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Efficiency of the Sophisticated DSMC Algorithm

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Direct Simulation Monte Carlo: Theory, Methods, and Applications
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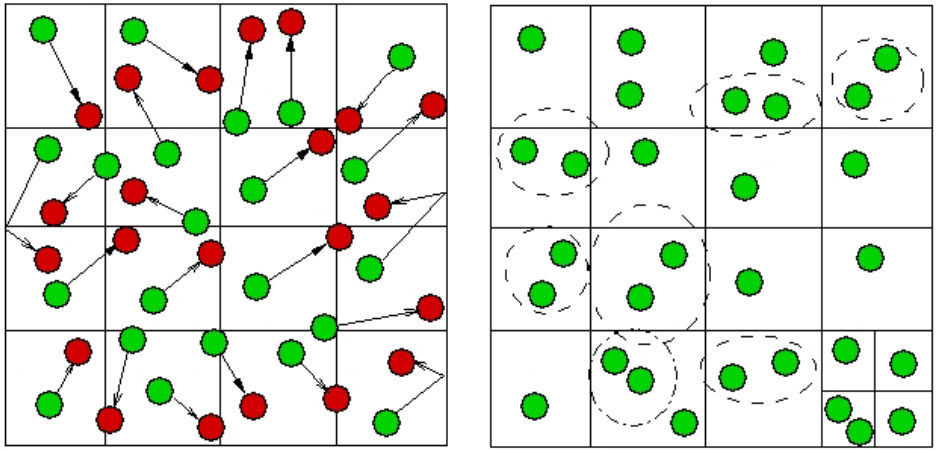
DSMC 1963-2009: The Quest for Speed

- DSMC, being a Monte Carlo method, is computationally intense.
- A new variant of DSMC has been proposed: "*Sophisticated DSMC".*
- The new method is purported to be more accurate but appears to be more expensive than the original method.
- Is the new method computationally more efficient than the old one?
- "Efficiency" is essentially the amount of time that can be simulated with a prescribed accuracy on the same computational platform.

Sophisticated DSMC (DSMC07)

- Basic features of DSMC algorithm retained
  - Move-collide separation, molecular models, collision frequency calculation
- Changes in collide
  - Virtual sub-cells (VSC): nearest-neighbor collisions, N^2 search operation
  - Adaptive transient sub-cells (TASC) based on a background grid (N>30)
  - Exclusion of latest collision partner: physically realistic requirement for VSC/TASC schemes
- Changes in temporal advection
  - Global time step
  - Cell-based time step
- Changes in time-tracking
  - Global time
  - Cell time
  - Molecule time
- Separate sampling and collision cells



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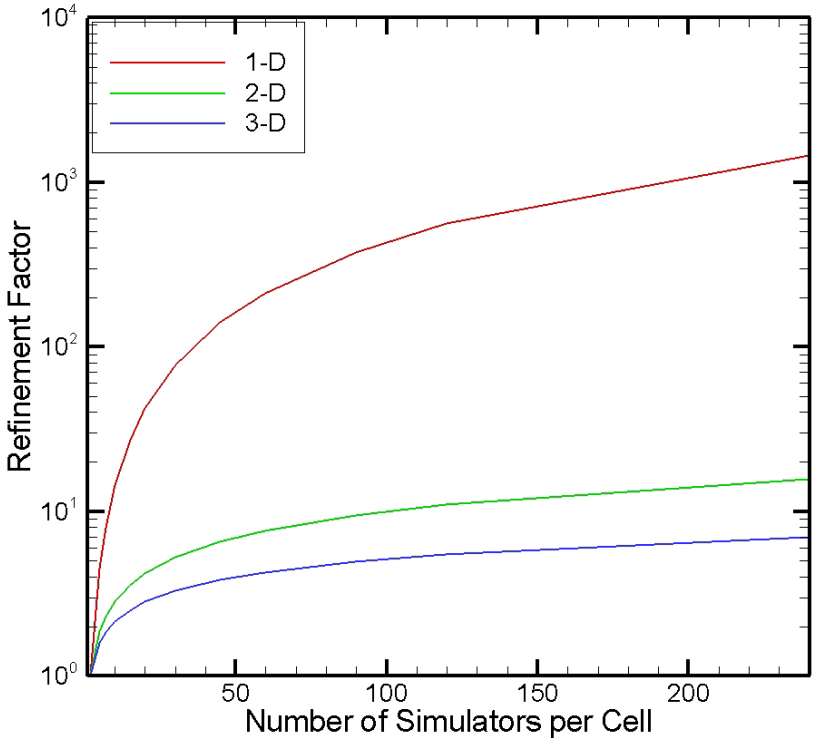
Spatial Discretization
Virtual Sub-Cell Refinement



- The goal of the new procedures is to minimize the MCS/MFP ratio at the lowest possible cost
  - "MCS" is mean collision separation, "MFP" is mean free path
- For DSMC94, MCS/MFP is independent of the number of simulators per cell
- Sub-cell resolution can be achieved using the Virtual Sub-Cell (VSC) collision partner selection method

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Temporal Discretization
DSMC07 Time-Step Properties

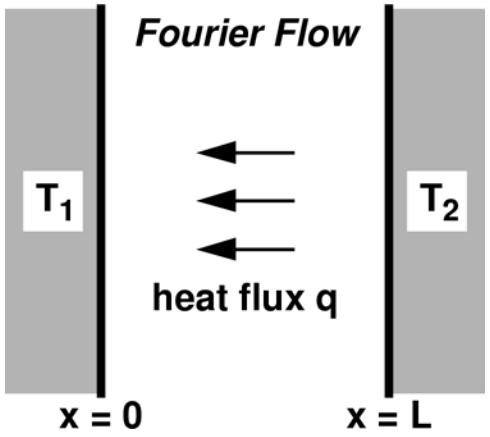
- Local: Cell-based time step (Δt_c): function of the local collision frequency and average molecular speed
- Adaptive: Global time step (Δt_g): function of the smallest Δt_c (adjusted during run)
- Dynamic: Move and collision phases are not synchronized for the whole domain (large low-collisionality regions)

- Collisions are considered for a collision cell
  Move is considered for a particular molecule

- Molecules cannot travel across a sampling cell in one move without considering collisions

- Same pair cannot have sequential collisions

Fourier Benchmark Flow



- Molecules VSS-Maxwell & HS “argon”
- Walls fully accommodating
- Width 0.001 m (1 mm)
- Pressure 264.9 Pa (~2 torr)
  - L/λ ~42
  - t_o 71 ns (at 273.15 K)
  - ΔT 100 K

