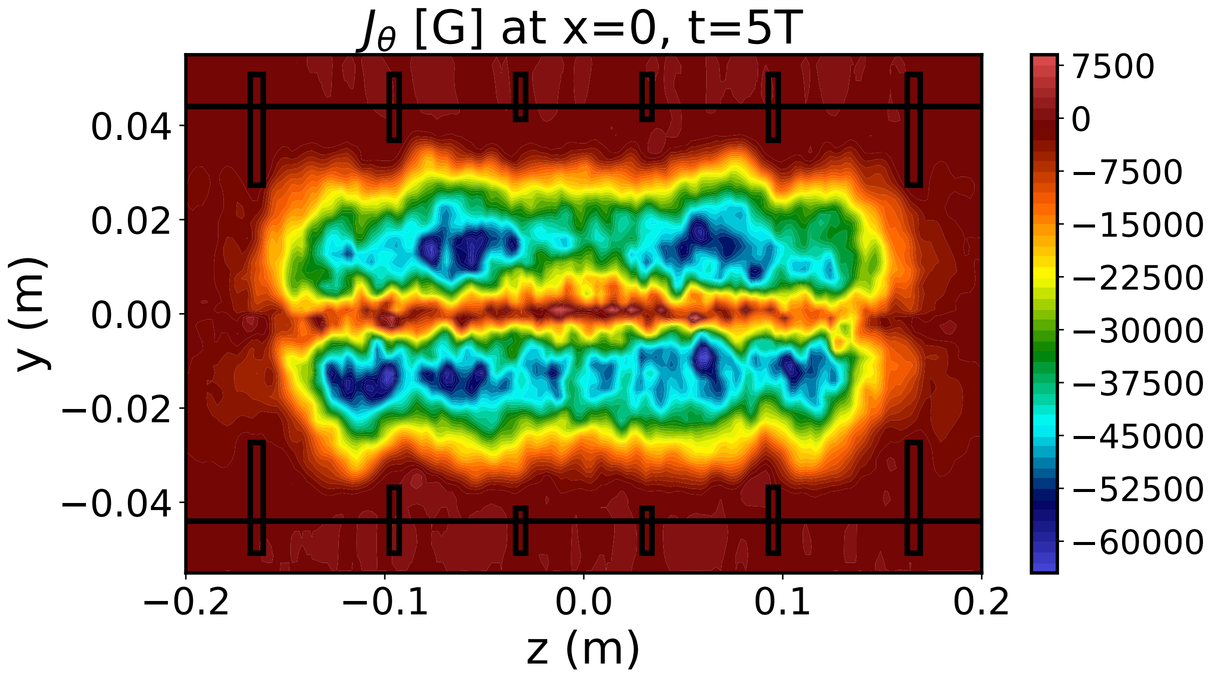
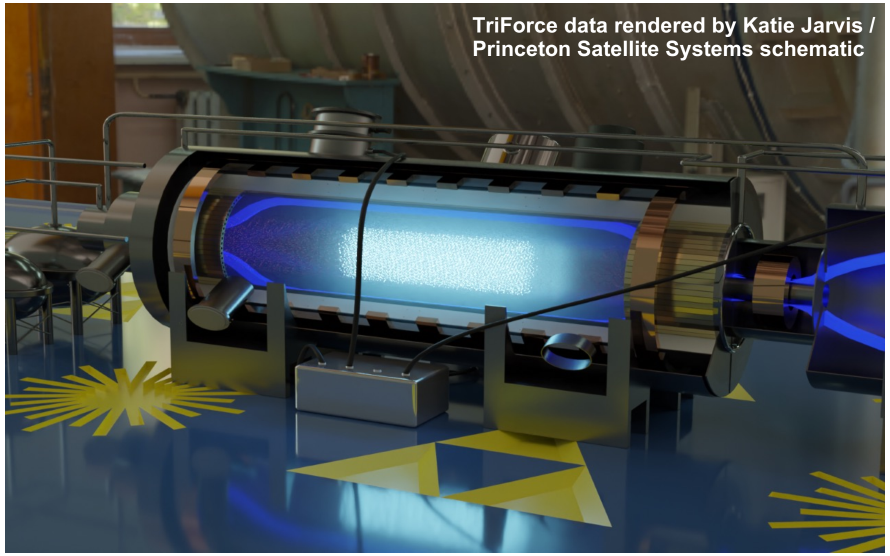
# Implementation and validation of collisions in a new PIC code




**Accurate scattering model required for simulating PFRC-1 heating and stability**

**M. J. Lavell**
**University of Rochester**
**Laboratory for Laser Energetics**
**APS DPP 2022**

# TriForce Center for Multiphysics Modeling Collaborators

A. Kish, A. Sexton, R. Masti, J. G. Shaw, A. Srinivasan, Prof. A. B. Sefkow (U of R)

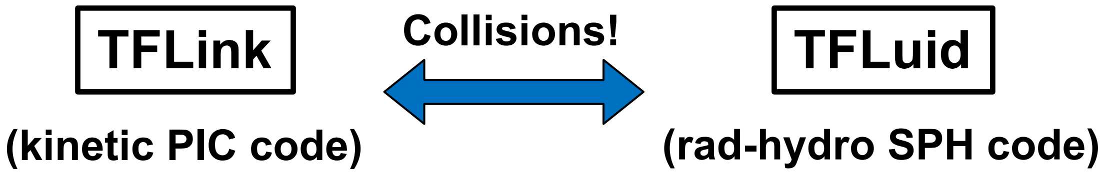
S. Thomas, M. Paluszek, C. Galea, E. Evans, S. Punjabi-Vinoth, Prof. S. Cohen (PPPL, PSS)

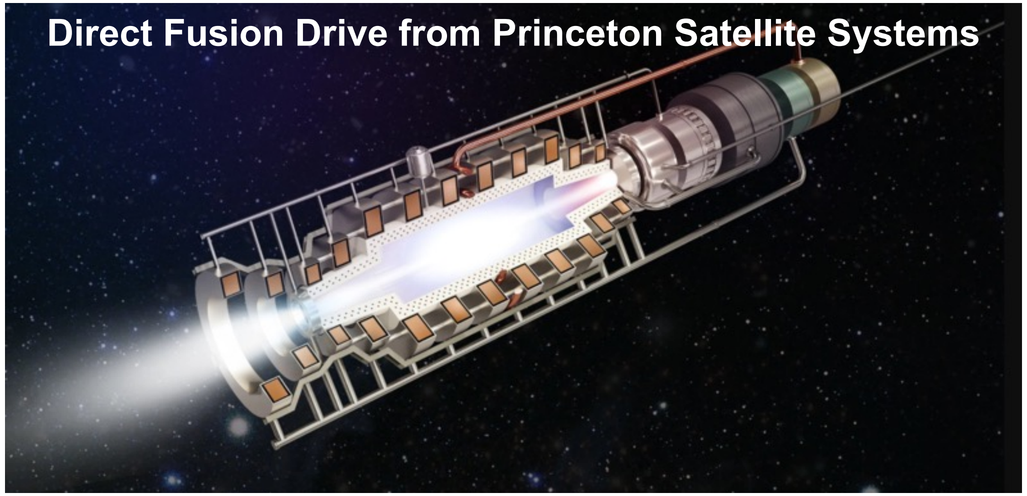
This material is based upon work supported by the U.S. DOE ARPA-E under Award No. DE-AR0001272, U.S. DOE OFES under Award No. DE-SC0017951, and U.S. DOE NNSA under Award No. DE-NA0003856.

