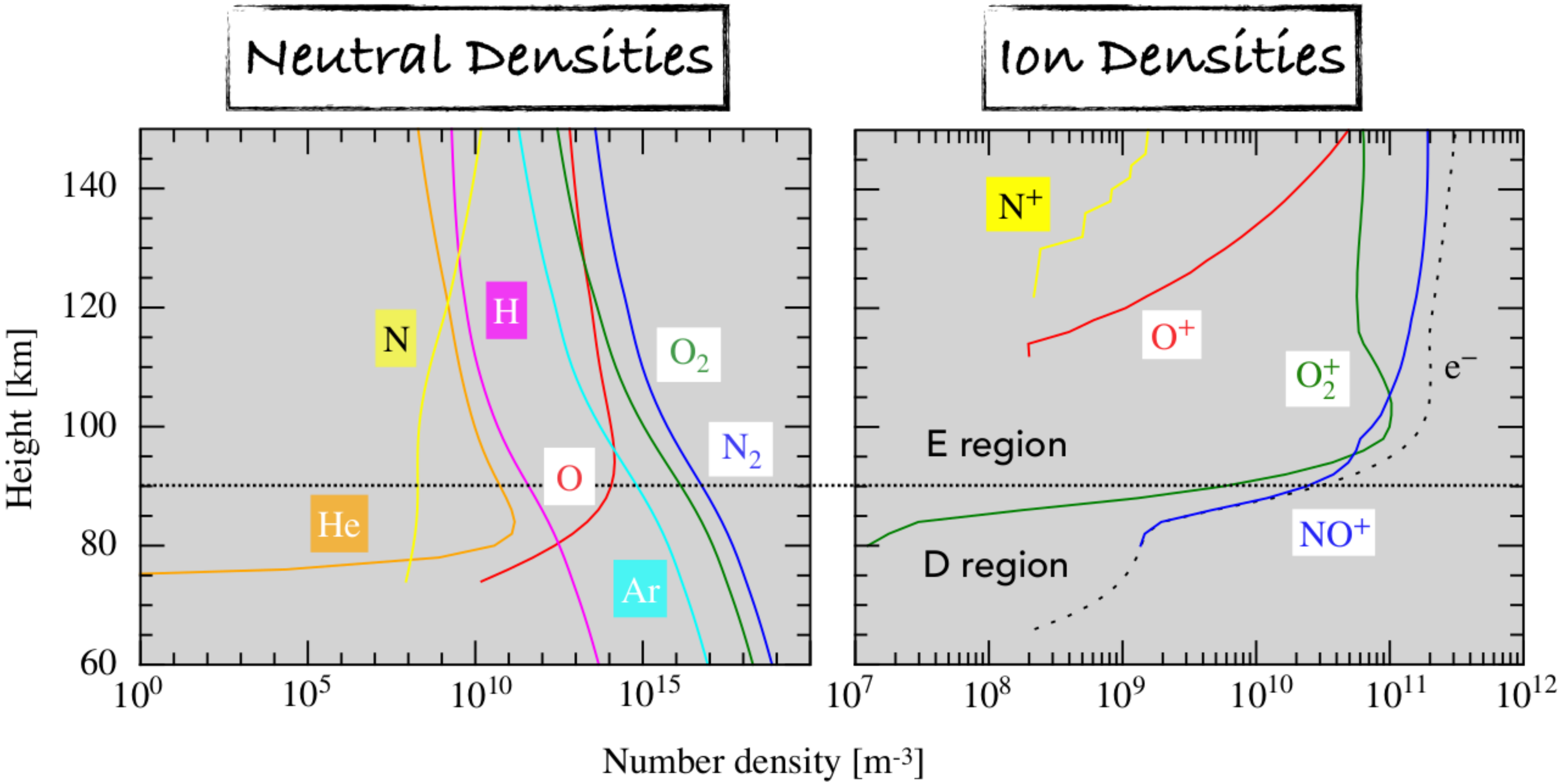
PETSc Users Meeting 2023

University of New Hampshire

The Ionosphere



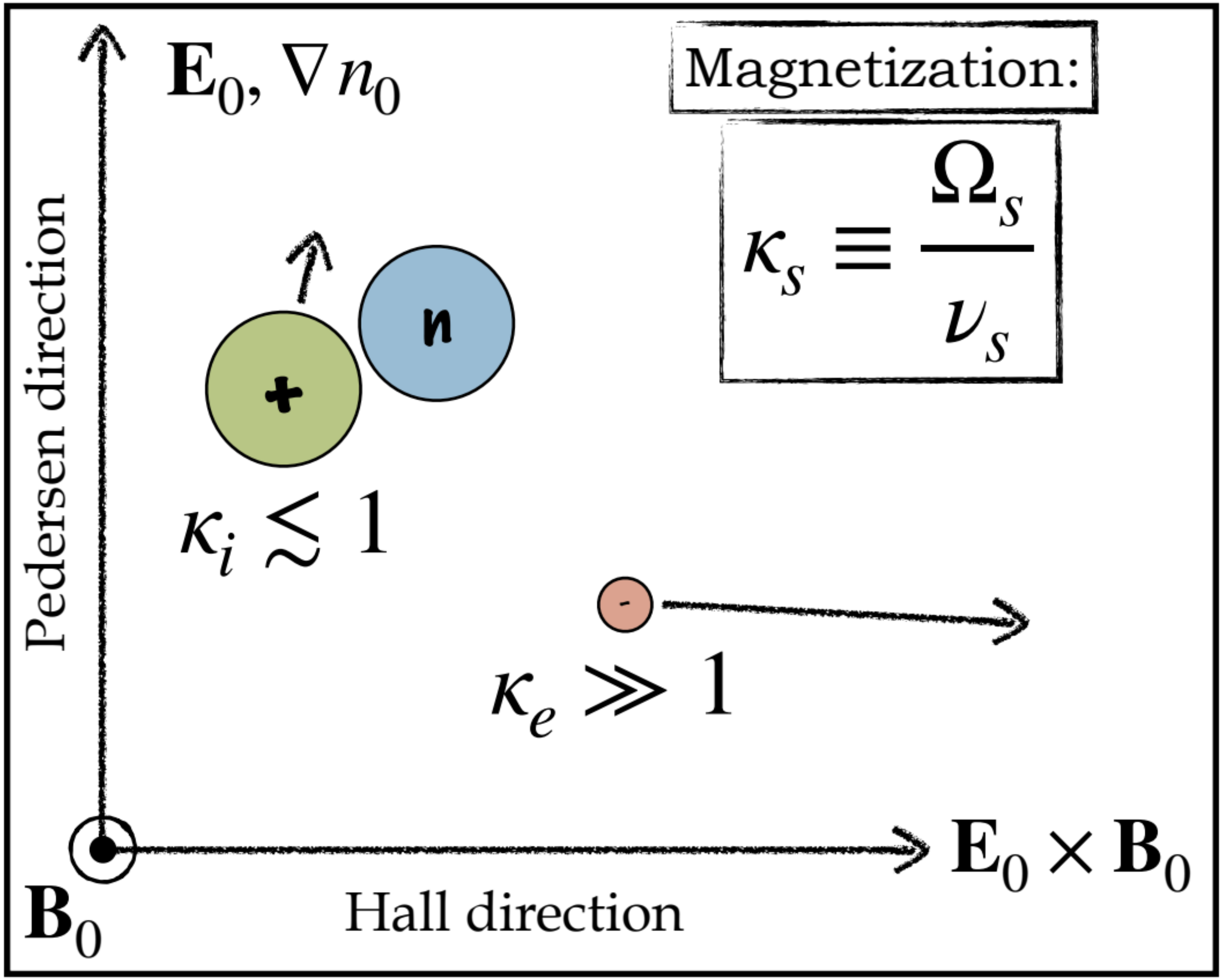
The Ionosphere



N_2 density ~ 10^6 times NO^+ or O_2^+ density

Physical Context

In the E-Region…



Physical Context

E-Region Instabilities

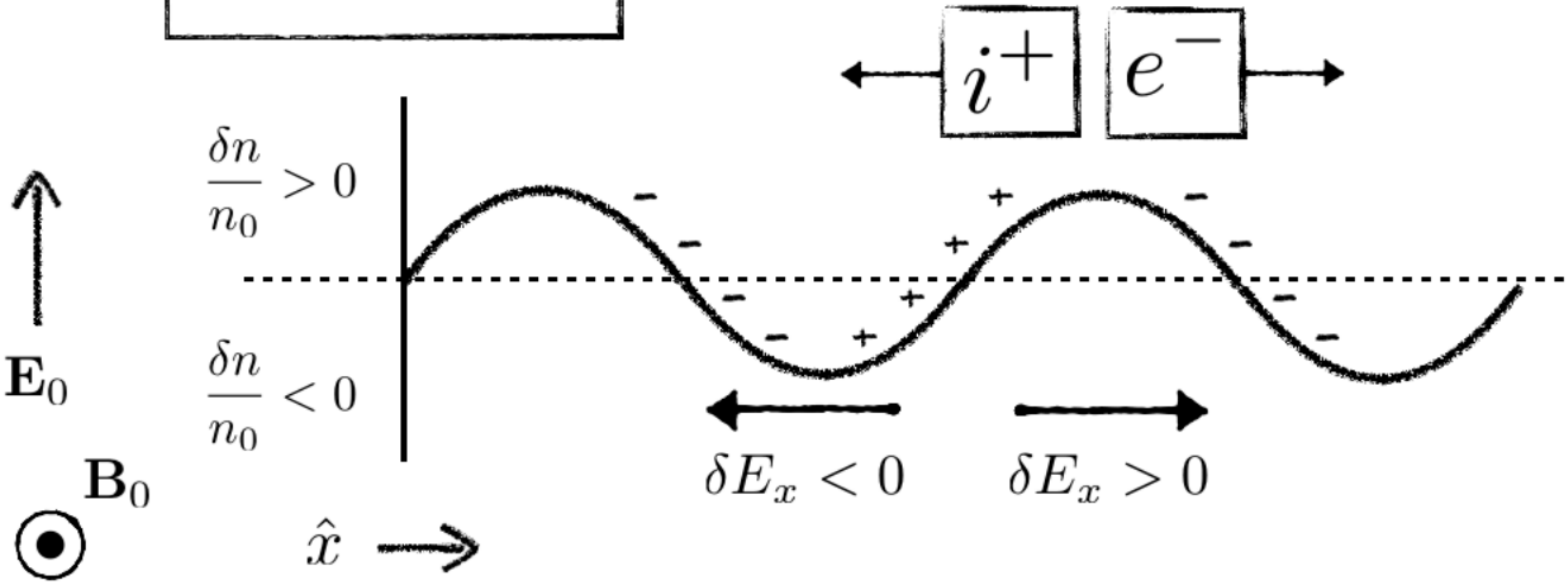
$\partial_t \mathbf{B} = \mathbf{0}$ (electrostatic)

