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Verification of Plasma Physics Codes

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Outline

Introduction

Cold diode Verification Study with Empire-PIC

Warm diode Verification Study with Empire-Fluid

Summary

Thanks to Sean Miller for helpful discussions

Introduction

Code V&V Efforts simultaneously with Code Development

- Advanced Technology Disruption Mitigation (ATDM) program aims at developing performant application codes for next generation hardware while also supporting a vigorous V&V effort
- EM plasma Grand Challenge Lab Directed R&D (GCLDRD) which aims is to improve modeling/simulation for Z power flow has a component focused on reproducible Science which includes V&V and Code Comparison Infrastructure (CCI)

EMPIRE Verification Topics to be Discussed in this Presentation

- Boundary condition and time integration verification of EMPIRE-PIC using a Cold Diode problem
- Space charge limited (SCL) and general inflow boundary conditions and EM/fluid coupling verification in EMPIRE-Fluid using a Warm Diode problem

Verification and Validation

- Code verification – Determination that mathematical description of the physical model is solved correctly (usually involves comparing to known solutions)
  - Often involves simplifications in order to obtain an exact or analytic solution
- Solution verification – Determination that the numerical solutions are converging under refinement (to a highly refined reference solution, or a nearby solution)
- Solution validation – Determine if the right model is being solved
  - Direct comparison of the numerical simulation solution data to experimental data

Empire-PIC Verification of a Cold Diode

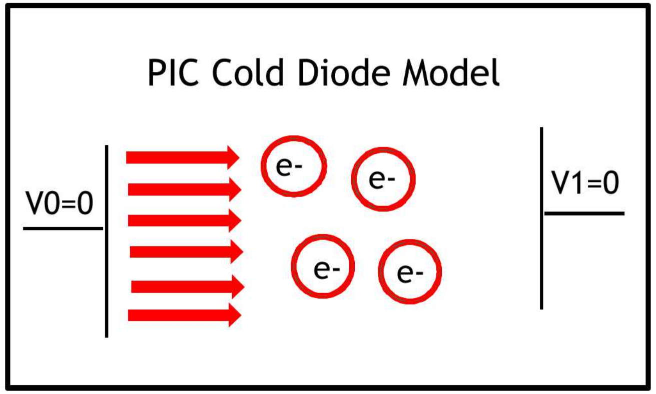
Cold Diode Problem (w. T. Pointon)

1D electrostatic system, $0 \le x \le d$, with applied voltage V

- Inject cold beam of particles with charge q and mass m at $x = 0$, with kinetic energy W and current density J
- BCs on the electrostatic potential: $\phi(0) = 0$, $\phi(d) = V$
- $qV < 0$ for net acceleration across the gap

Equilibrium solution published long ago: George Jaffe, Phys. Rev., **65**, 91 (1944)

- Space-charge-limited current: $J_{\max} = \frac{J_0}{4}\left[1+\left(1-\frac{qV}{W}\right)^{1/2}\right]^3$, where $J_0 = \frac{16}{9}\varepsilon_0\left(\frac{2q}{m}\right)^{1/2}\frac{(W/q)^{3/2}}{d^2}$
- J_{max} reduces to Child-Langmuir current for $W \to 0$
- $J_{max} = 2J_0$ for cold beam injected into a grounded box ($V = 0$)



For $J < J_{max}$, exact analytic profiles for $\phi(x)$, electric field $E(x)$, and particle velocity $v(x)$

Very clean verification problem for an electrostatic PIC code

Caveat for verification: must use a timestep that is an exact integer divisor of the particle transit time

- Otherwise, equilibrium PIC solution has a slight gap with no particles near $x = d$

Governing equations: charge conservation, energy conservation, Poisson's equation

Physical parameters: $\phi(0) = 0$, $\phi(d) = V$, d, W, J

Computational parameters: transit time, simulation time, particle count, timestep, mesh resolution

Cold diode verification problem (W. T. Pointon)

Formal verification of EMPIRE-PIC using Jaffe's solution for the cold diode

Electrostatic field solver with uniform and random particle emission tested

Leapfrog and Velocity-Verlet time integrators tested

Outcomes from verification study:

- Convergence rates for E-field exposed an issue at boundaries – which was corrected by development team, resulting in expected order of accuracy
- Convergence rates for velocity showed Leapfrog time integration scheme requires an error correction for staggered velocity/particle solutions in order achieve expected rates accuracy
- Velocity-Verlet time integration scheme, which alleviates the need for a correction, was implemented, tested and verified
- Velocity-Verlet time integration scheme velocity boundary conditions were implemented, tested and verified

Potential Error Norms

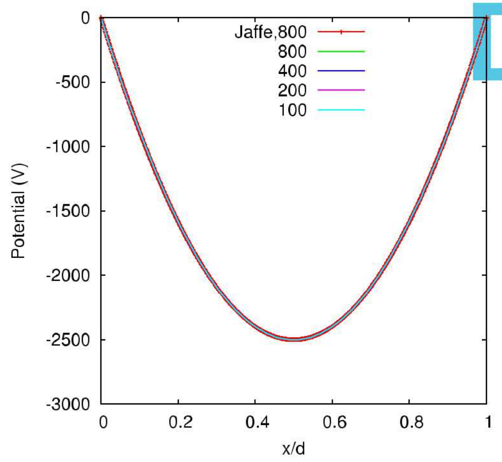
$Mesh$	L_1	L_2	L_∞
800	1.04e-04	1.16e-04	1.66e-04
400	3.95e-04	4.41e-04	6.30e-04
200	1.55e-03	1.73e-03	2.48e-03
100	6.02e-03	6.77e-03	9.83e-03

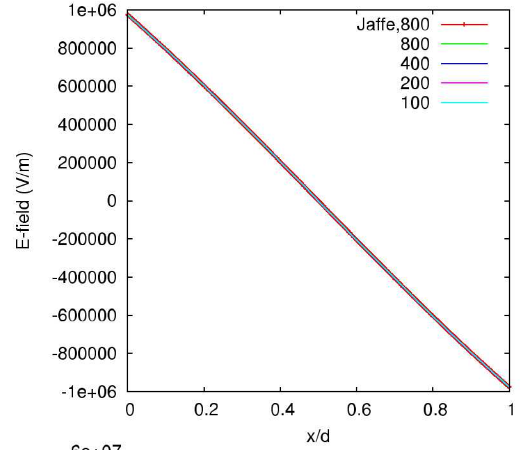
E-field Error Norms

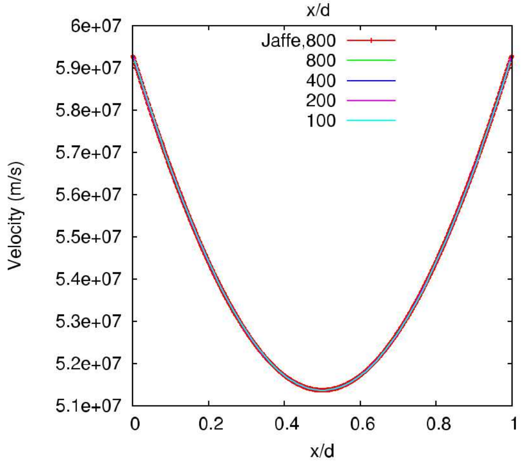
$Mesh$	L_1	L_2	L_∞
800	1.76e-01	1.95e-01	2.78e-01
400	6.95e-01	7.70e-01	1.11e+00
200	2.76e+00	3.06e+00	4.49e+00
100	1.09e+01	1.21e+01	1.79e+01

Electron Velocity Particle (Verlet) Error Norms

$Mesh$	L_1	L_2	L_∞
800	3.08e+00	3.34e+00	4.74e+00
400	1.15e+01	1.26e+01	1.82e+01
200	4.51e+01	4.97e+01	7.17e+01
100	1.79e+02	1.97e+02	2.83e+02