# The goal of the TriForce Center for Multiphysics Modeling is to develop a simulation framework for studying fluids and plasmas in a wide range of environments

<u>**TriForce**</u>

- **Open source particle code for studying HED and fusion relevant environments**
- **Massively parallel, GPU accelerated**
- **Smoothly transition between coexisting fluid and kinetic descriptions**



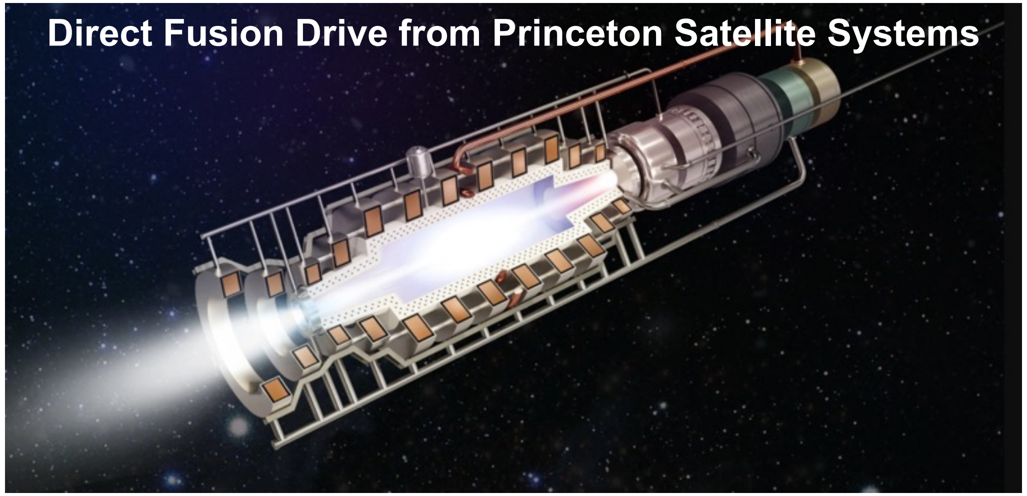



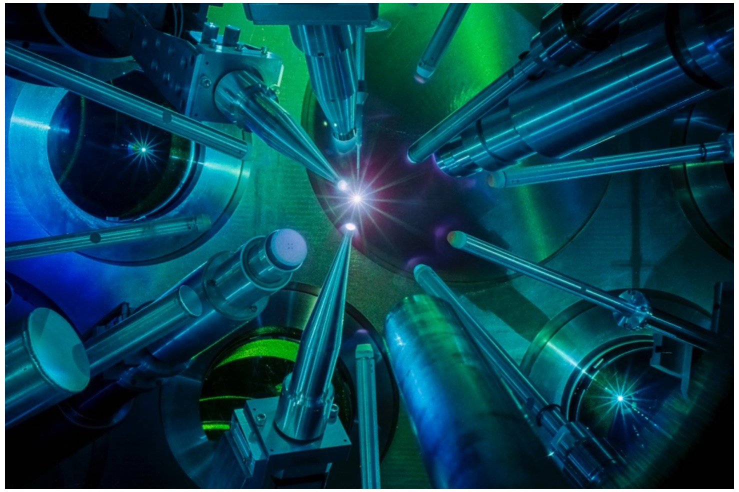
# The goal of the TriForce Center for Multiphysics Modeling is to develop a simulation framework for studying fluids and plasmas in a wide range of environments

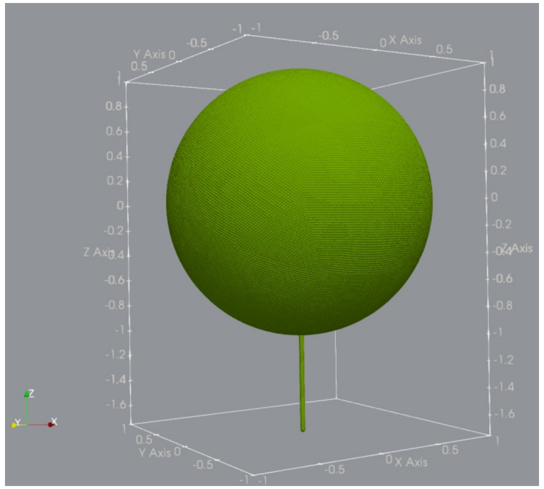
## TriForce

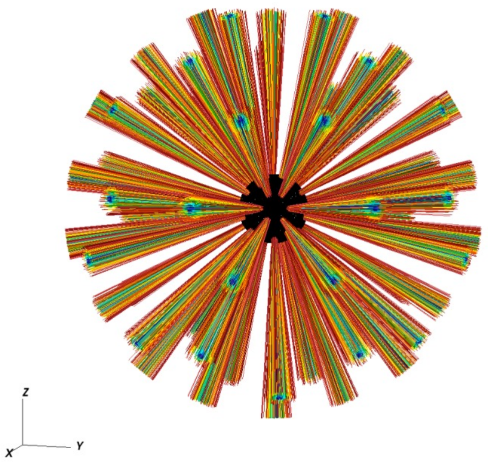
- Open source particle code for studying HED and fusion relevant environments
- Massively parallel, GPU accelerated
- Smoothly transition between coexisting fluid and kinetic descriptions

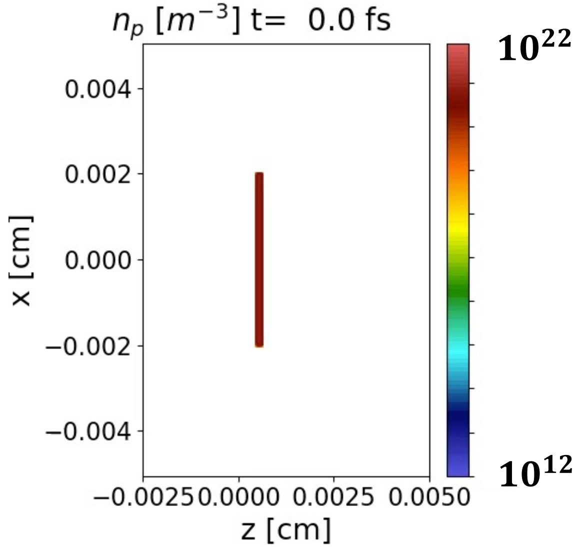
**TFLink** (kinetic PIC code) ⟷ **Collisions!** ⟷ **TFLuid** (rad-hydro SPH code)