Perturbed

Relative perturbed density: $\dfrac{\delta n}{n_0} = \dfrac{n_1 - n_0}{n_0}$

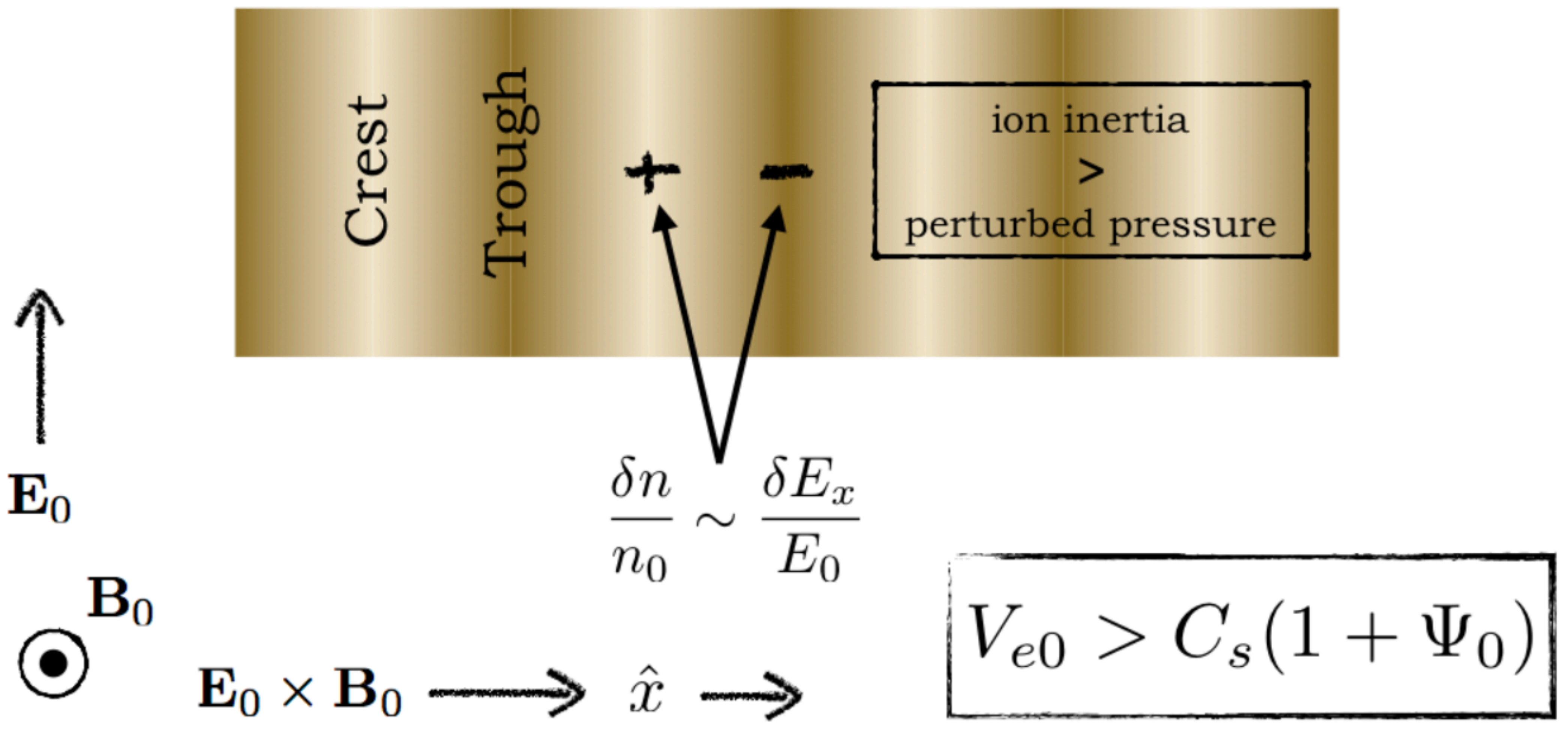
Background

In the wave frame

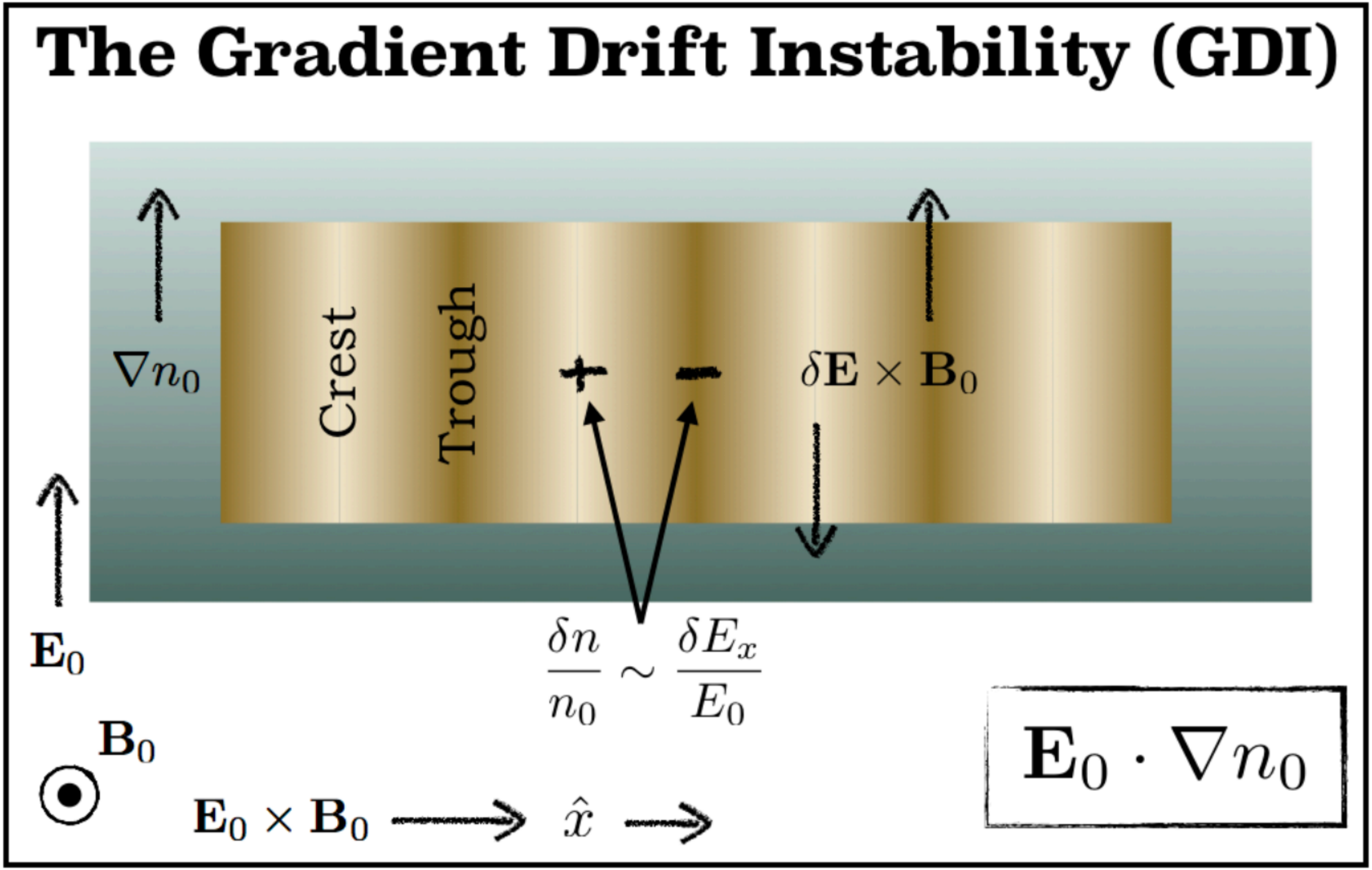


Physical Context

The Farley-Buneman Instability (FBI)



