Equation Free Projective Integration and its Applicability for Simulating Plasma

Results: 1D Ion Acoustic Wave

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Collaborators

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Abstract

We examine a novel simulation scheme called equation free projective integration[1] which has the potential to allow global simulations of plasmas while still including the global effects of microscale physics. These simulation codes would be ideal for such multiscale problems as the Earth's magnetosphere, tokamaks, and the solar corona. In this method, the global plasma variables stepped forward in time are not time-integrated directly using dynamical differential equations, hence the name "equation free." Instead, these variables are represented on a microgrid using a kinetic simulation. This microsimulation is integrated forward long enough to determine the time derivatives of the global plasma variables, which are then used to integrate forward the global variables with much larger time steps. We explore the feasibility of the method for simulating plasma by examining the propagation and steepening of an ion acoustic wave. The results are quite promising, as the equation free method has been demonstrated to provide at least a factor of 20 speedup in simulation time. The equation free ion acoustic wave produces results very similar to those of the fully kinetic particle code. The propagation speed and steepening is nearly identical, with only a small difference in the maximum amplitude of the wave.

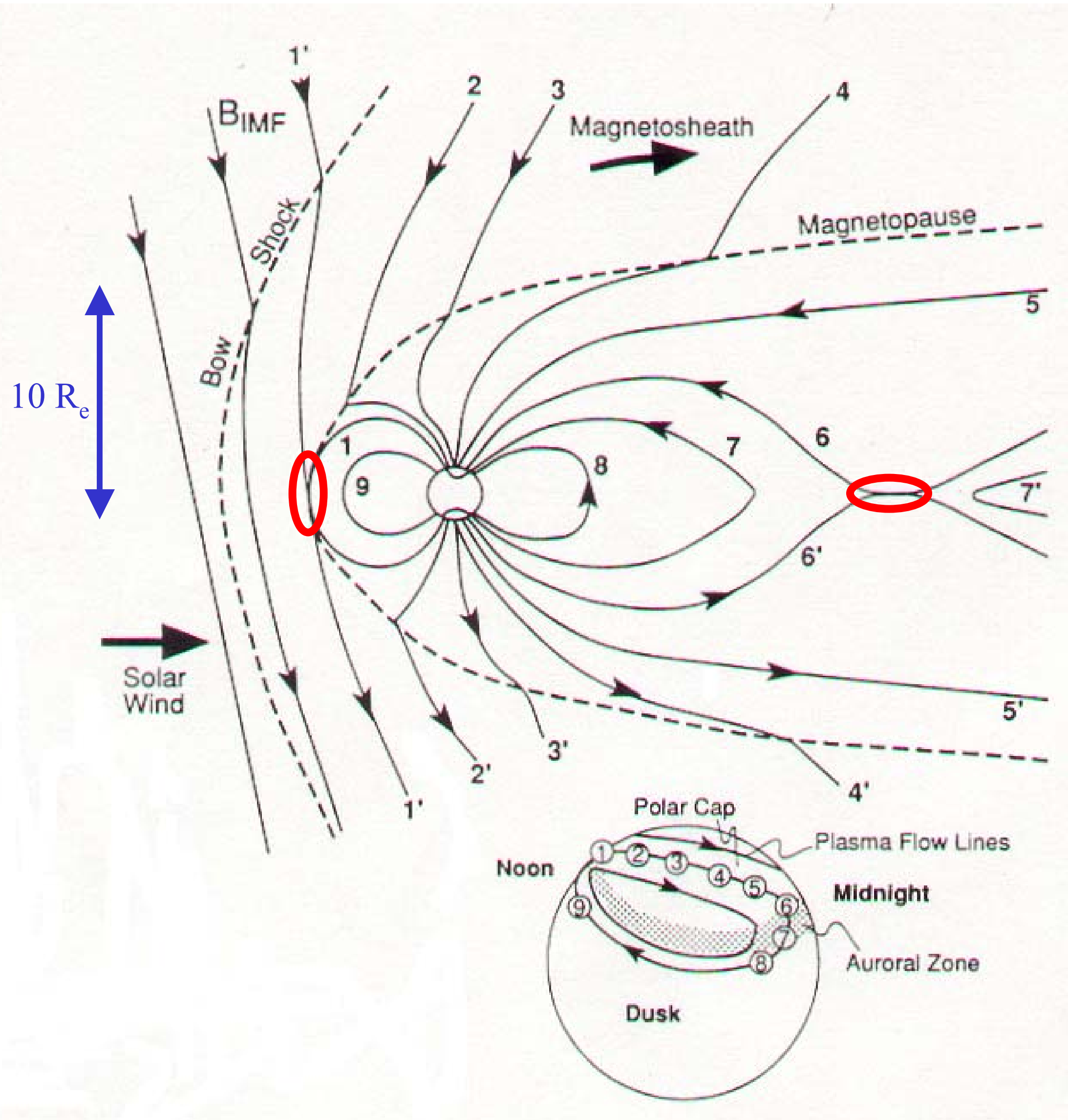
[1] I. G. Kevrekidis et. al., ``Equation-free multiscale computation: Enabling microscopic simulators to perform system-level tasks,'' **arXiv**:physics/0209043.

Overview

- Multiscale: A process that mixes micro and macro scales.
- What is Equation Free Projective Integration?
- efree
  - Application of Eq. Free Proj. Int.
- Test Problem: Ion-Acoustic Wave
  - 20 times speedup so far!

Reconnection: A Multiscale Problem

- Dayside of Magnetosphere
  - System size ~ 20 R_e
  - c/ω_{pi} ~ 1/60 R_e
  - c/ω_{pi} ~ 1/3000 R_e
- Best MHD Simulations:
  - grid scale ~ 1/10 R_e
- New physics decreases time step.
  - Whistler: $\omega \sim k^2$
  - $\Delta t \sim (1/\Delta x)^2$
- Brute force method impossible.