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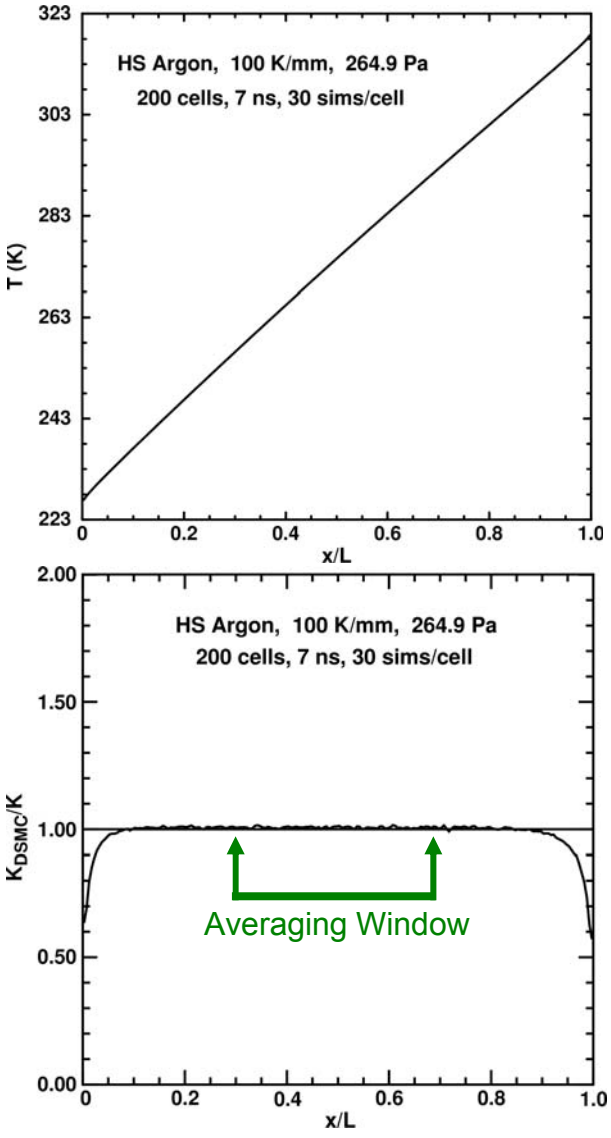
Assessing DSMC07 Requirements



Temperature Profile

- Nearly linear
- Near-continuum
- Small jumps near walls

Thermal conductivity from
CE theory and DSMC94 results

K $\qquad q = K_{DSMC}\left(\frac{\partial T}{\partial x}\right)$

Average over central 40% of domain to obtain a single convergence metric

K_{DSMC}/K

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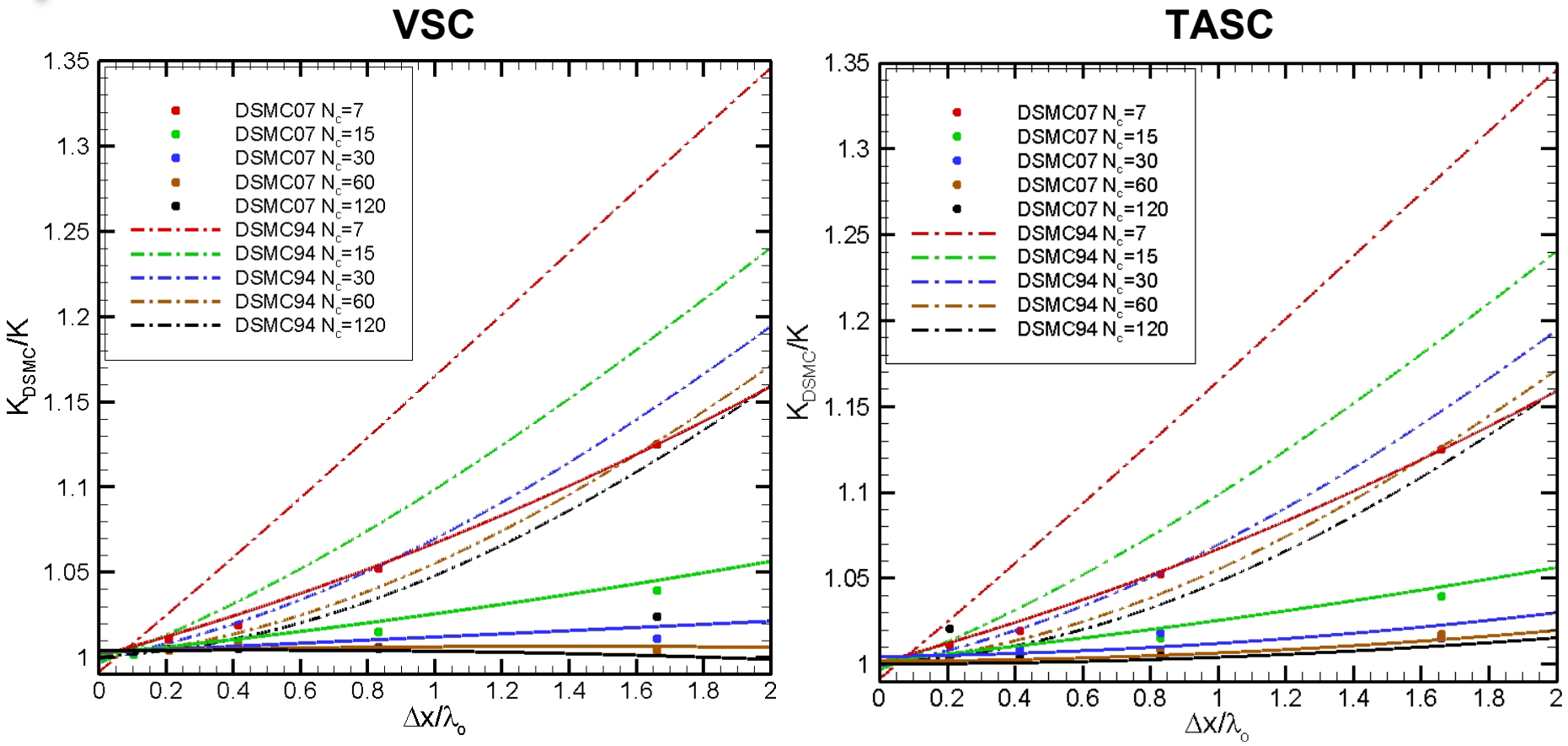
DSMC07 Convergence ($\Delta t/t_o$=10)



- VSC and TASC have similar performance for small Nc
- VSC is more accurate for determining the nearest neighbor for large Nc

