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Technical University of Crete
School of Production Engineering and Management

Sandia National Laboratories

Validation Simulations of the DSMC Code SPARTA

A. G. Klothakis
I. K. Nikolos
T. P. Koehler
M. A. Gallis
S. J. Plimpton

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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SPARTA DSMC Code

- SPARTA (Stochastic Parallel Rarefied-gas Time-accurate Analyzer), was created at Sandia National Laboratories. The main code developers are Michael Gallis and Steve Plimpton.
- Provides an interface in order to perform DSMC simulations. The code can be extended or "tuned" regarding the problems analyzed.
- The kernel is easily extendable in order to include more models and can run in a large number of processors.
- Code features include cell-weighting, grid-cutting for fast data exchange, and adapted grids
- VSS and VHS molecular models are implement in the code
- Recombination and dissociation chemical reactions can be handled
- Ambipolar model for low-density plasma modeling is included
- Multilevel Cartesian grids are used to divide the computational domain in cells.
- Code is parallelized to run efficient on large numbers of processors.
- Easily modifiable and extendable, can be used as a library.

Validation

- In order to stress test the code 4 common validation test cases where selected from literature:
  - Flow over a flat plate (2d)
  - Flow around a 70-degree blunt cone (2d axisymmetric and 3d)
  - Flow around a flared cylinder (2d axisymmetric)
  - Flow around a 25/55 degrees biconic (2d axisymmetric)

Flows past these geometries are complex and involve the following:

- Steep gradients of velocity and temperature and density
- Shock/shock and shock/boundary interactions
- Compression and rapid expansions

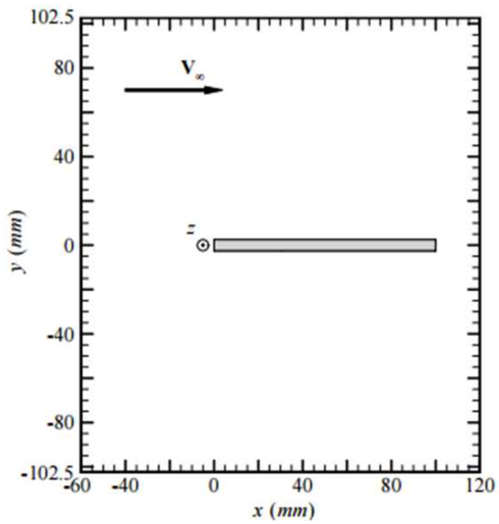
All these complicate the numerical simulation.

Hypersonic flow around a flat plate

- Geometry: Flat plate

  Length : 100mm

  Height : 50mm
- Flowfield Dimensions : 180mm x 205mm
- Grid size: 360 x 410 cells
- Cell size: 0.5mm x 0.5mm
- λ=1.6mm



➤ In this test case SPARTA is compared with DAC in order to verify the code's parallel efficiency and memory spread. The results quality is compared as well as the parallel efficiency and memory spread.

$$n_{ps} = \frac{t_s}{N_{proc} \times t_{parallel}}$$

$$s_{pm} = \frac{\sum_{proc} m_{proc}}{m_s}$$

n_{ps}: *Parallel efficiency*
t_s: *Serial execution time*
N_{proc}: *Number of processors*
$t_{parallel}$: *Time for parallel execution*
s_{pm}: *Memory spread*
Σ_{proc}: *Sum of processors*
m_{proc}: *Memory needed for parallel execution*
m_s: *Memory needed for serial execution*

J. F. Padilla, "Comparison of DAC and MONACO DSMC Codes with Flat Plate Simulation," 2010.

Hypersonic flow around a flat plate

Flow conditions				
$V_\infty\ (m/s)$	$T_\infty\ (K)$	$T_w\ (K)$	$n_\infty\ (m^{-3})$	F_{NUM}
1504	13.32	290	3.716×10^{20}	4.56×10^{11}

Simulation parameters	
Time-step	$3.102 \times 10^{-7}\ sec$
Transient period	8000 steps
Sampling period	8000 steps
Interval sample data	2 steps

Hypersonic flow around a flat plate

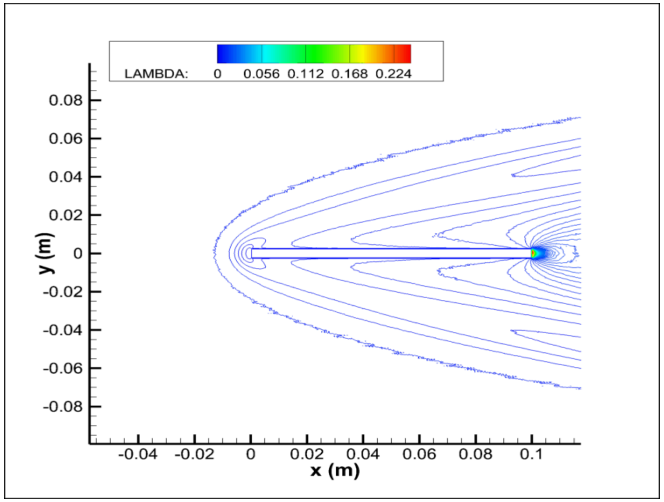


Figure 1. Mean free path contours.

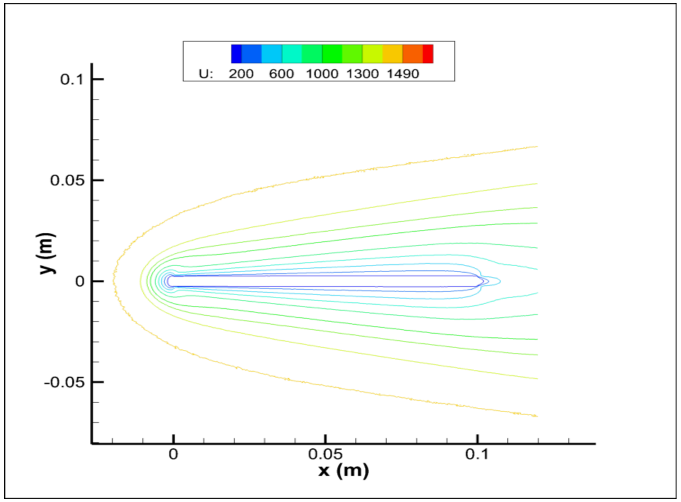


Figure 2. Velocity along x-axis.

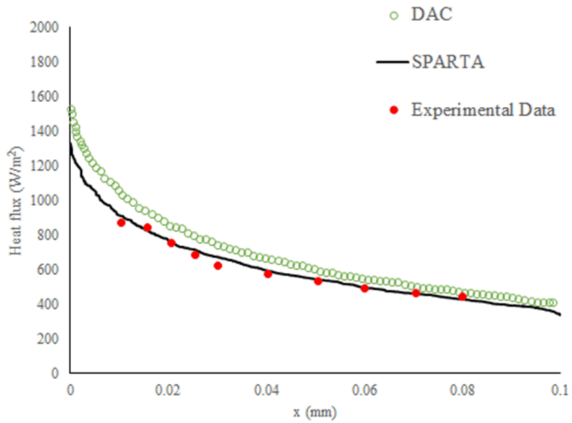


Figure 3. Surface heat flux.

