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Hybrid gas/plasma simulations using DSMC with the VORPAL code

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14. ABSTRACT

We are adding a Direct Simulation Monte Carlo model to the plasma simulations code VORPAL to model dilute (large Knudsen number) gases. This will allow VORPAL to run hybrid simulations of gas/plasma mixtures using the current plasma simulation capabilities of VORPAL along with the newly added DSMC capabilities. VORPAL is a multidimensional parallel Particle-in-Cell plasma simulation code that supports a variety of models for both the plasma and electromagnetic fields. The DSMC simulation model is built on the existing PIC model by adding a Monte-Carlo collision model and adding the capability to do ensemble averaging. We present here the results of validation tests by comparing VORPAL simulations with an established DSMC code. These include simulations of 1D thermal Couette flow, 1D high speed Couette flow, and 1D heat transfer rate in the transition regime.

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Abstract

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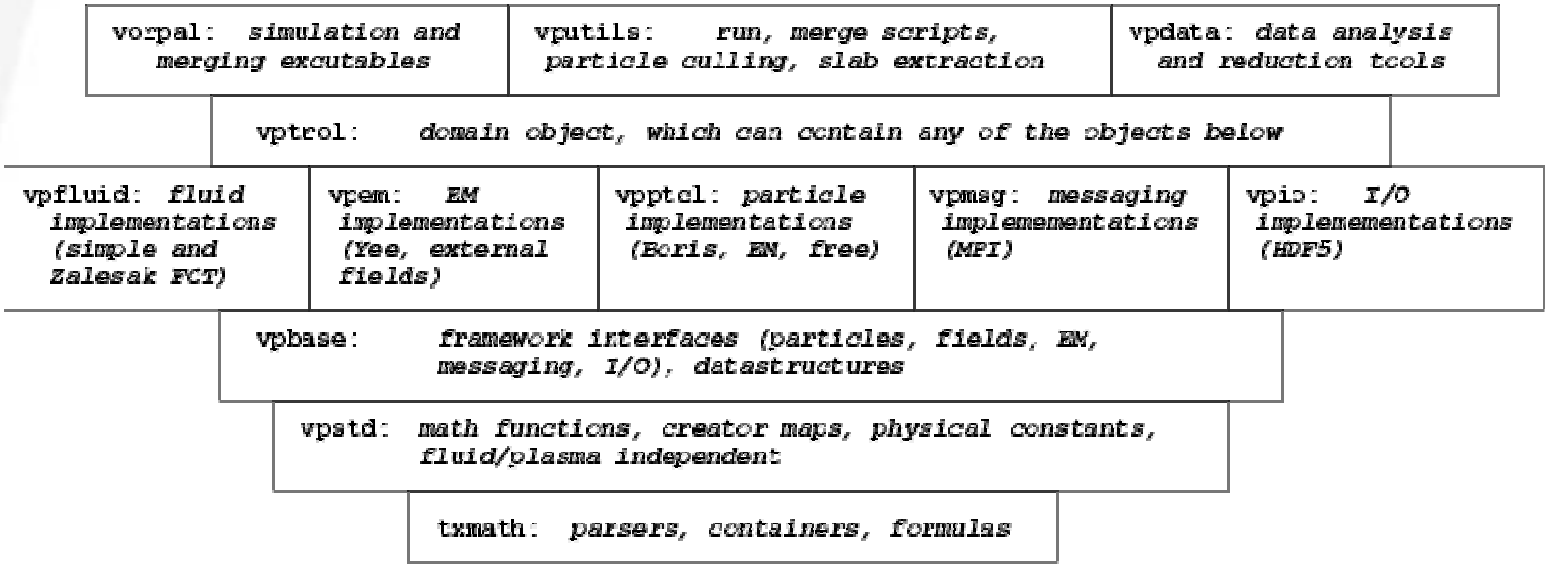
VORPAL's capabilities

- Flexible, object-oriented framework supports plasma simulations with electromagnetics, electrostatics, neutral flow, etc.
- Template meta-programming allows a single code base to support simulations of 1,2 or 3 dimensions.
- Overlap of communication and computational result and effective domain decomposition in good parallel scaling.
- Independent numerical libraries for physics processes (e.g. ionization or secondary emission) extend VORPAL capabilites and allow other codes to benefit.

