Algorithms for Enabling Long-Time-Scale Hybrid Fluid-Kinetic Plasma Simulations

Presenting: A. Kish

M. Lavell, R. Masti, A. Sexton, J. G. Shaw,
and Prof. A. B. Sefkow

TriForce Group for Multiphysics Modeling
University of Rochester
Laboratory for Laser Energetics

APS-DPP 2022
Spokane, WA
Mon, Oct. 17th, 2022

Acknowledgements & Collaborators

This material is based upon work supported by the US DOE ARPA-E under Award No. DE-AR0001272, US DOE OFES under Award No. DE-SC0017951, and US DOE NNSA under Award No. DE-NA0003856.

E. Evans, S. Thomas, M. Paluszek, C. Galea, S. Punjabi-Vinoth, Prof. S. Cohen (PPPL, PSS)

Multiple packages enabling long-time-scale simulation for the TriForce Library for Integrated Numerical Kinetics have been implemented

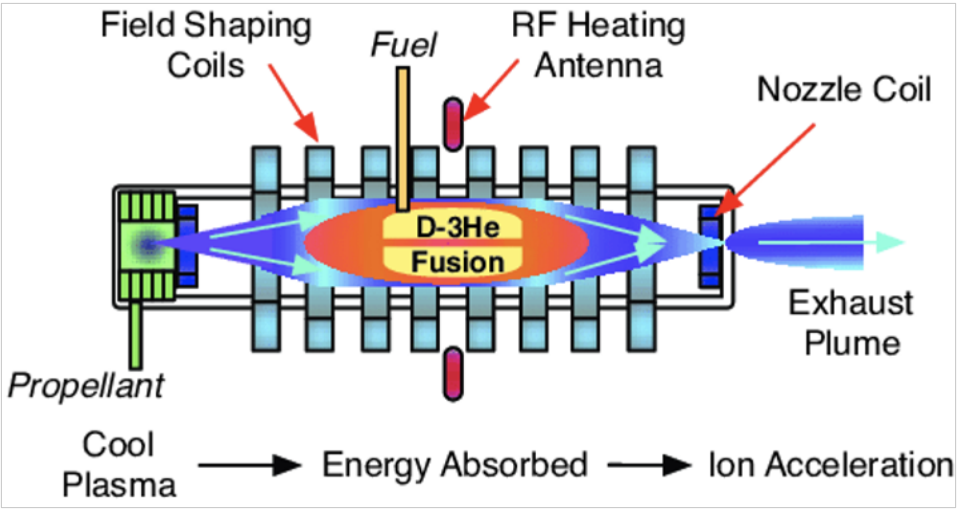
- **The "standard" explicit particle-in-cell (PIC) method requires careful monitoring of conserved quantities**

- **Errors in conserved quantities, as well as statistical noise, cause unphysical behavior and the build-up of errors over long-time-scales**

- **Algorithms for maintaining conservation of charge and energy/momentum, as well as particle statistics, have been implemented in TriForce's Library for Integrated Numerical Kinetics (TF-Link)**

- **These algorithms are being used toward higher-fidelity simulations of the Princeton Field-Reversed Configuration (pFRC)**

Obstacles to long-time-scale particle-in-cell (PIC) simulations



- Standard PIC schemes require careful monitoring of momentum, energy, and charge conservation
- Statistical noise due to low particle count can contribute to error
- Particle loss mechanisms include:
  - Surface absorption
  - Expansion into vacuum
  - Fusion
  - Recombination
- Particle gain mechanisms include:
  - Surface emission
  - Ionization

Figure adapted from: Thomas, S. J., Paluszek, M., Cohen, S., McGreivy, N., & Evans, E. (2017). Fusion-enabled pluto orbiter and Lander. In AIAA SPACE and Astronautics Forum and Exposition (p. 5276).

Where do conservation violations occur?