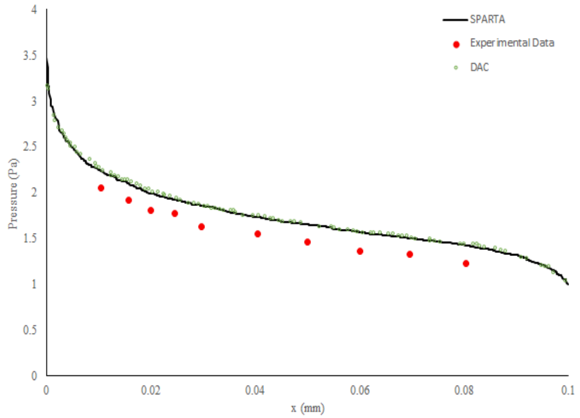
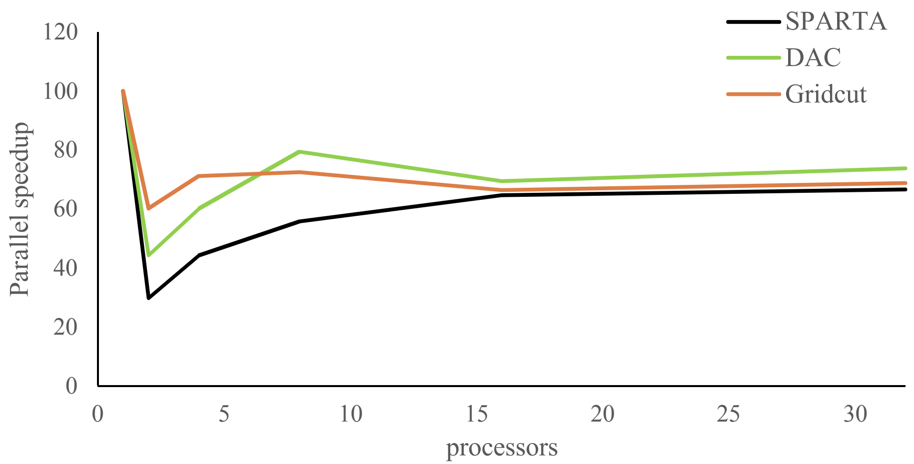
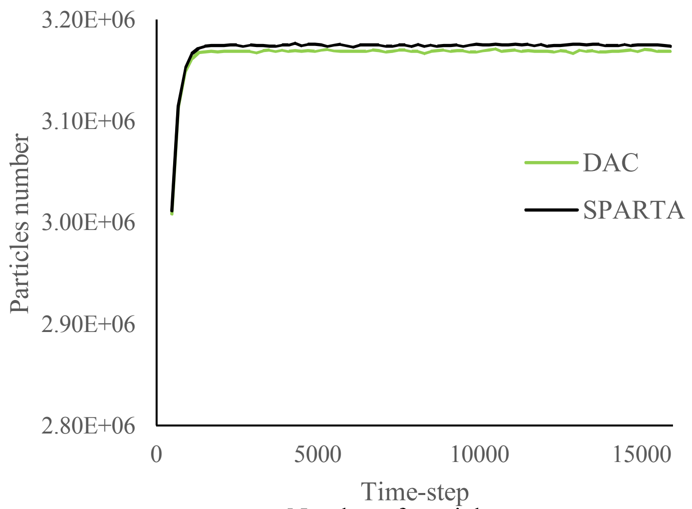


Figure 4. Pressure on the upper surface.

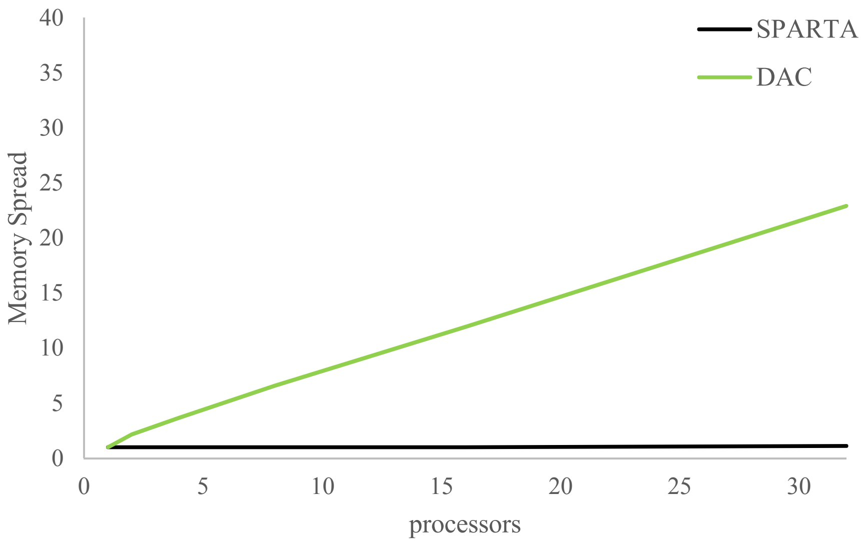
Hypersonic flow around a flat plate



Parallel speedup.



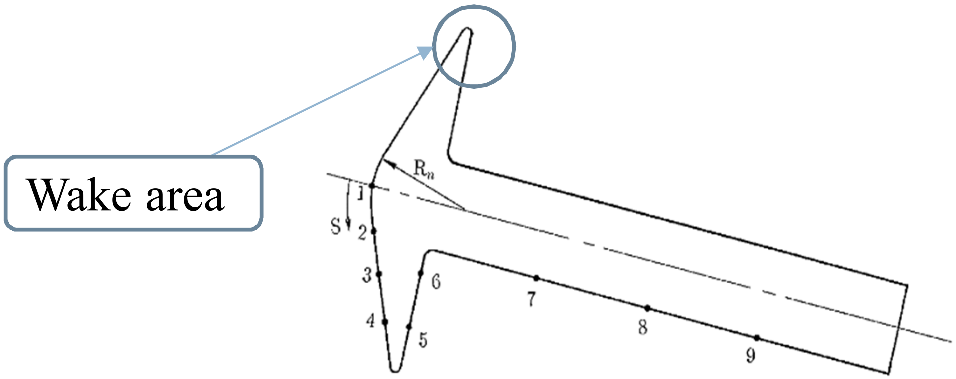
Number of particles.



Memory spread.

Hypersonic flow around a 70-degree blunt cone

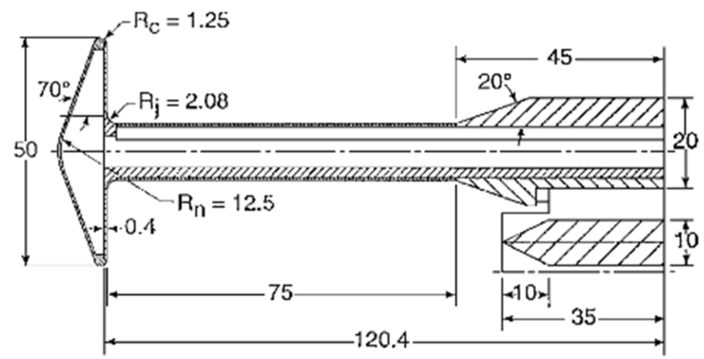
- This test case is one of the most common hypersonic rarefied flows used for validation of DSMC codes.
- This flow is used to assess the code's ability to resolve surface properties on the cone as well as the flow characteristics



Simulation parameters	
Time-step	$1.3 \times 10^{-7}\ sec$
F_{NUM}	7.2×10^{16}
Transient period	100,000 steps
Sampling period	20,000 steps
Interval sample data	2 steps

