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Towards a Hybrid Multi-fluid/PIC Plasma Capability

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ECP EXASCALE COMPUTING PROJECT

13th World Congress on Computational Mechanics

July 22-27, 2018 • New York City, USA

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration CCR Center for Computing Research

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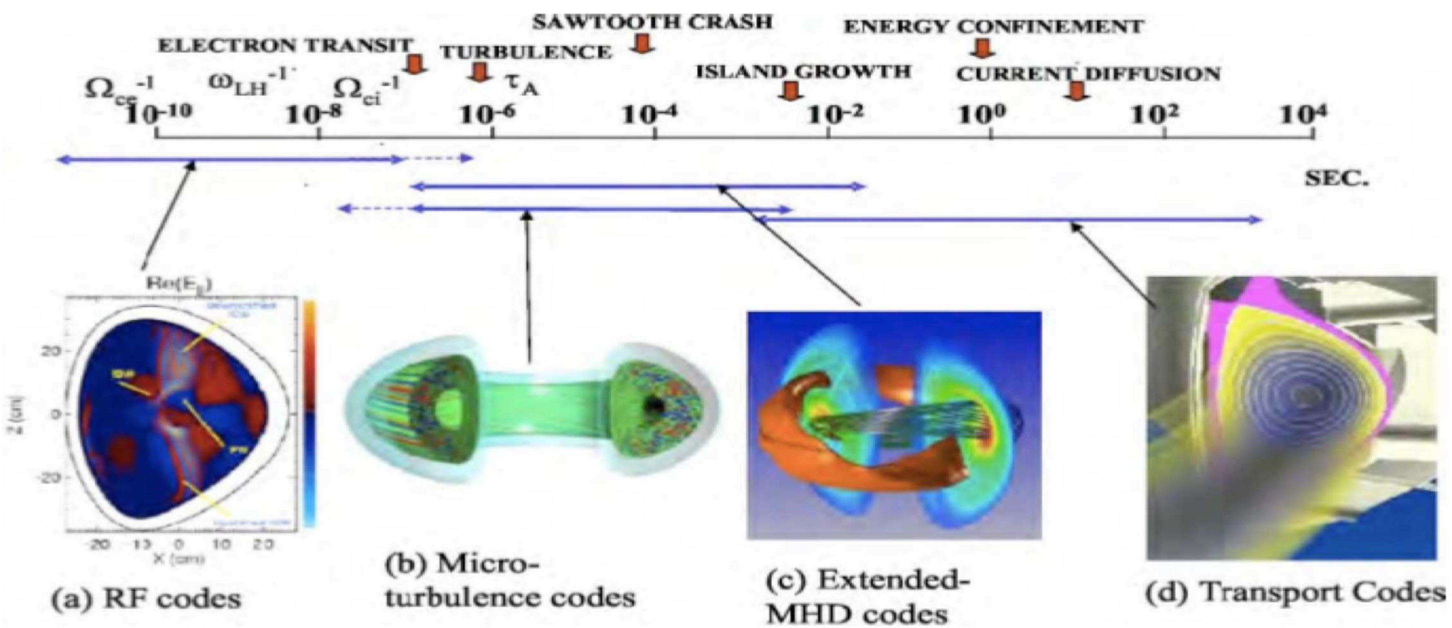
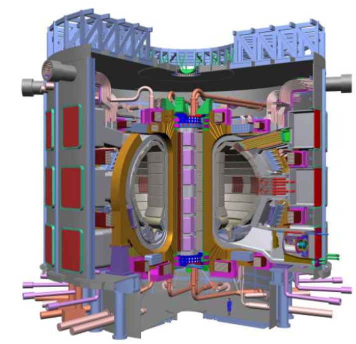
Outline

- Motivation
- Fluid Models and Solvers
- PIC and Coupled Model
- Current Results
- Software/Performance Portability
- Conclusions

ITER: Understanding and controlling instabilities in plasma confinement is critical.



(a) Time scales in fusion plasmas (FSP report)


ITER

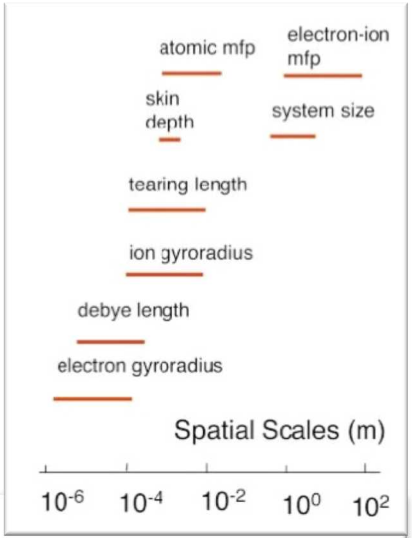
Strong external magnetics field used to:
- Confine the hot plasma and keep it from striking wall,
- Attempt is to achieve temperature of about 100M deg K (6x Sun temp.),
- Energy confinement times O(1 – 10) seconds is desired.

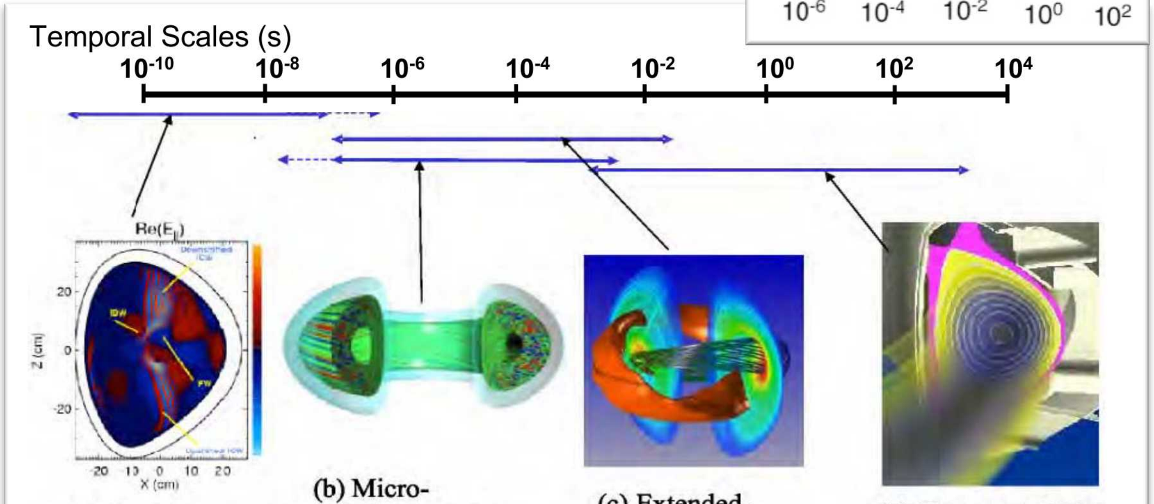
Plasma instabilities can cause break of confinement, huge energy loss, and discharge very large electrical currents (~20MA) into structure. ITER can sustain only a limited number of disruptions, O(1 – 5) significant instabilities.

DOE Office of Science ASCR/OFES Reports:
Fusion Simulation Project Workshop Report, 2007, Integrated System Modeling Workshop 2015

Multiphysics kinetic transport models are particularly ripe for algorithmic development

- **Physics models interact in strongly nonlinear way**
- **Models and/or regions in physical space require kinetic treatment (e.g., Boltzmann): transport in phase space**
- **Naturally hierarchical formulation: velocity moments contract phase space into macroscopic quantities (e.g., density, momentum, …)**
- **Longer length-scales / time-scales needed to understand macroscopic instabilities and performance**
- **Development of moment-based scale-bridging algorithms that embrace heterogeneous architectures is needed**





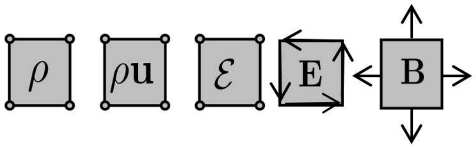
(a) RF codes
(b) Micro-turbulence codes
(c) Extended-MHD codes
(d) Transport Codes

Courtesy: Chacon, Hittinger, Shadid, Wildey (ASCR PI Meeting)

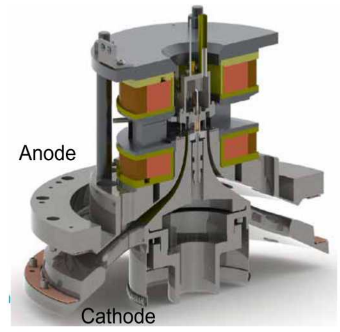
SNL's Mission Requires a Significant Range of Advanced Simulation Capabilities

<u>DOE/NNSA and many DOE/SC Mission Drivers are Characterized by:</u>

- Complex strongly coupled physical mechanisms (**multiphysics**)
  - Strongly coupled nonlinear solvers (**Newton methods**)
  - Physics-compatible discretizations

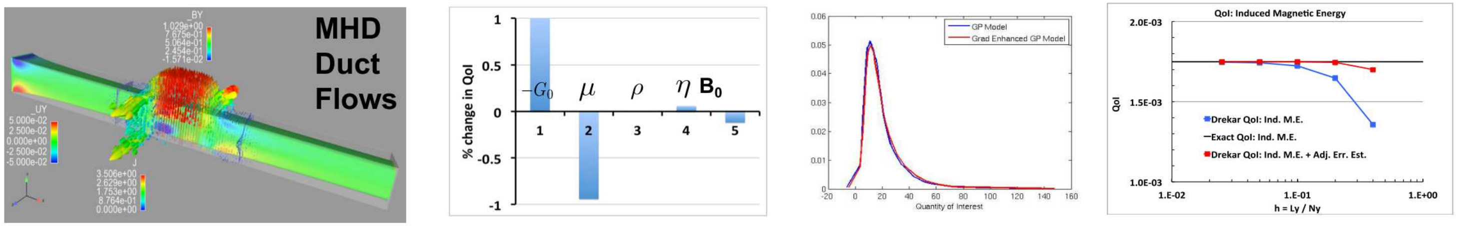


- Large range of interacting time-scales (Multiple-time-scales)
  - Implicitness (**fully-Implicit** or **implicit/explicit [IMEX]**)
- Complex geometries, multiple length-scales, high-resolution
  - Unstructured mesh FE (HEX and TET)
  - Scalable solution (**Krylov methods, physics-based prec., AMG**)



Z Convolute Power-feed

- High consequence decisions informed by modeling / simulation
  - Beyond forward simulation (**sensitivities, UQ, error est., design opt.**)



Adjoint-enabled Sensitivities, UQ surrogates, Error-estimates

Hybrid Code Design

- Goal: Develop a hybrid code with 5-Moment Fluid Model + Electromagnetics coupled to Particle-In-Cell (PIC) Model.

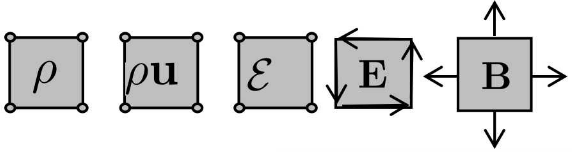
- Requirements
  - **Performance Portable** on emerging HPC architectures: HSW, KNL, CUDA, …
  - **Component-based**, heavily leverage Exascale Computing Project (ECP) software stack: Trilinos, Kokkos, …

- Two Scalable Fluid solvers
  - **Research code:** (Drekar):
    - CGFEM, FTC, HDG
    - Implicit, IMEX, Explicit
    - Turbulent CFD, turbulent MHD, Multispecies Plasma, …
  - **Production code**: DGFEM, Explicit, IMEX

- Scalable PIC solver
  - **Production code:** Currently explict, implicit under development

Fluid Model

Multi-fluid 5-Moment Plasma System Model



Density	$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a) = \sum_{b \neq a} (n_a \rho_b \bar{\nu}^+_{ab} - n_b \rho_a \bar{\nu}^-_{ab})$
Momentum	$\frac{\partial (\rho_a \mathbf{u}_a)}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a \otimes \mathbf{u}_a + p_a I + \Pi_a) = q_a n_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B})$ $- \sum_{b \neq a} [\rho_a (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^M_{ab} + \rho_b \mathbf{u}_b n_a \bar{\nu}^+_{ab} - \rho_a \mathbf{u}_a n_b \bar{\nu}^-_{ab}]$
Energy	$\frac{\partial \varepsilon_a}{\partial t} + \nabla \cdot ((\varepsilon_a + p_a) \mathbf{u}_a + \Pi_a \cdot \mathbf{u}_a + \mathbf{h}_a) = q_a n_a \mathbf{u}_a \cdot \mathbf{E} + Q^{src}_a$ $- \sum_{b \neq a} \left[(T_a - T_b) k \bar{\nu}^E_{ab} - \rho_a \mathbf{u}_a \cdot (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^M_{ab} - n_a \bar{\nu}^+_{ab} \varepsilon_b + n_b \bar{\nu}^-_{ab} \varepsilon_a \right]$
Charge and Current Density	$q = \sum_k q_k n_k \qquad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$
Maxwell's Equations	$\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0} \qquad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ $\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \nabla \cdot \mathbf{B} = 0$

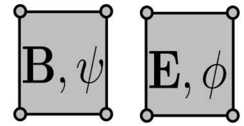
Electromagnetics Summarized Maxwell Formulation

$$\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} + \nabla \phi = 0$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} + \nabla \psi = 0$$

$$\frac{1}{c_h}\frac{\partial \phi}{\partial t} + \frac{1}{c_p}\phi + \left[\nabla \cdot \mathbf{E} - \frac{q}{\epsilon_0}\right] = 0$$

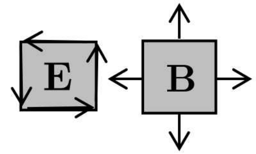
$$\frac{1}{c_h}\frac{\partial \psi}{\partial t} + \frac{1}{c_p}\psi + [\nabla \cdot \mathbf{B}] = 0$$



Or

$$\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = 0 \; ; \quad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$$

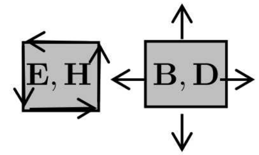
$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0 \; ; \quad \nabla \cdot \mathbf{B} = 0$$

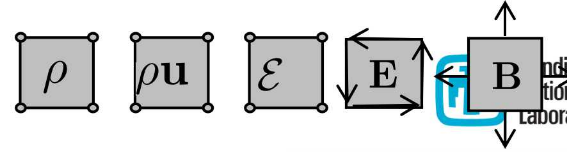


Or

$$\frac{\partial \mathbf{D}}{\partial t} - \nabla \times \mathbf{H} + \mathbf{J} = 0 \; ; \quad \nabla \cdot \mathbf{D} = q \; ; \quad \mathbf{E} = \epsilon^{-1}\mathbf{D}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0 \; ; \quad \nabla \cdot \mathbf{B} = 0 \; ; \quad \mathbf{H} = \mu_0^{-1}\mathbf{B}$$





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Energy	$\frac{\partial \varepsilon_a}{\partial t} + \nabla \cdot ((\varepsilon_a + p_a)\mathbf{u}_a + \Pi_a \cdot \mathbf{u}_a + \mathbf{h}_a) = q_a n_a \mathbf{u}_a \cdot \mathbf{E} + Q^{src}$ $- \sum_{b\neq a} \Big[(T_a - T_b) k \bar{\nu}^E_{ab} - \rho_a \mathbf{u}_a \cdot (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^M_{ab}$
Charge and Current Density	$q = \sum_k q_k n_k \qquad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$
Maxwell's Equations	$\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0} \qquad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ $\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \nabla \cdot \mathbf{B} = 0$

Cyclotron Frequency

Strong off diagonal coupling for plasma oscillation

Light wave

IMEX: Time Integration

$$\mathbf{M}\dot{\mathbf{U}} + \mathbf{F} + \mathbf{G} = 0$$

Explicit Hydrodynamics

Implicit EM, EM sources, sources for species $(\rho_a, \rho_a \mathbf{u}_a, \epsilon_a)$ interactions

E.g. Implicit / Explicit (IMEX) Methods and the Implicit Sub-problem

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

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

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

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

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

$$\begin{array}{c|c} \hat{\mathbf{c}} & \hat{\mathbf{a}} \\ \hline & \hat{\mathbf{b}}^T \end{array} \text{ is explicit, and } \begin{array}{c|c} \mathbf{c} & \mathbf{a} \\ \hline & \mathbf{b}^T \end{array} \text{ is implicit.}$$

High-order accuracy (e.g. 2nd – 5th), 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)

E.g. Implicit / Explicit (IMEX) Methods and the Implicit Sub-problem (contd.)