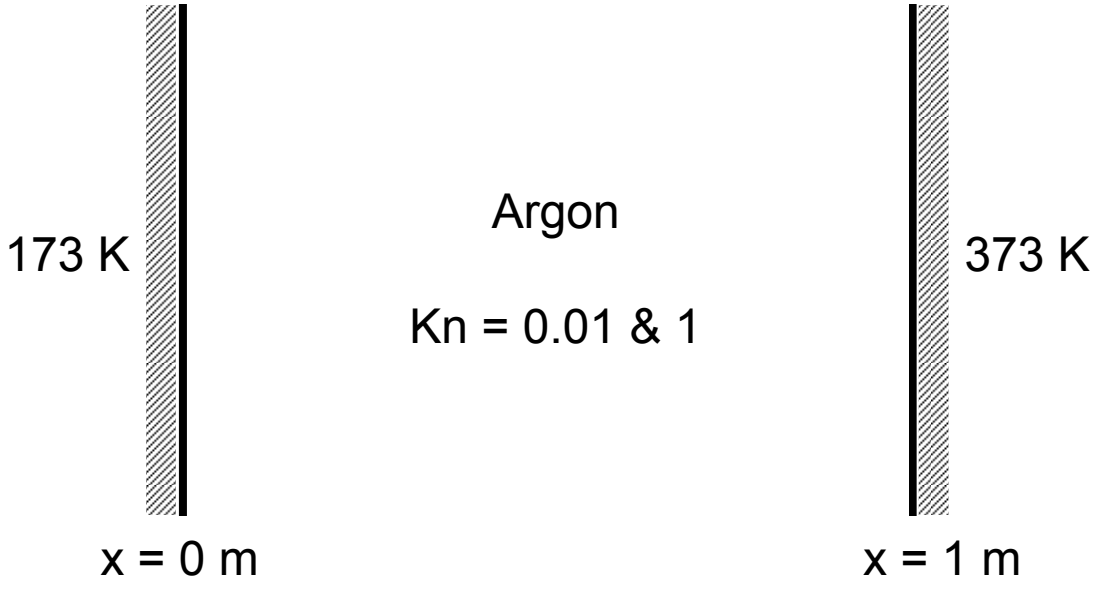
VORPAL's hierarchy



DSMC procedures

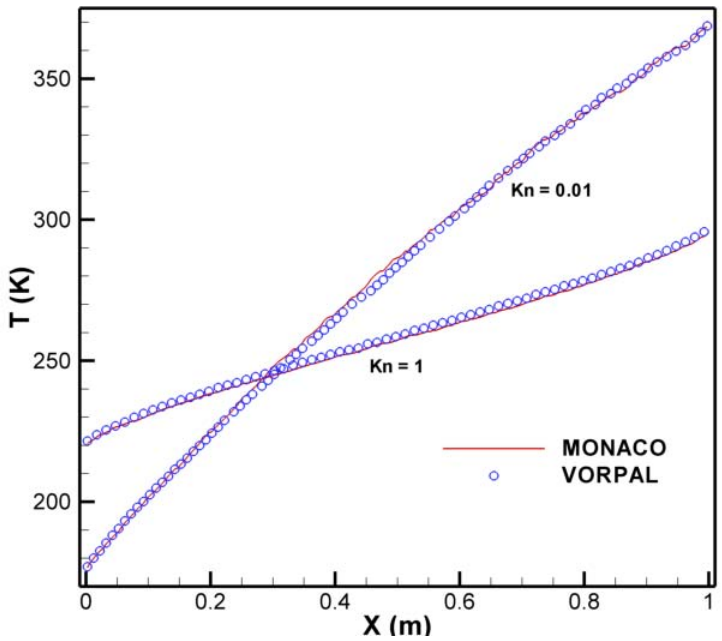
1. Pushing particles without collisions.
2. Performing particle collisions:
   - collision rate: No Time Counter (NTC)
   - collision model: Variable Hard Sphere (VHS)
3. Evolving to the steady (equilibrium) state.
4. Collecting the ensemble averages.

