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Hybrid gas/plasma simulations using DSMC with the VORPAL code

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ICOPS 2005 18 - 23 June 2005, Monterey, California
32nd IEEE International Conference on Plasma Science

Report Documentation Page			Form Approved OMB No. 0704-0188		
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1. REPORT DATE MAY 2005	2. REPORT TYPE	3. DATES COVERED -			
4. TITLE AND SUBTITLE Hybrid Gas/Plasma Simulations using DSMC with the VORPAL Code		5a. CONTRACT NUMBER FA8650-04-C-2511			
		5b. GRANT NUMBER			
		5c. PROGRAM ELEMENT NUMBER			
6. AUTHOR(S) Wen-Lan Wang; Chet Nieter; Peter Stoltz; Jean-Luc Cambier		5d. PROJECT NUMBER OSDB			
		5e. TASK NUMBER R4QP			
		5f. WORK UNIT NUMBER			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Tech-X Corp.,5621 Arapahoe Ave, Ste A,Boulder,CO,80303		8. PERFORMING ORGANIZATION REPORT NUMBER			
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)			
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)			
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES					
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.					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES 13	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

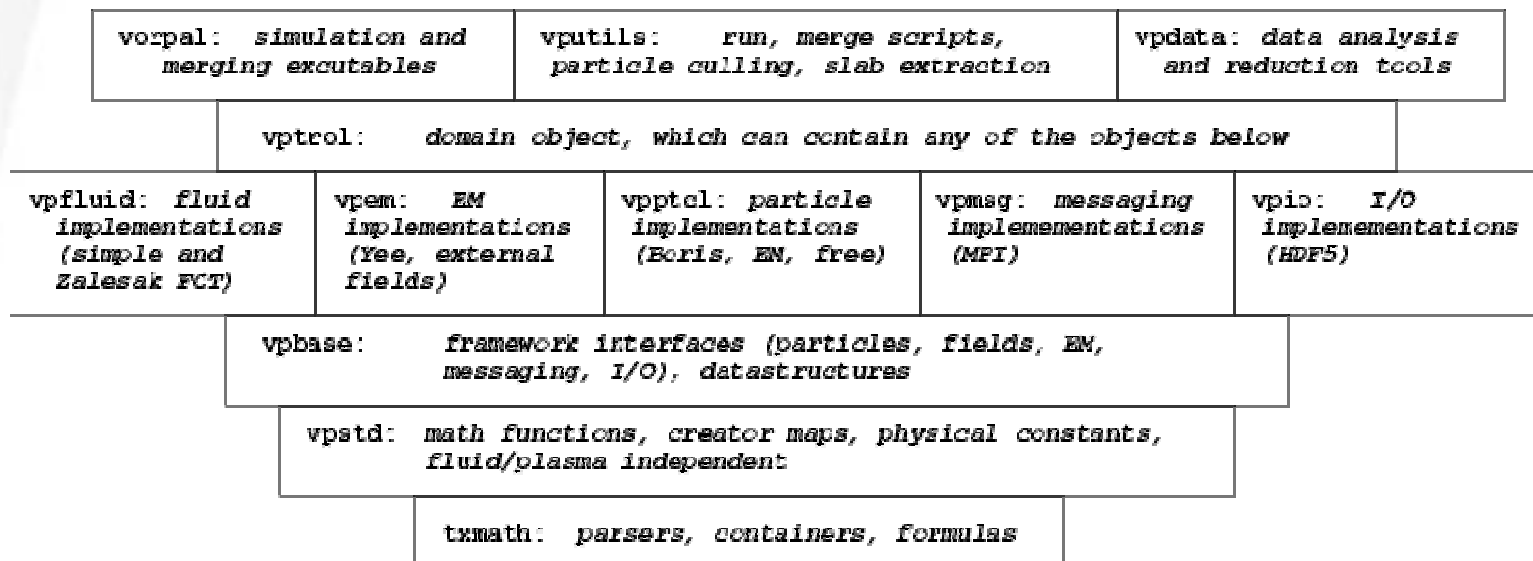
Abstract

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 multi-dimensional, 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.

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 capabilities and allow other codes to benefit.