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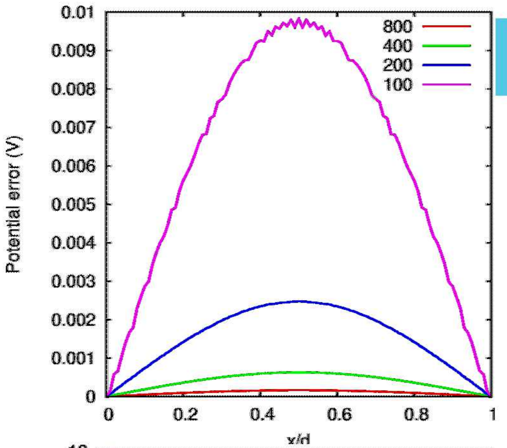

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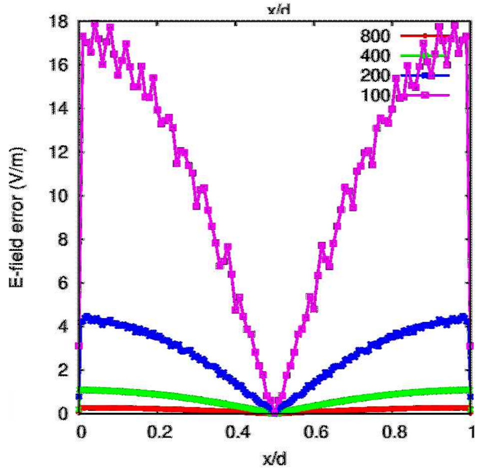

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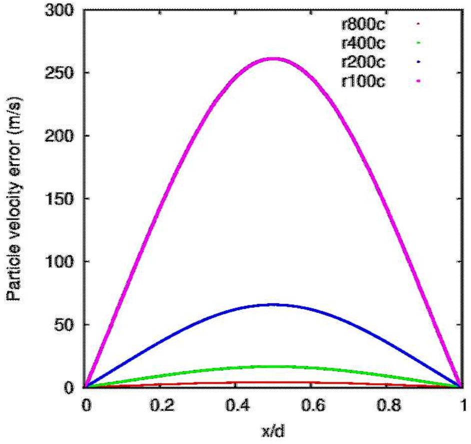
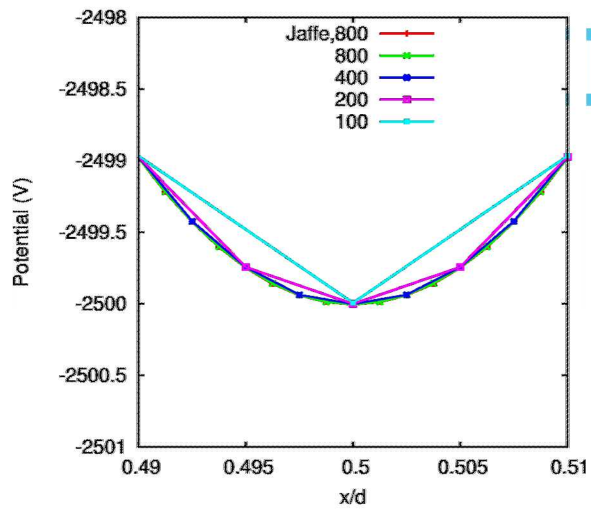
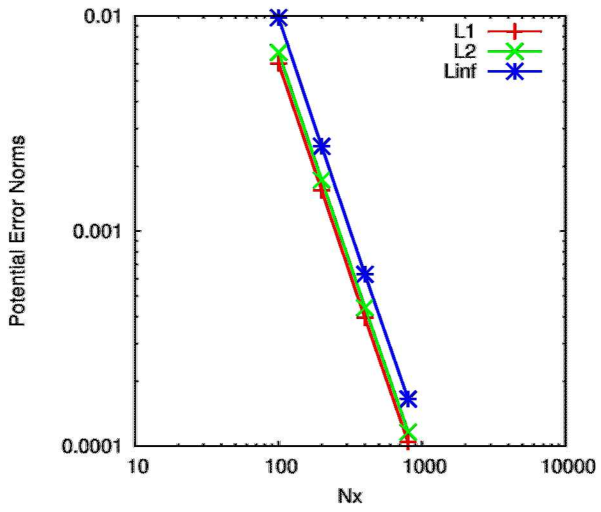


Cold diode error norm convergence (w. T. Pointon)

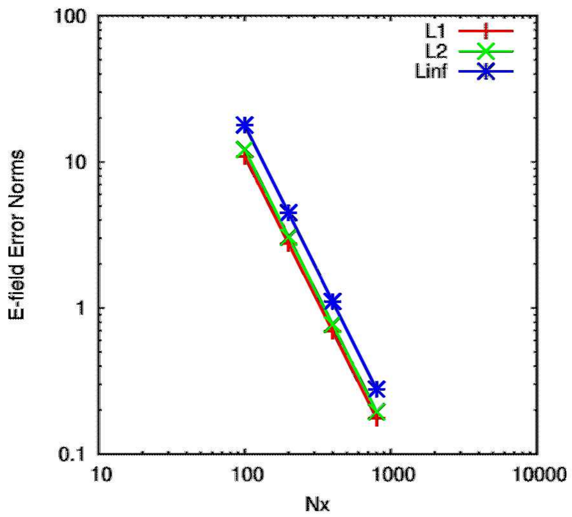


- L1, L2 and L_∞ spatial error norms of potential, electric field and particle velocity all converge at the expected rate ($p \approx 2$)
- **For the cold diode problem with conditions studied: electrostatic field solver, BCs and time integration algorithms were verified to expected order of accuracy**



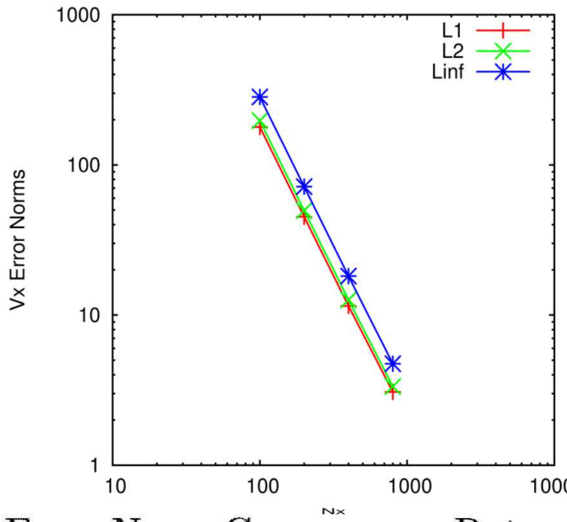
Potential Error Norm Convergence Rates

Mesh pair	L_1	L_2	L_∞
800-400	1.92	1.92	1.93
400-200	1.97	1.97	1.98
200-100	1.96	1.97	1.99



E-field Error Norm Convergence Rates

Mesh pair	L_1	L_2	L_∞
800-400	1.98	1.98	1.99
400-200	1.99	1.99	2.02
200-100	1.98	1.99	2.00



Velocity Error Norm Convergence Rates

Mesh pair	L_1	L_2	L_∞
800-400	1.90	1.92	1.94
400-200	1.97	1.98	1.98
200-100	1.99	1.99	1.98

Empire-Fluid Verification of a Warm Diode

EMPIRE-Fluid Warm Diode Verification

Similar to the cold diode:

- One dimensional
- Non-zero electron streaming velocity
- Physical parameters: $W, J_0, d,$
- Computational parameters: *simulation time, timestep, mesh resolution*

Unlike the cold diode:

- Temperature, internal energy and pressure and equation of state
- Additional physical parameters: E_0, T_{e0}, *adiabatic index, equation of state assumption*
- MF numerical formulation solves the conservation equations which includes total energy
- Do not use discrete particles