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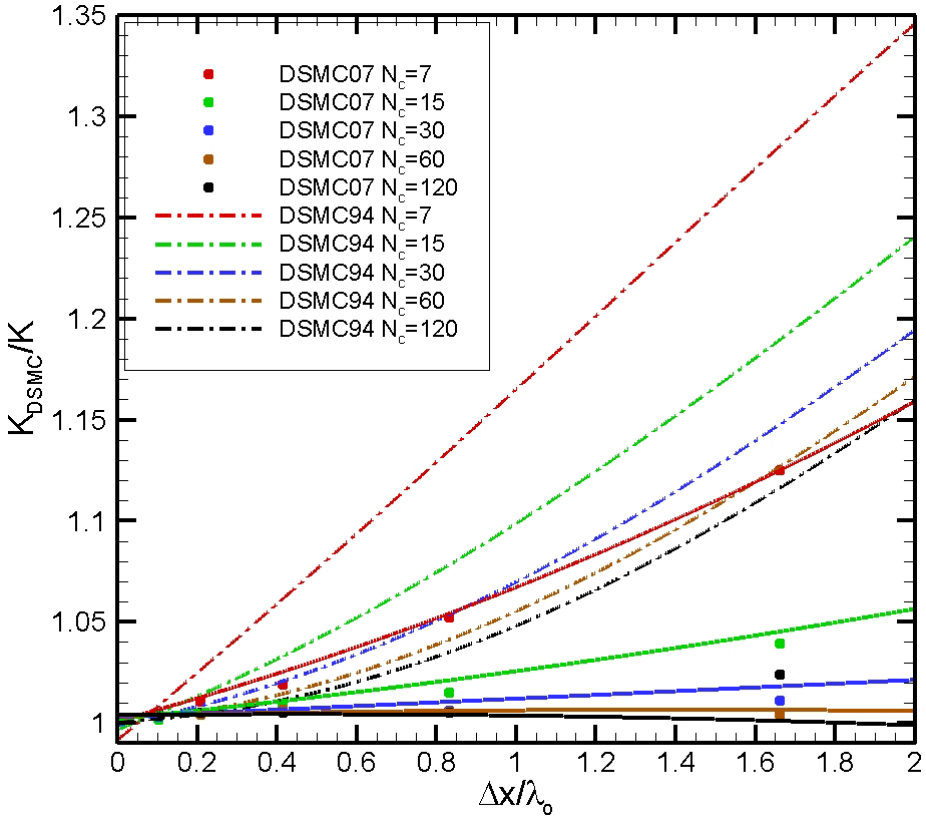
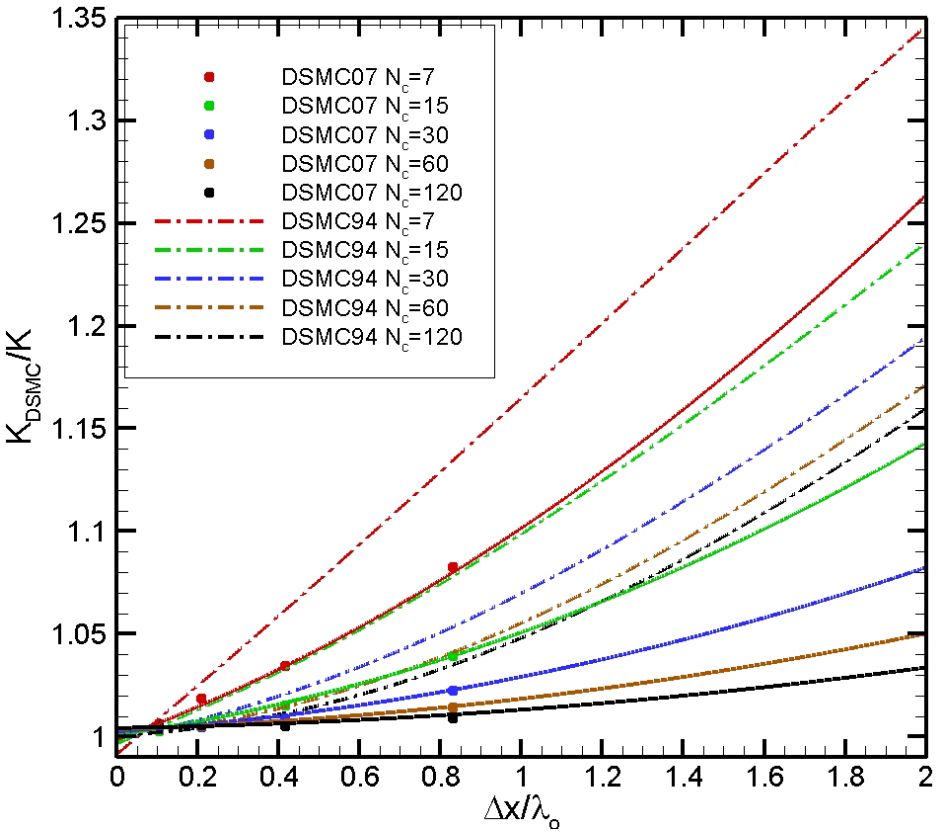
DSMC07-3D Convergence ($\Delta t/t_o$=10)

VSC-1D



VSC-3D



- The 1D domain is replaced with a 1D series of 3D cells.
- Nearest neighbors determined by $ds = \sqrt{dx^2 + dy^2 + dz^2}$
- Increased dimensionality reduces the effectiveness of the scheme.

