Particle-kinetic modeling of high speed shock boundary layer interactions and large separation bubbles

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2024 Frontera User Meeting

August 5–6, 2024, Austin, TX, US

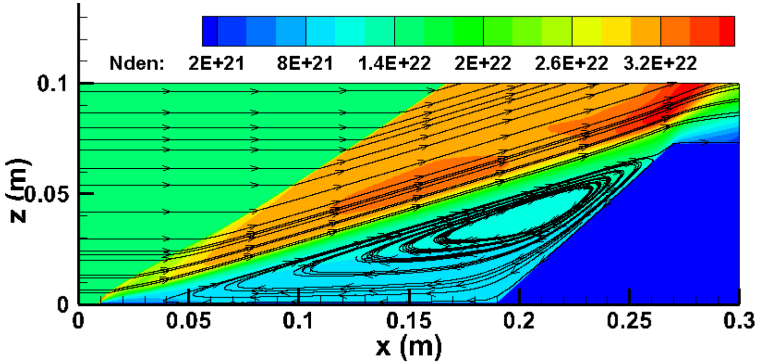
Funding: ONR Grant No. N000141202195

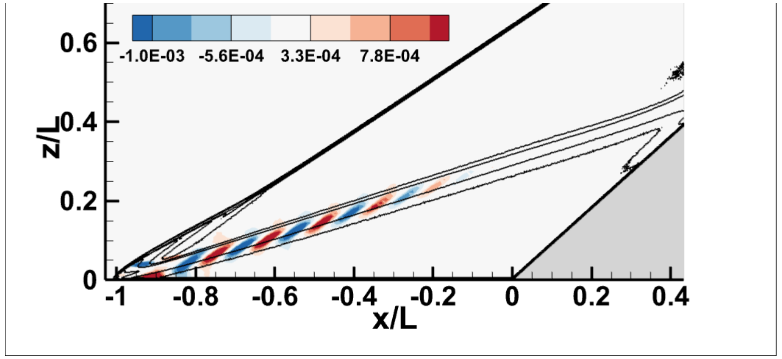
Computation Resources: NSF TACC Frontera Supercomputer, LRAC Project CTS23002

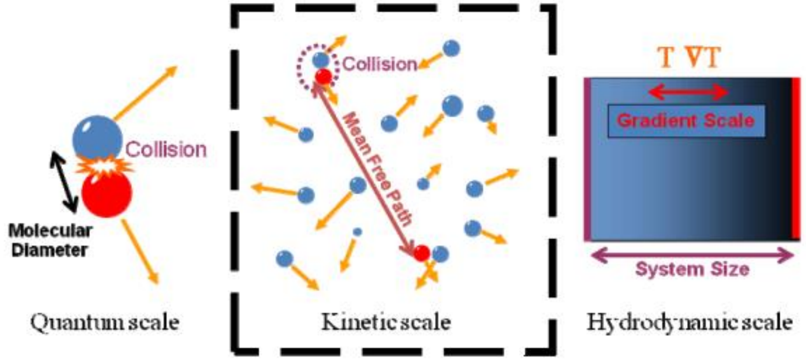
Outline

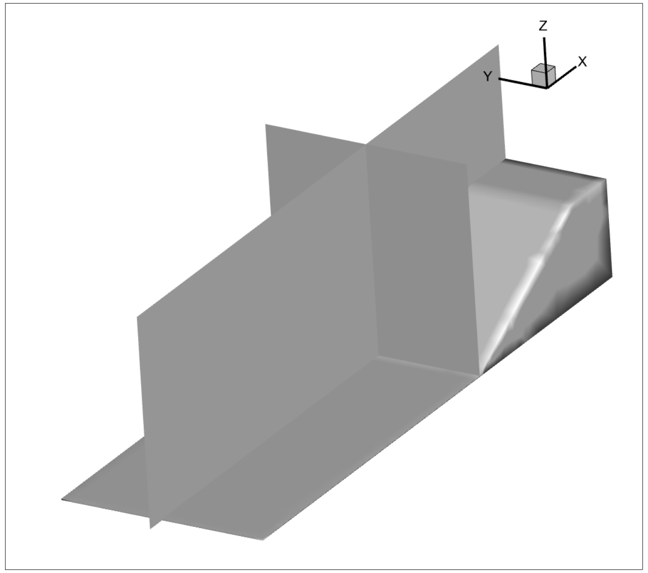
- **Introduction and Motivation**
- **Flow Domain and Numerical Methods**
- **3D SP simulations and BiGlobal Stability Analysis**

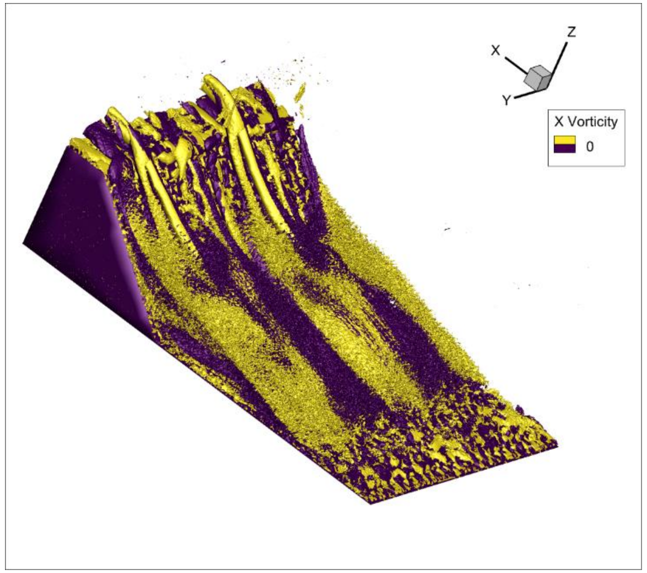
Conclusions





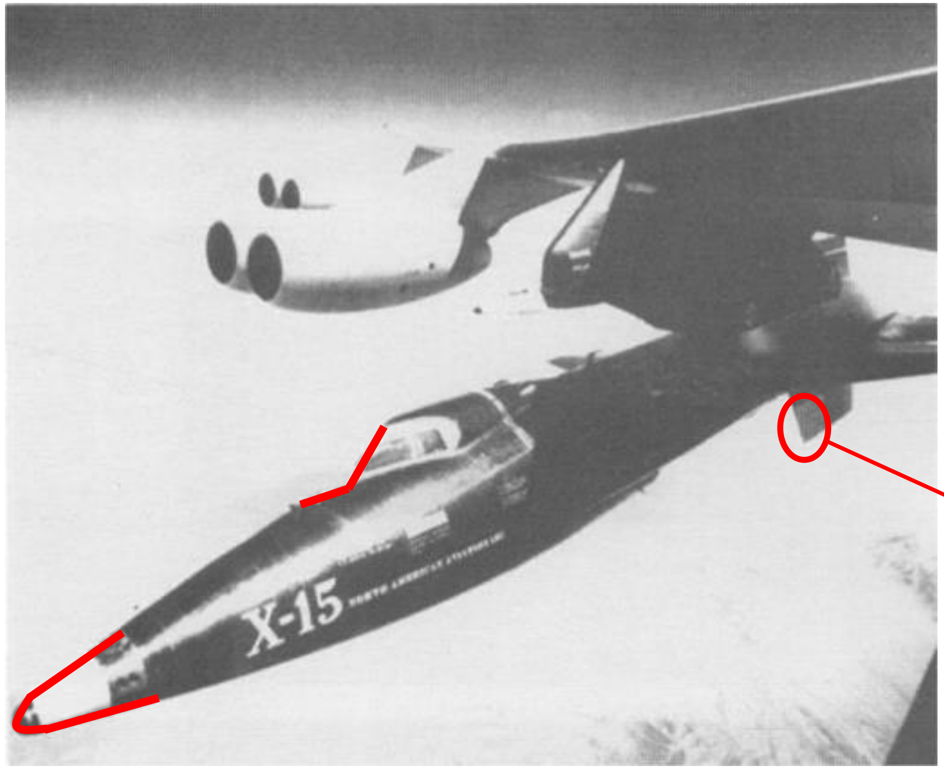




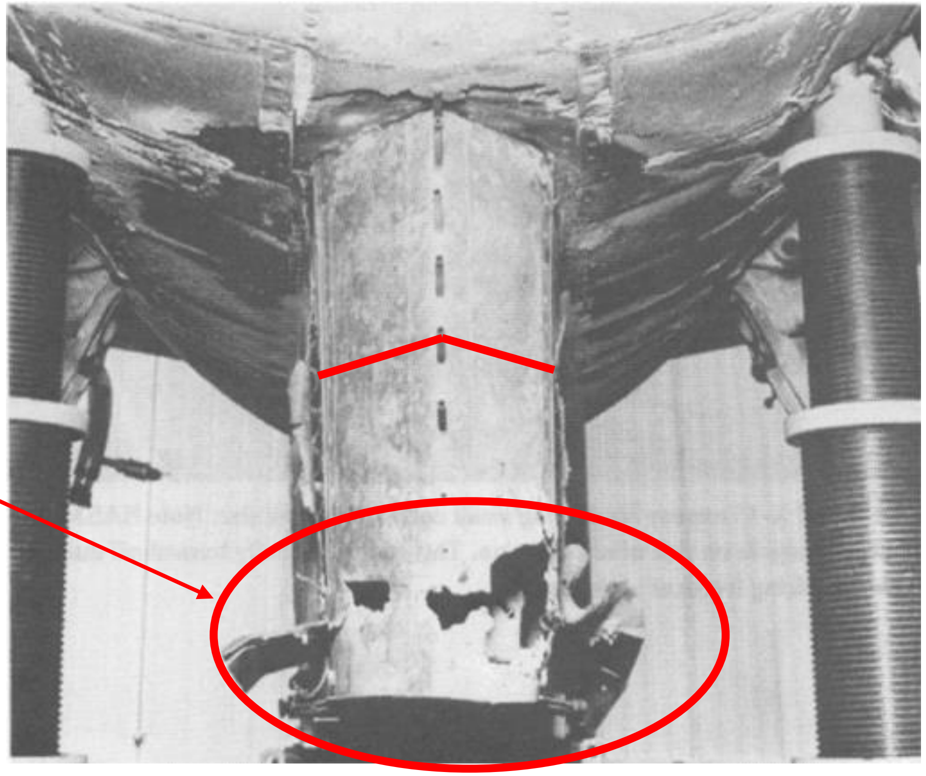


Fastest Piloted Hypersonic Flight X-15A-2

X-15 separates from B-52



Damage to lower ventral fin by shock impingement on flight 2-53-97



Pete Knight flew at Mach 6.7 at 31 km altitude (2021 m/s, i.e. > 2x speed of a bullet).

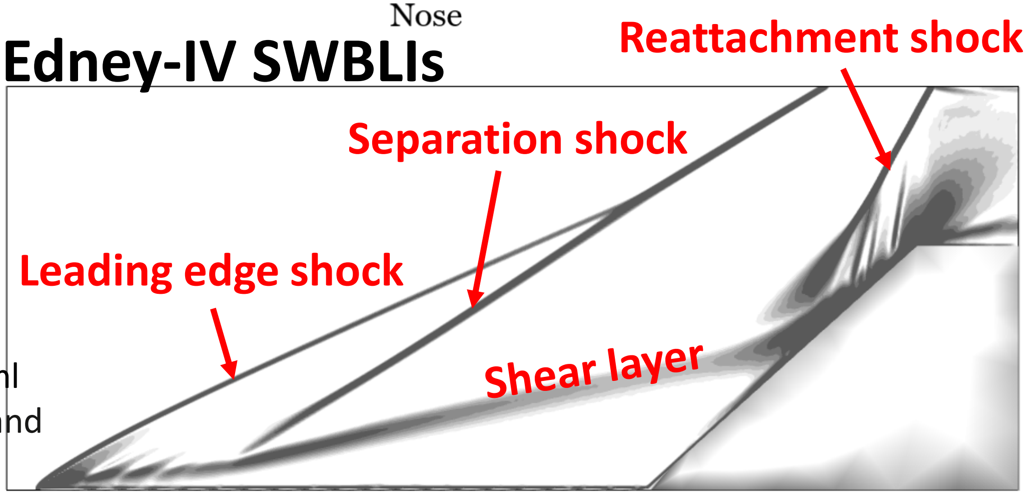
Thompson M. O. At the edge of space: The X-15 flight program. (1992) Smithsonian.