An analysis different than cold diode analysis is necessary to verify multi-fluid (MF) plasma physics codes

- Include pressure gradient terms
- Include equation of state
- Solving Maxwell's equations instead of using electrostatic assumption

Euler/Poisson Steady State Analysis (N.D. Hamlin)

Steady Euler/Poisson system provides a quasi-analytic solution for the warm diode

Assume adiabatic equation of state: $P_e = An_e^\Gamma$

System is transformed to IVP

- solved for ve(x) and dve/dx(x) -> Pe, ne, Te, Ex
- In limit as Te -> 0 and the pressure gradient term is neglected the Euler/Poisson solution recovers the cold diode solutions of Jaffe, (1944) and Rokhlenko and Lebowitz, (2013)
- Solved using Mathematica
- This solution method is similar to MF, solved with EM instead of ES, and both prescribing E0 at the inflow BC
- Initialization: $(v_{e0}, E_0, \Gamma, T_{e0}, J_0, d)$

$$m_e\left(v_{e0} - \frac{\Gamma v_{T_{e0}}^2}{v_{e0}}\right)\frac{dv_{e0}}{dx} = eE_0$$

Euler/Poisson System

$$\begin{aligned}
m_e n_e v_e \frac{\partial v_e}{\partial x} &= n_e e\frac{\partial \phi}{\partial x} - \frac{\partial P_e}{\partial x} \\
\frac{\partial^2 \phi}{\partial x} &= \frac{n_e e}{\epsilon_0} \\
P_e &= An_e^\Gamma \\
J_0 &= n_e e v_e = constant
\end{aligned}$$

IVP System

$$m_e\left[v_e - \Gamma v_{T_{e0}}^2 v_{e0}^{\Gamma-1}\left(\frac{1}{v_e^\Gamma}\right)\right]\frac{\partial^2 v_e}{\partial x^2} + m_e\left[1 + \Gamma v_{T_{e0}}^2 v_{e0}^{\Gamma-1}\left(\frac{1}{v_e^{\Gamma+1}}\right)\right]\left(\frac{dv_e}{dx}\right)^2 = \frac{eJ_0}{\epsilon_0 v_e}$$

Recover Pe, ne, Te, Ex

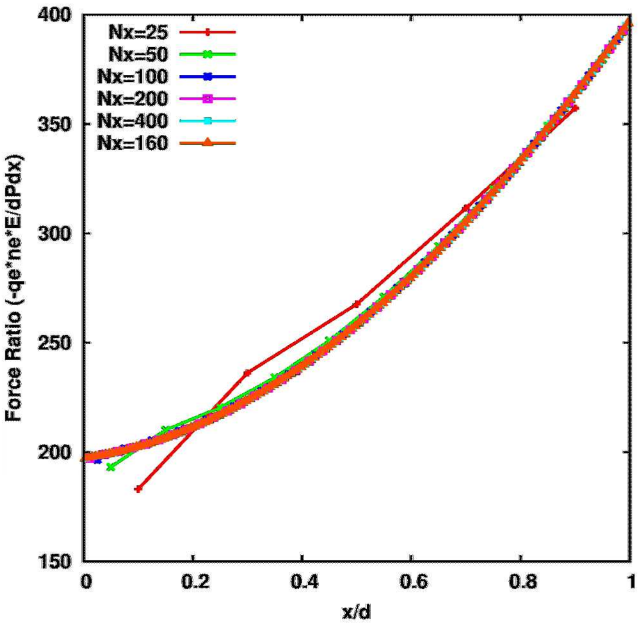
$$\begin{aligned}
v_{T_{e0}} &= \sqrt{k_B T_{e0}/m_e} \\
P_e &= An_e^\Gamma \\
A &= (m_e v_{T_{e0}}^2)(ev_{e0}/J_0)^{\Gamma-1} \\
n_e &= J_0/(ev_e) \\
T_e &= P_e/(k_B * n_e)
\end{aligned}$$

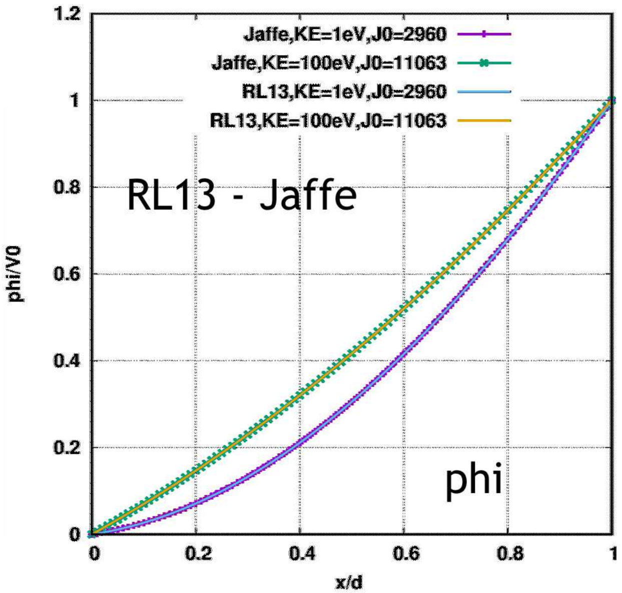
$$E(x) = \frac{m_e}{e}\left(v_e - \frac{\Gamma v_{T_{e0}}^2 v_{e0}^{\Gamma-1}}{v_e^\Gamma}\right)\frac{dv_e}{dx}$$