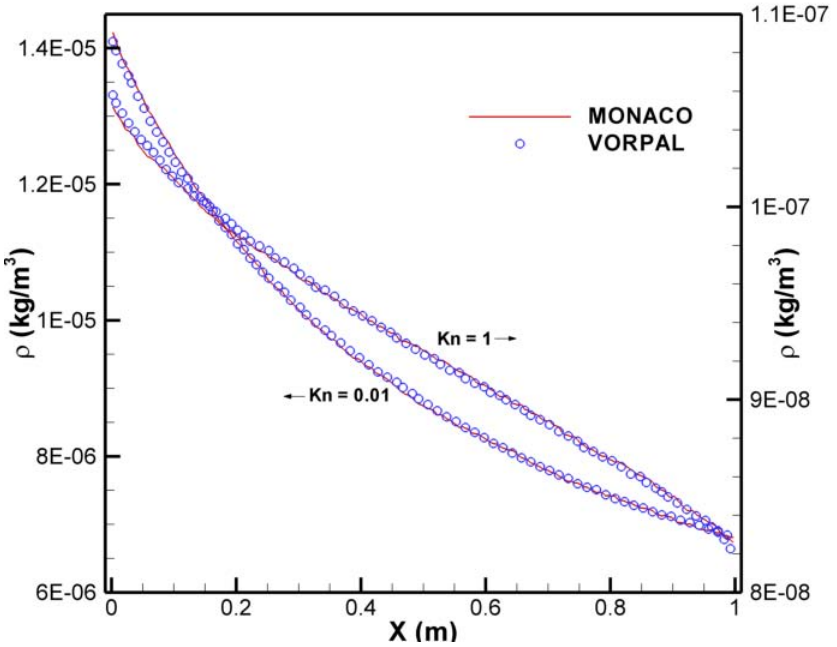
Simulations of 1-D thermal Couette flow



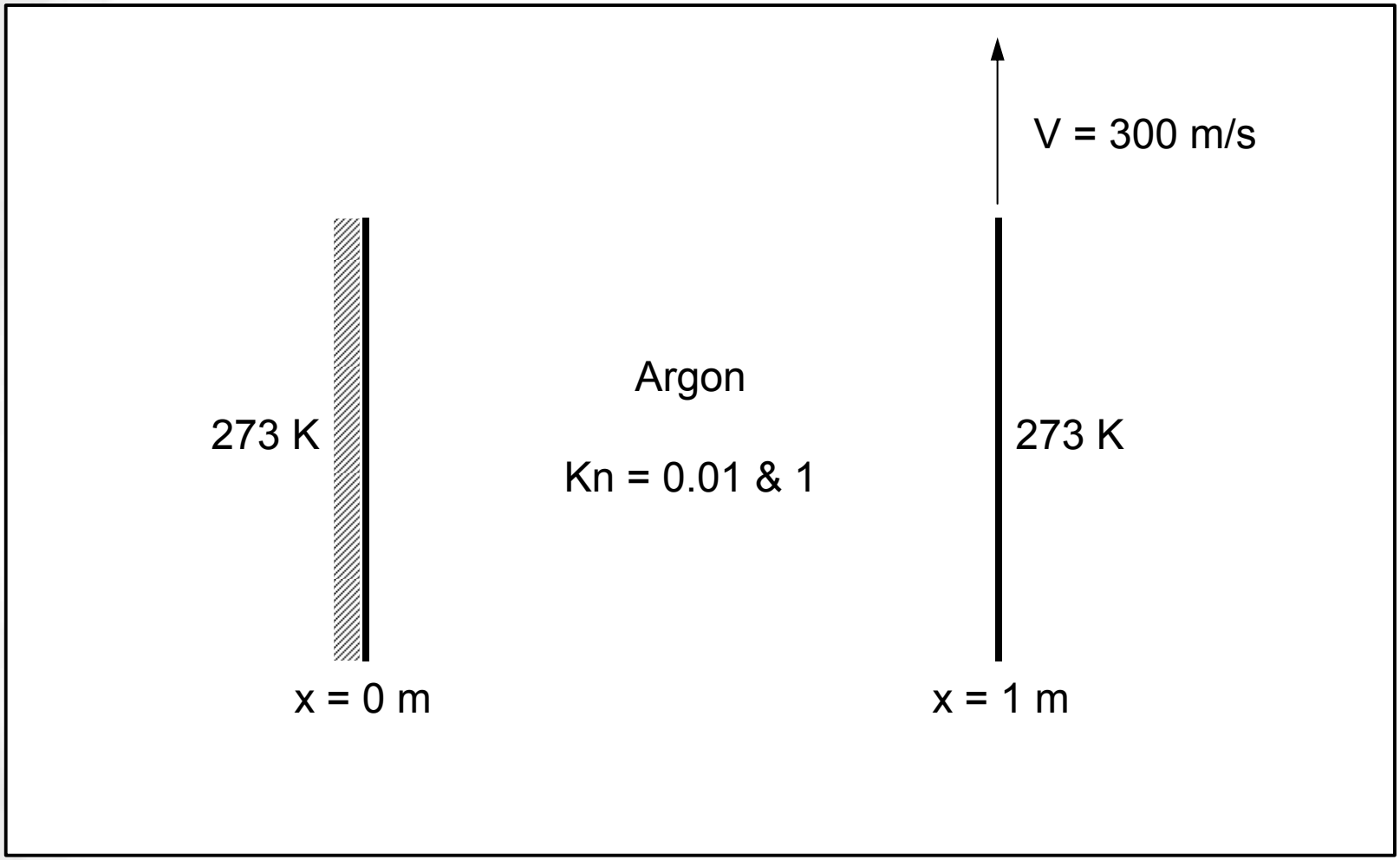
$$Kn \equiv \lambda / L$$

Comparisons of 1-D thermal Couette flow

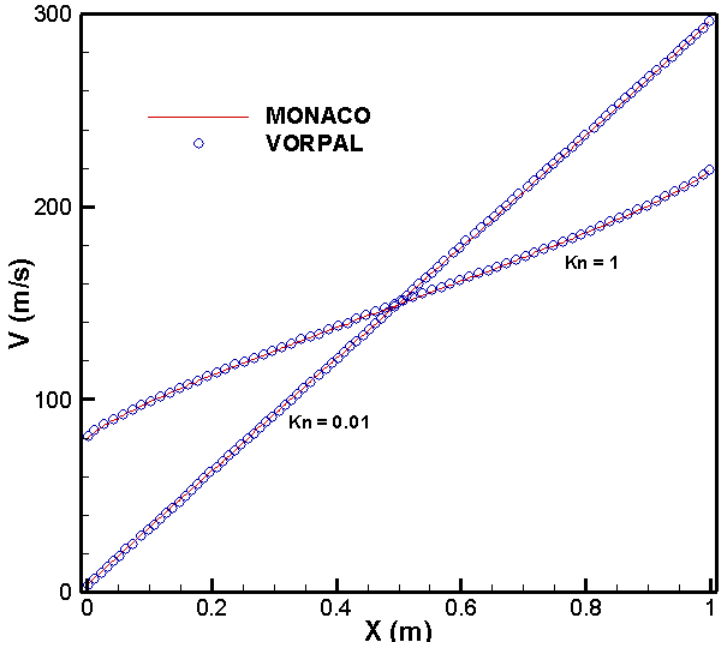


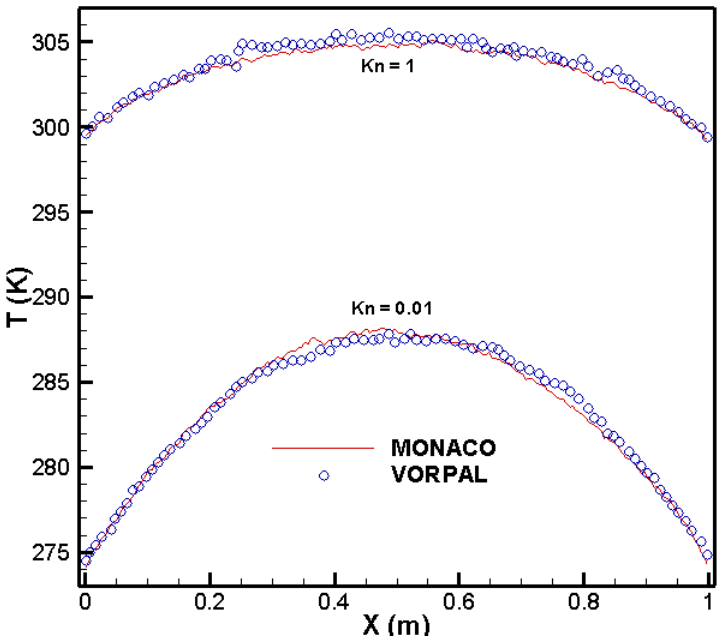


