Development of a Coupled Kinetic Plasma - Neutral Transport Code*

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Poster presented at the 21st US Transport Task Force Workshop, Boulder, CO

*This work supported by US DOE contract no. DE-AC02-76CH03073.

Abstract

Monte Carlo neutral transport codes have been run in conjunction with fluid plasma transport codes for more than a decade. The logical next step is to couple a Monte Carlo neutral transport package to a kinetic plasma transport code. The XGC neoclassical particle transport [1] does just this with a built-in, rudimentary Monte Carlo neutral transport routine. A primary objective of the Center for Plasma Edge Science project is the replacement of this routine with a more general routine based on the DEGAS 2 Monte Carlo neutral transport code. As was done by XGC's neutral routine, the DEGAS 2 neutrals collide off of a fluid plasma background with its moments computed from the kinetic XGC ions. The resulting neutral density, flow velocity and temperature profiles are passed back to XGC. XGC's ions and electrons collide off of this background using the same ionization and charge exchange rates employed in the neutral transport calculation.

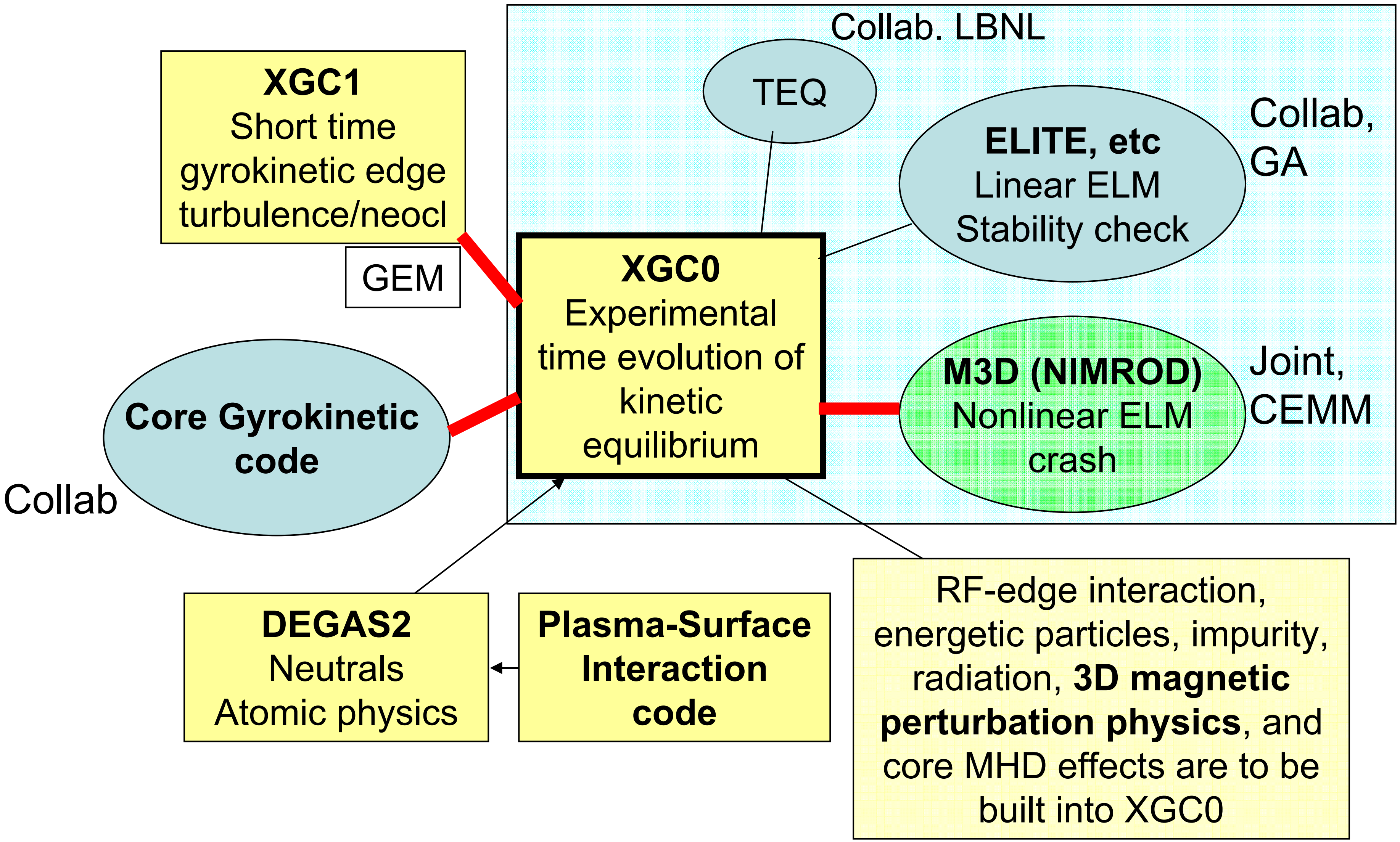
Efforts to obtain self-consistent solutions of Monte Carlo neutral and fluid plasma transport codes were complicated by subtle numerical and physical problems beyond those associated with finite Monte Carlo statistical noise [2,3]. Those convergence problems are less of a concern here since XGC uses a particle-based approach to solving its underlying equations. Nonetheless, we need to ensure overall conservation of particles, momentum, and energy in the exchanges between plasma and neutral populations. Not doing so could lead to spurious sources that could accumulate throughout the simulation, compromising the accuracy of the final result. We will describe an approach to the coupling designed to avoid this problem.