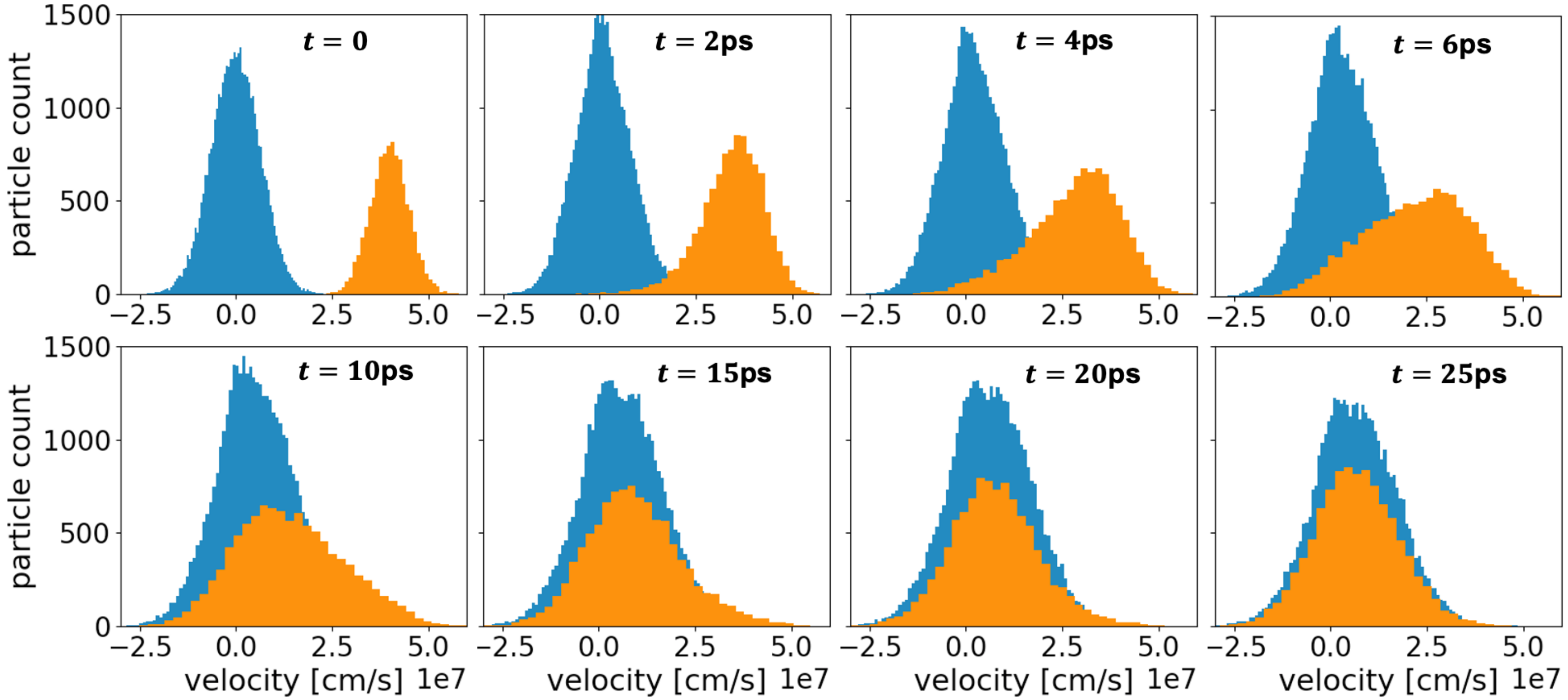


# PIC solves the Maxwell-Boltzmann system with operator splitting, allowing the particle push and collisions to be treated separately

- **Solve Maxwell-Boltzmann system by discretizing $f(x,v,t)$ onto a set of macroparticles**
- **Compute particle push (global fields) and collisions (particle-particle interactions) separately**

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{q}{m}\left(E + \frac{v \times B}{c}\right) \cdot \nabla_v f = \left(\frac{\partial f}{\partial t}\right)_c$$

$$f = \sum_i w_i \delta(x - x_i)\delta(v - v_i) \qquad w_i \sim \frac{nV_{cell}}{N_{ppc}}$$



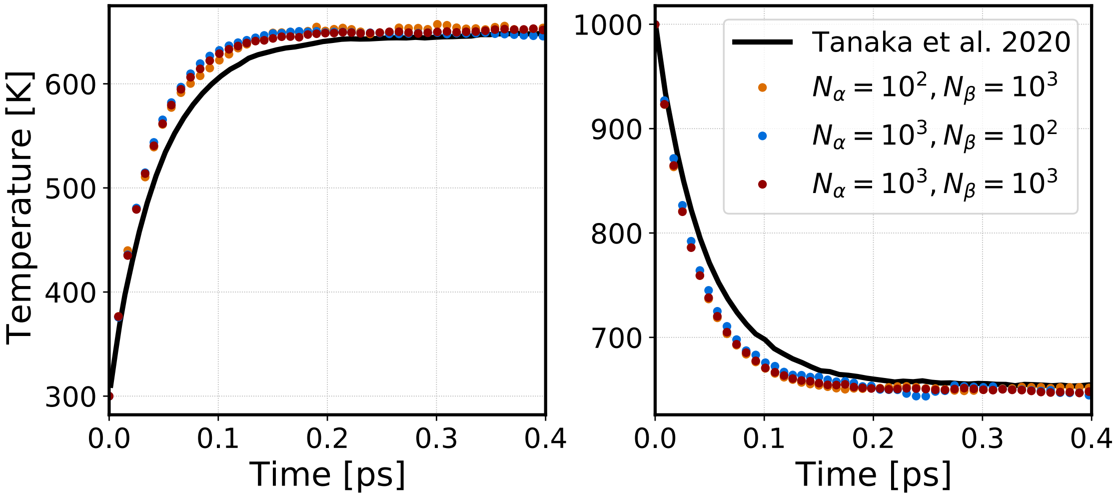
# In the binary Monte Carlo scattering model, particles are paired with a computational cell and perform a representative scatter for arbitrary distributions

- **Neutral collisions** - sample collision frequency

$$P_{\text{scatter}} = \nu \Delta t < 1$$

if $(U < P_{\text{scatter}})$ particles collide

**Two-temperature water mixture thermal relaxation**




† Higginson, D. P., Holod, I., & Link, A. (2020). *JCP*, *413*, 109450.
* Nanbu, K., & Yonemura, S. (1998). *JCP*, *145*(2), 639-654.
** Nanbu, K. (2000). *IEEE*, *28*(3), 971-990.
‡ Pérez, F., et al. (2012). *PoP*, *19*(8), 083104
\+ Takizuka, T., & Abe, H. (1977). *JCP*, *25*(3), 205-219.
* Tanaka, S., & Shimamura, K. (2020). *J. of Chemical Phys*, *153*(3), 034114.

