Towards Modeling and Simulation of Particulate Interactions with High-Speed Transitional Boundary-Layer Flows

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Collaborators and Funding

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- External collaborators: **Prof. Hermann Fasel** (University of Arizona), **Anthony Haas** (University of Arizona), fruitful discussions on particle modeling with **Prof. Anatoli Tumin** (University of Arizona)

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- An extended form of this presentation will be given at AIAA Aviation conference in Dallas, Texas, 17th – 21st June 2019

Outline

Particle Flow Simulations Background

Background, prior research and findings.

Numerical Methods

BitCart, Dual-Mesh Approach, and AMR.

Simulations Results

Validation, and 2D/3D patricle flow simulations results.

Summary, Outlook, & Research Interest

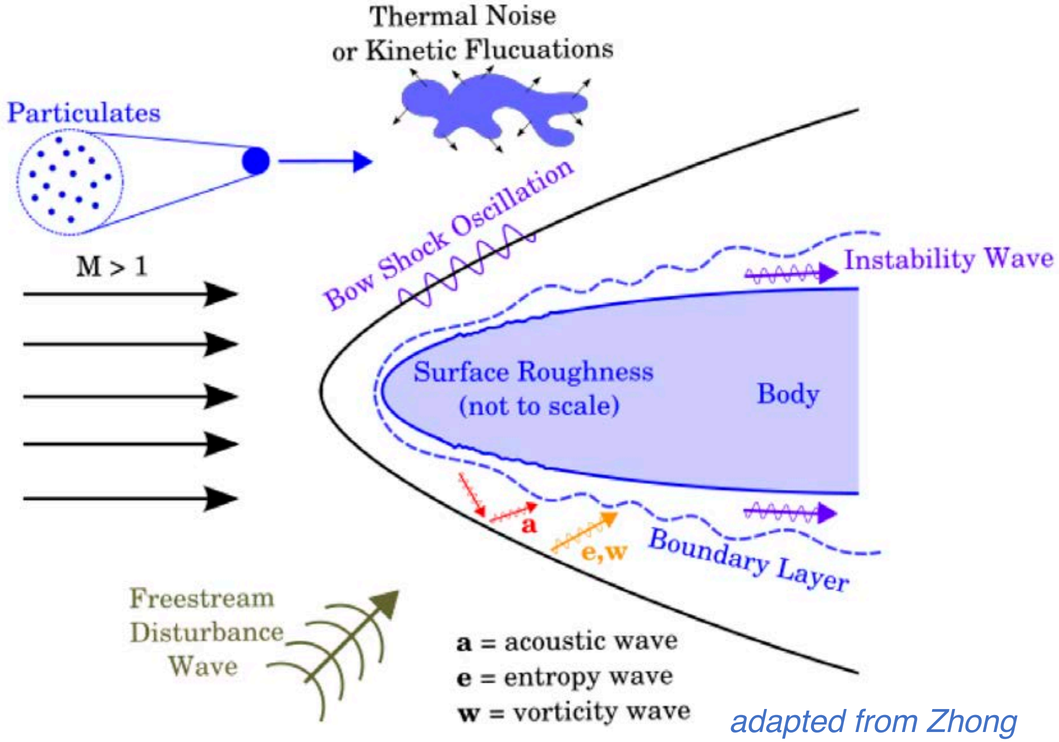
Summary of presented research

Hypersonic Free Flight Disturbance Environment

- Understanding of the relevant physics is essential to **reduce design margins** and **systems uncertainties** and, ultimately, guide the development of novel innovative designs

Artist's concepts of hypersonic cruise hardware

Wave field in a hypersonic flow induced by disturbance sources



adapted from Zhong

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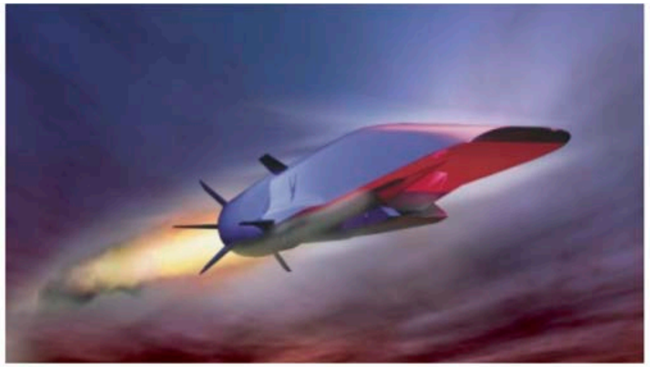

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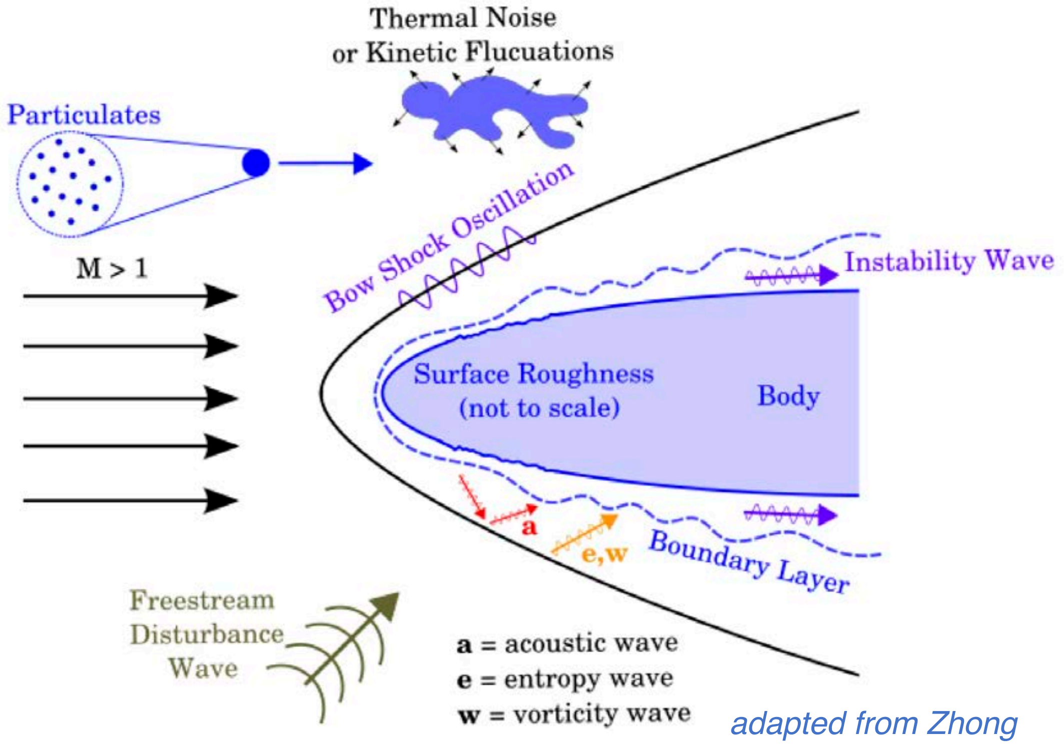

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- Consider **flow conditions** at altitude of **15-45 km** (stratosphere) with a free-stream temperature range of 217 to 260 K and free-stream Mach numbers between **6-18**

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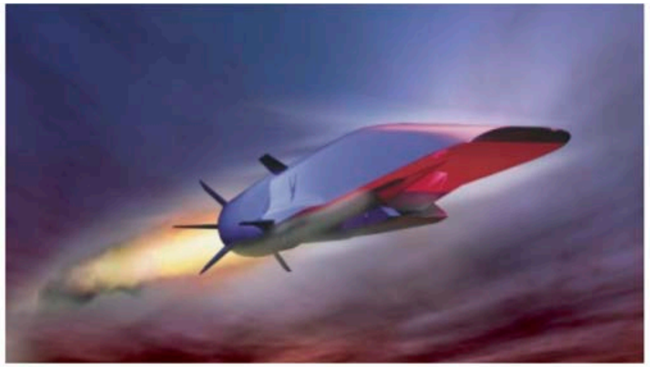

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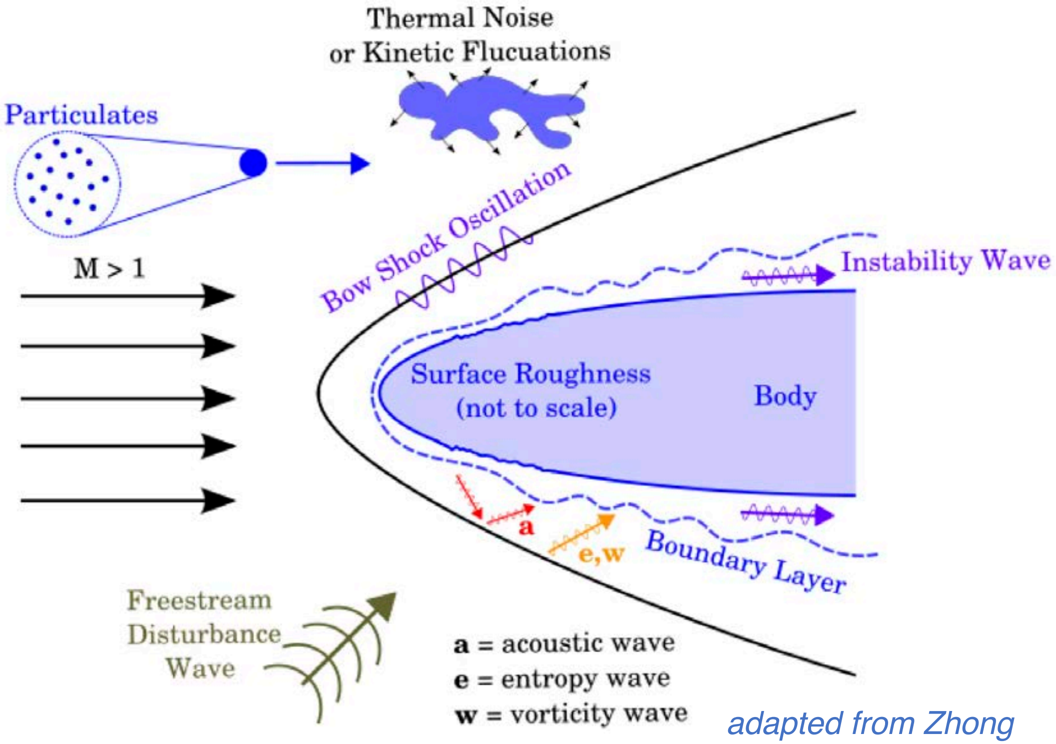

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- **Different types of particulates** can be found with ice clouds, a non-negligible amount of exhaust products from rockets, volcanic eruptions, terrestrial and cosmic dust, *etc*.