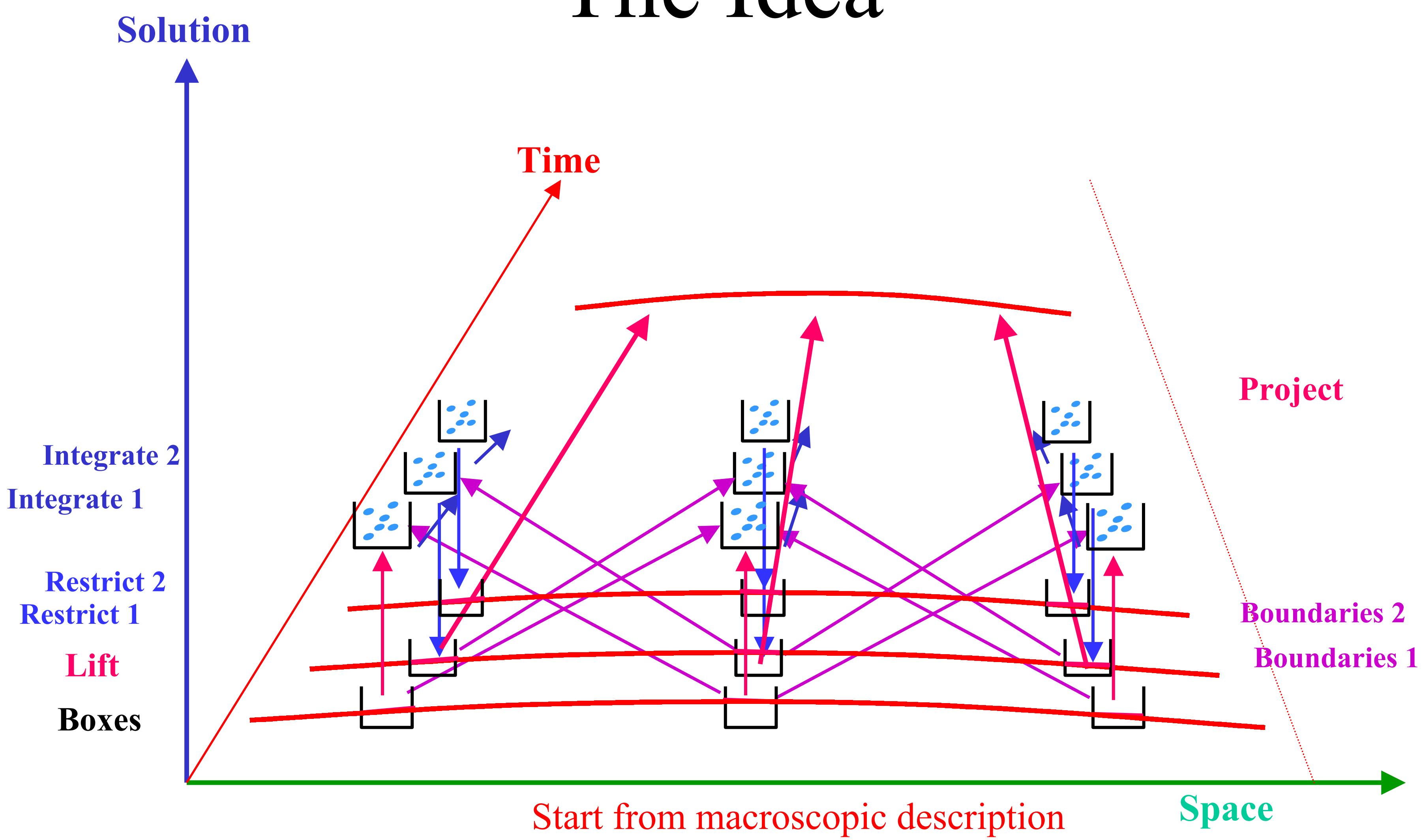


Kivelson et al., 1995

The Idea

- Equation Free Projective Integration
  - (Kevrekidis et al., 2002, Gear et al., 2003)
- Goal: Determine the time behavior of variables at large scales (Coarse Variables)
  - B, n, V, E
- Need time derivative:
  - $B_{t+1} = B_t + \Delta t\,(dB_t/dt)$
  - Normally use PDEs.
  - Use an "experiment" instead.

The Idea



One full step finished

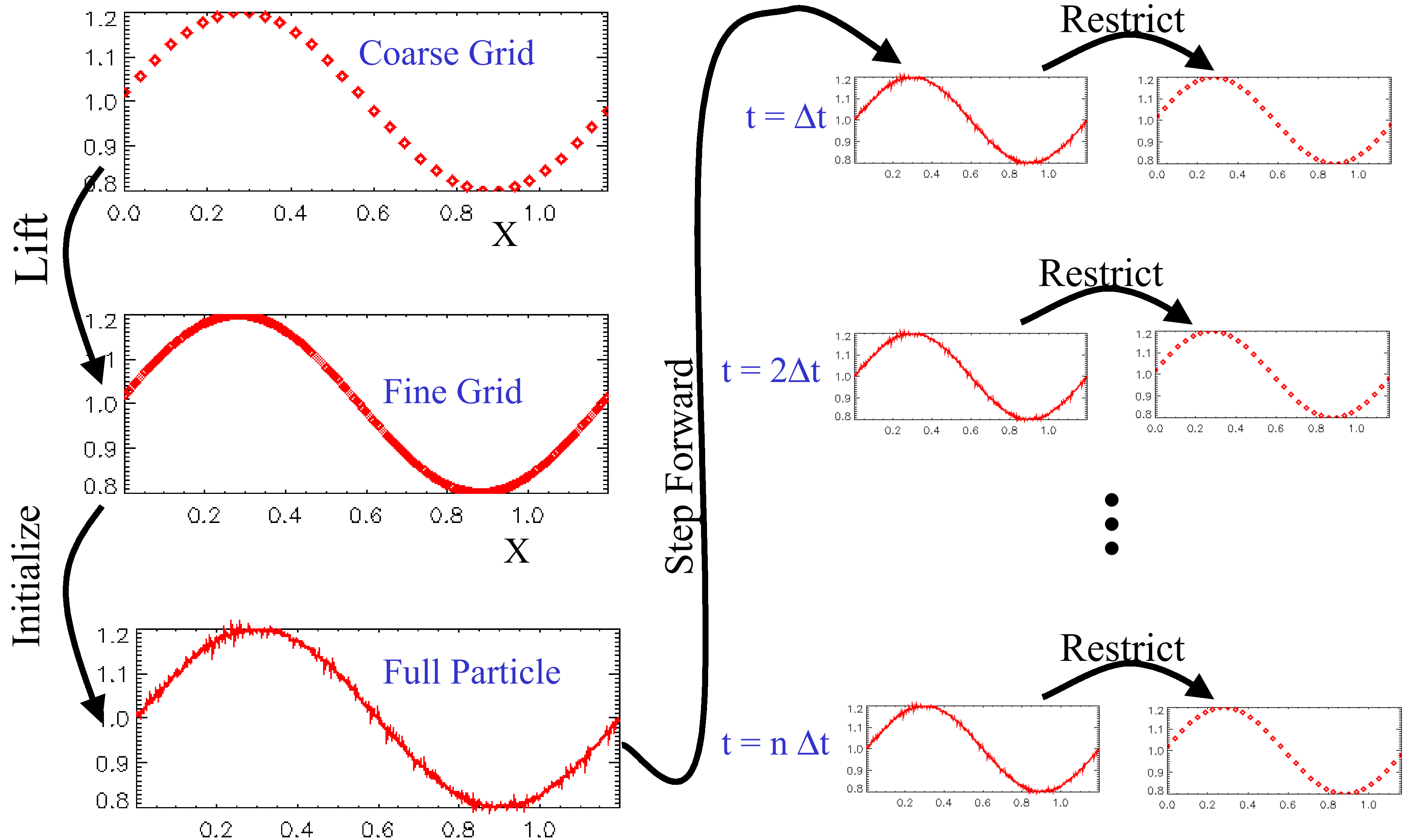
Concerns

- The art is determining which coarse variables to interpolate forward in time.
  - Physics will guide us.
- Noise
  - Must reduce noise level to allow accurate determination of time derivative.

Introducing: efree

- Equation free projective integration stepper.
- Envelopes p3d (Univ. of MD full particle code)
  - (Shay et al., 1998), (Zeiler et al., 2002)
- Parallel with MPI message passing.
- Only 1D for now.
- Projective Integration:
  - Least Squares fit in time to determine time derivative.
  - 2nd order trapezoidal leapfrog time integration.