# In the binary Monte Carlo scattering model, particles are paired with a computational cell and perform a representative scatter for arbitrary distributions

- **Neutral collisions** - sample collision frequency

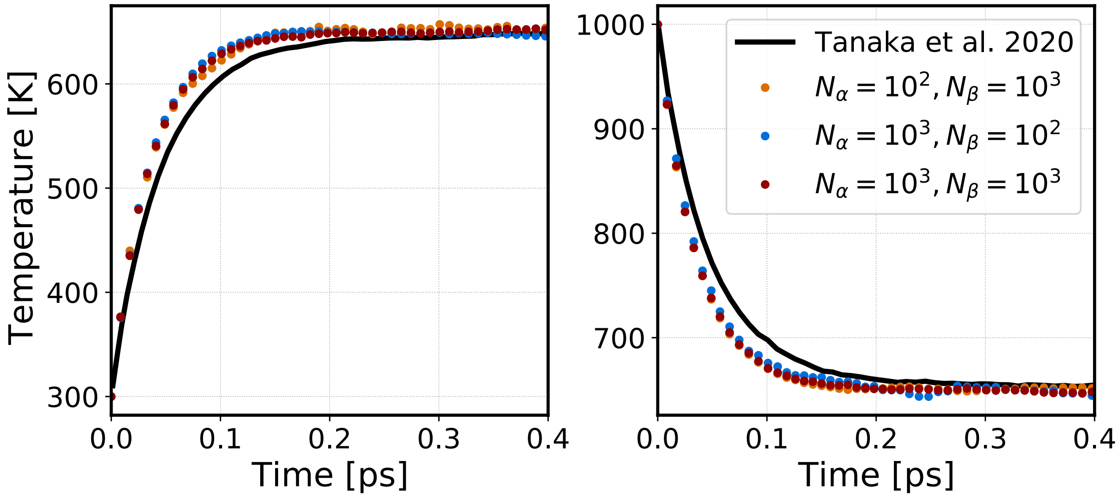
$$P_{\text{scatter}} = \nu\Delta t < 1$$

if $(U < P_{\text{scatter}})$ particles collide

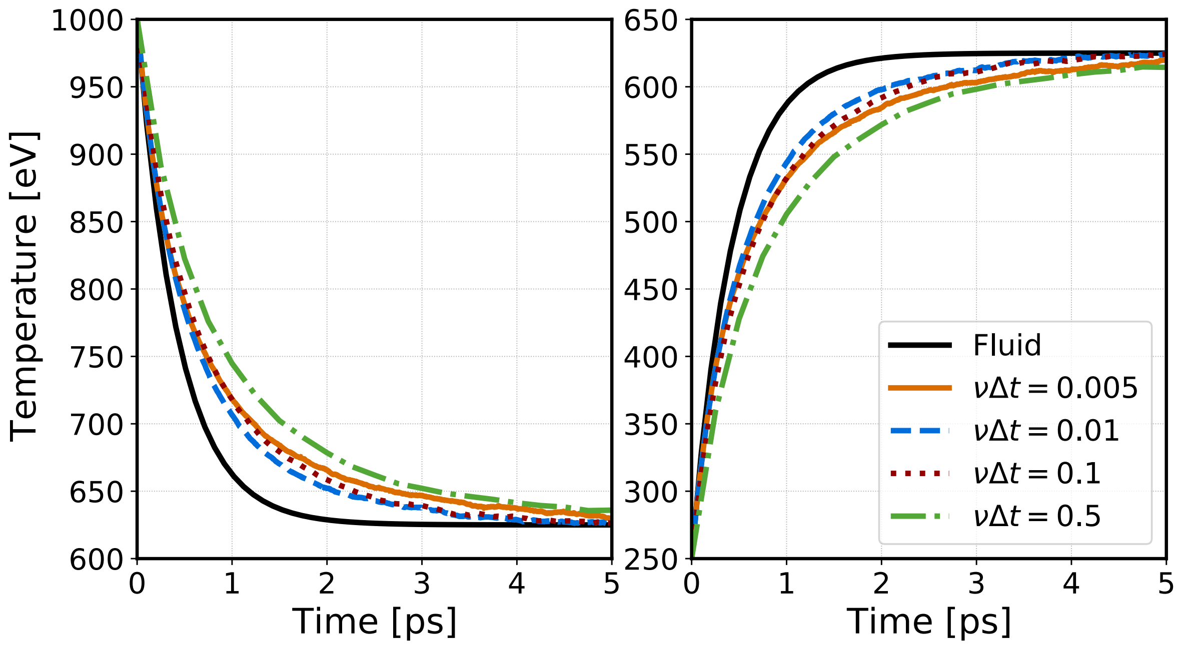
- **Coulomb collisions** - sample scattering distribution

$$\cos\theta = 1 + \frac{1}{A}\ln\left[1 - U_\theta\left(1 - e^{-2A}\right)\right] \qquad A = A(s) \sim 1/s \qquad s = \nu\Delta t$$