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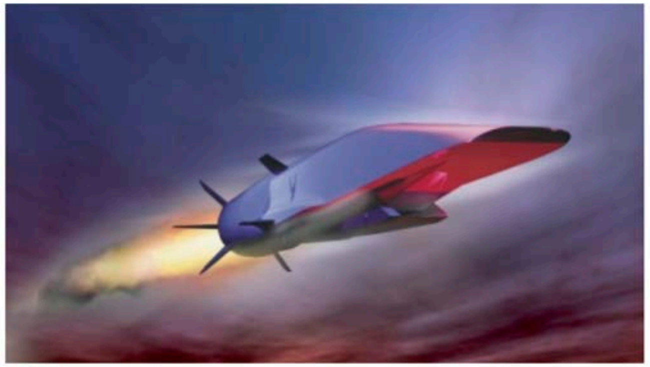

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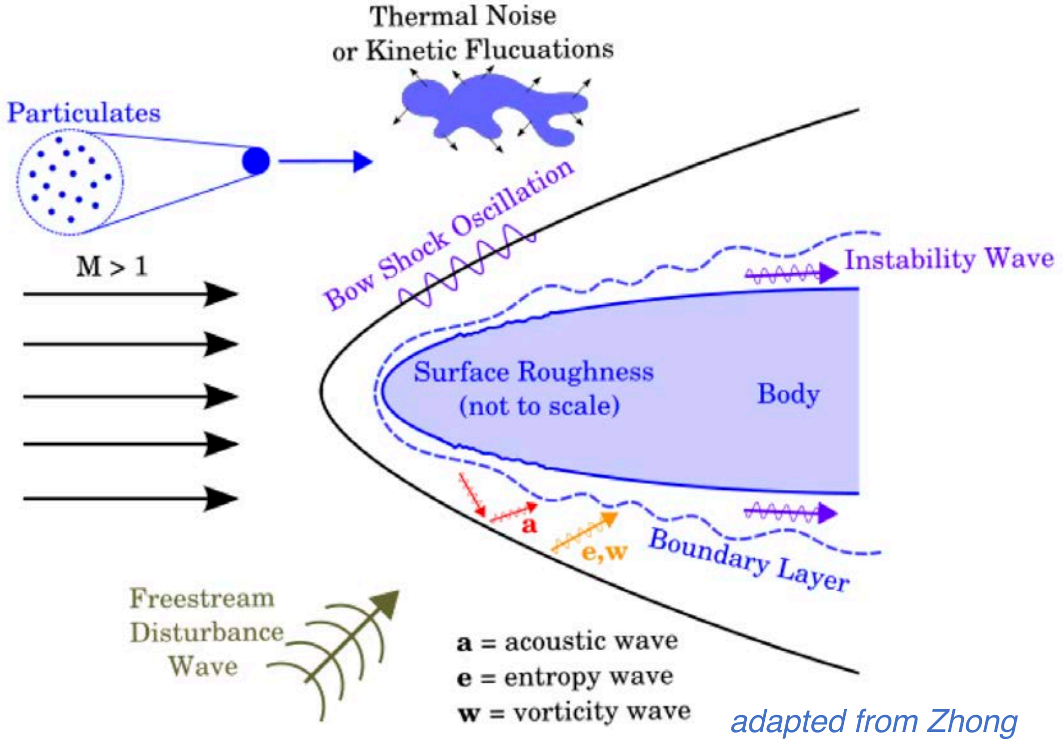

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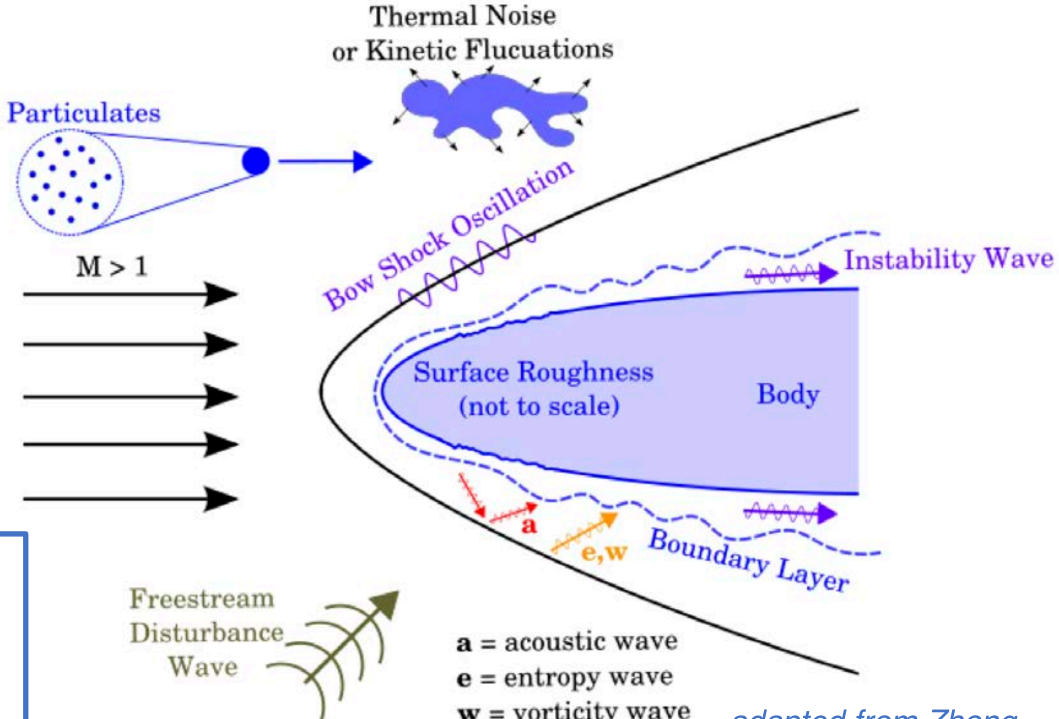

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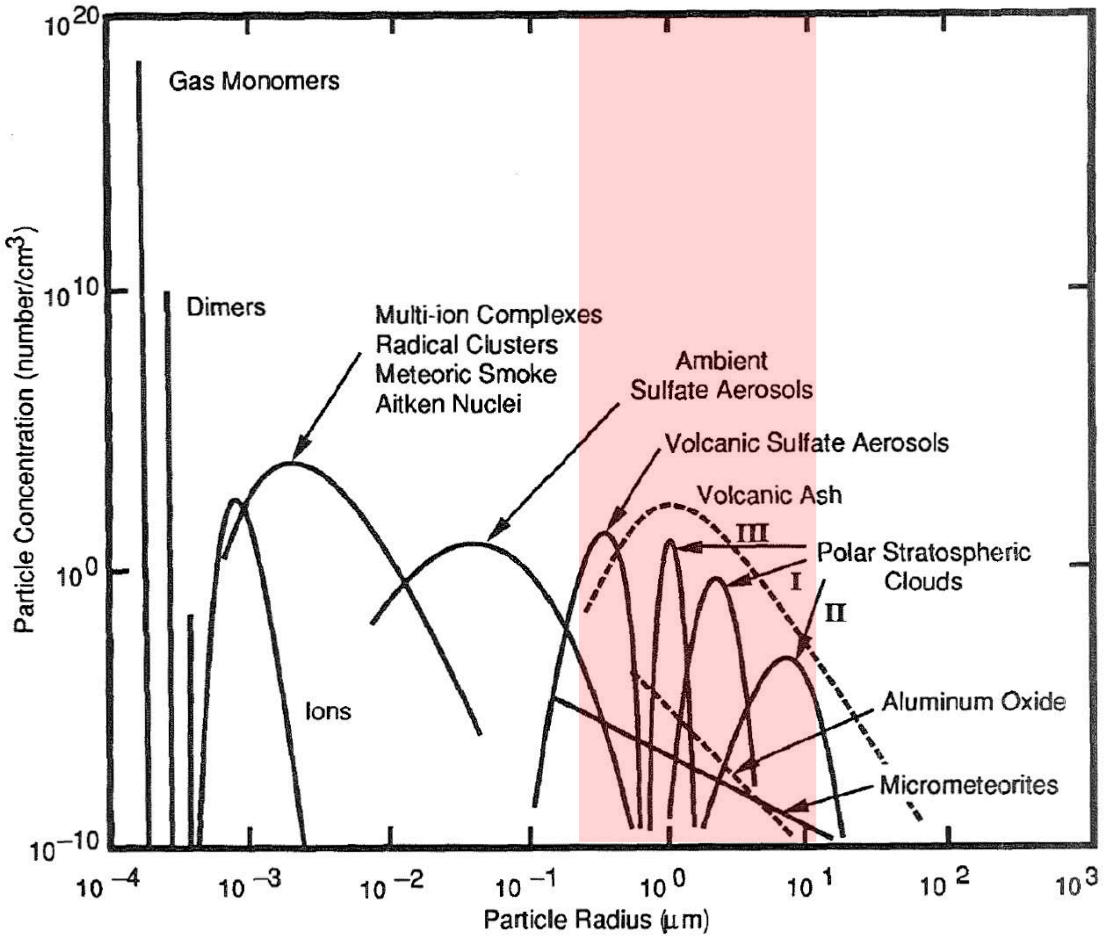
Research Objective: Provide physical insight into the interaction of the disturbance environment, in particular particulates, on the flow field during realistic high-speed flight conditions

Particle Properties in Atmosphere

- **Particulates are inevitably present** in the atmosphere as well as in wind tunnels (unless careful cleaning technique), and they can be a major source of disturbance energy
- Properties and concentration of particles in the atmosphere are documented in the literature (also see **Hypersonic Flight In the Turbulent Stratosphere Research Team at UCB**)
- **Highly variable and seasonably dependent**
- High concentration of particles can be obtained in **ice clouds** (mostly in troposphere, regular crystalline shaped $\mathcal{O}$(10-1000μm)))
- Large amount of particulates are related to **exhaust products from rockets** ($\mathcal{O}$(10μm))
- Another important source of particulates is **volcanic eruptions** ($\mathcal{O}$(1-20μm))

It is not a question of whether a flight vehicle encounters particles but rather how these particles affect the flow field around them!