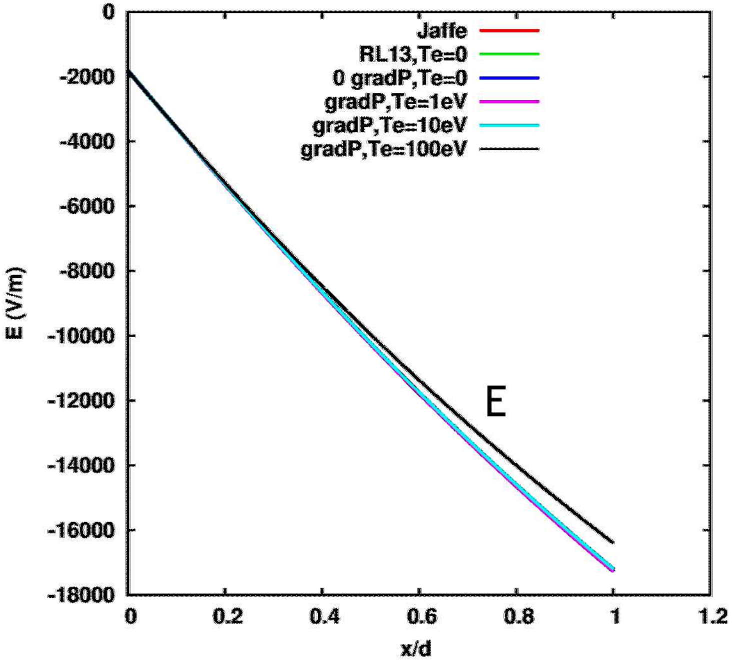
Comparing Cold and Warm Diode Analyses

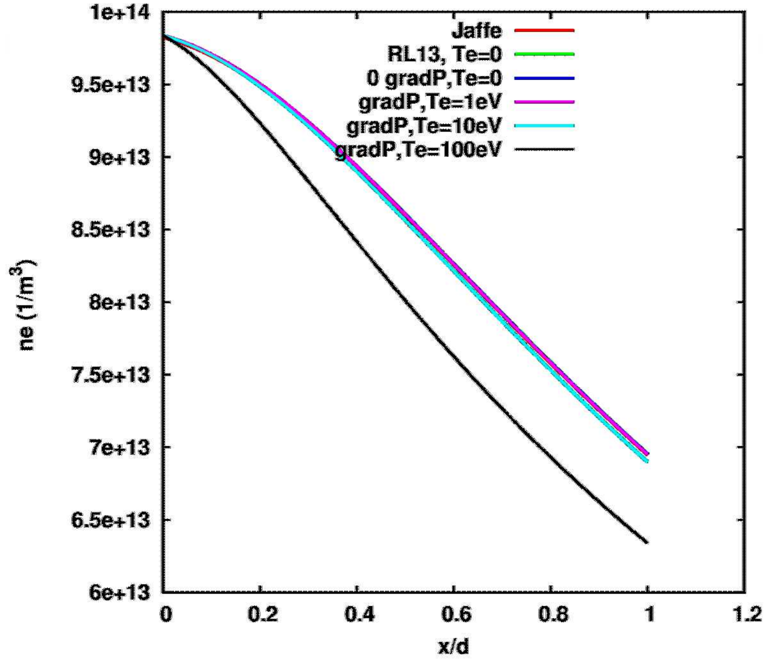
Analytical and quasi-analytical models

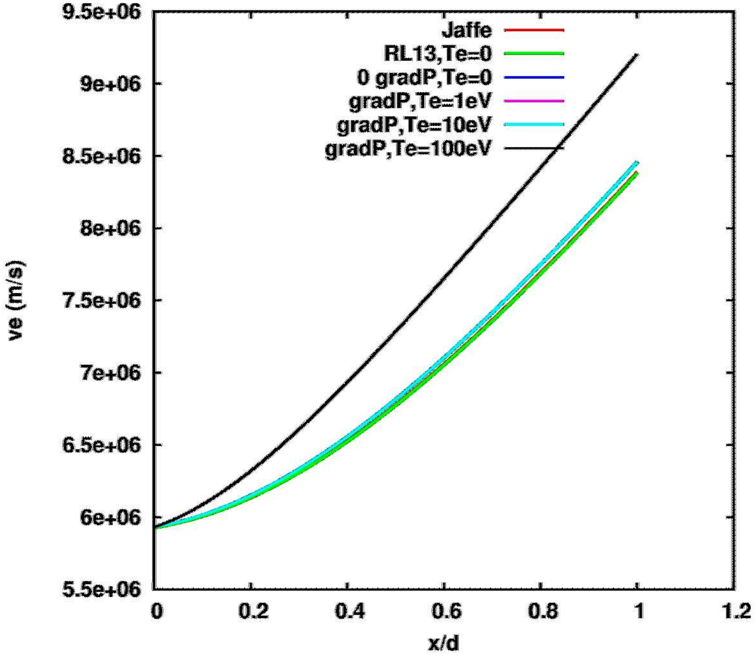
- Jaffe Cold Diode, 1944: (**Jaffe**)
- Rokhlenko and Lebowitz Cold Diode, 2013: (**RL13**)
- Euler/Poisson IVP, adiabatic eos: (**gradP**)





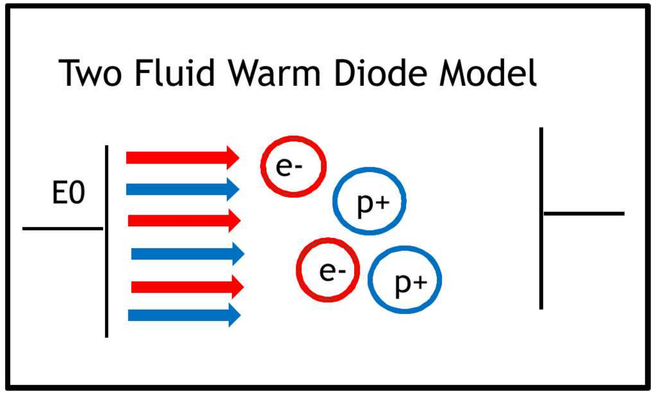






Fluid Model of Warm Diode

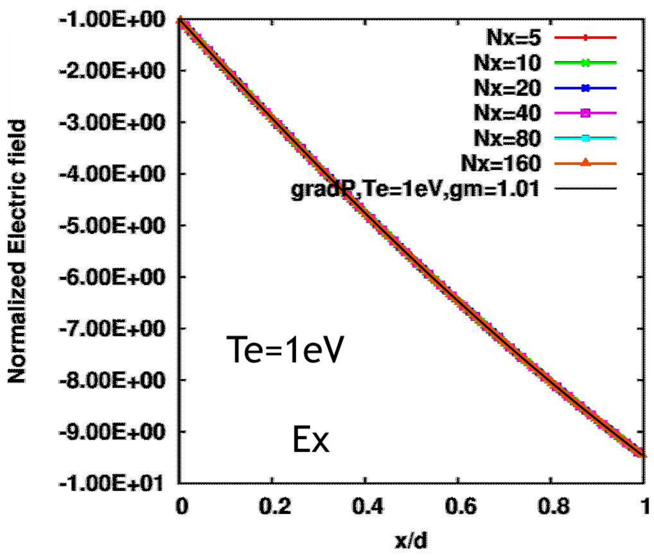
- Fluid Model has additional parameters
  - Background temperature
  - adiabatic index
  - Electric field offset E_0 instead of Voltage

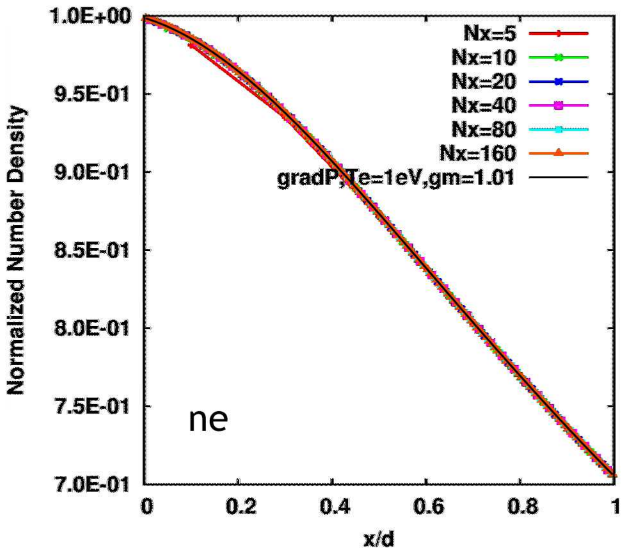


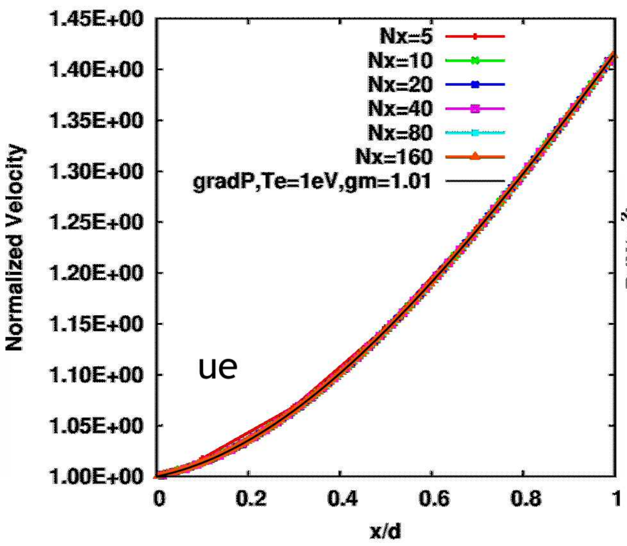
- Numerical details:
  - Two fluids: electrons and positrons
  - Current neutralization using heavy positrons
  - IMEX time integration
  - Implicit CG electromagnetics
  - Explicit DG fluids
  - Supersonic inflow fluid BCs
  - Conducting wall EM-field BCs
  - Fluid ICs are uniform,
  - Initial charge density is zero

