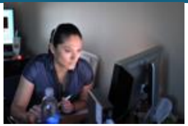
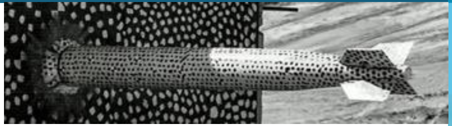
SAND2021-14833C

Fluid Plasma Model Development in Drekar





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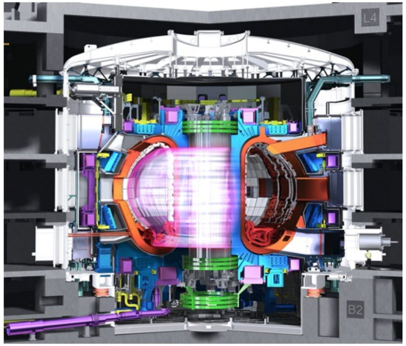
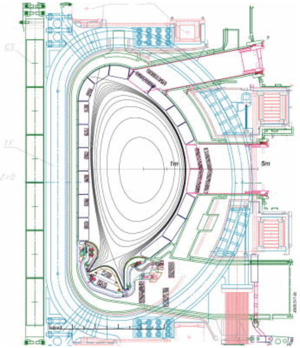
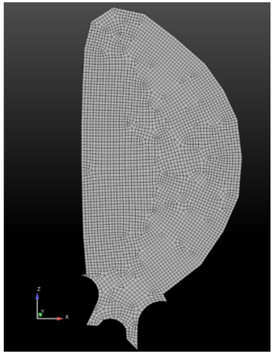
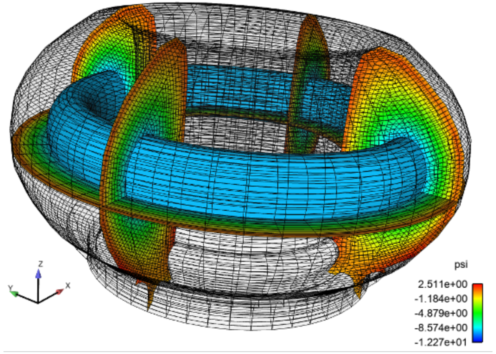
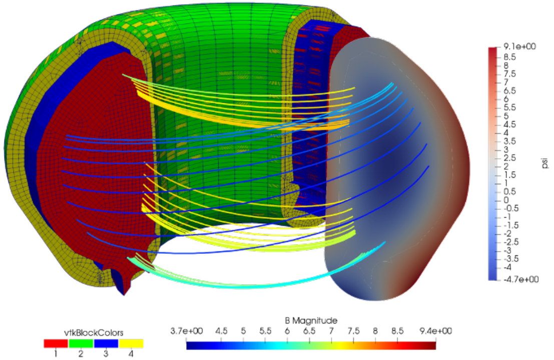
Motivation: Tokamak Disruption Simulation (TDS) ASCR/OFES SciDAC Center







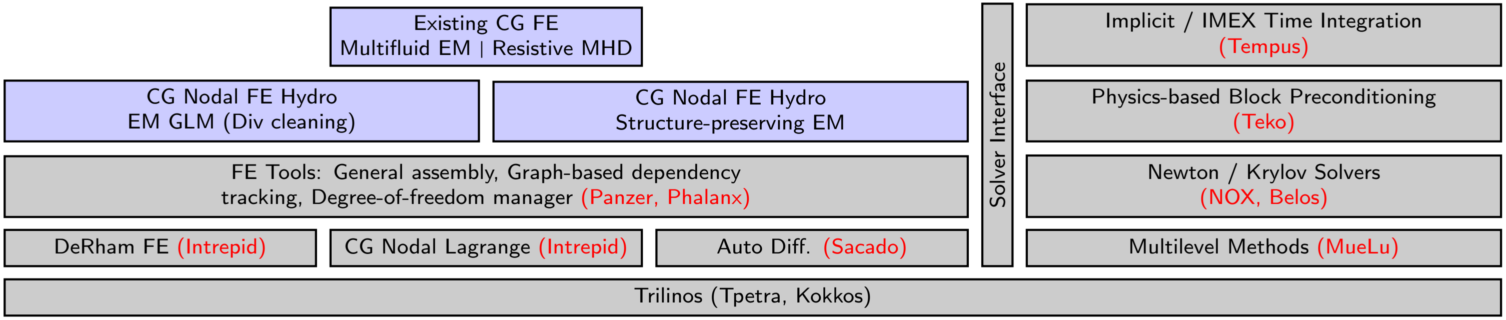




Context

Drekar: Resistive MHD / Multifluid with Coupled Multiphysics

- Arbitrarily many equations describing physics (continuity, momentum, energy, electromagnetics).
- ERK, DIRK, IMEX time integration (Tempus).
- 2D & 3D unstructured finite element (Intrepid):
  - Stabilized Q1/P1 elements (high-order possible).
  - Physics compatible discretizations (node, edge, face).
  - High-resolution positivity-preserving methods.
- Advanced software capabilities:
  - MPI+X (Kokkos).
  - Linear/non-linear solvers (NOX, Belos) with robust, scalable preconditioning (Teko, MueLu).
  - Jacobians computed through automatic differentiation (Sacado).
  - Asynchronous dependency manages multiphysics complexity (Phalanx).