Hypersonic flow around a 70-degree blunt cone

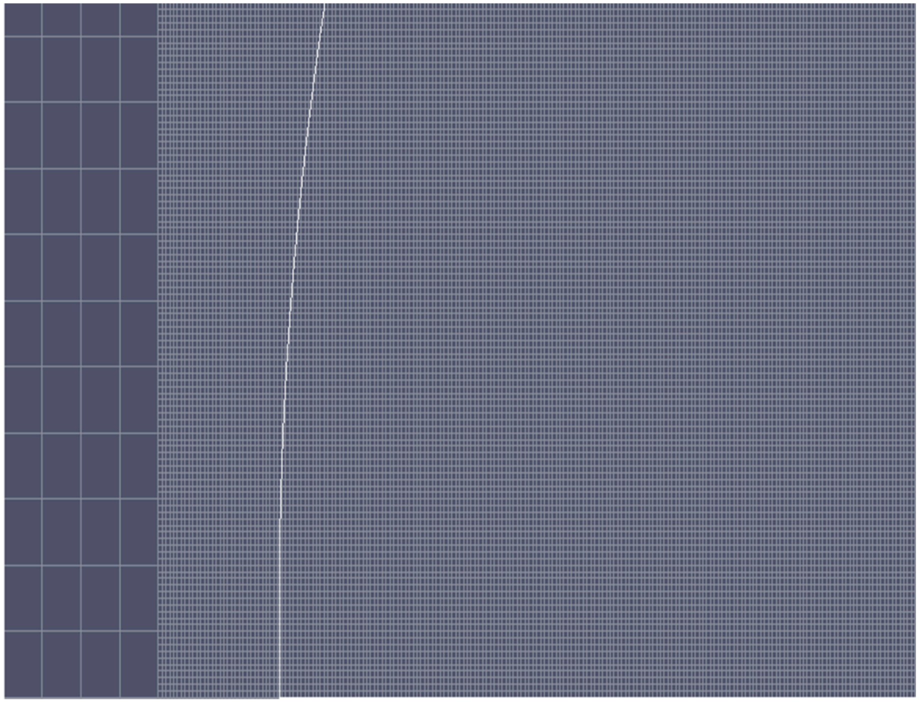
- Geometry: AGARD Group Mars Pathfinder
- Flowfield dimensions: 10cm x 15cm
- Grid: 800x800 cells, 2-level 10x10 cells around the cone area



Flow conditions	Gas	Ma	T_0, K	$p_0, bars$	Re_d	$\overline{V}$
1	N_2	20.2	1100	3.5	1420	0.53
2	N_2	20	1100	10	4175	0.31
3	N_2	20.5	1300	120	36265	0.11

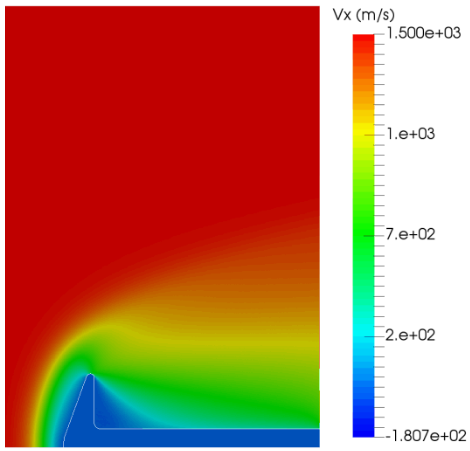
J. Allègre, D. Bisch, D., J.C. Lengrand, Journal of Spacecraft and Rockets, 34 (6), 724-728 (1997).
J. Allègre, D. Bisch, J. C. Lengrand, Journal of Spacecraft and Rockets, 34, (6), 714-718 (1997).

Hypersonic flow around a 70-degree blunt cone

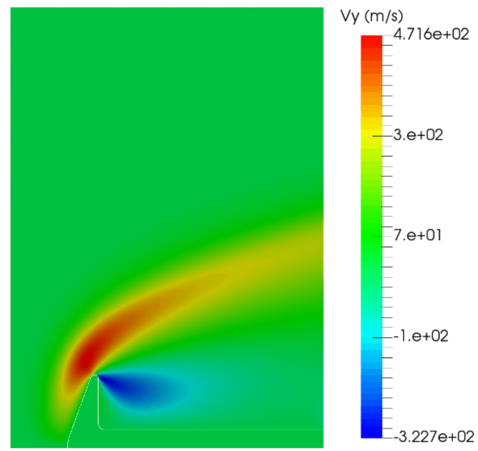


Grid refinement area.

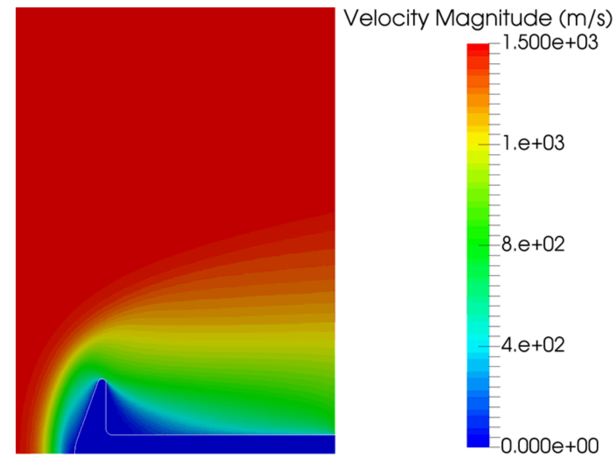
Hypersonic flow around a 70-degree blunt cone



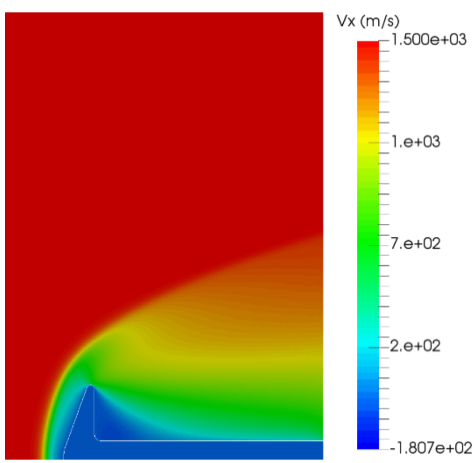
Velocity along x-axis (Case 1)



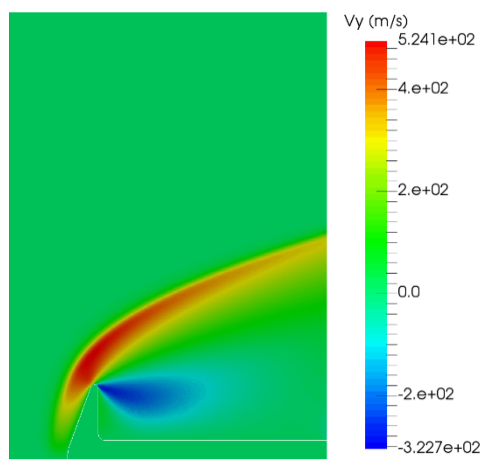
Velocity along y-axis (Case 1)



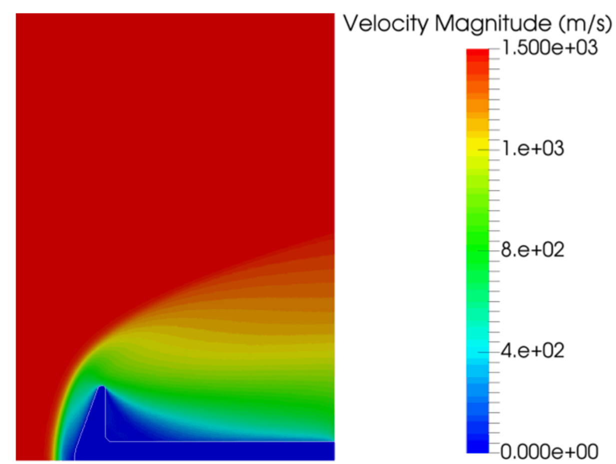
Total Velocity (Case 1)



Velocity along x-axis (Case 2)