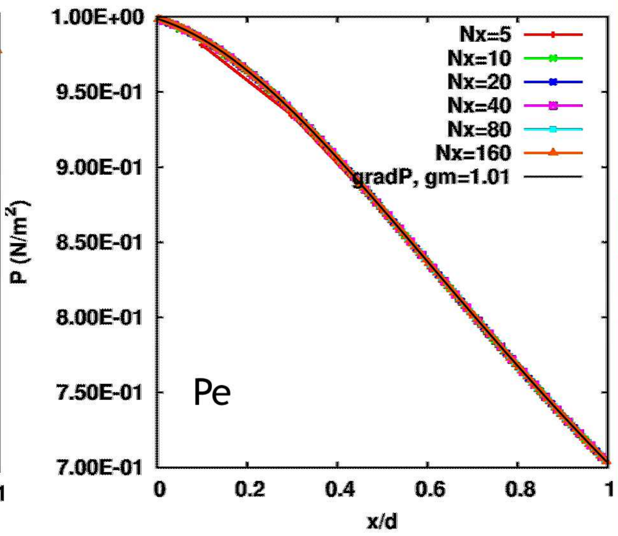
One example:

- d=0.01 (m)
- V1 ~100 (V) -> E0~-1821.2 (V/m)
- J=J0 = 93.35807793 (A/m^2)
- W = 1.60217662e-17 (eV)
- T0 = 1, 10, 100 (eV)
- gamma=1.01
- Mach=14, 4.4, 1.4
- EM-Field ICs: B=0, *E=-e*n0*x/eps0* + *E0*





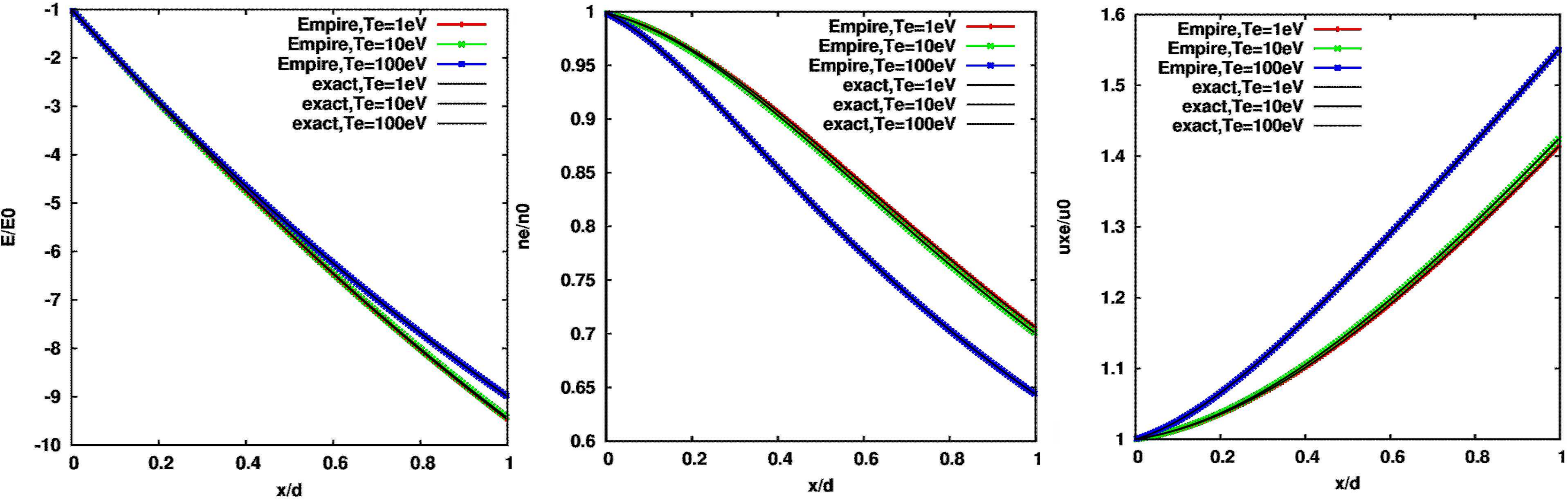




Multi-Fluid Code Verification: Warm Diode Behavior

Solution for warm diode deviates from cold diode as temperature increases

- Relatively small deviation from cold behavior for Te=1eV and 10eV
- Empire-Fluid MF code tracks exact solution of electric field, number density and velocity for all three temperatures



Multi-Fluid Code Verification: Warm Diode Behavior

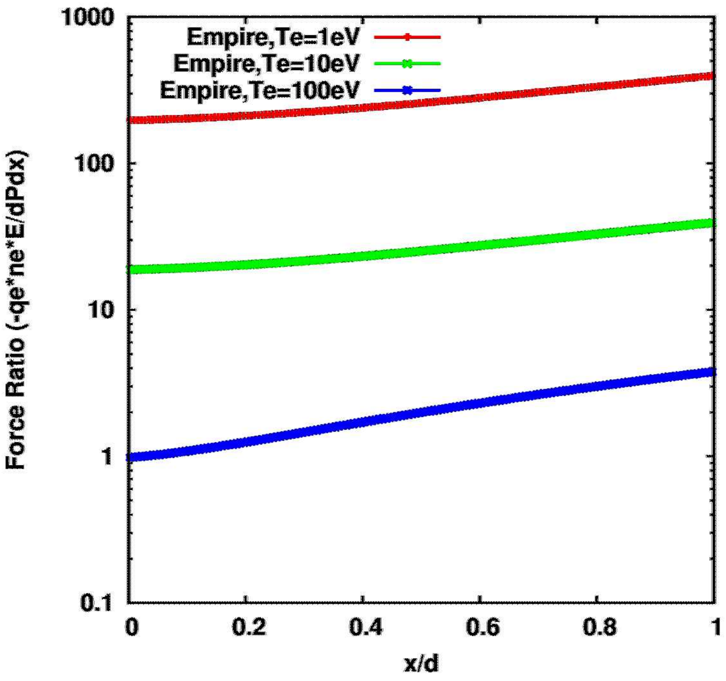
Force ratio is the ratio of EM to pressure forces

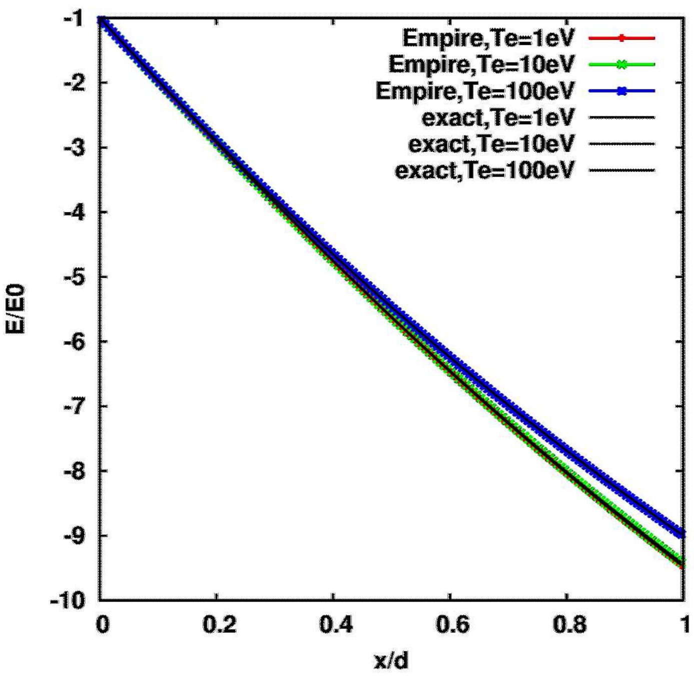
- EM forces dominate at low temperature (cold diode behavior)
- As temperature increases pressure force becomes important (warm diode behavior)