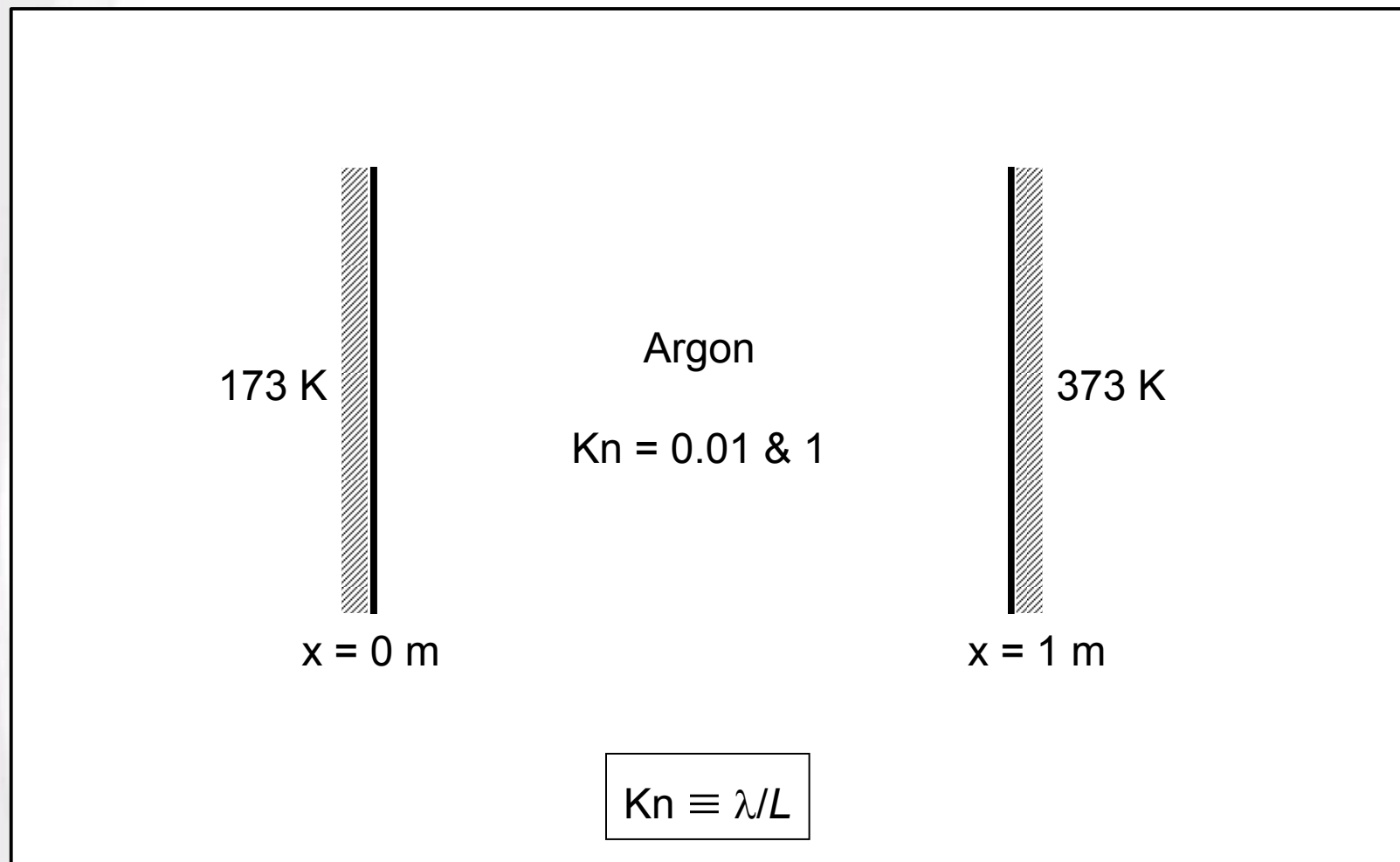
VORPAL's hierarchy



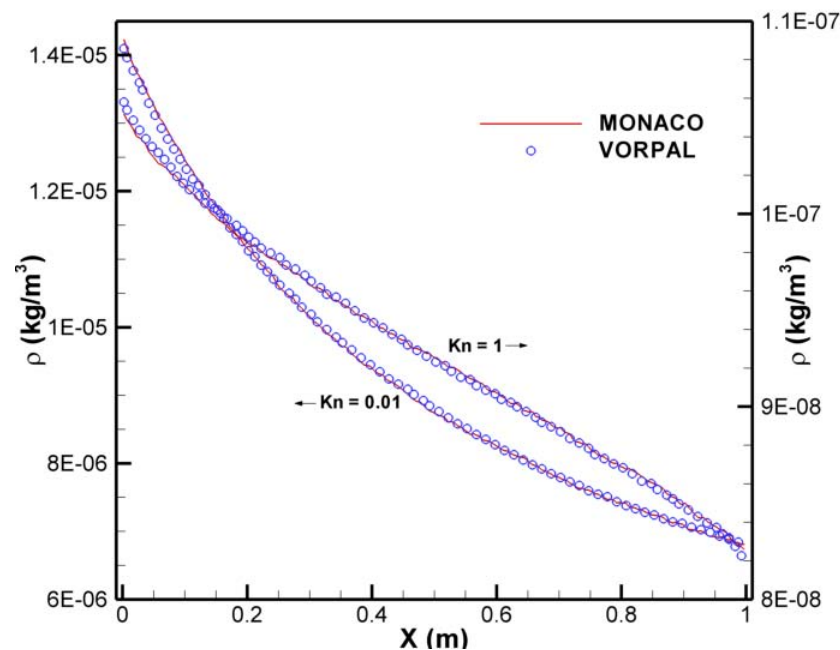