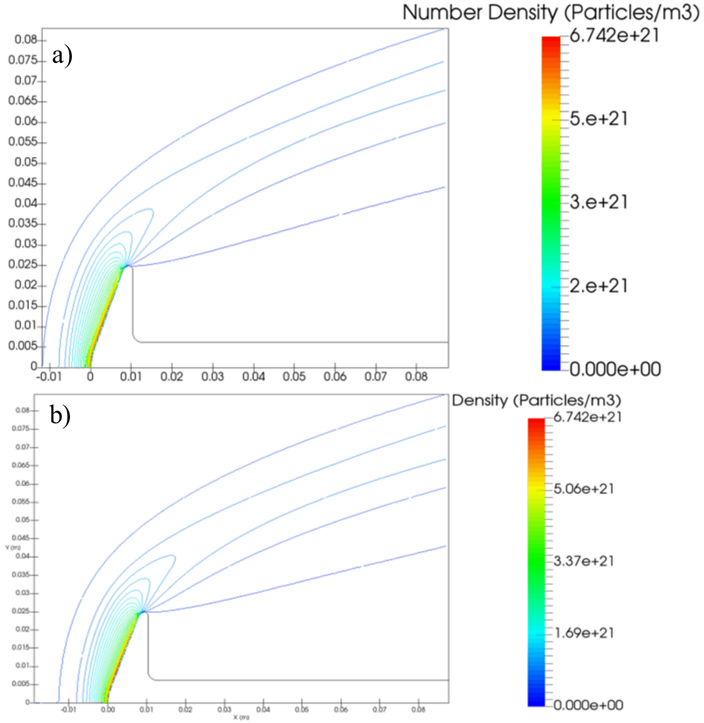
Velocity along y-axis (Case 2)



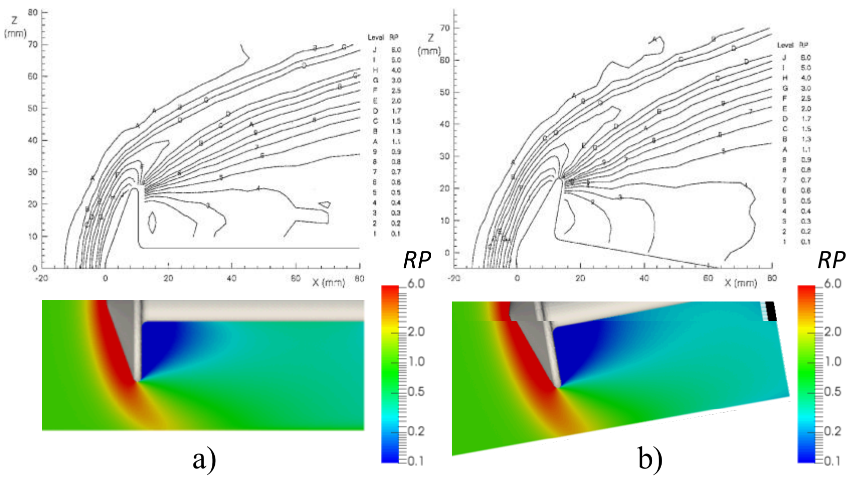
Total Velocity (Case 2)

Hypersonic flow around a 70-degree blunt cone

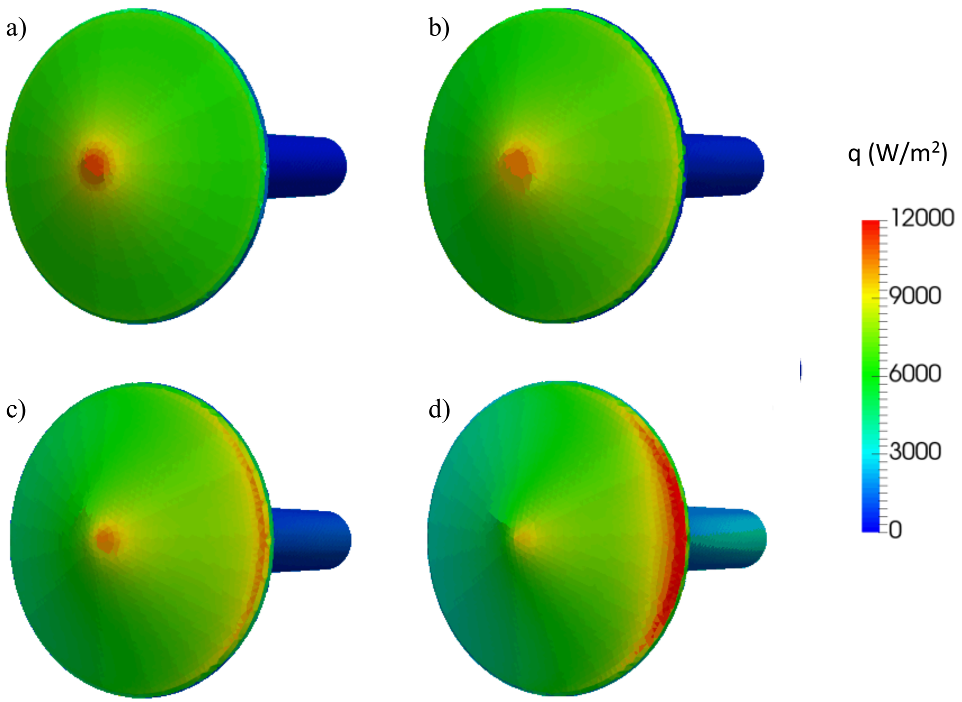
Density flowfields around the 70-degree blunted cone at 0° for a) first set and b) second set of flow conditions.



Relative density ($RP = \frac{\rho}{\rho_\infty}$) flowfields around the 70-degree blunted cone at a) 0° and b) 10° angles of attack for the first set of flow conditions.



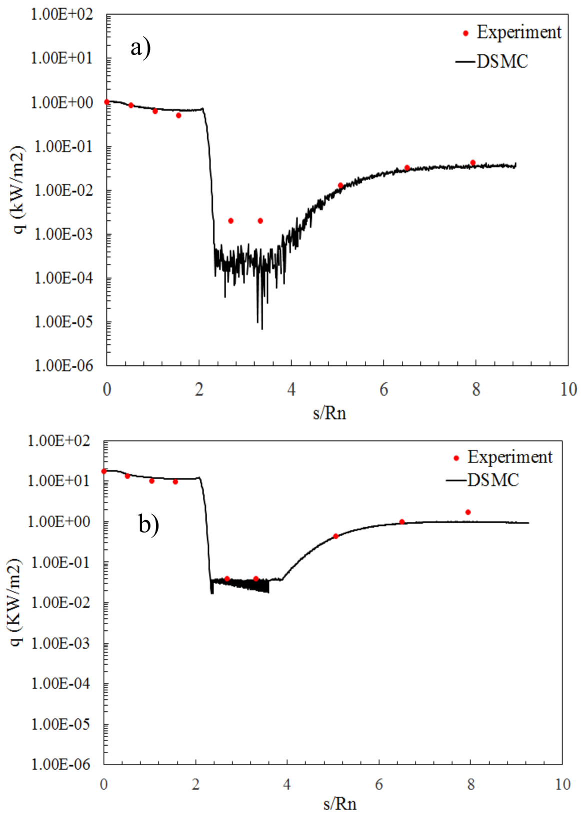
Hypersonic flow around a 70-degree blunt cone