Simulations of 1-D high-speed Couette flow

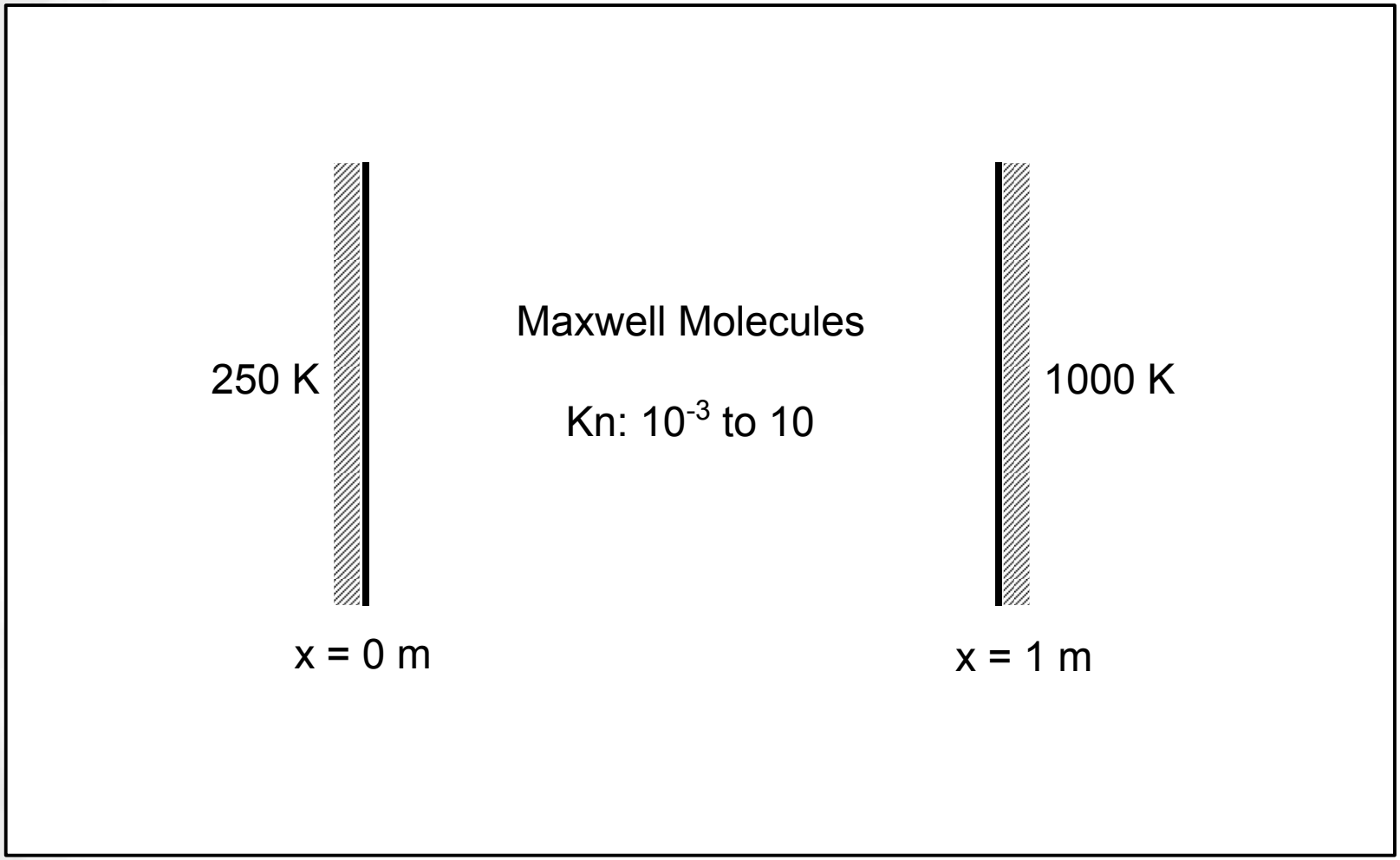


Comparisons of 1-D high-speed Couette flow





Simulations of heat transfer rate in transition regime



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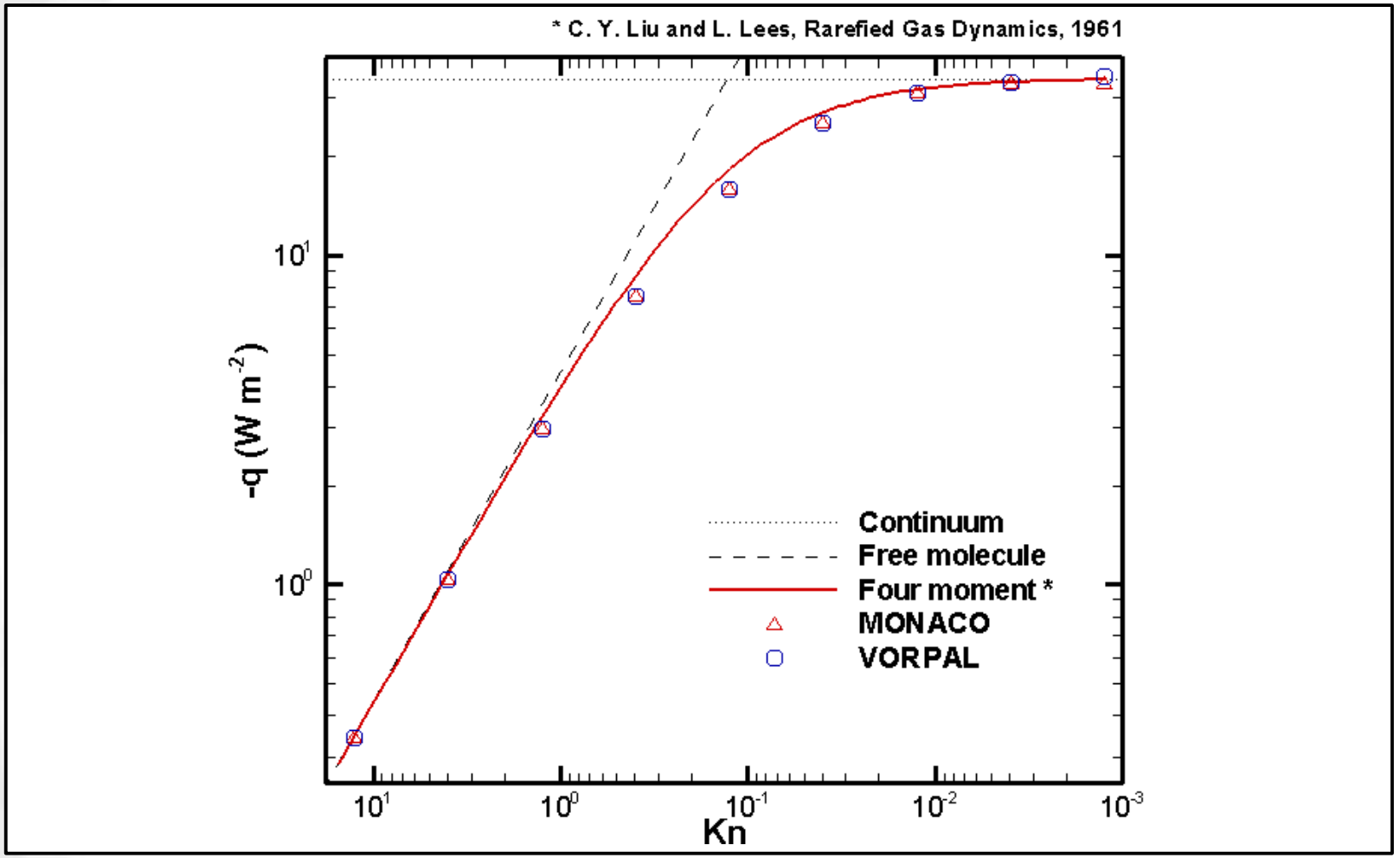

Summary & Conclusions

- Integration of DSMC capability into VORPAL is proceeding well.
- Added capability will result into a highly capable platform for hybrid gas/plasma simulations.
- Numerical experiments for argon gas at high Knudsen numbers have been conducted.
- Verification & validation is being achieved through excellent agreement with a well-established DSMC code.

Future Work

- Performance optimization
- Implementation of internal mode relaxation and chemical reactions
- Continued validation
- Application to selected gas discharges