SAND2015-9791C

# Solution of Eulerian Frame MHD Simulations with Multi-stage RK Implicit / Explicit (IMEX) Time integration

**John N. Shadid**

***Computational Mathematics Department***
***Center for Computational Research***
***Sandia National Laboratories***

**Collaborators:**

**Eric C. Cyr, Roger P. Pawlowski, Edward G. Phillips**
***Sandia National Laboratories***

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

# Outline

- General Scientific and Mathematical/Computational Motivation
- Motivation for Considering IMEX Methods (Multiphysics, time-scales)
- Some Very Recent – Preliminary Experience
  - Diffusion Reaction, Convection-Diffusion-Reaction
  - CFD
  - MHD (just beginning for IMEX)
    - Low Mach number resistive MHD (2D Tearing Mode)
    - Euler-Maxwell (electron, ion-electron two fluid)
- Preliminary Conclusions

## Motivation: Science/Technology and Mathematical / Computational

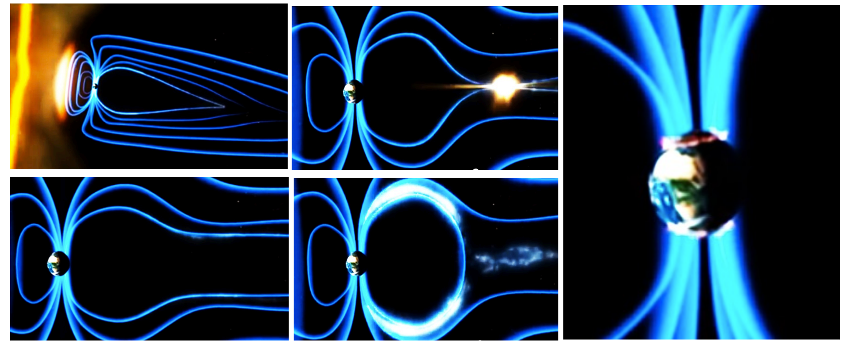
### *Science / Technology Motivation:*

**Resistive and extended MHD models important plasma physics systems**

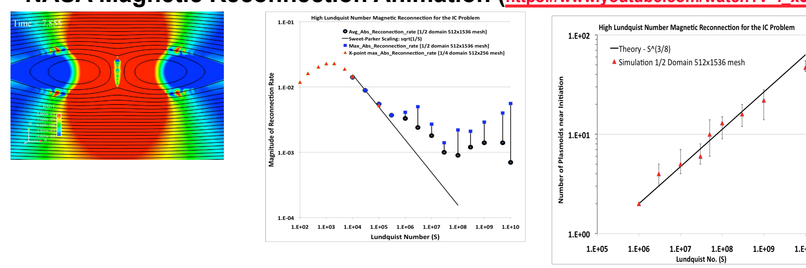
- **Astrophysics:** Magnetic reconnection, solar flares, ..
- **Planetary-physics:** Earth's magnetospheric sub-storms, Aurora, geo-dynamo, planetary-dynamos
- **Fusion:** Magnetic Confinement [MCF] (e.g. ITER), Inertial Conf. [ICF] (e.g. NIF, Z-pinch)

### *Mathematical/Computational Motivation:*

Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multiphysics Systems to Enable Scientific Discovery and Engineering Design/Optimization



NASA Magnetic Reconnection Animation (https://www.youtube.com/watch?v=i_x3s8ODaKg)




Magnetic Reconnection: S = 1e+9 (left), Reconn. Rate vs. SP theory (right)

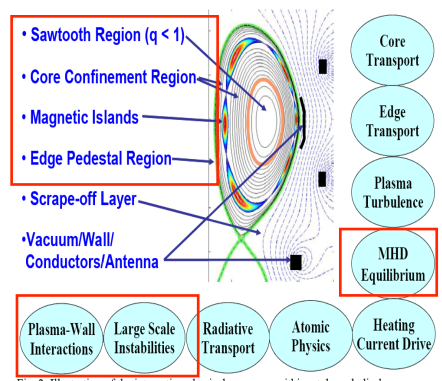
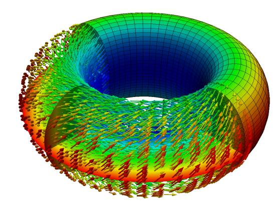
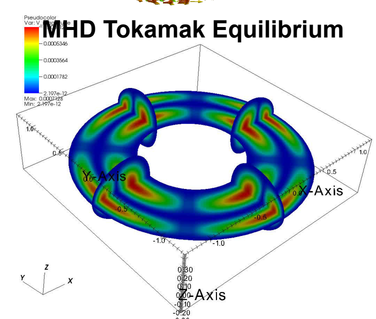



Fig. 2: Illustration of the interacting physical processes within a tokamak discharge.



MHD Tokamak Equilibrium




MHD Equilibrium Instability

## What are multi-physics systems? (A multiple-time-scale perspective)

**These systems are characterized by a myriad of complex, interacting, nonlinear multiple time- and length-scale physical mechanisms.**

**These mechanisms:**

- **can be dominated by one, or a few processes, that drive a short dynamical time-scale consistent with these dominating modes,**

- **consist of a set of widely separated time-scales that produce a stiff system response,**
- **nearly balance to evolve a solution on a dynamical time-scale that is long relative to the component time scales,**
- **or balance to produce steady-state behavior.**

Sandia National Laboratories

## A Subjective view of Desired Characteristics for Multiphysics Time Integration

- **Stable, accurate, and efficient integration of multiple-time-scale multiphysics systems (time-steps consistent with the dynamical time-scales of interest)**
- **Higher-order (e.g. $2^{nd}$ – $5^{th}$); A-, L-stability, SSP, ..**
- **Flexible algorithmic structure for time-accurate & robust pseudo-transient**
- **Consistent nonlinear residual-based description facilitating**
    - **Robust scalable nonlinear / linear solution of strongly coupled implicit multiphysics operators (e.g. Newton-Krylov-AMG)**
    - **Beyond forward simulations (optimization, inversion, UQ, ..)**
- **Mathematical structure enabling the use of adjoint-enhanced methods**
    - **Integrated local sensitivity analysis,**
    - **Reduction of effective UQ parameter space exploration**
    - **Efficient UQ surrogate construction**
    - **Dual weighted a posteriori error-estimation**
- **Mathematical structure consistent with enforcing nonlinear stability constraints (e.g. positivity / monotonicity preservation, TVD, LED, ….)**

Sandia National Laboratories

# Implicit / Explicit (IMEX) Methods Appear Promising (in this context)

Governing PDE Semi-discretized in Space (e.g. FV, FD, FE) written as an ODE system

$$\mathbf{u}_t + \underbrace{\mathbf{F}(\mathbf{u})}_{\textbf{Slow, Explicit}} + \underbrace{\mathbf{G}(\mathbf{u})}_{\textbf{Fast, Implicit}} = \mathbf{0}$$

IMEX Multistep Methods (e.g. BDF type methods) form the consistent nonlinear residual:

$$\sum_{j=0}^{k} a_j \mathbf{u}_{n-j} + \sum_{j=1}^{k} \hat{b}_j \Delta t \mathbf{F}(\mathbf{u}_{n-j}) + \sum_{j=0}^{k} b_j \Delta t \mathbf{G}(\mathbf{u}_{n-j}) = \mathbf{0}.$$

High-order accuracy (e.g. $2^{nd}$ – $5^{th}$), various stability properties have been demonstrated A-, L-stability, Strong Stability Preserving (SSP), TVB, ….