Introduction and Motivation (1/2)

- Compression ramps are widely used in:
  - Control Surfaces
  - Inlets
- Compression ramps in supersonic and hypersonic flow creates
  - Separation shock
  - Shear layers
  - Reattachment shock
  - Expansion waves
- Triple Deck Theory [2] to predict transition
  - Scaled Angle(Re,M,α,..)
- DSMC provides higher fidelity for regions with high gradients
  - Previous effort for the base flows are done with DNS of Navier-Stokes Equations
- Linear Stability Theory (LST) [3] is used to predict transition in compression ramp flows

SR71 Blackbird [1]

Edney-IV SWBLIs

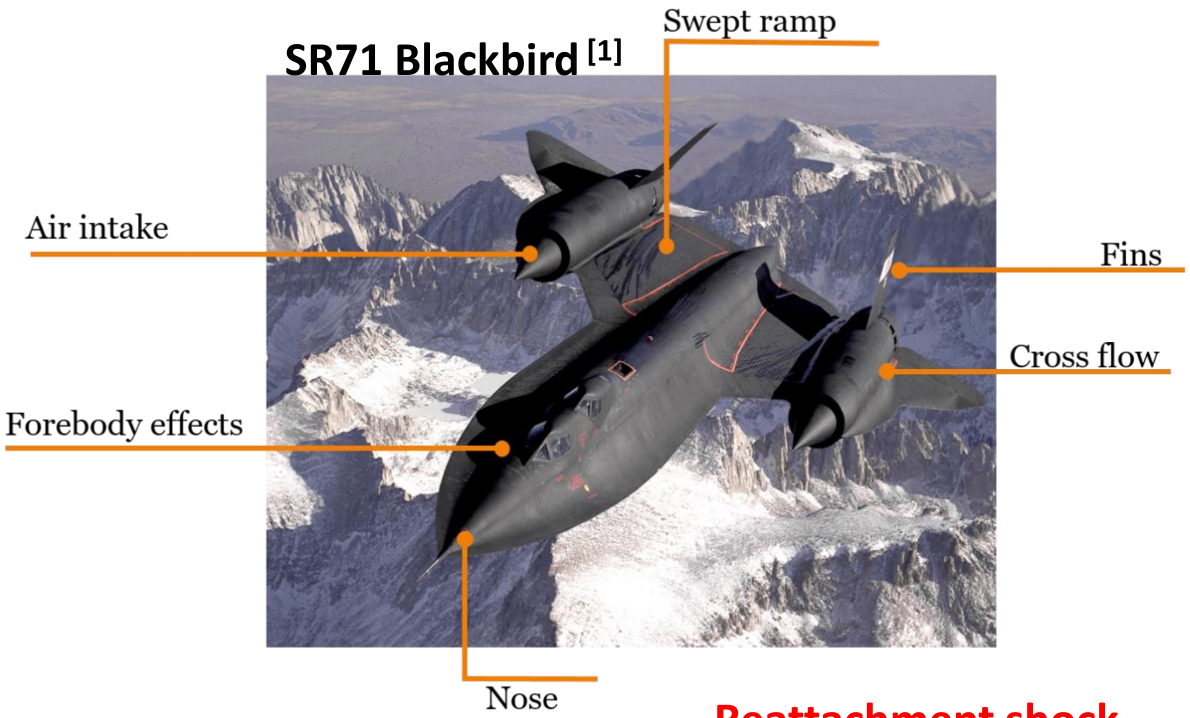


[1] https://www.nasa.gov/centers/dryden/multimedia/imagegallery/SR-71/EC94-42883-4.html
[2] Rizzetta, D., Burggraf, O., & Jenson, R. (1978). Triple-deck solutions for viscous supersonic and hypersonic flow past corners. *Journal of Fluid Mechanics, 89*(3), 535-552. doi:10.1017/S0022112078002724
[3] Theofilis, V. (2011) “Global linear instability,” Annual Review of Fluid Mechanics 43, 319–352 (2011), https://doi.org/10.1146/annurev-fluid-122109-160705

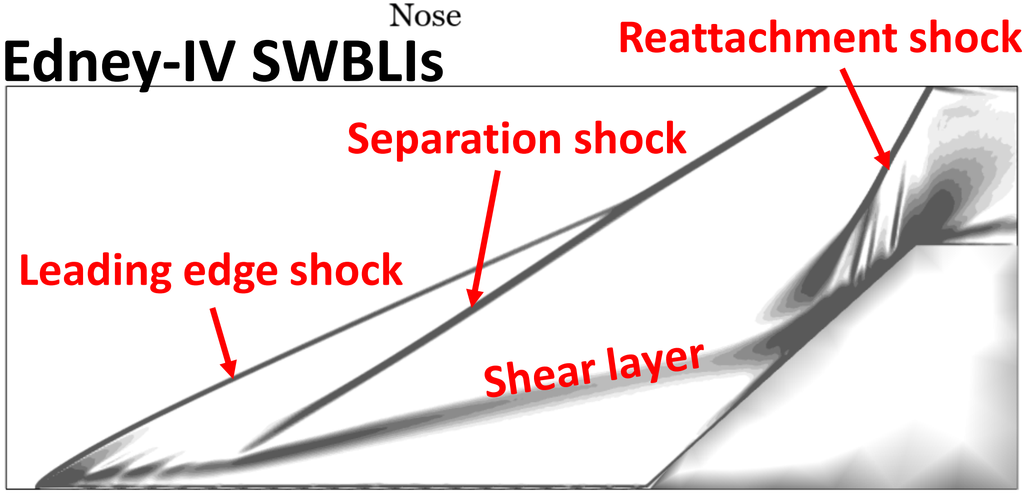
Introduction and Motivation (2/2)

- In this work we will use:
  - Linear Stability Theory to predict transition characteristics for compression ramp flows
  - DSMC solutions for the base flow
- The ramp angles will be chosen with the help of the triple deck theory
  - Appearance of the secondary recirculation regions
  - Laminar separation bubble might breakdown to a 3D structure
- 3D spanwise periodic DSMC simulations to test the predictions of linear stability theory

SR71 Blackbird [1]



Edney-IV SWBLIs



[1] https://www.nasa.gov/centers/dryden/multimedia/imagegallery/SR-71/EC94-42883-4.html

Computational Fluid Dynamics

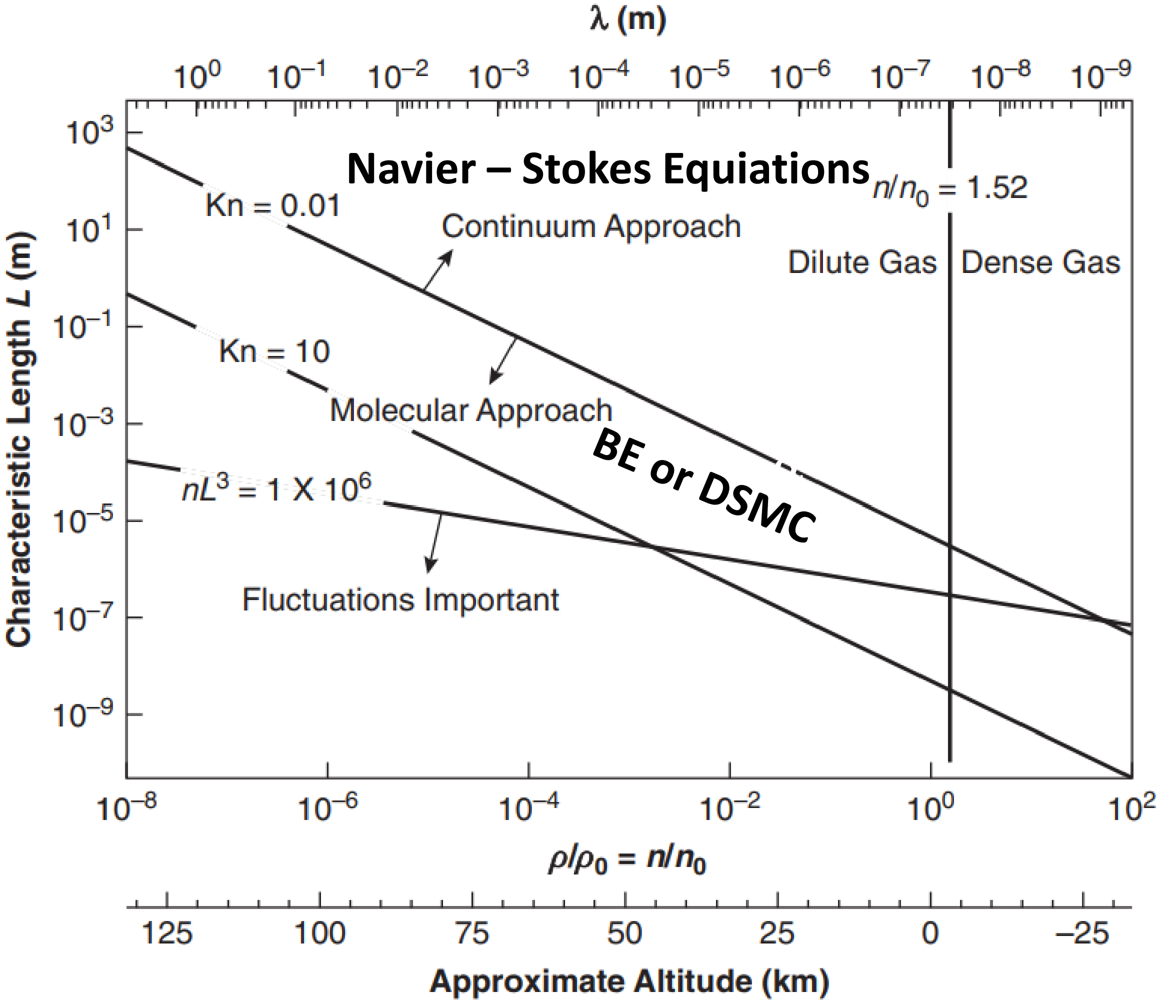
Fluid flows can be defined in the most general form by the Boltzmann Equation;

$$\frac{\partial f}{\partial t} + \vec{\xi} \bullet \frac{\partial f}{\partial \vec{r}} = \Omega(f) \qquad f = f(r, \xi, t)$$

$$\Omega(f)(\xi) = \int_{\xi^*} d\xi^* \int_{\Sigma} B(\Sigma, \xi^*)[G(\xi, \xi^*, \Sigma) - F(\xi, \xi^*, \Sigma)] d\Sigma$$

Some of the most common ways to handle the collision operator and the equation are;