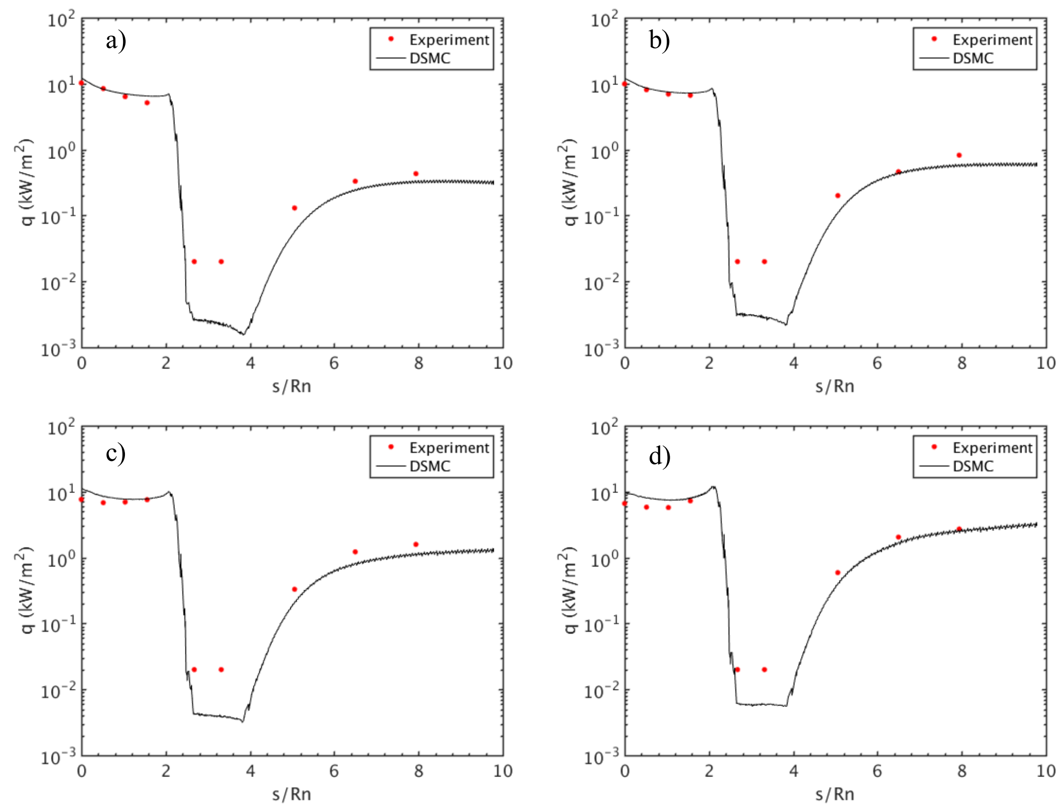
Surface heat flux contours on the 70-degree blunted cone at a) 0°, b) 10°, c) 20°, and d) 30° angles of attack for the first set of flow conditions.

Hypersonic flow around a 70-degree blunt cone

Surface heat flux on the 70-degree blunted cone for a) the first and b) the second sets of flow conditions (2d-axisymmetric).

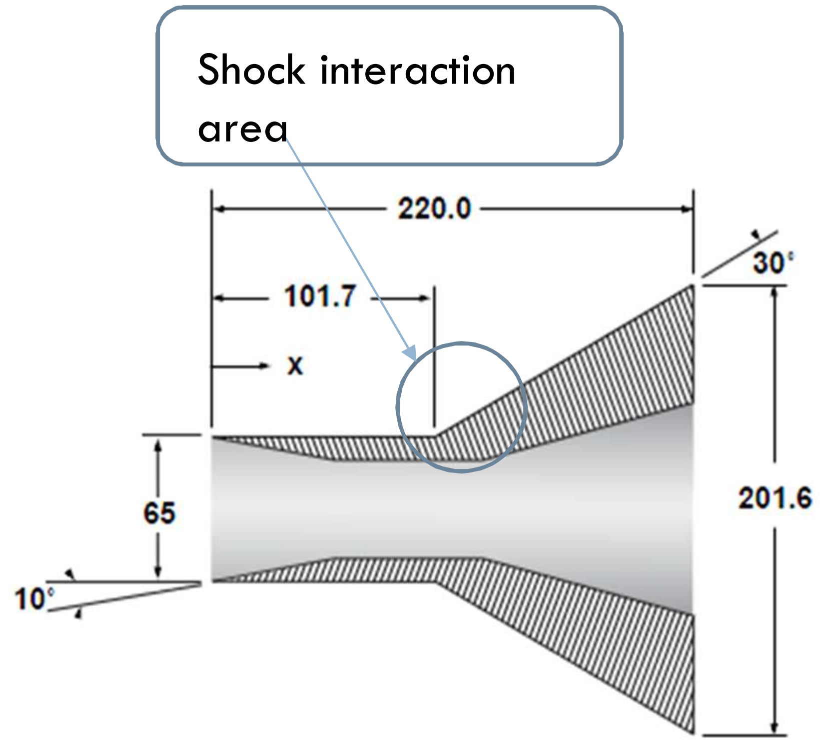


Heat flux along the surface of the 70-degree blunted cone at a) 0°, b) 10°, c) 20°, and d) 30° angles of attack for the first set of flow conditions (3d).



Hypersonic flow around a flared cylinder

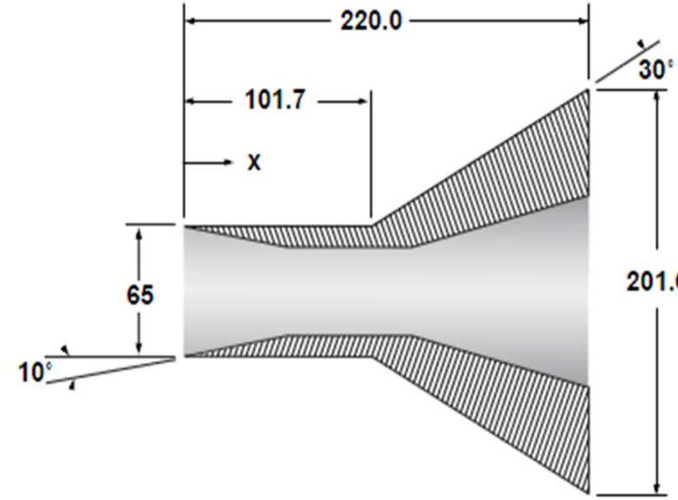
- The purpose of this test case is to test SPARTA and the Cartesian grid in interacting shock waves conditions.
- Simulation results are compared with experimental results from literature.



Simulation parameters	
Time-step	$2.0 \times 10^{-8}\ sec$
F_{NUM}	4.4×10^{18}
Transient period	246000 steps
Sampling period	12000 steps
Interval sample data	2 steps

Hypersonic flow around a flared cylinder

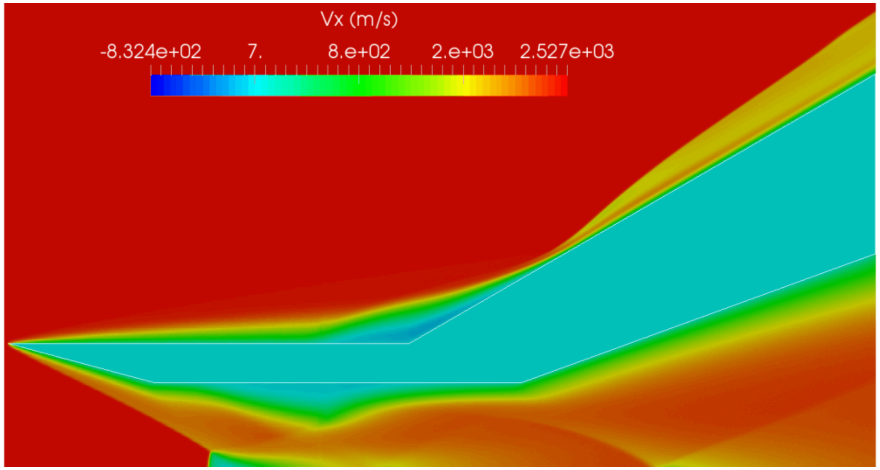
- Geometry: NATO Research Technology Organization
- Flowfield dimensions: 22cm x 12cm
- Grids : Uniform 1000x1800 cells, 2-Level 957x440 cells second level 10x10 cells