**Two-temperature water mixture thermal relaxation**




**Charged particle thermal relaxation**

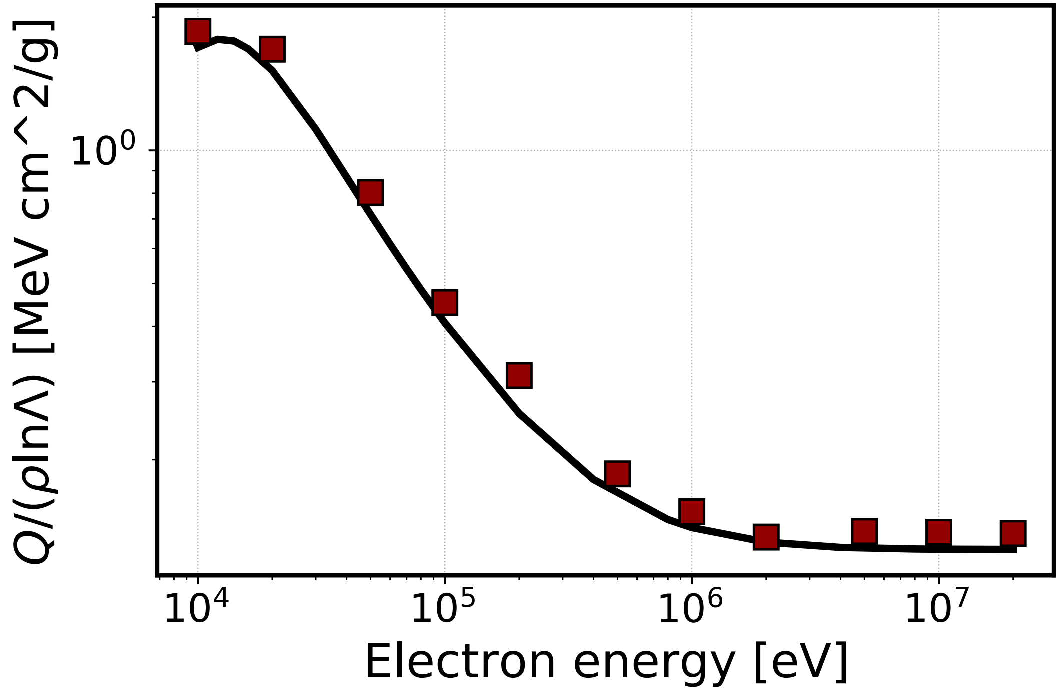




† Higginson, D. P., Holod, I., & Link, A. (2020). *JCP*, *413*, 109450.
* Nanbu, K., & Yonemura, S. (1998). *JCP*, *145*(2), 639-654.
** Nanbu, K. (2000). *IEEE*, *28*(3), 971-990.
‡ Pérez, F., et al. (2012). *PoP*, *19*(8), 083104
\+ Takizuka, T., & Abe, H. (1977). *JCP*, *25*(3), 205-219.
* Tanaka, S., & Shimamura, K. (2020). *J. of Chemical Phys*, *153*(3), 034114.

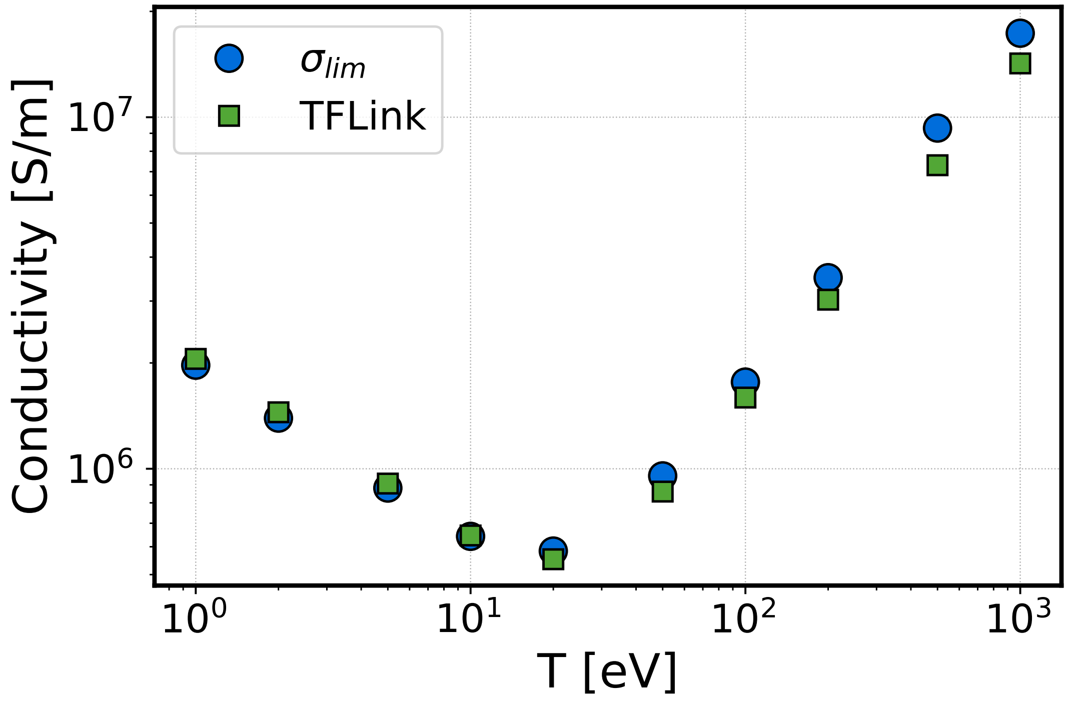
# Simulated measurements of plasma properties