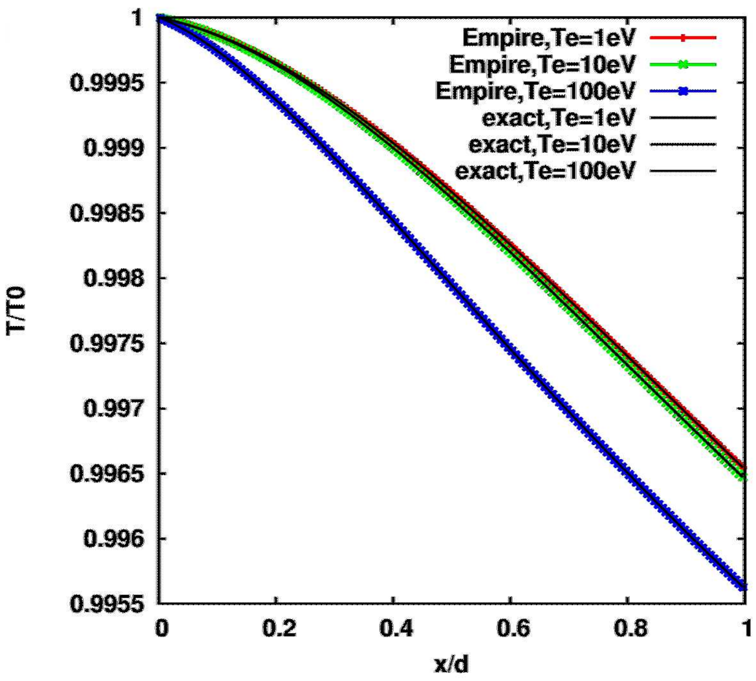
Study of Euler/Poisson system showed solutions not sensitive to adiabatic index for range [1, 1.1]

For this initial study adiabatic index = 1.01 to approach isothermal conditions and minimize pressure gradient effects

These results for temperature range [1eV, 100 eV] show that the MF solution track temperature dependence of the analytic solution







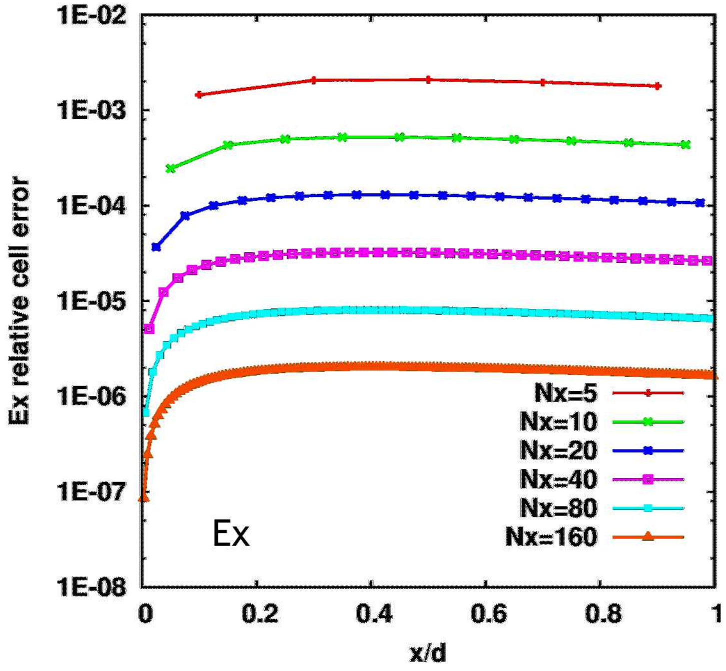
Multi-Fluid Code Verification: Relative Cell Based Error for Te=1eV

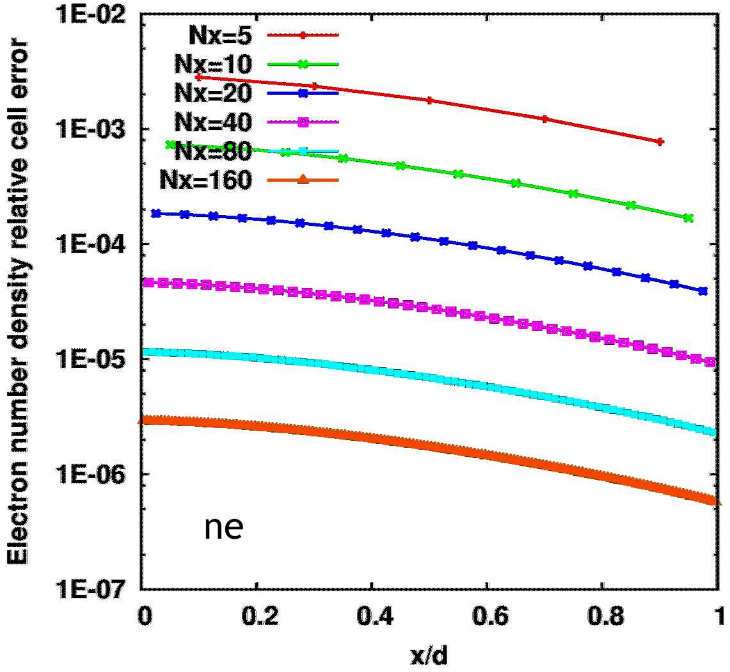
Relative error profiles for the electric field, electron number density and velocity

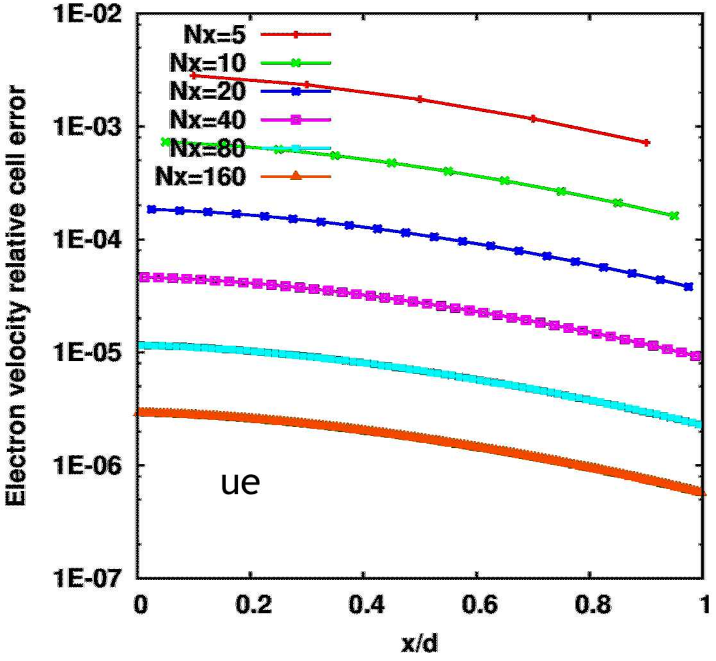
- Monotonic reduction in error under mesh refinement for all three quantities

$$\mathrm{error}_i^{Rel} = \frac{| < f(x) >_i - < f^h >_i |}{| < f(x) >_i |}$$

$<f(x)>_i$ is the hex centered integrated table value
$<f^h>_i$ is the hex centered simulation value