Approximate size distributions for particles with different origins in the Earth's middle atmosphere

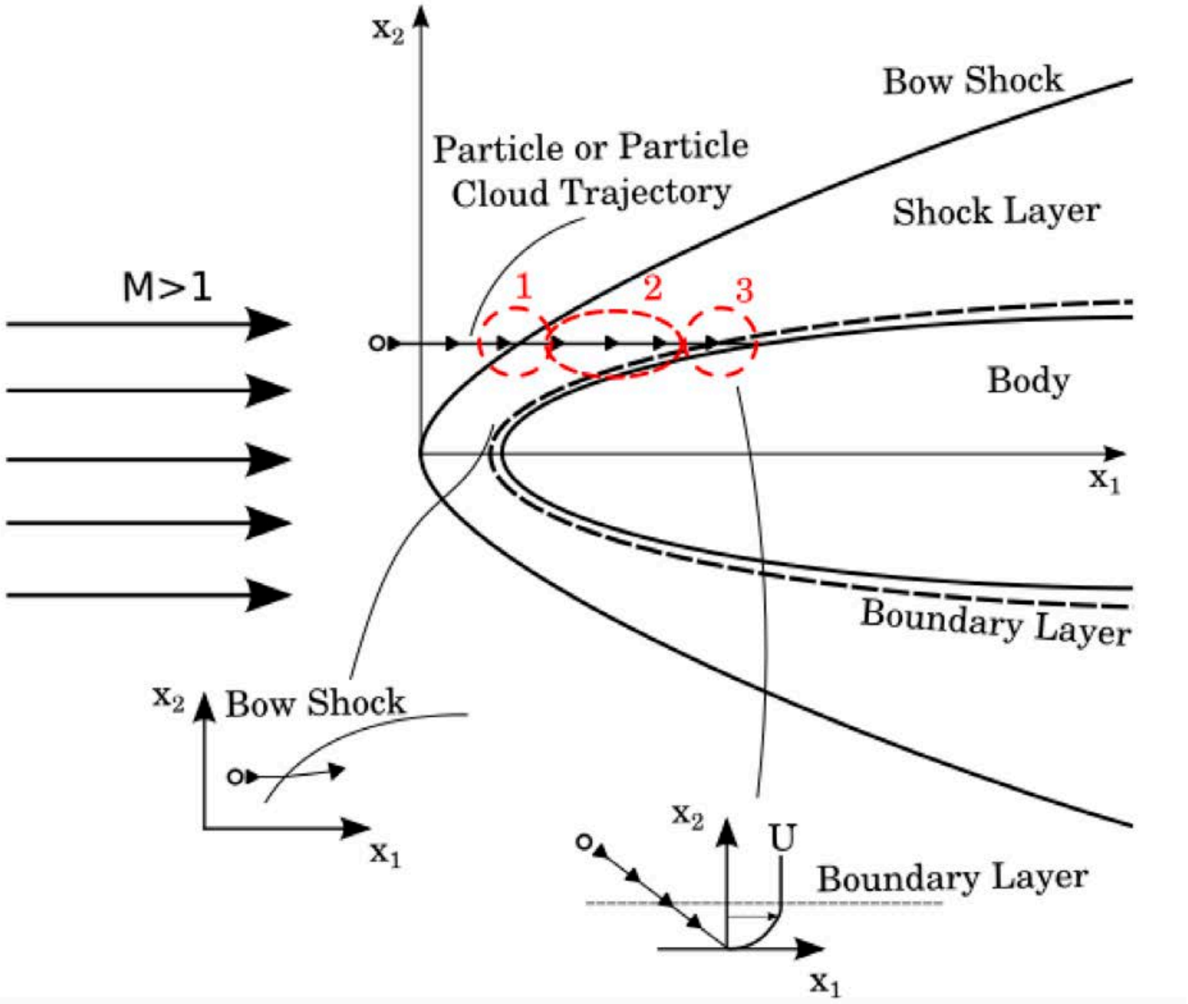


(adjusted from Turco, data before 1992)

Particle Flow Interaction Mechanisms

Different mechanisms of how particles affect low and high-speed transition were summarized in Bushnell (1990):

1) **roughness** generation via impacting or sticking to the surface,



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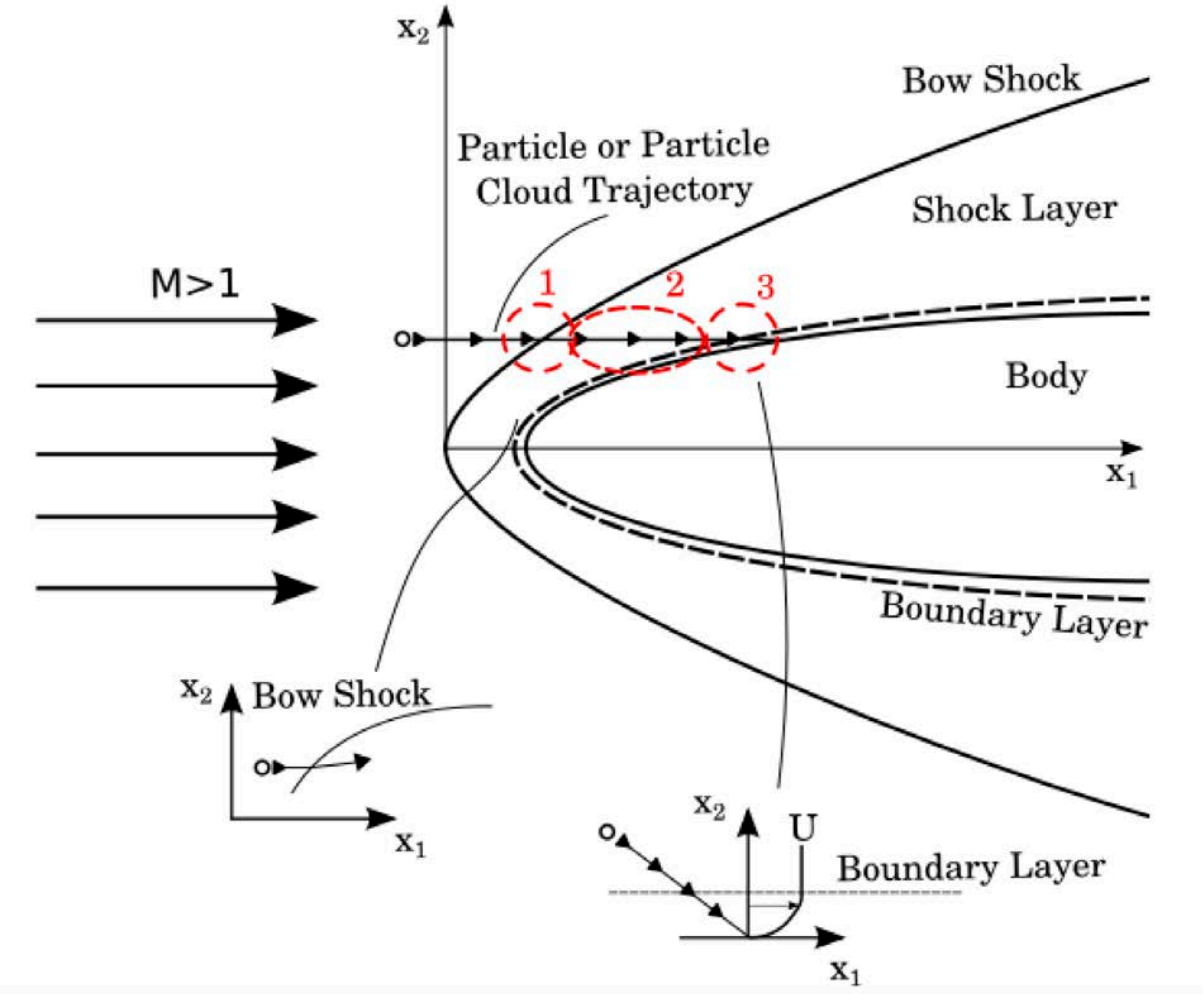

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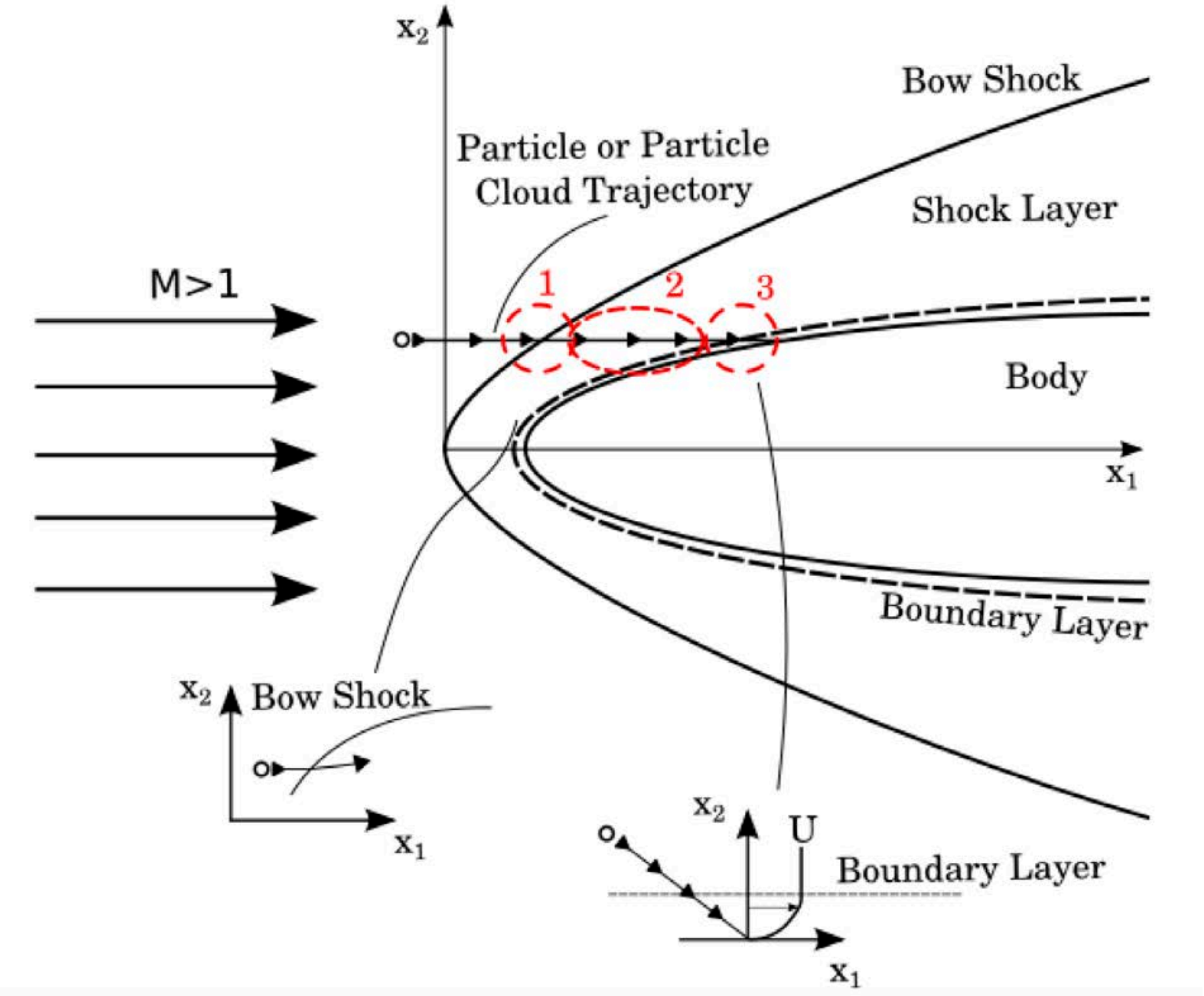