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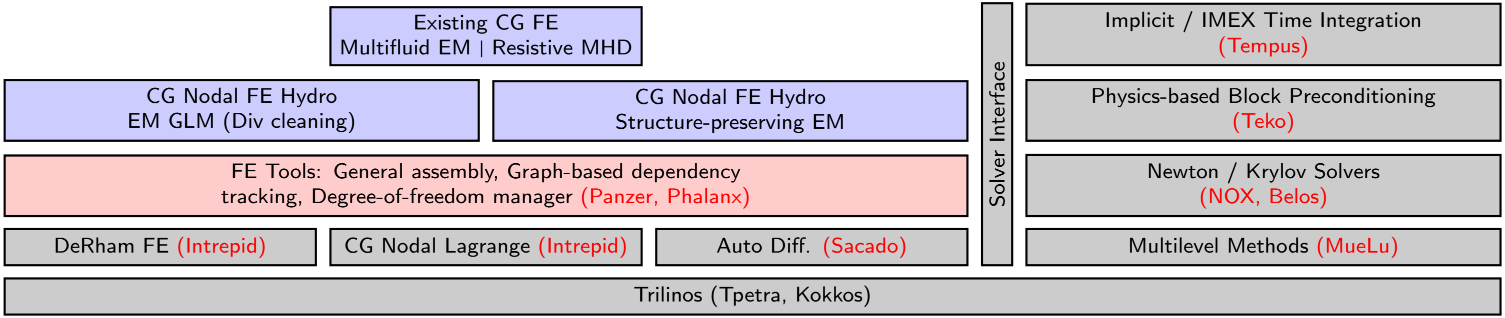

Trilinos Assembly/Evaluation Engines

Panzer: Multiphysics finite element assembly engine.

- Implement models using *equation set* classes to describe physics in residual form (eg., weak form residual).
- Manages arbitrary assignments of physics models (*equation sets*) to mesh regions (*element blocks*) with various discretizations.
- Handles indexing of solution fields into global solution vectors, Jacobian matrices, etc.

Phalanx: DAG-based expression evaluation.

- Each node (*evaluator*) maps input fields to output fields (Ideal gas EoS: $(\rho, \rho\mathbf{u}, \mathcal{E}) \mapsto (p, T)$).
- Written using *evaluate* strategy ($\text{output} = f(\text{input})$) or *contribute* strategy ($\text{output} += f(\text{input})$).
- Simple closure relations (eg., equation of state) leverage *evaluate* strategy for flexibility: just replace with a different evaluation.
- *Contribute* strategy allows for flexibility in model construction: *evaluate* a base model, then *contribute* specialized components for specific models.
- Template evaluators on scalar type to support generation of Jacobian matrices through automatic differentiation (AD).

Plasma Model Components

Typical plasma fluid models are composed of three main parts:

Fluid Equations:

- Euler system(s).
- MHD fluxes.
- Viscous terms, etc.

Electromagnetics:

- Magnetic induction (MHD)
- Electrostatics.
- Magnetostatics.
- Nodal Maxwell + cleaning.
- Nodal Maxwell w/ potentials.
- De Rham Maxwell.

Closures/Material Models:

- Equation of state.
- EM sources (Lorentz force).
- Ohm's law.
- Elastic collisions.
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Fluid Equations

Generic form:

$$
\begin{aligned}
\partial_t \rho_s + \nabla \cdot \mathbf{F}_s^{[0]} &= \mathcal{S}_s^{[0]} \\
\partial_t \left(\rho_s \mathbf{u}_s \right) + \nabla \cdot \underline{\mathbf{F}}_s^{[1]} &= \boldsymbol{\mathcal{S}}_s^{[1]} \\
\partial_t \mathcal{E}_s + \nabla \cdot \mathbf{F}_s^{[2]} &= \mathcal{S}_s^{[2]}
\end{aligned}
$$

Examples:

Euler fluid equations:

$$
\begin{aligned}
\mathbf{F}_s^{[0]} &= \rho_s \mathbf{u}_s \\
\underline{\mathbf{F}}_s^{[1]} &= \rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} \\
\mathbf{F}_s^{[2]} &= \left(\mathcal{E}_s + p_s \right) \mathbf{u}_s
\end{aligned}
$$

Magnetics terms for MHD:

$$
\begin{aligned}
\underline{\mathbf{F}}_s^{[1]} &= -\frac{1}{\mu_0} \mathbf{B} \otimes \mathbf{B} + \frac{1}{2\mu_0} \|\mathbf{B}\|^2 \underline{\mathbf{I}} \\
\mathbf{F}_s^{[2]} &= -\frac{1}{2\mu_0} \|\mathbf{B}\|^2 \mathbf{u}_s + \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B}
\end{aligned}
$$

or

$$
\begin{aligned}
\boldsymbol{\mathcal{S}}_s^{[1]} &= \mathbf{J} \times \mathbf{B} \\
\mathcal{S}_s^{[2]} &= \mathbf{J} \cdot \mathbf{E}
\end{aligned}
$$