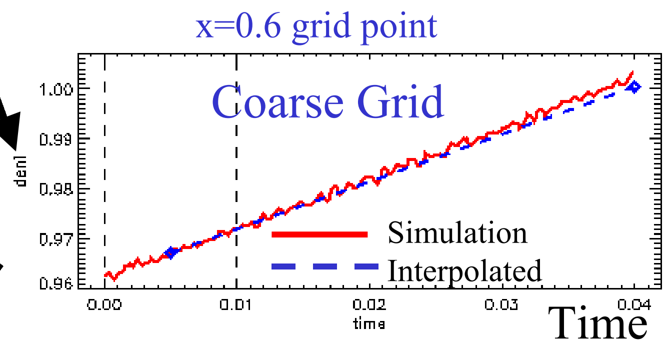
Projective Integration Cycle

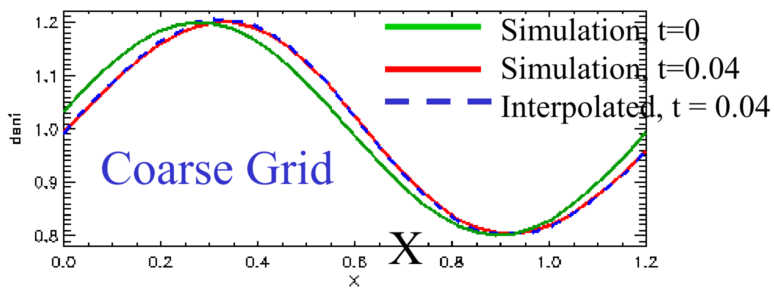


Projective Integration Cycle

Examine each coarse grid point

Extrapolate forward





Initial Study: Ion Acoustic Mode

- Nice Simple 1D problem.
- Linear solution known.

Linear Theory

- Electrostatic limit.
- $T_e >> T_i$
- $(k\lambda_{de})^2 >> m_e/m_i$

$$\frac{\partial n_i}{\partial t} = -\partial_x n_i V_{ix}$$

$$m_i \frac{dV_{ix}}{dt} \approx eE_x$$

$$0 \approx -eE_x - \frac{T_e \partial_x n_e}{n_e}$$

$$\partial_x E_x = 4\pi e(n_i - n_e)$$

$$\omega^2 = \frac{k^2 c_s^2}{1 + k^2 \lambda_{de}^2} \qquad c_s^2 = \frac{T_e}{m_i}$$