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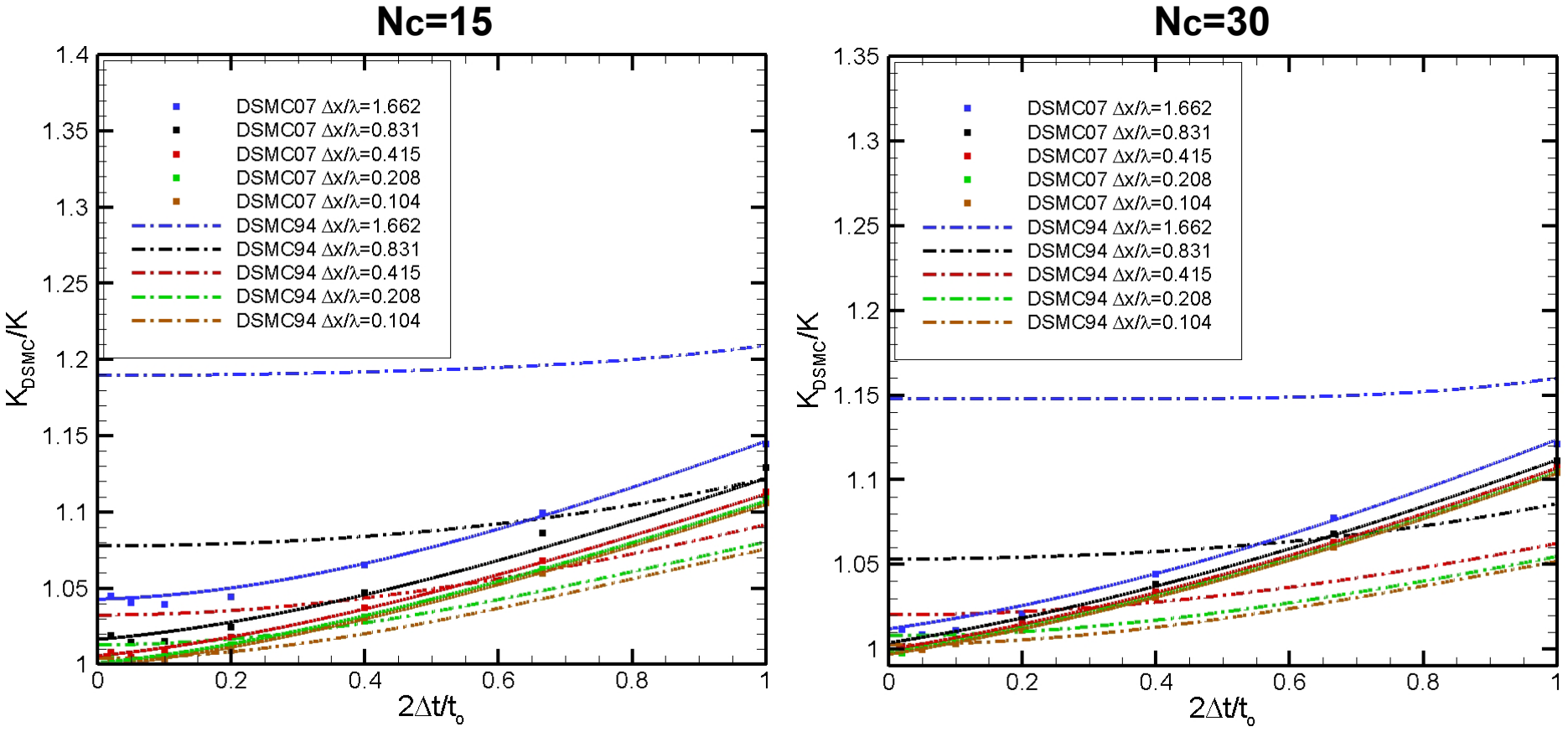
Convergence Behavior for N_c = 15,30
Effect of Time Step



- The algorithm exhibits a near-linear dependence on time step.
- For nearest-neighbor schemes, time step should conform to the effective spatial resolution.

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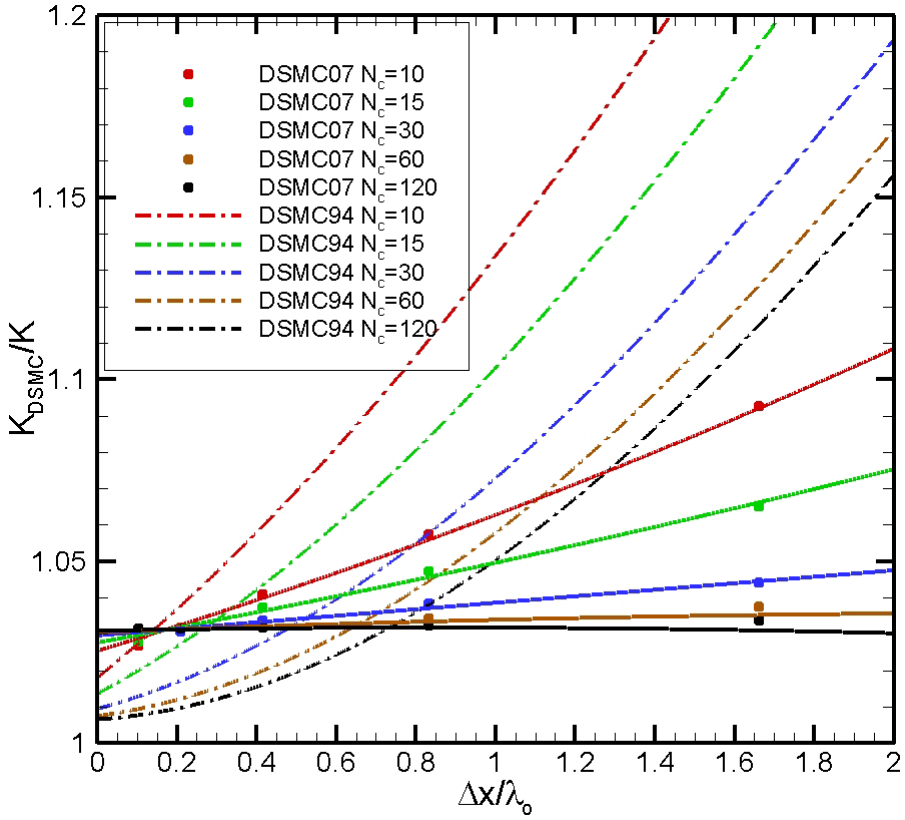
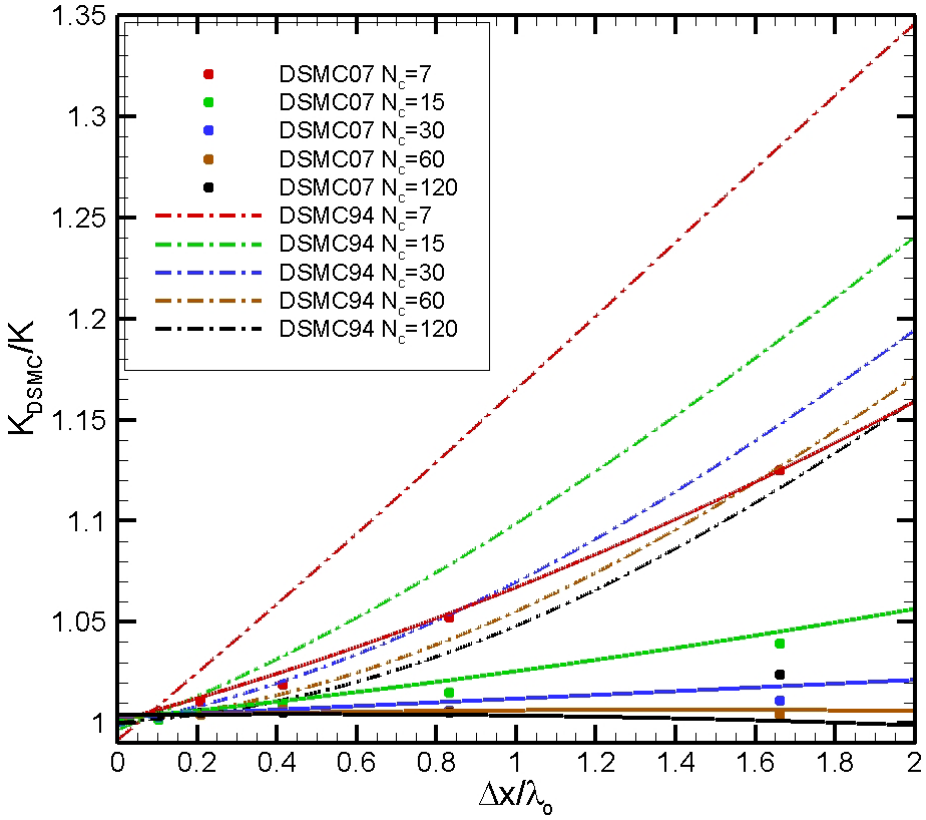
Effect of Time-Step Selection