Viscous stress, heat flux:

$$
\begin{aligned}
\underline{\mathbf{F}}_s^{[1]} &= \underline{\boldsymbol{\Pi}}_s \\
\mathbf{F}_s^{[2]} &= \mathbf{u}_s \cdot \underline{\boldsymbol{\Pi}}_s + \mathbf{h}_s
\end{aligned}
$$

with

$$
\begin{aligned}
\underline{\boldsymbol{\Pi}}_s &= -\mu_s \left(\nabla \mathbf{u}_s + \nabla \mathbf{u}_s^T - \frac{3}{2} \underline{\mathbf{I}} \nabla \cdot \mathbf{u}_s \right) \\
\mathbf{h}_s &= -\kappa_s \nabla T_s
\end{aligned}
$$

CG Finite Element Discretization

Hyperbolic system for each fluid:

$$\partial_t \mathbf{U}_s + \nabla \cdot \mathbf{F}_s(\mathbf{U}_s) = \mathbf{S}_s, \qquad \mathbf{U}_s = \left(\rho_s, \rho_s \mathbf{u}_s, \mathcal{E}_s\right)^T.$$

Semi-discrete scheme:

$$\underline{\boldsymbol{\mathcal{M}}}_{\mathrm{C}} \cdot \partial_t \boldsymbol{\mathcal{U}}_s^h + \boldsymbol{\mathcal{K}}_s(\boldsymbol{\mathcal{U}}_s^h) + \boldsymbol{\mathcal{B}}_s(\boldsymbol{\mathcal{U}}_s^h) + \boldsymbol{\mathcal{S}}_s = \mathbf{0},$$

where

$$\underline{\boldsymbol{\mathcal{M}}}_{\mathrm{C}} = \left[m_{k,\ell}\right]_{k,\ell=1}^{N_h} \otimes \underline{\mathbf{I}}_{N\times N} \qquad m_{k,\ell} = \int_\Omega \phi_k \phi_\ell \, d\mathbf{x}$$

$$\boldsymbol{\mathcal{K}}_s(\boldsymbol{\mathcal{U}}_s^h) = \left[\mathbf{K}_{s,1}, \ldots, \mathbf{K}_{s,N_h}\right]^T \qquad \mathbf{K}_{s,k} = -\int_\Omega \nabla\phi_k \cdot \mathbf{F}_s(\mathbf{U}_s)\, d\mathbf{x}$$

$$\boldsymbol{\mathcal{B}}_s(\boldsymbol{\mathcal{U}}_s^h) = \left[\mathbf{B}_{s,1}, \ldots, \mathbf{B}_{s,N_h}\right]^T \qquad \mathbf{B}_{s,k} = \int_\Gamma \phi_k \mathbf{F}_s(\mathbf{U}_s) \cdot \mathbf{n}\, d\Gamma$$

$$\boldsymbol{\mathcal{S}}_s = \left[\mathbf{S}_{s,1}, \ldots, \mathbf{S}_{s,N_h}\right]^T \qquad \mathbf{S}_{s,k} = -\int_\Omega \phi_k \mathbf{S}_s \, d\mathbf{x}$$

AFC Stabilization

Stabilized system:

$$\underline{\mathcal{M}}_{\mathrm{L}} \cdot \partial_t \mathcal{U}_s^h + \mathcal{K}_s(\mathcal{U}_s^h) + \mathcal{B}_s(\mathcal{U}_s^h) + \mathcal{S}_s + \underline{\mathcal{D}}_s \cdot \mathcal{U}_s^h - \mathcal{A}_{s,\alpha}(\mathcal{U}^h) = \mathbf{0},$$

where

$\underline{\mathcal{D}}_s$: Artificial diffusion

$\alpha_s^{(e)} \in [0,1]$: Element limiter

$$\mathcal{A}_{s,\alpha} = \sum_e \alpha_s^{(e)} \mathcal{A}_s^{(e)}(\mathcal{U}^h),$$

$$\mathcal{A}_s^{(e)} = (\underline{\mathcal{M}}_{\mathrm{C}} - \underline{\mathcal{M}}_{\mathrm{L}}) \cdot \partial_t \mathcal{U}_s^h + \underline{\mathcal{D}}_s^{(e)} \cdot \mathcal{U}_s^h,$$

- Artificial diffusion $\underline{\mathcal{D}}_s$ uses the mesh graph ⇒ support general unstructured meshes (quad, hex, tri, tet).
- Limiters require knowledge of the “patch” around each element, but FE assembly engine separates each elements (use “response-as-parameter”).

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Electromagnetics

Divergence constraints *must* be adequately satisfied: $\nabla \cdot \mathbf{B} = 0, \quad \epsilon_0 \nabla \cdot \mathbf{E} = q.$

Can we do this using a fully-nodal discretization? (This is not straightforward to do.)