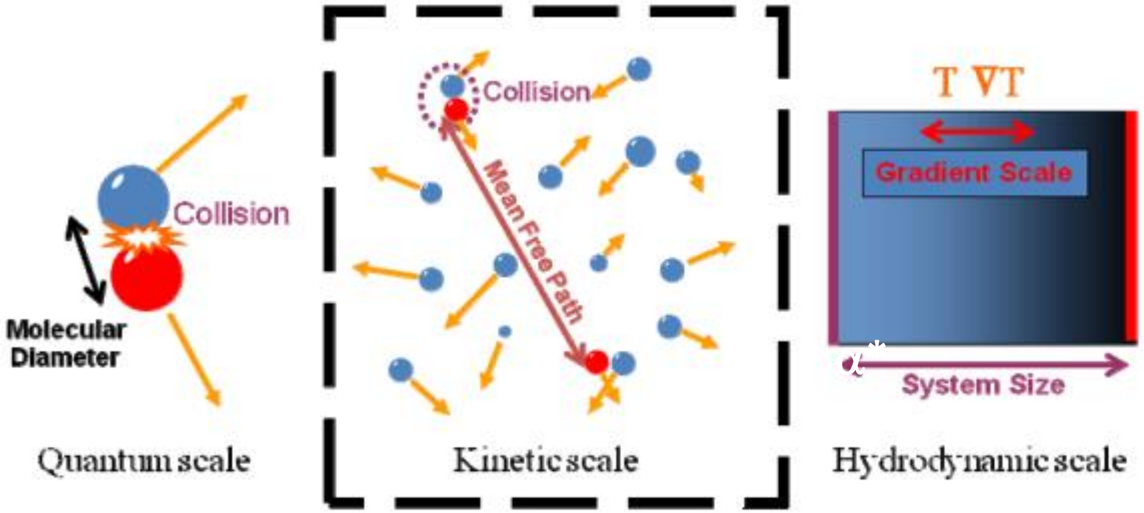
- Navier-Stokes equations can be obtained by taking moments of BE
- Define a Hamiltonian-like equilibrium term for the collision operator (BGK/ESBGK)
- **Use gas particles**
  - **Direct Simulation Monte Carlo**



I. D. Boyd & T. E. Schwartzentruber, Nonequilibrium Gas Dynamics and Molecular Simulation, 2017, Cambridge University Press

Direct Simulation Monte Carlo – General

- Direct Simulation Monte Carlo (**DSMC**) is a particle based kinetic method [1]
- Each simulation particle represents some number of real gas particles
  - Parameter FNUM, generally a big number, 10^8, 10^{14} etc.
- A **stochastic** approach
  - First physics based probability of an event is calculated
  - Then a random number is generated to decide whether or not that event takes place
- **Naturally resolves high gradient layers without any extra modeling**
- **Inherently time accurate**



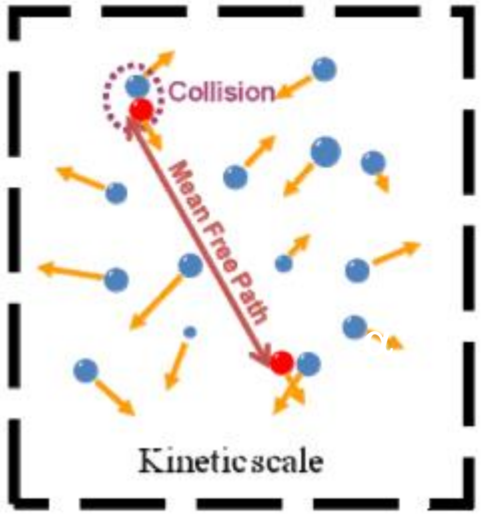
Alejandro L. Garcia, “ Direct Simulation Monte Carlo: Theory, Methods, and Open Challenges “, RTO-EN-AVT-194

[1] Bird, G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon, Oxford, England, U.K., 1994.

Direct Simulation Monte Carlo – Parameters

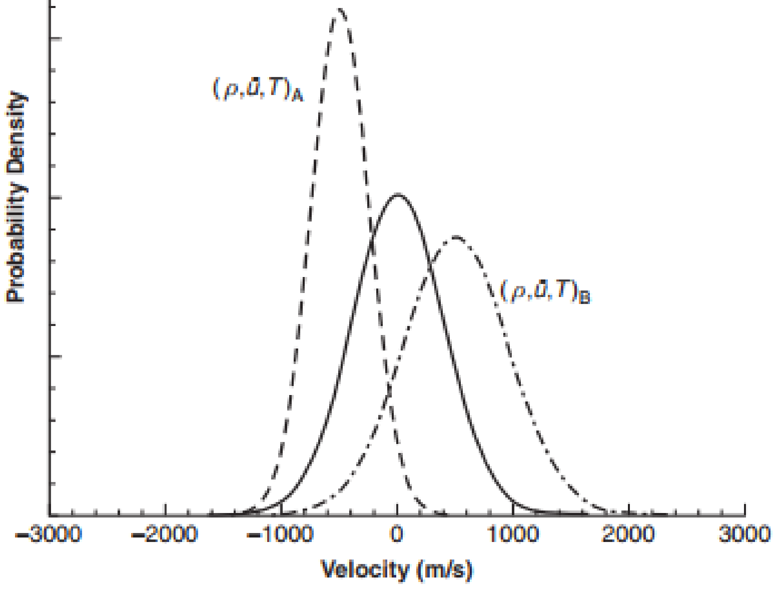
- The variables are the location (x, y, z), velocity (V_x, V_y, V_z) and the internal energy (E_{rot}, E_{vib}) of the gas particles
- Initialized with Maxwellian distributions
  - Collisions move the system towards equilibrium
- Macroparameters needed to be sampled,
  - Density, bulk velocity, temperature, etc.

A sampling cell with particles

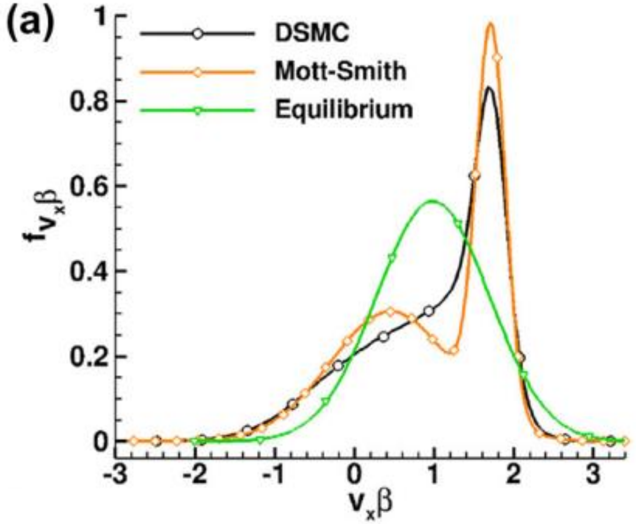


Alejandro L. Garcia, " Direct Simulation Monte Carlo: Theory, Methods, and Open Challenges ", RTO-EN-AVT-194

Two VDFs moving towards equilibrium [1]



Non-Maxwellian VDFs compared to Maxwellian [2]



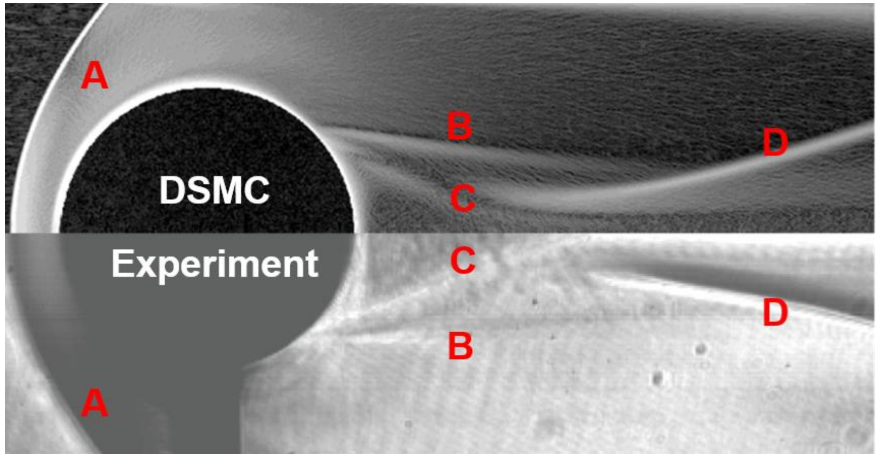
[1] I. D. Boyd & T. E. Schwartzentruber, Nonequilibrium Gas Dynamics and Molecular Simulation, 2017, Cambridge University Press

[2] Sawant, S. S., Levin, D. A., and Theofilis, V., "Analytical prediction of low-frequency fluctuations inside a one-dimensional shock," *Theoretical and Computational Fluid Dynamics*, Vol. 36, No. 1, 2022, pp. 25–40.

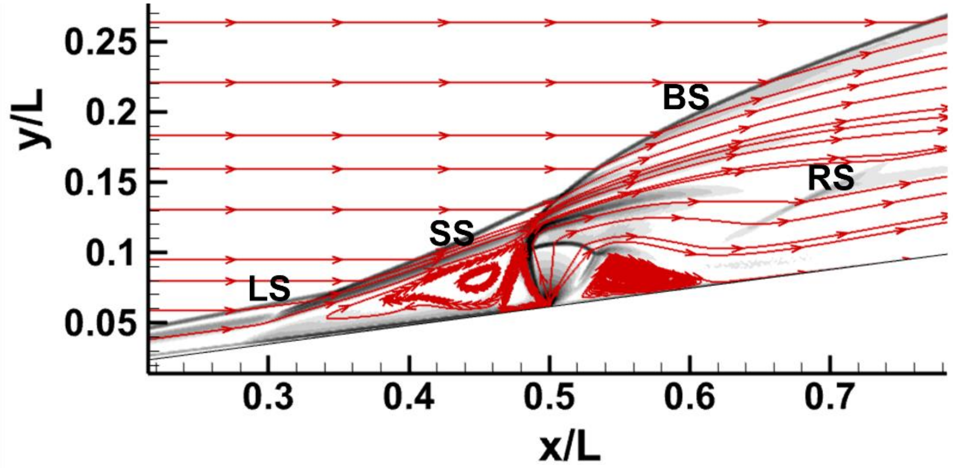
Direct Simulation Monte Carlo – Utilization

- Conventional use – "hot flows"
  - Re-entry, high altitude hypersonic flights
  - Thermochemistry
  - Rarefied Flows
  - Microchannel flows
  - Expansion to vacuum

- Novel use – "cold flows"
  - Shock boundary layer interactions
  - Flow Unsteadiness
  - Continuum breakdown
  - Base Flows for Linear Stability Analysis
  - Transition Studies



Karpuzcu, I. T., Jouffray, M. P., and Levin, D. A., "Effect of Oxygen Dissociation on Nitric Oxide Ultraviolet Emissions," *Journal of Thermophysics and Heat Transfer*, Vol. 37, No. 1, 2023, pp. 147–160.