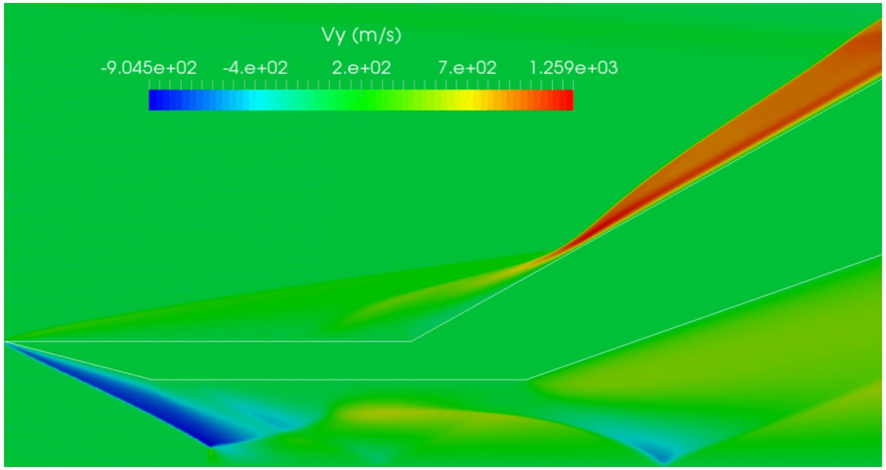
Condition	Flow Velocity (m/s)	Number Density, m^{-3}	Flow temperature (K)	Gas	Surface Temperature (K)
LENS Run 11	2484	1.187×10^{22}	95.6	N_2	297.2

J. N. Moss and G. A. Bird, "Direct simulation Monte Carlo simulations of hypersonic flows with shock interactions," *AIAA J.*, vol. 43, no. 12, pp. 2565–2573, 2005.

Hypersonic flow around a flared cylinder



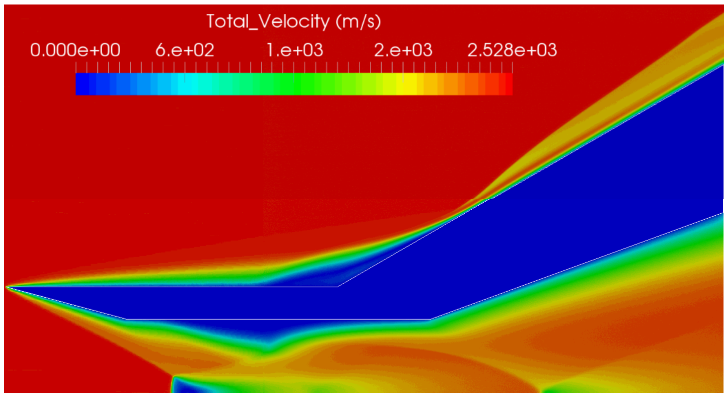
a)



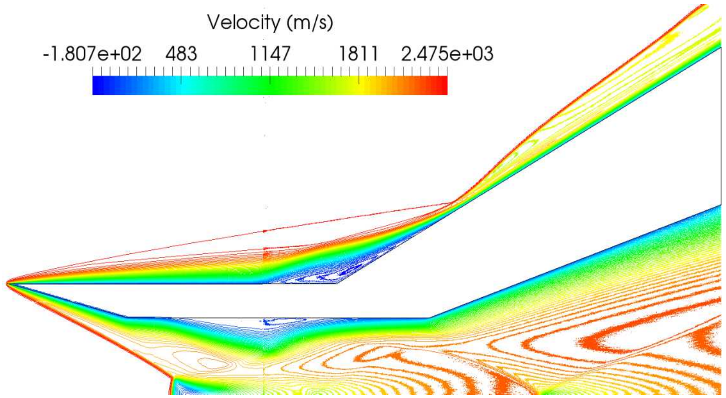
b)

Flared cylinder contours of a) Velocity along x-axis, b) Velocity along y-axis.

Hypersonic flow around a flared cylinder

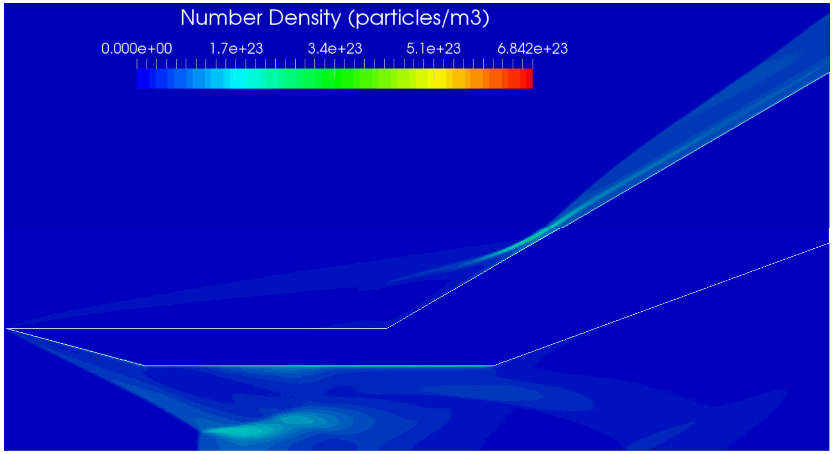


a)



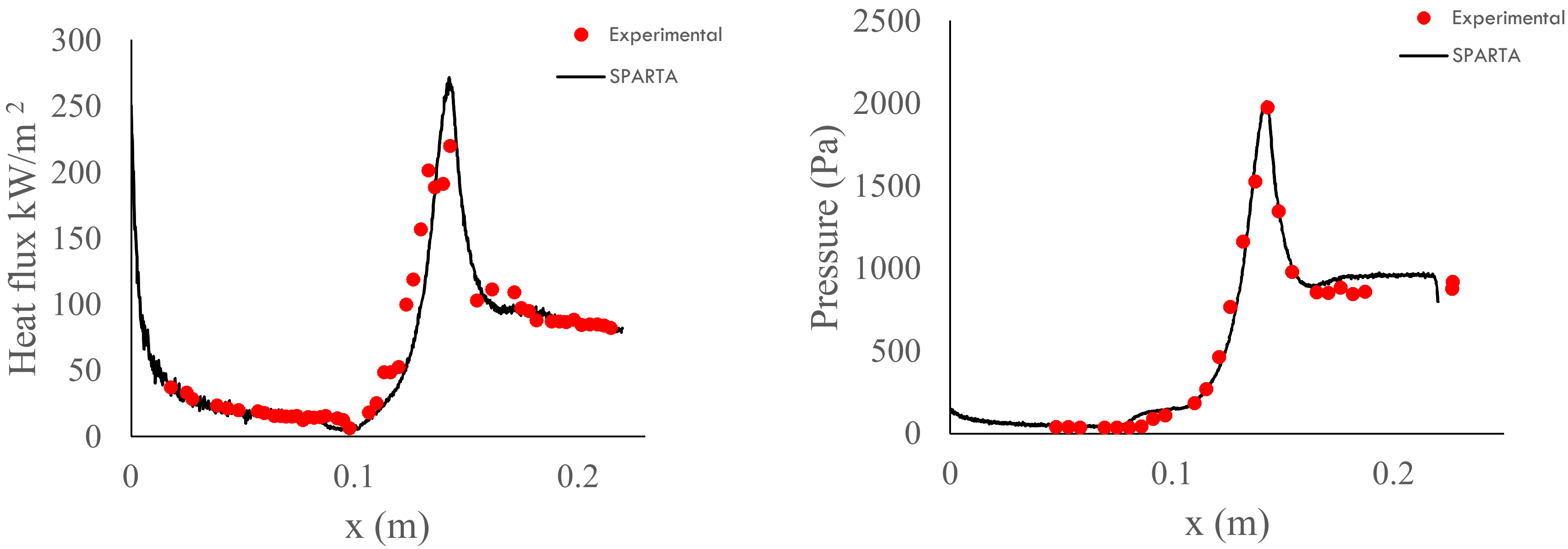
b)

Flared cylinder contours of a) Total velocity, b) Velocity contour lines along x-axis.