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Discrete Nonlinear Sub-problem – Newton's Method

$$\mathcal{F}(\mathbf{u}^{(\mathbf{i})}) = \mathbf{u}^{(i)} - \mathbf{u}^{n} - \Delta t \sum_{j=1}^{i-1} \hat{a}_{ij} \mathbf{F}(\mathbf{u}^{(j)}) + \Delta t \sum_{j=1}^{i} a_{ij} \mathbf{G}(\mathbf{u}^{(j)}) = 0$$

/* Find u* such that $\mathcal{F}(\mathbf{u}^*) = \mathbf{0}$*/

Until Nonlinear Convergence {

Iteratively solve linear sub-problem (e.g. AMG preconditioned Krylov method)

$$\mathcal{F}'(\mathbf{u_k})\mathbf{s_k} = -\mathcal{F}(\mathbf{u_k}) \quad \text{until} \quad \frac{\|\mathcal{F}'(\mathbf{u_k})\mathbf{s_k} + \mathcal{F}(\mathbf{u_k})\|}{\|\mathcal{F}(\mathbf{u_k})\|} \leq \eta^L$$

Update Sequence $\mathbf{u_{k+1}} = \mathbf{u_k} + \mathbf{s_k}$

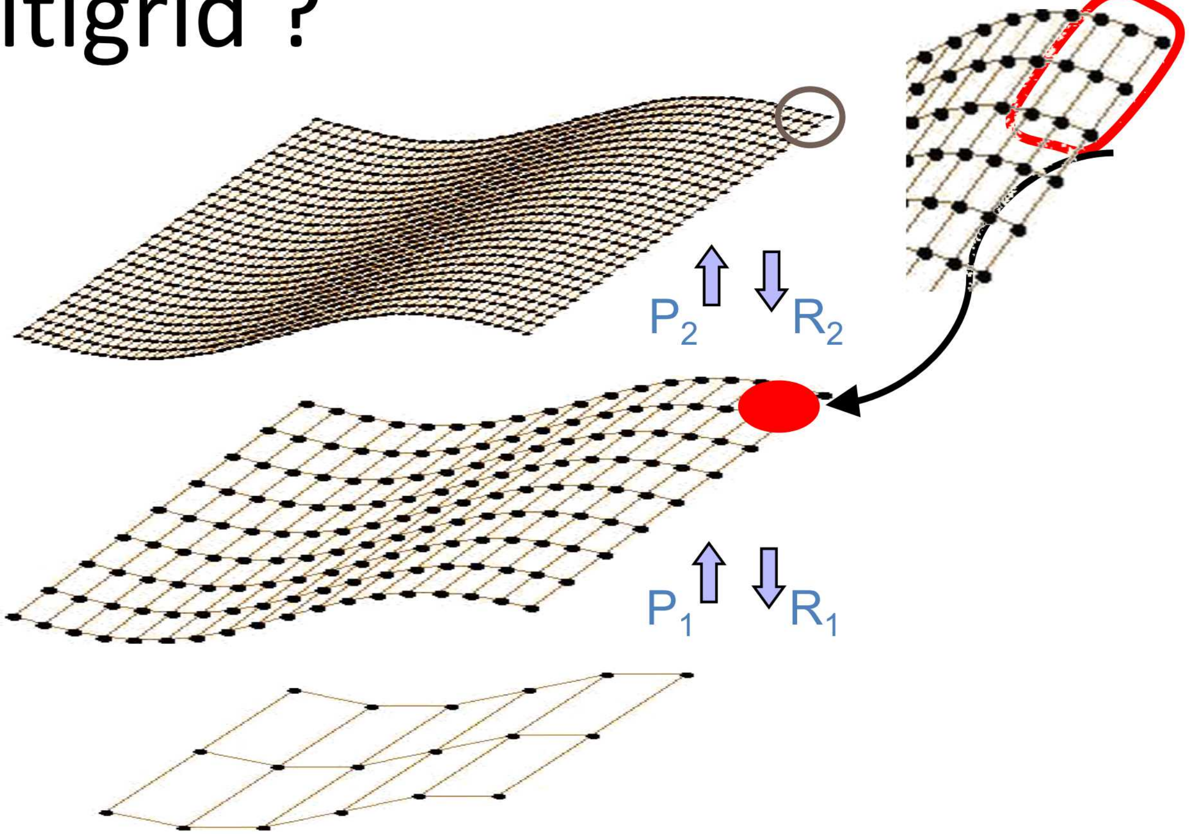
Check nonlinear norms for convergence ($\|\mathcal{F}(\mathbf{u_{k+1}})\|$, $\frac{\|\mathcal{F}(\mathbf{u_{k+1}})\|}{\|\mathcal{F}(\mathbf{u_0})\|}$, $\|\mathbf{s_k}\|_{WRMS}$, nan, max iter);

}

A key technology for implicit/IMEX is AD for Jacobian evaluation!

What is Multigrid ?

Solve $A_3 u_3 = f_3$



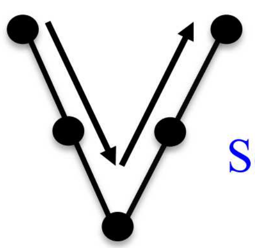
Basic idea:

- Develop coarse approximations on multiple levels (e.g discretize)
- Define prolongation P_i and restriction operator R_i (e.g. for P -FE interpolation)
- Accelerate convergence via coarse iterations to efficiently propagate information across domain

Smooth $A_3 u_3 = f_3$. Set $f_2 = R_2 r_3$.

Smooth $A_2 u_2 = f_2$. Set $f_1 = R_1 r_2$.

Solve $A_1 u_1 = f_1$ directly.



Set $u_3 = u_3 + P_2 u_2$. Smooth $A_3 u_3 = f_3$.

Set $u_2 = u_2 + P_1 u_1$. Smooth $A_2 u_2 = f_2$.

Large-scale Scaling Studies for Cray XK7 AND BG/Q; VMS 3D FE MHD

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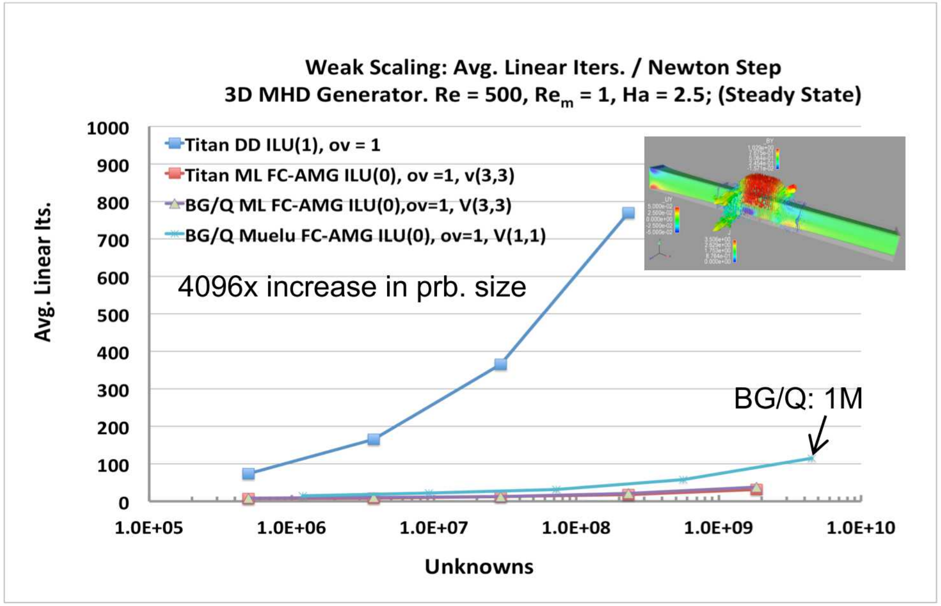
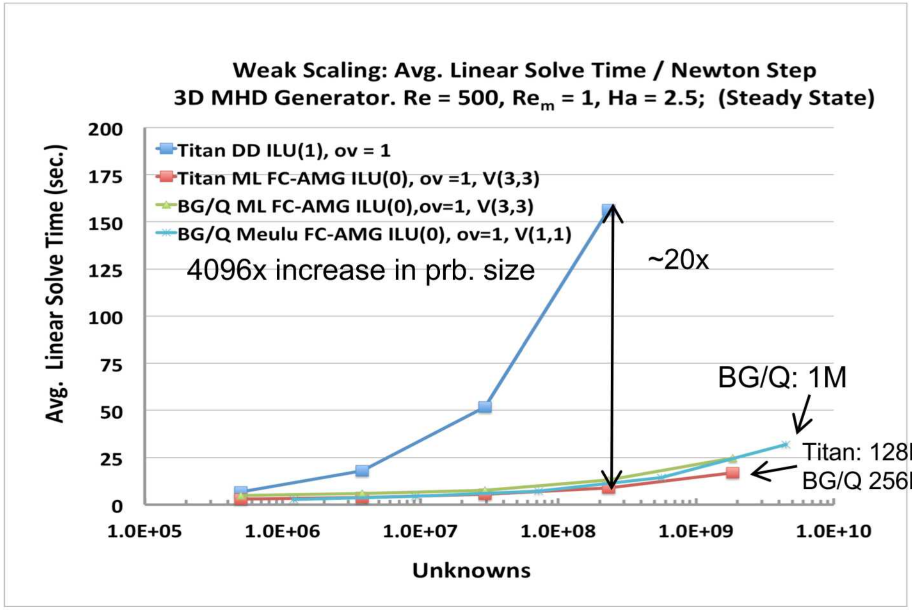
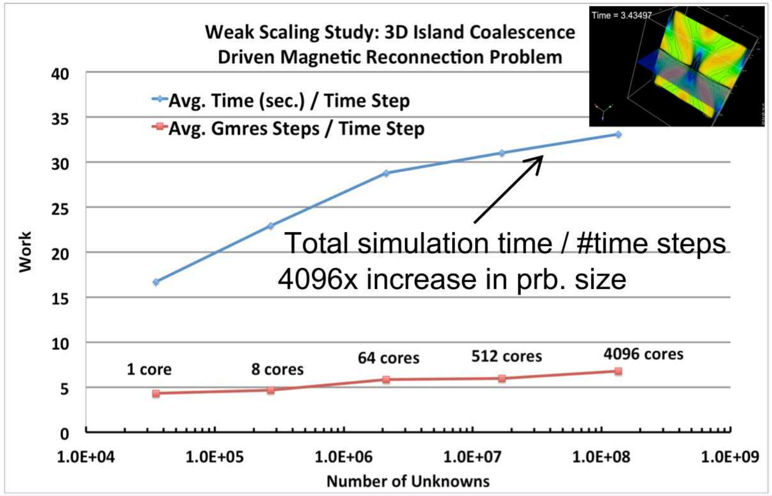
u P B r (similar discretizations for all variables, fully-coupled H(grad) AMG)







Largest fully-coupled unstructured FE MHD solves demo. to date:

MHD (steady) weak scaling studies to 128K Cray XK7, 1M BG/Q
Large demonstration computations

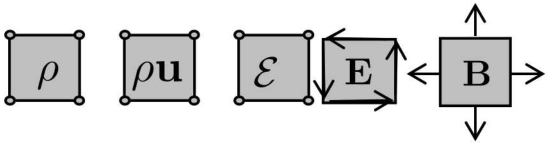
- MHD (steady): 13B DoF, 1.625B elem, on 128K cores
- CFD (Transient): 40B DoF, 10.0B elem, on 128K cores

Poisson sub-block solvers: 4.1B DoF, 4.1B elem, on 1.6M cores

Scalable Physics-based Preconditioners for Physics-compatible Discretizations

$$
\begin{bmatrix}
\mathbf{D}_{\rho_i} & \mathbf{K}^{\rho_i}_{\rho_i u_i} & 0 & \mathbf{Q}^{\rho_i}_{\rho_e} & 0 & 0 & 0 & 0 \\
\mathbf{D}^{\rho_i u_i}_{\rho_i} & \mathbf{D}_{\rho_i u_i} & 0 & \mathbf{Q}^{\rho_i u_i}_{\rho_e} & \mathbf{Q}^{\rho_i u_i}_{\rho_e u_e} & 0 & \mathbf{Q}^{\rho_i u_i}_{E} & \mathbf{Q}^{\rho_i u_i}_{B} \\
\mathbf{D}^{\mathcal{E}_i}_{\rho_i} & \mathbf{D}^{\mathcal{E}_i}_{\rho_i u_i} & \mathbf{D}_{\mathcal{E}_i} & \mathbf{Q}^{\mathcal{E}_i}_{\rho_e} & \mathbf{Q}^{\mathcal{E}_i}_{\rho_e u_e} & \mathbf{Q}^{\mathcal{E}_i}_{\mathcal{E}_e} & \mathbf{Q}^{\mathcal{E}_i}_{E} & 0 \\
\mathbf{Q}^{\rho_e}_{\rho_i} & 0 & 0 & \mathbf{D}_{\rho_e} & \mathbf{K}^{\rho_e}_{\rho_e u_e} & 0 & 0 & 0 \\
\mathbf{Q}^{\rho_e u_e}_{\rho_i} & \mathbf{Q}^{\rho_e u_e}_{\rho_i u_i} & 0 & \mathbf{D}^{\rho_e u_e}_{\rho_e} & \mathbf{D}_{\rho_e u_e} & 0 & \mathbf{Q}^{\rho_e u_e}_{E} & \mathbf{Q}^{\rho_e u_e}_{B} \\
\mathbf{Q}^{\mathcal{E}_e}_{\rho_i} & \mathbf{Q}^{\mathcal{E}_e}_{\rho_i u_i} & \mathbf{Q}^{\mathcal{E}_e}_{\mathcal{E}_i} & \mathbf{D}^{\mathcal{E}_e}_{\rho_e} & \mathbf{D}^{\mathcal{E}_e}_{\rho_e u_e} & \mathbf{D}_{\mathcal{E}_e} & \mathbf{Q}^{\mathcal{E}_e}_{E} & 0 \\
0 & \mathbf{Q}^{E}_{\rho_i u_i} & 0 & 0 & \mathbf{Q}^{E}_{\rho_e u_e} & 0 & \mathbf{Q}_{E} & \mathbf{K}^{E}_{B} \\
0 & 0 & 0 & 0 & 0 & 0 & \mathbf{K}^{B}_{E} & \mathbf{Q}_{B}
\end{bmatrix}
\begin{bmatrix}
\rho_i \\ \rho_i \mathbf{u}_i \\ \mathcal{E}_i \\ \rho_e \\ \rho_e \mathbf{u}_e \\ \mathcal{E}_e \\ \mathbf{E} \\ \mathbf{B}
\end{bmatrix}
$$

16 Coupled Nonlinear PDEs



Group the hydrodynamic variables together (similar discretization)

$$\mathbf{F} = (\rho_i, \rho_i \mathbf{u}_i, \mathcal{E}_i, \rho_e, \rho_e \mathbf{u}_e, \mathcal{E}_e)$$

Resulting 3x3 block system

$$
\begin{bmatrix}
\mathbf{D}_F & \mathbf{Q}^F_E & \mathbf{Q}^F_B \\
\mathbf{Q}^E_F & \mathbf{Q}_E & \mathbf{K}^E_B \\
0 & \mathbf{K}^B_E & \mathbf{Q}_B
\end{bmatrix}
\begin{bmatrix}
\mathbf{F} \\ \mathbf{E} \\ \mathbf{B}
\end{bmatrix}
$$

Reordered 3x3

$$
\begin{bmatrix}
\mathbf{Q}_B & \mathbf{K}^B_E & 0 \\
\mathbf{K}^E_B & \mathbf{Q}_E & \mathbf{Q}^E_F \\
\mathbf{Q}^F_B & \mathbf{Q}^F_E & \mathbf{D}_F
\end{bmatrix}
\begin{bmatrix}
\mathbf{B} \\ \mathbf{E} \\ \mathbf{F}
\end{bmatrix}
$$

Physics-based Approach Enables Optimal AMG Sub-block Solvers

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$$\begin{bmatrix} \mathbf{Q}_B & \mathbf{K}_E^B & 0 \\ 0 & \hat{\mathcal{D}}_E & \mathbf{Q}_F^E \\ 0 & 0 & \hat{\mathbf{S}}_F \end{bmatrix} \begin{bmatrix} \mathbf{B} \\ \mathbf{E} \\ \mathbf{F} \end{bmatrix}$$

$$\hat{\mathbf{S}}_F = \mathbf{D}_F - \mathcal{K}_E^F \tilde{\tilde{\mathcal{D}}}_E^{-1} Q_F^E$$

CFD type system
node-based coupled
ML: H(grad) AMG
(SIMPLEC: Schur-compl.)