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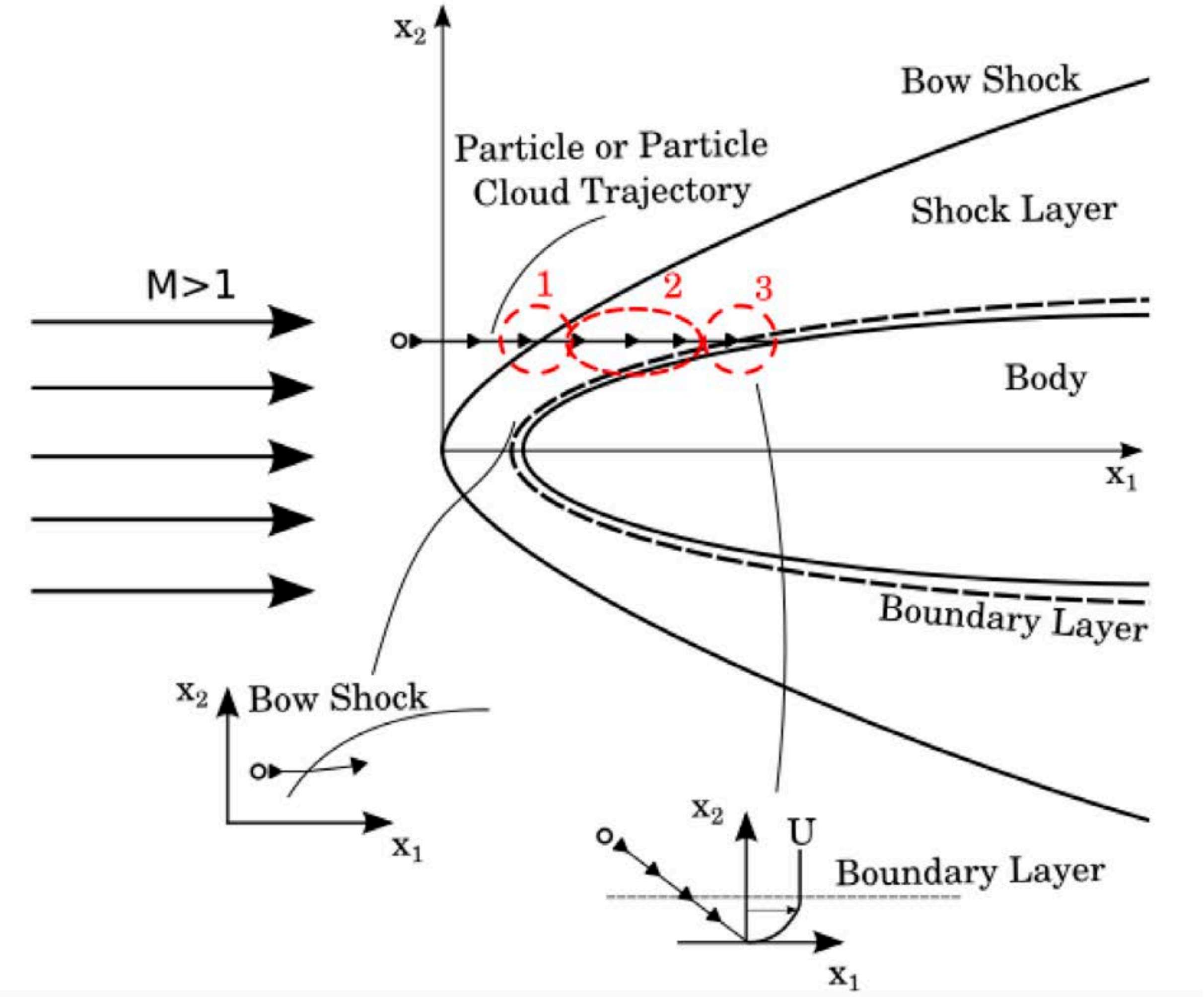

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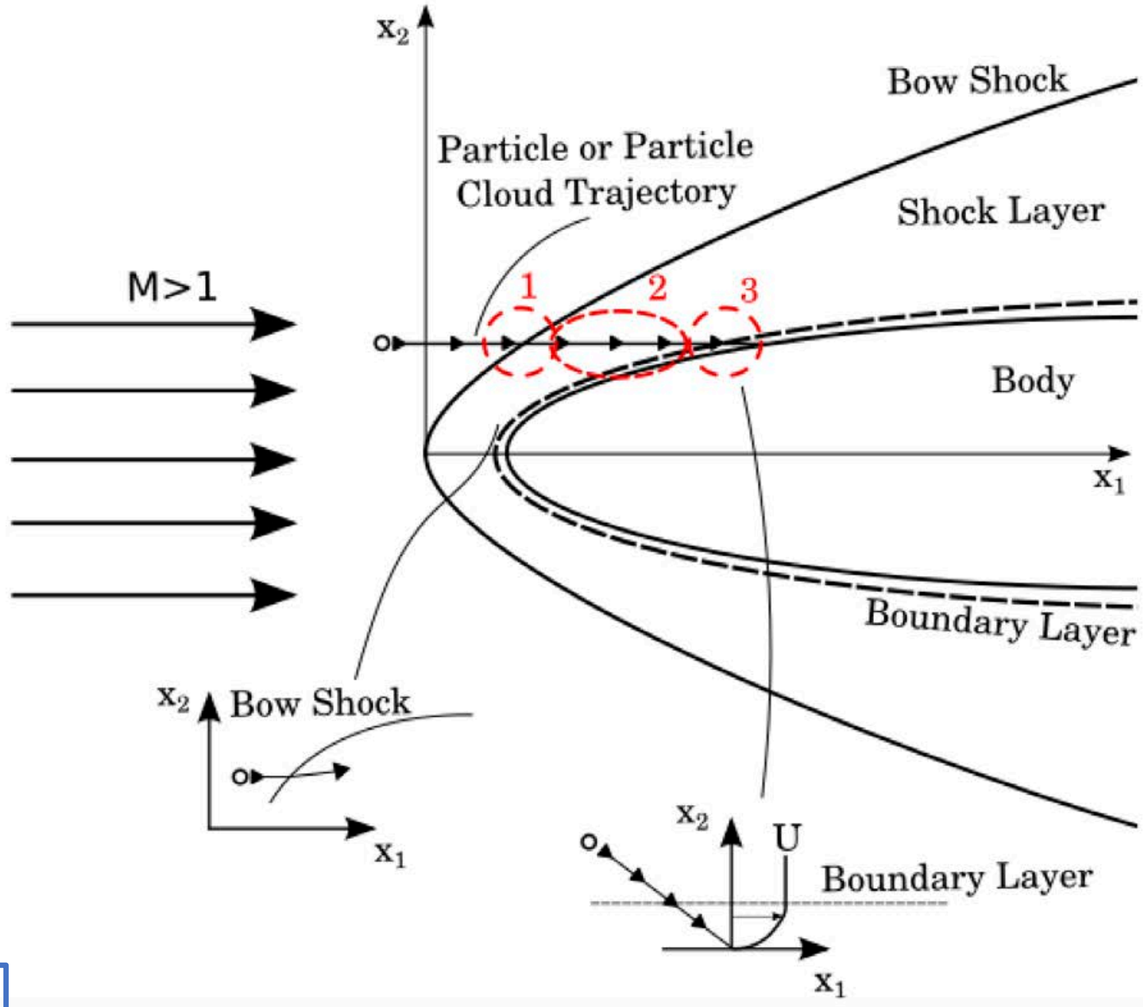
5) after particle impacts the surface it can rebound and **dynamically interact with the bow shock** induced by the vehicle causing the **formation of jets and shear-layers**.



➢ **Not a complete list very few fundamental studies have been conducted, especially for hypersonic flow.**

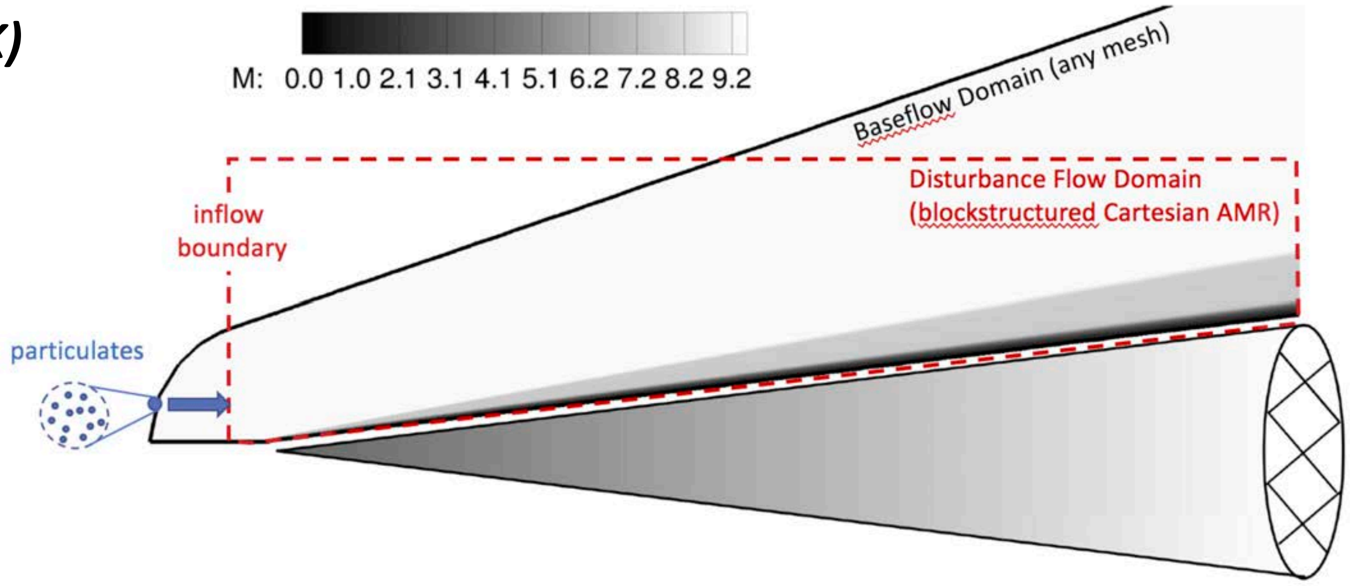
Solver Overview & Simulation Approach

- **Solving compressible Navier-Stokes equations with in-house multi-physics solver *BitCart* *(developed at UK)***
  - Conservative FD scheme
  - **Higher-order shock capturing (CWENO-6) for convective terms**
  - 4^{th}-order accurate treatment of viscous terms
  - Higher-order explicit and implicit time-discretization
  - **Higher-order immersed boundary method (IBM)**
  - Multi-species, gas chemistry, multi-phase, etc.
  - Fluid-structure interaction (FEM CSD solver)
  - Particle solver
  - Grid: generalized curvilinear, block-structured**, adaptive mesh refinement (AMR) Cartesian, dual-mesh overset**

- DNS of particle flows: **solve nonlinear disturbance equations with IBM, AMR, and dual-mesh approach**

- **Motivation was to develop method that has fidelity of DNS but at a reduced computational cost.**