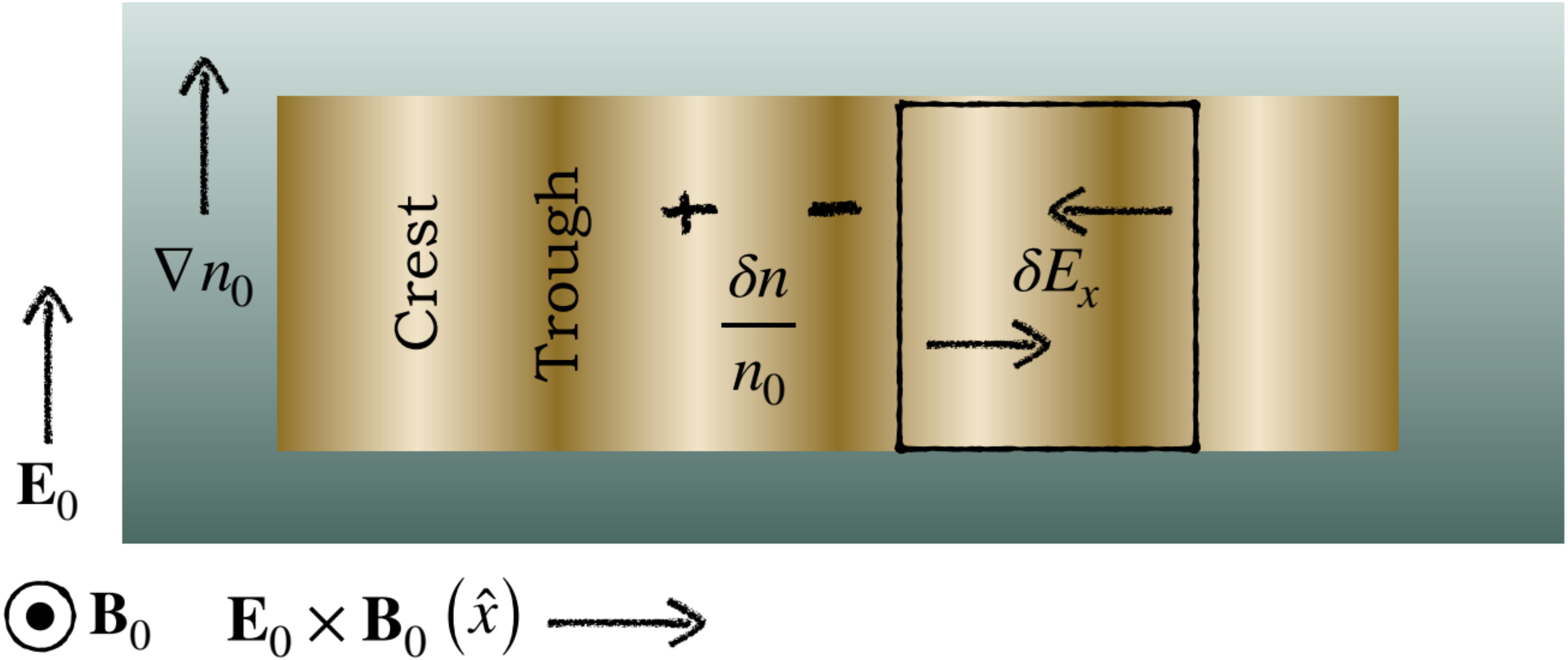
Physical Context



Physical Context

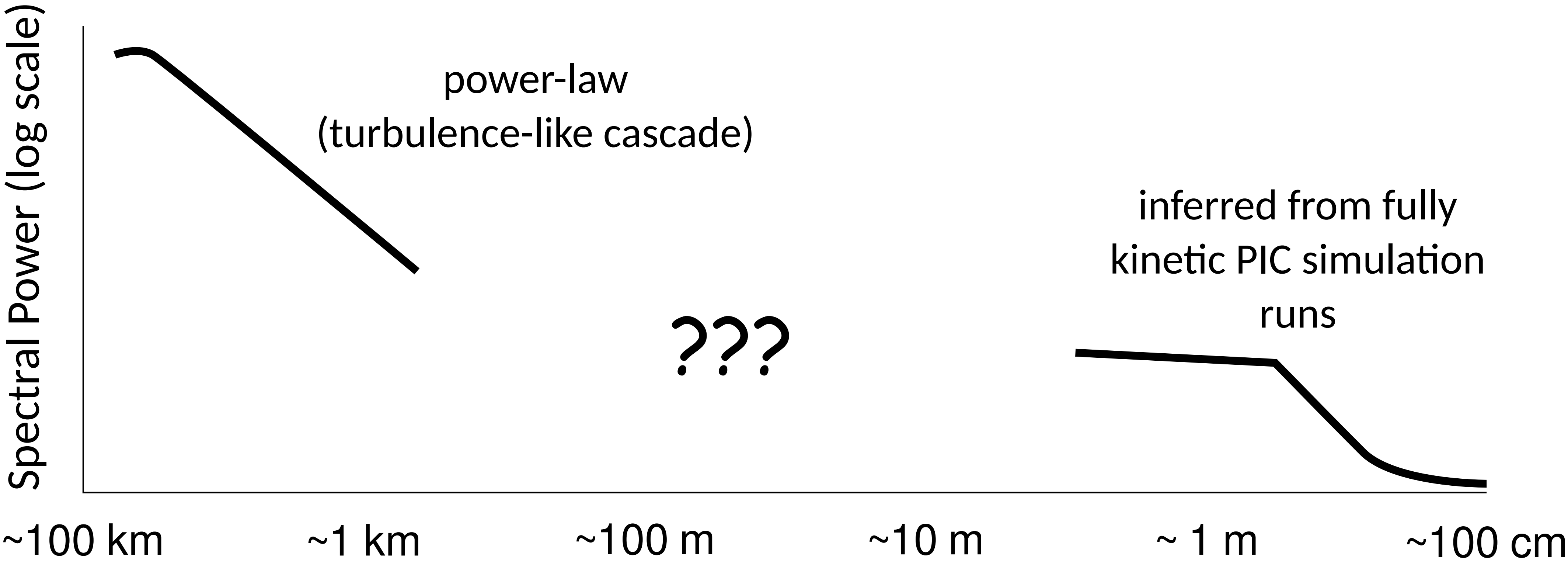
Secondary FBI from GDI

$$\boxed{\frac{\delta n}{n_0} \sim \frac{\delta E_x}{E_0}}$$



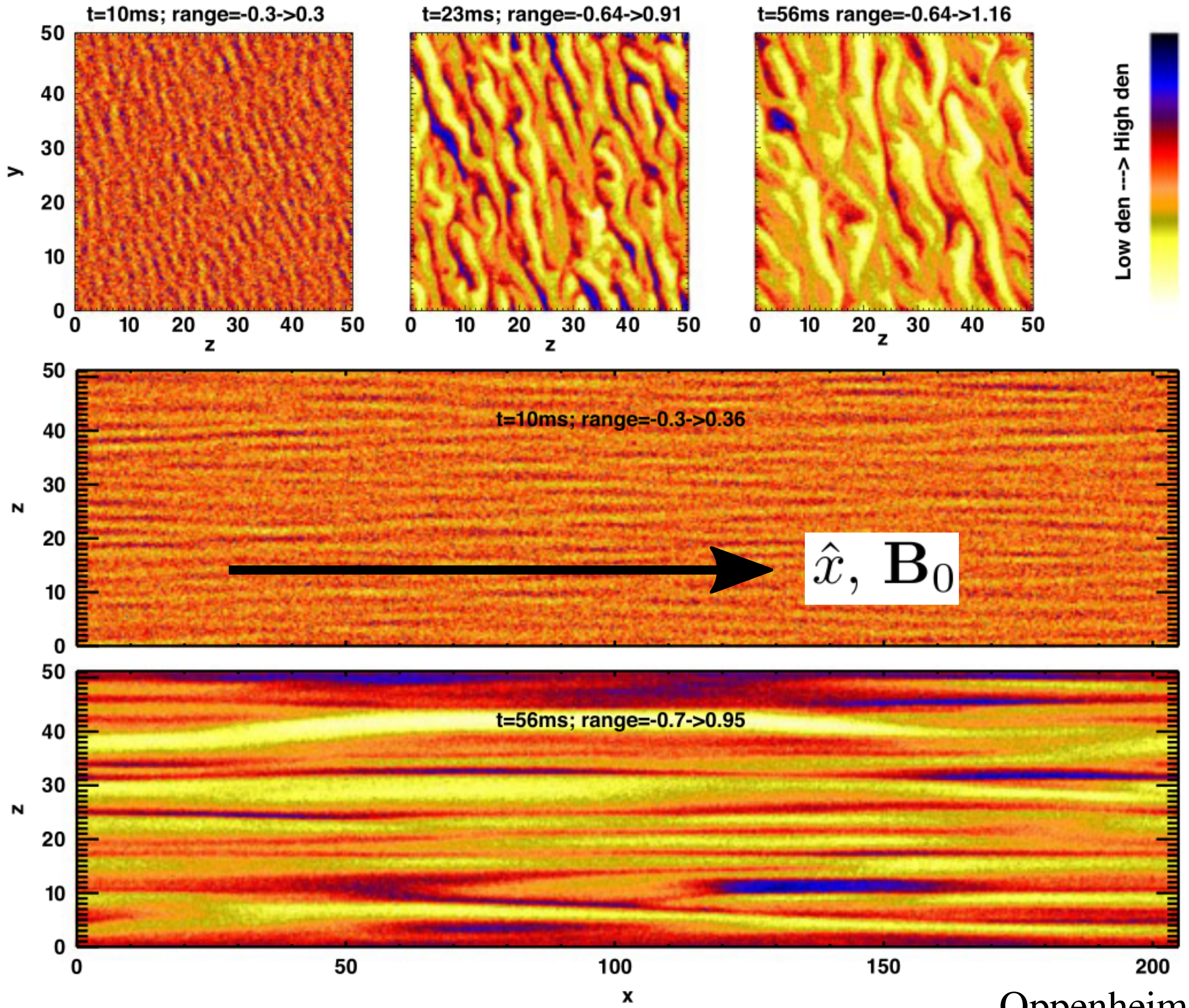
Irregularity Spectrum

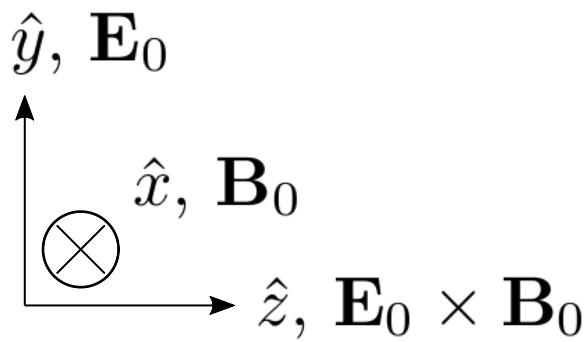
The high-level goal is to understand the spectrum of density irregularities in the ionosphere because they cause electromagnetic (e.g., GPS) scintillation.