$\Delta t/t_o=5$



$\Delta t/t_o=10$



- Time-step selection must be based on both
  - Local collision time
  - Local transit time

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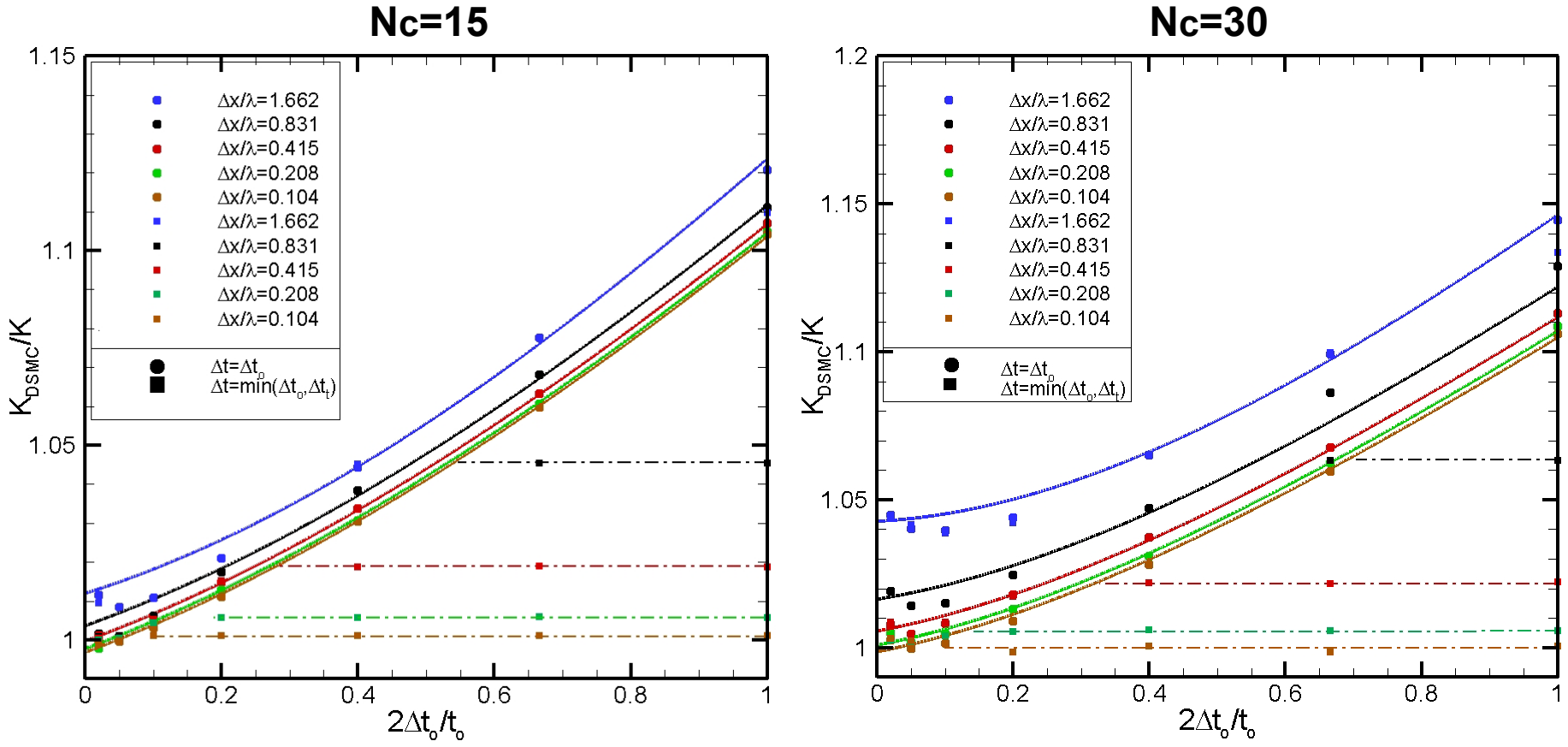
Convergence Behavior for N_c = 15,30
Effect of Time Step



The DSMC07 time step Δt is based on both

- mean collision time t_o, via $\Delta t_o \propto t_o$
- mean cell-transit time t_t, via $\Delta t_t \propto t_t$

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Efficiency of DSMC07-1D

Algorithm	N_c	$\Delta t/t_o$	$\Delta x/\lambda$	Accuracy	Efficiency
DSMC94	15	0.2	0.4	5%	1
DSMC07-VSC	15	0.2	0.8	5%	2
DSMC94-TASC	15	0.2	0.8	5%	3

Algorithm	N_c	$\Delta t/t_o$	$\Delta x/\lambda$	Accuracy	Efficiency
DSMC94	15	0.2	0.01	1%	1
DSMC07-VSC	15	0.2	0.4	1%	4
DSMC94-TASC	15	0.2	0.4	1%	5

- DSMC07 can simulate more physical time when the same accuracy is achieved.
- The high efficiency of TASC relative to VSC is partly due to the 1D nature of the case.
- DSMC07 can achieve the same accuracy as DSMC94 with less resources.

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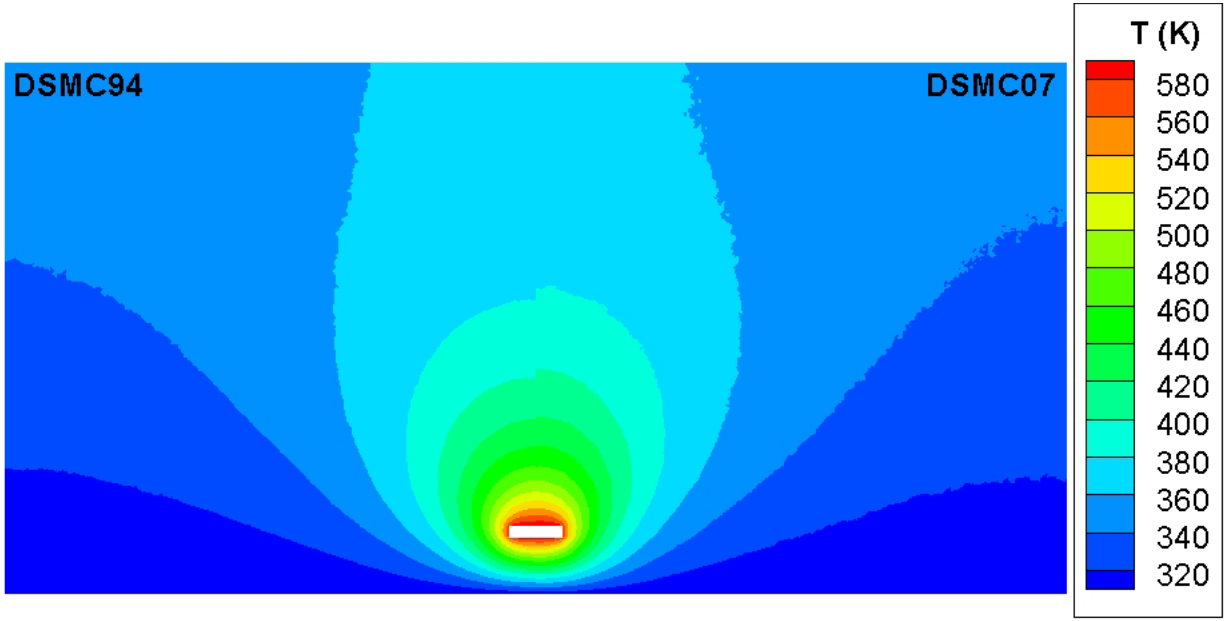
Micro-Fluidic Simulation