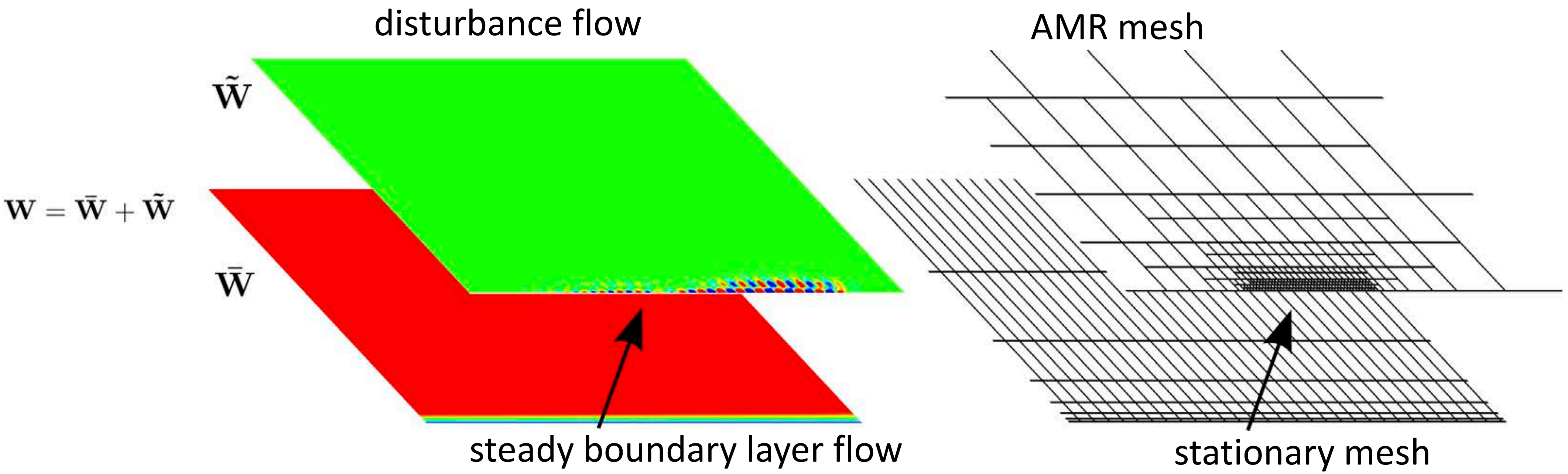
Simulation Domain



Nonlinear Disturbance Flow Solver

$$\mathbf{W} = \bar{\mathbf{W}} + \tilde{\mathbf{W}} = \underbrace{\begin{bmatrix} \bar{\rho} \\ \bar{\rho}\bar{u} \\ \bar{\rho}\bar{v} \\ \bar{\rho}\bar{w} \\ \bar{\rho}\bar{E}_t \end{bmatrix}}_{\text{baseflow}} + \underbrace{\begin{bmatrix} \tilde{\rho} \\ \tilde{\rho}\bar{u} + \bar{\rho}\tilde{u} \\ \tilde{\rho}\bar{v} + \bar{\rho}\tilde{v} \\ \tilde{\rho}\bar{w} + \bar{\rho}\tilde{w} \\ \bar{\rho}\tilde{E}_t + \tilde{\rho}\bar{E}_t \end{bmatrix}}_{\text{linear disturbance}} + \underbrace{\begin{bmatrix} \tilde{\rho}\tilde{u} \\ \tilde{\rho}\tilde{v} \\ \tilde{\rho}\tilde{w} \\ \tilde{\rho}\tilde{E}_t \end{bmatrix}}_{\text{nonlinear disturbance}}$$

AMR Dual-Mesh Approach

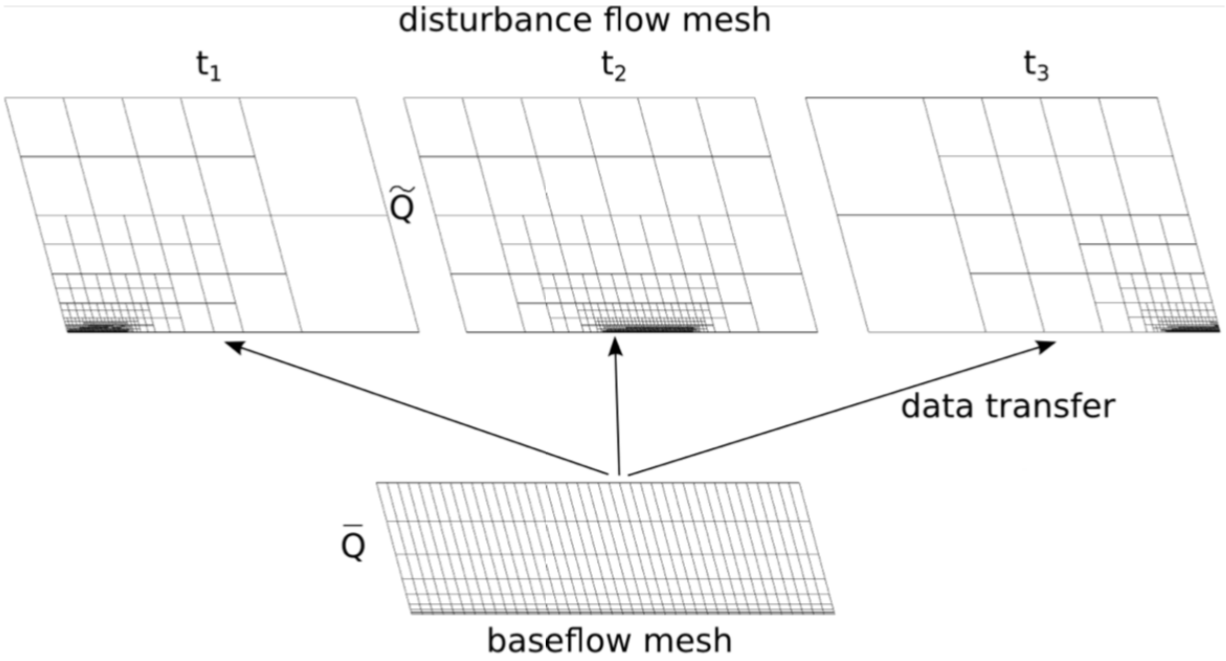


- **AMR is a proven methodology for multi-scale problems** with an extensive existing mathematical and software knowledge base
- **Higher-order accurate inter-level operators** (implementation is similar to Kiris *et al*. (2018))
- Octree-based donor cell search algorithm for **dual-mesh approach**
- **Sensitivity parameter $\boldsymbol{\varphi}$** controls mesh refinement/derefinement

$$\varphi = max\left(\frac{|\phi_1'|}{max(|\phi_1'|)}, \frac{|\phi_2'|}{max(|\phi_2'|)}, \dots\right)$$ based on tracking variable $\phi'(\boldsymbol{x}, t, \boldsymbol{Q}')$

- What is the best set of tracking variables? **Compromise between efficiency vs. accuracy!**

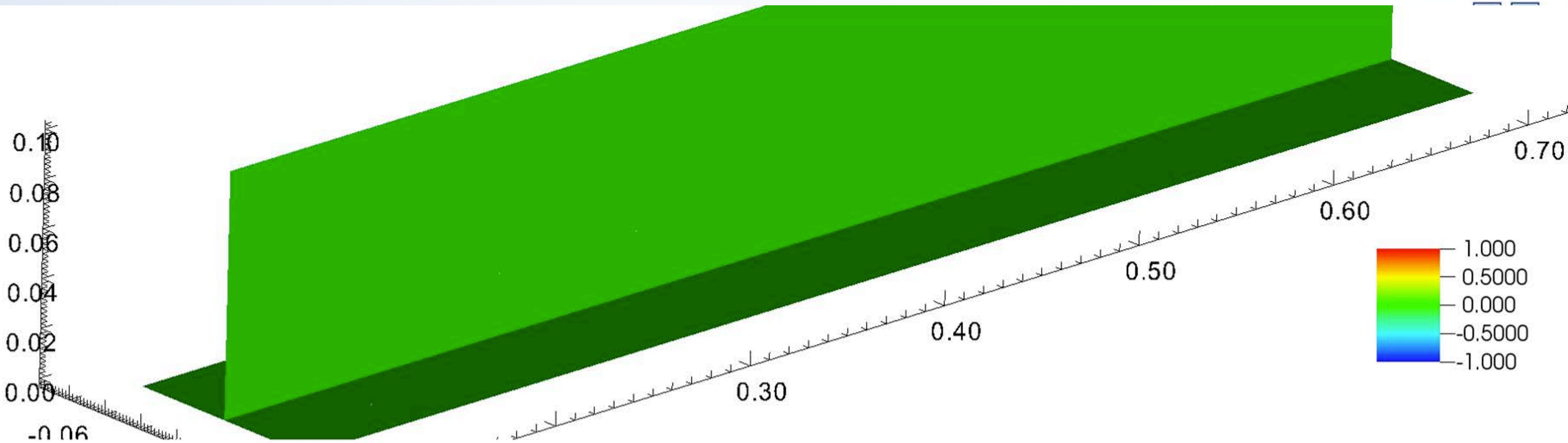
AMR Dual-Mesh Approach

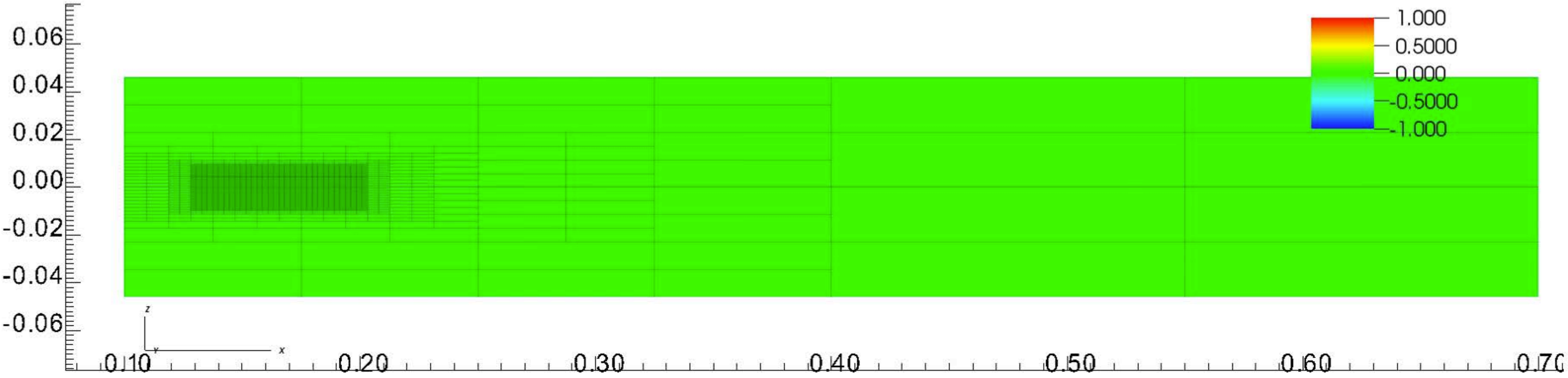


Disturbance flow formulation of 3D compressible Navier-Stokes Equations

$$\frac{\partial \tilde{\mathbf{W}}}{\partial t} + \frac{\partial \tilde{\mathbf{E}}}{\partial x} + \frac{\partial \tilde{\mathbf{F}}}{\partial y} + \frac{\partial \tilde{\mathbf{G}}}{\partial z} = 0.$$

- **High grid resolution is only required locally,** and temporal sub-cycling on the octree-based block-structured Cartesian mesh allows to efficiently simulate particles over time.