Previous Simulations

plasma density



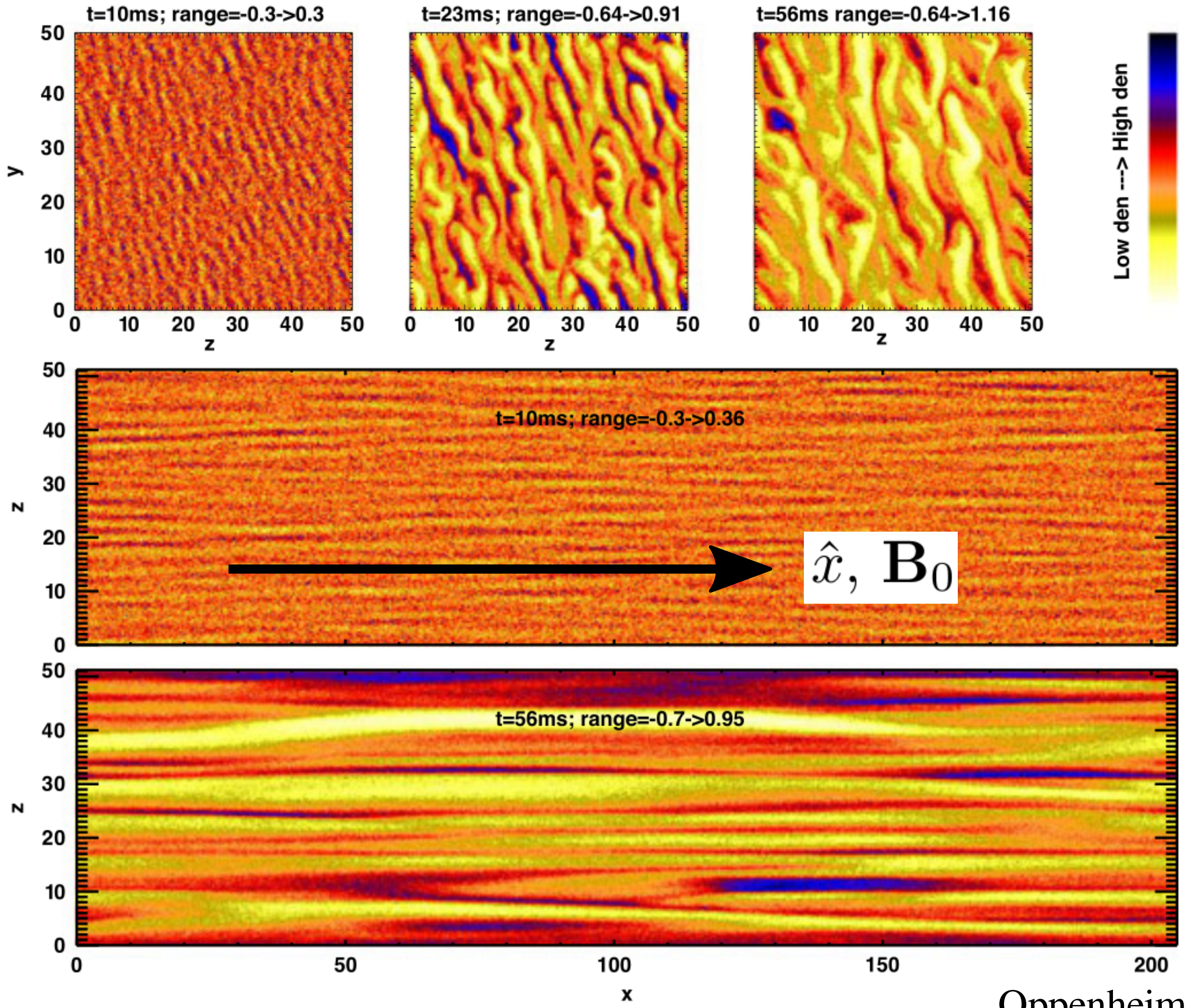


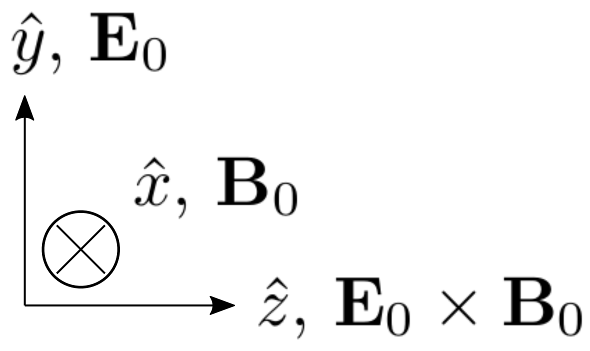
EPPIC:
Electrostatic
Parallel
PIC

Oppenheim & Dimant (2013); doi: 10.1002/jgra.50196

Previous Simulations

plasma density

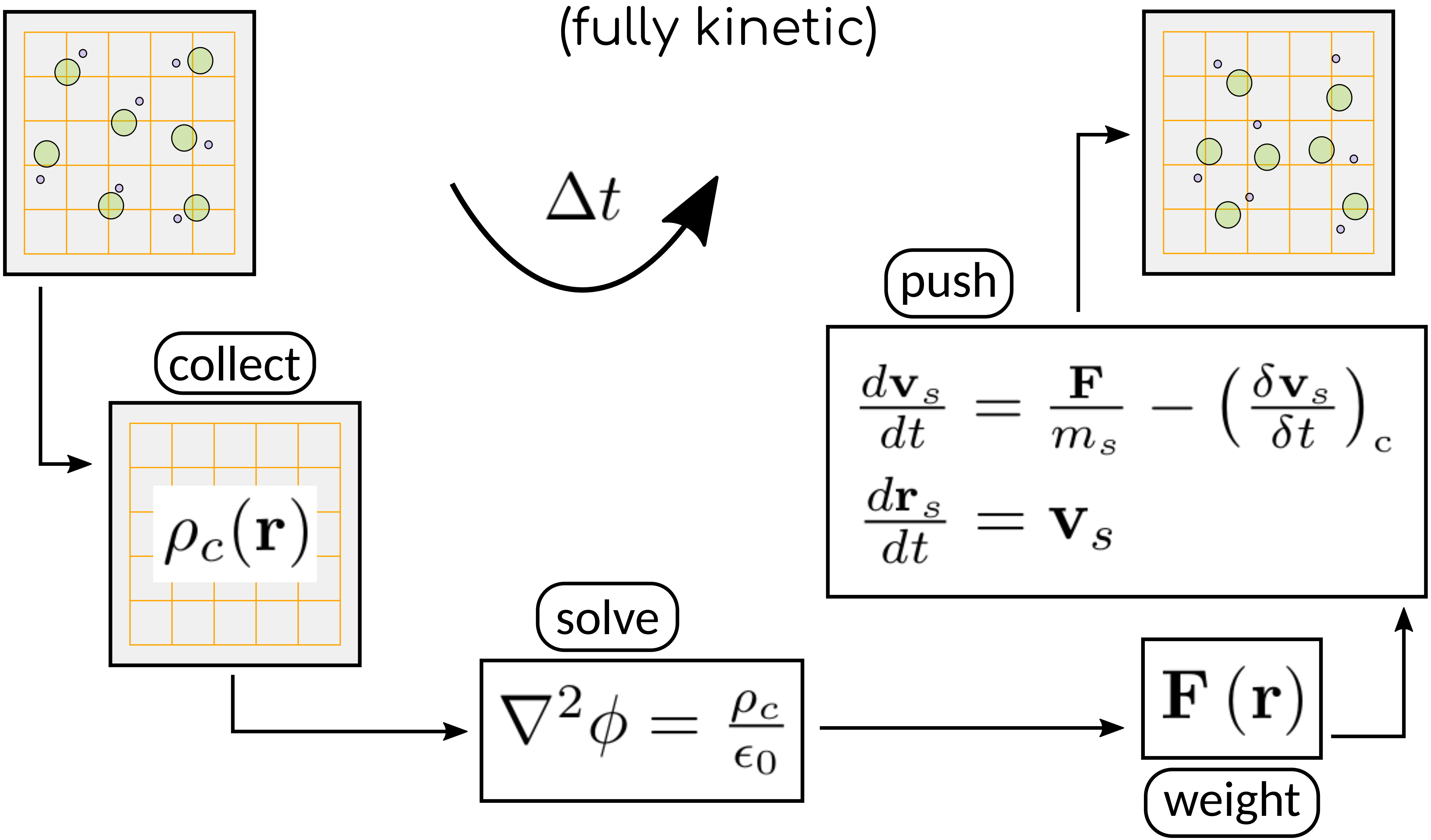




- Full PIC
- Box size 76.8 × 76.8 × 307.2 m^3
- No large-scale gradient
- Periodic BC everywhere
- Farley-Buneman irregularities initially develop with wavelengths of a few meters
- Irregularities are elongated parallel to the large-scale magnetic field

Oppenheim & Dimant (2013); doi: 10.1002/jgra.50196

The PIC Cycle



Quasineutral Hybrid Model

Full PIC

- Must resolve electron dynamical scales
  - plasma frequency
  - Debye length
- Allows non-Maxwellian electrons and ions

Hybrid PIC

- Must resolve ion dynamical scales
  - ion-neutral collision frequency
  - ion mean free path
- Assumes fluid electrons

Plasma frequency: the fundamental oscillation frequency of electrons about their neighboring ions.

$$\omega_{pe} \equiv \sqrt{\frac{ne^2}{\epsilon_0 m_e}}$$

Debye length: the length beyond which electrons shield the positive charge of ions.

$$\lambda_{De} \equiv \sqrt{\frac{\epsilon_0 k_B T_e}{ne^2}}$$

Quasineutral Hybrid Model

Kinetic Model

Poisson's equation provides the electrostatic potential

$$\nabla^2\phi = \frac{\rho_c}{\epsilon_0} = \frac{1}{\epsilon_0}\sum_s q_s n_s$$

Quasineutral Model

$$\nabla^2\phi = 0$$ (not useful)

We assume electrons are inertialess, then solve for potential

$$0 = -ne\left(\mathbf{E}_0 - \nabla\phi + \mathbf{u}_e \times \mathbf{B}_0\right) - \nabla\cdot\mathsf{P}_e - nm_e\nu_e\mathbf{u}_e$$

Quasineutral Potential Equation

ion flux

electron

pressure mass collision frequency

plasma density

large-scale electric field

$$\nabla \cdot (n\mathsf{R}\nabla\phi) = \nabla \cdot \left[n\mathsf{R}\mathbf{E_0} + \mathsf{R}\left(\frac{\nabla \cdot \mathsf{P_e}}{e}\right) + (1+\kappa^2)\left(\frac{m_e \nu_e}{e}\right)\mathbf{\Gamma}_i \right]$$

