Coupling plasma and neutral kinetic models: Considerations and solutions

G. J. Wilkie, D. P. Stotler, R. M. Churchill, C.-S. Chang

Princeton Plasma Physics Laboratory

gwilkie@pppl.gov

Summary

- Neutral interactions with the plasma in the scrape-off layer and divertor regions are critical for predicting wall load and detachment.[1]
- The edge gyrokinetic code XGC[2,3] is coupled to the DEGAS2 neutral transport solver[4]
- Ensuring conservation and accuracy for charge exchange interactions is a major challenge due to the non-Maxwellian nature of both ions and neutrals.[5]
- A method for nonlinear interactions (charge exchange and elastic scattering) has been identified and is being implemented.

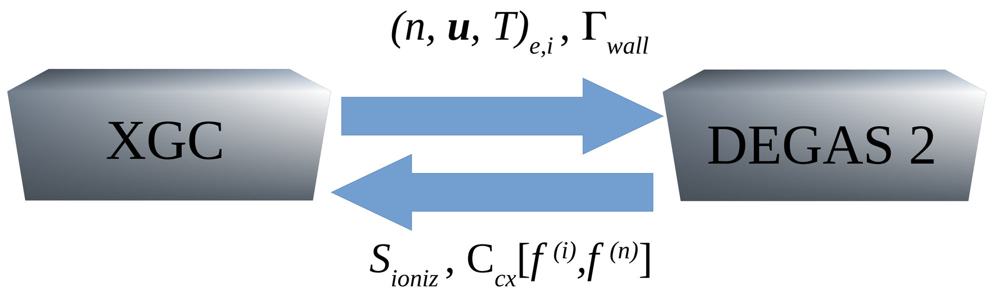
Coupled plasma and neutral kinetic simulation

DEGAS2 solves the Boltzmann equation for moments of the neutral distribution function $f^{(n)}$ with a model BGK operator for nonlinear elastic scattering:

$$\frac{\partial f^{(n)}}{\partial t} + \mathbf{v}\cdot\nabla f^{(n)} = S_{\rm rec} - L_{\rm ioniz} f^{(n)} + C_{\rm el}\left[f^{(n)}\right] + \sum_{s'\neq n}\int\int u\sigma_k(u)\left[f^{(n)}(\mathbf{v}')f^{(s')}(\mathbf{w}') - f^{(n)}(\mathbf{v})f^{(s')}(\mathbf{w})\right]\,\mathrm{d}^2\Omega\,\mathrm{d}^3\mathbf{w},$$

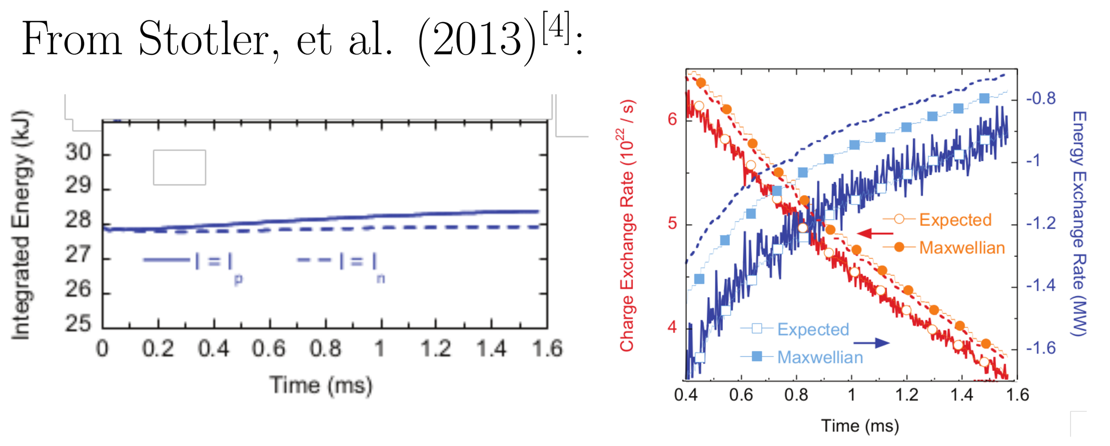
where σ is a scattering cross section, $\mathbf{u} = \mathbf{v} - \mathbf{w}$ is the relative velocity, $S_{\rm rec}$ is the recombination source rate either at the wall or within the plasma, and $L_{\rm ioniz}$ is the ionization loss rate.

DEGAS2 is coupled with modern versions of the XGC gyrokinetic edge code.



Although both are fully kinetic solvers, collisions between plasma and neutrals are treated with Maxwellian targets.