- **Electrostatics:** $\varepsilon_0 \nabla^2 \phi + q = 0$; $\mathbf{E} = -\nabla \phi$.
- **Magnetostatics:** $\nabla \times (\nabla \times \mathbf{A}) - \nabla (\nabla \cdot \mathbf{A}) - \mu_0 \mathbf{J} = 0$; $\mathbf{B} = \nabla \times \mathbf{A}$.
- **Magnetic Induction:**

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} - \nabla \cdot \left[c_p^2 (\nabla \cdot \mathbf{B}) \underline{\mathbf{I}} \right] = 0, \qquad \mu_0 \mathbf{J} = \nabla \times \mathbf{B}, \qquad \mathbf{E} = -\mathbf{u} \times \mathbf{B} + \frac{1}{\sigma} \mathbf{J} + \frac{1}{n_e \mathrm{e}} \mathbf{J} \times \mathbf{B}.$$

- **Nodal Maxwell + Cleaning:**

$$\partial_t \mathbf{E} - c^2 \nabla \times \mathbf{B} + \frac{1}{\varepsilon_0} \mathbf{J} - \nabla \cdot \left[c_p^2 \left(\nabla \cdot \mathbf{E} - \frac{q}{\varepsilon_0} \right) \underline{\mathbf{I}} \right] = 0, \qquad \partial_t \mathbf{B} + \nabla \times \mathbf{E} - \nabla \cdot \left[c_p^2 (\nabla \cdot \mathbf{B}) \underline{\mathbf{I}} \right] = 0$$

- **Nodal Maxwell with Potentials:**

$$\partial_t^2 \mathbf{A}^2 + c^2 \nabla \times (\nabla \times \mathbf{A}) - c^2 \nabla (\nabla \cdot \mathbf{A}) - \frac{1}{\varepsilon_0} \mathbf{J} = 0, \qquad \mathbf{E} = -\nabla \phi - \partial_t \mathbf{A},$$

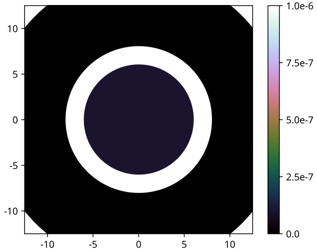
$$-\nabla \cdot \left(\nabla \phi - \partial_t \mathbf{A} \right) - \frac{q}{\varepsilon_0} = 0, \qquad \mathbf{B} = \nabla \times \mathbf{A}.$$

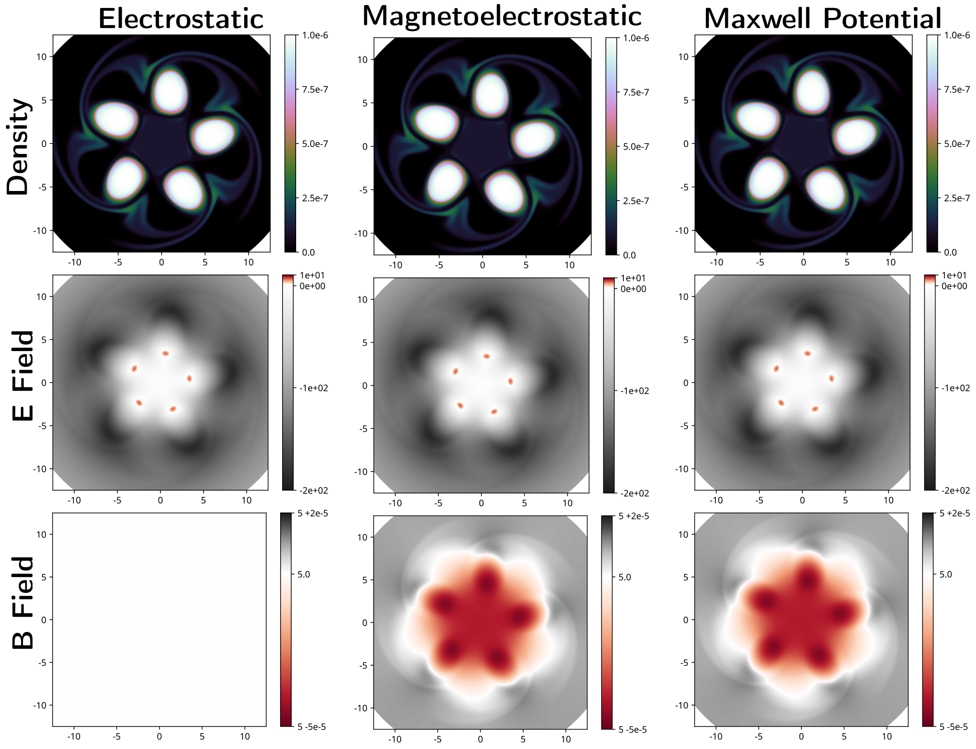
Electromagnetics

Problem setup:

- Cylindrical electron beam within axial magnetic field ($B_z = 5.0$).
- Drift instability develops due to:
  $\Rightarrow$ Non-monotonic radial profile.
  $\Rightarrow$ Guiding center motion: $\mathbf{v} \propto \mathbf{E} \times \mathbf{B}$.