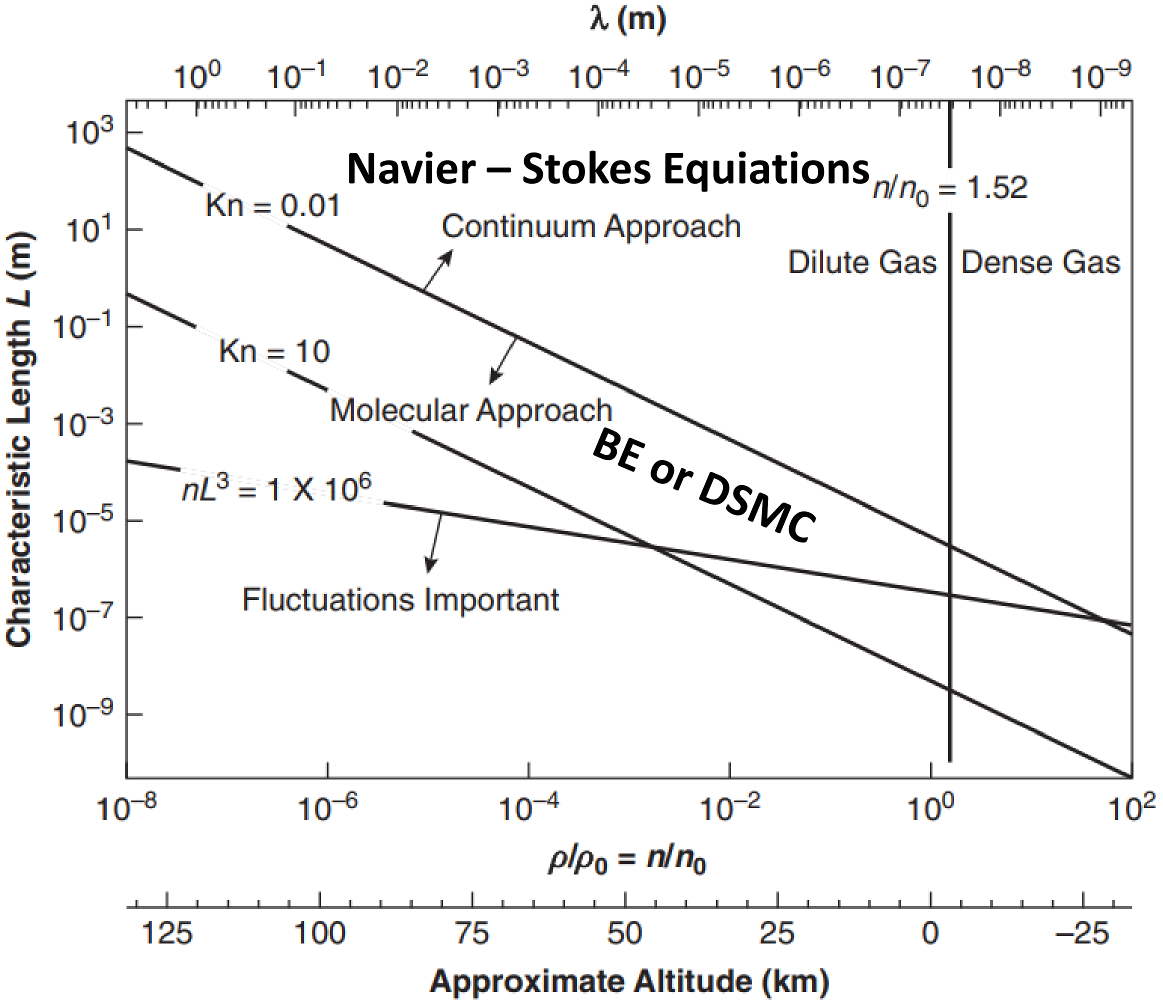
Karpuzcu, I. T., and Levin, D. A., "Study of Side-Jet Interactions over a Hypersonic Cone Flow Using Kinetic Methods," AIAA Journal, Vol. 61, No. 11, 2023, pp. 4741–4751.

Summary – Fidelity Offered by DSMC Method

- Resolves high gradient layers in the flow
  - Shocks, shear layers, expansion waves
  - Anistropic stresses and heat flux vector
- Captures rarefaction effects
  - Slip velocity and temperature jump
  - Finite thickness shocks
- Inherently time accurate
- Captures non-equilibrium with well tested collision models
  - Translational, rotational, vibrational nonequilibrium

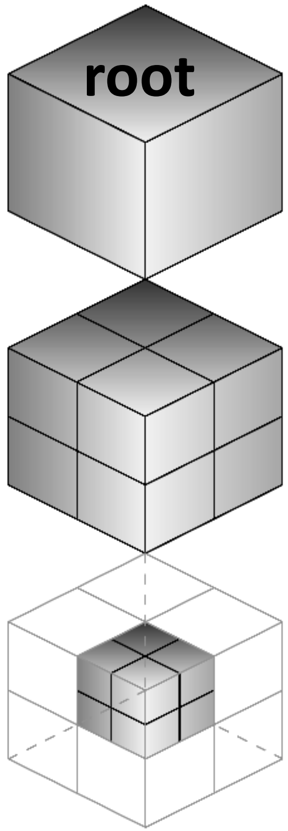
DSMC – Computational Challenges

- Collisions is the main cost
  - Majorant frequency scheme
- Sampling cells & collision cells
  - Sampling cells to see the flowfield
  - Collision cells for handling collisions
- Collision cell volume ~ λ_{local}^3
- If enough particles in collision cell, can resolv all scales
  - At least 4 particles in a collision cell
- Time step requirement
  - $\Delta t \leq$ local mean-collision-time
- Near continuum flows are computationally expensive
  - SUGAR – an efficiently parallelized DSMC solver
  - Frontera – a very powerful supercomputer

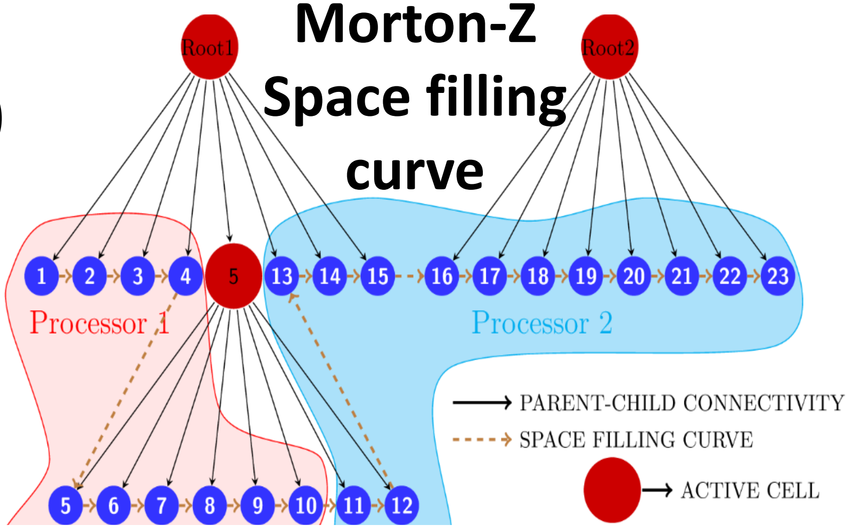


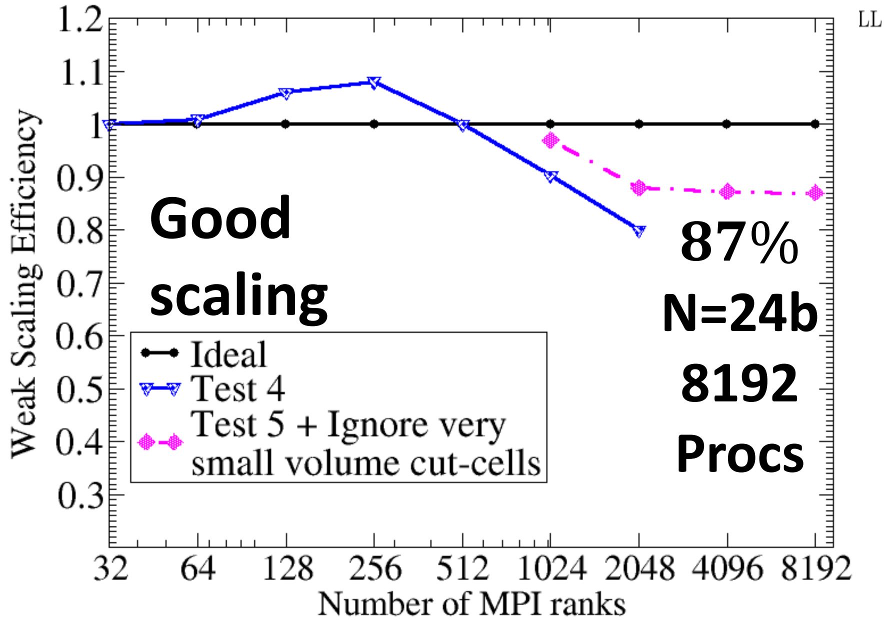
Key Strategies in SUGAR[1]

Adaptive Mesh Refinement (AMR)

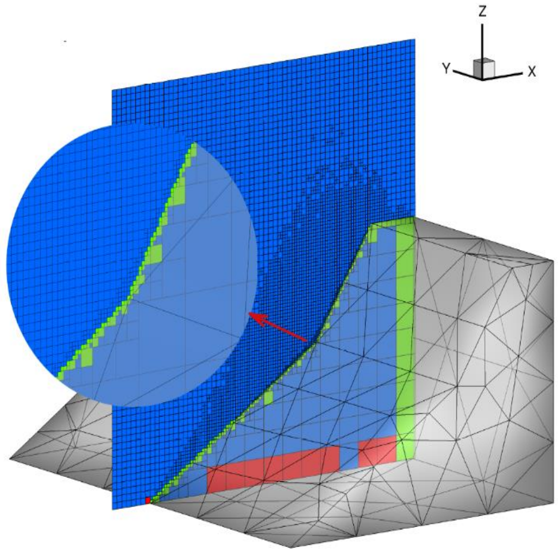


Morton-Z Space filling curve





A cutcell algorithm

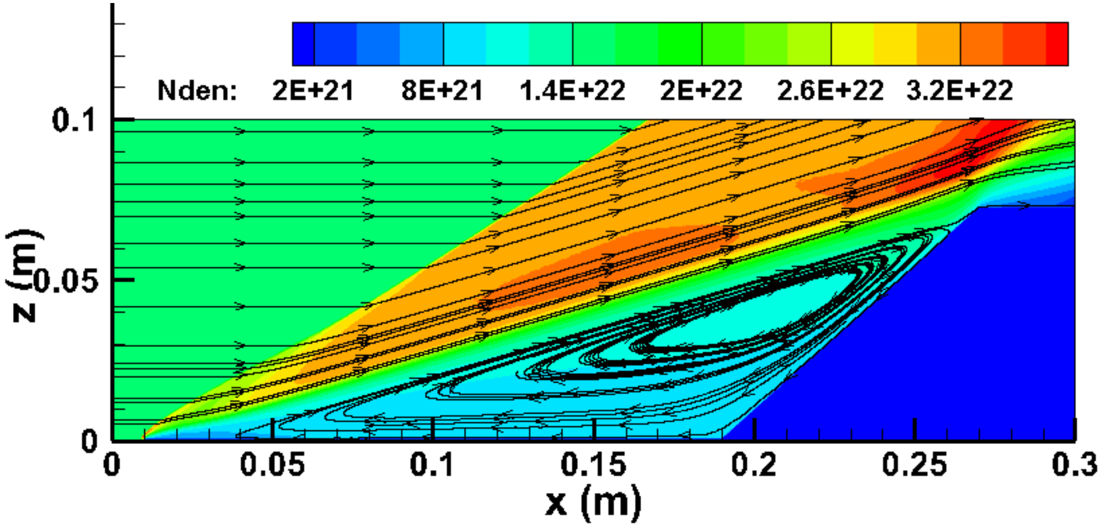


- Load balance scheme
- Efficient communication
- Collision schemes
- Energy relaxation models
- Gas-surface interactions
- Boundary conditions

[1]Sawant, S. S., Tumuklu, O., Jambunathan, R., and Levin, D. A., "Application of adaptively refined unstructured grids in DSMC to shock wave simulations," *Computers and Fluids*, Vol. 170, 2018, pp. 197–212. Viewgraph adapted from Dr. S. Sawant's PhD Thesis presentation.