0.10
0.08
0.06
0.04
0.02
0.00
-0.06
0.30
0.40
0.50
0.60
0.70
1.000
0.5000
0.000
-0.5000
-1.000


0.06
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-0.04
-0.06
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0.20
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0.40
0.50
0.60
0.70
1.000
0.5000
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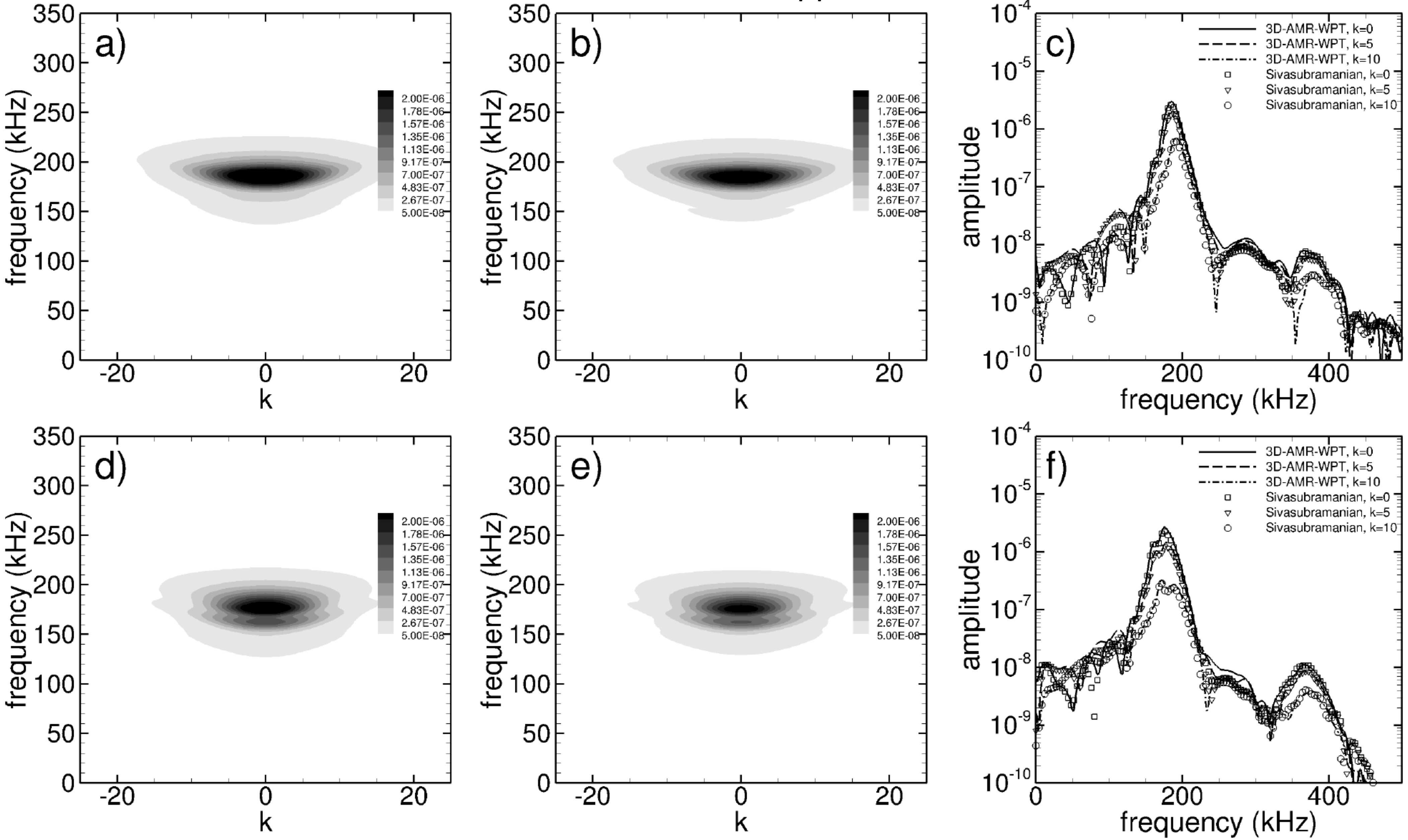
-0.5000
-1.000
z
x

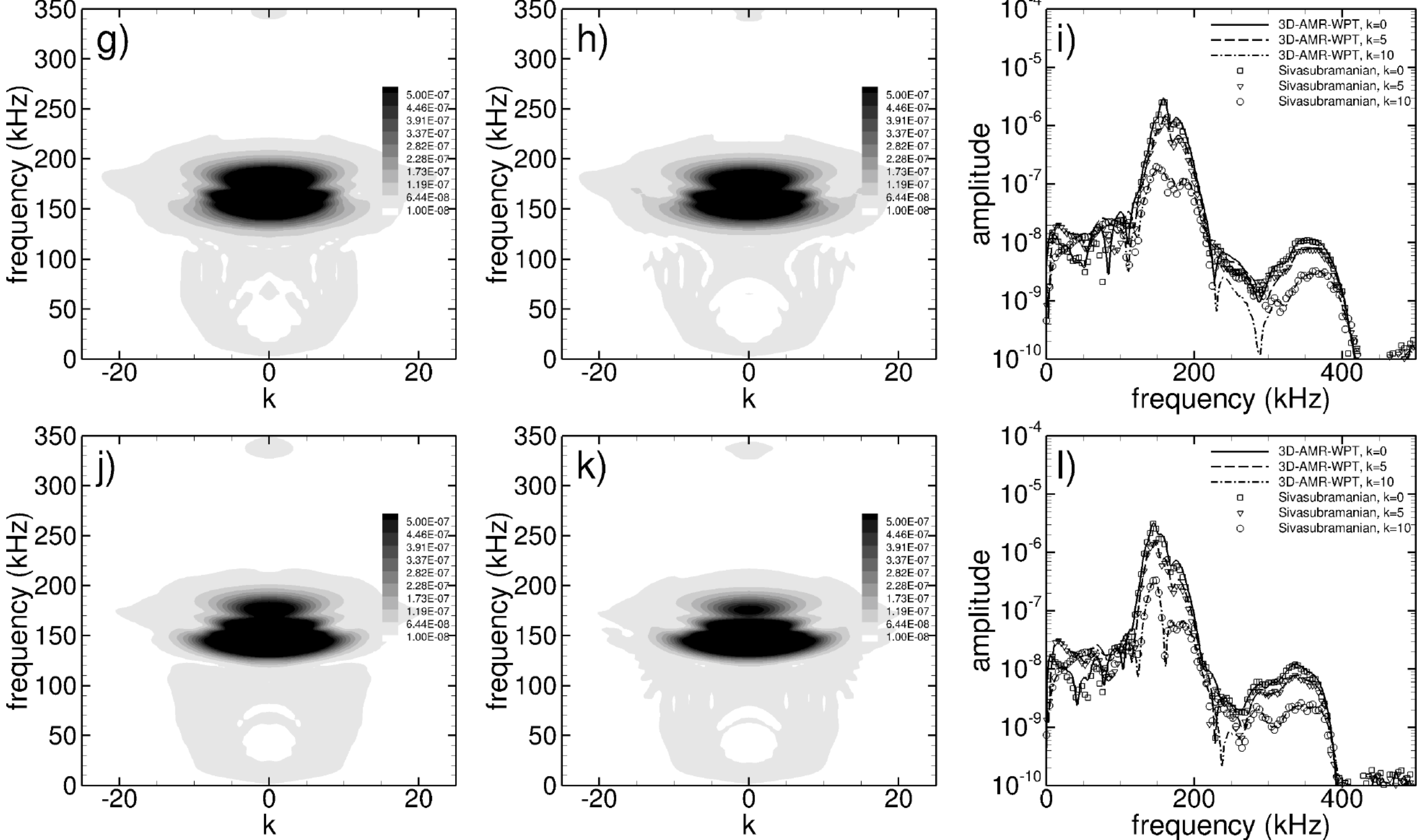
Comparison Against Standard DNS Approach

Sivasubramanian & Fasel 2016 Current AMR Approach



Comparison Against Standard DNS Approach

Sivasubramanian & Fasel 2016 | Current AMR Approach



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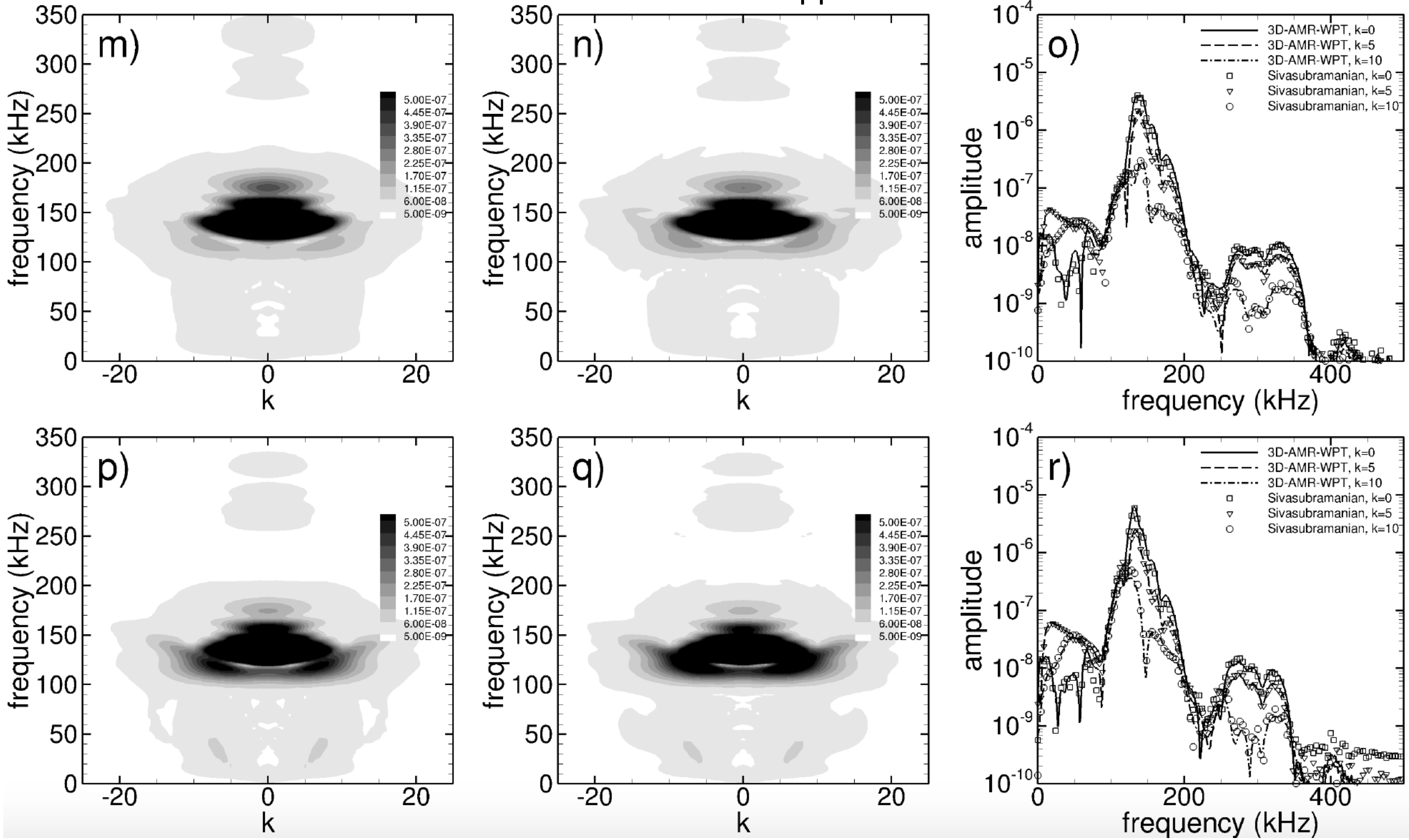