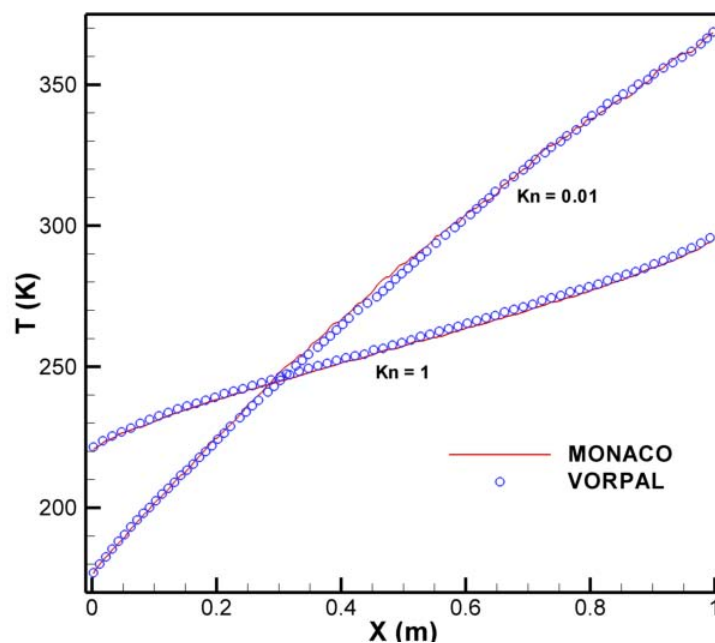
DSMC procedures

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.