[1] C. S. Chang et al., Phys. Plasmas **11** 2649 (2004).
[2] G. P. Maddison and D. Reiter, KFA Jülich Report Jül-2872 (1994).
[3] D. P. Stotler et al., Contrib. Plasma Phys. **40** 221 (2000).

The Center for Plasma Edge Simulation Devoted to Understanding H-Mode Pedestal & ELM Physics

- Multi-institutional prototype Fusion Simulation Project funded in 2005.
- Goal is to understand:
  - Pedestal build-up,
  - L-H mode transition,
  - ELM crash & cycle.
- Involves multiple codes covering different physics, time & length scales:
  - Neoclassical & turbulent plasma transport,
  - Open & closed flux surfaces,
  - Large scale instabilities (ELM's),
  - Neutral transport,
  - Plasma-wall interactions

CPES Code Integration Framework



Kinetic Character of Both Plasma & Neutrals Essential in Edge

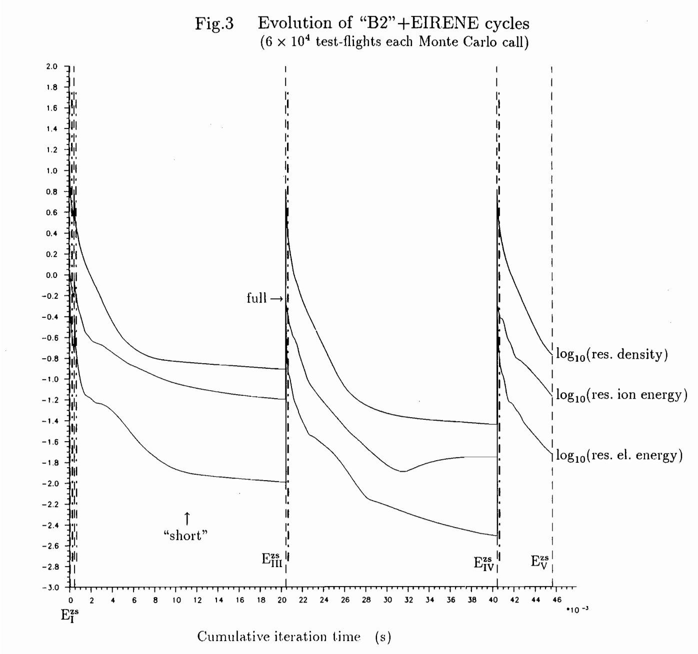
- For plasma:
  - Low collisionality,
  - Steep gradients,
  - Large particle orbits,
  - Non-Maxwellian distributions.
- For neutrals:
  - Atoms & molecules recycled from wall,
  - Uncollided dissociation products,
  - CX with non-Maxwellian ions.

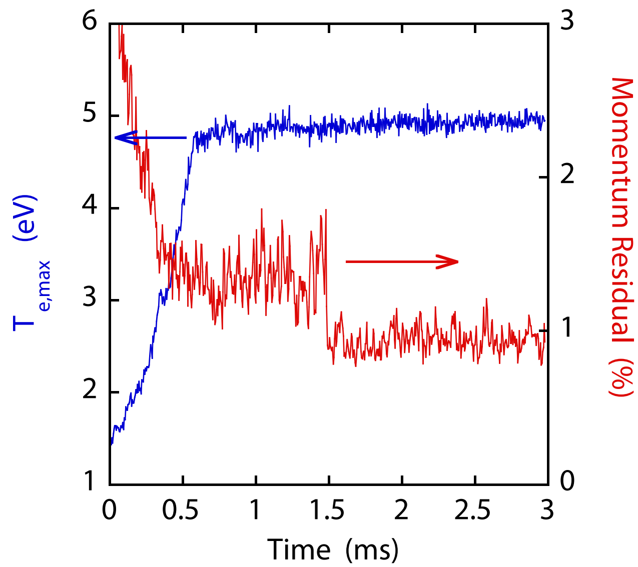
CPES Pursuing Fully Kinetic Plasma-Neutral Simulation

- Original XGC-0 had rudimentary MC neutral transport routine.
- Replacing with one based on DEGAS 2.
- How to verify the resulting code?
  - Verification of XGC-0 NC plasma transport presented at 20th TTF.
  - Focus here on conservation of mass, momentum, and energy in plasma-neutral interactions.
  - Other verification tests will follow.