$$\hat{\mathcal{D}}_E = \mathbf{Q}_E - \mathbf{K}_B^E \bar{\mathbf{Q}}_B^{-1} \mathbf{K}_E^B$$

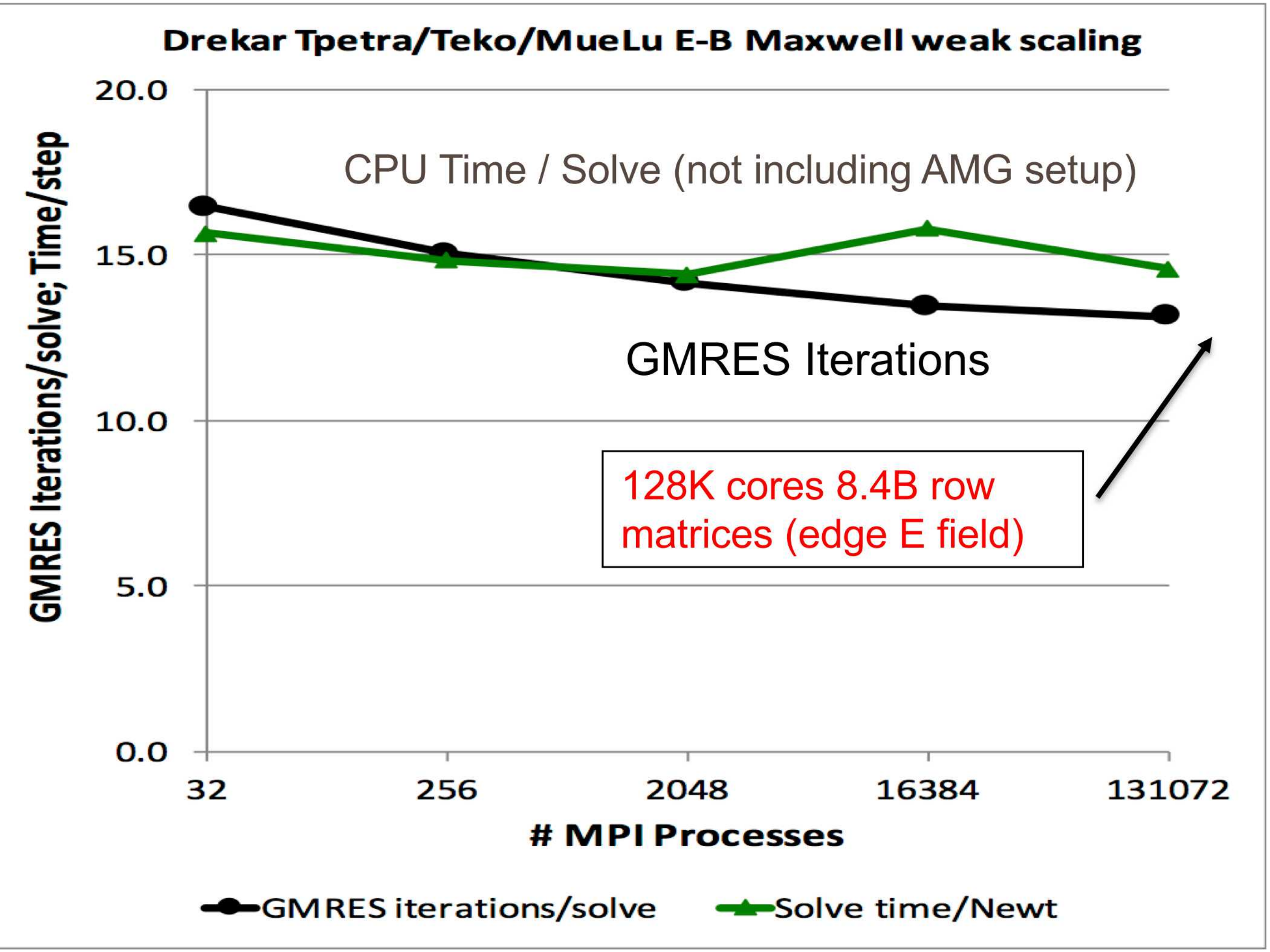
Compare to: $\dfrac{\partial^2 \mathbf{E}}{\partial t^2} - \dfrac{1}{\sigma \mu_0} \nabla \times \nabla \times \mathbf{E} = \mathbf{0}$

Electric field system
Edge-based curl-curl type
ML: H(curl) AMG
(lumped mass)

$$\mathbf{B} = -\bar{\mathbf{Q}}_B^{-1} \mathbf{K}_E^B \ \mathbf{E}$$

Face-based simple
mass matrix Inversion.

Weak Scaling for 3D Electro Magnetic Pulse with Block Maxwell Eq. Preconditioners on Trinity



$$\mathcal{D}^E = \mathbf{Q}_E - \mathbf{K}_B^E \bar{\mathbf{Q}}_B^{-1} \mathbf{K}_E^B$$

Maxwell subsystem: electric field Edge-based curl-curl type system.

Good scaling on block solves (at least for solve; setup needs improvement)

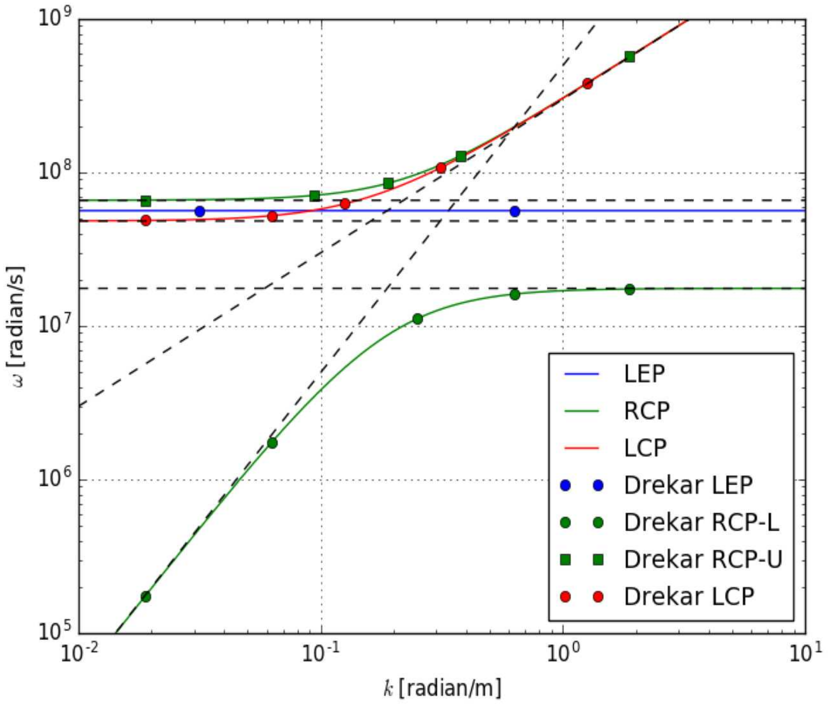
Demonstrated to $CFL_c > 10^4$

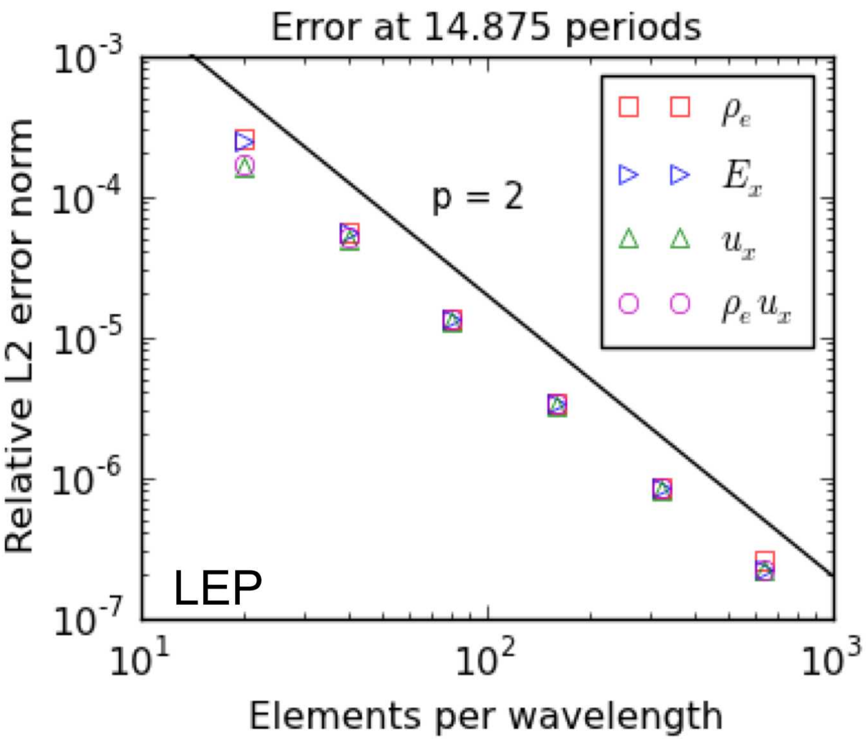
Drekar

GS smoother with H(grad) AMG

Max $CFL_c \sim 200$

Demonstration / Verification of Implicit Solution for Longitudinal Electron Plasma (LEP) Oscillation with Under-resolved EM Waves



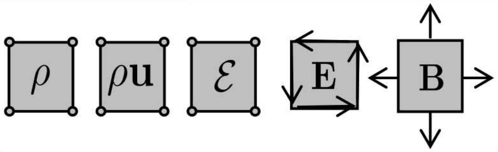


LEP: Longitudinal Electron Plasma Wave
RCP: Right Hand Circularly Polarized Wave
LCP: Left Hand Circularly Polarized Wave
(Cold plasma)

Verification effort with Niederhaus, Radtke, Bettencourt, Cartwright, Kramer, Robinson and ATDM EMPIRE Team

Initial Weak Scaling for Longitudinal Electron / Ion Plasma Oscillation and Under-resolved TEM Wave Results (Full Maxwell – two-fluid)

$$\Delta t = 1.1 \times 10^{-11} \approx 0.023\ \tau_{\omega_{pi}} \approx 0.1\ \tau_{\omega_{pe}} \geq 3 \times 10^{2}\ \tau_{c}$$



Structure-preserving discretization

N	P	Linear its / Newton	Solve time / linear solve	$\frac{\Delta t_{imp}}{\Delta t_{exp}}$
100	1	4.18	0.2	300
200	2	4.21	0.22	600
400	4	4.27	0.23	1.2E+3
800	8	4.4	0.26	2.4E+3
1600	16	4.51	0.35	4.8E+3
3200	32	4.89	0.42	9.6E+3
6400	64	6.21	0.61	1.9e+4

$$\mu = \frac{m_i}{m_e} = 1836.57 \qquad \Delta x \approx 1 \mu m$$

Initial weak scaling of ABF preconditioner

- Domain [0,0.01]x[0,0.0004]x[0,0.0004]; Periodic BCs in all directions
- N elements in x-direction;
- Fixed time step size for SDIRK (2,2): (not resolving TEM wave)

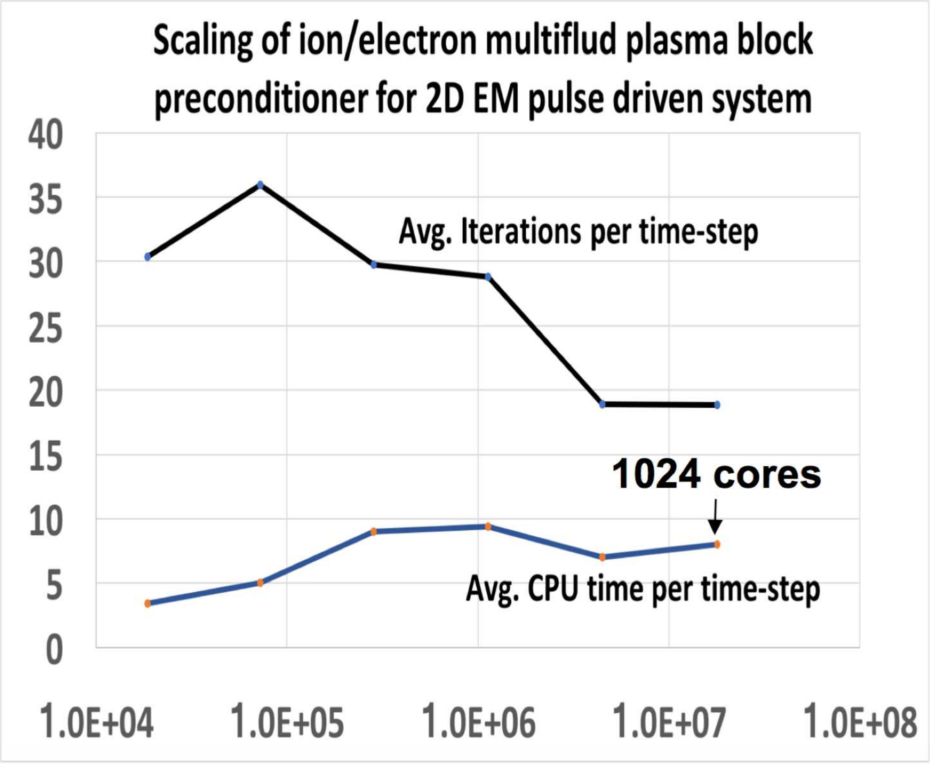
Proof of Principle

SimpleC on fluid Schur-complement
DD-ILU for Euler Eqns.
DD-LU curl-curl

A MORE REALISTIC TEST PROBLEM

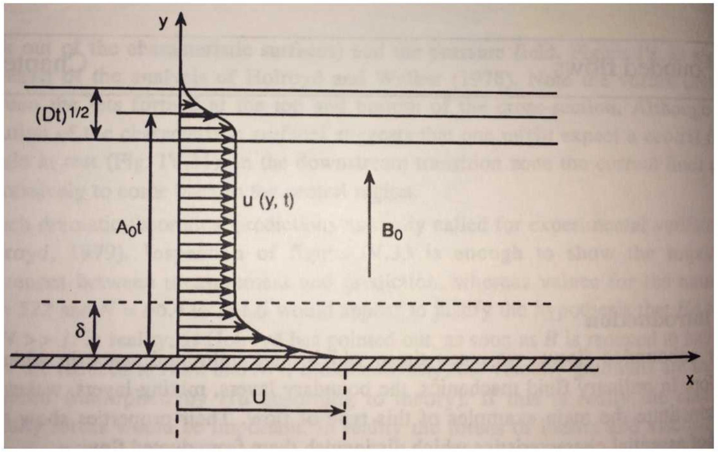
- 2D electron/ion plasma driven by an external current pulse with background magnetic field and density gradient
- Simulation resolves current source

Time-scale	Pulse Problem
CFL_{EM}	$[6.25 \times 10^{-2}, 2.0]$
$CFL_{\mathbf{u}_e}$	$[3.75 \times 10^{-2}, 1.2]$
$CFL_{\mathbf{u}_i}$	$[3.75 \times 10^{-5}, 1.2 \times 10^{-3}]$
CFL_{s_e}	0
CFL_{s_i}	0
$CFL_{\omega_{p,e}}$	1.2×10^2
$CFL_{\omega_{p,i}}$	3.8
$CFL_{\omega_{c,e}}$	2.7
$CFL_{\omega_{c,i}}$	2.7×10^{-3}



Resistive Alfven wave problem

- Solution is derived from resistive/viscous MHD which **ignores Hall effects:**
  - Hall parameter $\mathrm{H} = \frac{\omega_{ce}}{\nu_{ei}} = \frac{\eta\, B}{n_e e} \ll 1$
  - Reducing Hall effects in magnetized multi-fluid model is tricky - requires large collision frequency
- Problem used for verifying resistive, Lorentz force, and viscous operators:
  - Impulse shear due to a moving wall drives a **Hartmann layer**
  - Hartmann layer shear excites **Alfven wave** traveling along magnetic field
  - Alfven wave front diffuses due to momentum and magnetic diffusivity
  - Profile depends on the effective **Lundquist number** $S = \frac{L\, v_A}{\lambda}$



R. Moreau, Magnetohydrodynamics, 1990

$$u_x = \frac{U}{4}\left(1 + \exp\left(\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_+) + \frac{U}{4}\left(1 + \exp\left(-\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_-)$$

$$B_x = \sqrt{\mu_0 \rho}\,\frac{U}{4}\left(1 - \exp\left(\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_+) - \sqrt{\mu_0 \rho}\,\frac{U}{4}\left(1 - \exp\left(-\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_-)$$

$$\eta_\pm = \frac{y \pm v_A t}{2\sqrt{\lambda t}}$$

Asymptotic Solution of multifluid in MHD Limit:

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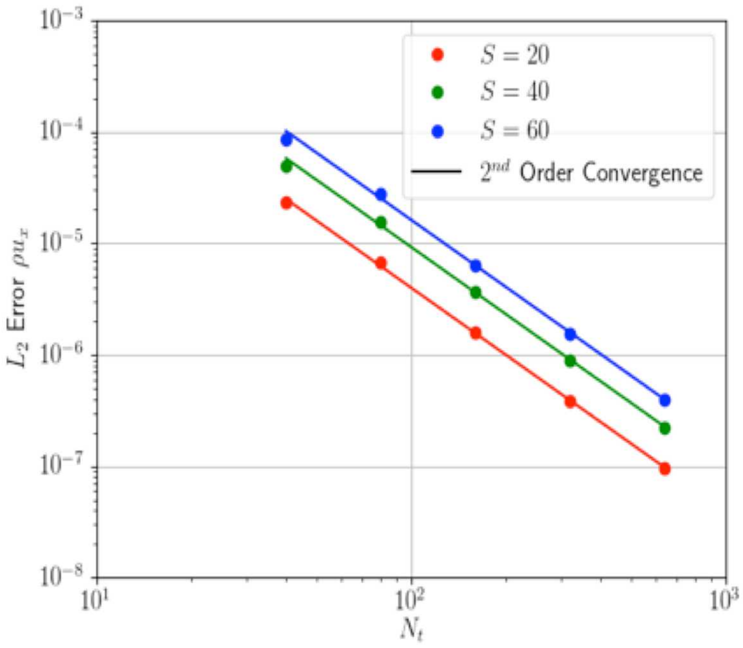
Implicit L-stable and IMEX SSP/L-stable time integration and block preconditioners enable solution of multifluid EM plasma model in the asymptotic resistive MHD limit.
(Simple Visco-resistive Alfven wave)



Accuracy in MHD limit (IMEX)

Plasma Scales for S = 60		
	Electrons	Ions
$\omega_p \Delta t$	10^7 - 10^9	10^6 - 10^7
$\omega_c \Delta t$	10^6 - 10^7	10^3 - 10^4
$\nu_{\alpha\beta} \Delta t$	10^{10} - 10^{11}	10^7 - 10^8
$\nu_S \Delta t / \Delta x$	10^{-2}	10^{-4}
$u \Delta t / \Delta x$	10^{-4}	10^{-4}
$\mu \Delta t / \rho \Delta x^2$	10^{-1} - 10^1	10^{-2} - 10^0
$c \Delta t / \Delta x$	10^2	

IMEX terms: implicit/explicit

EM-PIC Model

Kinetic equation (Klimontovich) for phase space density of each plasma species N_s

$$\frac{\partial N_s(\boldsymbol{x},\boldsymbol{u},t)}{\partial t} + \boldsymbol{v}\cdot\nabla_x N_s + \frac{q_s}{m_s}\left(\mathbf{E} + \frac{\boldsymbol{v}}{c}\times\mathbf{B}\right)\cdot\nabla_u N_s = \left.\frac{\partial N_s(\boldsymbol{x},\boldsymbol{u},t)}{\partial t}\right|_c$$

$$\rho(\boldsymbol{x},t) = \sum_{species} q_s \int d\boldsymbol{u} N_s(\boldsymbol{x},\boldsymbol{u},t)$$

$$\boldsymbol{J}(\boldsymbol{x},t) = \sum_{species} q_s \int d\boldsymbol{u}\boldsymbol{u} N_s(\boldsymbol{x},\boldsymbol{u},t)$$

Maxwell's Equations

$$\nabla\cdot\boldsymbol{D}(\boldsymbol{x},t) = \frac{\rho(\boldsymbol{x},t)}{\epsilon_0}$$

$$\nabla\cdot\mathbf{B}(\boldsymbol{x},t) = 0$$

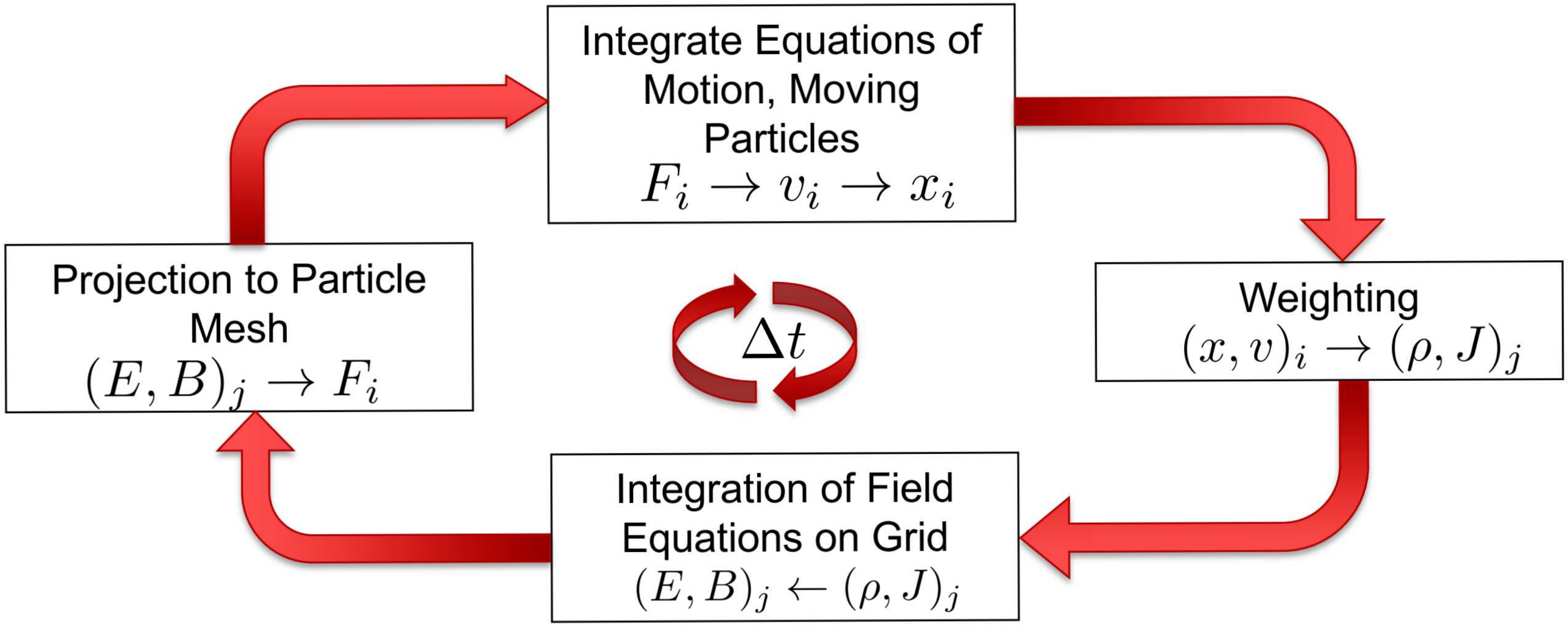
$$\nabla\times\mathbf{E}(\boldsymbol{x},t) = -\frac{\partial\mathbf{B}(\boldsymbol{x},t)}{\partial t}$$

$$\nabla\times\boldsymbol{H}(\boldsymbol{x},t) = \mu_0\boldsymbol{J}(\boldsymbol{x},t) + \mu_0\epsilon_0\frac{\partial\boldsymbol{D}(\boldsymbol{x},t)}{\partial t}$$

- Lagrangian particles updated by F=ma
- Currently solved with explicit time integration
- PIC code contains its own EM field solver

Operator Split Coupled Model

$$m_s \frac{d}{dt}\left(\boldsymbol{V}_i(t)\gamma_i(t)\right) = q_s\left(\mathbf{E}(\boldsymbol{X}_i(t),t) + \boldsymbol{V}_i(t) \times \mathbf{B}(\boldsymbol{X}_i(t),t)\right) \qquad \gamma_i(t) = 1/\sqrt{1 - \boldsymbol{V}_i^2(t)/c^2}$$



$$\nabla \cdot \boldsymbol{D}(\boldsymbol{x},t) = \frac{\rho(\boldsymbol{x},t)}{\epsilon_0}$$

$$\nabla \cdot \mathbf{B}(\boldsymbol{x},t) = 0$$

$$\nabla \times \mathbf{E}(\boldsymbol{x},t) = -\frac{\partial \mathbf{B}(\boldsymbol{x},t)}{\partial t}$$

$$\nabla \times \boldsymbol{H}(\boldsymbol{x},t) = \mu_0 \boldsymbol{J}(\boldsymbol{x},t) + \mu_0\epsilon_0 \frac{\partial \boldsymbol{D}(\boldsymbol{x},t)}{\partial t}$$

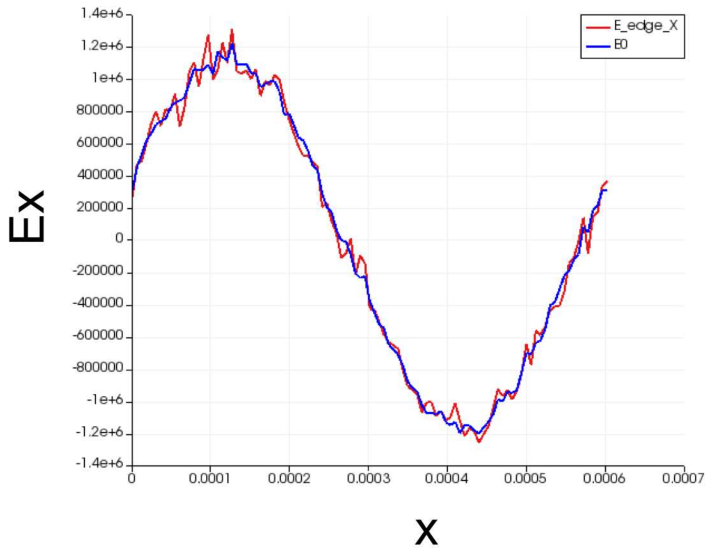
$$\rho(\boldsymbol{x},t) = \sum_{species} q_s \int d\boldsymbol{u} N_s(\boldsymbol{x},\boldsymbol{u},t)$$

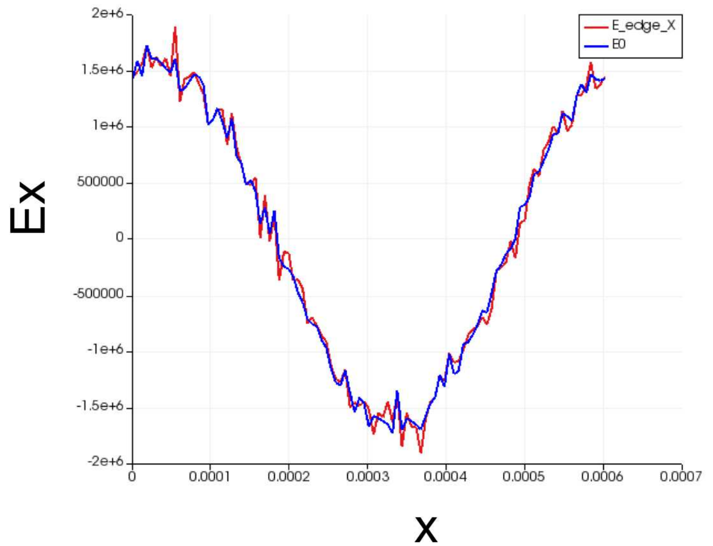
$$\boldsymbol{J}(\boldsymbol{x},t) = \sum_{species} q_s \int d\boldsymbol{u}\boldsymbol{u} N_s(\boldsymbol{x},\boldsymbol{u},t)$$

Coupled System Results

Drekar-PIC Coupling Demonstration

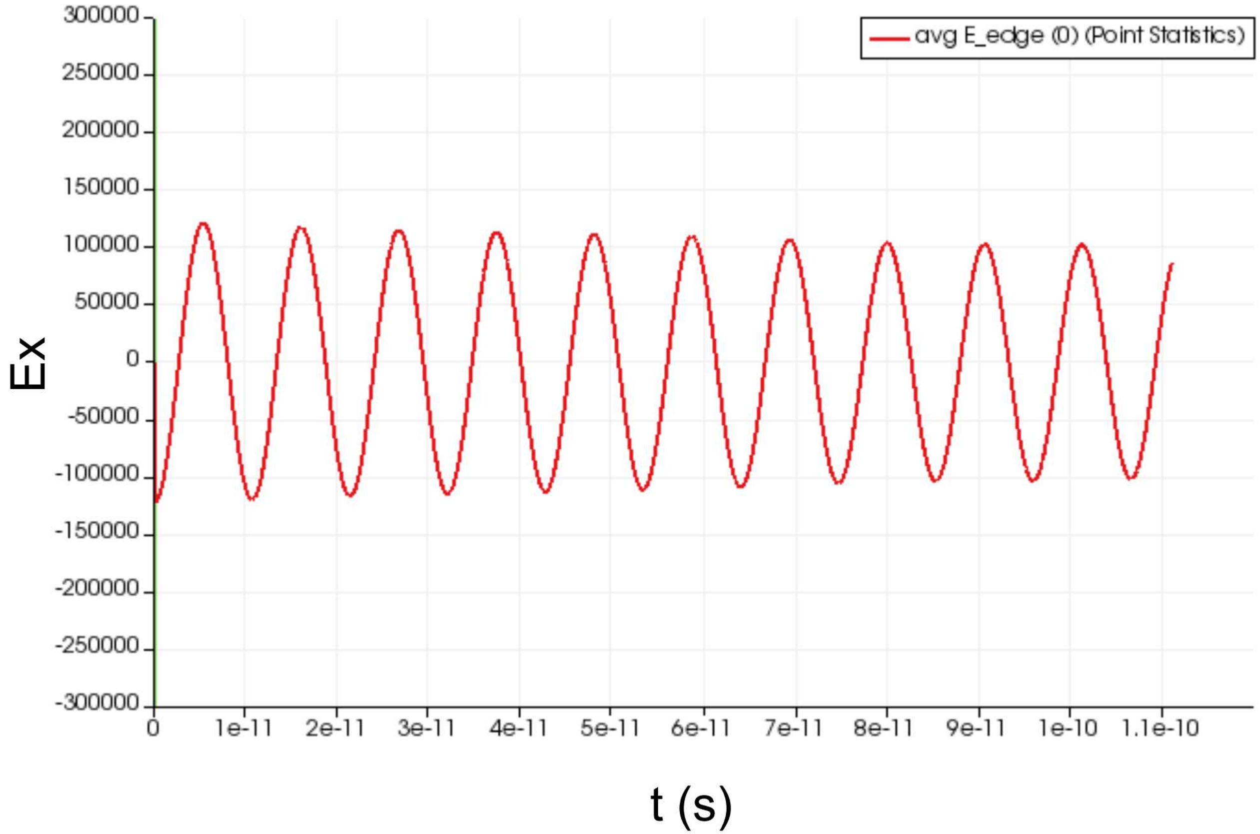
- First coupling of Drekar to EMPIRE-PIC for a Langmuir Wave
- Simple proof-of-principle (Drekar Electrostatic potential, EMPIRE-PIC electrons)
- Replace PIC EM Solver with Drekar EM
- CG fluid, 1024 cells, 9K particles
- Plots show Ex line plot over spatial domain: red is coupled solution (cell avg.), blue is EM-PIC standalone solution at nodes.
- Good agreement





Verification Example: Ion/Electron Plasma Oscillation

- Coupled fluid (electrons) and PIC (ions)
  - N = 1e+20
  - 16384 particles
  - 32x2 mesh
- Simplified problem for ES formulation
- Theory period: 1.06192e-11
- Simulation period: 1.0593e-11
  - 0.25% error
- New results, just delving into accuracy