$$\tilde{n}_i$$

$$\tilde{V}_i = \frac{\tilde{n}_i}{n_0} \frac{\omega}{k}$$

$$\tilde{n}_e = \tilde{n}_i \frac{1}{1 + k^2 \lambda_{de}^2}$$

$$\tilde{E}_x = -i \frac{m_i}{e} \frac{\tilde{n}_i}{n_0} \frac{\omega^2}{k}$$

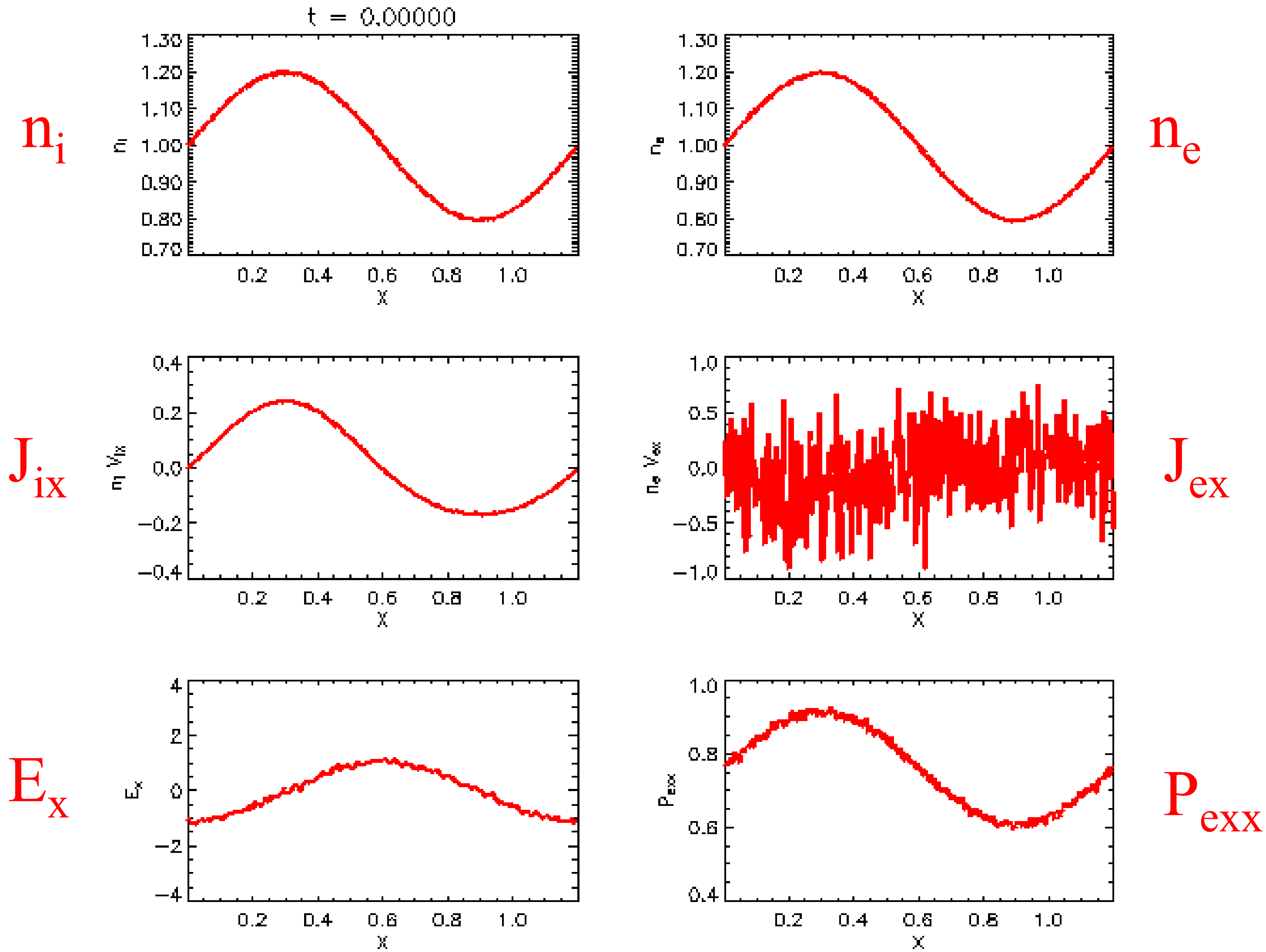
Important Variables

n_i J_{ix} E_x

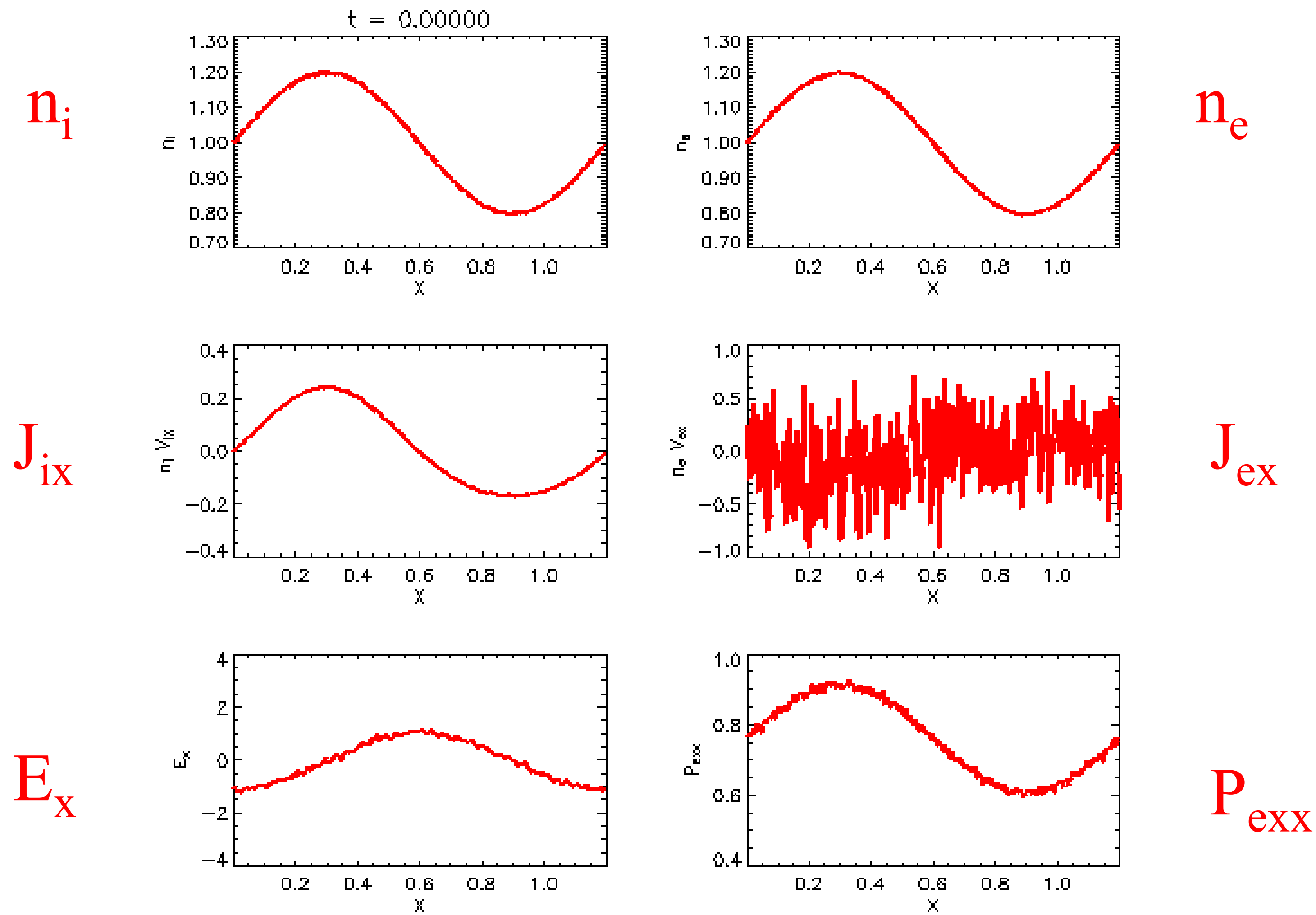
Full Particle Simulations

- Time normalized to Ω_i^{-1}, Length to c/ω_{pi}.
- 1D: Variation along x.
- $n_x = 512$, $L_x = 1.2$, $\Delta_x = 0.00234$
- 5000 particles per cell, 3 million electrons/ions
- 16 processors on IBM SP II
- Initial conditions:
  - $n_i = 1.0 + 0.2 \sin(2\pi x/L_x)$
  - $T_e = 1.0$, $T_i = 0.05$
  - $m_e/m_i = 1800$
  - $c = 120$
- Resultant Plasma parameters
  - $\lambda_{de} = 0.00833$, $\lambda_{di} = 0.00186$
  - $\omega_{pi} = 120$, $\omega_{pi} = 5091$
  - $V_{thi} = 0.22$, $V_{the} = 42.5$
- Time step: $dt = 0.0001$