Initial density:





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Multifluid Models

Euler subsystem for each species, with Lorentz force sources:

$$\partial_t \rho_s + \nabla \cdot \mathbf{F}_s^{[0]} = \mathcal{S}_s^{[0]} \qquad \mathbf{F}_s^{[0]} = \rho_s \mathbf{u}_s$$

$$\partial_t \left(\rho_s \mathbf{u}_s\right) + \nabla \cdot \underline{\mathbf{F}}_s^{[1]} = \boldsymbol{\mathcal{S}}_s^{[1]} \qquad \underline{\mathbf{F}}_s^{[1]} = \rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} \qquad \boldsymbol{\mathcal{S}}_s^{[1]} = q_s n_s \left(\mathbf{E} + \mathbf{u}_s \times \mathbf{B}\right)$$

$$\partial_t \mathcal{E}_s + \nabla \cdot \mathbf{F}_s^{[2]} = \mathcal{S}_s^{[2]} \qquad \mathbf{F}_s^{[2]} = \left(\mathcal{E}_s + p_s\right) \mathbf{u}_s \qquad \mathcal{S}_s^{[2]} = q_s n_s \mathbf{u}_s \cdot \mathbf{E}$$

- General multifluid models use a separate set of fluid equations for each charge state of each atomic species in the system, plus electrons:

$$s \in \Lambda = \left\{(\alpha, k) : \alpha = 1, \ldots, N_A; k = 0, \ldots, z_\alpha\right\} \cup \{e\}$$

- Couple to desired description of electromagnetics (electrostatic, magnetoelectrostatic, full Maxwell).
- Add source terms for more advanced models: elastic scattering, ionization, recombination, charge exchange, radiative loss, etc. **Many are highly nonlinear.**
- Timescales require implicit treatment of source terms: Assembly engines and solver infrastructure are crucial.

Elastic Scattering[1,2]

$$\mathcal{S}_s^{[1]} = + \sum_{t \in \Lambda_G \setminus s} \mathbf{R}_{s;t}, \qquad \mathbf{R}_{s;t} = \alpha_{s;t} \rho_s \rho_t \left(\mathbf{u}_t - \mathbf{u}_s\right) \Phi_{s;t},$$

$$\mathcal{S}_s^{[2]} = \sum_{t \in \Lambda_G \setminus s} \left(\mathbf{u}_s \cdot \mathbf{R}_{s;t} + Q_{s;t}\right), \qquad Q_{s;t} = \frac{\alpha_{s;t} \rho_s \rho_t}{m_s + m_t} \left[A_{s;t} k_B \left(T_t - T_s\right) \Psi_{s;t} + m_t \left(\mathbf{u}_t - \mathbf{u}_s\right)^2 \Phi_{s;t} \right],$$

- Charge-charge (Coulomb):

$$\alpha_{s;t} = \frac{Z_s^2 Z_t^2 |q_e|^4 \ln \Lambda_{s;t}}{6\pi \sqrt{2\pi} \epsilon_0^2 m_s m_t m_{s;t} \left(k_B T_s / m_s + k_B T_t / m_t\right)^{3/2}},$$

- Charge-neutral/Neutral-neutral:

$$\alpha_{s;t} = \frac{1}{m_s + m_t} \frac{4}{3} \left[\frac{8}{\pi} \left(\frac{k_B T_s}{m_s} + \frac{k_B T_t}{m_t} \right) \right]^{1/2} \sigma_{s;t}.$$

⇒ Using constant cross-sections for now (most computed using hard-sphere approximation, some from QM calculations).

[1] D. Martínez-Gómez, R. Soler, and J. Terradas, *Multi-fluid approach to high-frequency waves in plasmas. I. Small-amplitude regime in fully ionized media*, The Astrophysical Journal, 832 (2016), p. 101, doi:10.3847/0004-637X/832/2/101.

[2] D. Martínez-Gómez, R. Soler, and J. Terradas, *Multi-fluid approach to high-frequency waves in plasmas. II. Small-amplitude regime in partially ionized media*, The Astrophysical Journal, 837 (2017), p. 80, doi:10.3847/1538-4357/aa5eab.

Reactions: Ionization & Recombination

$$\mathcal{S}^{[0]}_{(\alpha,k)} = \frac{m_{(\alpha,k)}}{m_{(\alpha,k-1)}} n_e \rho_{(\alpha,k-1)} I_{(\alpha,k-1)} - n_e \rho_{(\alpha,k)} I_{(\alpha,k)} + \frac{m_{(\alpha,k)}}{m_{(\alpha,k+1)}} n_e \rho_{(\alpha,k+1)} R_{(\alpha,k+1)} - n_e \rho_{(\alpha,k)} R_{(\alpha,k)}$$

$$\boldsymbol{\mathcal{S}}^{[1]}_{(\alpha,k)} = \frac{m_{(\alpha,k)}}{m_{(\alpha,k-1)}} n_e (\rho\mathbf{u})_{(\alpha,k-1)} I_{(\alpha,k-1)} - n_e (\rho\mathbf{u})_{(\alpha,k)} I_{(\alpha,k)} + \left(n_e (\rho\mathbf{u})_{(\alpha,k+1)} + n_{(\alpha,k+1)} (\rho\mathbf{u})_e\right) R_{(\alpha,k+1)} - n_e (\rho\mathbf{u})_{(\alpha,k)} R_{(\alpha,k)}$$

$$\mathcal{S}^{[2]}_{(\alpha,k)} = \frac{m_{(\alpha,k)}}{m_{(\alpha,k-1)}} n_e \mathcal{E}_{(\alpha,k-1)} I_{(\alpha,k-1)} - n_e \mathcal{E}_{(\alpha,k)} I_{(\alpha,k)} + \left(n_e \mathcal{E}_{(\alpha,k+1)} + n_{(\alpha,k+1)} \mathcal{E}_e\right) R_{(\alpha,k+1)} - n_e \mathcal{E}_{(\alpha,k)} R_{(\alpha,k)}$$

- Assume a coronal ionization model (simpler than full collisional-radiative model).
- Need rate coefficients $I_{(\alpha,k)}$ and $R_{(\alpha,k)}$ for each charge state.
- Rates are nonlinear functions of electron temperature.
- Sometimes models have to be combined from different sources to obtain a complete set.