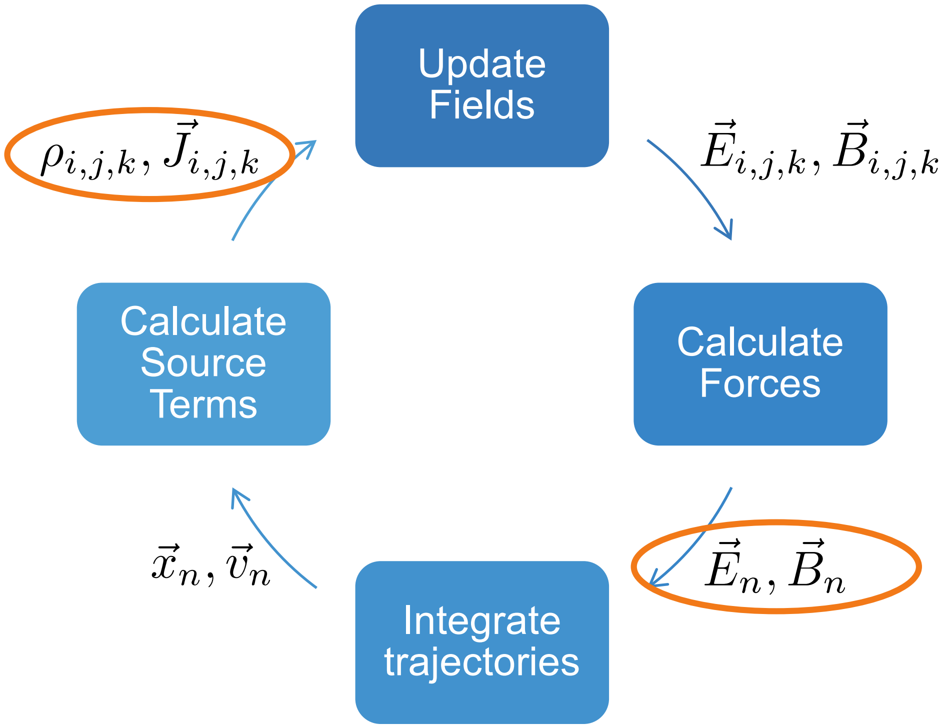


Figure 1: The basic structure of the particle-in-cell (PIC) method. i, j, k subscripts denote grid quantities, while n subscripts denote particle quantities.

Charge Conserving Algorithm

- **Because Gauss' law is not explicitly satisfied by the electromagnetic field solver, charge conservation must be built into the definition of current density**

$$\frac{\rho_{i,j,k}^{n+1} - \rho_{i,j,k}^{n}}{dt} + \frac{J_{i+1/2,j,k}^{(x)} - J_{i-1/2,j,k}^{(x)}}{dx} + \frac{J_{i,j+1/2,k}^{(y)} - J_{i,j-1/2,k}^{(y)}}{dy} + \frac{J_{i,j,k+1/2}^{(z)} - J_{i,j,k-1/2}^{(z)}}{dz} = 0$$

- **TF-Link implements Esirkepov's* definition of current density, which is derived directly from the charge continuity equation**

$$J_{i+1/2,j,k}^{(x)} - J_{i-1/2,j,k}^{(x)} = -q\frac{dx}{dt}W_{i,j,k}^{(x)}$$

$$W_{i,j,k}^{(x)} \sim S_{i,j,k}\left(\vec{x}_n + \Delta x\right) - S_{i,j,k}\left(\vec{x}_n\right)$$

***T. Z. Esirkepov, "Exact charge conservation scheme for Particle-in-Cell simulation with an arbitrary form-factor," Computer Physics Communications 135, 144–153 (2001).**

Conservation of Momentum/Energy

- **TF-Link implements both the standard momentum-conserving algorithm, as well as Lewis'[†] energy-conserving algorithm**

- **Lewis' algorithm is derived from variational principles and conserves energy intrinsically**

$$F_n = -q_n \sum_i \phi_i \frac{\partial S_i(x_i)}{\partial x} = q_n E_n$$

$$\frac{1}{4\pi} \sum_i \phi_i \int dx \frac{\partial S_{i'}(x_n)}{\partial x} \frac{\partial S_i(x_n)}{\partial x} = q_n \sum_n S_i(x_n)$$

† H. R. Lewis, "Energy-conserving numerical approximations for vlasov plasmas," Journal of Computational Physics 6 (1970).

Maintaining Statistical Significance

- **Many physical processes of interest can inflate/deflate particle counts**
  - **Processes like expansion into vacuum or particle absorption/fusion may deflate particle counts**
  - **Processes like ionization or surface emission may inflate particle counts**

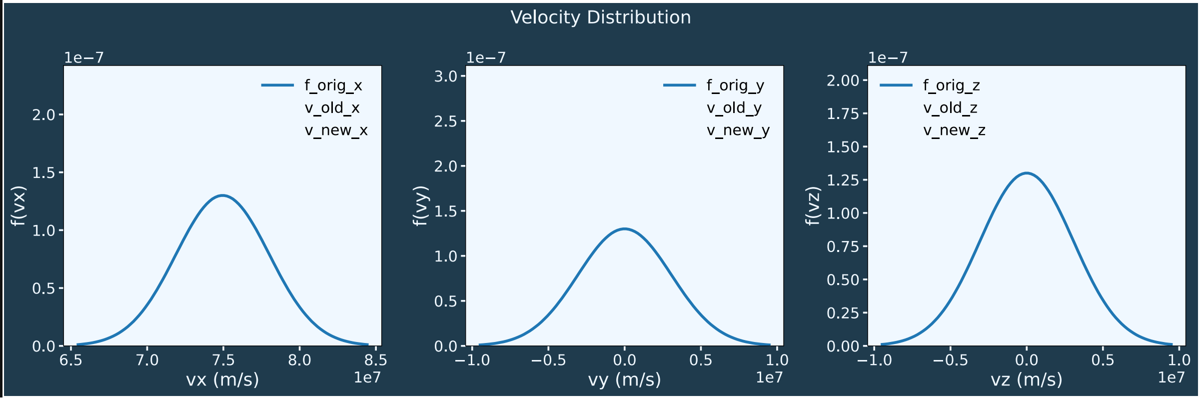
- **TF-Link implements an algorithm for 'adaptive particle management', first used in the LSP code*, to dynamically resample the cell-wise particle distribution and maintain consistent sample count**