Geometry and Free Stream Conditions

- Direct Simulation Monte Carlo (**DSMC**) method was used to simulate the flowfields
- SUGAR was used as the DSMC solver
- BiGlobal Stability analysis was done using LiGHT code
- Free stream conditions:
  - Re_L number=11,200
  - **Kn_L number=3x10^{-4}**
  - Mach number=3.0
  - Flat plate length(L)=0.18 m
  - Wall temperatures=300K
- A scaling including boundary layer and Mach number effects for the angle
- α*=42°, corresponding to α=5.7

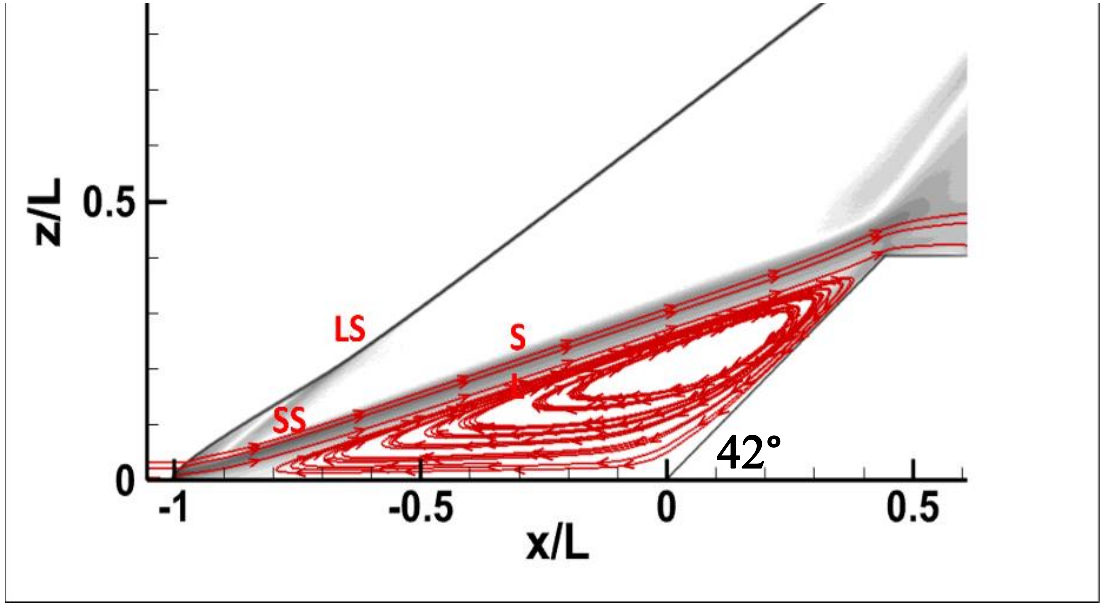


Formula for scaled angle[1]=

$$\alpha = \alpha^* \frac{Re^{\frac{1}{4}}}{0.332^{\frac{1}{2}} C^{\frac{1}{4}} (M_\infty^2 - 1)^{\frac{1}{4}}},$$

[1]Stewartson, K., “On laminar boundary layers near corners,” *The Quarterly Journal of Mechanics and Applied Mathematics*, Vol. 23, No. 2, 1970, pp. 137–152.

2D Computations for the Base Flow



- Steady state results are shown
- Separation bubble is more than 80% of the flat plate length
- There is no strong reattachment shock present
- For Δv>10%, the separation bubble is expected to become three dimensional[1]

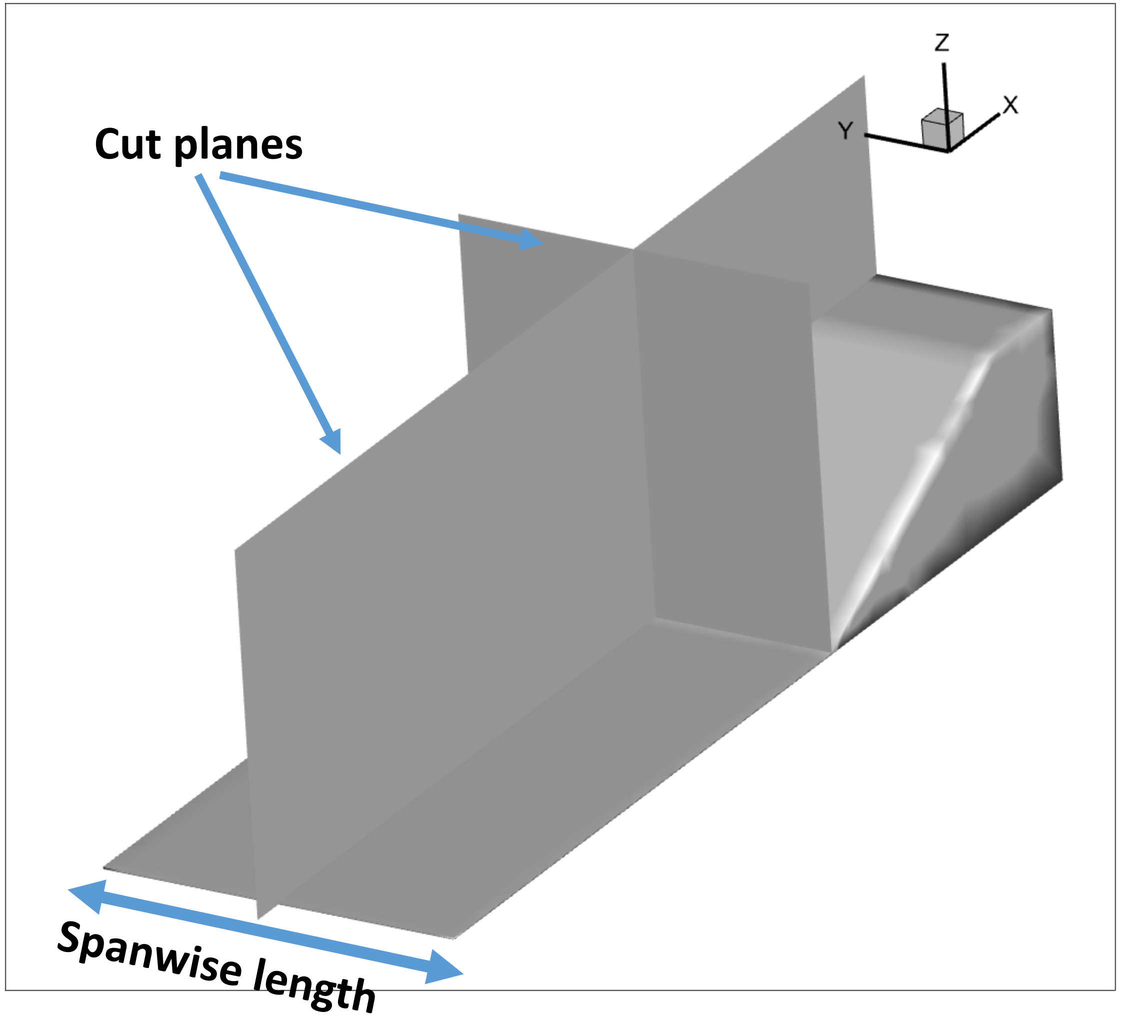
Ramp Angle	Scaled Angle using L-L_sep	Scaled Angle using L	L_sep/L	Recirculation Strength (Δv) [2]
42°	5.7	8.6	0.86	16.3%

[1]Theoflis, V., Hein, S., and Dallmann, U., "On the origins of unsteadiness and three-dimensionality in a laminar separation bubble," *Philosophical Transactions of the Royal Society of London*, Vol. 358, 2000, pp. 3229–3324.

Karpuzcu, I. T., Theofilis, V., and Levin, D. A., "On linear stability of supersonic flow over a short compression corner at large ramp angles," , 2024. https://doi.org/10.48550/arXiv.2405.06775

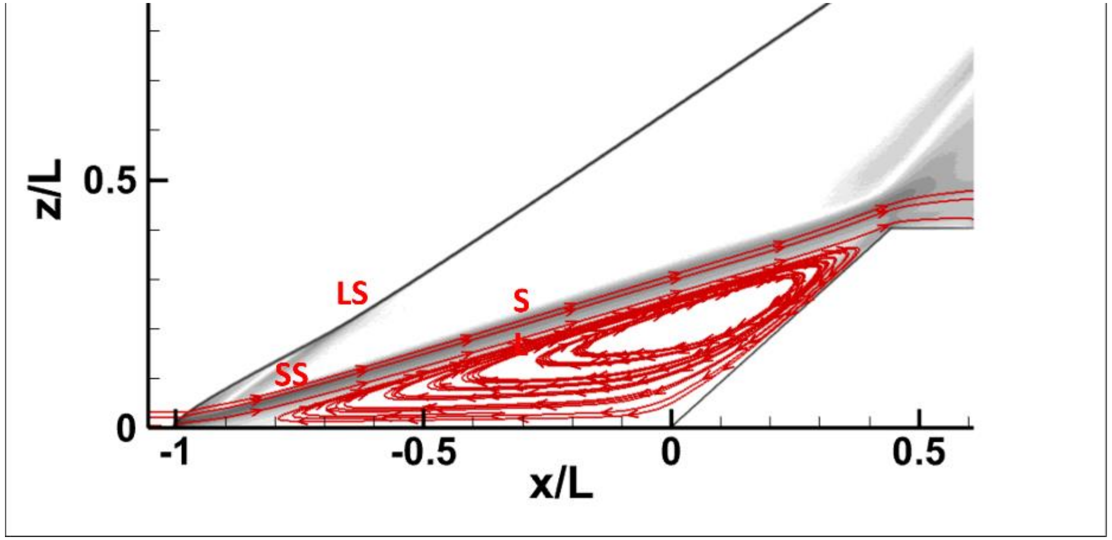
3D Spanwise Periodic DSMC Simulations – Case Setup

- 42° Ramp angle case is simulated with spanwise periodic (SP) boundaries
- Sampling cell size and time step are the same as the 2D case
- Spanwise length is selected as 1.12L
  - BiGlobal stability analysis showed that most unstable mode is occurring ~0.56L
- **30 billion computational gas particles**
- **85×10^{12} collisions /τ_{flow}**
- **Frontera cost: 7200 SUs/τ_{flow}**
- **About 20 τ_{flow} needed to capture the unsteady flow physics**