Ionization

Voronov:[a]

$$I_{(\alpha,k)} = A_{(\alpha,k)} \frac{1 + P_{(\alpha,k)}\sqrt{U_{(\alpha,k)}}}{X_{(\alpha,k)} + U_{(\alpha,k)}} \left(U_{(\alpha,k)}\right)^{K_{(\alpha,k)}} \exp\left(-U_{(\alpha,k)}\right), \qquad U_{(\alpha,k)} = \frac{\phi^{\text{ion}}_{(\alpha,k)}}{T_e}.$$

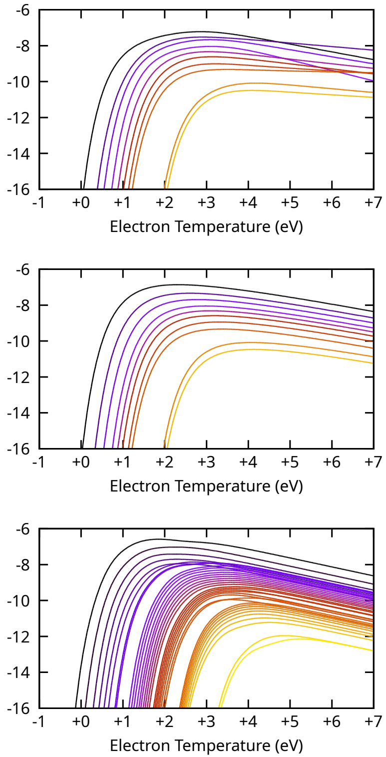
- Available for H to Ni^{27+}.
- Accurate to within 10% for T_e between 1 eV and 20 KeV.

Lotz:[b,c]

$$I_{(\alpha,k)} = (2.97\text{E}{-6}) \frac{\xi_{(\alpha,k)}}{\phi^{\text{ion}}_{(\alpha,k)}\sqrt{T_e}} E_1\left(U_{(\alpha,k)}\right),$$

- $\xi_{(\alpha,k)}$ is the number of outer electrons in the ionizing atom.
- General analytic model for any atomic species.
- Compatible with ionization potential depression models.

Others: Other sources for specific higher Z elements; eg., Mattioli, et al.[d] for Kr.



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[a] G. Voronov, *A practical fit formula for ionization rate coefficients of atoms and ions by electron impact: z=1-28*, Atomic Data and Nuclear Data Tables, 65 (1997), pp. 1–35, doi:10.1006/adnd.1997.0732.

[b] W. Lotz, *Electron-impact ionization cross-sections and ionization rate coefficients for atoms and ions from hydrogen to calcium*, Zeitschrift für Physik, 216 (1968), pp. 241–247, doi:10.1007/BF01392963.

[c] W. Lotz, *Electron-impact ionization cross-sections and ionization rate coefficients for atoms and ions from scandium to zinc*, Zeitschrift für Physik, 220 (1969), pp. 466–472, doi:10.1007/BF01394789.

[d] M. Mattioli, G. Mazzitelli, K. B. Fournier, M. Finkenthal, and L. Carraro, *Updating of atomic data needed for ionization balance evaluations of krypton and molybdenum*, Journal of Physics B: Atomic, Molecular and Optical Physics, 39 (2006), pp. 4457–4489, doi:10.1088/0953-4075/39/21/010.

Radiative Recombination

Badnell, et al.:[a]

$$R^{\text{rad}}_{(\alpha,k)} = A_{(\alpha,k)} \left[\sqrt{T_e / T_0^{(\alpha,k)}} \left(1 + \sqrt{T_e / T_0^{(\alpha,k)}}\right)^{1-D_{(\alpha,k)}} \left(1 + \sqrt{T_e / T_1^{(\alpha,k)}}\right)^{1+D_{(\alpha,k)}} \right]^{-1},$$

$$D_{(\alpha,k)} = B_{(\alpha,k)} + C_{(\alpha,k)} \exp\left(-T_2^{(\alpha,k)} / T_e\right)$$

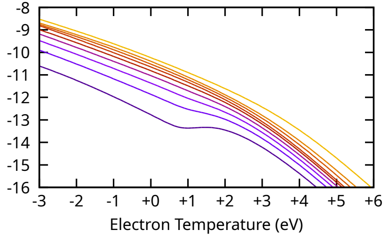
- Available for H through Zn, plus Kr, Mo, Xe.
- Fits of calculated data from AUTOSTRUCTURE code.