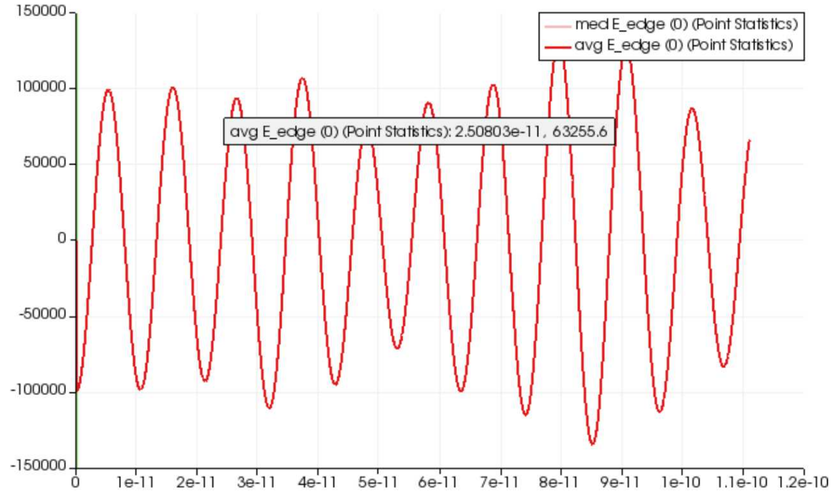


Period Computation

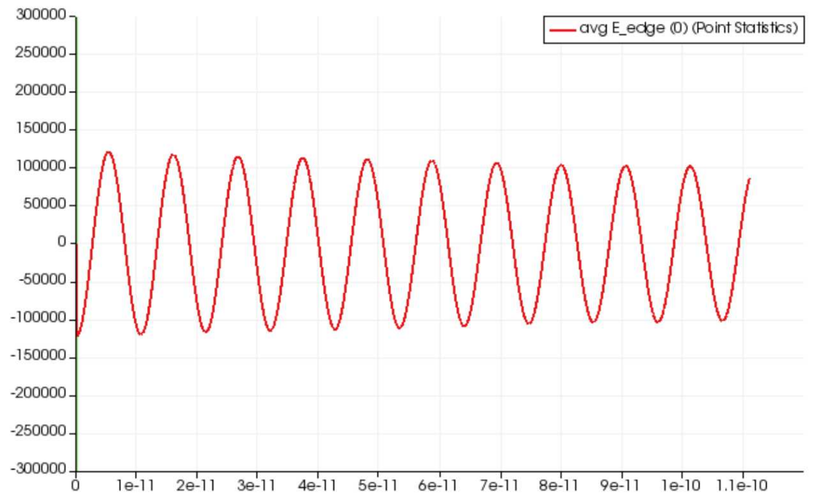
- Frequency/Period values computed using FFT

- Time history data can be sampled from a single point in space or using average value from line across mesh (half plane)
  - 1D problem in a 2D code

Single Point (0.000175, 0.0)

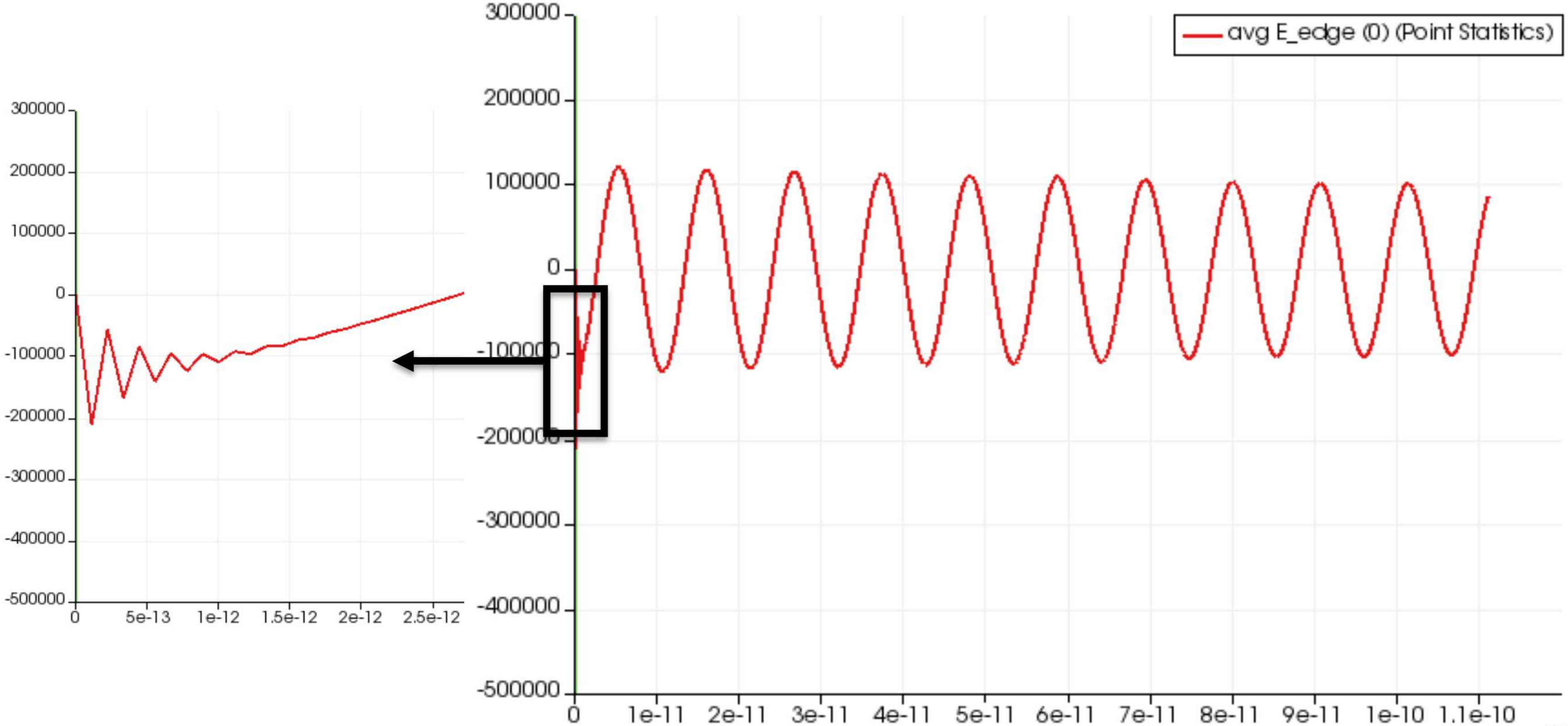


Line Average (center to edge)



Time Integration Effects

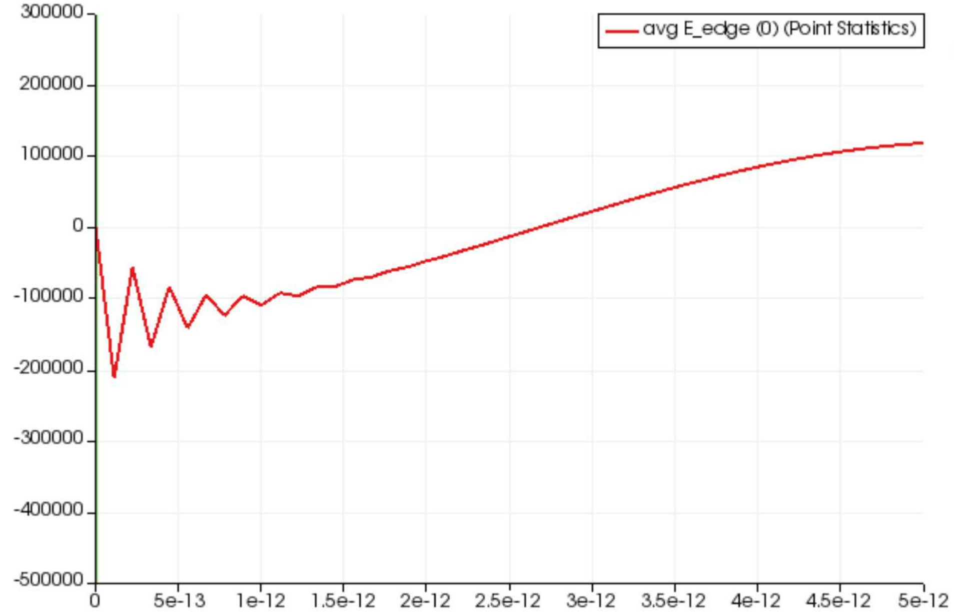
- Can we control stability in fluid solver for coupled system?

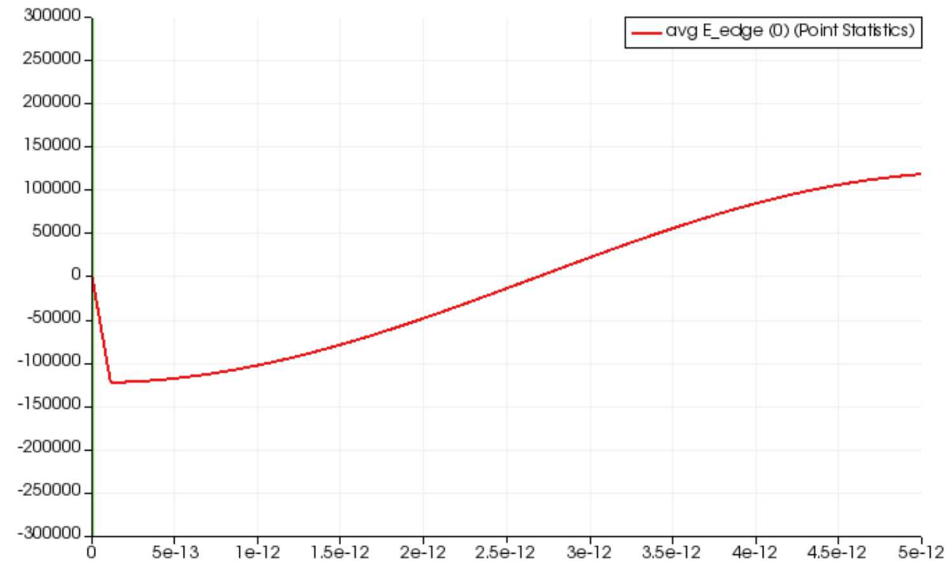


Time Integrator

- Try an L-Stable integrator
  - DIRK 2 stage,2nd Order: L-Stable
  - DIRK 2 stage, 3rd Order: A-Stable
- L-Stability damps out startup oscillations in E-Field
- Simulations are indistinguishable except for short startup.
- Same period values from FFT
- Confidence that we can control part of stability for the fluid and EM

Integrator	Stability	Period	% Error
DIRK 2nd Order, 2 stage	L-Stable	1.1111E-11	4.63E+00
DIRK 3rd Order, 2 stage	A-Stable	1.1111E-11	4.63E+00





Time Step Size

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- Operator split solve with implicit electons (fluid) and explicit ions (PIC)
- Stability of ion plasma frequency
- Coupling of Ion Momentum and Energy to Ampere's law
- Failure exhibited by divergence of the Nonlinear solver

Fluid: Implicit Electrons → w_p_e * dt

PIC: Explicit Ions → w_p_i * dt

dt	Result	w_p_e * dt	w_p_i * dt
1.11E-13	Converged	6.26E-02	1.98E-02
2.22E-13	Converged	1.25E-01	3.96E-02
4.44E-13	Converged	2.50E-01	7.92E-02
8.88E-13	Converged	5.01E-01	1.58E-01
2.22E-12	Converged	1.25E+00	3.96E-01
4.44E-12	Converged	2.50E+00	7.92E-01
8.88E-12	Failed	5.01E+00	1.58E+00

Production Code (DG) Verification: Temporal Plasma Oscillation (No Spatial Variation)

- A plasma oscillation can be setup assuming an neutralizing background fluid by setting an initial electric field to **E=0**. Writing the momentum and Ampere equations gives:

$$\partial_t \mathbf{v}_1 = \frac{q_1}{m_1}\mathbf{E}$$

$$\partial_t \mathbf{v}_2 = \frac{q_2}{m_2}\mathbf{E}$$

$$\epsilon_0 \partial_t \mathbf{E} = -q_1 n_1 \mathbf{v}_1 - q_2 n_2 \mathbf{v}_2$$

- One can show that:

$$E = C sin(\gamma t)$$

$$v_1 = -\frac{q_1}{m_1 \gamma} C cos(\gamma t) + A$$

$$v_2 = -\frac{q_2}{m_2 \gamma} C cos(\gamma t) - \xi A$$

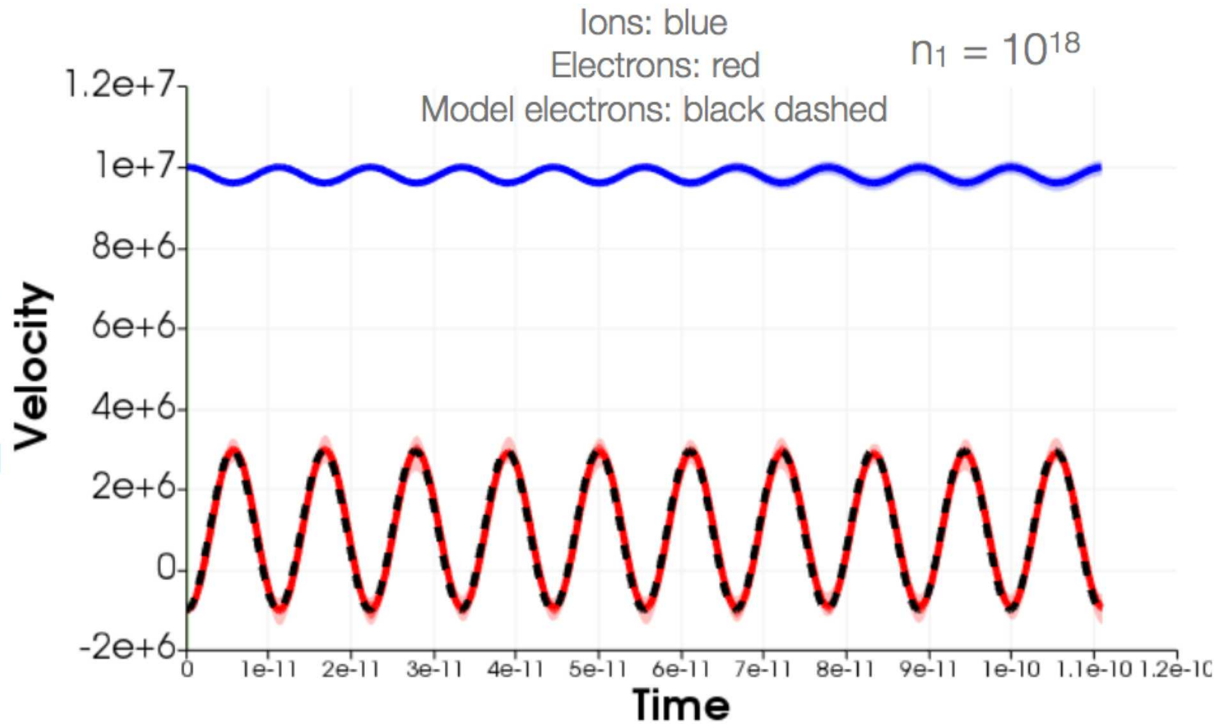
- With:

$$\gamma = \sqrt{\frac{q_1^2 n_1}{\epsilon_0 m_1} + \frac{q_2^2 n_2}{\epsilon_0 m_2}},\ \xi = \frac{q_1 n_1}{q_2 n_2},\ C = -\gamma \frac{\tilde{\mathbf{v}}_2 + \xi \tilde{\mathbf{v}}_1}{\left(\frac{q_2}{m_2} + \xi \frac{q_1}{m_1}\right)},\ A = \tilde{\mathbf{v}}_1 + \frac{q_1}{m_1 \gamma} C.$$

Low Number Density: Good Match between Simulation/Analytic Model

- Simulation setup:
  - Kinetic (PIC) ions; fluid (DG) electrons; Maxwell (DG) with cleaning
  - Resolution: 4x4 mesh, with 1000 particles (total); 50 time steps per plasma oscillation
  - *Spatially constant* by construction, though the fluid and PIC solvers are definitely not constrained in that way.
  - The time integration is explicit SSPRK3 for the fluid+Maxwell; operator split with the particle update.
  - The particles are initially randomly distributed throughout the domain

$q_1 = -10q_e, m_1 = 100m_e, \mathbf{v}_1 = 1e7, n_2 = 1e20, q_2 = q_e, m_2 = m_e, \mathbf{v}_2 = -1e6$



Experiment: increase particle # density
Measure: how electrons respond
Result: **At low ion number density, simulation reproduces model expectation**