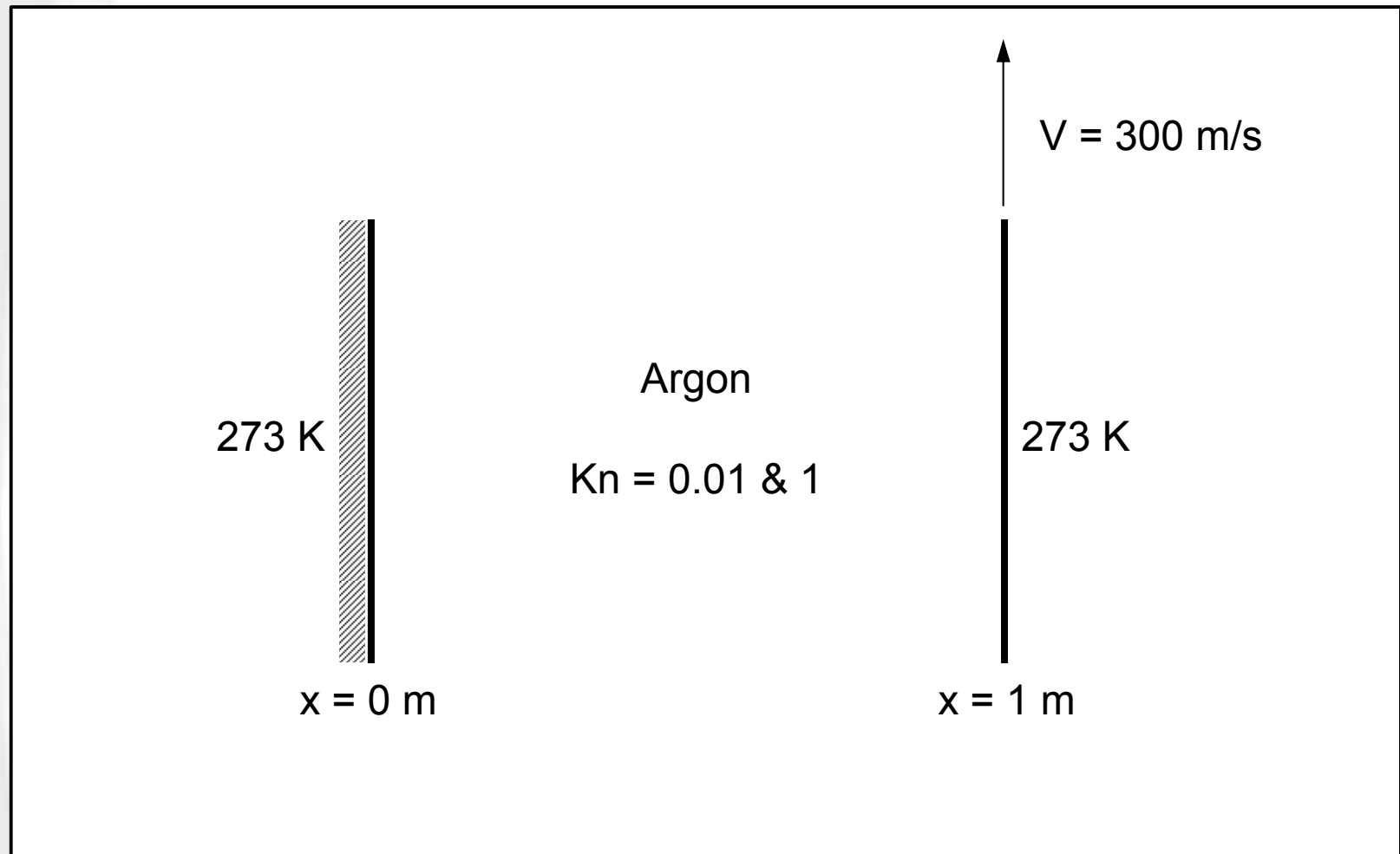
Simulations of 1-D thermal Couette flow



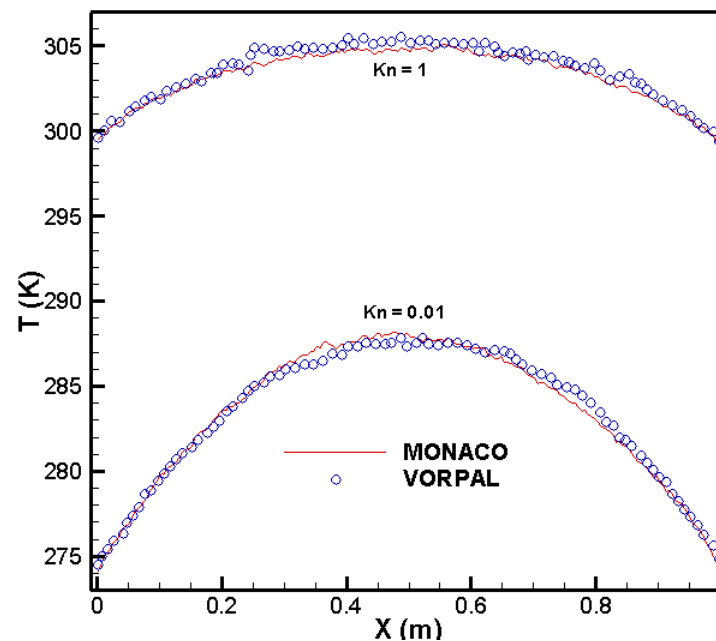
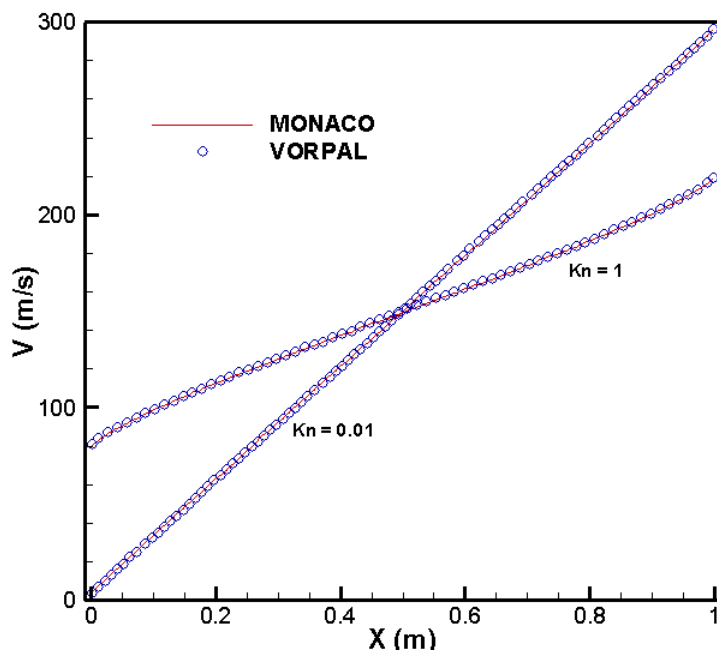
Comparisons of 1-D thermal Couette flow