Particle Model

A. Particle-Source-In-Cell Method Simulation Approach

Kinematic equations:

$$\frac{d\boldsymbol{x_p}}{dt} = \boldsymbol{v_p}$$

Newton's second law:

$$m_p \frac{d\boldsymbol{v_p}}{dt} = \sum_{n=1}^{N_b} \boldsymbol{F_{b,n}} + \sum_{n=1}^{N_s} \boldsymbol{F_{s,n}}$$

Surface force by Boiko (1997):

$$\boldsymbol{F_S} = f_1\left(\frac{\boldsymbol{v_f} - \boldsymbol{v_p}}{\tau_p}\right) - \frac{1}{\rho_p}\boldsymbol{\nabla} p$$

where $f_1 = \frac{3}{4}\left(24 + 0.38Ref + 4\sqrt{Ref}\right)\left(1 + exp\left(-0.43/M_f^{4.67}\right)\right)$

Coupling with the fluid domain:

$$\boldsymbol{S}_m = \sum_{n=1}^{N_p} \boldsymbol{K}(\boldsymbol{x}_p, \boldsymbol{x})\boldsymbol{W}_m \text{ and } \boldsymbol{S}_e = \sum_{n=1}^{N_p} \boldsymbol{K}(\boldsymbol{x}_p, \boldsymbol{x})\left(\boldsymbol{W}_m \cdot \boldsymbol{v}_p + W_e\right),$$

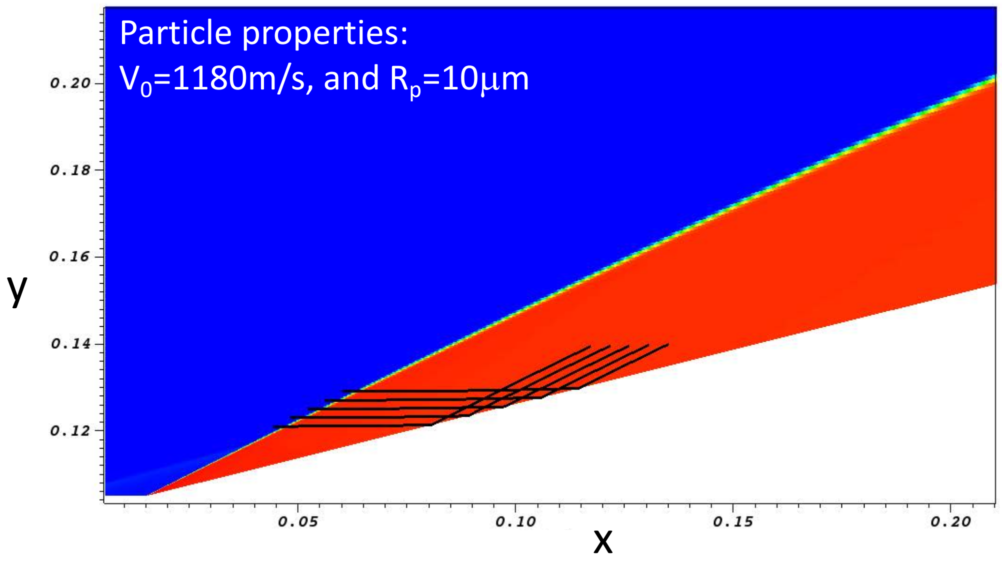
$\mathbf{x_p}$: particle position
$\mathbf{v_p}$: particle velocity
$\mathbf{F_b}$: body force
$\mathbf{F_b}$: surface force

$Re_f=|v_f - v_p|d_p/\nu$ is relative particle Reynolds number

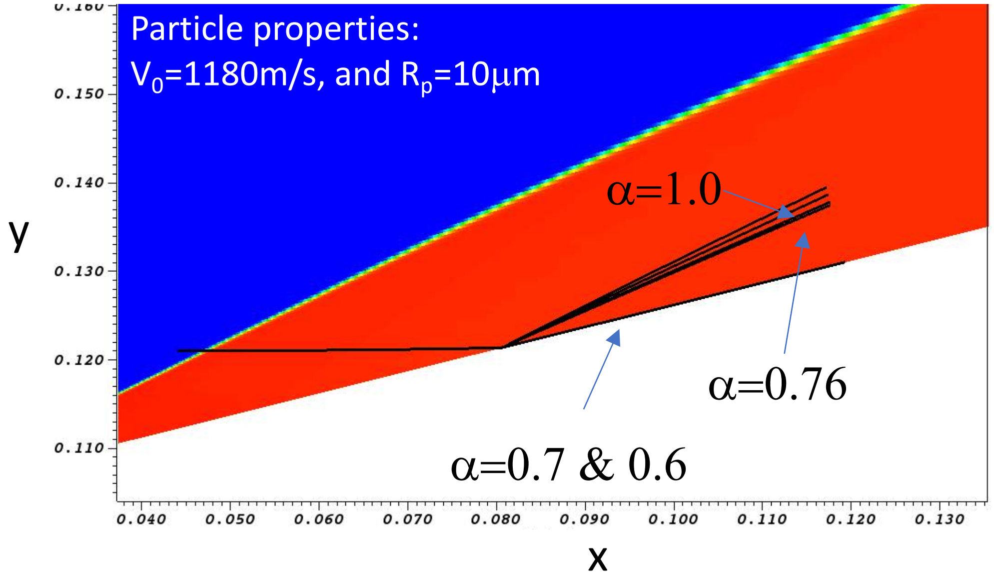
$\tau_p = Re_p R_p^2 \rho_p / 9$

$\mathbf{S_m}$: momentum source term
$\mathbf{S_e}$: energy source term

Different Positions



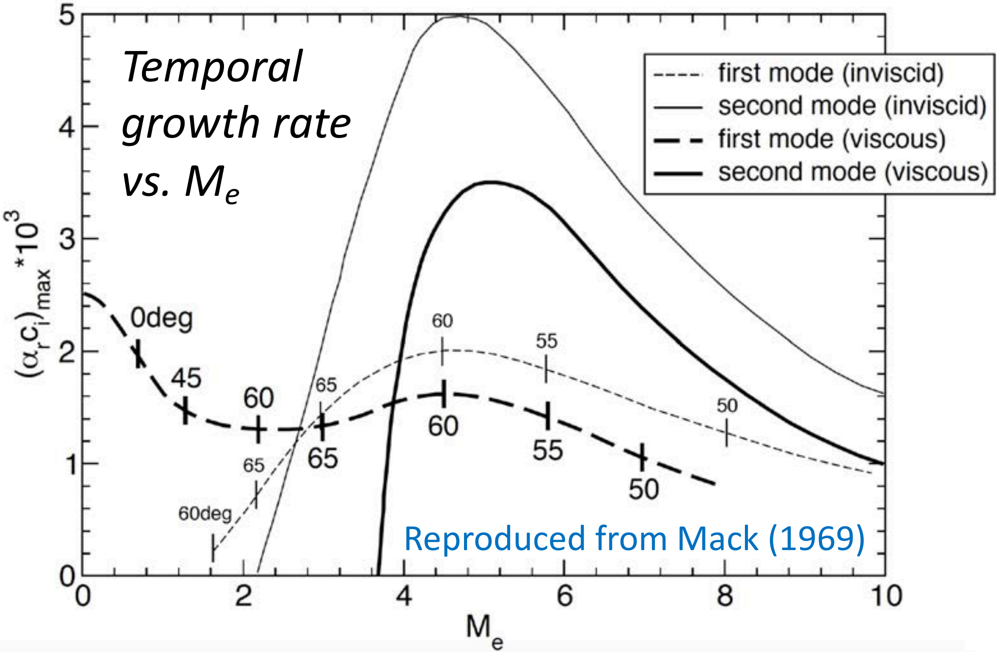
Different Values of Collision Coefficient



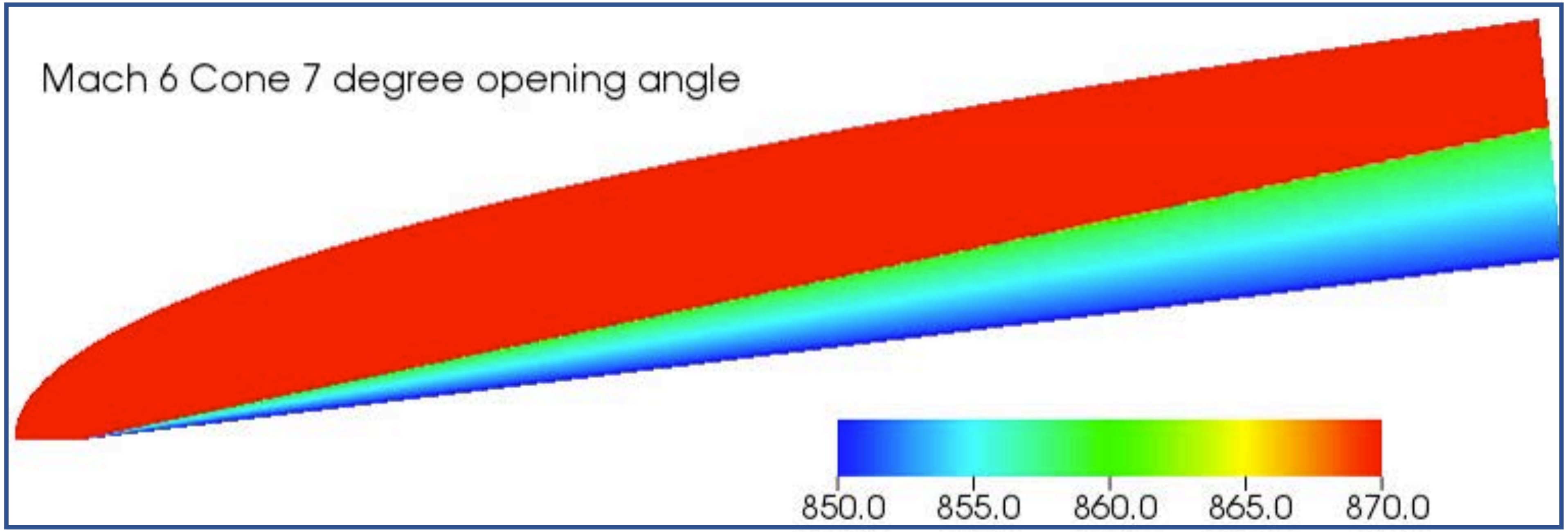
B. Direct Particle Simulation via Immersed Boundary Method

- Comparison in AIAA summer conference paper.