Software: Critical Technology

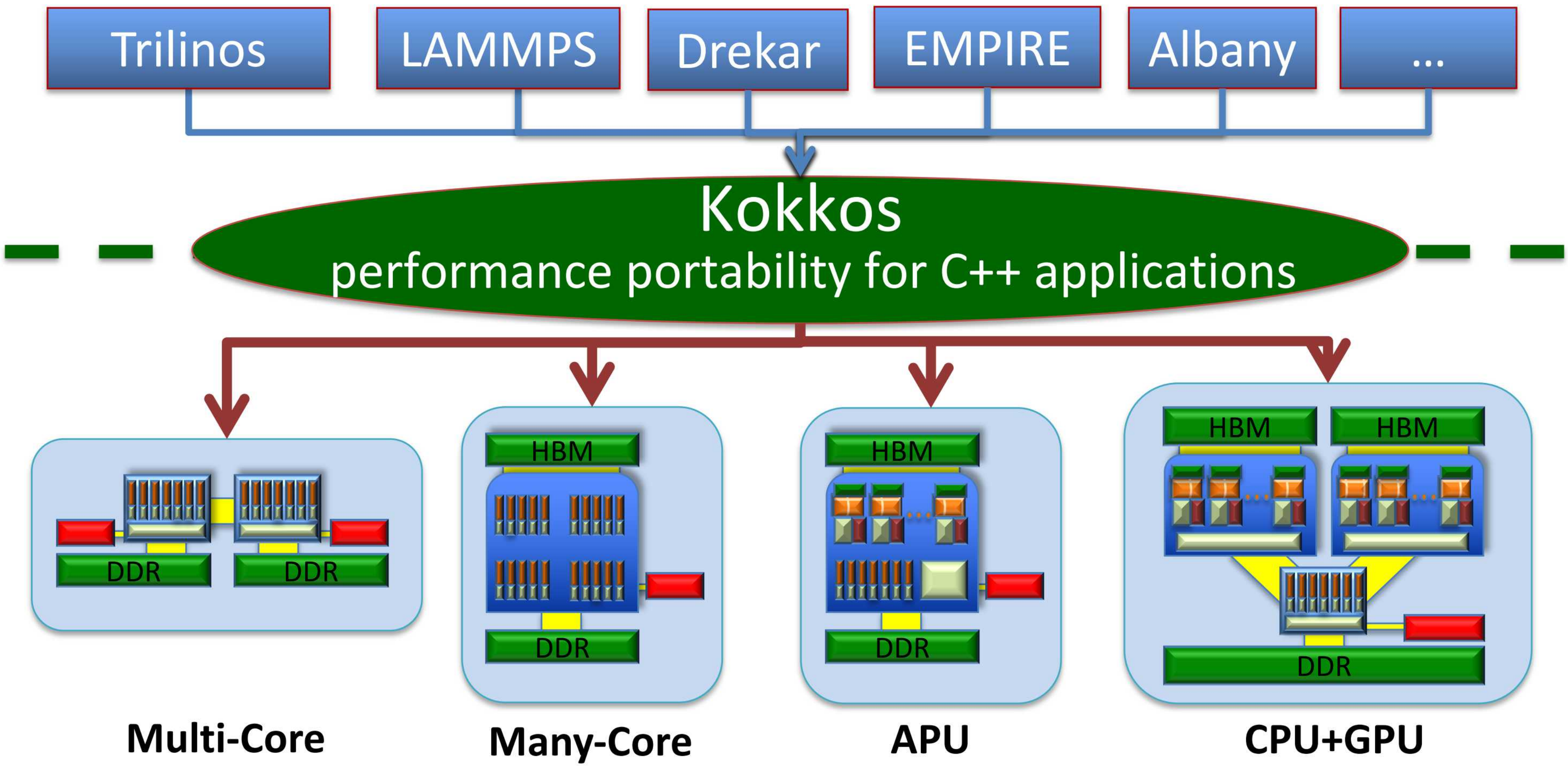
- Performance portability on next generation architectures
  - CPU, PHI, GPU, …
  - Easy for application teams to code

- Sensitivities
  - Implicit and IMEX time integrators, parametric sensitivity analysis, optimization, stability, bifurcation analysis
  - Combinatorial explosion of sensitivity requirements → AD is only viable solution!
  - Do not burden analysts/physics experts with analysis algorithm requirements

- Handle complexity in multiphysics PDE systems:
  - Complex interdependent coupled physics
  - Multiple proposed mathematical models
  - Different numerical formulations (e.g. space-time discretizations)
    - CG, DG, mixed CG-DG
    - Implicit, IMEX
    - Stabilized, Compatible
  - Supporting multiplicity in models and solution techniques often leads to complex code with ***complicated logic*** and ***fragile software designs***

Performance Portability: Kokkos

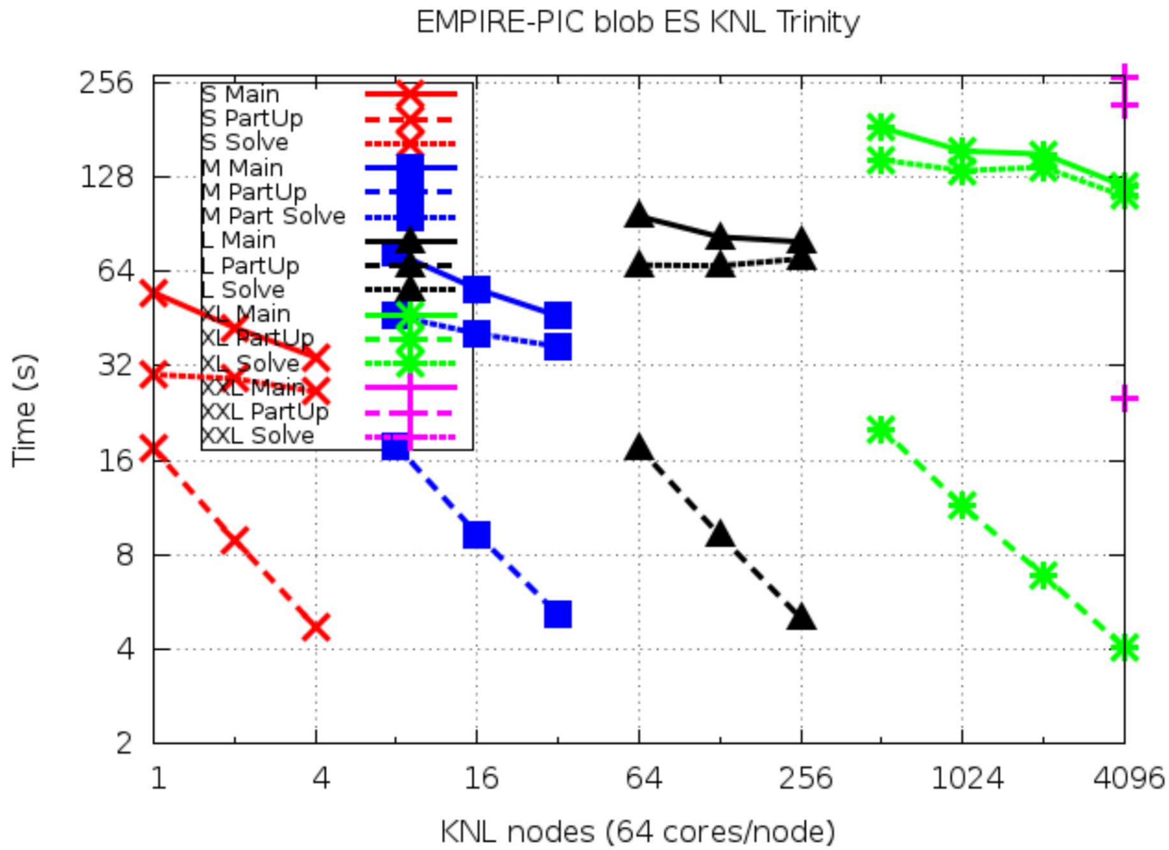
- Performance Portable Thread-Parallel Programming Model in C++
- Multidimensional Array
- Compiletime polymorphic memory layouts: cached vs coalesced memory
- Asynchronous Many Tasking



https://github.com/kokkos/kokkos

Performance Portability (EM-PIC)

ES Simulation on Trinity: 4 MPI x 16 OMP (1 HT) per KNL node.



size	elements	particles
S	337k	9.6M
M	2.68M	77.1M
L	20.7M	617M
XL	166M	4.94B
XXL	1332M	39.5B

Solvers are under active development for Performance Portability

Sacado: Template-based Automatic Differentiation

- Implement equations templated on the scalar type
- Libraries provide new scalar types that ***overload the math operators*** to propagate embedded quantities
  - Expression templates for performance
  - Derivatives: FAD, RAD
  - Hessians
  - Stochastic Galerkin: PCE
  - Multipoint: Ensemble (Stokhos)
- Analytic Values (NO FD involved)!

```
template <typename ScalarT>
void computeF(ScalarT* x, ScalarT* f)
{
  f[0] = 2.0 * x[0] + x[1] * x[1];
  f[1] = x[0] * x[0] * x[0] + sin(x[1]);
}
```

double **Fad<double>**

Operation	Forward AD rule
$c = a \pm b$	$\dot{c} = \dot{a} \pm \dot{b}$
$c = ab$	$\dot{c} = a\dot{b} + \dot{a}b$
$c = a/b$	$\dot{c} = (\dot{a} - c\dot{b})/b$
$c = a^r$	$\dot{c} = ra^{r-1}\dot{a}$
$c = \sin(a)$	$\dot{c} = \cos(a)\dot{a}$
$c = \cos(a)$	$\dot{c} = -\sin(a)\dot{a}$
$c = \exp(a)$	$\dot{c} = c\dot{a}$
$c = \log(a)$	$\dot{c} = \dot{a}/a$

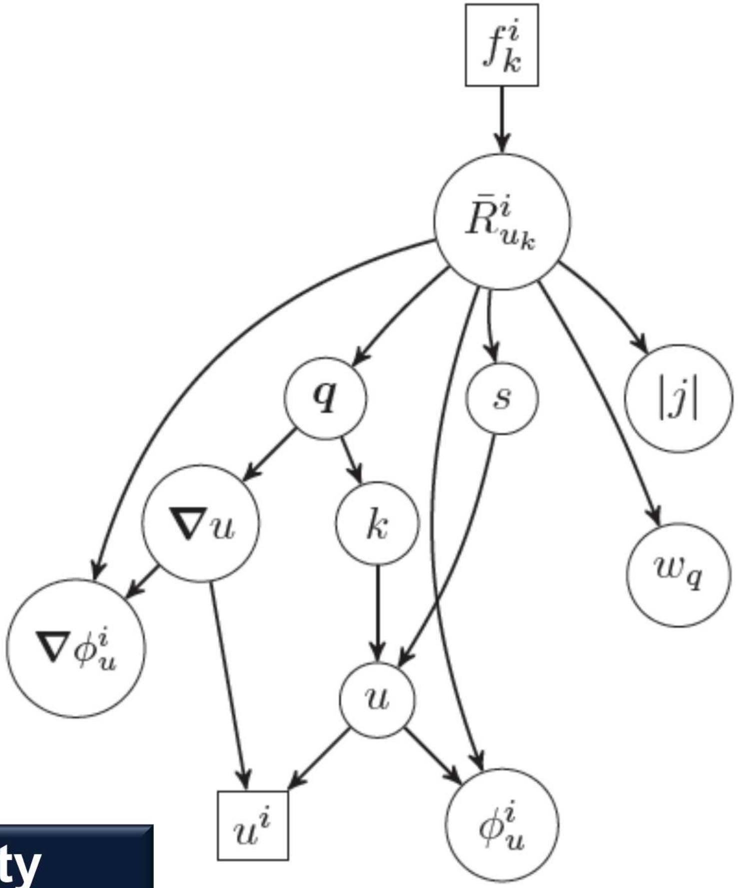
```
double* x;
double* f;
…
computeF(x,f);
```

```
DFad<double>* x;
DFad<double>* dfdx;
…
computeF(x,dfdx);
```

Phalanx: Lightweight DAG-based Expression Evaluation

$$R_u^i = \int_\Omega \left[\phi_u^i \dot{u} - \boldsymbol{\nabla}\phi_u^i \cdot \boldsymbol{q} + \phi_u^i s\right] \, d\Omega$$

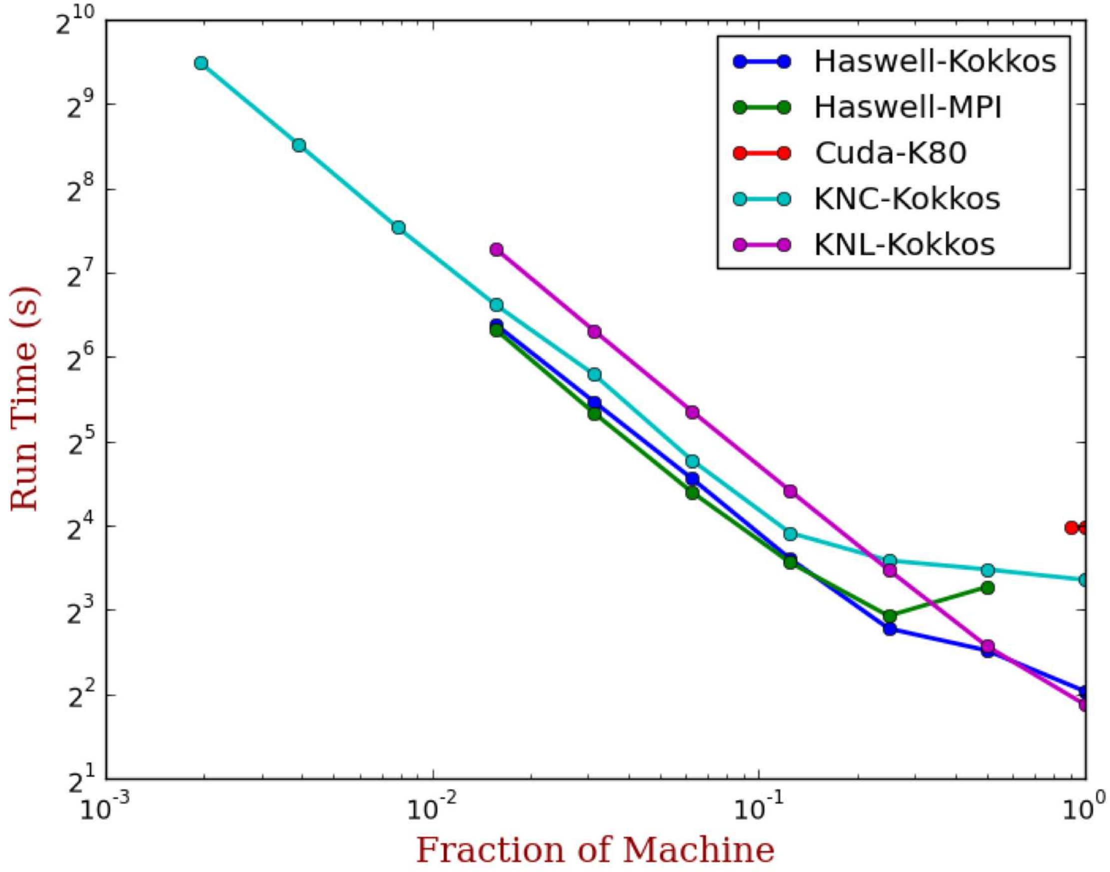
- Decompose a complex model into a graph of simple kernels (functors)
- A node in the graph evaluates one or more temporary **fields (memory for flexibility)**
- Runtime DAG construction of graph
- Supports rapid development, separation of concerns and extensibility.
- Achieves flexible multiphysics assembly
- Leverages Sacado scalar types for non-invasive Jacobian, Hessian, …
- Combine kernels for performance



DAG-Based Assembly → flexibility

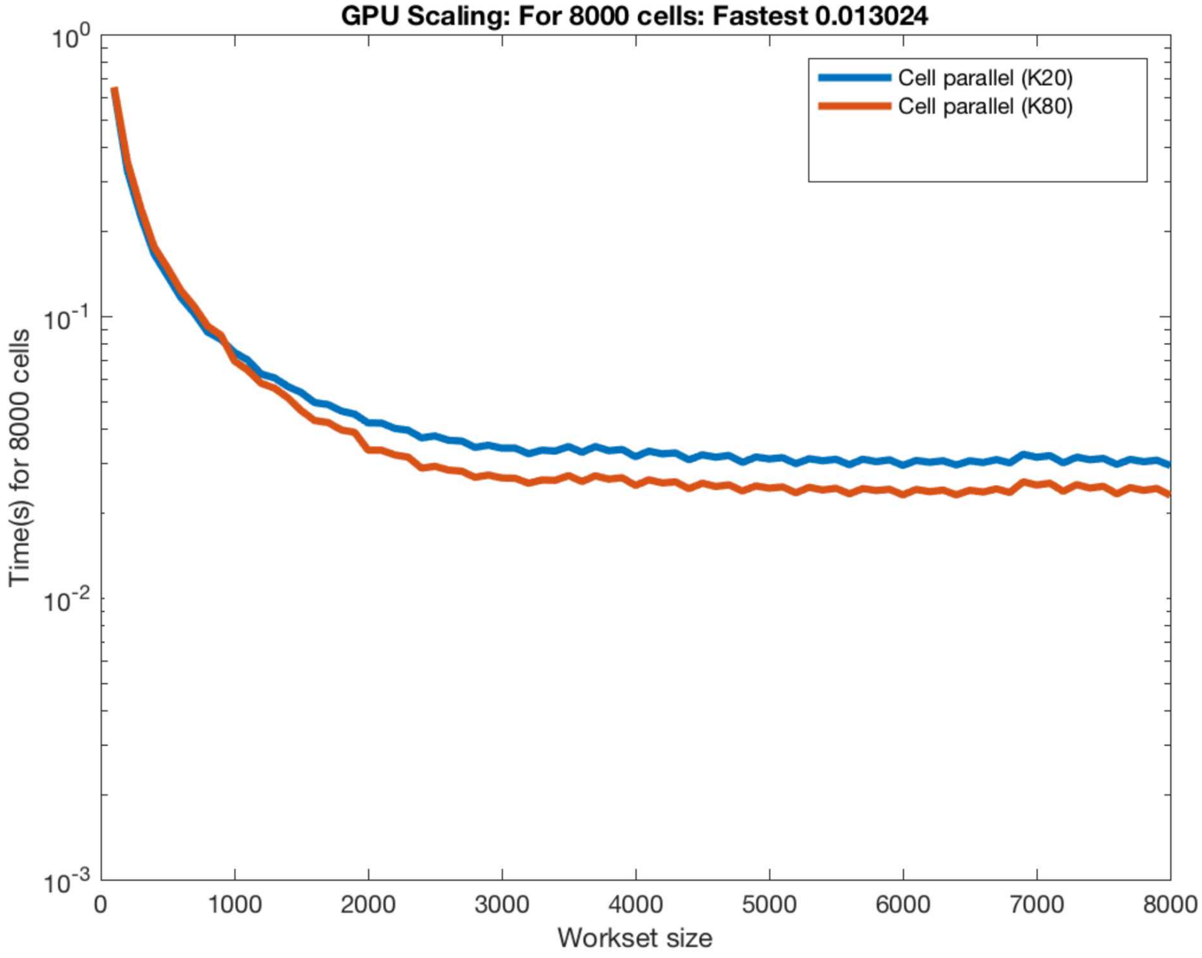
Initial Port for Jacobian Assembly

- 2016 Milestone to demonstrate the "ecosystem"
- 16K elements
- Flat/Single level data parallelism (loop over cells)
- Basic MPI (no thread spec.)