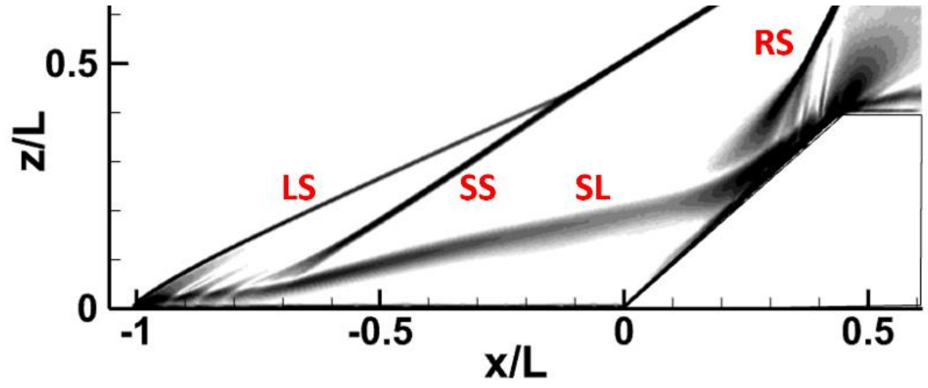


Comparison of 3D SP vs 2D Cases

2D simulations



3D simulations, middle y plane cut



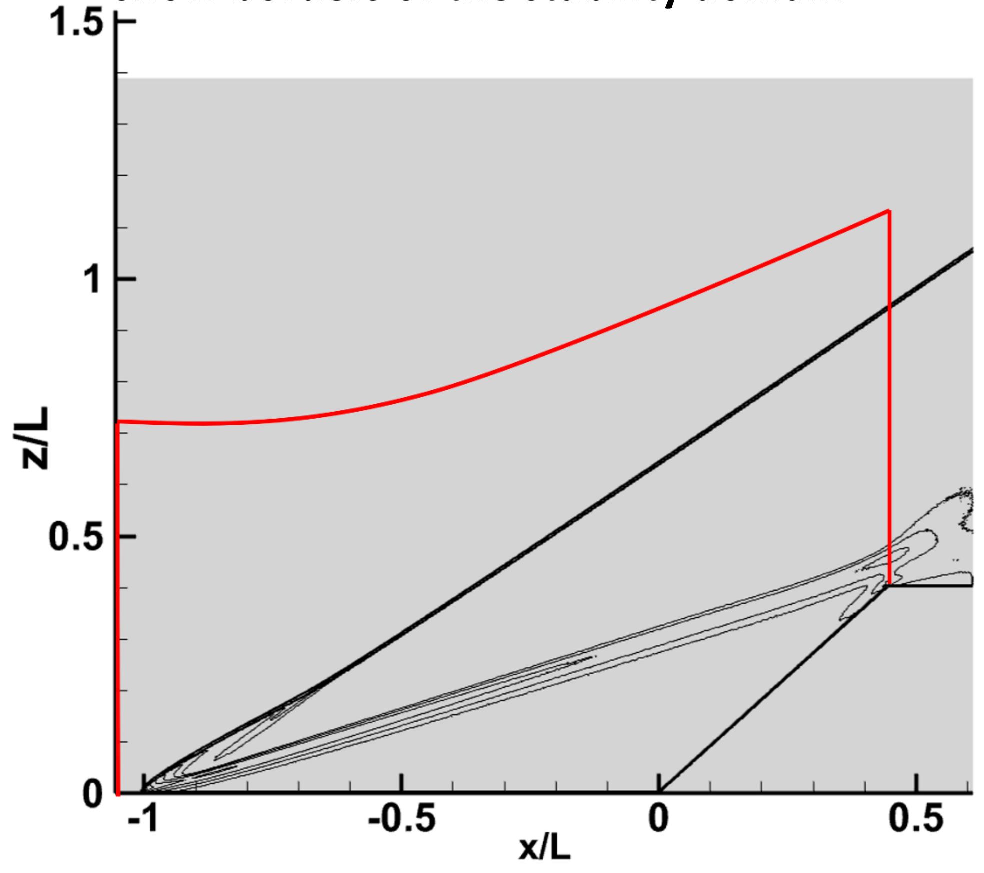
- 42 ramp angle case resulted in very different flowfields for 2D and 3D SP simulations;
  - Separation bubble is smaller
  - A very strong separation shock appears
  - **Flow is three dimensional**

BiGlobal Stability Analysis – Case Setup

- DSMC domain is the full flow solution from SUGAR, shown by the grey area
- Stability domain is shown with red lines
- Dirichlet BC: perturbations are set zero
- Extrapolation BC: gradient of perturbations are constant
- Ansatz are given as follows:

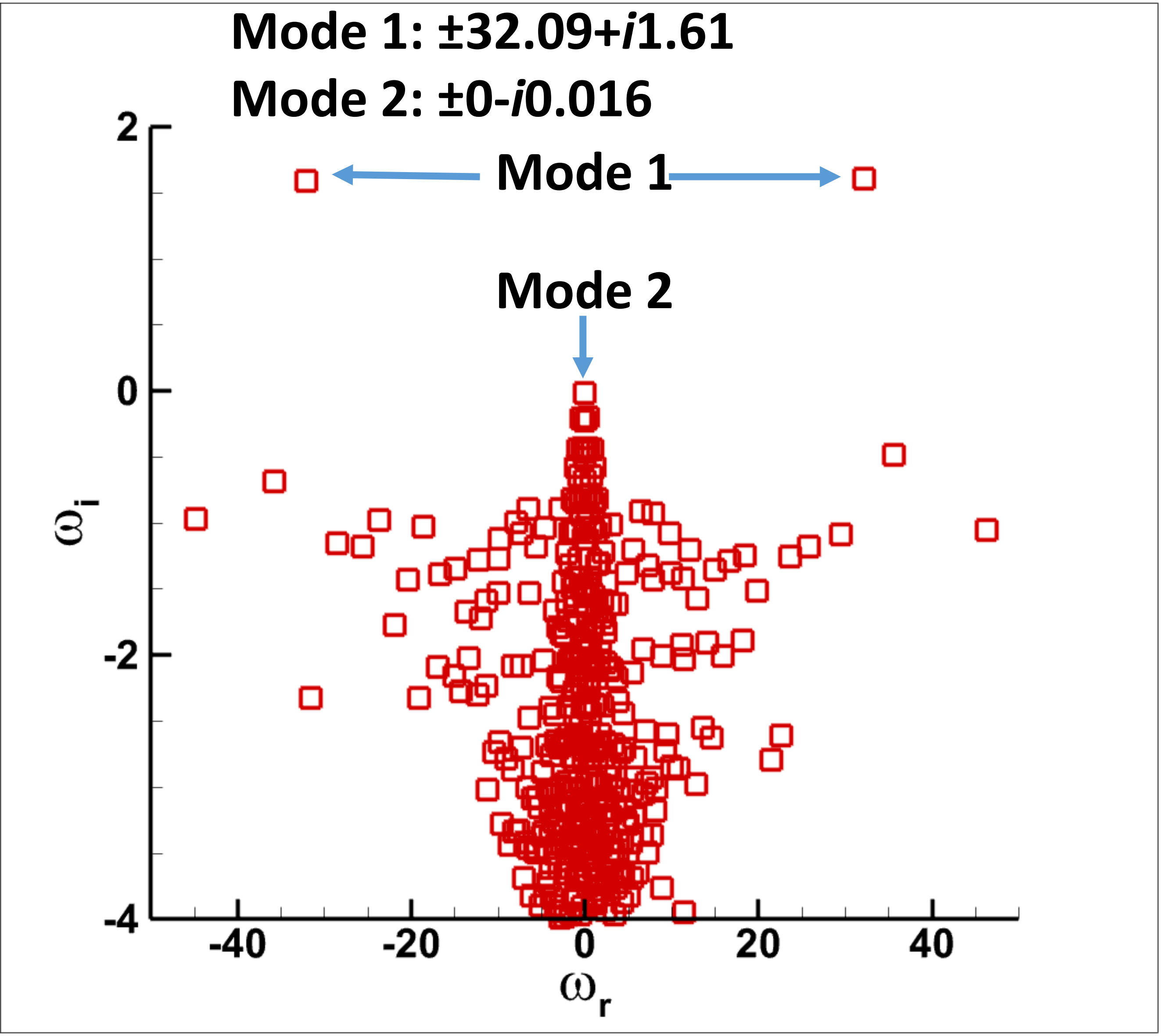
$$q(x,y,z,t) = \bar{q}(x,y,z) + \varepsilon\tilde{q}(x,y,z,t)$$
$$\tilde{q}(x,y,z,t) = \hat{q}(x,z)e^{i(\beta y-\omega t)}$$
$$\lambda = \frac{2\pi}{\beta} \quad \lambda^* = \frac{\lambda}{L}$$

Contour lines show gradient of density, red line show borders of the stability domain

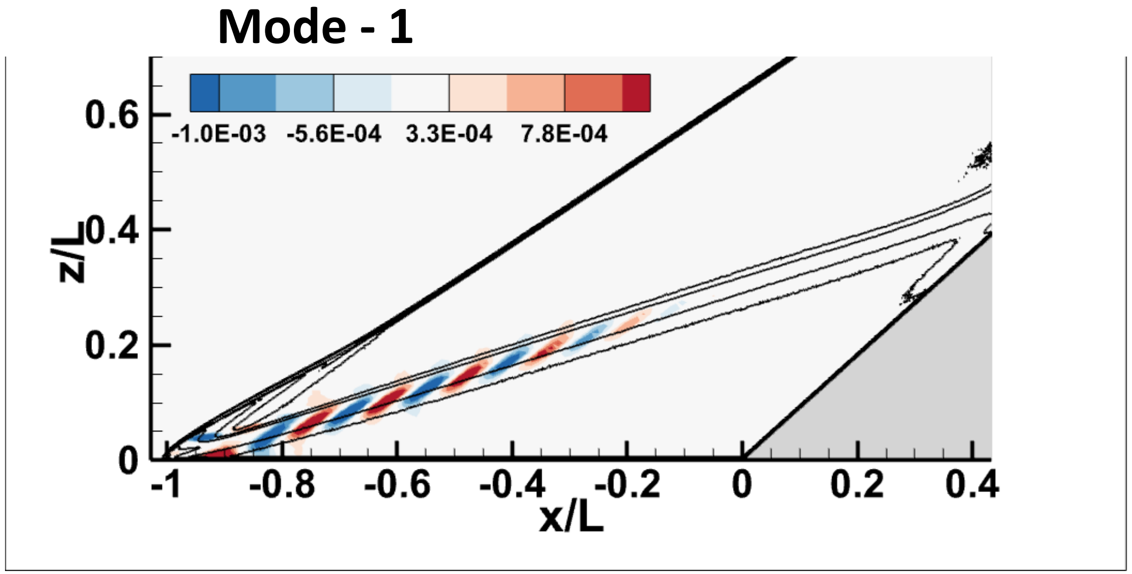


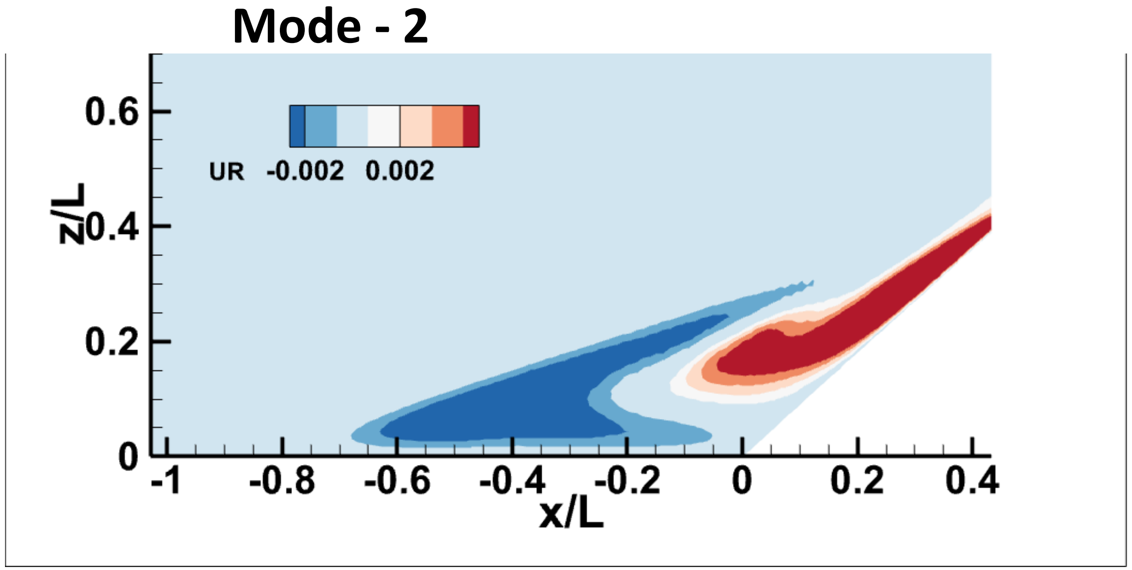
- β is the spanwise wavenumber.
- Assuming β real and ω complex, eigenvalue problem is solved for complex ω for given β values.