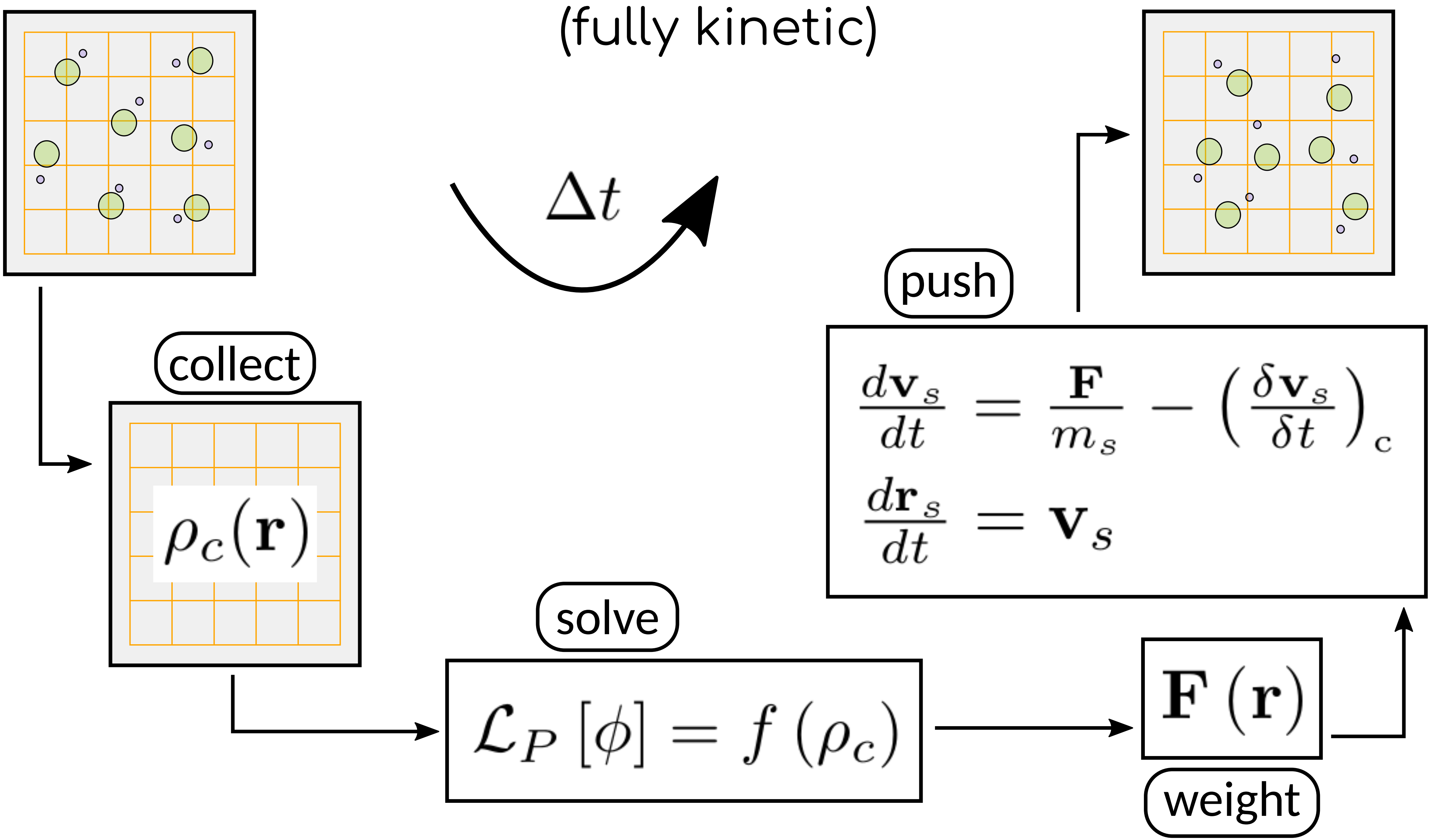
$$\mathsf{R} \equiv \begin{pmatrix} 1+\kappa_x^2 & \kappa_y\kappa_x - \kappa_z & \kappa_z\kappa_x + \kappa_y \\ \kappa_x\kappa_y + \kappa_z & 1+\kappa_y^2 & \kappa_z\kappa_y - \kappa_x \\ \kappa_x\kappa_z - \kappa_y & \kappa_y\kappa_z + \kappa_x & 1+\kappa_z^2 \end{pmatrix}$$

magnetization tensor

$$\kappa_j \equiv \frac{\Omega_j}{\nu_e} = \frac{eB_j}{m_e\nu_e} = \frac{\text{average number of gyro-orbits}}{\text{average number of collisions}}$$

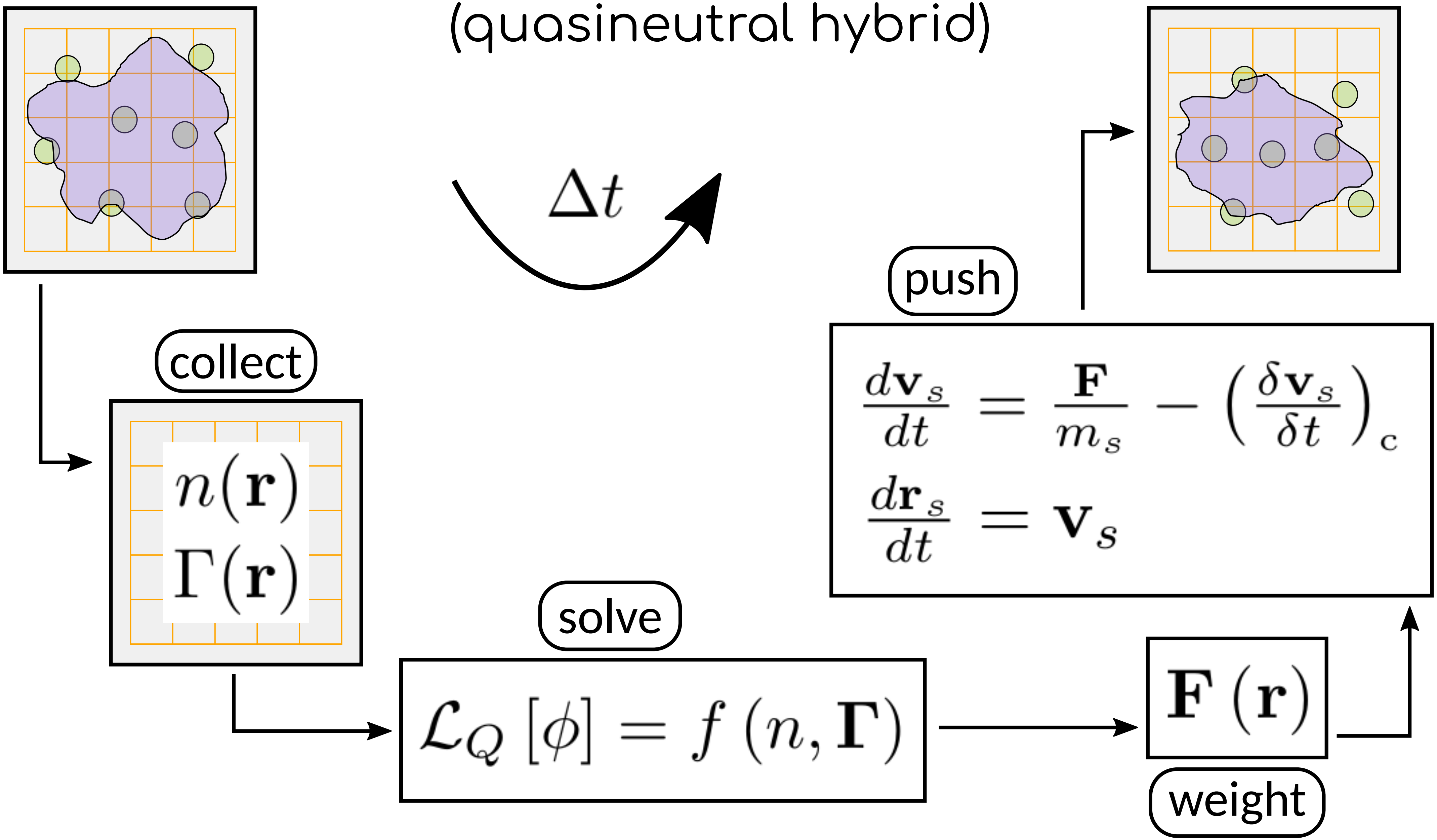
magnetization definition

The PIC Cycle



The PIC Cycle

(quasineutral hybrid)

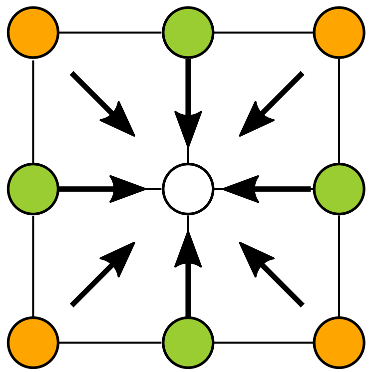


Discrete Potential Equation

$$\nabla \cdot (n\mathsf{R}\nabla\phi) = f\left(n, \mathbf{\Gamma}, \dots\right) \longrightarrow \mathbf{A}\mathbf{x} = \mathbf{b}$$

$$\begin{aligned}\nabla \cdot (n\mathsf{R}\nabla\phi) \approx \; & \frac{\left[(n\mathsf{R}\nabla\phi)\cdot\hat{x}\right]_{i+1/2} - \left[(n\mathsf{R}\nabla\phi)\cdot\hat{x}\right]_{i-1/2}}{\Delta x} \\ & + \frac{\left[(n\mathsf{R}\nabla\phi)\cdot\hat{y}\right]_{j+1/2} - \left[(n\mathsf{R}\nabla\phi)\cdot\hat{y}\right]_{j-1/2}}{\Delta y} \\ & + \frac{\left[(n\mathsf{R}\nabla\phi)\cdot\hat{z}\right]_{k+1/2} - \left[(n\mathsf{R}\nabla\phi)\cdot\hat{z}\right]_{k-1/2}}{\Delta z}\end{aligned}$$

$$\begin{aligned}&\left[n\left(r_{xx}\partial_x\phi + r_{xy}\partial_y\phi + r_{xz}\partial_z\phi\right)\right]_{i+1/2} \\ &= n_{i+1/2}\left(\boxed{r_{xx}\left[\partial_x\phi\right]_{i+1/2}} + \boxed{r_{xy}\left[\partial_y\phi\right]_{i+1/2}} + \boxed{r_{xz}\left[\partial_z\phi\right]_{i+1/2}}\right)\end{aligned}$$