### Stopping in solid density fully-ionized Al




$$Q = \left(\frac{dE}{dx}\right)_0 = \frac{1}{v_0}\left(\frac{dE}{dt}\right)_0$$

### Electrical conduction in solid copper

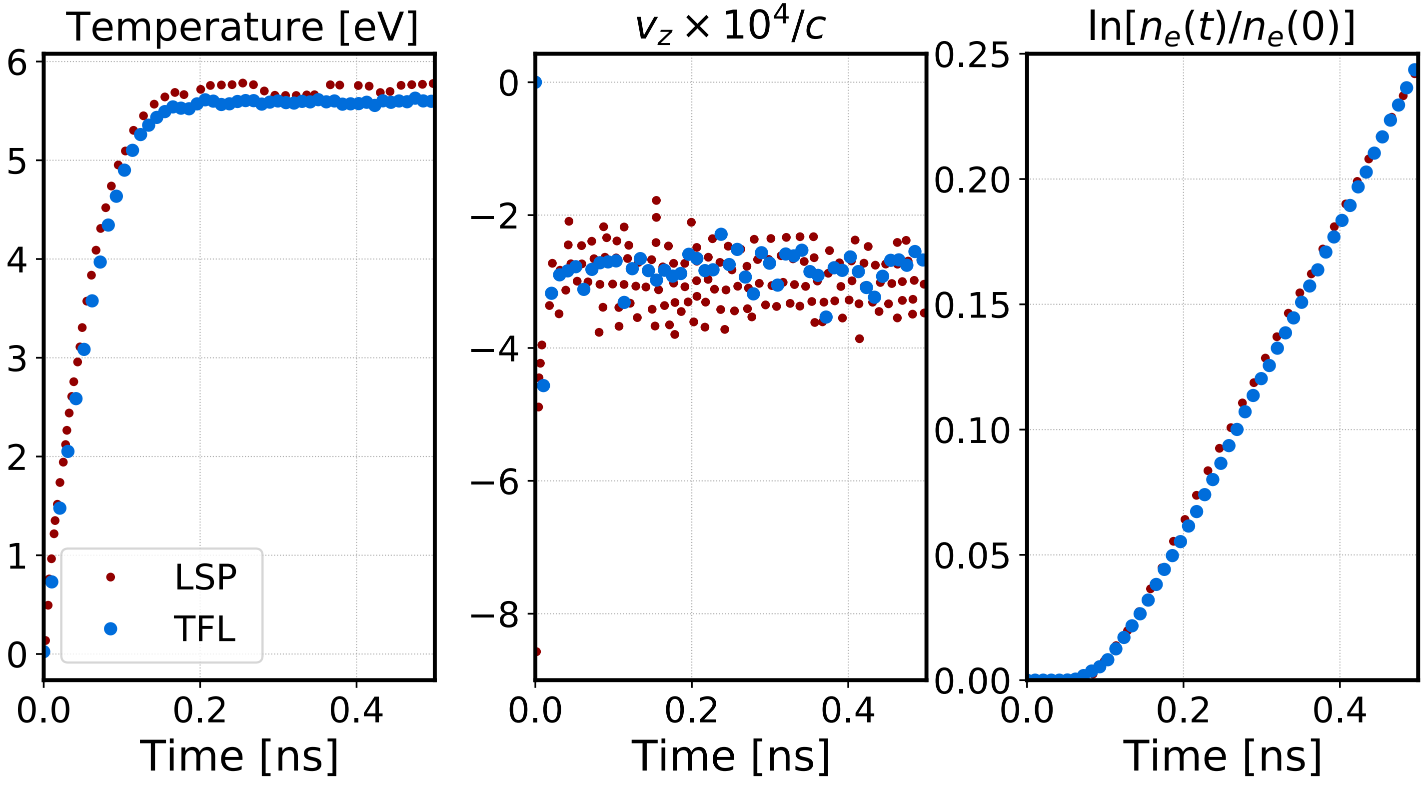



$$v(t) \sim at + v_f\left(1 - \exp\left(-{}^{t}/_{\tau}\right)\right) \qquad \sigma = \frac{env_f}{E}$$

* Pérez, F., Gremillet, L., Decoster, A., Drouin, M., & Lefebvre, E. (2012). *Physics of Plasmas*, *19*(8), 083104.

# Combined electron-neutral scattering model – plasma breakdown

**Helium breakdown in applied electric field**




- **Helium gas ($2e19$ $\mathrm{cm}^{-3}$) and seed plasma ($1e10$ $\mathrm{cm}^{-3}$) subject to 10 kV/cm field**
- **Scattering channels include:**
  - **Direct elastic collisions**
  - **Excitation**
  - **Electron impact ionization**
- **Agrees with original LSP simulation by Thoma et al. 2006**

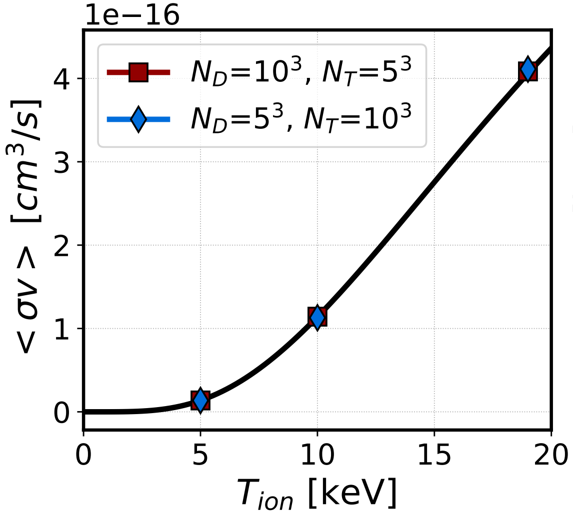
* Thoma, C., Hughes, T. P., Bruner, N. L., Genoni, T. C., Welch, D. R., & Clark, R. E. (2006). IEEE *34*(3), 910-919.

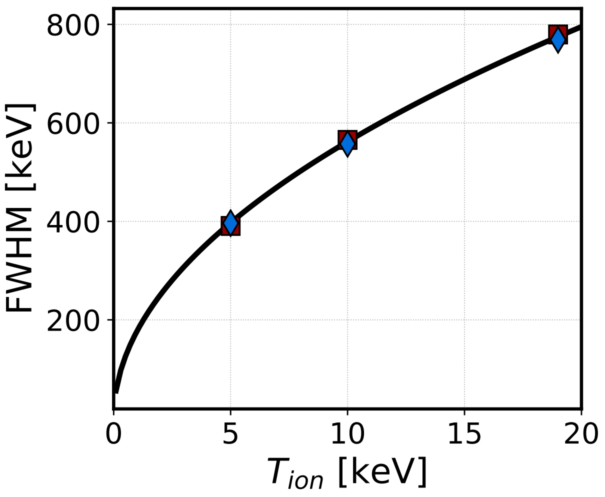
# Thermonuclear and beam-target fusion

### Treat fusion yield as probability

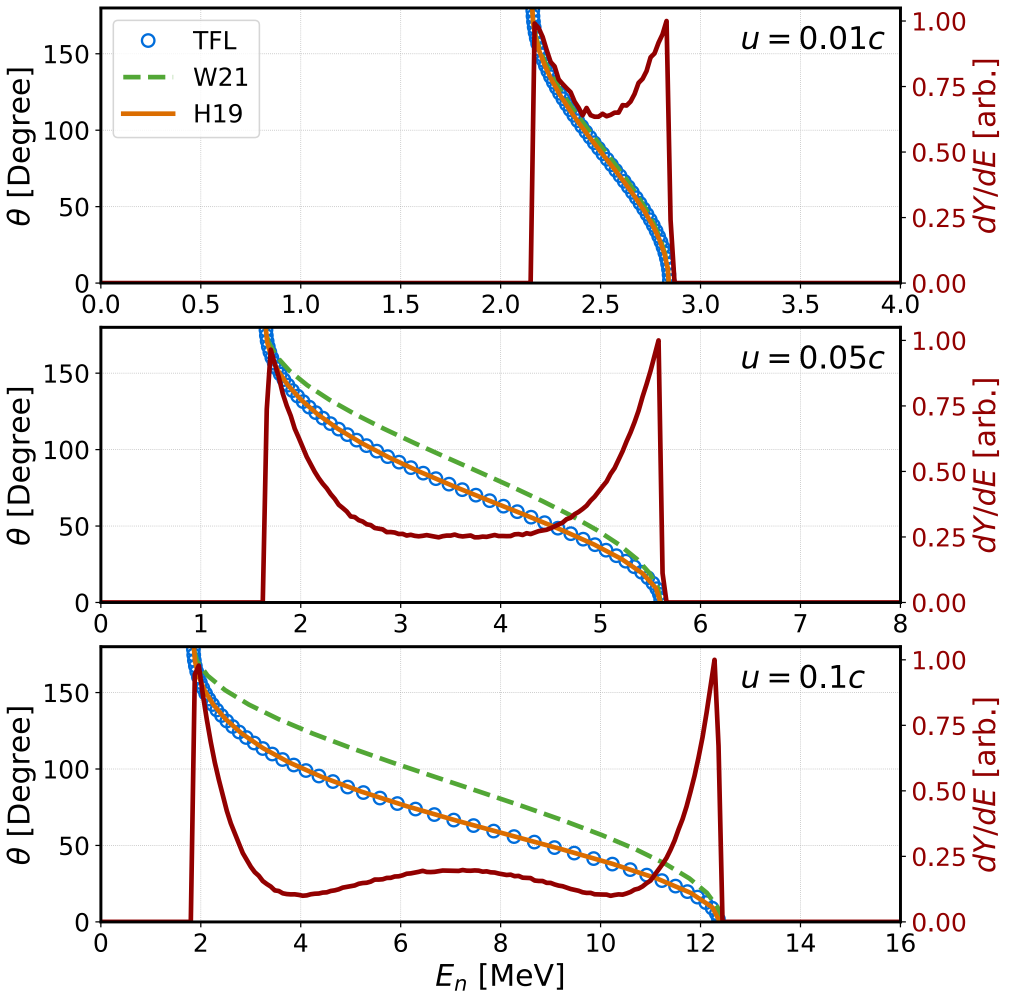
$$a + b \rightarrow c + d + Q \qquad Y \sim \frac{\mathbf{w_a w_b}}{\mathbf{V}} \sigma_{ab} v_{ab} \Delta \mathbf{t}$$