See for e.g. Hundsdorfer and Ruuth (2007)

# Implicit / Explicit (IMEX) Methods Appear Promising (in this context)

Governing PDE Semi-discretized in Space (e.g. FV, FD, FE) written as an ODE system

$$\mathbf{u}_t + \underbrace{\mathbf{F}(\mathbf{u})}_{\textbf{Slow, Explicit}} + \underbrace{\mathbf{G}(\mathbf{u})}_{\textbf{Fast, Implicit}} = \mathbf{0}$$

IMEX Multi-stage Methods (RK-type) form a consistent set of nonlinear residuals:

$$\mathbf{u}^{(i)} = \mathbf{u}^n + \Delta t \sum_{j=1}^{i-1} \hat{a}_{ij} \mathbf{F}(\mathbf{u}^{(j)}) - \Delta t \sum_{j=1}^{i} a_{ij} \mathbf{G}(\mathbf{u}^{(j)}) \qquad \text{for } i = 1 \ldots s,$$

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \sum_{i=1}^{s} \hat{b}_i \mathbf{F}(\mathbf{u}^{(i)}) - \Delta t \sum_{i=1}^{s} b_i \mathbf{G}(\mathbf{u}^{(i)}).$$

High-order accuracy (e.g. $2^{nd}$ – $5^{th}$), with various stability properties have demonstrated A-, L-stability, Strong Stability Preserving (SSP), TVB, ….

See for e.g. Ascher, Ruuth and Wetton (1997), Ascher, Ruuth and Spiteri (1997), Carpenter, Kennedy, et. al (2005), Higueras et. al. (2011)

Sandia National Laboratories

# A Heuristic Discussion of Time Scales (as a reminder)

**Coupled transport physics:** Consider a linearized transient convection-diffusion-reaction equation, performing a Von Neumann stability analysis (amplification factor) for explicit time integration for specific discrete systems will essentially identify the following time-scales

$$\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u - D \nabla^2 u + S u = 0$$

$$\tau_c \approx \frac{h}{\|\mathbf{w}\|} \quad \tau_D \approx \frac{h^2}{D} \quad \tau_S \approx \frac{1}{|S|}$$

# A Heuristic Discussion of Time Scales (as a reminder)

**Coupled 1st order wave interaction physics,** (e.g. Maxwell's Eq. in a vacuum, $\mathbf{J} = \mathbf{0}; \rho_c = 0$ ).
Coupling time scale is illustrated by derivation of the 2nd order system from 1st order system

$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = \mathbf{0}, \quad \nabla \cdot \mathbf{B} = 0$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}\,, \quad \nabla \cdot \mathbf{E} = 0$$

**Taking curl of Faraday's Law and using** $\nabla \times \nabla \times \mathbf{E} = -\nabla^2 \mathbf{E} + \nabla(\nabla \cdot \mathbf{E})$

$$\frac{\partial^2 \mathbf{E}}{\partial t^2} - \frac{1}{\epsilon_0 \mu_0} \nabla^2 \mathbf{E} = \mathbf{0}$$

Von Neumann stability analysis (amplification factor) for explicit time integration for specific discrete systems will essentially identify the following time-scale

$$\tau_{EM} = \frac{h}{c} \quad \text{where } c = \frac{1}{\sqrt{\epsilon_0 \mu_0}}$$

# A Heuristic Discussion of Time Scales (as a reminder)

**Desire to select dynamical time scale of interest** $\Delta t_{dyn}$
**and take stable time steps. Of course stable does not imply accurate.**

$$\tau_c \approx \underbrace{\frac{h}{\|\mathbf{w}\|}}_{\Delta t_{dyn}}, \; \tau_S \approx \underbrace{\frac{1}{|S|}}_{\Delta t_{dyn}}, \; \tau_D \approx \frac{h^2}{D}, \; \ldots\ldots, \; \tau_{EM} = \frac{h}{c}$$

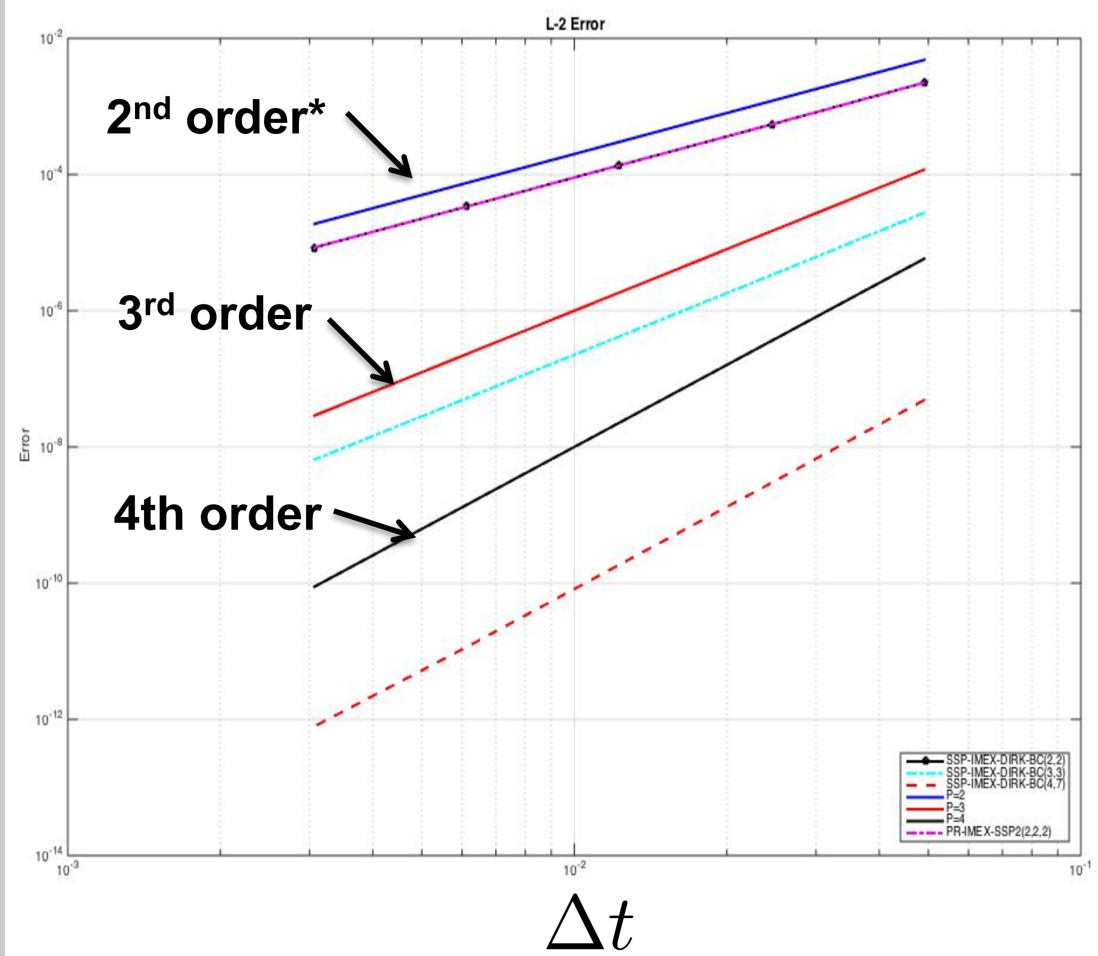
# Illustrative IMEX accuracy results (Convection-diffusion)

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$

$$u(x,t) = A\exp(-\nu k^2 t)\sin\left(2\pi k(x - at)\right)$$

- **Explicit Convection**
- **Implicit Diffusion**

- **Fixed CFL**




**New set of IMEX SSP/L-stable methods (with S. Conde and S. Gottlieb, U Mass - Dartmouth)**
**Both explicit and implicit part are SSP/L-stable and overall IMEX is SSP/L-stable**