Gas	Nitrogen
Pressure	Atmospheric
Substrate Temp.	300 K
Beam Temp.	600 K
Domain Size	100x100 μm

Heat flux between microbeam and substrate is used as the convergence metric

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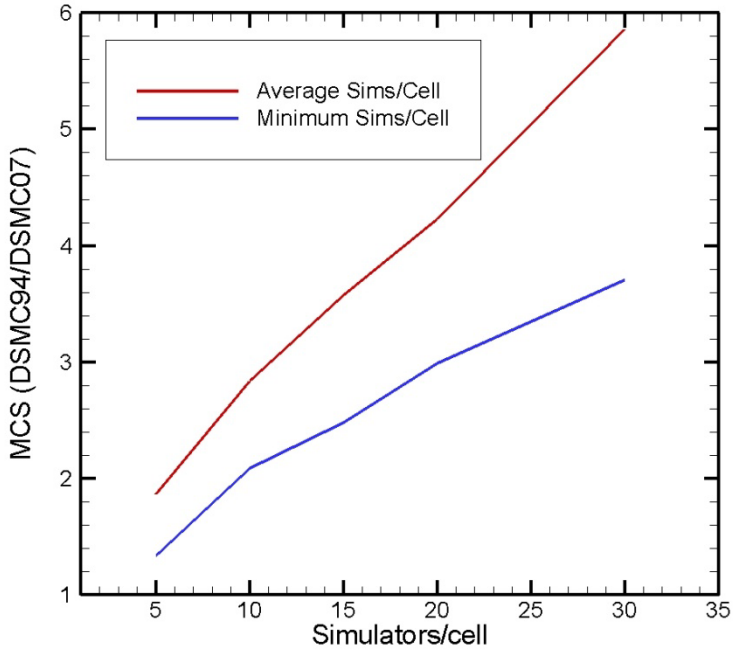
Spatial Refinement Using Cells and Simulators

Number of Cells	Simulators/Cell
160,000	5
160,000	10
160,000	15
160,000	20
160,000	30
160,000	10
640,000	10
2,400,000	10



Goal: minimize MCS for the lowest computational cost

The calculation was refined using as a parameter:

- **Simulators per cell (DSMC94 indifferent, DSMC07 strongly influenced)**
- **Number of cells (both DSMC94 and DSMC07 similarly influenced)**

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DSMC94 and DSMC07 Simulation Speed when Achieving Equal Accuracy

DSMC94 MCS = DSMC07 MCS							
DSMC94				DSMC07			
# Cells	Sims/cell	W/m	ns/proc-hr	# Cells	Sims/cell	W/m	ns/proc-hr
640,000	10	17.34	18.50	160,000	10	17.47	45.54
2,400,000	10	14.94	3.12	160,000	30	15.04	10.43

Accuracy is largely controlled by Mean Collision Separation (MCS)

- DSMC94: MCS is set by cell size alone
- DSMC07: MCS is set by cell size and sims/cell

DSMC07 simulates 2-3 times as much physical time as DSMC94

- At the same level of accuracy (equal MCS values) per processor-hour
  - Same heat flux obtained by both algorithms for each case
- With much smaller memory/machine requirements (fewer simulators)

Many other cases (not shown) confirm this observation

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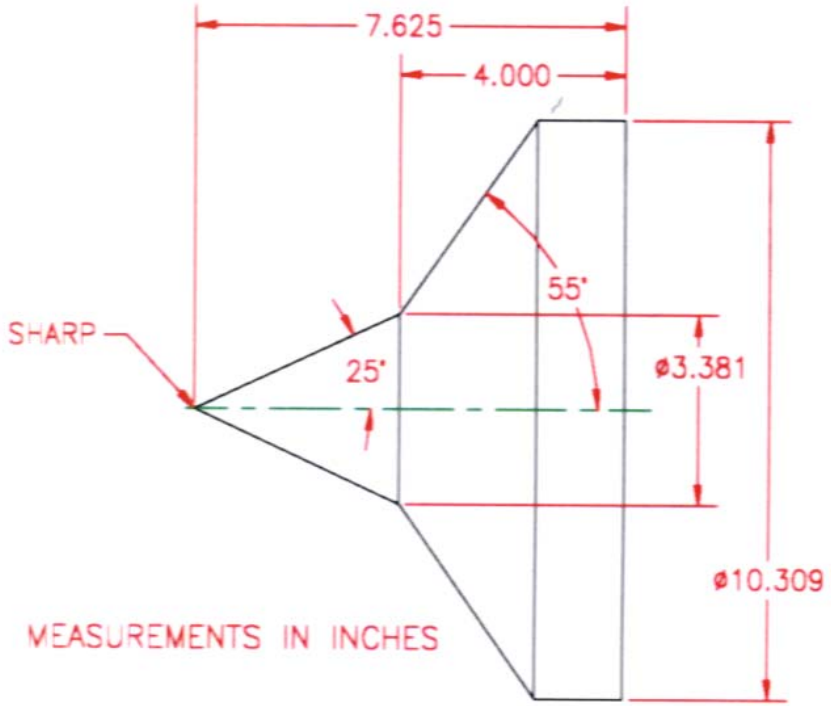
Hypersonics Simulation
Mach 11, 25-55 Biconic

Flow Conditions

- Nitrogen gas
- *Re* = 140,000/m
- T_0 = 3280 K
- *V* = 2072 m/s
- *Kn* = 0.02
- *M* = 11.3
- *T* = 42 K
- T_{vib} = 1983 K