Coupling MC Neutral Transport Codes to Fluid Plasma Transport Codes Has Been Challenging

- Conservation of mass, momentum, and energy straightforward since plasma code takes integrated sources / sinks.
  - In principle!
- More complicated in practice!
  - “Short” vs. “full” cycle in B2-EIRENE designed to reduce simulation time,
  - Incomplete UEDGE convergence due to finite MC noise.
- Such problems can dramatically affect code convergence / behavior.





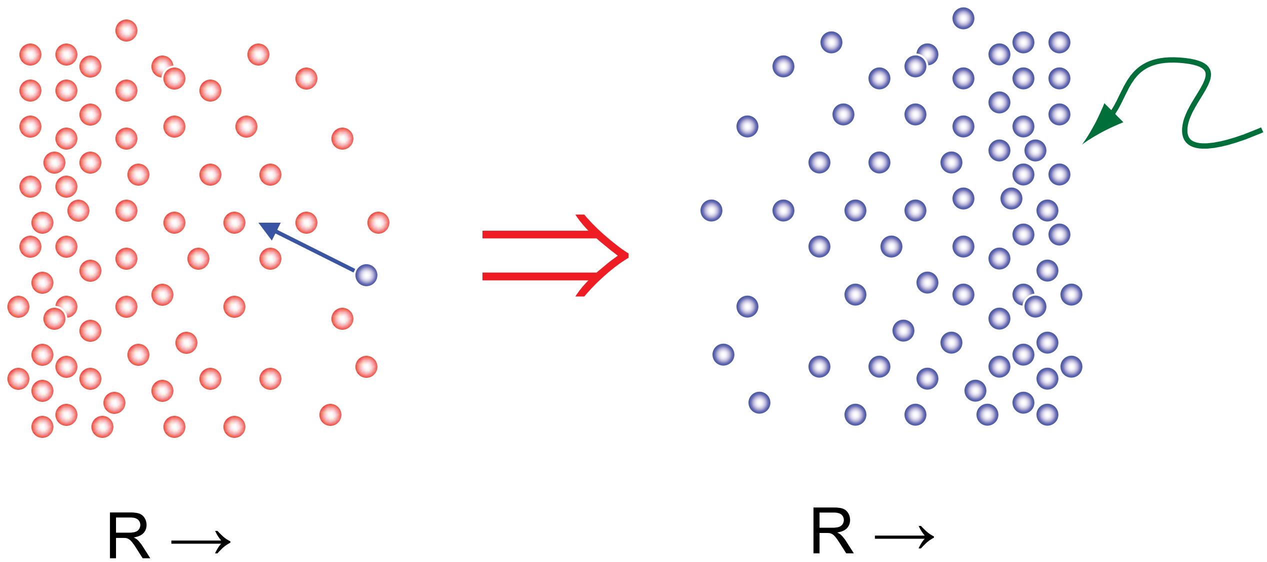
What Challenges Await a Coupled MC Neutral - Kinetic Plasma Code?

- XGC-0 is a particle code,
  - Will yield a “solution” with few requirements on neutral transport data.
  - $\Rightarrow$ conservation errors could easily escape detection,
  - Accumulated errors could compromise simulation result.
  - $\Rightarrow$ explicit conservation checks required.
- Specifying neutral sources complex,
  - Should develop kinetic characterization of ions striking wall,
  - And consistently determine sheath parameters.
- Reexmaine ionization & other atomic physics rates?
  - Entire database invokes averages over Maxwellian distributions.