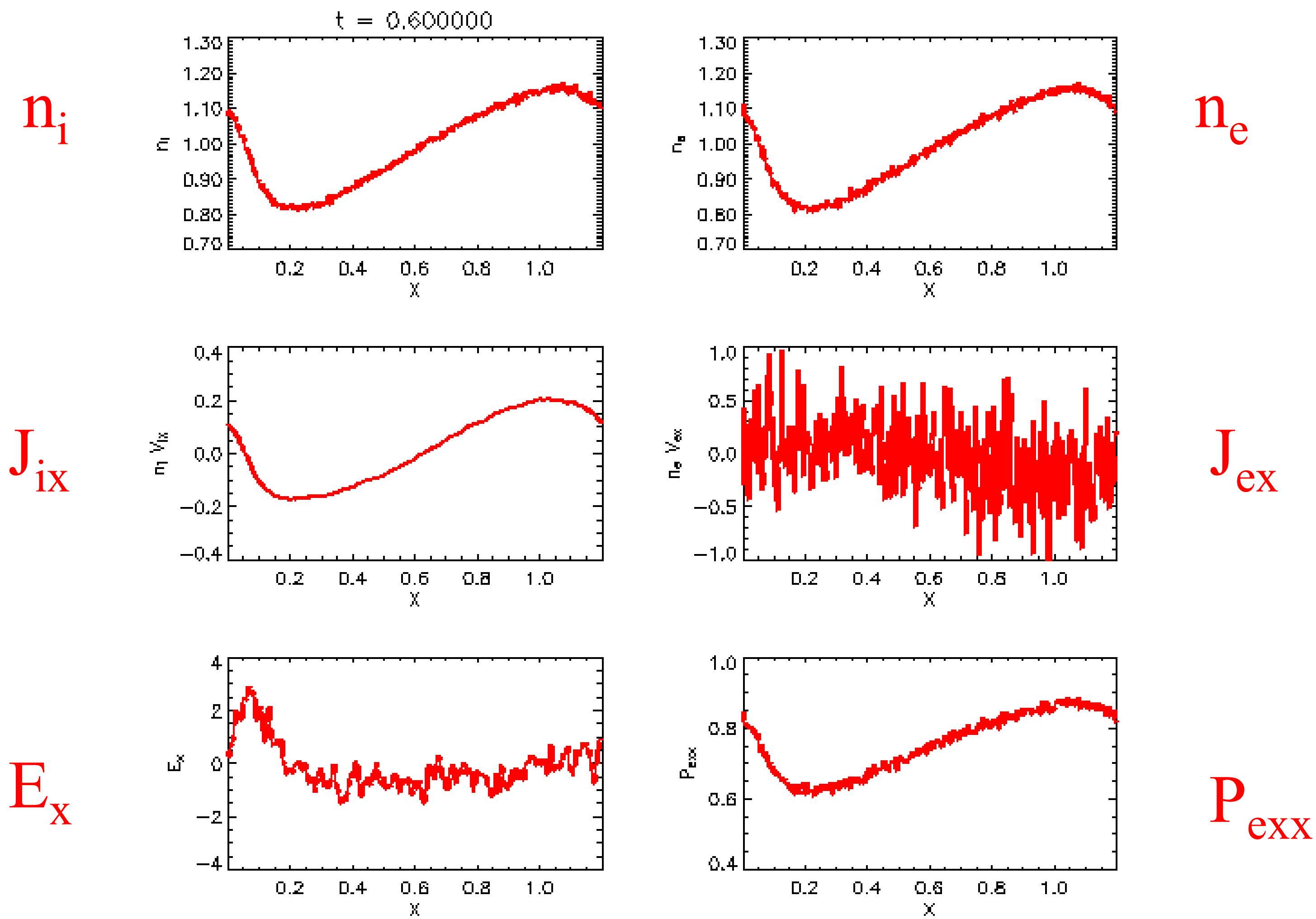
Full Particle Simulations



Full Particle Simulations

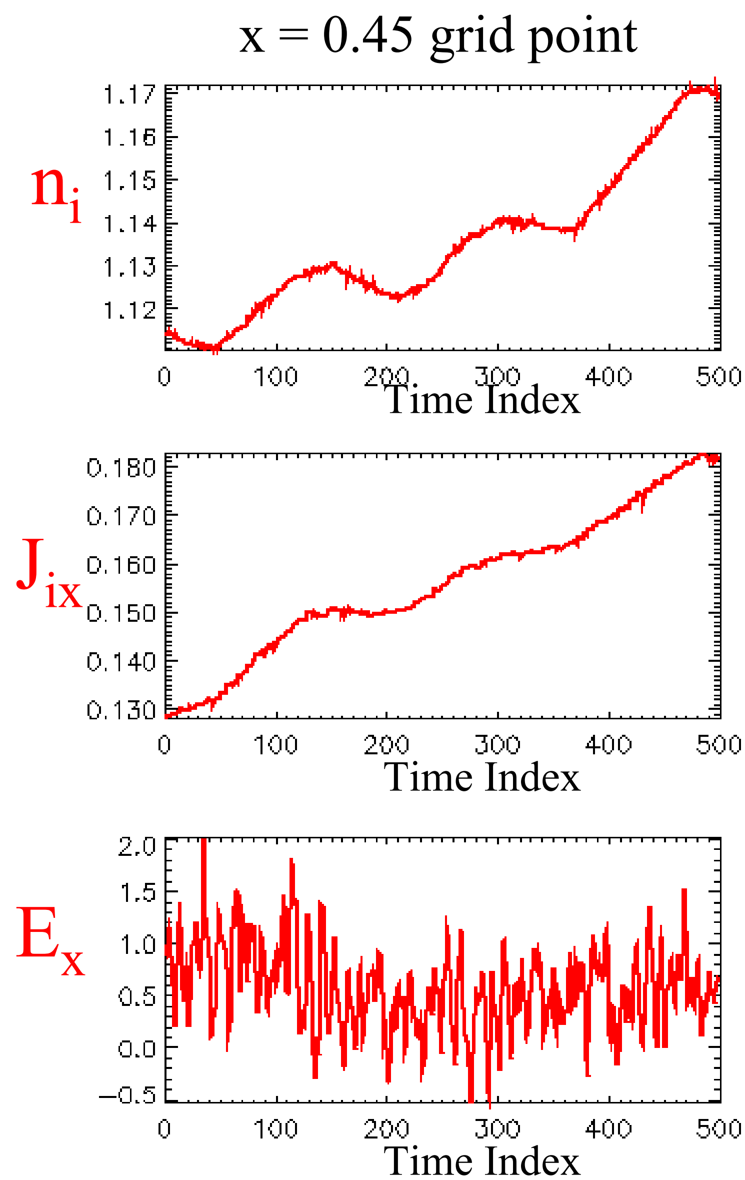


Full Particle Simulations



Equation Free Ion Acoustic

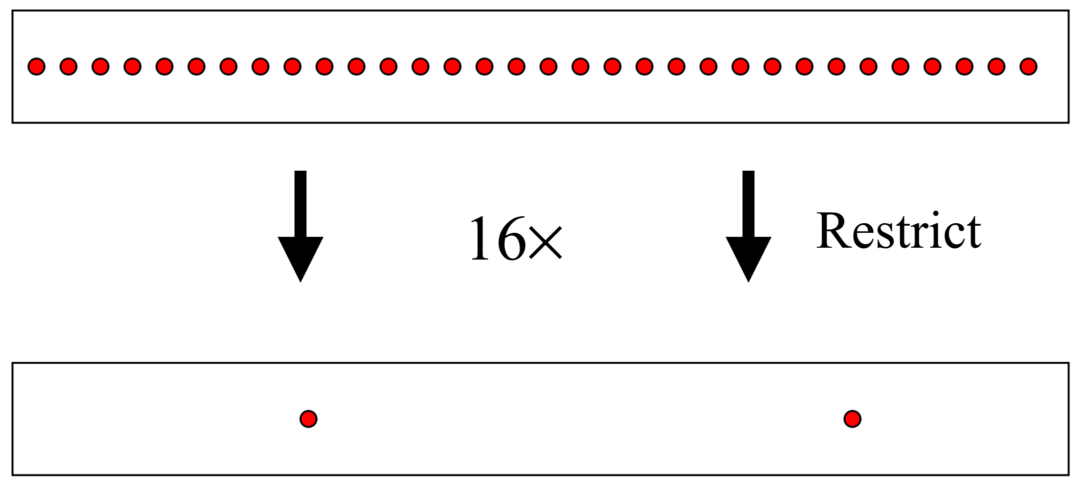
- Minimum: Need n_i, J_{ix}, E_x
- Problem: Noise
  - Especially plasma waves
- Multiscale context:
  - Only need macroscale solution.
  - Coarsen grid.