Flared cylinder number density contours

Hypersonic flow around a flared cylinder

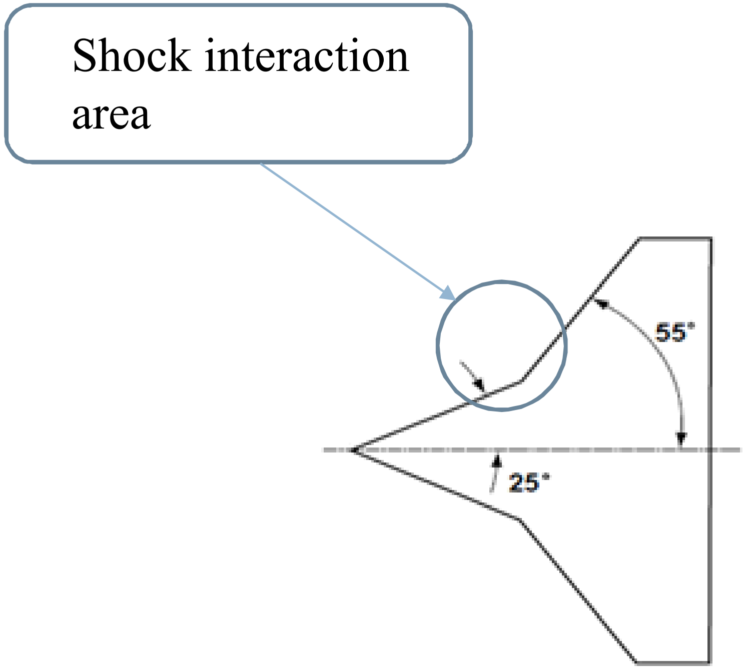


Surface heat flux and surface pressure plots.

Hypersonic flow around a 25/55 degree biconic

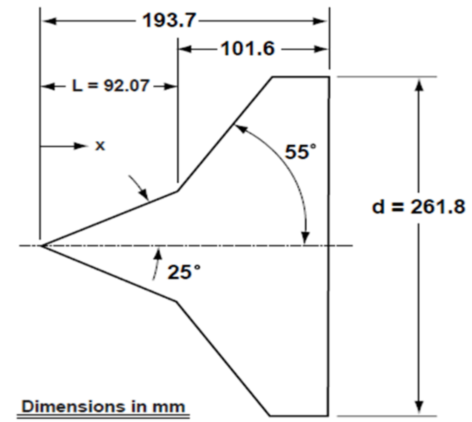
- This test case was selected to test SPARTA on flows with strong shock/shock interactions.
- In the biconic geometry, the attached shock from the first cone interacts with the detached shock bow shock of the second cone.
- The outer shocks are also modified by separation and reattachment shocks.

Simulation parameters	
Time-step	$6.0 \times 10^{-7}\ sec$
F_{NUM}	1.0×10^{18}
Transient period	250000 steps
Sampling period	60000 steps
Interval sample data	2 steps



Hypersonic flow around a 25/55 degree biconic

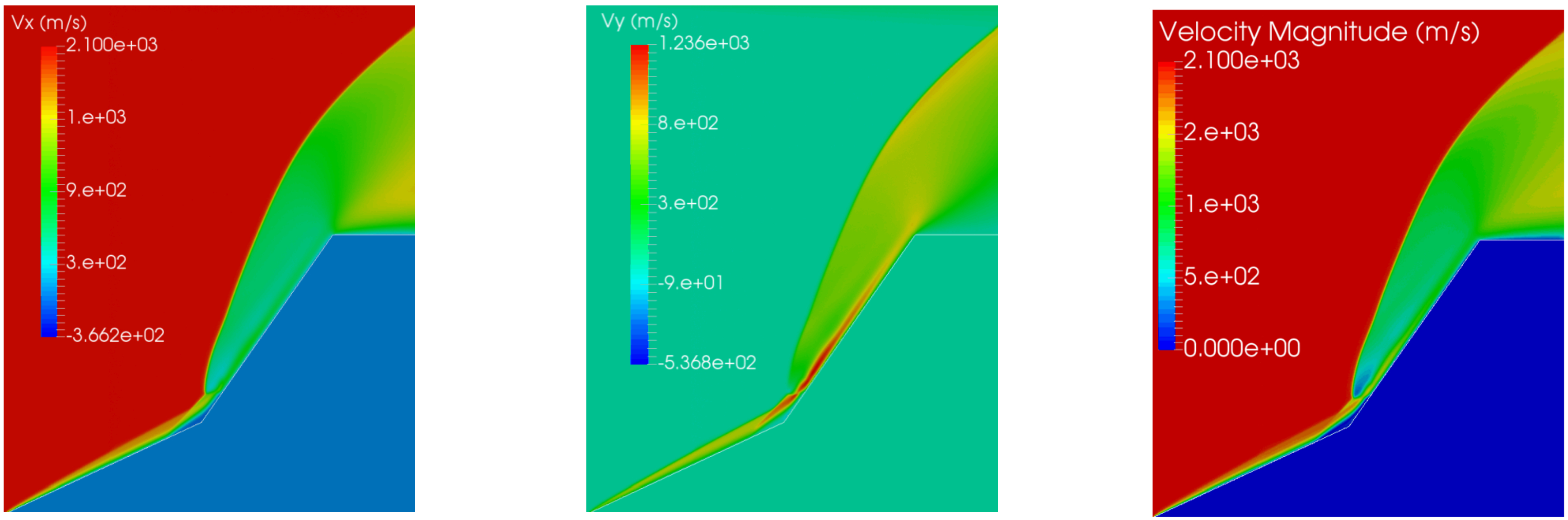
- Geometry: NATO Research Organization in collaboration with the Working Group 10
- Flowfield dimensions: 19.47cm x 24cm
- Grid: 2-level grid. 1st level 870x870 cells, 2nd level refinement 10x10 of the 1st level 50 mm after the biconic's sharp leading edge to 20 mm prior



Condition	Flow Velocity (m/s)	Number Density, m^{-3}	Flow temperature (K)	Gas	Surface Temperature (K)
ONERA	2073	$3{,}779 \times 10^{21}$	42,6	N_2	293

D. Knight, AIAA Paper 2002-0433, American Institute of Aeronautics and Astronautics (2002).
S. Walker and J. D. Schmisseur, AIAA Paper 2002-0436, American Institute of Aeronautics and Astronautics (2002).

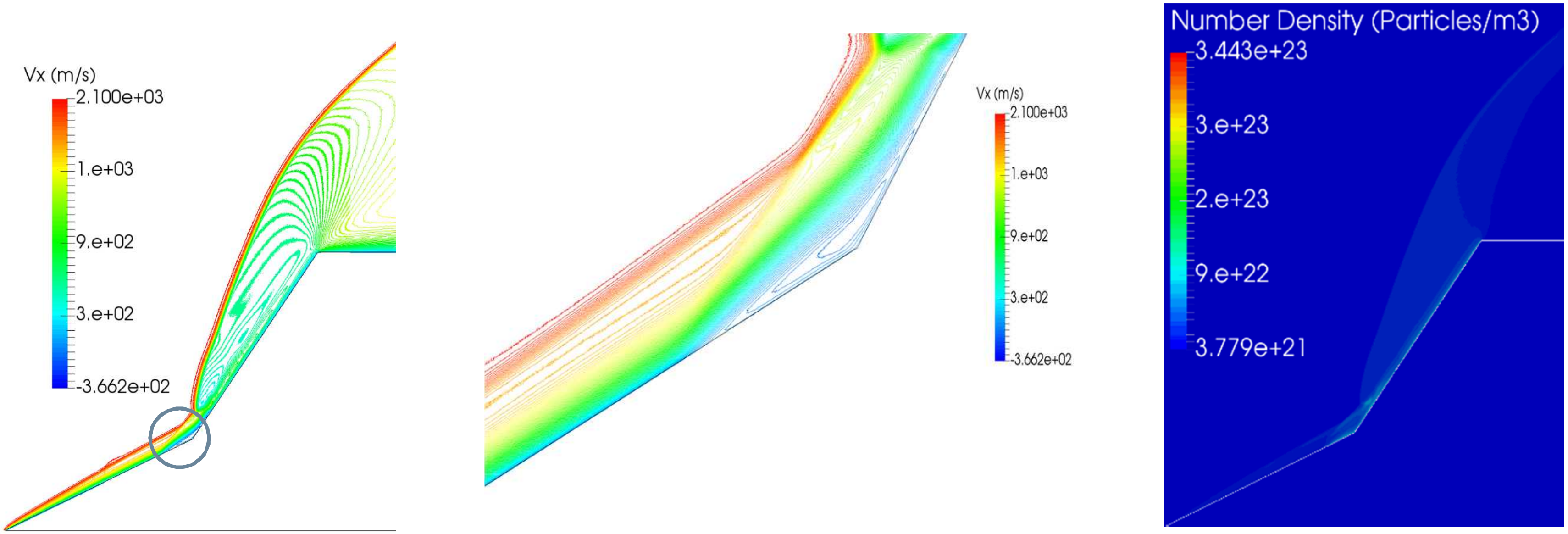
Hypersonic flow around a 25/55 degree biconic