***Comparison with 2nd order SSP3(3,3,2) [Pareschi and Russo (2000,2005)]**

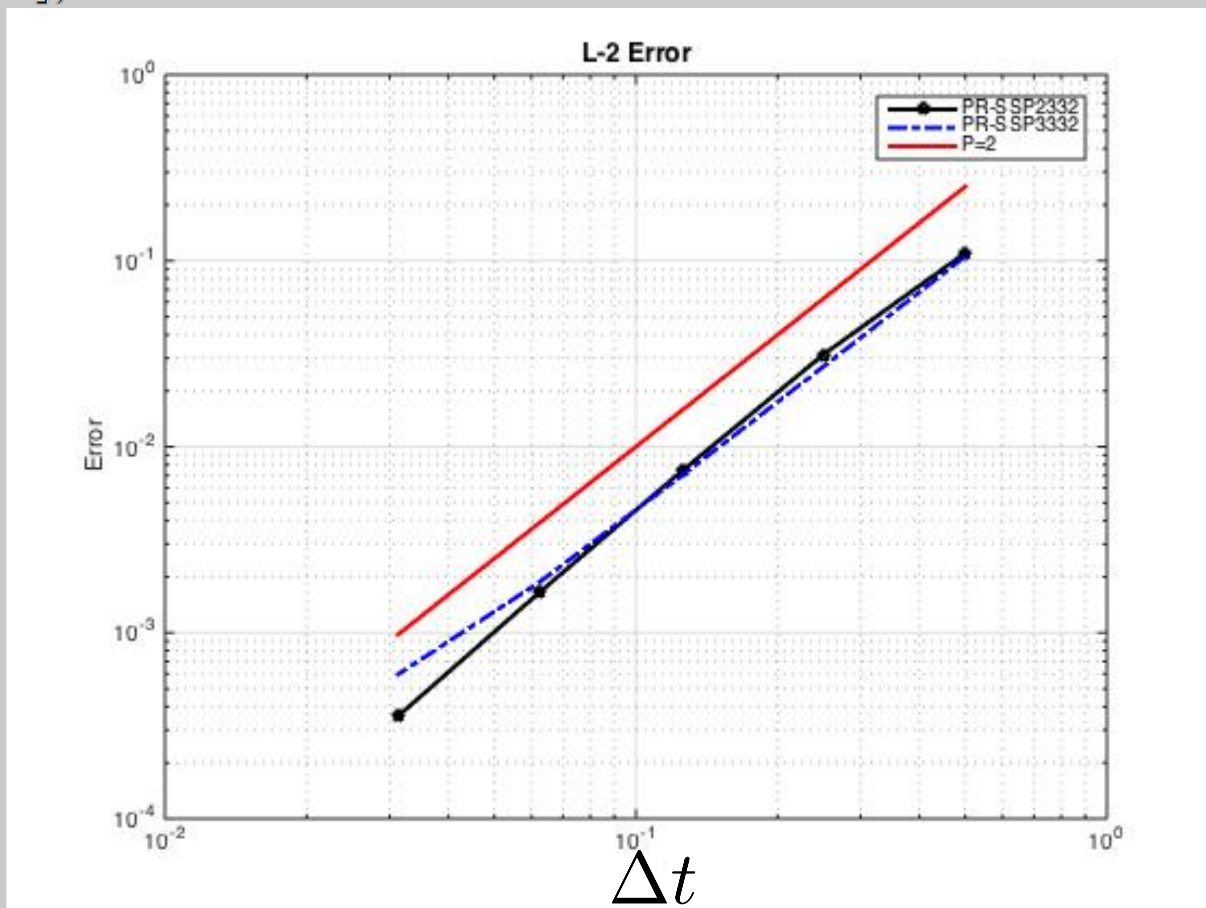
Sandia National Laboratories

Illustrative IMEX accuracy results (Convection-Diffusion-Nonlinear Reaction)

$$\frac{\partial T}{\partial t} = \nu \frac{\partial^2 T}{\partial x^2} + \frac{\epsilon}{\delta}\frac{\partial T}{\partial x} + \frac{8\nu}{\delta^2} T^2 (1 - T)$$

$$T(x,t) = \frac{1}{2}\left(1 - \tanh\left[\frac{x - (2\nu - \epsilon)t/\delta}{\delta}\right]\right)$$

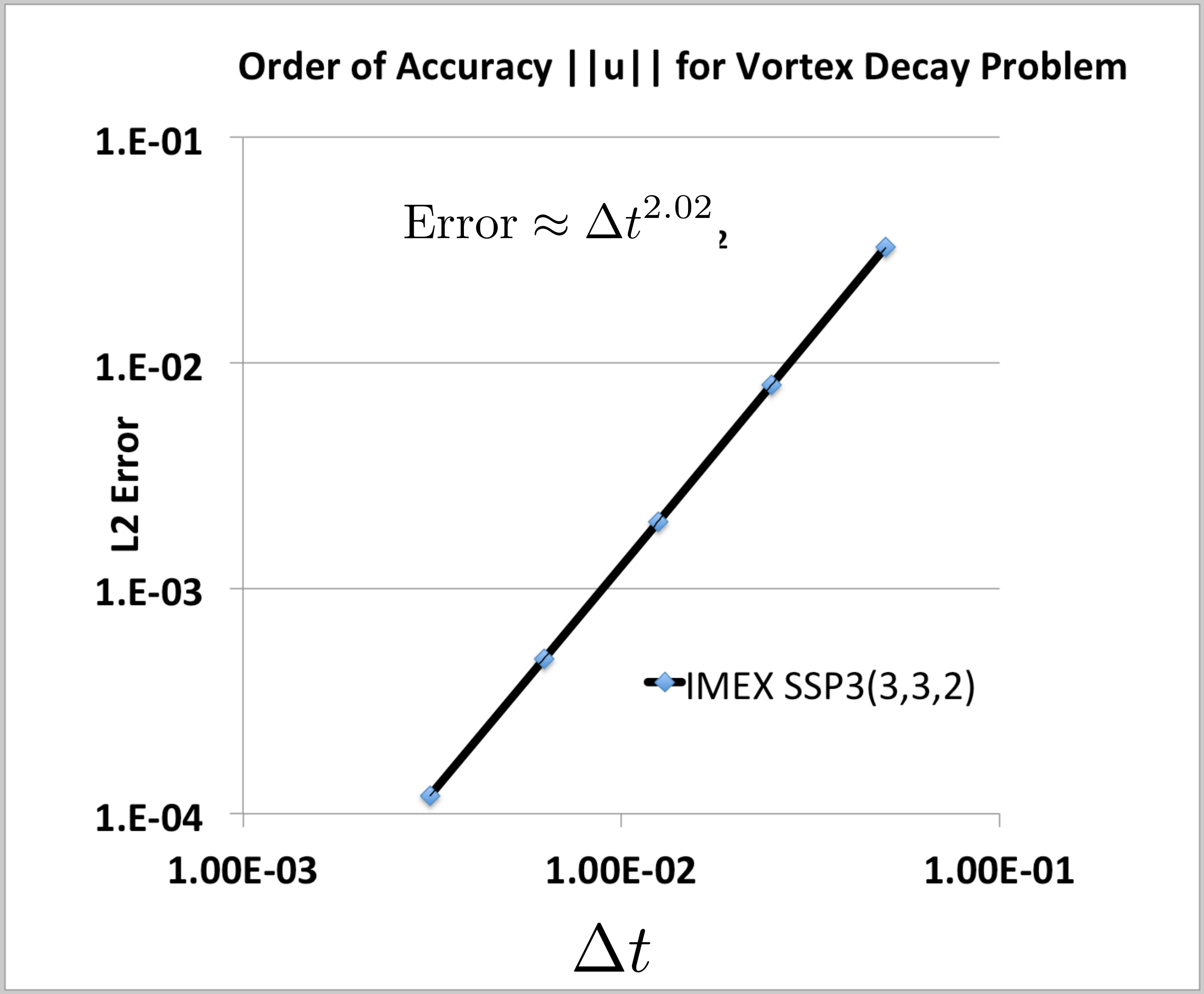
- **Explicit Convection**
- **Implicit Diffusion, Reaction**
- **Fixed CFL**




**$2^{nd}$ order Pareschi and Russo (2000,2005) SSP3(3,3,2), SSP2(3,3,2)**

# Illustrative IMEX accuracy results (Navier-Stokes - Incompressible)

Exact Solution to
Navier-Stokes:
Decaying Vortex




CR Ethier and DA Steinman (1994)