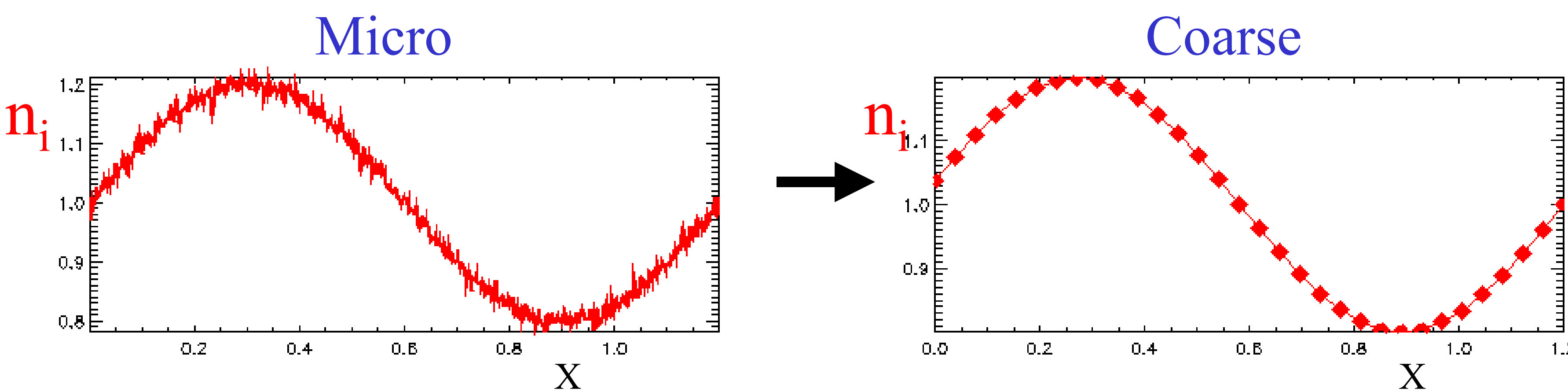


Micro-grid to Coarse-grid

nxmicro = 512
$\Delta_x = 0.00234$

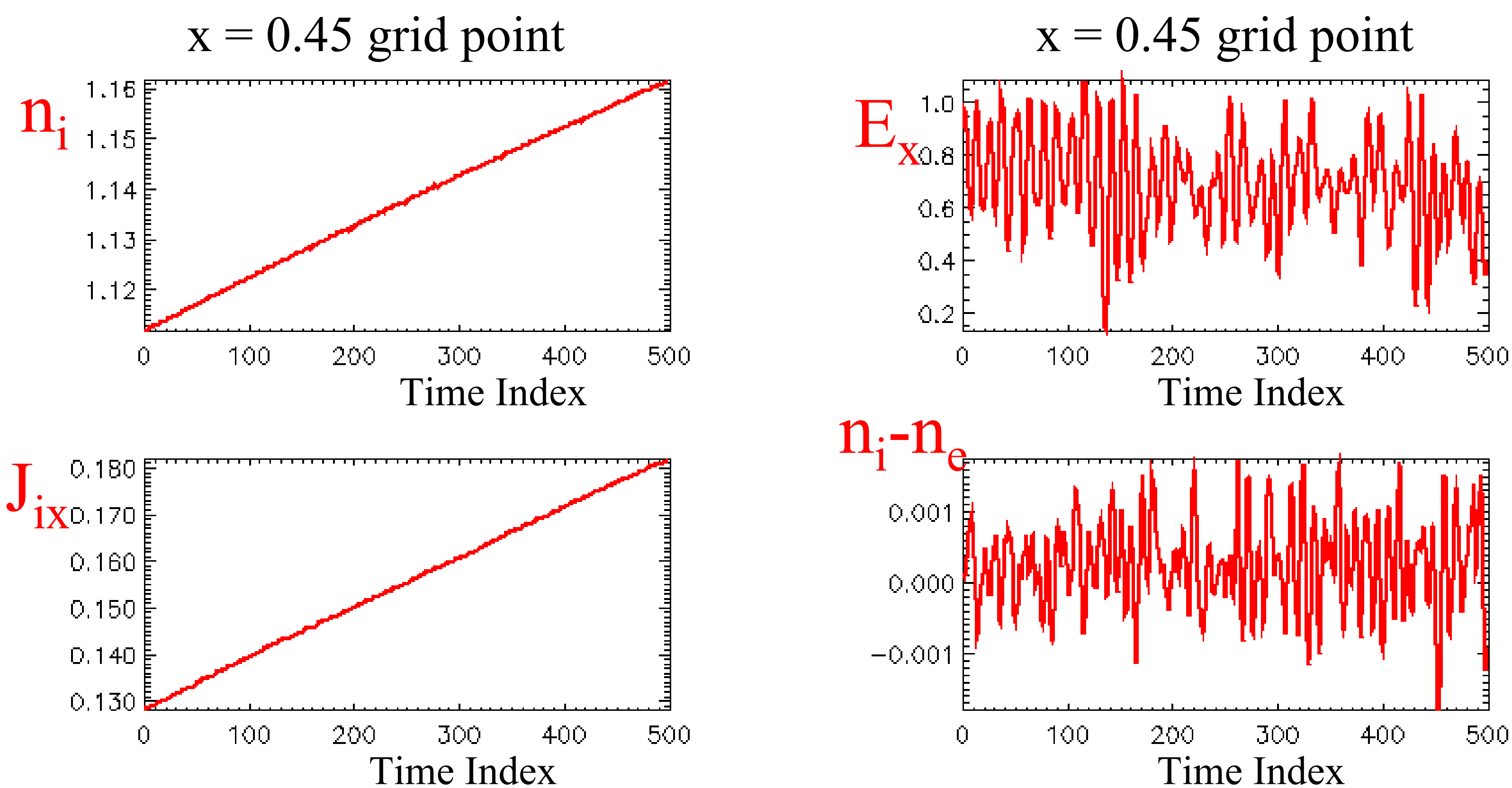
nxcoarse= 32
$\Delta_x = 0.0375$





Coarse Grid Time Extrapolation

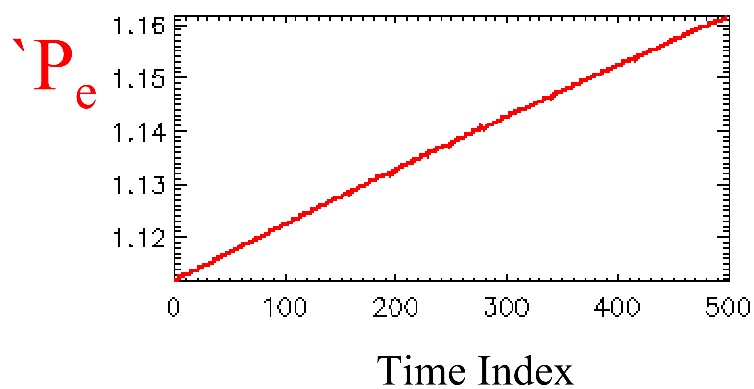
- Problem: E_x still too noisy.
  - Global plasma wave (no k dependence).



Solution: Assume Isothermal

- Use $P_e \approx T_e n_i$, $E_x \approx -\partial_x P_e/n_i$

x = 0.45 grid point

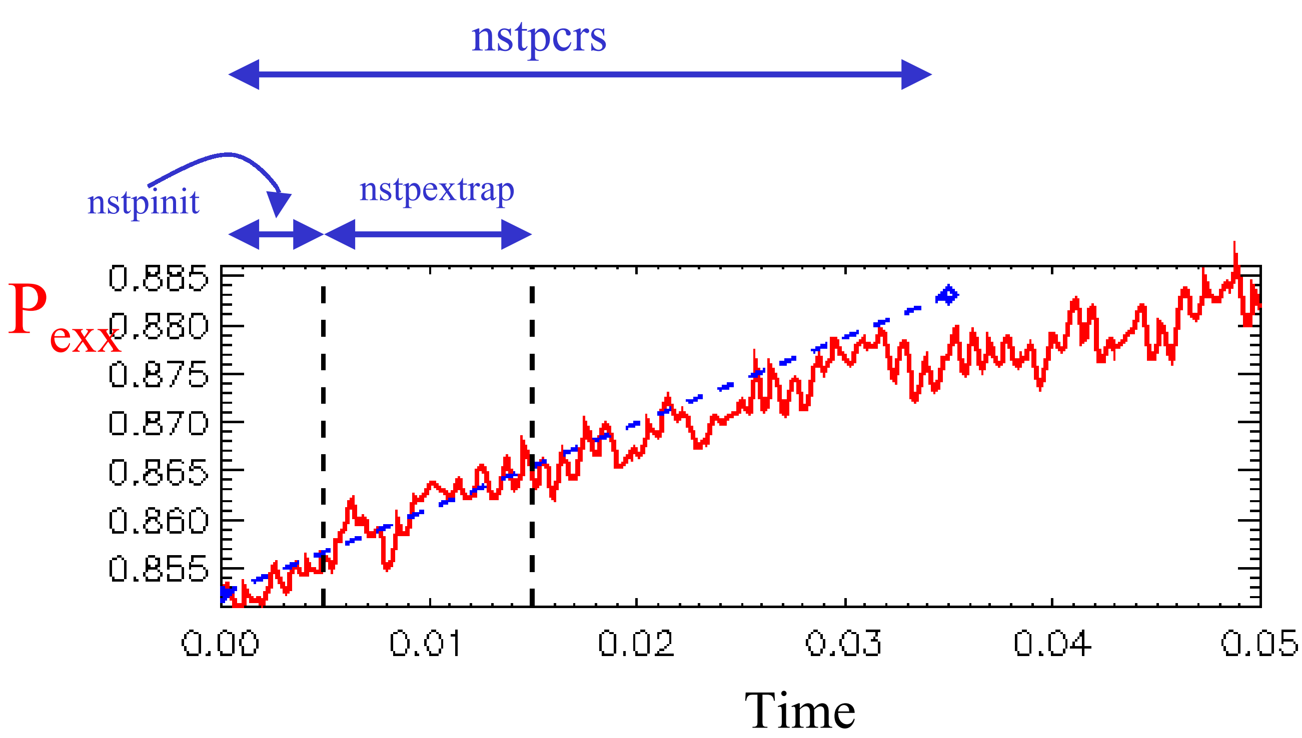


Projecting Forward in Time

- Use least squares fit.
- Skip nstpinit steps,   fit to nstpextrap steps
- Extrapolate forward nstpcrs steps.
- Use predictor corrector (trapezoidal leapfrog)
  - 2nd order accurate in time