*** D. R. Welch, T. C. Genoni, R. E. Clark, and D. V. Rose, "Adaptive particle management in a particle-in-cell code," Tech. Rep. SAND2007-1344J (Voss Scientific, 2007).**

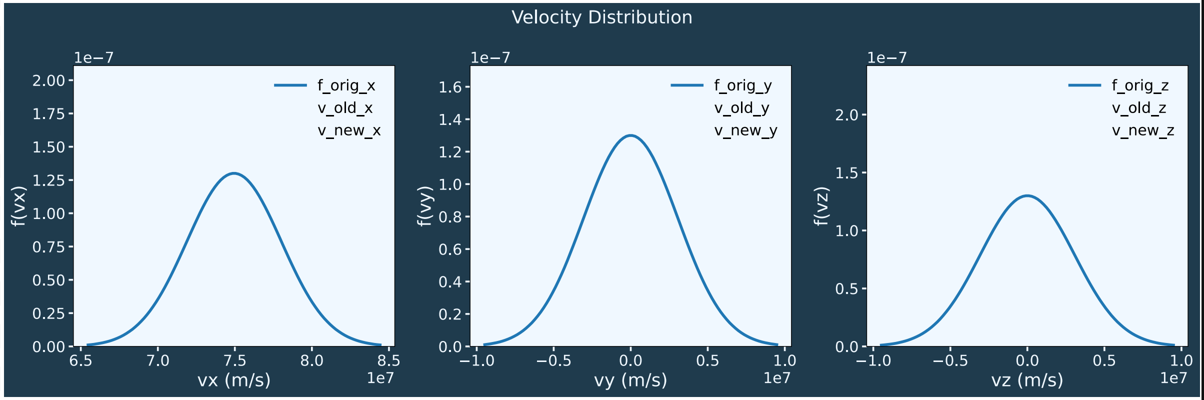
Adaptive Particle Management Examples

```
--------------- Pre APM Routine ---------------
PPC:  216

Total:
            Weight:  1.000e+19
          Momentum: ( 1.295e+00,  1.718e-05,  1.097e-05) kg*m/s
            Energy:  1.553e+09 J


--------------- Post APM Routine ---------------
PPC:  64
        (Change:  0.296 times)

Total:
            Weight:  1.0000e+19
               (Change:  0.0000e+00)

          Momentum: ( 1.2951e+00,  1.7184e-05,  1.0966e-05) kg*m/s
               (Change: -4.4409e-16, -1.6975e-18, -2.8460e-18 kg*m/s)

            Energy:  1.5529e+09 J
               (Change:  0.0000e+00 J [ 0.0000e+00 %])

 kT in: 2.063e+07 eV
kT out: 2.063e+07 eV
```

216 to 64 parts/cell



64 to 216 parts/cell




```
--------------- Pre APM Routine ---------------
PPC:  64

Total:
            Weight:  1.000e+19
          Momentum: ( 1.295e+00, -6.400e-07,  8.025e-06) kg*m/s
            Energy:  1.553e+09 J


--------------- Post APM Routine ---------------
PPC:  192
        (Change:  3.000 times)

Total:
            Weight:  1.0000e+19
               (Change:  0.0000e+00)

          Momentum: ( 1.2951e+00, -6.4002e-07,  8.0252e-06) kg*m/s
               (Change:  0.0000e+00, -3.5237e-19, -9.3241e-18 kg*m/s)

            Energy:  1.5529e+09 J
               (Change: -2.4983e+00 J [-1.6088e-07 %])

 kT in: 2.063e+07 eV
kT out: 2.063e+07 eV
```

Multiple packages enabling long-time-scale simulation for the TriForce Library for Integrated Numerical Kinetics (TF-Link) have been implemented

- **The "standard" explicit particle-in-cell (PIC) method requires careful monitoring of conserved quantities**
- **Errors in conserved quantities, as well as statistical noise, cause unphysical behavior and the build-up of errors over long-time-scales**
- **Algorithms for maintaining conservation of charge and energy/momentum, as well as particle statistics, have been implemented in TriForce's Library for Integrated Numerical Kinetics (TF-Link)**
- **These algorithms are being used toward higher-fidelity simulations of the Princeton Field-Reversed Configuration (pFRC)**

Future Work

- Implementation and testing of (semi-)implicit algorithms to address computational resource requirements
  - Implicit particle pushers capable of under-resolving the cyclotron frequency would enable fast simulations of highly-magnetized systems
  - *See Thursday morning's poster session for A. Sexton's work on explicit and implicit EM field solvers for TFLink (TP11.00049)*
- Improving APM performance with very-low initial particle counts
- Continued work toward simulations in support of current pFRC experiments, and design of future experiments (larger, higher density, larger magnetic field)