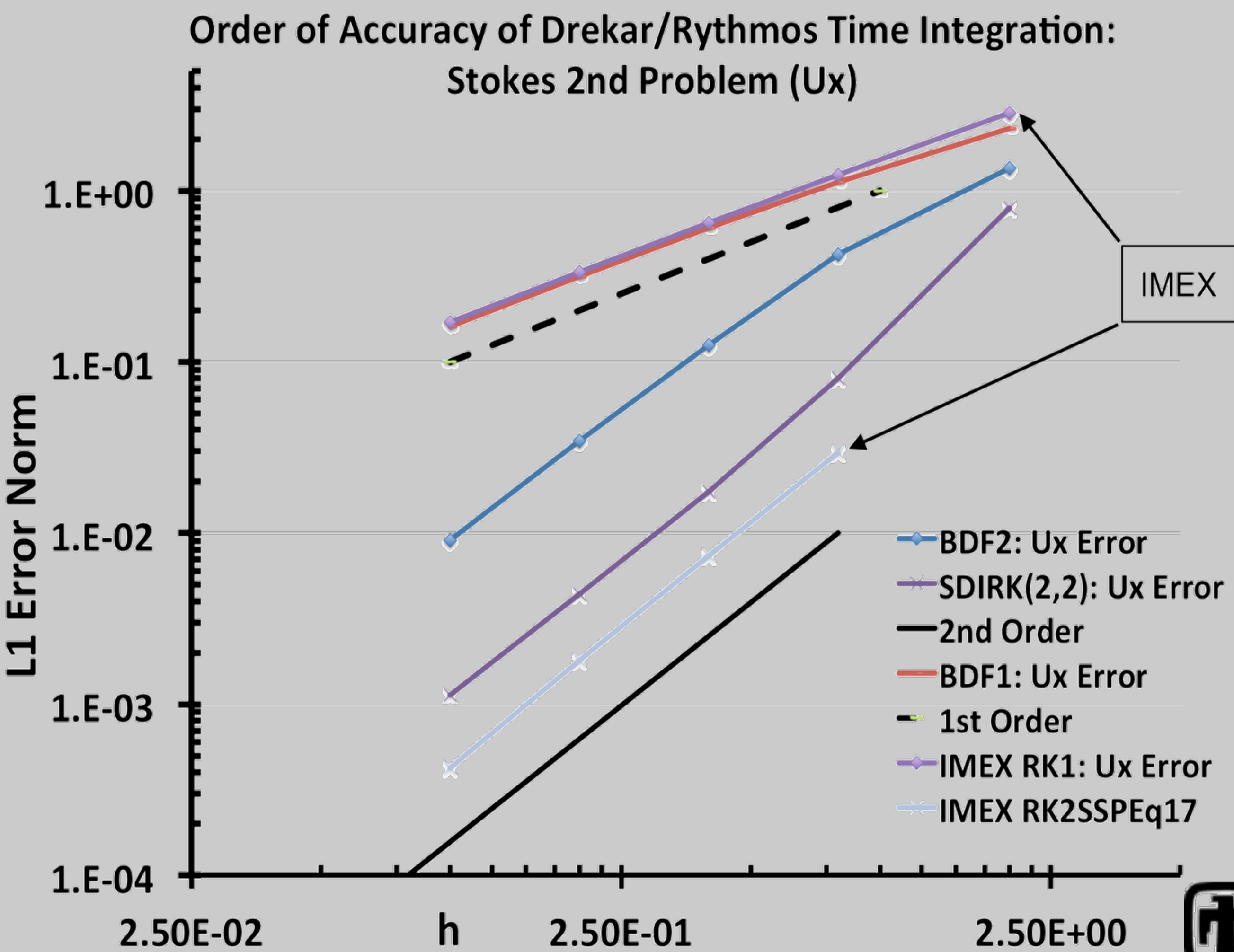
Sandia National Laboratories

# Illustrative IMEX Stability Results (Navier-Stokes – Low Mach number)

Convergence in time for Stokes 2nd Problem (Low-Mach version, fixed CFL)

- Explicit advection
- Implicit diffusion, Implicit sound wave operators

**Error in velocity**




Sandia National Laboratories

# 3D Resistive MHD Equations: VMS FE Formulation

**Resistive MHD Model in Residual Notation**

$$\mathbf{R_v} = \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v} - (\mathbf{T} + \mathbf{T}_M)] + 2\rho\Omega \times \mathbf{v} - \rho \mathbf{g} = \mathbf{0}$$

$$R_P = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\mathbf{T} = -[P - \frac{2}{3}\mu(\nabla \cdot \mathbf{v})]\mathbf{I} + \mu[\nabla \mathbf{v} + \nabla \mathbf{v}^T]$$

$$\mathbf{T_M} = \frac{1}{\mu_0}\mathbf{B} \otimes \mathbf{B} - \frac{1}{2\mu_0}\|\mathbf{B}\|^2 \mathbf{I}$$

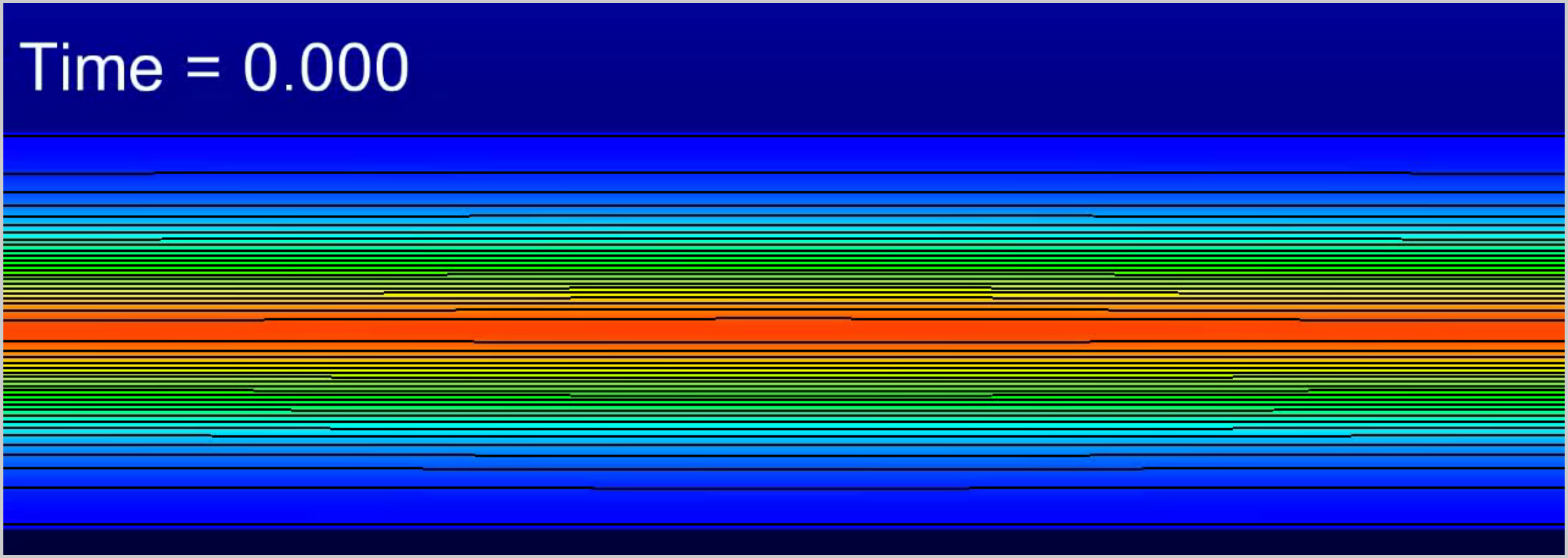
$$R_e = \frac{\partial (\rho e)}{\partial t} + \nabla \cdot [\rho \mathbf{v} e + \mathbf{q}] - \mathbf{T} : \nabla \mathbf{v} - \eta \| \frac{1}{\mu_0} \nabla \times \mathbf{B} \|^2 = 0$$

$$\mathbf{R_B} = \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot \left[\mathbf{B} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{B} - \frac{\eta}{\mu_0}\left(\nabla \mathbf{B} - (\nabla \mathbf{B})^T\right) + \psi \mathbf{I}\right] = \mathbf{0}$$

$$R_\psi = \nabla \cdot \mathbf{B} = 0$$

Multiple-time-scale systems: E.g. 2D Tearing Mode

Low Mach number compressible; M ~ $10^{-4}$; Fully-implicit (BDF2), IMEX (SSP3)