42° Ramp BiGlobal Stability Results at β=11



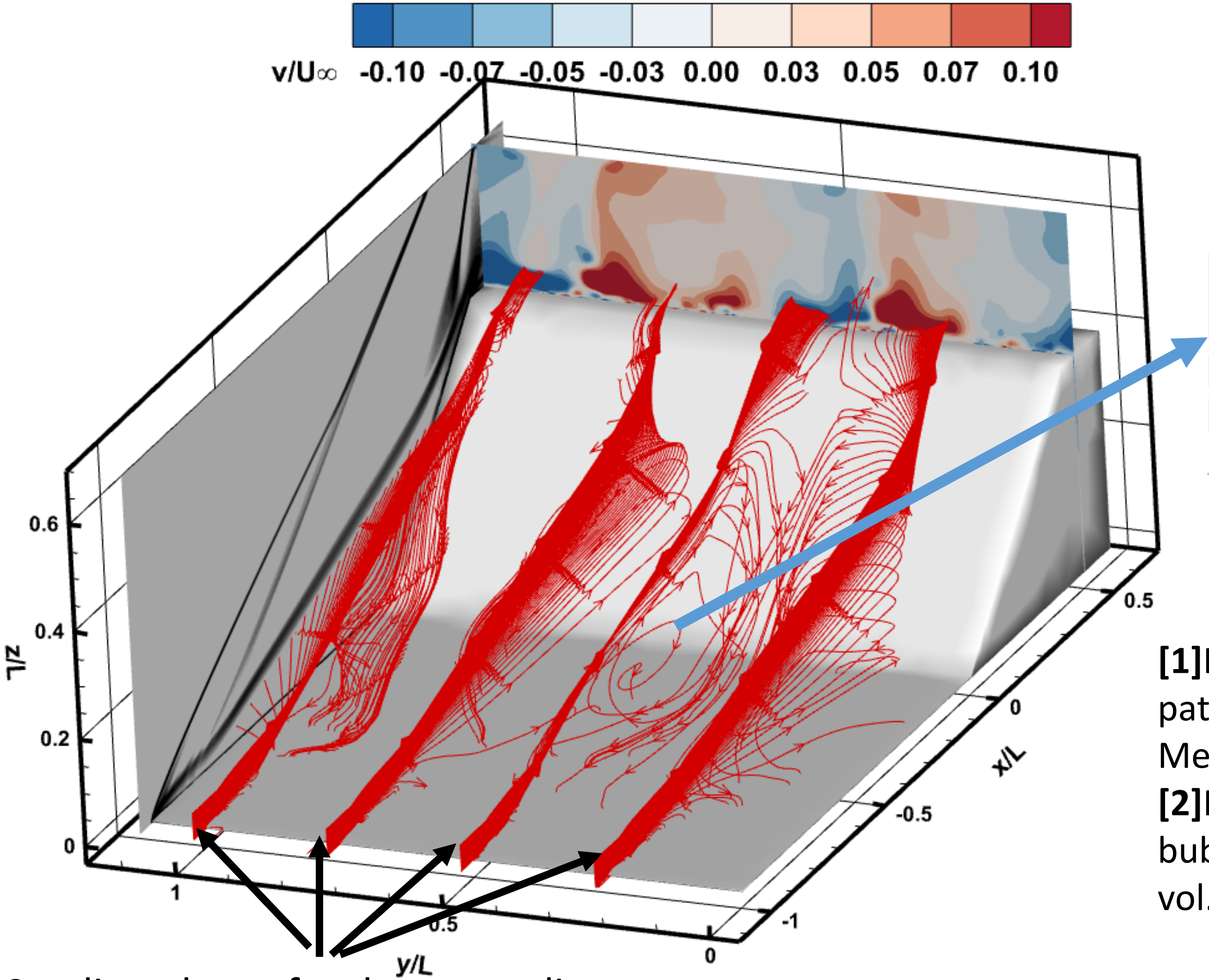
Real part of the eigenvector for the spanwise velocity



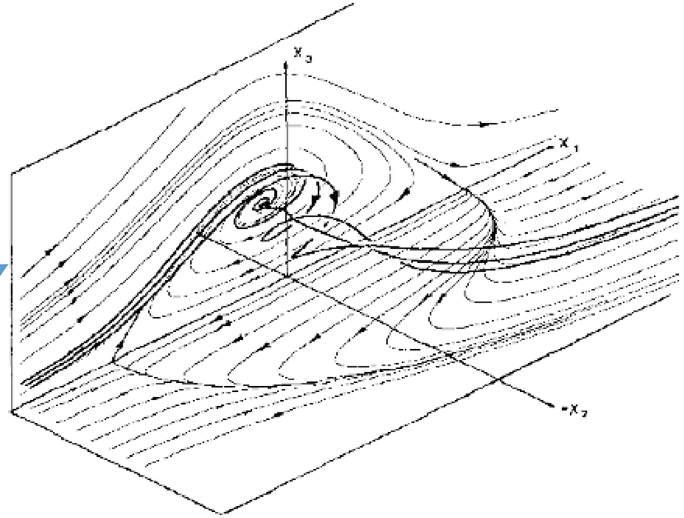


Streamlines within the Separation Bubble for 3D SP Computations

- Separation region flow topology is highly 3D
- Quite similar to the U separation[1,2], originating from the growth of the 3D perturbations



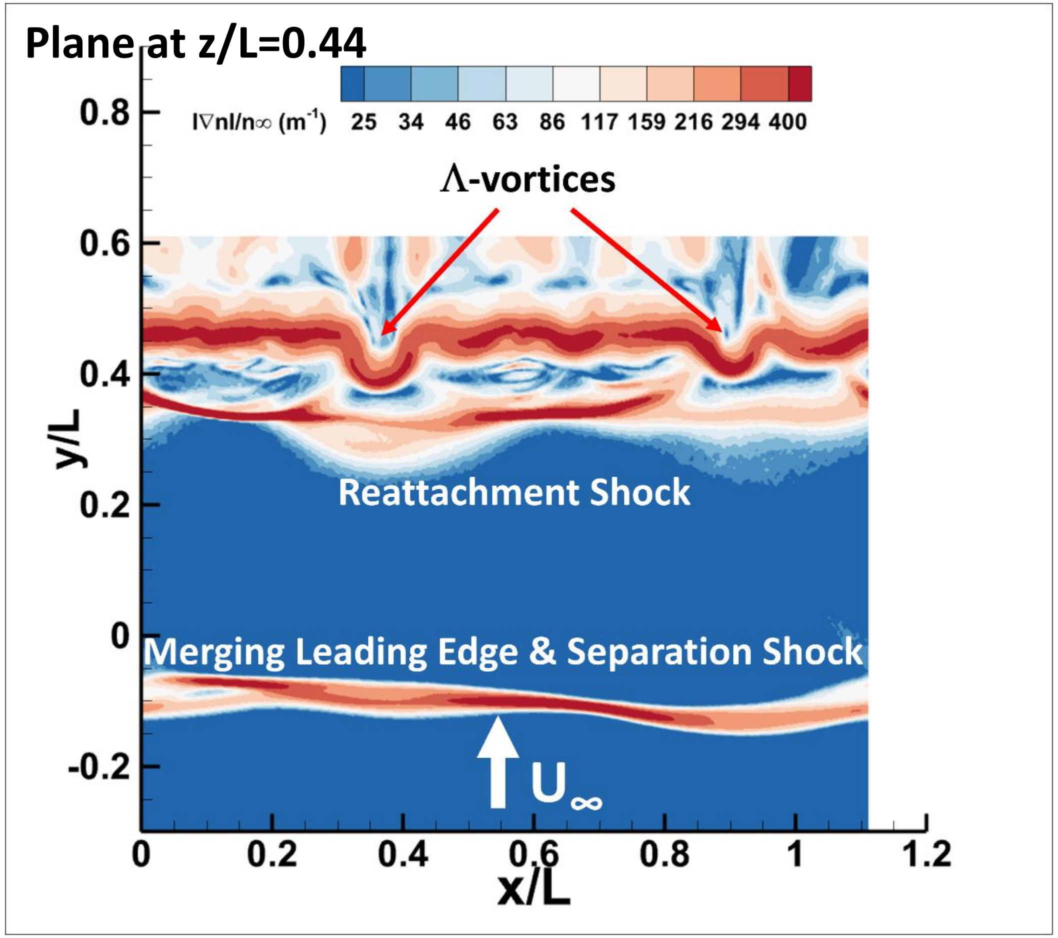
Seeding planes for the streamlines

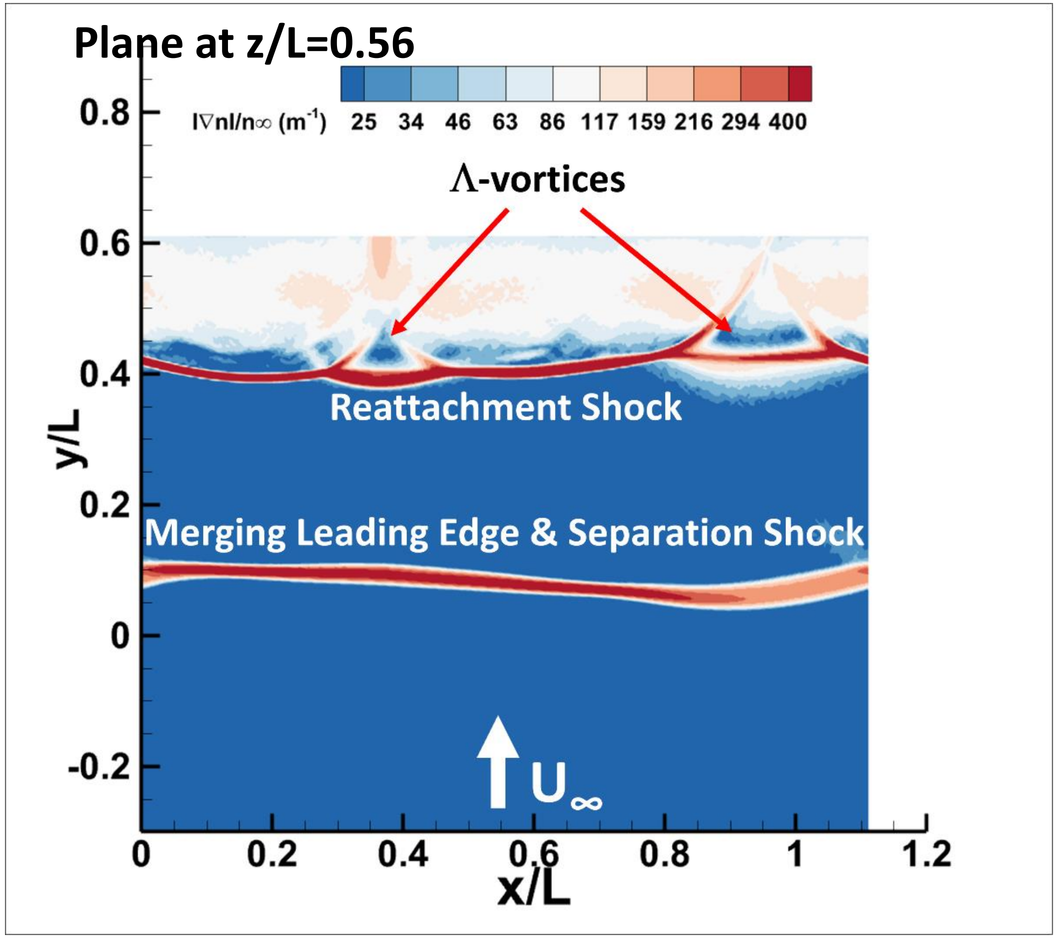


[1]Perry AE, Chong MS, "A description of eddying motions and flow patterns using critical-point concepts", Annual Review of Fluid Mechanics, vol. 19, pp. 125 – 155, 1987