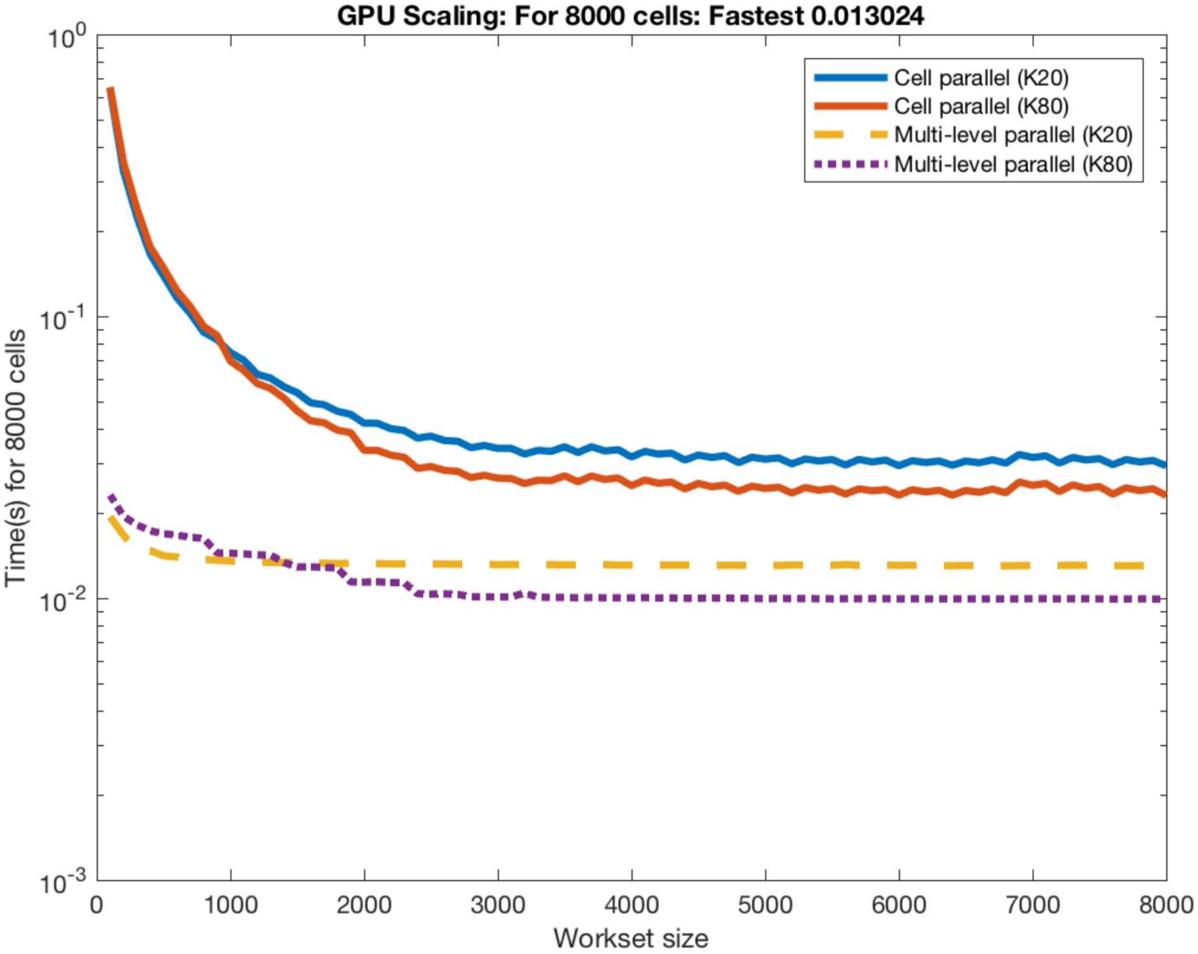
Single CFD Kernel GPU Performance Assessment

- Single level parallelism is insufficient
- Does not expose enough parallelism



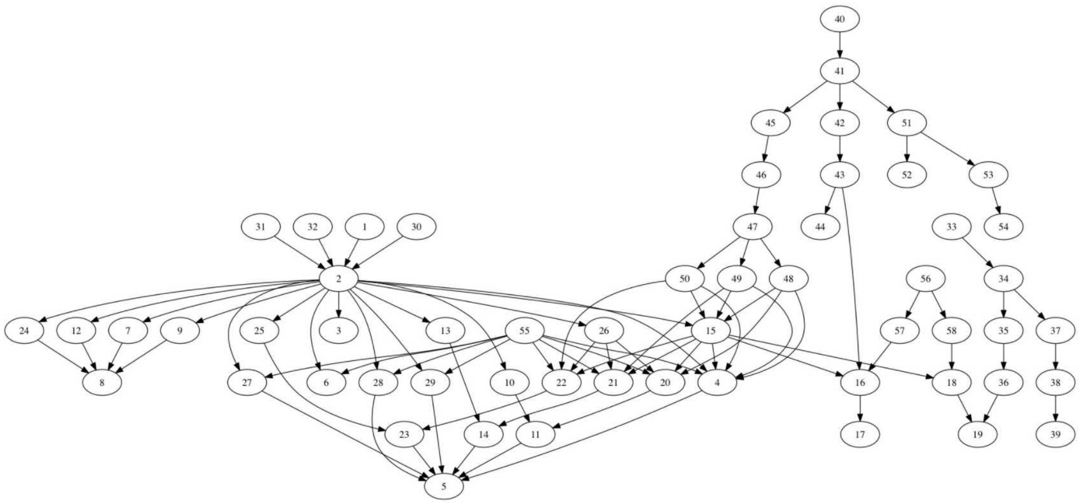
Single CFD Kernel GPU Performance Assessment

- Single level parallelism is insufficient
- Does not expose enough parallelism
- 3-level hierarchical parallelism shows significant improvement
- Hand coded sensitivity array outside libraries
- ***Key is to parallelize (vectorize) over FAD derivative dimension***



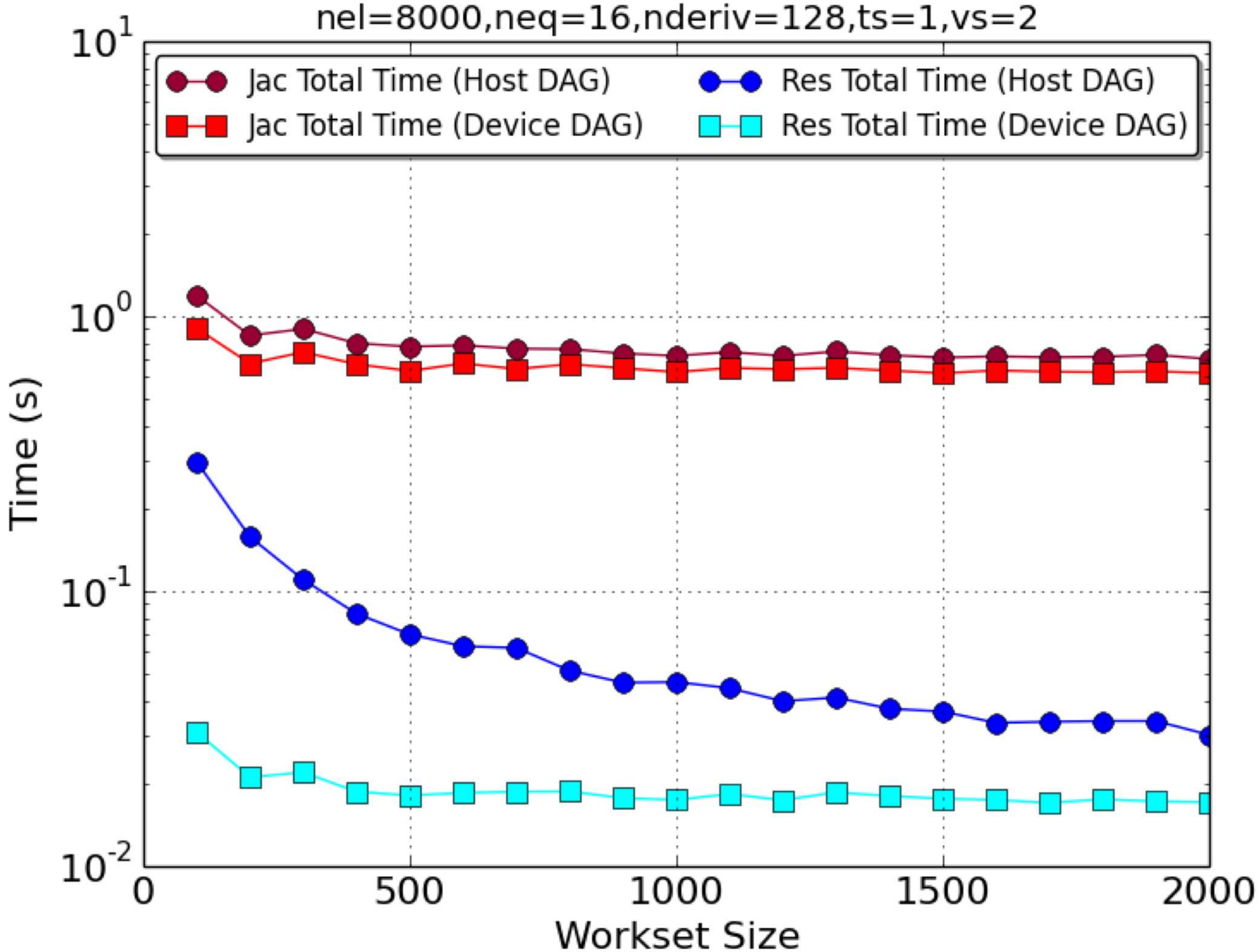
Host vs Device DAG

- **Host DAG:**
  - Each node in DAG launches its own device kernel via parallel_for from host
- **Device DAG:**
  - Single parallel_for for entire DAG
  - Goal: keep values in cache for next functor evaluation
- Device DAG implementation:
  - Need a virtual function call to run through a runtime generated list of functors
  - Copy all functors to device and instantiate
  - Requires relocatable device code (RDC) for CUDA



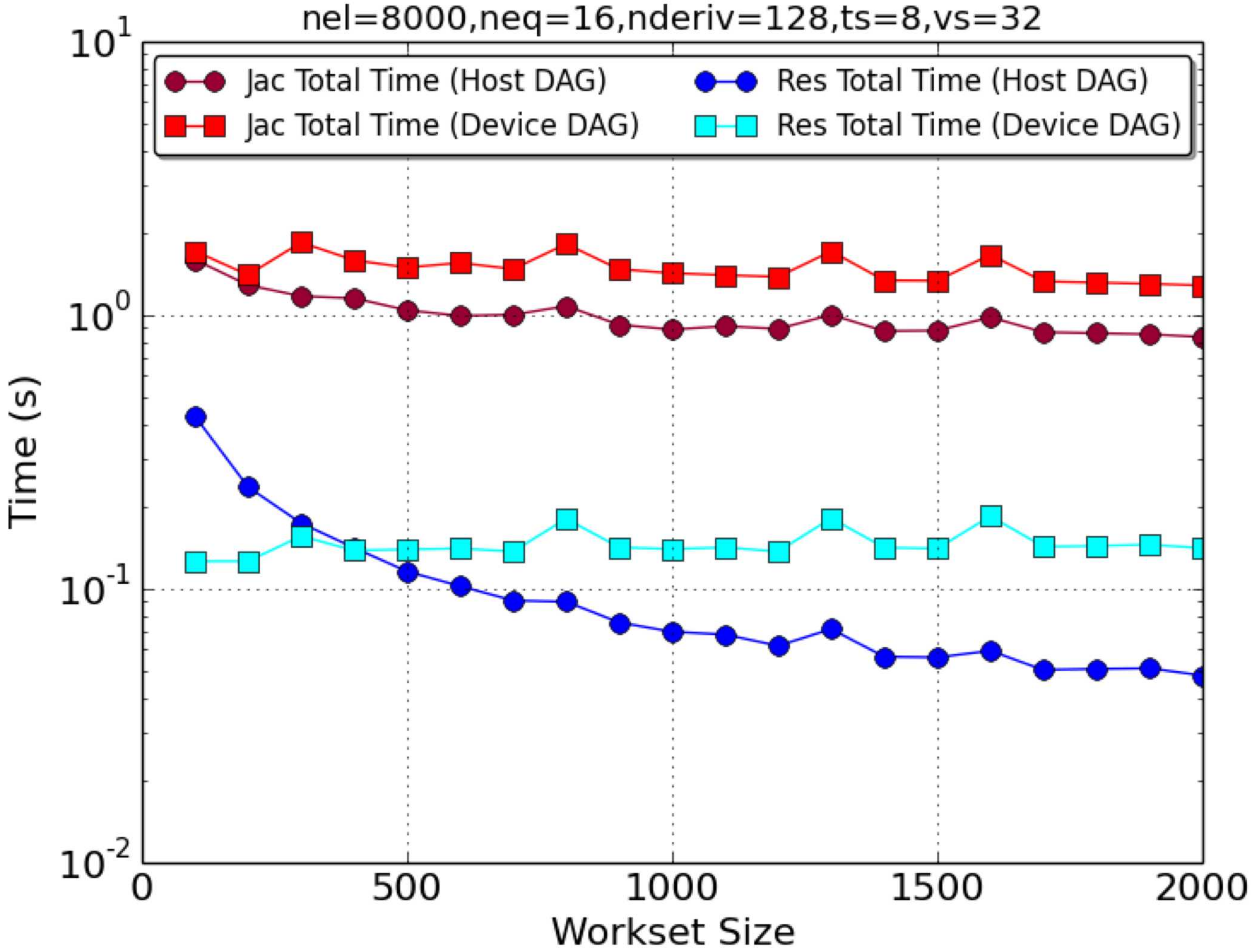
```
template<typename Traits>
struct RunDeviceDag {

  Kokkos::View<PHX::DeviceEvaluatorPtr<Traits>*,PHX::Device> evaluators_;

  ...

  KOKKOS_INLINE_FUNCTION
  void operator()(const TeamPolicy<exec_space>::member_type& team) const
  {
    const int num_evaluators = static_cast<int>(evaluators_.extent(0));
    for (int e=0; e < num_evaluators; ++e) {
      evaluators_(e).ptr->prepareForRecompute(team,data_);
      evaluators_(e).ptr->evaluate(team,data_);

    }
  }

};
```

Host vs Device DAG Performance, 16 Equations



- **OpenMP on Broadwell** node, team size=1, vector size = 2
- Performance gains for residual (significant) and Jacobian (minor)

Host vs Device DAG Performance, 16 Equations



- CUDA P100, team size=8, vector size = 32, 128 derivatives
- Significant performance loss

Conclusions

- Progress towards a hybrid code
  - Developing new set of codes for Fluid and PIC
  - Verification test suite for individual codes in place
  - Initial coupling of codes performed
  - Getting a feel for initial test problems for coupled simulation
- Performance portability and scalability assessment underway
  - PIC shows excellent strong and weak scaling
  - Fluid assembly shows good scaling
  - Preconditioners and solvers are being assessed
- Multiphysics heterogeneity
  - DAG Assembly provides flexible environment and removes fragile logic
  - AD is essential to prevent combinatorial explosion of code for sensitivities
  - Hybrid parallelism essential for AD tools on next-gen architectures

Extra Slides

Multi-fluid plasma model

- Continuity equation:

$$\partial_t \rho_\alpha + \nabla \cdot (\rho_\alpha \boldsymbol{u}_\alpha) = S_\alpha$$

Each species α is represented by a separate density ρ, momentum $\rho\boldsymbol{u}$, and isotropic energy ϵ.