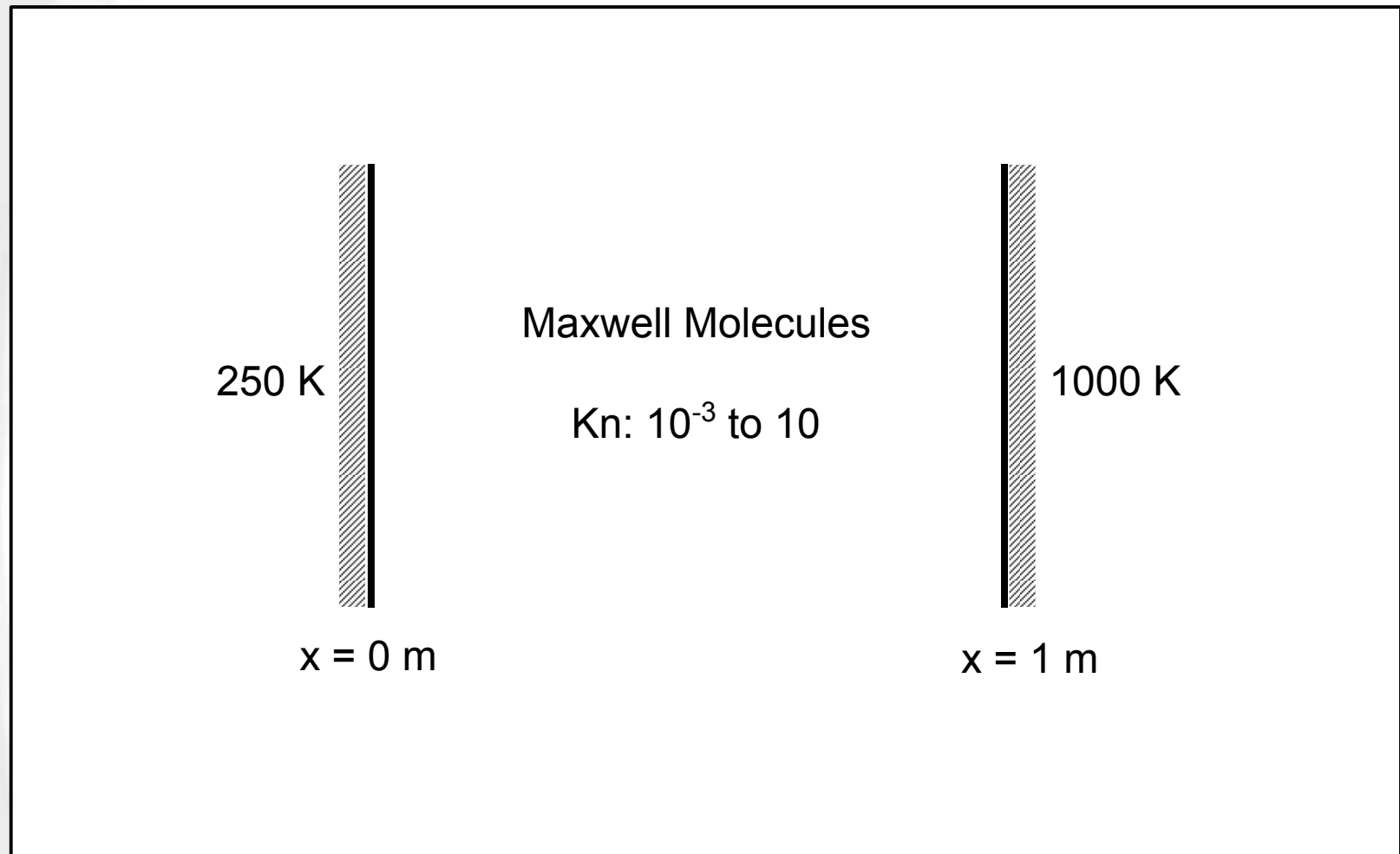
Simulations of 1-D high-speed Couette flow