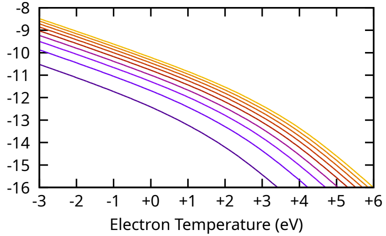
Kotelnikov, et al.:[b]

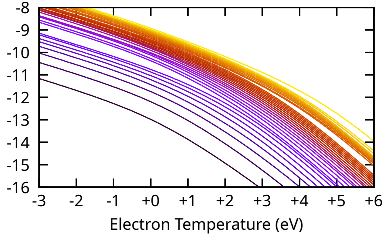
$$R^{\text{rad}}_{(\alpha,k)} = \frac{8.414 k \alpha^4 c a_0^2 \left[\ln(1+\lambda) + 3.499\right]}{(1/\lambda)^{1/2} + 0.6517\,(1/\lambda) + 0.2138\,(1/\lambda)^{3/2}}, \qquad \lambda = \frac{h R_\infty c k^2}{k_{\text{B}} T_e}$$

- Generic hydrogenic approximation.
- Valid in both high- and low-temperature limits.

Others: Other sources for specific higher Z elements; eg., Mattioli, et al.[c] for Kr.







[a] N. R. Badnell, *Radiative recombination data for modeling dynamic finite-density plasmas*, The Astrophysical Journal Supplement Series, 167 (2006), pp. 334–342, doi:10.1086/508465.

[b] I. A. Kotelnikov and A. I. Milstein, *Electron radiative recombination with a hydrogen-like ion*, Physica Scripta, 94 (2019), p. 055403, doi:10.1088/1402-4896/ab060a.

[c] M. Mattioli, G. Mazzitelli, K. B. Fournier, M. Finkenthal, and L. Carraro, *Updating of atomic data needed for ionization balance evaluations of krypton and molybdenum*, Journal of Physics B: Atomic, Molecular and Optical Physics, 39 (2006), pp. 4457–4489, doi:10.1088/0953-4075/39/21/010.

Dielectronic Recombination

Badnell, et al.:[a]

$$R^{\text{die}}_{(\alpha,k)} = T_e^{-3/2} \sum_{i=1}^{N_{(\alpha,k)}} c_i^{(\alpha,k)} \exp\left(-E_i^{(\alpha,k)} / T_e\right)$$

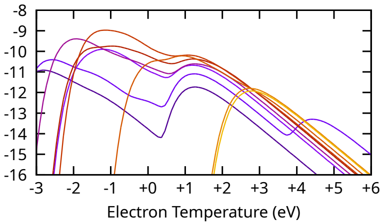
- Available by isoelectronic sequence, through Si sequence.
- Fits of calculated data from AUTOSTRUCTURE code.

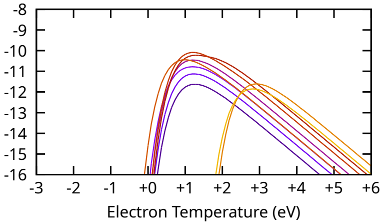
Landini, et al.:[b]

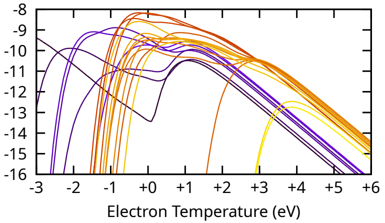
$$R^{\text{die}}_{(\alpha,k)} = A_{(\alpha,k)} T_e^{-3/2} \exp\left(-T_0^{(\alpha,k)} / T_e\right) \left(1 + B_{(\alpha,k)} \exp\left(-T_1^{(\alpha,k)} / T_e\right)\right)$$

- Less resolved, but data available for a wider range of species (eg., low charge states of Ar).

Others: Other sources for specific higher Z elements; eg., Mattioli, et al.[c] or Sterling[d] for Kr.







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[a] N. R. Badnell, M. G. O'Mullane, H. P. Summers, Z. Altun, M. A. Bautista, J. Colgan, T. W. Gorczyca, D. M. Mitnik, M. S. Pindzola, and O. Zatsarinny, *Dielectronic recombination data for dynamic finite-density plasmas: I. Goals and methodology*, Astronomy & Astrophysics, 406 (2003), pp. 1151–1165, doi:10.1051/0004-6361:20030816.