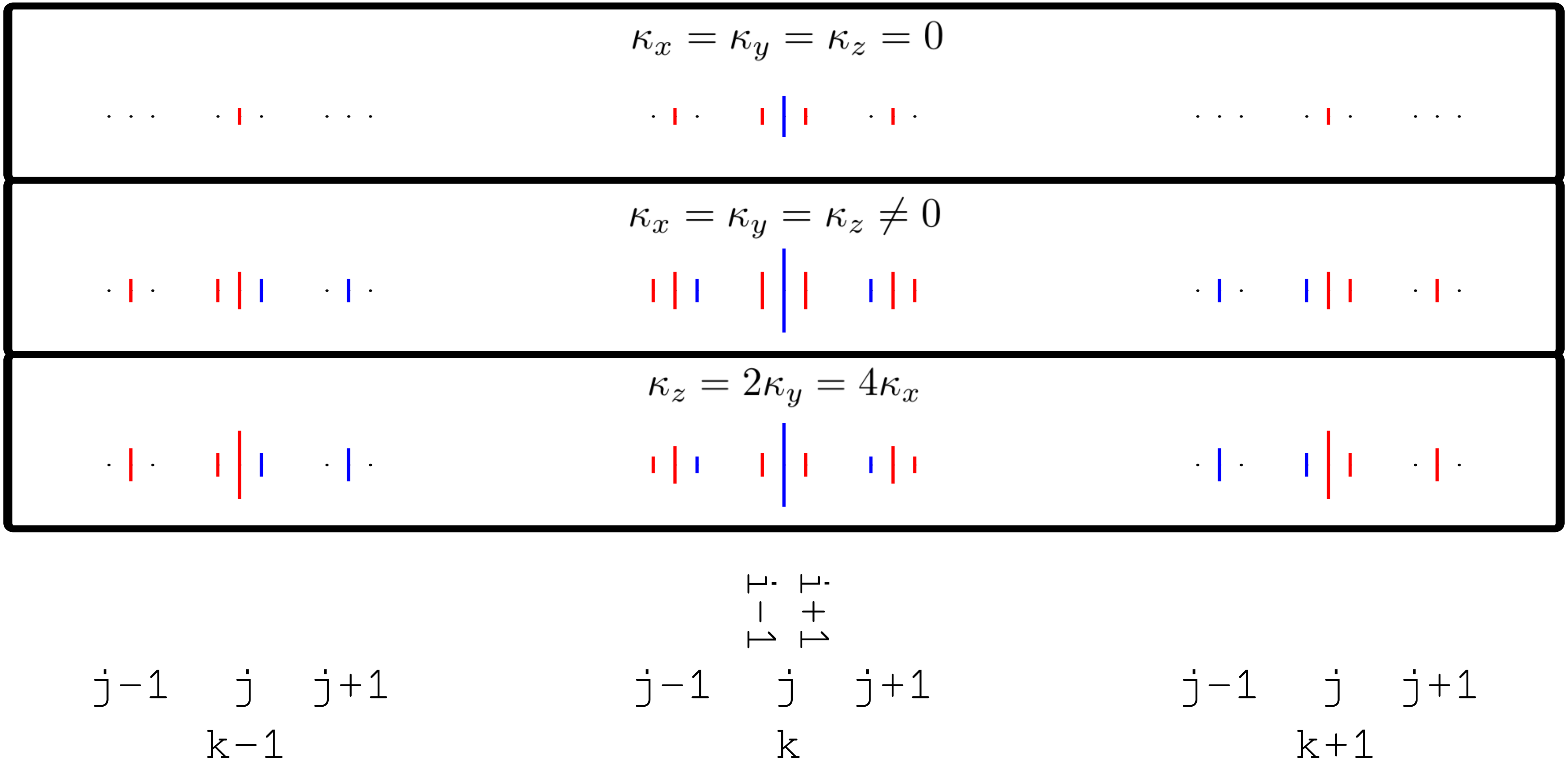


$$\left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} \begin{matrix} x \times y \\ y \times z \\ x \times z \end{matrix}$$

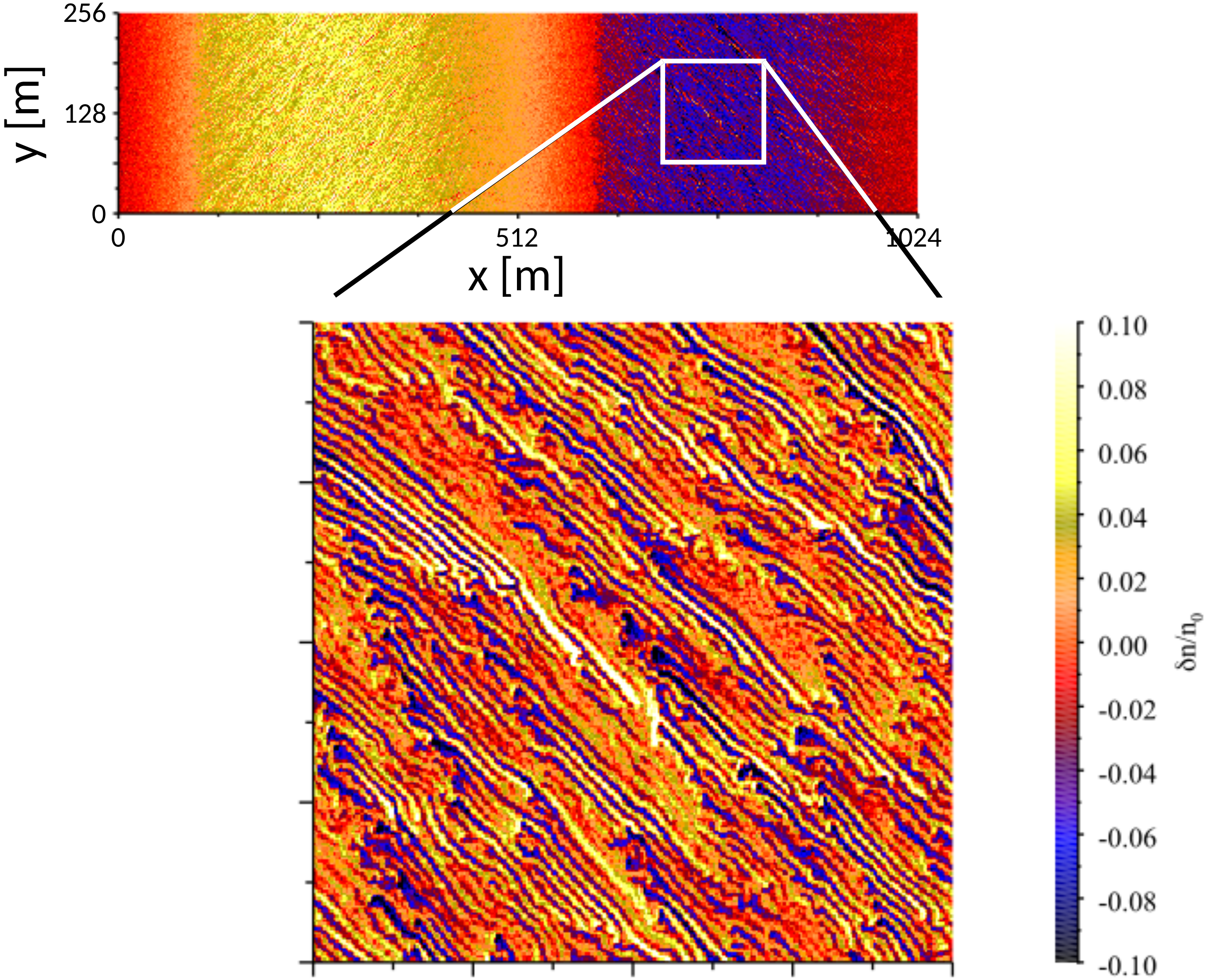
19-point stencil

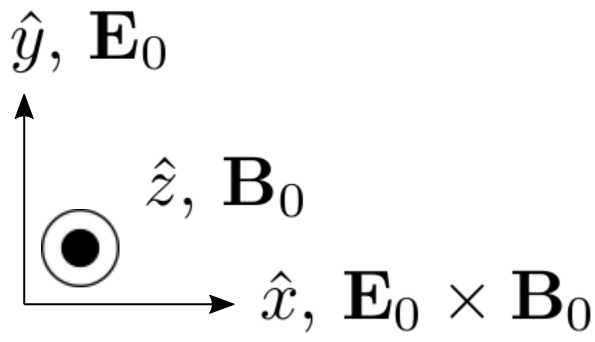
Discrete Stencil

$$\nabla \cdot (n\mathrm{R}\nabla\phi) = f\,(n, \mathbf{\Gamma}, \ldots) \longrightarrow \mathbf{Ax} = \mathbf{b}$$