**Approx. Computational Time Scales:**

- **Divergence Constraint ($\nabla \cdot \mathrm{B} = 0$): 1/ $\infty$ = 0**
- **Fast Magnetosonic Wave ($c_f$): $10^{-4}$ to $10^{-2}$**
- **Alfven Wave ($c_a$): $10^{-4}$ to $10^{-2}$**
- **Slow Magnetosonic Wave ($c_s$): $10^{-2}$ to $10^{-1}$**
- **Sound Wave (c): $10^{-2}$**
- **Advection ($c_v$): $\infty$ to $10^{1}$**
- **Diffusion: $10^{-4}$ to $10^{-2}$**
- **Macroscopic Tearing Mode: $10^{2}$**

**Fully-implicit (BDF2) / IMEX SSP3**
**Max CFL:**

$CFL_{div} = \infty$

$CFL_{cf}$ ~ $10^5$ to $10^4$

$CFL_{cA}$ ~ $10^5$ to $10^4$

$CFL_{cs}$ ~ $10^3$ to $10^2$

$CFL_{c}$ ~ $10^3$ to $10^2$

$CFL_{cv}$ ~ 1 to 0.1

**Wave speeds**

$$\|\mathbf{u}\|, \|\mathbf{u}\| \pm c_s, \|\mathbf{u}\| \pm c_a, \|\mathbf{u}\| \pm c_f, \pm c_h$$