A First Approach to Kinetic-Kinetic Coupling: Two Complementary Collision Routines

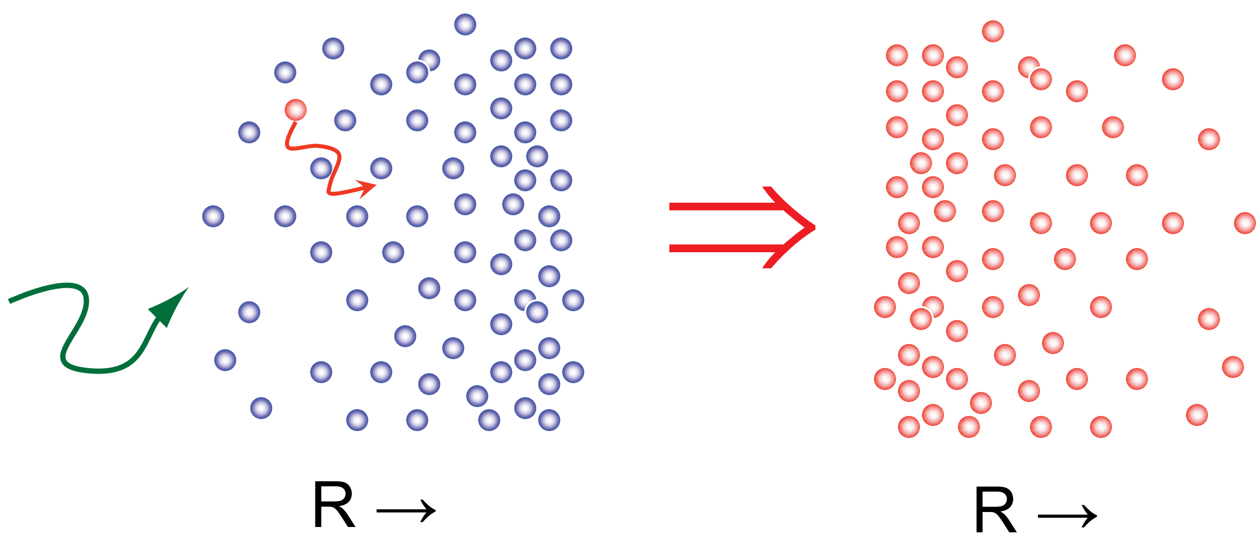
- Used in original XGC-0.
- Kinetic neutrals colliding with fluid plasma background,
- Kinetic ions & electrons colliding with fluid neutral background.
- Use same reaction rates for both.
- Spatial domain restricted to flux surfaces,
  - I.e., does not go to wall,
  - Multiple meshes used.
- “Fluids” characterized by density & temperature,
  - $\Rightarrow$ no momentum exchange.
- Neutral source has arbitrary spatial variation,
  - Magnitude adjusted to yield specified recycling rate.

Complementary Collision Routines



Neutral atoms are tracked through & collide with a fluid plasma background. The resulting neutral distribution is characterized by a density & temperature.