### Diagnose thermonuclear DT fusion neutron emission



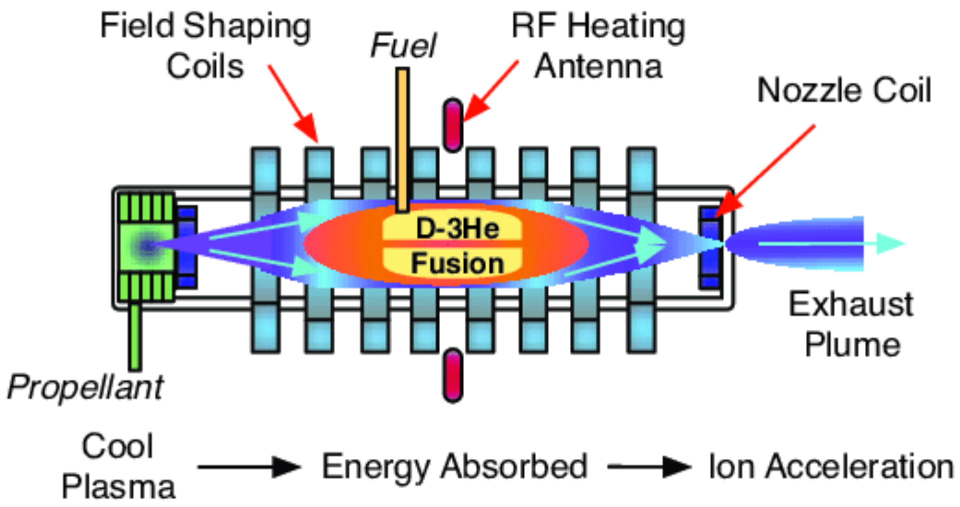

### Beam-target DD fusion

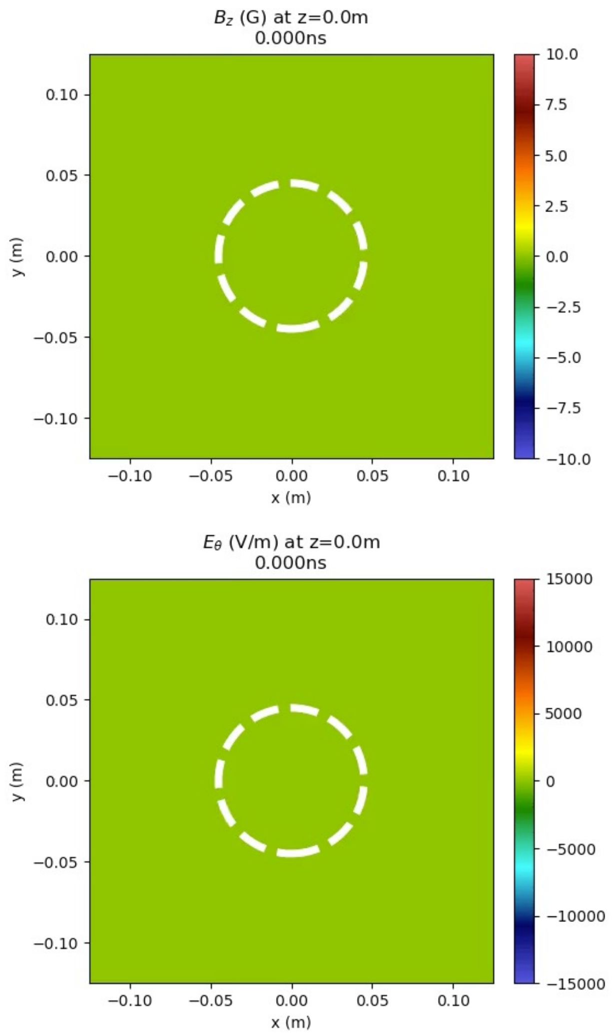



* Higginson, D. P., Link, A., & Schmidt, A. (2019). *JCP*, *388*, 439-453.
** Wu, D., Sheng, Z. M., Yu, W., Fritzsche, S., & He, X. T. (2021). *AIP Advances*, *11*(7), 075003.