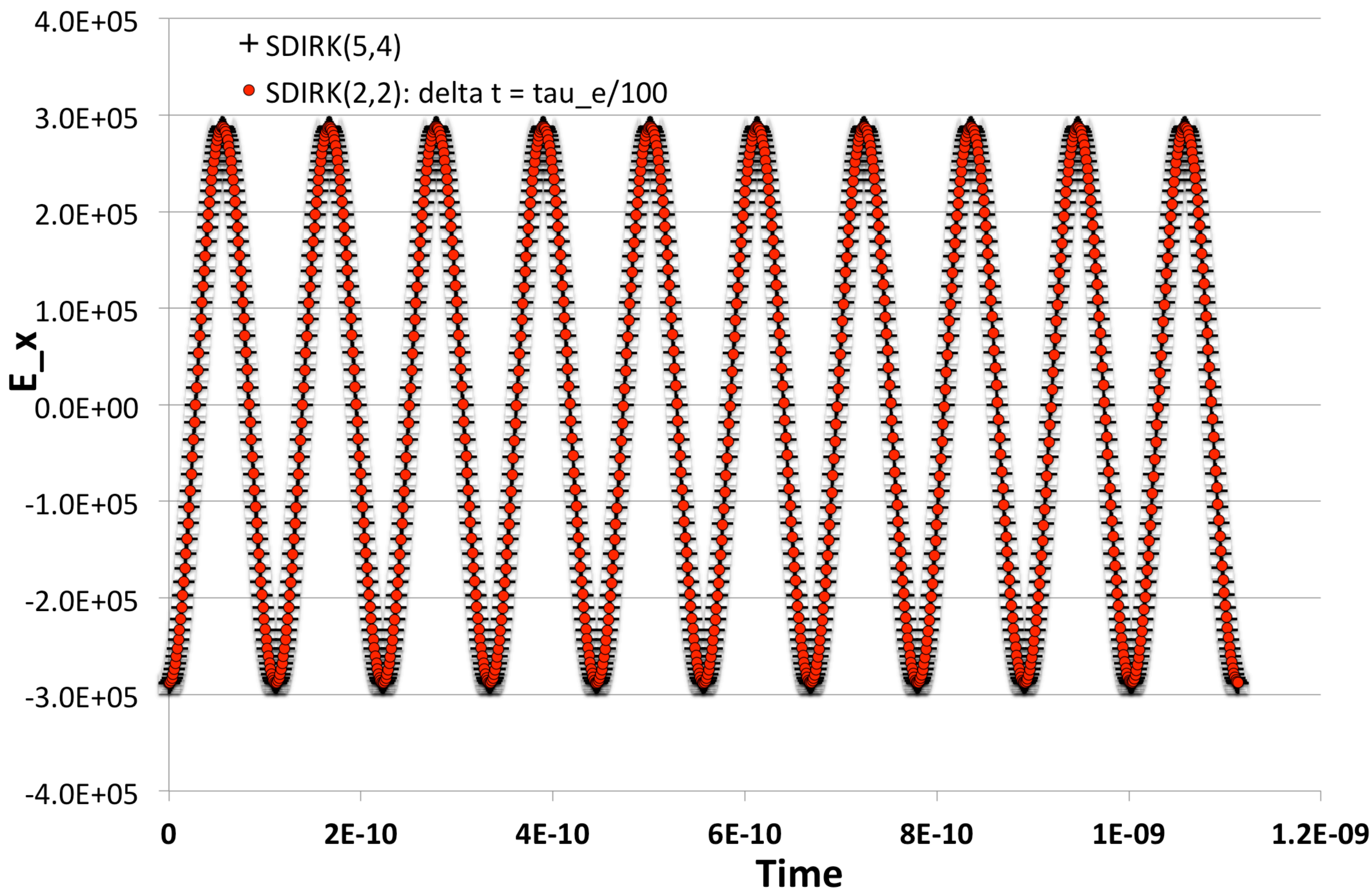
Sandia National Laboratories

# Target – Multi-fluid 5 Moment Plasma System Models

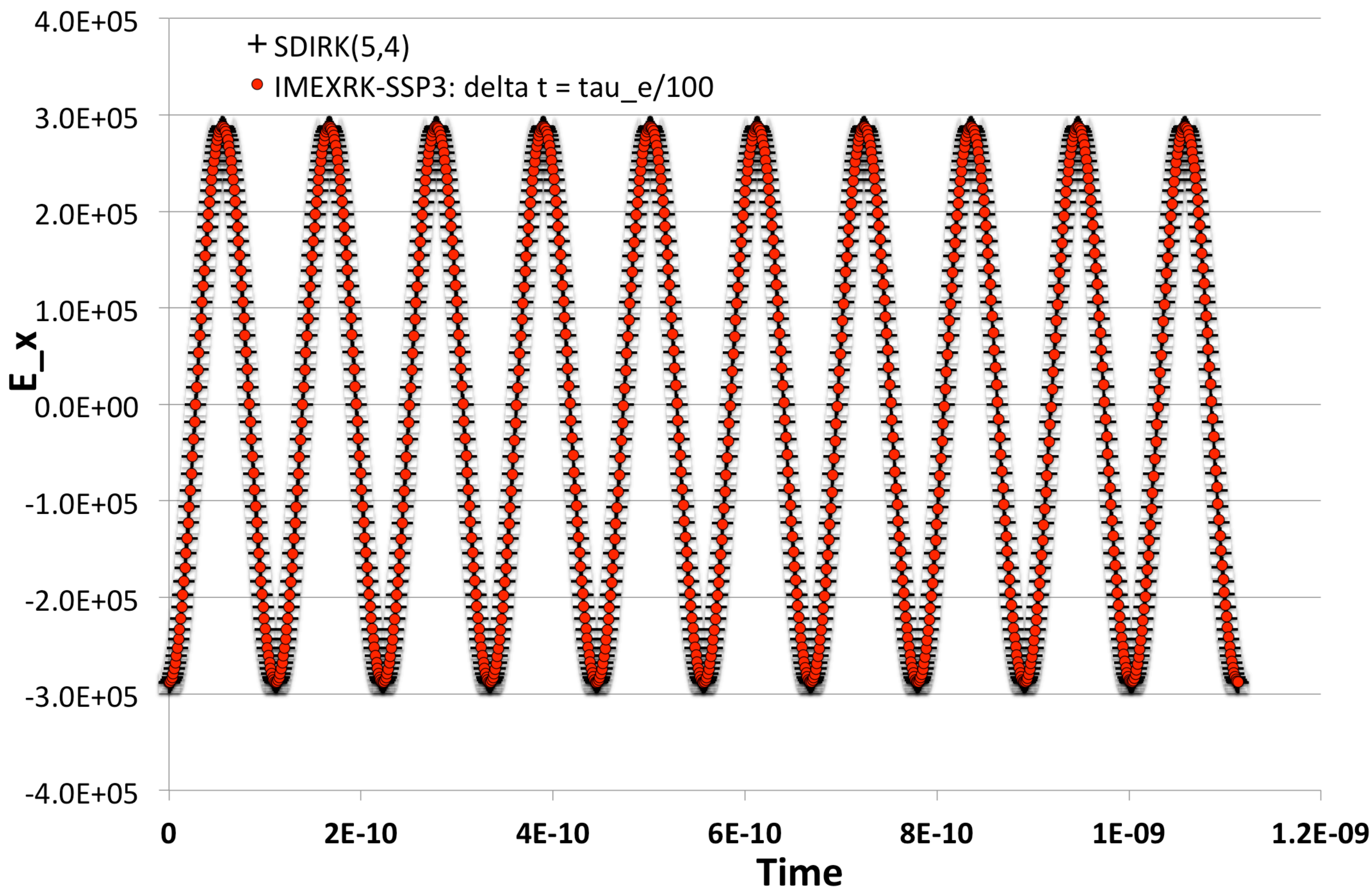
| | |
|---|---|
| Density | $\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a) = 0$ |
| Momentum | $\frac{\partial (\rho_a \mathbf{u}_a)}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a \otimes \mathbf{u}_a + p_a I + \Pi_a) = q_a n_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B})$ |
| Energy | |
| Charge and Current Density | $q = \sum_k q_k n_k$ $\quad$ $\mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$ |
| Maxwell's Equations | $\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$ $\quad$ $\nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ <br> $\nabla \cdot \mathbf{B} = 0$ $\quad$ $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$ |
| Eq. of State | $\varepsilon_a = \frac{p_a}{\gamma - 1} + \frac{1}{2} \rho_j u_a^2$ |

Sandia National Laboratories

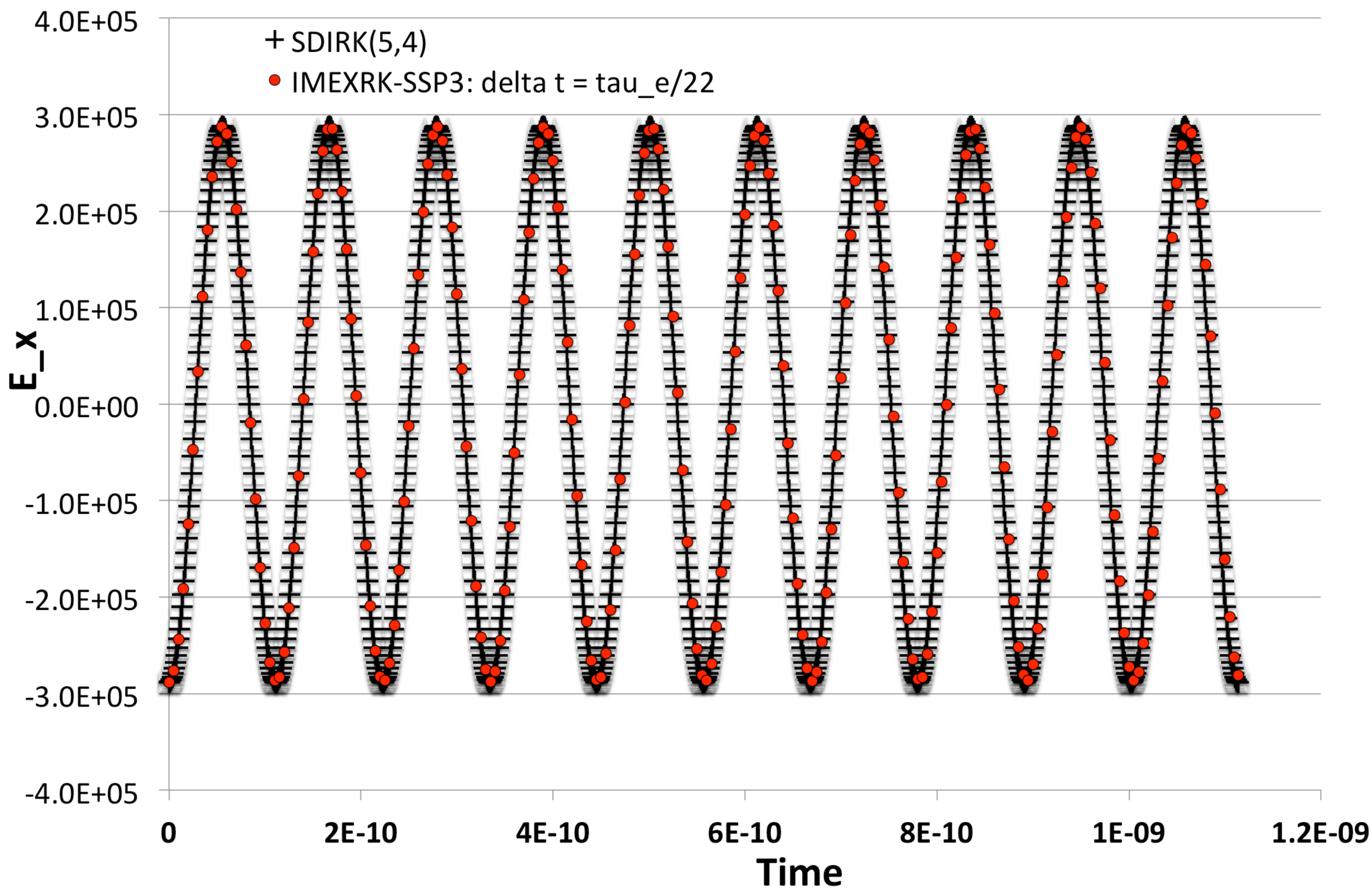
# Illustrative IMEX accuracy results (Full Maxwell – Electron Plasma Oscillation)