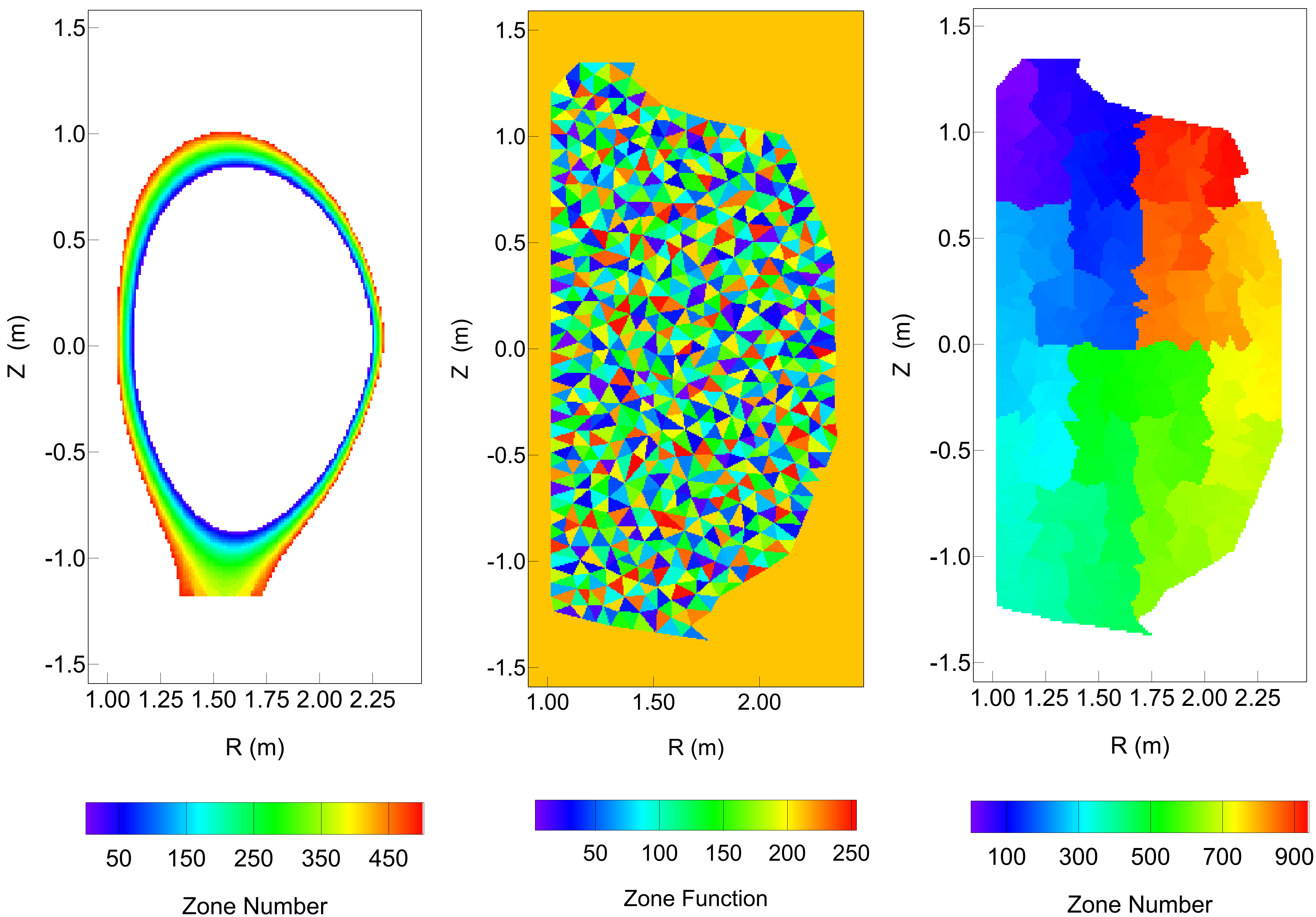
Subsequently, plasma ions are collided with this neutral atom distribution. Ionization creates new ion & electron; CX results in velocity exchange with atom ⇒ updated ion distribution function.



Envisioned Improvements Will Mitigate Shortcomings

- Will be using DEGAS 2 for this work,
  - $\Rightarrow$ more sophisticated atomic physics.
- Vacuum vessel filling mesh $\Rightarrow$ invoke real PMI.
  - Neutral source can be directly tied to ion losses to wall.
  - Can consistently incorporate D_2.
- Include flow velocity $\Rightarrow$ can exchange momentum.
- Make time intervals consistent in both collision routines.

Replace Structured, Flux Surface Constrained Mesh with Unstructured, Vessel Filling Mesh



Design Mesh & Associated Interpolation Scheme to Ensure Mass Conservation

- Use same mesh in both collision routines,
- All quantities scored as integrals over mesh zone volume.
- Ionization rate in a given zone same in both routines:

$$N_{\mathrm{ion}} = \int_{\Delta t} dt \int_{\Delta V} d^3x \, n_e \langle \sigma v \rangle_{\mathrm{ion}} n_0$$

$$\Rightarrow \Delta t \Delta v \langle \sigma v \rangle_{\mathrm{ion}} \left(\sum_{j \in \Delta V} \frac{w_j}{\Delta V} \right) \left(\sum_{k \in \Delta V} \frac{w_{0,k}}{\Delta V} \right) .$$

  - Apart from ion / neutral density variations over time interval between collision routine calls.
  - And statistical deviations due to finite number of particles.
- Careful treatment of time variation & neutral sources also essential.

Other Considerations

- What happens to mass conservation when we introduce D_2?
  - What about adding an impurity (e.g., C)?
- Conservation of momentum & energy?
  - Examining basic equations.
  - Suspect conservation ensured only for simple reaction rates,
  - Can we bound resulting sources / sinks?
- What role does ion diamagnetic drift play?
  - *Not* included in fluid calculations because is nearly divergence-free.
  - Nor does it contribute to currents through sheath in the fluid case.
  - But what about this (kinetic) case?

- XGC-0 can now do electron transport,
  - Describe collisions with cross section rather than reaction rate?
  - Time scales may be $\ll$ atomic collisional / radiative times.
    - $\Rightarrow$ track atomic excited states?
- Investigate completely different approaches?
  - DSMC: track neutrals & ions together; one collision routine.
    - Concerned with statistics.
  - Something else?

Conclusions

- This is a work in progress.

- Will also need verification tests of spatial & temporal discretization.

- And some benchmark verification tests,

  - E.g., from UEDGE.

  - Or Method of Manufactured Solutions?

- Will examine physics results en route.