From Stotler, et al. (2013)[4]:



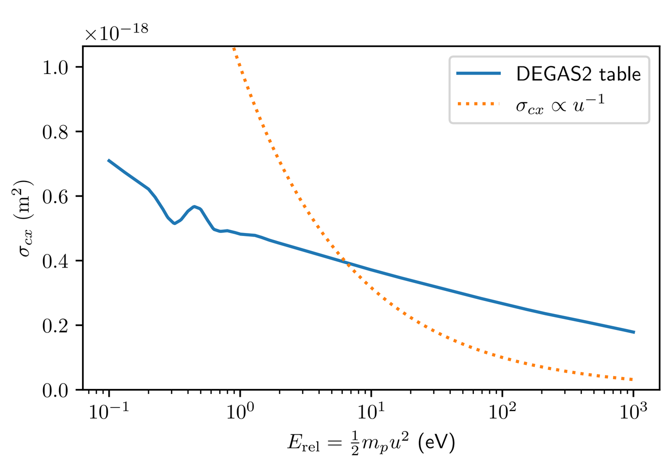
Charge exchange with Maxwellian targets results in lack of energy conservation.

Error in the energy moment for ions colliding off of neutrals represented as an "effective" neutral Maxwellian $F_M^{(n)}$:

$$\mathrm{Err}\left[v^2\right] = \int\int u\sigma_{cx}(u) f^{(i)}(\mathbf{w})\left[f^{(n)}(\mathbf{v}) - F_M^{(n)}(\mathbf{v})\right]\left[w^2 - v^2\right]\,\mathrm{d}^3\mathbf{w}\,\mathrm{d}^3\mathbf{v}.$$

To eliminate this error, the collision kernel $u\sigma_{cx}$ must not depend on neutral velocity $\mathbf{v}$. Possible options:

- Assume ion velocity is much greater than neutral velocity so that $u \approx w$. Even at sufficiently high ion temperatures, this is only satisfied for a subset of neutrals: those newly formed from molecular dissociation that are undergoing their first charge exchange.
- Use a fictitious cross section $\sigma_{cx} \propto u^{-1}$. Inevitably under-estimates interactions at high energy and/or over-estimates at low energy.



Neutral density and mean velocity/energy is not sufficient to inform the ion-neutral collision operator (and vice-versa).

Conservative spectral moment method

Expand the distribution function in an orthogonal basis with $N = M^3$ spectral coefficients:

$$f_\alpha^{(s)}(\mathbf{v}) = \sum_{\alpha=1}^{N} f_\alpha^{(s)}\phi_\alpha(\mathbf{v})$$

where $\alpha = (k_\alpha, l_\alpha, m_\alpha)$ is a compound index and

$$\phi_\alpha(v,\theta,\phi) = A_{k_\alpha l_\alpha} e^{-v^2/2v_{\rm ref}^2}\left(\frac{v}{v_{\rm ref}}\right)^{l_\alpha} L_{k_\alpha}^{l_\alpha+1/2}\left(\frac{v^2}{v_{\rm ref}^2}\right) Y_{l_\alpha m_\alpha}(\theta,\phi)$$

$$f_\alpha^{(s)} = \int \phi_\alpha(\mathbf{v})\, f^{(s)}(\mathbf{v})\,\mathrm{d}^3\mathbf{v} \qquad (1)$$

This basis has been verified for nonlinear Boltzmann collisions in the LightningBoltz prototype, using the Galerkin-Petrov algorithm of Gamba & Rjasanow[6]. It provides an efficient framework for rigorous nonlinear elastic scattering.

To use this basis for conservative charge exchange interactions between ions and neutrals:

- XGC estimates the ion moments (1) from quadrature on the total-f velocity space mesh. Use these to find the total reaction rate.
- DEGAS2 estimates the neutral moments and subsequent changes to the ion moments using Monte Carlo integration.

Set of moments for gyrokinetic ions for a spectral resolution of $N = 27$:

- $\int f^{(i)}\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v^2\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v^4\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v_\parallel\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v_\parallel v^2\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v_\parallel v^4\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v_\parallel^2\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v_\parallel^2 v^2\,\mathrm{d}^3\mathbf{v}$
- $\int f^{(i)}v_\parallel^2 v^4\,\mathrm{d}^3\mathbf{v}$