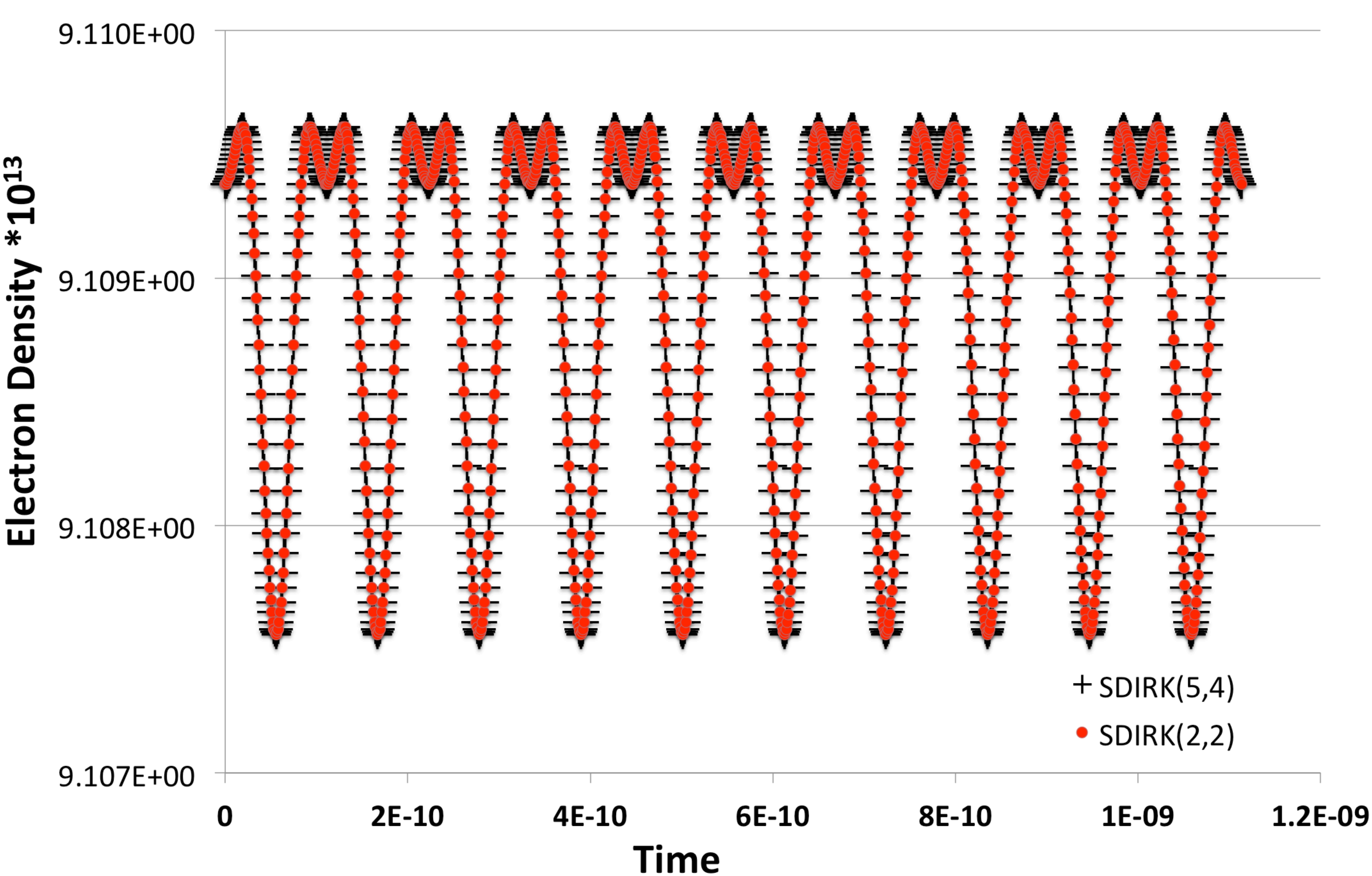
# Illustrative IMEX accuracy results (Full Maxwell – Electron Plasma Oscillation)



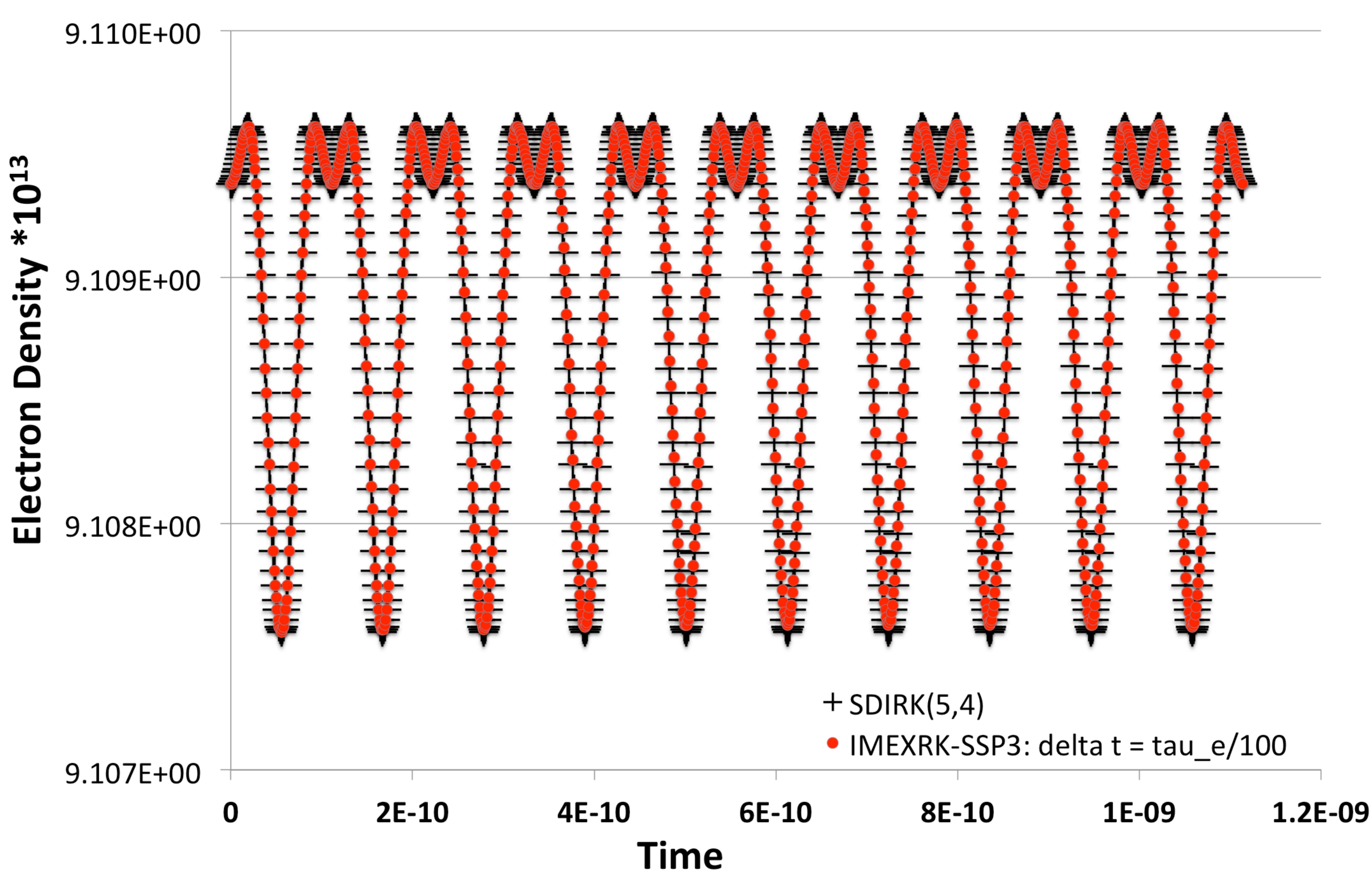
# Illustrative IMEX accuracy results (Full Maxwell – Electron Plasma Oscillation)