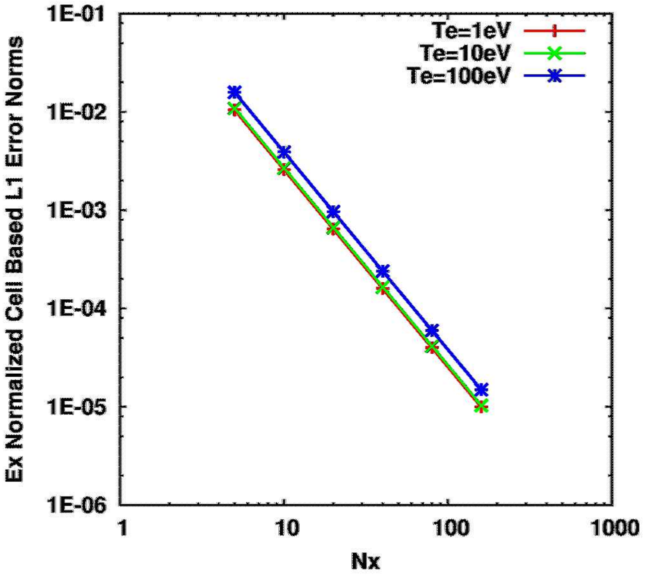


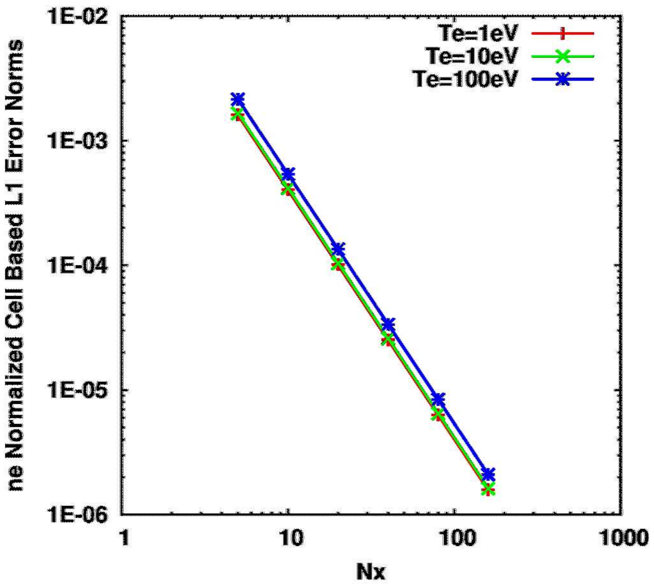
Multi-Fluid Code Verification: Warm Diode (Cell averaged)

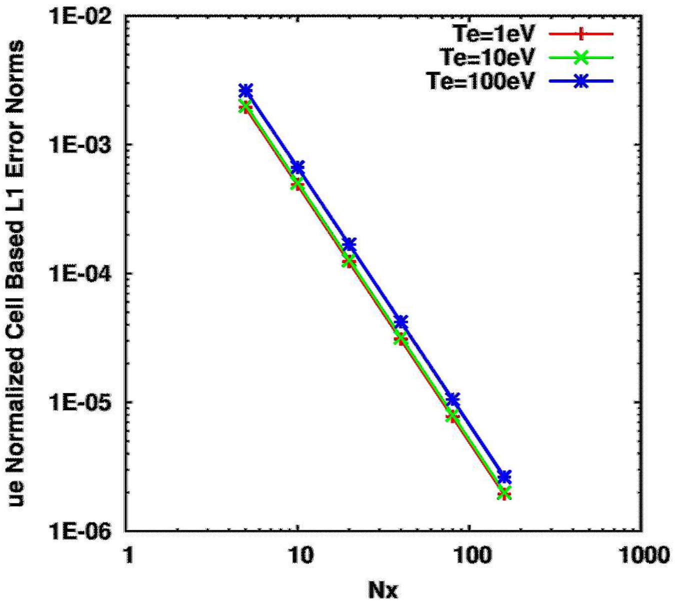
Consistent convergence rates for all three temperatures:

- Electric field, number density and velocity converge at expected rate

L1 norm definition: $\mathcal{E}_{L1} = \frac{1}{N_x}\sum_{i=1}^{N_x} | < f(x) >_i - < f^h >_i |$







Nx	E_L1_slope	n_L1_slope	ux_L1_slope
5-10	2.014e+00	1.996e+00	1.986e+00
10-20	2.010e+00	2.000e+00	1.993e+00
20-40	2.006e+00	2.000e+00	1.997e+00
40-80	2.003e+00	2.000e+00	1.999e+00
80-160	2.002e+00	2.000e+00	2.000e+00

Te=1eV

Nx	E_L1_slope	n_L1_slope	ux_L1_slope
5-10	2.014e+00	1.986e+00	1.993e+00
10-20	2.011e+00	1.993e+00	1.998e+00
20-40	2.006e+00	1.997e+00	2.000e+00
40-80	2.003e+00	1.998e+00	2.000e+00
80-160	2.002e+00	1.999e+00	2.000e+00

Te=10eV

Nx	E_L1_slope	n_L1_slope	ux_L1_slope
5-10	2.015e+00	1.995e+00	1.980e+00
10-20	2.015e+00	2.002e+00	1.991e+00
20-40	2.009e+00	2.002e+00	1.996e+00
40-80	2.005e+00	2.000e+00	1.997e+00
80-160	2.003e+00	2.001e+00	2.000e+00

Te=100eV

Summary

Summary

Cold diode verification (SAND2019-9384)

- Analytic solution was developed based on Jaffe (1944)
- This is a very good choice for verifying a PIC code
- Expected orders of accuracy were observed
- Several boundary condition issues were exposed and remedied
- New Velocity-Verlet time integration scheme was verified

Warm diode

- A quasi-analytic solution to the Euler/Poisson system including pressure gradient effects has been developed
- EMPIRE-Fluid solutions compare reasonably well with the quasi-analytic solutions capturing both structure and temperature sensitivity
- Several code issues have been exposed and addressed
- Expected rates of convergence based on cell integrated/averaged quantities has been demonstrated

Next Steps

- Continue improving diagnostics in EMPIRE-Fluid
- Develop an automated version for faster turn-around
- Drive this problem to more realistic temperatures and adiabatic index
- Develop relativistic versions of the diode for verification in EMPIRE-PIC and -Fluid

Thank you!

Are there any questions?

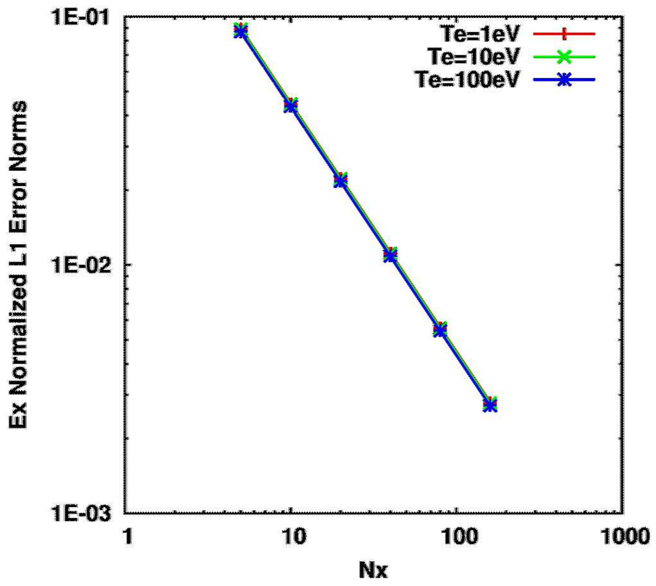
Backup Slides

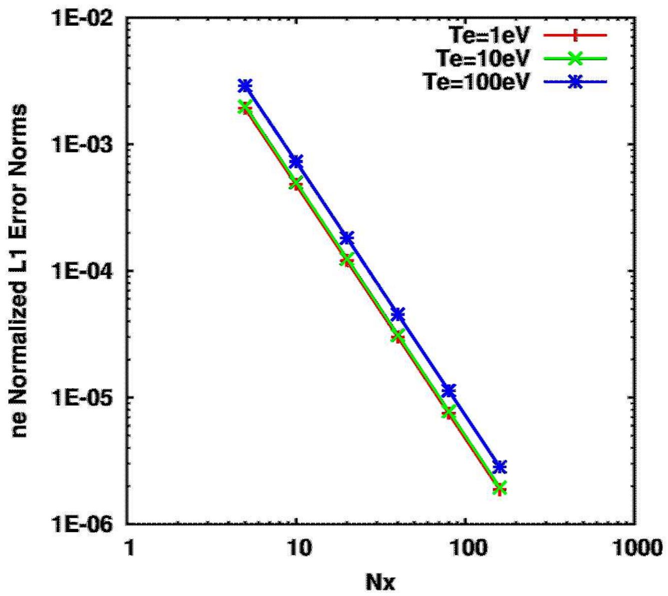
Multi-Fluid Code Verification: Warm Diode (Internal norms)