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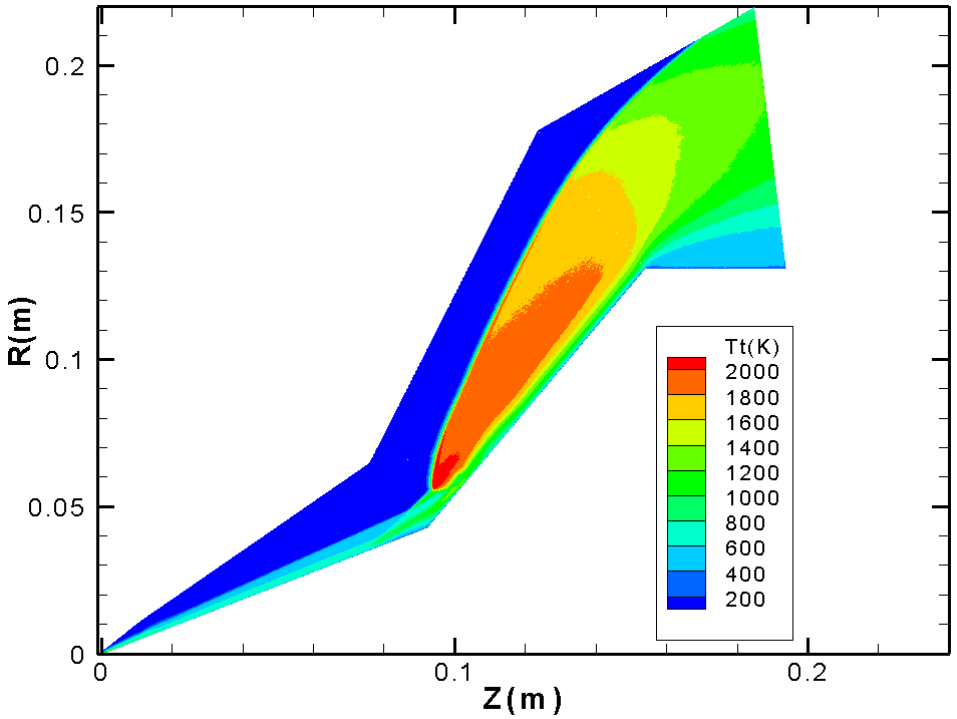
Simulation Details



Goal: optimize simulation at the lowest computational cost

The calculation was refined using the number of cells as a parameter.

Simulation Parameters:

Sims per cell:	**10**
Time step:	**2.5 ns (min)**
Cells:	**10^6, 2.5×10^5**

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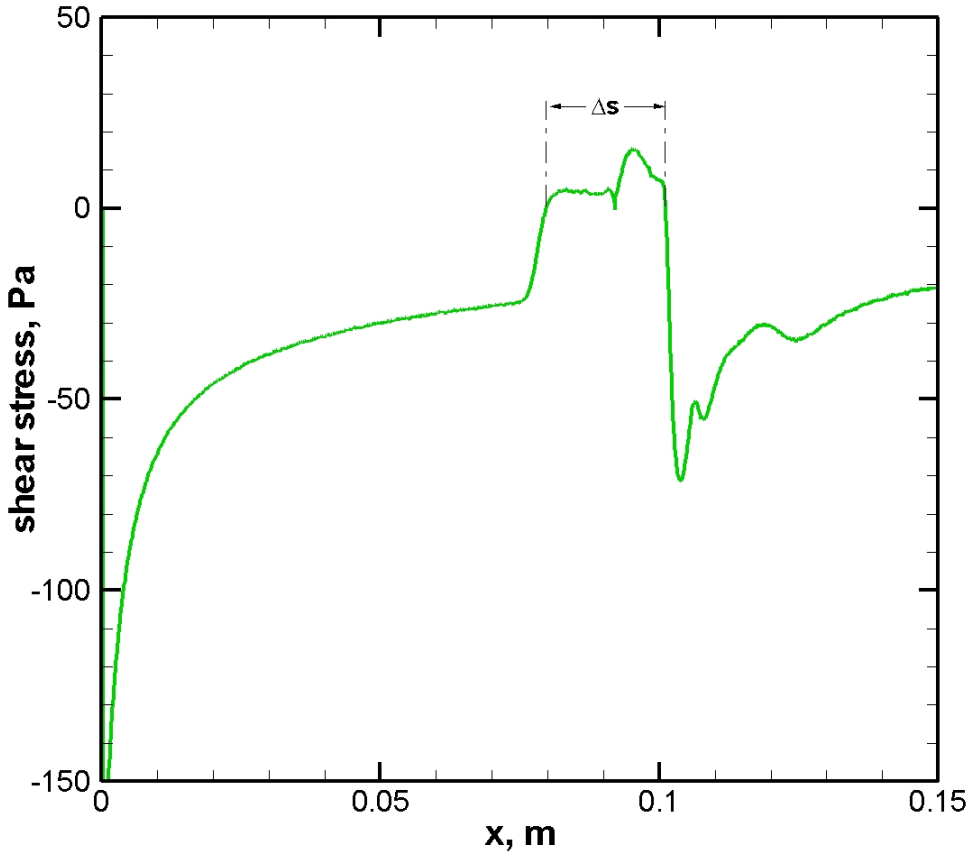
Recirculation Zone



Extensive studies (Moss, Markelov) indicate that the extent of the recirculation zone is Δs = 21.5 mm.

Δs is sensitive to discretization parameters and is used as a convergence criterion.