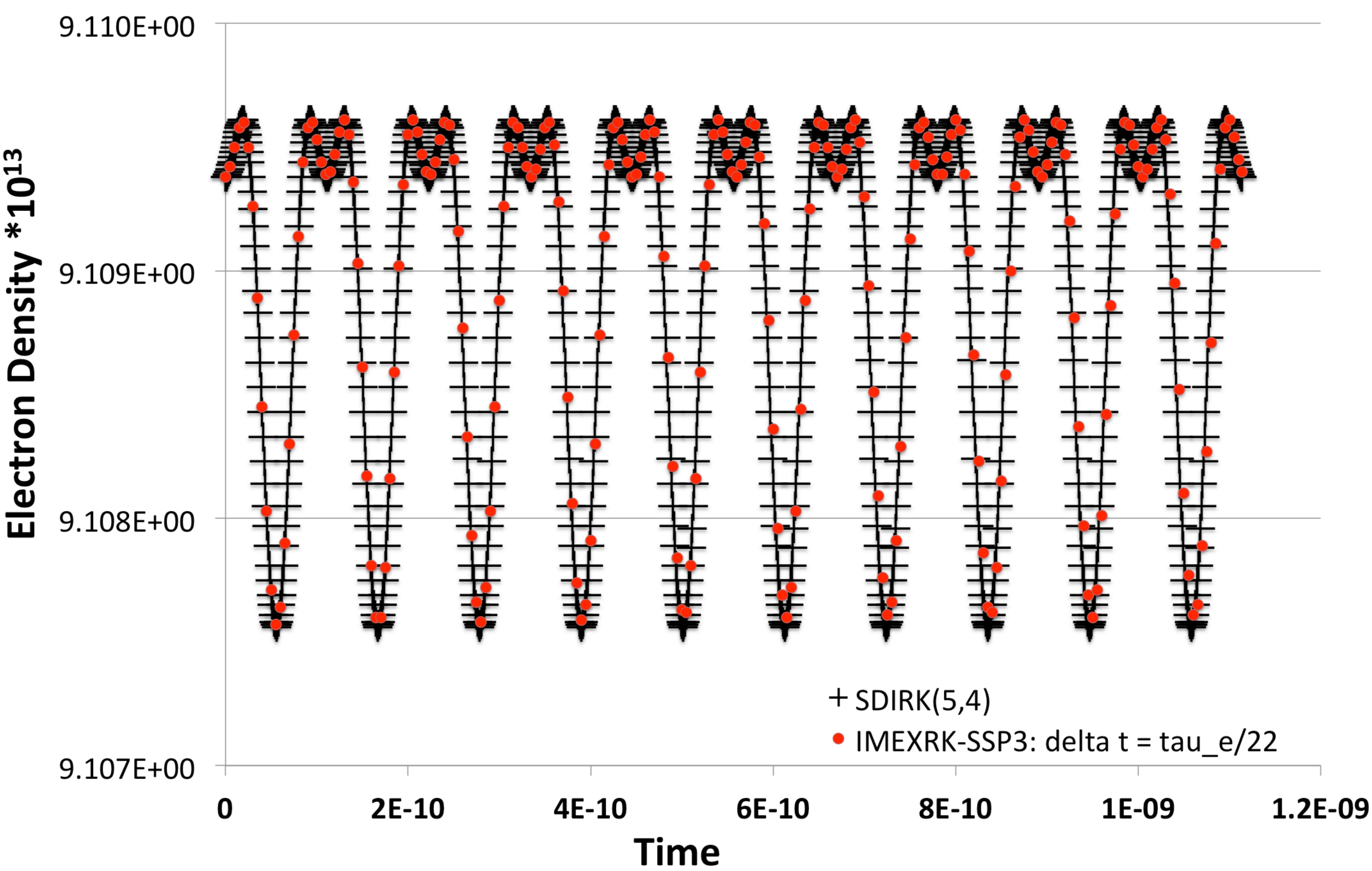
# Illustrative IMEX accuracy results (Full Maxwell – Electron Plasma Oscillation)



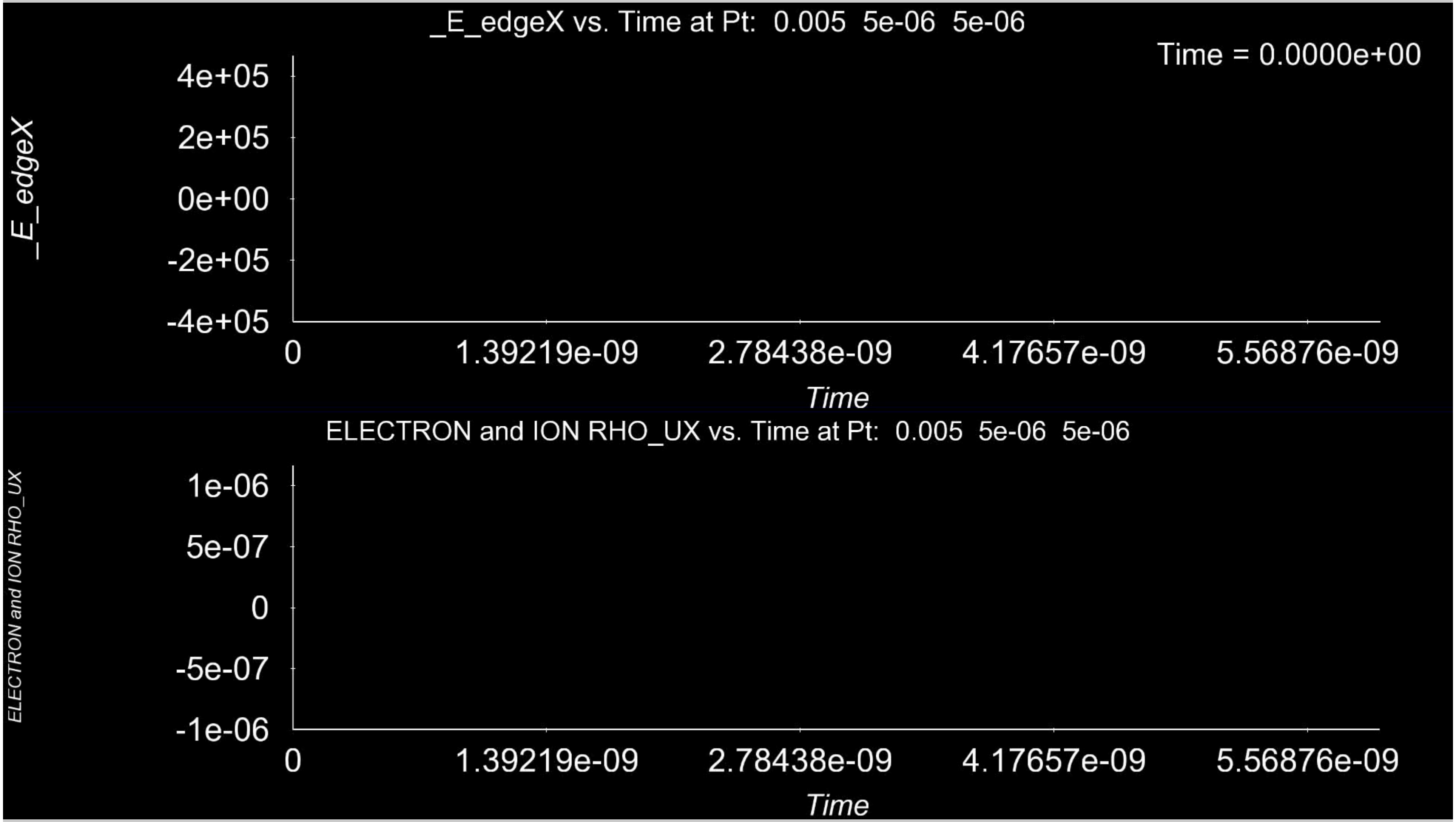
# Illustrative IMEX accuracy results (Full Maxwell – Electron Plasma Oscillation)



# Illustrative IMEX accuracy results (Full Maxwell – Electron Plasma Oscillation)



# Illustrative IMEX (Full Maxwell – ion/Electron Plasma Oscillation)




Sandia National Laboratories

# Conclusions

- **Preliminary  results for IMEX multistage RK type methods is encouraging. Accuracy and stability.**

- **Flexibility of assignment of equations / operators as explicit or implicit is very useful in multiphysics simulations to deal with multiple-time-scale and choices of dynamic time scales of interest.**

- **Code structure to support IMEX methods and dynamic assigment requires significant abstractions to facilitate this approach (e.g. Phalanx, Panzer – package from Trilinos (Pawlowski, Cyr) , and Degree of Freedom Manager (Cyr)**

- **New IMEX RK SSP/L-stable methods appear promising.**

- **Next Steps**

    - **More quantitative  analysis of the stability and accuracy of the methods on prototype problems for MHD.**

    - **More extensive evaluation of methods on important MHD and multi-fluid / Full Maxwell.**

    - **Demonstration and evaluation of adjoint-enhanced methods for sensitivity, UQ tools (active-subspaces, surrogate construction, etc.,) error-estimation**