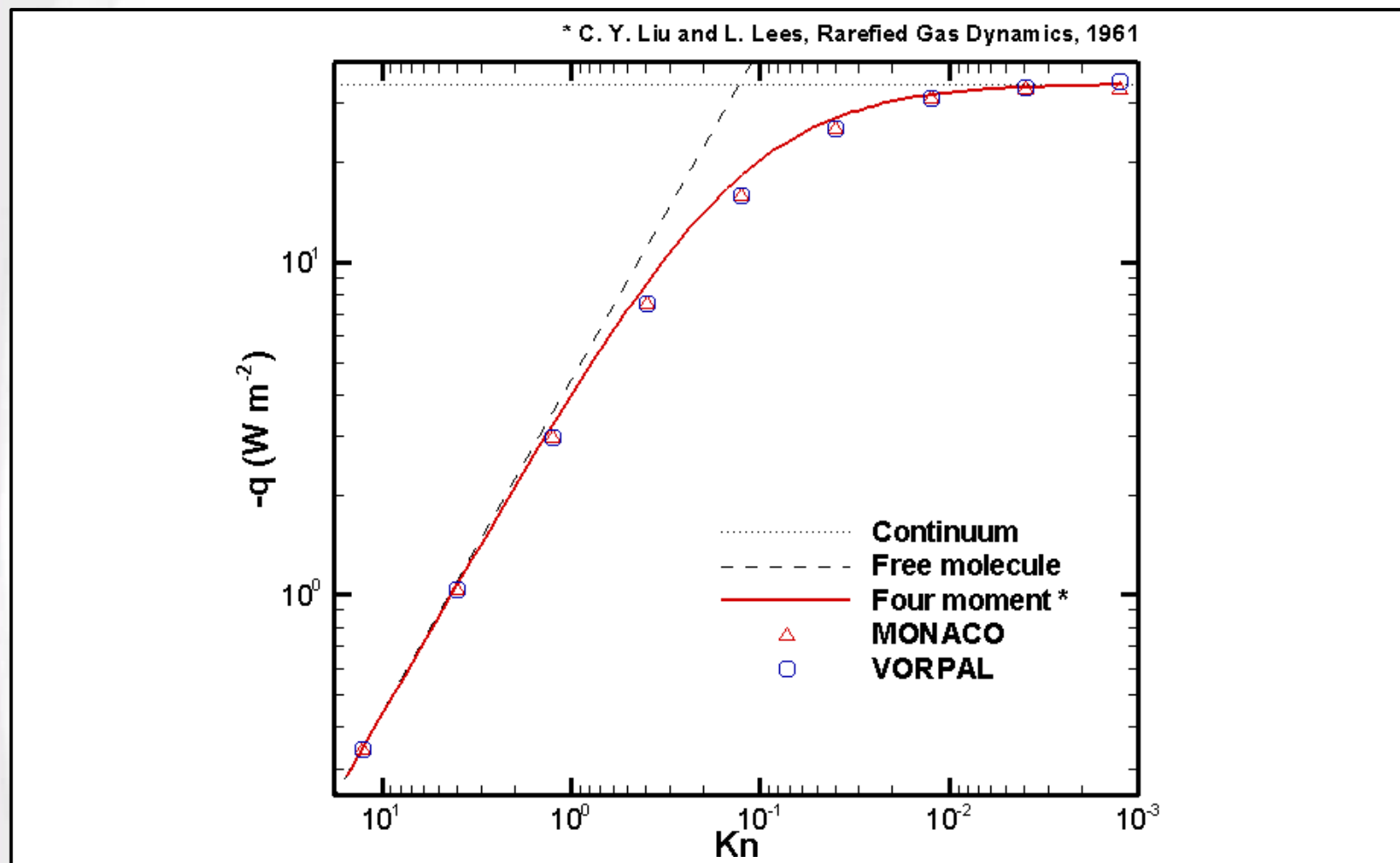
Comparisons of 1-D high-speed Couette flow



Simulations of heat transfer rate in transition regime



Comparisons of heat transfer rate in transition regime



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