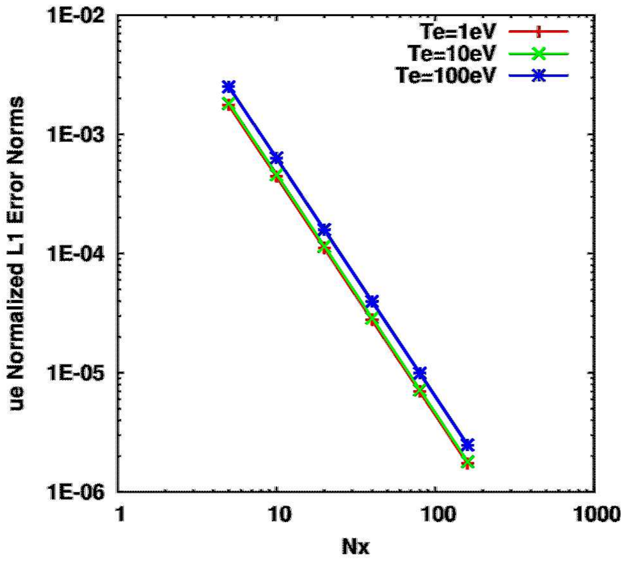
Consistent convergence rates for all three temperatures:

- Electric field converges at expected rate
- Electron number density and velocity convergence stalls

L1 norm definition: $\mathcal{E}_{L1}^{Rel} = \frac{\int_\Omega |f - f^h| dV}{\int_\Omega |f| dV}$







Nx	E_L1_slope	n_L1_slope	ux_L1_slope
5-10	1.000e+00	1.990e+00	1.980e+00
10-20	1.000e+00	2.003e+00	1.997e+00
20-40	1.000e+00	2.003e+00	1.999e+00
40-80	1.000e+00	2.002e+00	2.000e+00
80-160	1.000e+00	2.001e+00	2.000e+00

Te=100eV

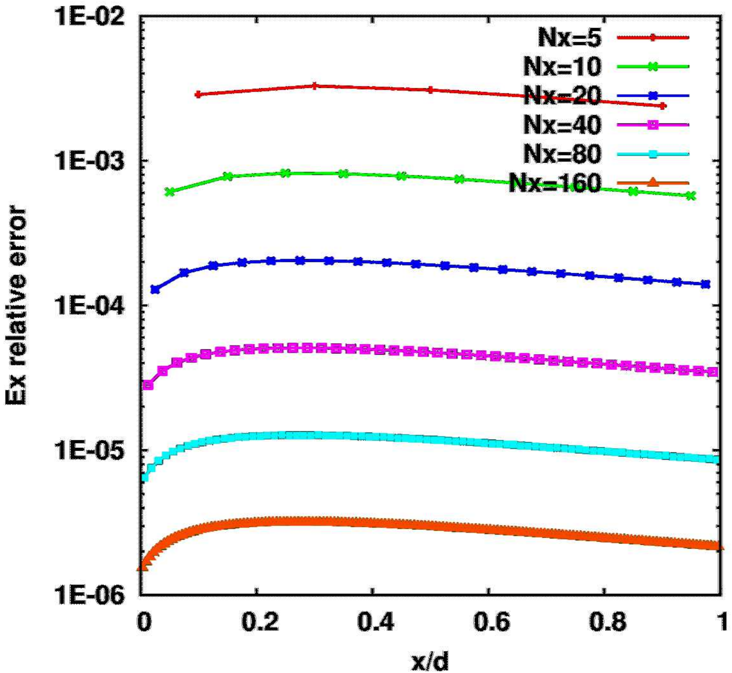
Multi-Fluid Code Verification: Relative Error from Interpolated analytic Table Te=1eV

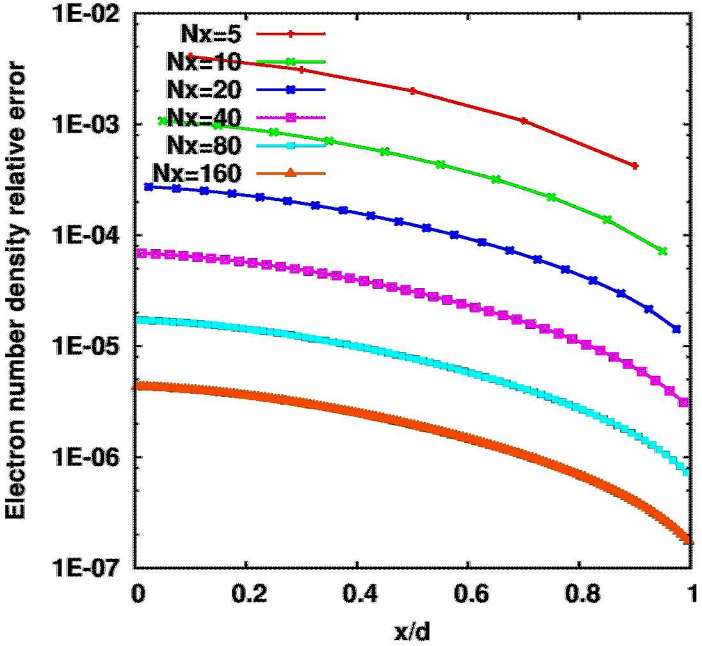
Relative error profiles for the electric field, electron number density and velocity

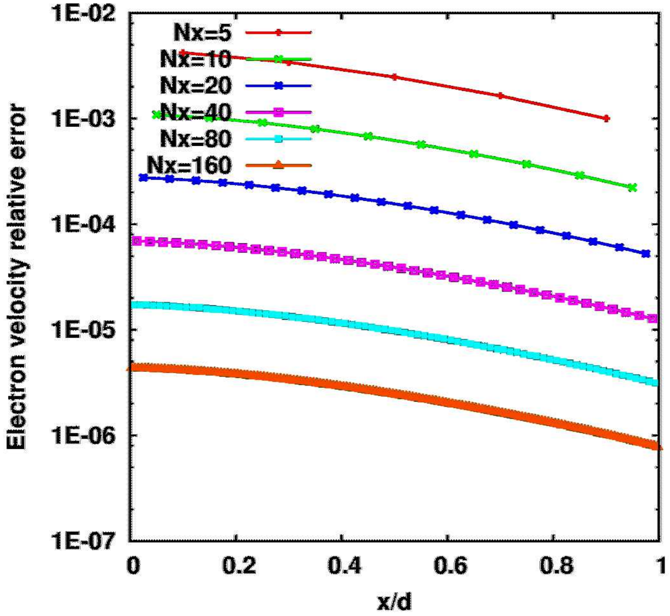
- Non-monotonic behavior for the electric field
- Errors are converging to a different solution

$$\text{error}_i^{Rel} = \frac{|f(x_i) - < f^h >_i|}{|f(x_i)|}$$

$f(x_i)$ is the interpolated table value at the hex centroid
$<f^h>_i$ is the hex centered average value







Multi-Fluid Code Verification: Warm Diode (Interpolated table values norms)

Consistent convergence rates for all three temperatures:

- Electric field converges at expected rate
- Electron number density and velocity converge at expected rates