# Application of the fully-integrated PIC code - the Princeton Field Reversed Configuration and Direct Fusion Drive

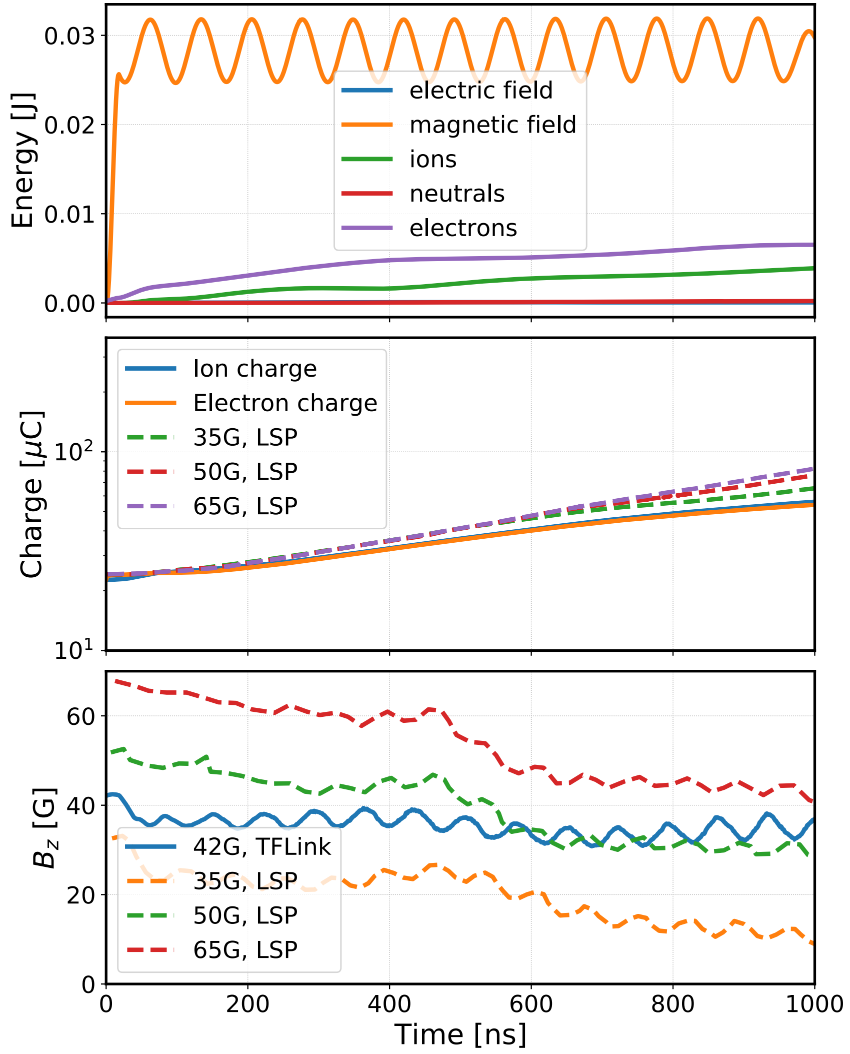
- **An invention of Dr. Samuel Cohen, the concept uses odd-parity rotating magnetic fields to drive the azimuthal current that sustains the FRC**
  - **Simple compact linear design**
  - **Kinetic device less prone to fluid instabilities**
  - **Efficient heating - low energy particles are preferentially trapped and accelerated in the rotating electric potentials**
  - **Efficient removal of tritium ash reduces neutron flux**

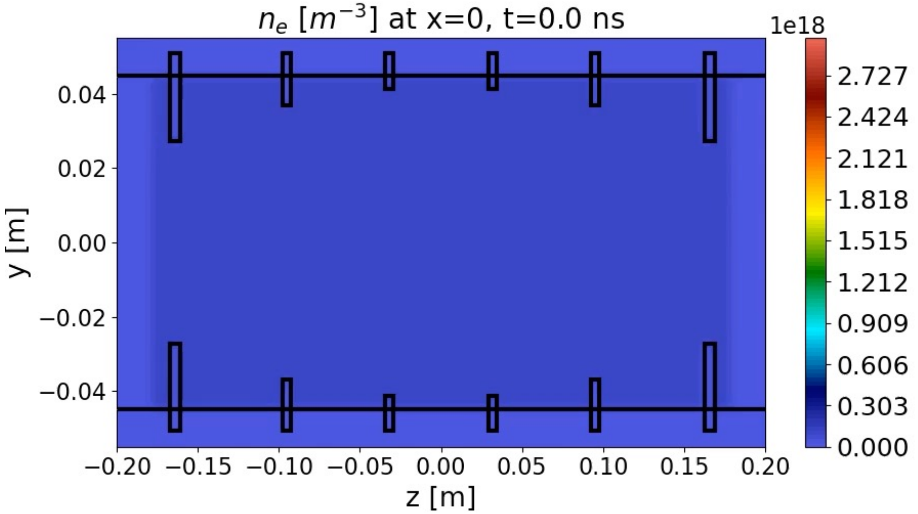


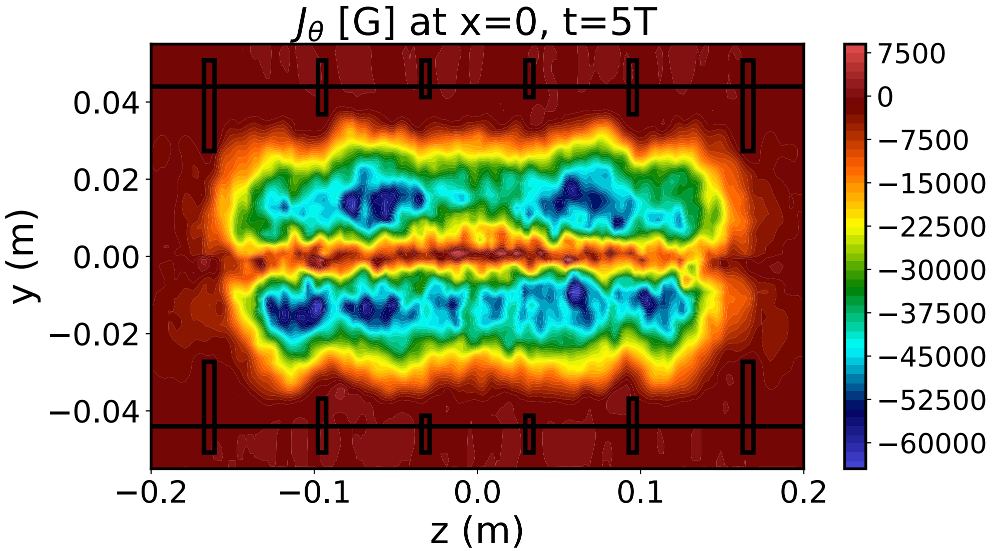




* Cohen, S. A., et al. (2007). *PRL*, *98*(14), 145002.
** Thomas, S. J., et al. (2017). *AIAA* (p. 5276).

# Fully-integrated kinetic electromagnetic simulations of PFRC-1 in development




* Cohen, S. A., et al. (2007). *PRL*, *98*(14), 145002.

** Welch, D. R., et al. (2010). *PRL*, *105*(1), 015002.

# Collisions validated for general plasma modeling



- **Particle collisions were implemented in a PIC code using the binary scattering method**
  - **Coulomb scattering, impact electron ionization, direct elastic collisions, excitation, fusion**
- **Validation tests include stopping and conduction measurements, plasma breakdown, and thermonuclear and beam-target fusion**
- **We are actively benchmarking a fully-integrated simulation of PFRC-1 before exploring the parameter space relevant to PFRC-2 and beyond**

**Thank you**