Hybrid Simulations





- Hybrid PIC
- Box size 1024 × 256 m^2
- Quasineutral to first order
- Large-scale wave
- Farley-Buneman irregularities develop in the crest and trough
- Driving electric field comes from large-scale wave
- Farley-Buneman irregularities reduce driving field to just above threshold

Hybrid Simulations

In EPPIC main:

```
... non-PETSc setup
#if HAVE_PETSC
  PetscInitialize(...);
  KSPCreate(...);
  KSPGetPC(...);
  PCSetFromOptions(...);
  KSPSetFromOptions(...);
#endif
... more non-PETSc stuff
#if HAVE_PETSC
  MatCreate(..., &A);
  MatSetSizes(...);
  MatSetType(...);
  MatSetFromOptions(...);
#endif
```

Hybrid Simulations

In EPPIC field solver:

```
VecCreate(..., &b);
VecSetSizes(...);
VecSetFromOptions(...);
VecDuplicate(b, &x);
... call custom function to fill b
... call custom function to fill A
KSPSetOperators(...);
KSPSolve(...);
... copy x to potential array
```

LHS

```
MatGetOwnershipRange(A, ...);
for local row in A {
  ... get density at local nodes
  ... define indices and values
  MatSetValues(A, ...);
}
... assemble A
```

RHS

```
VecGetOwnershipRange(b, ...);
for local row in b {
  ... get node density and flux
  ... compute value
  VecSetValue(b, ...);
}
... assemble b
```

Hybrid Simulations

- This is all fine, but PETSc functionality is hacked in as an afterthought.
- Non-periodic boundary conditions in EPPIC are not as well developed as periodic BC.
- There is limited documentation

- EPPIC only supports domain decomposition along the x dimension
- The EPPIC source code and build system are not especially approachable to new users
- EPPIC is not truly open source
- There have been multiple development philosophies with limited coordination

Hybrid Simulations

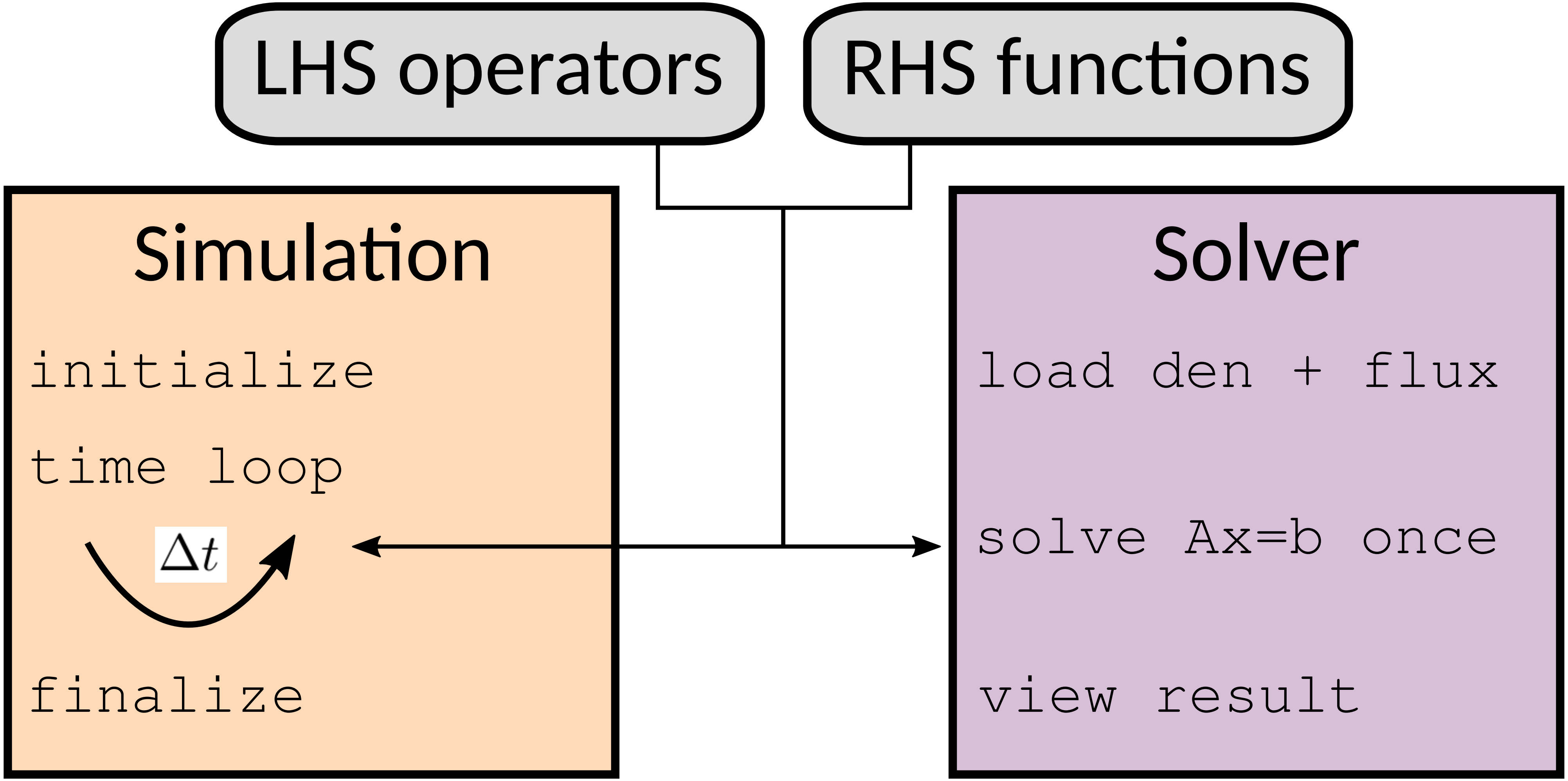
Recent development of a hybrid simulation built on PETSc's `DMDA` and `DMSWARM` objects:

- Use a `DMSWARM` to manage ions
- Use one `DMDA` to manage density and flux (collected from ion distribution)
- Use another `DMDA` to manage electrostatic potential (computed from density and flux)
- Separate executables for full simulation and stand-alone potential solver
- Eventually support multiple fluid electron models and ion-neutral collision models

Hybrid Simulations

```
PetscCall(SetUpVlasovDM(&ctx));
PetscCall(SetUpIonsDM(&ctx));
PetscCall(InitializePositions(&ctx));
PetscCall(InitializeVelocities(&ctx));
PetscCall(CollectVlasovQuantities(&ctx));
PetscCall(SetUpPotentialDM(&pdm, &ctx));
PetscCall(KSPCreate(PETSC_COMM_WORLD, &ksp));
... standard KSP setup
PetscCall(ComputePotential(ksp, &ctx));
... begin time-step loop
  PetscCall(UpdateVelocities(ksp, &ctx));
  PetscCall(UpdatePositions(&ctx));
  PetscCall(CollectVlasovQuantities(&ctx));
  PetscCall(ComputePotential(ksp, &ctx));
```

Hybrid Simulations



Stand-alone solver will allow us to test algorithms on a set of reference inputs.

Summary

- The collisionality of the ionospheric E region leads to unique plasma instabilities
- The Farley-Buneman and gradient drift instabilities couple energy across spatial scales
- A hybrid PIC simulation allows us to focus on ion temporal and spatial scales
- A new PETSc-based implementation of the hybrid code is in development

Acknowledgements

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Thank You

Appendix