Example

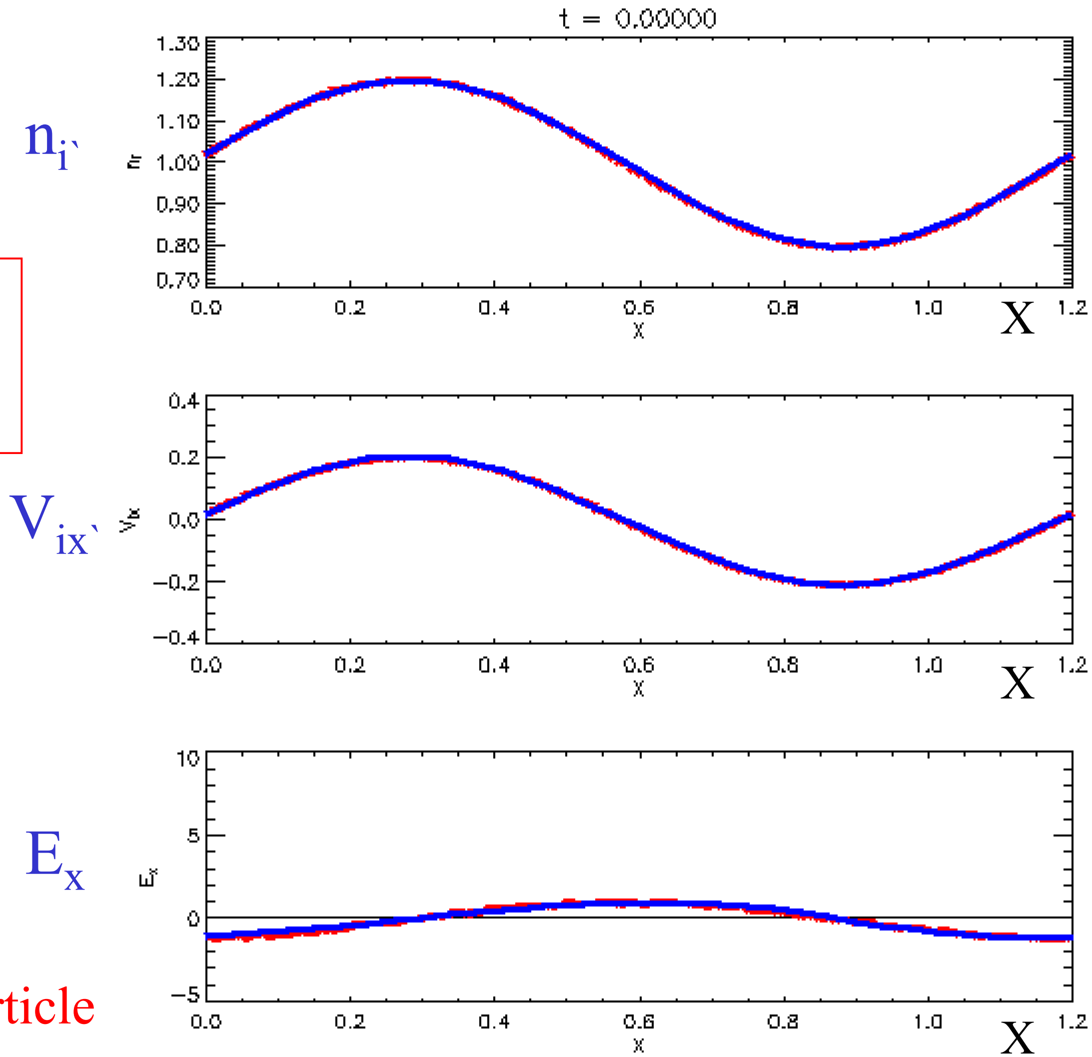
nstpinit = 50
nstpextrap = 100
nstpcrs = 350



Compare Eq. Free and Full Particle

- Pretty Good!

nstpinit = 0
nstpextrap = 20
nstpcrs = 200



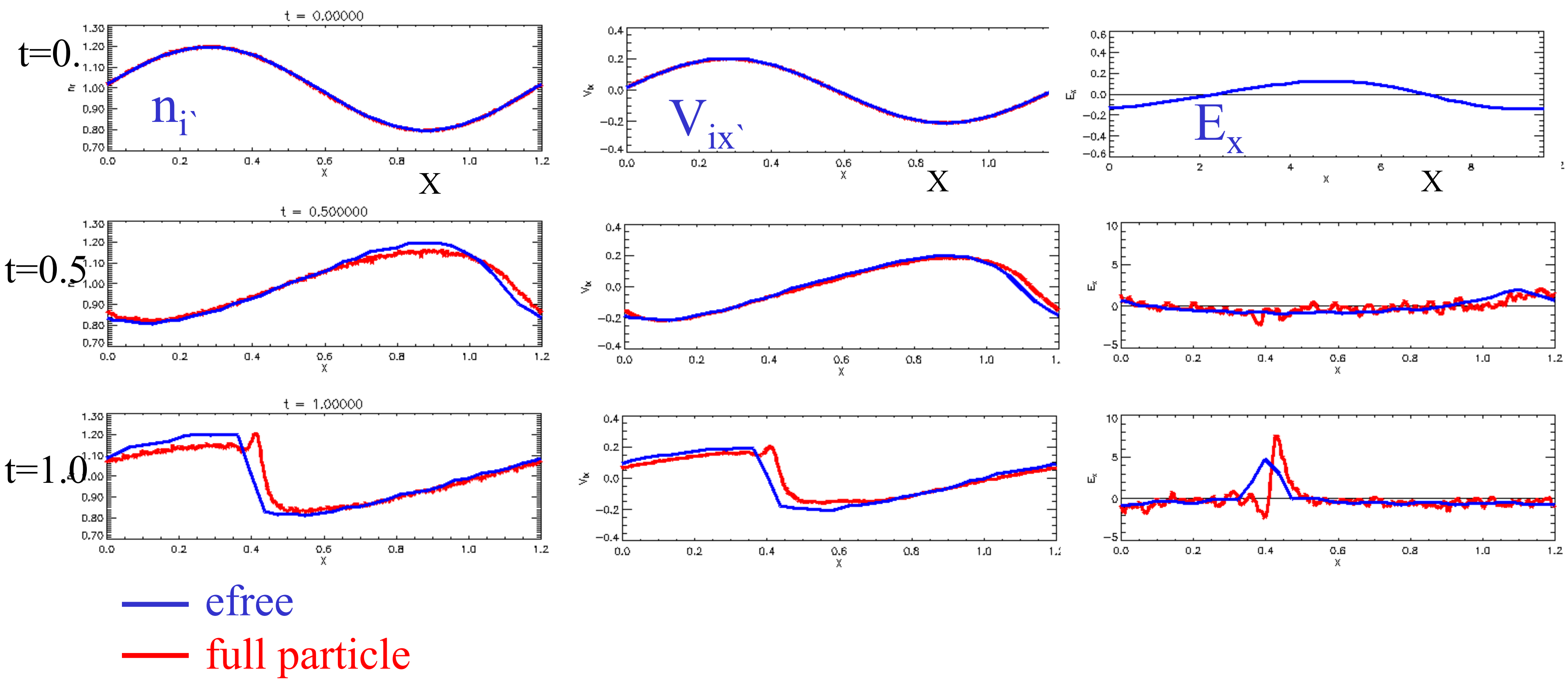
efree

full particle

Comare Eq. Free and Full Particle

- Pretty good!
  - Small difference as wave steepens.
    - Debeye length effect?