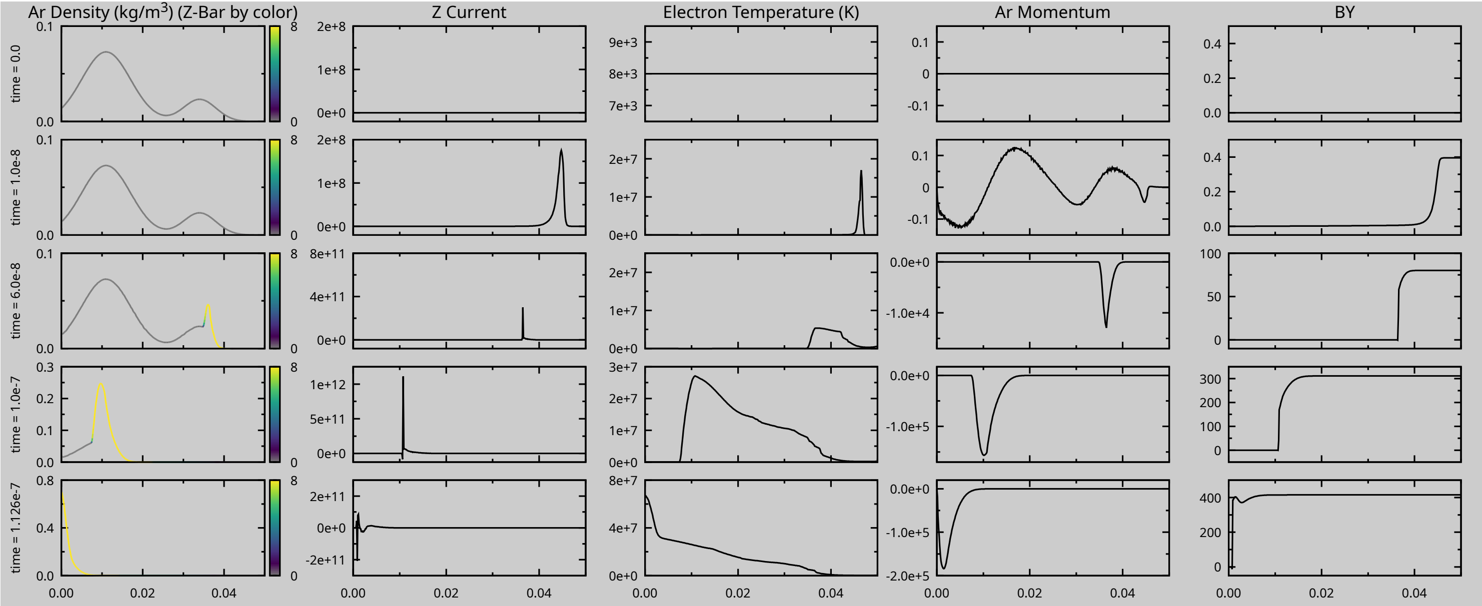
[b] M. Landini and B. C. Monsignori Fossi, *The X-UV spectrum of thin plasmas*, Astronomy & Astrophysics Supplement Series, 82 (1990), pp. 229–260.

[c] M. Mattioli, G. Mazzitelli, K. B. Fournier, M. Finkenthal, and L. Carraro, *Updating of atomic data needed for ionization balance evaluations of krypton and molybdenum*, Journal of Physics B: Atomic, Molecular and Optical Physics, 39 (2006), pp. 4457–4489, doi:10.1088/0953-4075/39/21/010.

[d] N. C. Sterling, *Atomic data for neutron-capture elements II. photoionization and recombination properties of low-charge krypton ions*, Astronomy & Astrophysics, 533 (2011), p. A62, doi:10.1051/0004-6361/201117471.

1D Argon Gas Puff (Proof of Concept)

- Argon gas ($z = 0$ to 8^+) plus electrons (58 eqs.)
- Potential form of Maxwell's equations.
- Driven by EM field applied at the boundary.
- Ionization + collisions yields resistive heating.
- Implicit time integration follows ion fluid CFL.
- Use black-box AMG GMRES preconditioners.



Ongoing work: Consistent material models for MHD

- Want to make comparisons between different fluid plasma models (resistive MHD, Hall/extended MHD, multifluid).
- **Goal:** Compute electrical conductivity using multifluid collision models.

Resistive MHD:

$$\partial_t \rho_s + \nabla \cdot \mathbf{F}_s^{[0]} = \mathcal{S}_s^{[0]} \qquad \mathbf{F}_s^{[0]} = \rho_s \mathbf{u}_s$$

$$\partial_t \left(\rho_s \mathbf{u}_s\right) + \nabla \cdot \underline{\mathbf{F}}_s^{[1]} = \boldsymbol{\mathcal{S}}_s^{[1]} \qquad \underline{\mathbf{F}}_s^{[1]} = \rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} \qquad \underline{\mathbf{F}}_s^{[1]} = -\frac{1}{\mu_0}\mathbf{B} \otimes \mathbf{B} + \frac{1}{2\mu_0}\|\mathbf{B}\|^2 \underline{\mathbf{I}}$$

$$\partial_t \mathcal{E}_s + \nabla \cdot \mathbf{F}_s^{[2]} = \mathcal{S}_s^{[2]} \qquad \mathbf{F}_s^{[2]} = \left(\mathcal{E}_s + p_s\right)\mathbf{u}_s \qquad \mathbf{F}_s^{[2]} = -\frac{1}{2\mu_0}\|\mathbf{B}\|^2 \mathbf{u}_s + \frac{1}{\mu_0}\mathbf{E} \times \mathbf{B}$$

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0 \qquad \mu_0 \mathbf{J} = \nabla \times \mathbf{B} \qquad \mathbf{E} = -\mathbf{u} \times \mathbf{B} + \frac{1}{\sigma}\mathbf{J}$$

- Conductivity depends on *all* ionization and recombination rates $\left(I_{(\alpha,k)},\ R_{(\alpha,k)}\right)$ and *all* pair-wise elastic collision rates $\alpha_{s;t}$.
- No closed form expression: Need point-wise linear/non-linear solve for conductivity.
- Use assembly engines with automatic differentiation (AD) to obtain exact Jacobian for these models.

Thank you