- Momentum equation:

$$\partial_t(\rho_\alpha \boldsymbol{u}_\alpha) + \nabla \cdot (\rho_\alpha \boldsymbol{u}_\alpha \otimes \boldsymbol{u}_\alpha + \boldsymbol{P}_\alpha) = \frac{q_\alpha}{m_\alpha}\rho_\alpha(\boldsymbol{E} + \boldsymbol{u}_\alpha \times \boldsymbol{B}) + \boldsymbol{R}_\alpha + \boldsymbol{u}_\alpha S_\alpha$$

- Energy equation:

$$\partial_t \epsilon_\alpha + \nabla \cdot (\boldsymbol{u}_\alpha \cdot (\epsilon_\alpha \boldsymbol{I} + \boldsymbol{P}_\alpha) + \boldsymbol{q}_\alpha) = \frac{q_\alpha}{m_\alpha}\rho_\alpha \boldsymbol{u}_\alpha \cdot \boldsymbol{E} + Q_\alpha + \boldsymbol{u}_\alpha \cdot \boldsymbol{R}_\alpha + \frac{1}{2}\boldsymbol{u}_\alpha^2 S_\alpha$$

- Ampere's Law:

$$\partial_t \boldsymbol{E} - c^2 \nabla \times \boldsymbol{B} = -\frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\rho_\alpha \boldsymbol{u}_\alpha$$

Spatial operators are discretized using a finite element method.

- Faraday's Law:

$$\partial_t \boldsymbol{B} + \nabla \times \boldsymbol{E} = 0$$

Fluid
Electromagnetic
Inter-fluid

IMEX time integration

- IMEX gives a framework for splitting the model up into implicit and explicit terms:
  - Explicit for slow, non-stiff terms
  - Implicit for fast, stiff terms

Implicit tableau

$$\begin{array}{c|c} c & A \\ \hline & b^t \end{array}$$

Explicit tableau

$$\begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^t \end{array}$$

$$\partial_t u = f(u,t) + g(u,t)$$

$$u^{(i)} = u^n + \Delta t \sum_{j=0}^{j<i} \hat{A}_{ij} f\left(u^{(j)}, t_n + \hat{c}_j \Delta t\right) + \Delta t \sum_{j=0}^{j\leq i} A_{ij} g\left(u^{(j)}, t_n + c_j \Delta t\right)$$

$$u^{n+1} = u^n + \Delta t \sum_{i=0}^{i<s} \hat{b}_i f\left(u^{(i)}, t_n + \hat{c}_i \Delta t\right) + \Delta t \sum_{i=0}^{i\leq s} b_i g\left(u^{(i)}, t_n + c_i \Delta t\right)$$

- **Objective**: Combine the advantages of implicit and explicit solvers.
  - Take advantage of expensive implicit solver to overstep fast scales, and explicit solver to resolve slow scales.

IMEX splitting for CG

$$\partial_t \rho_\alpha + \boldsymbol{u}_\alpha \cdot \nabla \rho_\alpha = -\rho_\alpha \nabla \cdot \boldsymbol{u}_\alpha$$

$$u_\alpha < \frac{\Delta x}{\Delta t}$$

Each operator is associated with one or more plasma scales, which are grouped by color representing their approximate explicit stability limits.

$$\partial_t \boldsymbol{u}_\alpha + \boldsymbol{u}_\alpha \cdot \nabla \boldsymbol{u}_\alpha = -\boldsymbol{u}_\alpha \nabla \cdot \boldsymbol{u}_\alpha - \frac{1}{\rho_\alpha} \nabla P_\alpha + \frac{1}{\rho_\alpha} \nabla \cdot \left(\mu_\alpha \left(\nabla \boldsymbol{u}_\alpha + \nabla \boldsymbol{u}_\alpha^T - \frac{2}{3} \boldsymbol{I} \nabla \cdot \boldsymbol{u}_\alpha \right) \right)$$

$$u_\alpha < \frac{\Delta x}{\Delta t} \qquad v_{s\alpha} < \frac{\Delta x}{\Delta t} \qquad \upsilon_\alpha < \frac{\Delta x^2}{\Delta t}$$

$$+ \frac{q_\alpha}{m_\alpha} \boldsymbol{E} + \frac{q_\alpha}{m_\alpha} \boldsymbol{u}_\alpha \times \boldsymbol{B} - \sum_\beta \nu_{\alpha\beta} \left(\boldsymbol{u}_\alpha - \boldsymbol{u}_\beta \right)$$

$$\omega_{p\alpha} \Delta t < 1 \qquad \omega_{c\alpha} \Delta t < 1 \qquad \nu_{\alpha\beta} \Delta t < 1$$

$$\partial_t P_\alpha + \boldsymbol{u}_\alpha \cdot \nabla P_\alpha = -\gamma P_\alpha \nabla \cdot \boldsymbol{u}_\alpha + \nabla \cdot \left((\gamma - 1) k_\alpha \nabla T_\alpha \right) - \sum_\beta \frac{(\gamma - 1) \nu_{\alpha\beta} \rho_\alpha}{m_\alpha + m_\beta} \left(3 \left(T_\alpha - T_\beta \right) - m_\beta \left(\boldsymbol{u}_\alpha - \boldsymbol{u}_\beta \right)^2 \right)$$

$$u_\alpha < \frac{\Delta x}{\Delta t} \qquad \kappa_\alpha < \frac{\Delta x^2}{\Delta t} \qquad \nu_{\alpha\beta} \Delta t < 1$$

$$\partial_t \boldsymbol{E} - c^2 \nabla \times \boldsymbol{B} = -\frac{1}{\epsilon_0} \sum_\alpha \frac{q_\alpha}{m_\alpha} \rho_\alpha \boldsymbol{u}_\alpha$$

$$c < \frac{\Delta x}{\Delta t} \qquad \omega_{p\alpha} \Delta t < 1$$

$$\partial_t \boldsymbol{B} + \nabla \times \boldsymbol{E} = 0$$

For IMEX-CG each operator can be moved between implicit and explicit evaluation depending on the explicit stability limits.

Compatible discretization for EM

- A physics compatible finite element discretization is used to enforce the divergence constraints for the electric and magnetic fields.
- Fluids are represented by an **HGrad** (node) basis $\rho \in V_{\nabla}$.
- The electric field is represented by an **HCurl** (edge) vector basis $\mathbf{E} \in \boldsymbol{V}_{\nabla\times}$.
- The magnetic field is represented by an **HDiv** (face) vector basis $\mathbf{B} \in \boldsymbol{V}_{\nabla\cdot}$.
- Compatibility is defined by the discrete preservation of the **De Rham Complex**:

$$\nabla \phi_{\nabla} \in \boldsymbol{V}_{\nabla\times} \longrightarrow \nabla\times\boldsymbol{\phi}_{\nabla\times} \in \boldsymbol{V}_{\nabla\cdot} \longrightarrow \nabla\cdot\boldsymbol{\phi}_{\nabla\cdot} \in V_{\mathrm{L}_2}$$

- For Faraday's law, we choose a basis for the electric field such that its curl is fully represented by the basis used by the magnetic field.

$$\partial_t \boldsymbol{B} + \nabla\times\boldsymbol{E} = 0 \qquad \nabla\cdot\boldsymbol{B} = 0$$

- Since the curl of the electric field is 'globally continuous' w.r.t. a divergence operator, the divergence of that curl is zero over the domain:

$$\nabla\cdot(\partial_t \boldsymbol{B} + \nabla\times\boldsymbol{E}) = \partial_t(\nabla\cdot\boldsymbol{B}) + \nabla\cdot\nabla\times\boldsymbol{E} = \partial_t(\nabla\cdot\boldsymbol{B}) + \sum_i E_i \underbrace{\nabla\cdot\nabla\times\boldsymbol{\phi}^i_{\nabla\times}}_{0} = \partial_t(\nabla\cdot\boldsymbol{B}) = 0$$

- **Result**: The curl operator does not add divergence errors to the magnetic field

Satisfying Gauss' laws in plasmas

- **Goal**: Solve plasma-coupled Maxwell's equations and satisfy a divergence constraint:

$$\partial_t \boldsymbol{E} - c^2 \nabla \times \boldsymbol{B} = -\frac{1}{\epsilon_0} \boldsymbol{j} \qquad \partial_t \rho_c + \nabla \cdot \boldsymbol{j} = 0$$

$$\nabla \cdot \boldsymbol{E} = \frac{1}{\epsilon_0} \rho_c$$

- In the **strong, non-discretized form**:

$$\nabla \cdot \left(\partial_t \boldsymbol{E} + \frac{1}{\epsilon_0} \boldsymbol{j} - c^2 \nabla \times \boldsymbol{B} \right) = \partial_t \nabla \cdot \boldsymbol{E} + \frac{1}{\epsilon_0} \nabla \cdot \boldsymbol{j} = \partial_t \left(\nabla \cdot \boldsymbol{E} - \frac{1}{\epsilon_0} \rho_c \right) = 0$$

- In the **weak form**: Choose a basis that supports the divergence constraint as HCurl does not support the divergence operation:

$$\int_\Omega \left(\partial_t \boldsymbol{E} - c^2 \nabla \times \boldsymbol{B} + \frac{1}{\epsilon_0} \boldsymbol{j} \right) \cdot \nabla \phi_\nabla \, dV = \int_\Omega \left(\partial_t \boldsymbol{E} \cdot \nabla \phi_\nabla + \frac{1}{\epsilon_0} \nabla \cdot \boldsymbol{j} \, \phi_\nabla \right) dV + c^2 \int_\Omega \boldsymbol{B} \cdot \underbrace{\nabla \times \nabla \phi_\nabla}_{0} dV$$

$$= \int_\Omega \partial_t \left(\boldsymbol{E} \cdot \nabla \phi_\nabla - \frac{1}{\epsilon_0} \rho_c \, \phi_\nabla \right) dV = 0$$

- Assumes that continuity equation is weakly satisfied:

$$\int_\Omega (\partial_t \rho_c - \nabla \cdot \boldsymbol{j}) \phi_\nabla \, dV = \int_\Omega (\partial_t \rho_c \phi_\nabla + \boldsymbol{j} \cdot \nabla \phi_\nabla) dV = 0 \rightarrow \int_\Omega \partial_t \rho_c \phi_\nabla \, dV = -\int_\Omega \boldsymbol{j} \cdot \nabla \phi_\nabla \, dV$$

Discontinuous Galerkin method

- Discontinuous Galerkin FEM does not assume a globally continuous test function:

Weak form

$$\int_{\Omega} \phi \partial_t u \, dV + \int_{\Omega} \phi \, \nabla \cdot \boldsymbol{f} \, dV - \int_{\Omega} \phi s \, dV = 0$$

Break into elements $\mathrm{K} \in \Omega$ with discontinuous element test function ϕ_i^{K}

$$\sum_{K} \left[\int_{\mathrm{K}} \phi_i^K \partial_t u \, dV + \int_{\mathrm{K}} \phi_i^K \nabla \cdot \boldsymbol{f} dV - \int_{\mathrm{K}} \phi_i^K s \, dV \right] = 0$$

Apply divergence theorem to flux integral

$$\int_{\mathrm{K}} \phi_i^K \partial_t u \, dV + \oint_{\partial \mathrm{K}} \phi_i^K \hat{\boldsymbol{n}} \cdot \boldsymbol{f} \, dS - \int_{\mathrm{K}} \boldsymbol{f} \cdot \nabla \phi_i^K dV - \int_{\mathrm{K}} \phi_i^K s \, dV = 0$$

- **Consistency**: Fluxes must be single valued on interfaces between elements.
  - **Numerical Flux**: Solution to Riemann problem to generate consistent flux on interfaces.

Drekar: Software Infrastructure Pushing Limits of Component Integration

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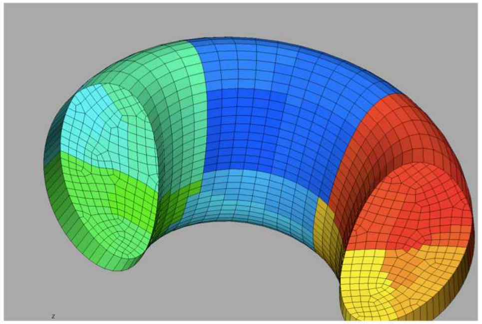
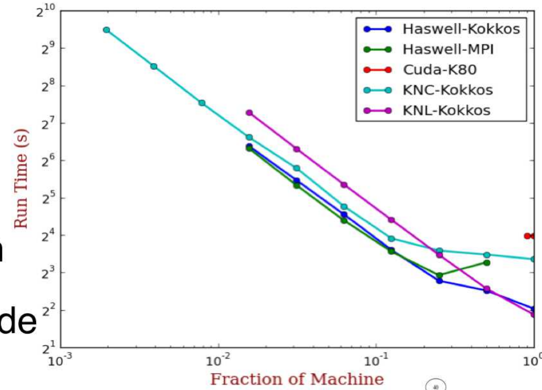
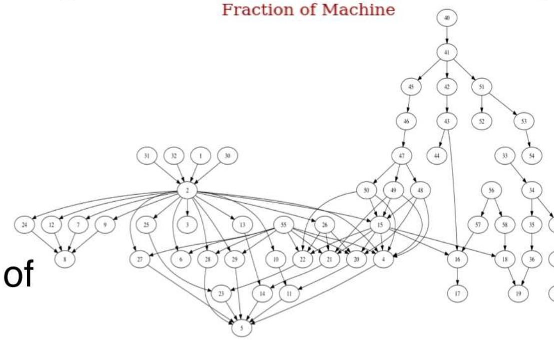
- 1st-5th order fully-implicit and implicit / explicit (IMEX) [Tempus]
- 2D & 3D Unstructured finite elements (FE), HEX and Tet with nodal FE and physics compatible (node, edge, face, …) methods [Drekar, Intrepid]
- Fully coupled globalized Newton-Krylov (NK) solver
  - Residuals are Programed and Automatic Differentiation (AD generates Jacobian for NK, Sensitivities, Adjoints, etc. [SACADO]
  - GMRES Krylov solvers using compressed sparse row (CSR)
  - Scalable Preconditioners: Fully-coupled system AMG, Physics-based block preconditioners with AMG [ML, Muelu, Teko]



- Software architecture:
  - Massively parallel R&D code:
    - MPI version demonstrated weak scaling to 1M cores; sub-block solvers to 1.6M cores
    - MPI+X. Employs Trilinos/Kokkos performance portability abstraction layer interface. FE assembly and linear algebra gather / scatter to CSR global distributed sparse matrix kernels, demonstrated on a wide variation of advanced node architectures (see figure). Solvers in process.
    - Asynchronous many Tasking (AMT) possible in future with DAG [Phalanx]





  - Solvers/Linear Alg. tools based on Trilinos packages (Aztec/Belos, ML/Muelu, Epetra/TPetra, Teko, etc.)
  - Template-based generic programming with automatic differentiation [AD] of FE weak forms (Sacado)
  - Core FE assembly capability (Panzer, Intrepid, Kokkos)
  - Asynchronous dependency graphs (DAG) used for multiphysics complexity management and possible AMT capability (Phalanx)

[Drekar: Shadid, Pawlowski, Cyr, Phillips, Lin, Smith, Conde, **Mabuza, Miller]**

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