nstpinit = 0
nstpextrap = 20
nstpcrs = 200



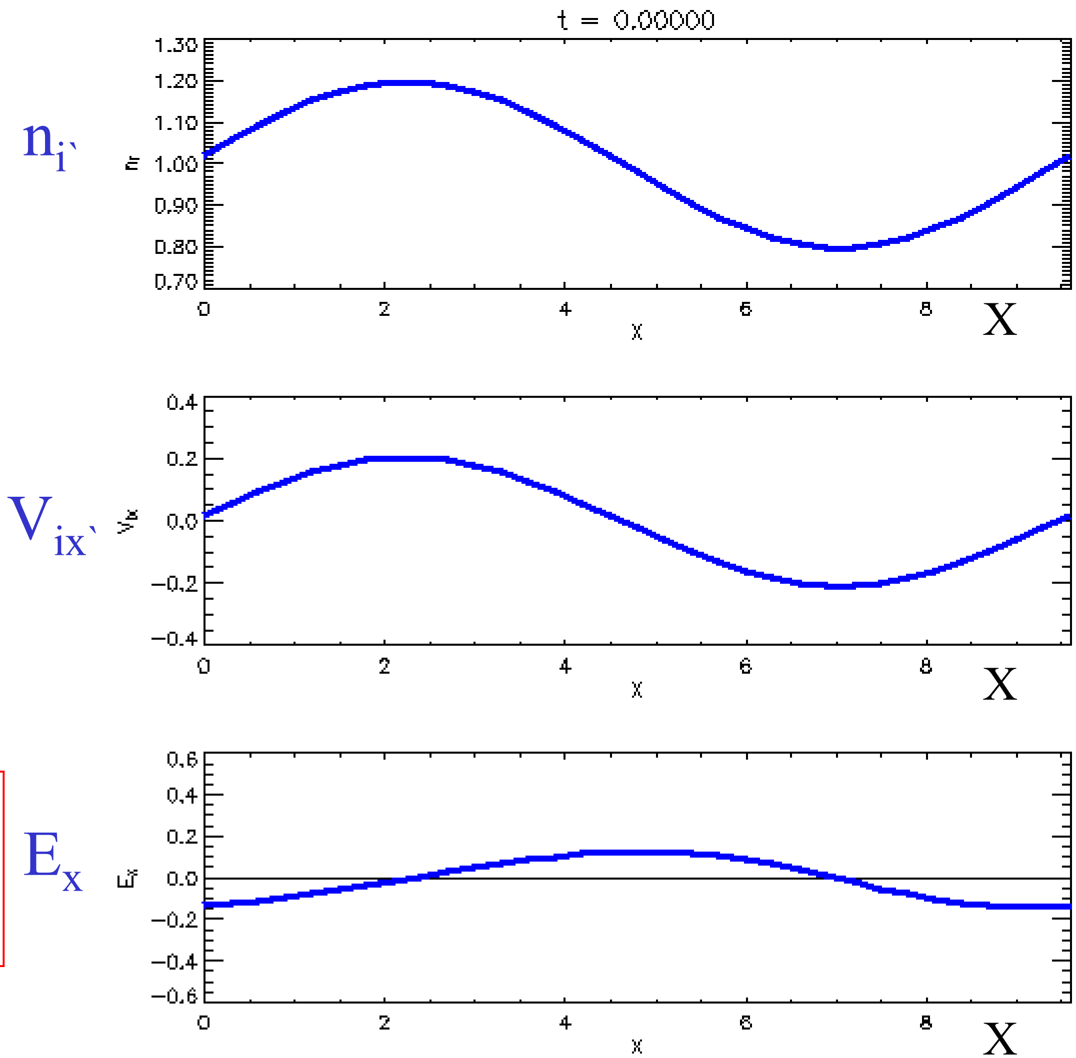
Much Larger Simulation

- As system size increases, increases time saved in equation free.
  - About 20 × speedup so far.

L_x	nstpextrap	nstpmicro	Full Particle (runtime/t_0)	Eq. Free (runtime/t_0)	Time Saved (p3d/efree)
1.2	20	200	11.1	1.6	6.9
9.6	40	800	63.9	3.3	19.3

Efree: Large Simulation

- $L_x = 9.6$
- 20 times faster than full particle



nstpinit = 0
nstpextrap = 40
nstpcrs = 800

Efree: Large Simulation

- $L_x = 9.6$
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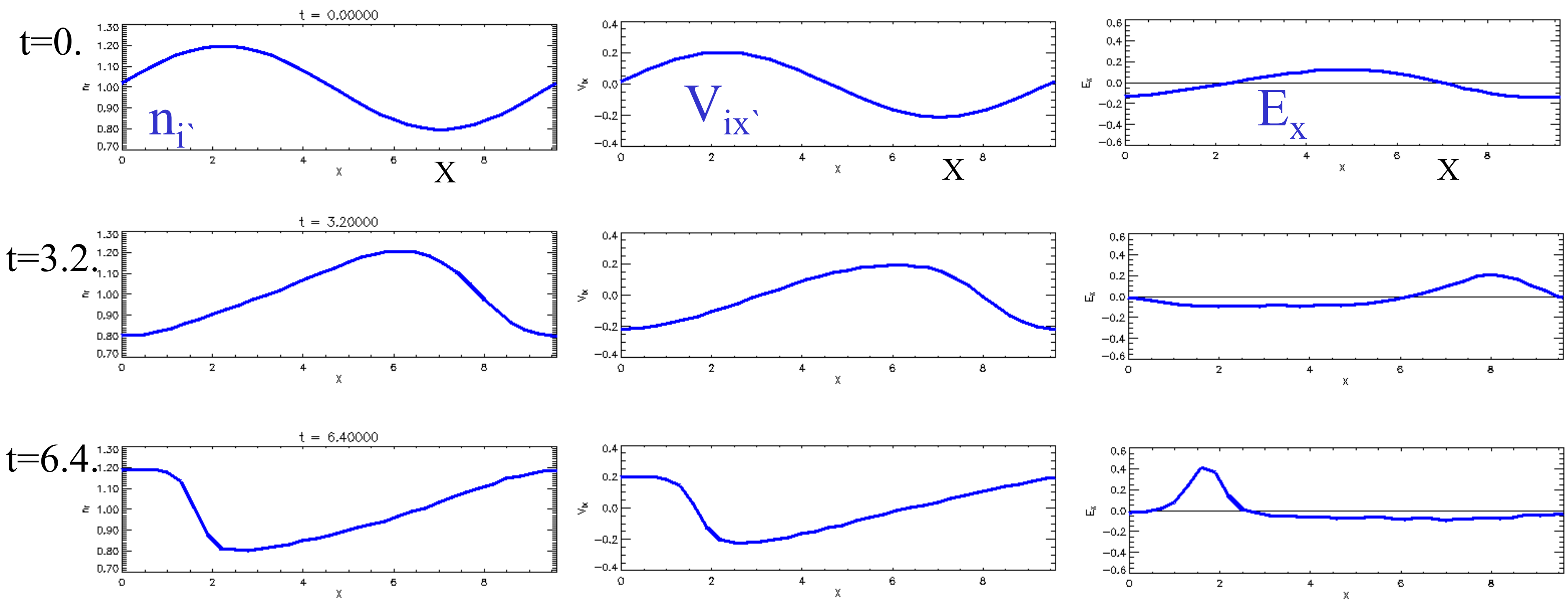

Conclusions

- Equation Free Projective Integration
  - May be useful tool for studying multiscale problems.
- efree: Equation free with kinetic PIC code for "experiment"
- Test Case: Ion Acoustic Wave
  - 20 time speedup over full particle!
  - Slight differences as wave approaches a shock.
    - Debeye length effects?