a) b) c)

Velocity contours a) Velocity along x-axis, b) Velocity along y-axis, c) Velocity Magnitude

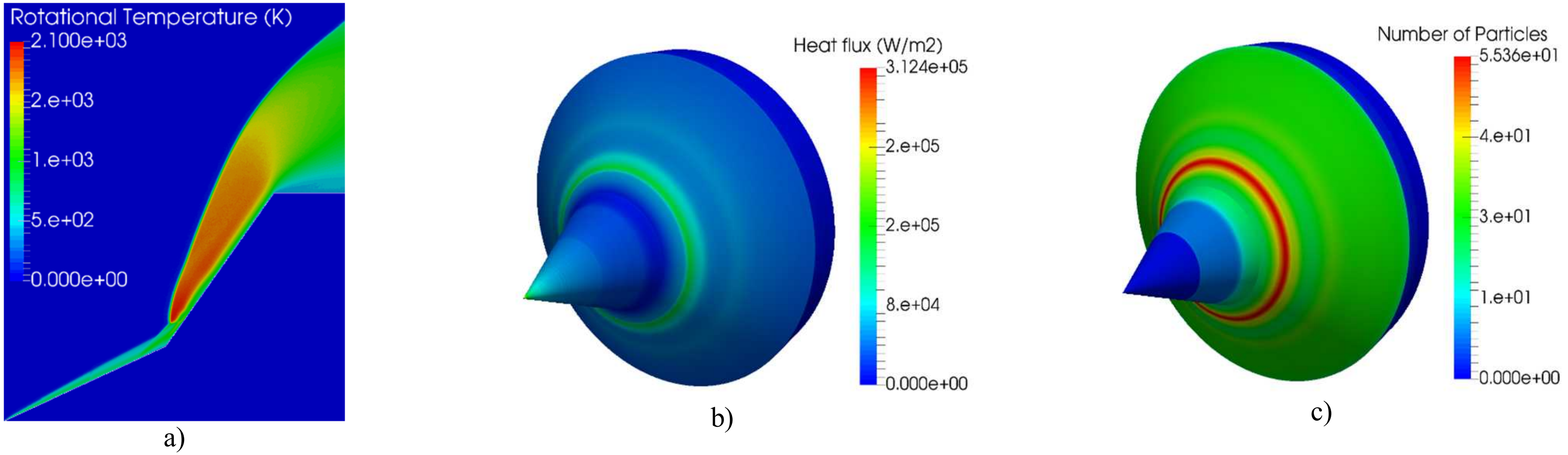
Hypersonic flow around a 25/55 degree biconic



a) b) c)

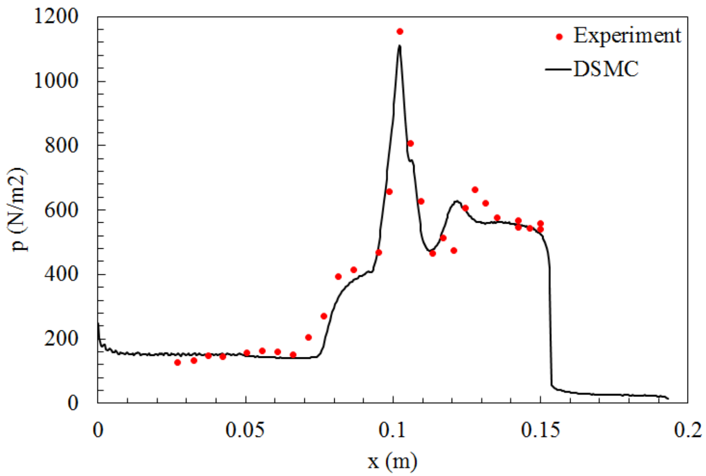
a) Velocity contours along x-axis, b) Recirculation area, c) Number density.

Hypersonic flow around a 25/55 degree biconic

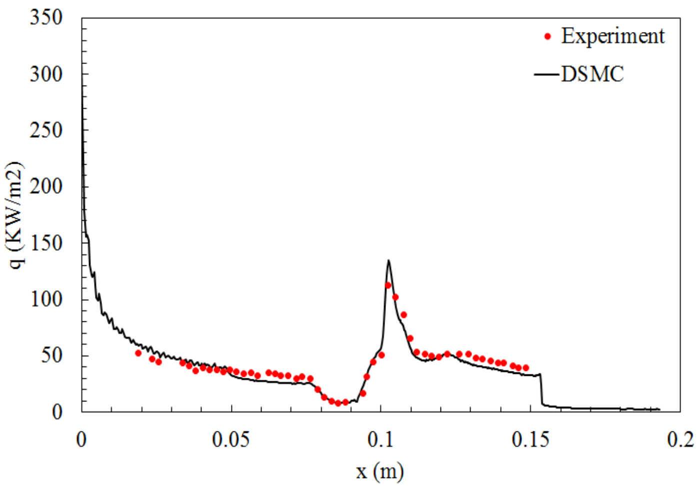


a) Rotational temperature contours, b) Surface heat flux, c) Number of particle/surface interactions

Hypersonic flow around a 25/55 degree biconic



a)



b)

a) Pressure on the surface, b) Surface heat flux.

Conclusions

- In this work several validation simulations were performed using the SPARTA DSMC code, for four challenging hypersonic test cases.
- The 70-degree blunt cone provided the opportunity to test the parallel efficiency of SPARTA while validating its capability to provide accurate three-dimensional calculations.
- The axisymmetric application of SPARTA was mainly validated with the 25/55 biconic and the flared cylinder geometries which produce flows in which shock-shock interactions can be difficult to resolve with DSMC codes.
- The SPARTA calculations for the 70-degree blunted cone included both axisymmetric and three-dimensional approaches, which enabled the simulation of two incident flow conditions and multiple angles of attack, all of which resulted in very good agreement with experimental measurements of the density flowfield and surface heat flux. Moreover vortices were observed at the back of the blunted cone for both flow conditions; however, the recirculation zone was better resolved for the higher density flow. The surface heat flux provided quantitative validation of SPARTA results, showing good agreement with experimental measurements for all angles of attack.
- The 25/55 biconic and the flared cylinder geometries provided some very challenging flow effects to simulate; both produce very strong shock-shock interactions due to an immediate change in the angle between the first and the second cone for the biconic and between the straight part and the inclined part on the flared cylinder, which generate regions of high density which is computationally burdensome for the DSMC method. However, with appropriately sized grid and solver parameters, SPARTA was shown to produce surface pressures and heat fluxes in good agreement with experimental measurements even with a not so huge number of particles.

Thank you for your attention!

Questions…??