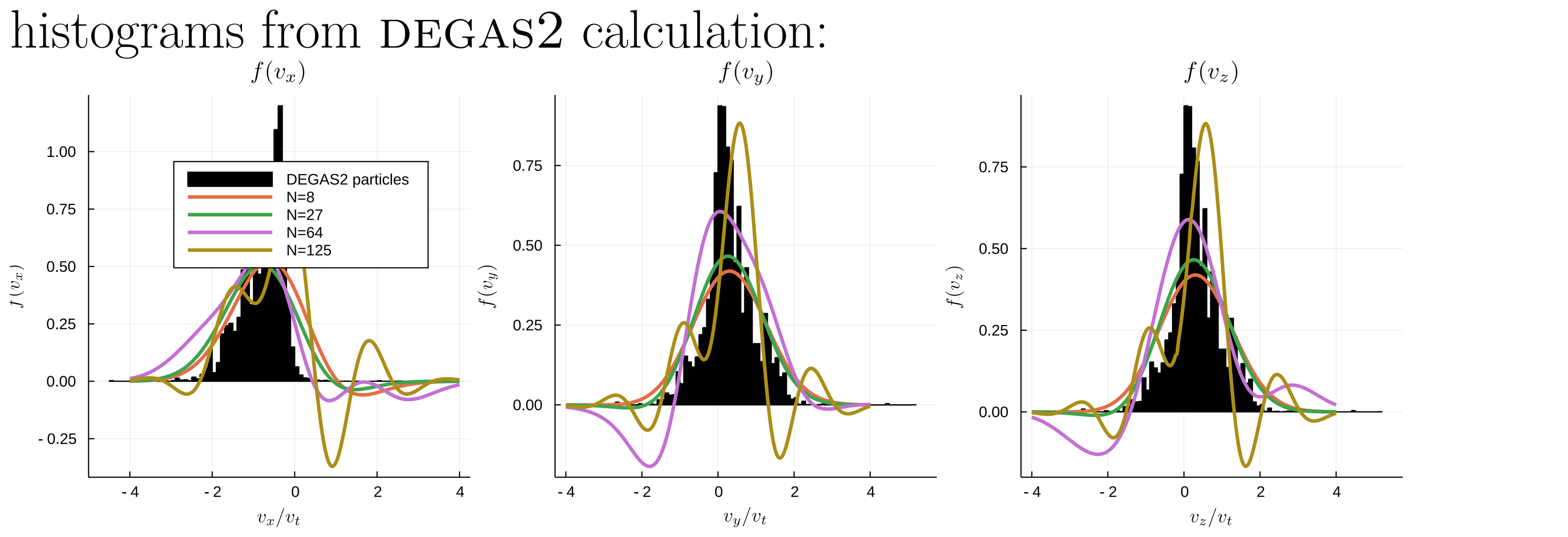
Transform basis to the lab frame and calculate the reaction rate for charge exchange:

$$\nu_{cx}(\mathbf{v}) = \sum_\alpha f_\alpha^{(i)}\int u\sigma_{cx}(u)\phi_{klm}(\mathbf{v}-\mathbf{u})\,\mathrm{d}^3\mathbf{u}$$

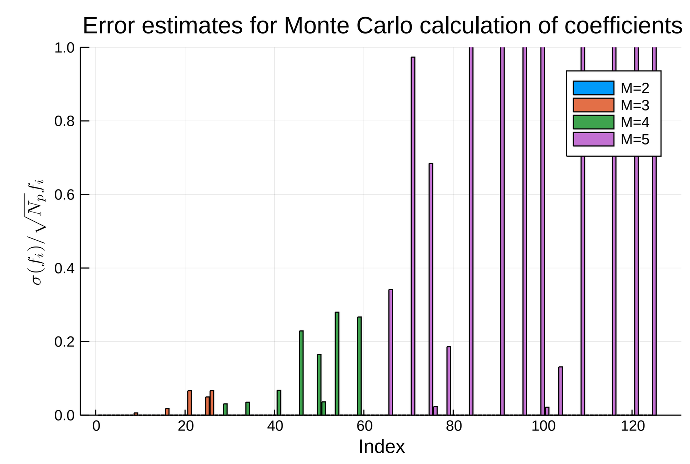
with pre-calculated Gaussian quadrature rules weighted by $u\sigma_{cx}$.[7]

Test feasibility with a sample of 15k neutral trajectories in the vicinity of a C-Mod gas puff.[8]

Reconstructed distributions from moments (1) compared to projected histograms from DEGAS2 calculation:



Relative Monte Carlo error increases for higher-order moments. Estimates accurate to within 10% for $N = 27$.



- Use *equation-free projective integration*[9] (originally developed for transport timescale integration) to find the change to $f^{(i)}(\mathbf{v})$ consistent with changes to the moments $f_{klm}^{(i)}$.

References

[1] Krasheninnikov and Kukushkin. *Journal of Plasma Physics* **83**:155830501 (2017)
[2] Ku, et al. *Journal of Compuational Physics* **315**:467 (2016)
[3] Churchill, et al. *Nuclear Materials and Energy* **12**:978 (2017)
[4] Stotler and Karney. *Contributions to Plasma Physics* **34**:392 (1994)
[5] Stotler, et al. *Computational Science and Discovery* **6**:015006 (2013)
[6] Gamba and Rjasanow. *Journal of Computational Physics* **366**:341 (2018)
[7] Wilkie. PhD thesis, Appendix C (2015)
[8] Stotler, et al. *Journal of Nuclear Materials* **313**:1066 (2003)
[9] Sturdevant, et al. *Physics of Plasmas* **27**:032505 (2020)