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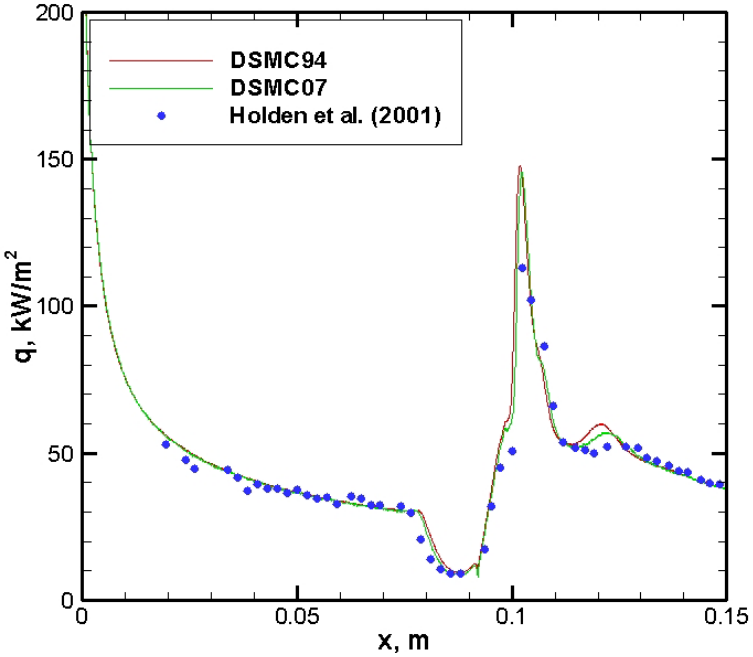
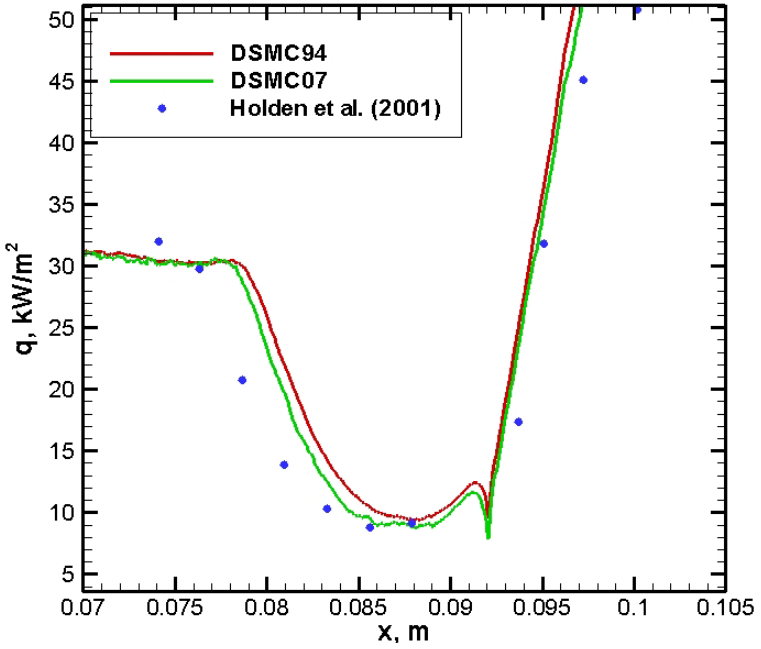
DSMC94 and DSMC07 Simulation Speed when Achieving Equal Accuracy





DSMC94 MCS = DSMC07 MCS							
DSMC94				DSMC07			
# Cells	Sims/cell	Δs Error (%)	ns/proc-min	# Cells	Sims/cell	Δs Error (%)	ns/proc-min
250,000	10	24.19	8.72	250,000	10	5.58	5.61
1,000,000	10	5.58	1.48	1,000,000	10	0.00	1.01

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Conclusions

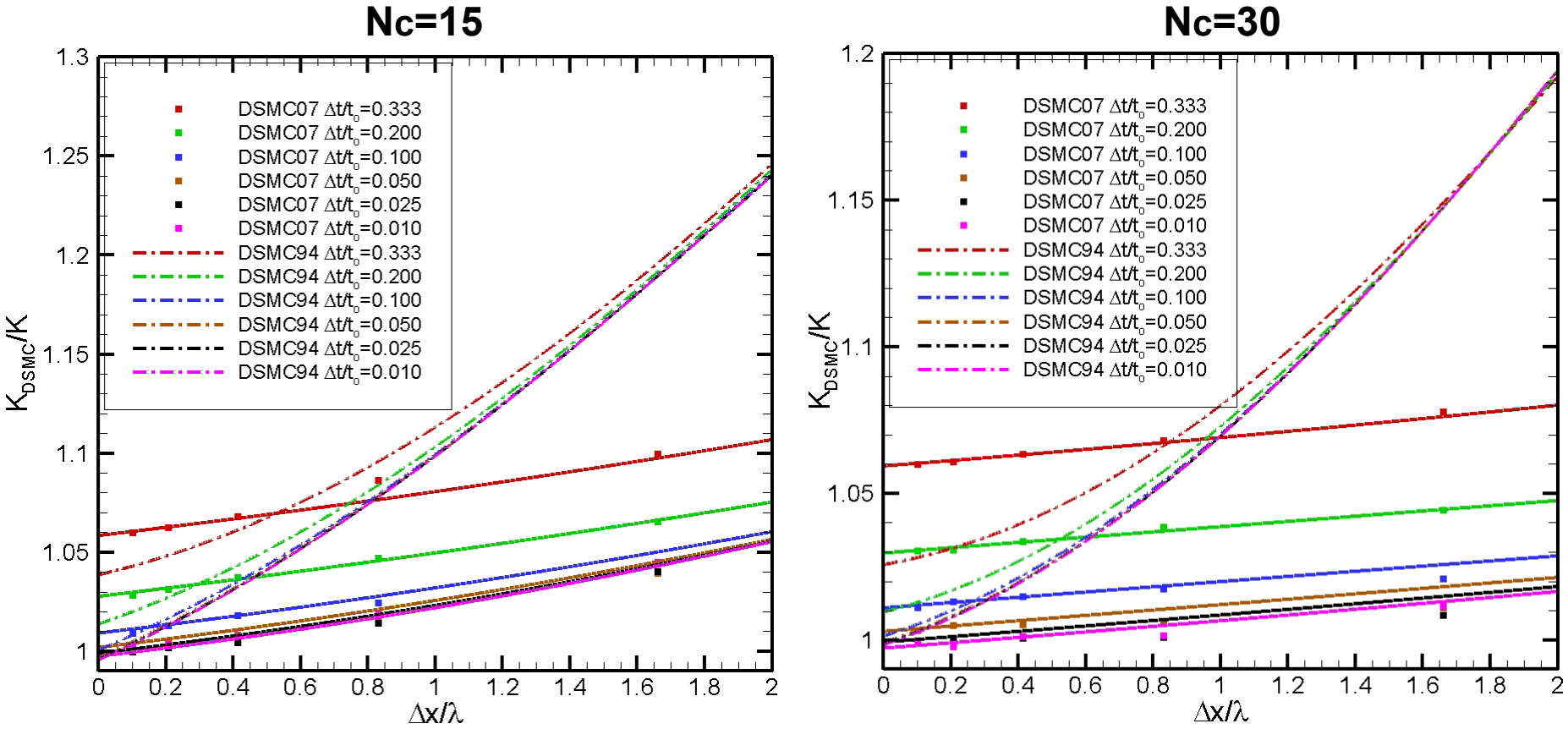
The efficiency of the new DSMC algorithm was investigated.

- Error has weak dependence on cell size (~10% of GK theory).
- Error has strong linear dependence on time step.
- Particular attention must be paid to the selection of time-step.
  - Local time-stepping may be the only viable alternative.

Efficiency is improved by a factor of

- 4-5 for 1-D
- 2-3 for 2-D
- 2-3 for 2-D axi-symmetric

Convergence Behavior for N_c = 15,30
Effect of Cell Size



- For finite number of simulators, the algorithm is
  - Insensitive to spatial resolution.
  - DSMC07 error is lower than DSMC94 when
  - $\Delta t/t_o \leq 0.1$ (N_C=15), $\Delta t/t_o \leq 0.05$ (N_C=30).

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