[2]Rodríguez D, Theofilis V, "Structural changes of laminar separation bubbles induced by global linear instability", Journal of Fluid Mechanics, vol. 655, pp. 280 – 305, 2010

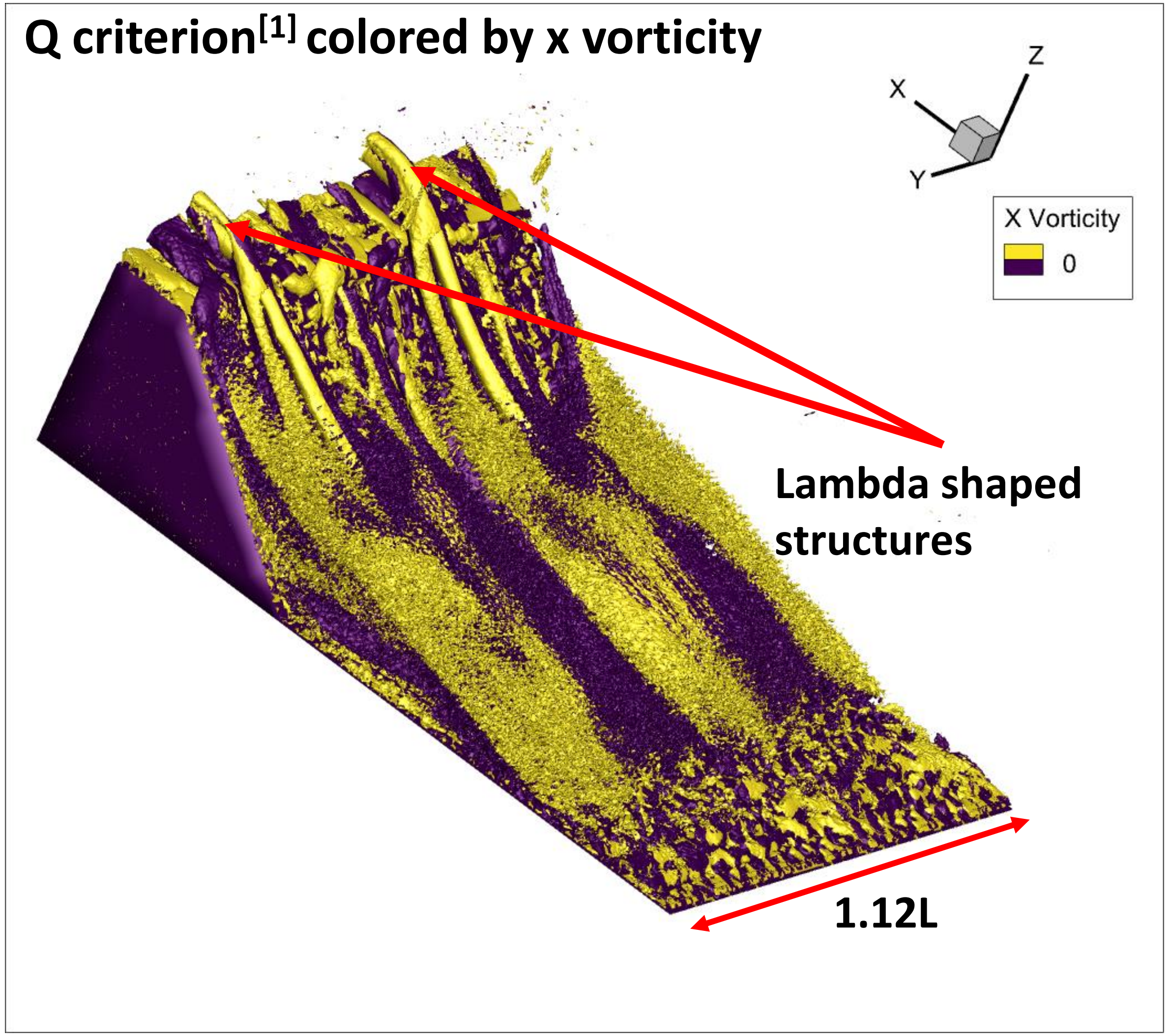
Three Dimensionality of the Shock Layers





- Both reattachment shock and separation shock has spanwise periodicity
  - Same periodicity as the interacting shear layer
- Analogous to the findings of Sawant et. al. JFM, 2022

Coherent Structures from Spanwise Periodic DSMC Simulations

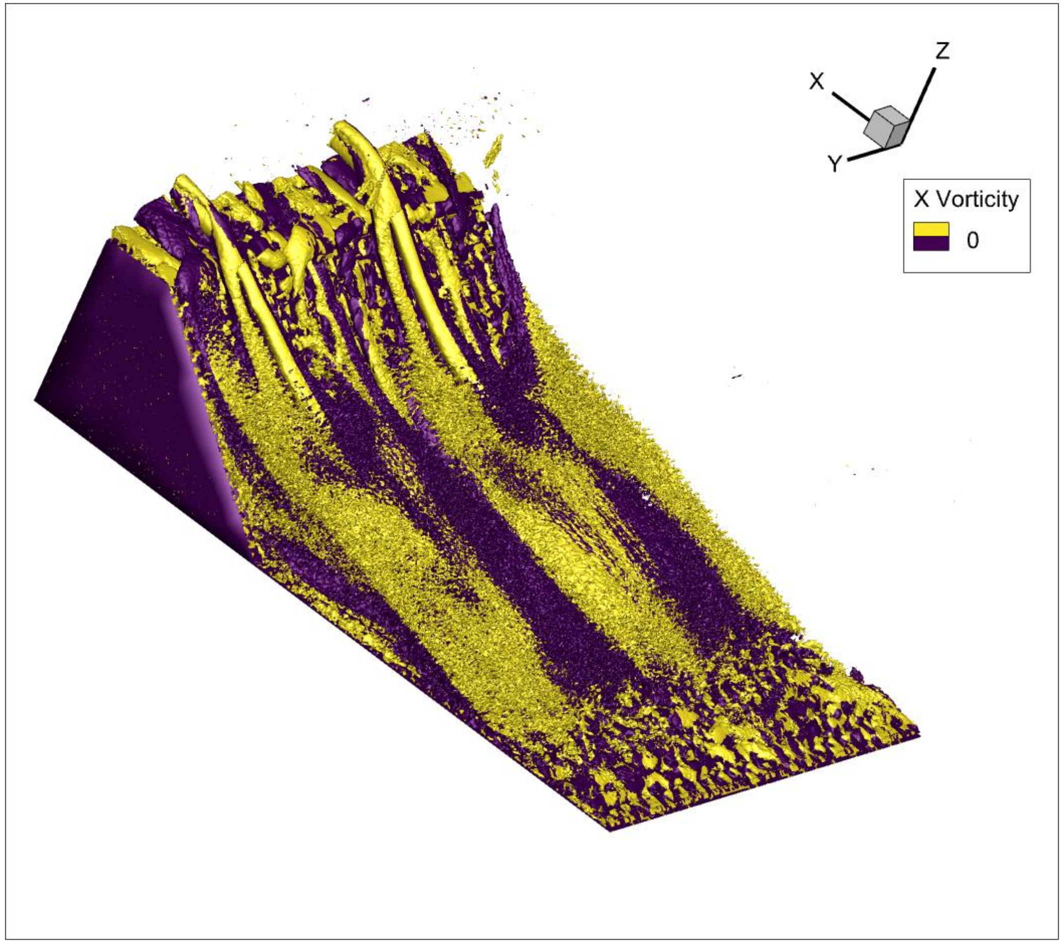


- Q criterion colored by x vorticity is shown
- Two coherent structures are observable at the ramp
  - So called lambda vortices
  - Also known as causing transition to turbulence downstream of the flow
- X vorticity values are also alternating starting from the separation point
  - Indicator of counter rotating vortices

[1]Hussain, F.: On the identification of a vortex. JFM 285, 69-94

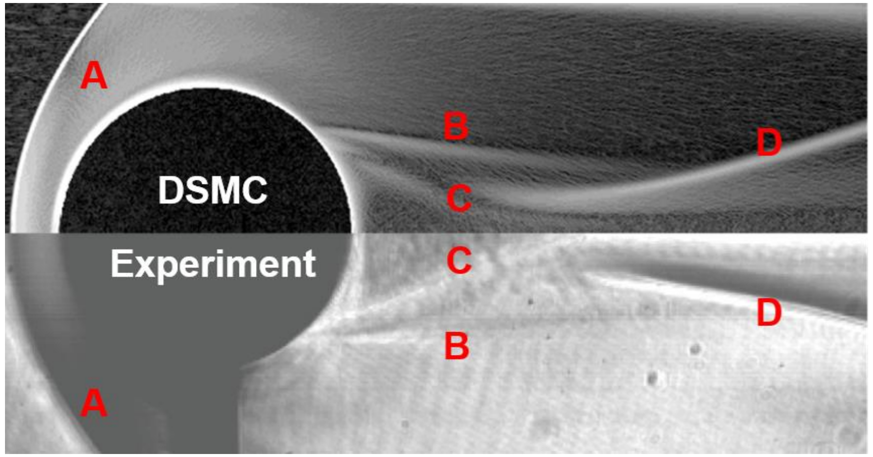
Summary for Flow Physics

- BiGlobal Stability analysis for the base case showed:
  - The leading unstable mode is **originating from the shocks and not from the recirculation**, captured for the first time
  - Made possible by accurately resolving the leading edge and separation shocks with DSMC
- DSMC for the 3D periodic ramp simulations confirmed these predictions:
  - Flow 3D and unsteady for the 42° ramp angle case
  - Separation bubble becomes a 3D structure
  - **Non-linear evolution of the delta vortices captured**



Future Directions for SUGAR – Challenging problems

- Experimental efforts on-going for High Mach number
  - Flow over blunt bodies[1]
  - Mach stem[2]
- Both type of flow has
  - Thermochemistry and non-equilibrium in 3D
  - Unsteadiness due to shock interactions
- Estimated cost for the flow over a cylinder at M=7.2 and 60 km altitude, with a domain of 2.5 cm x 15.0 cm x 5.0 cm;
  - **100 billion simulation particles, 84000 SUs/τ_{flow}**
- Capturing natural transition to turbulence;
  - Fully 3D simulations
  - Higher Reynolds Numbers, $O(10^7)\ m^{-1}$
  - At least two orders of magnitude improvement for the computational efficiency needed



[1]Kearney S. et. al., 2023, Burst-mode planar laser-induced fluorescence of Nitric Oxide in the Sandia Free-Pistion Shock Tunnel

[2] Boris S. Leonov, et. al.,2023, High-speed planar laser-induced fluorescence investigation of nitric oxide generated by hypersonic Mach reflections for computational fluid dynamics validation. Physics of Fluids 1 June 2023; 35 (6): 066102

Future Directions for SUGAR – Improvements to the code

- Better load balancing schemes
  - Most of the collisions happening in high density regions
- Utilizing High fidelity I/O libraries
  - Writing / reading information of billions of particles
  - Hdf5 libraries
- Improve weak scaling

Acknowledgments

The research conducted in this work is supported by the Office of Naval Research under Grant No. N000141202195 titled “Multi-scale modelling of unsteady shock-boundary layer hypersonic flow instabilities,” with Dr. Eric Marineau as the Program Officer. This research is also supported by NSF TACC Frontera supercomputer with the project number CTS23002. The authors also thank TACC Frontera for the travel support provided.