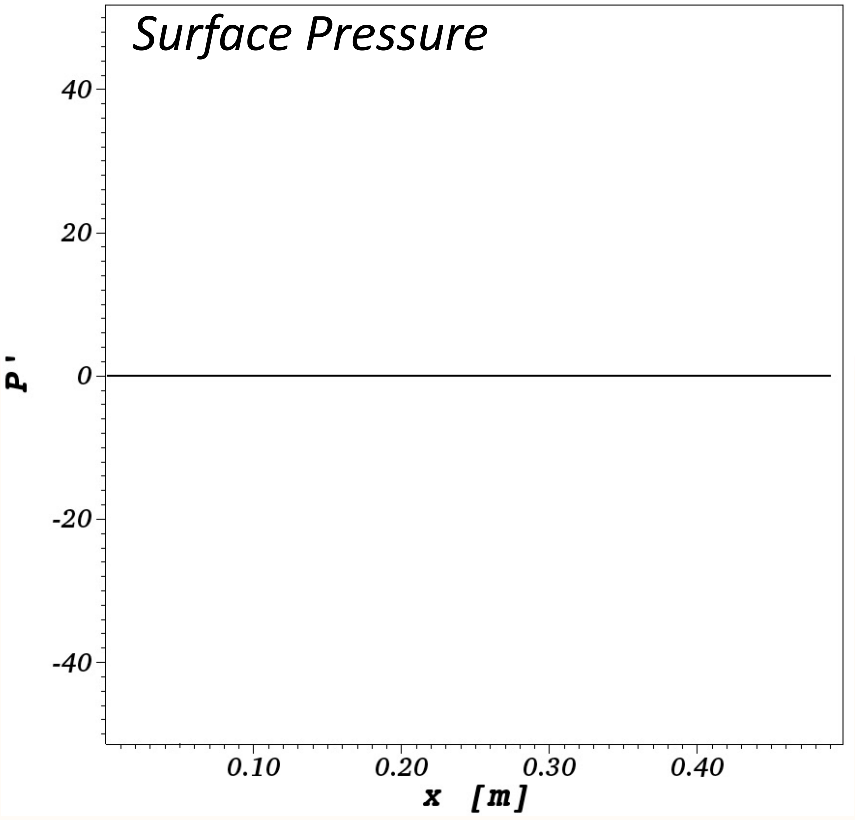
DNS of Particle Impingement for Mach 6 Flow



- Two-Step Simulation Approach:
  1.) baseflow computation & 2.) AMR particle tracking simulation
- Particle flow simulation approach was initially tested in 2-D (or axisymmetric) flows
- Initial 2-D simulations involve flows where second mode is the most dominant instability mechanism
- 3-D simulations of are currently conducted and analysis will be presented at AIAA summer meeting



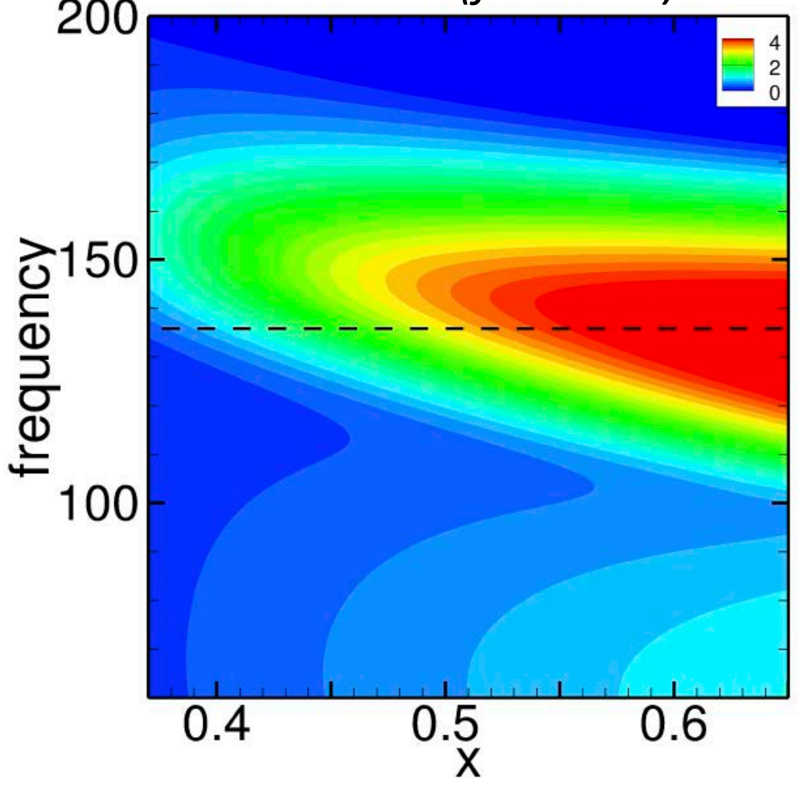
Flow Visualization – Disturbance Pressure



- Mach 5.35 Boundary Layer Flow
  After shock conditions:
  p_∞=1297 Pa, ρ_∞ =0.071 kg/m^3,
  T_∞ =63.9 K & Re=14.6·10^{6}m^{-1}

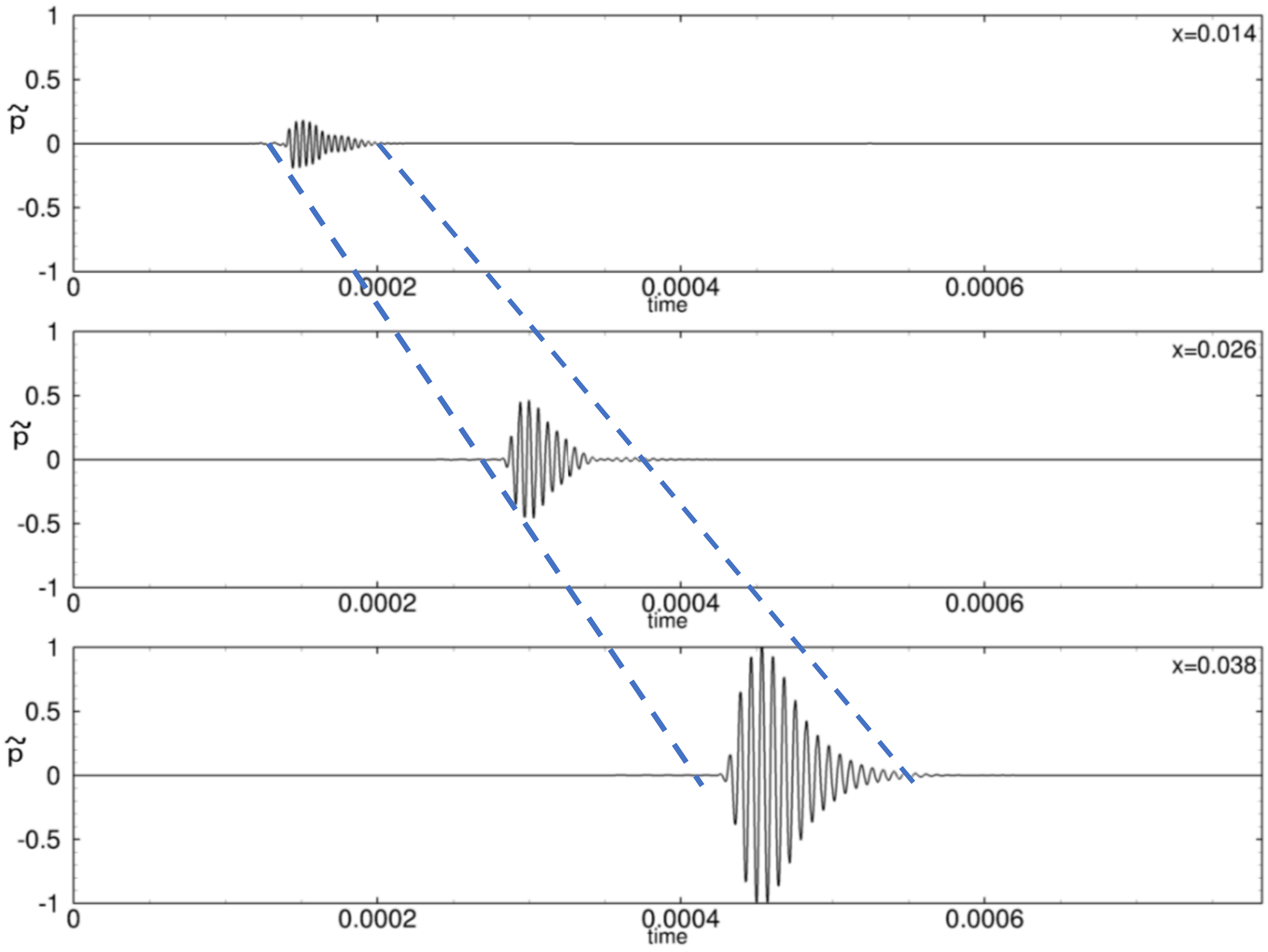
- Particle properties:
  ρ_p=1000 kg/m^3, R_p=5 μm
  $\mathbf{V_p}$=[cos(7°),sin(7°)] 871 m/s
  $\mathbf{x_p}$=[0.11,0.004] m & Re_p≈146

N-Factor (from LST)



Contours of Disturbance Pressure

Pressure Signature

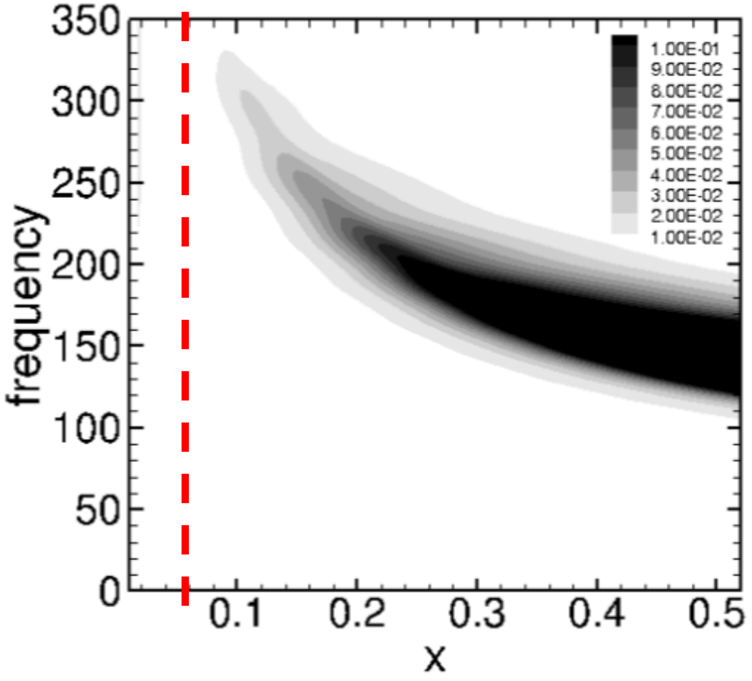


- Disturbance pressure signal is sampled at the wall via point probes,
- After performing an FFT on the signals, the dominant and amplified wavenumbers/frequencies can be obtained,
- The type of instability (first, second, higher-modes, cross-flow etc) that is introduced can be identified,
- Calculating N-factors can be used to predict transition location,

Pressure Signature

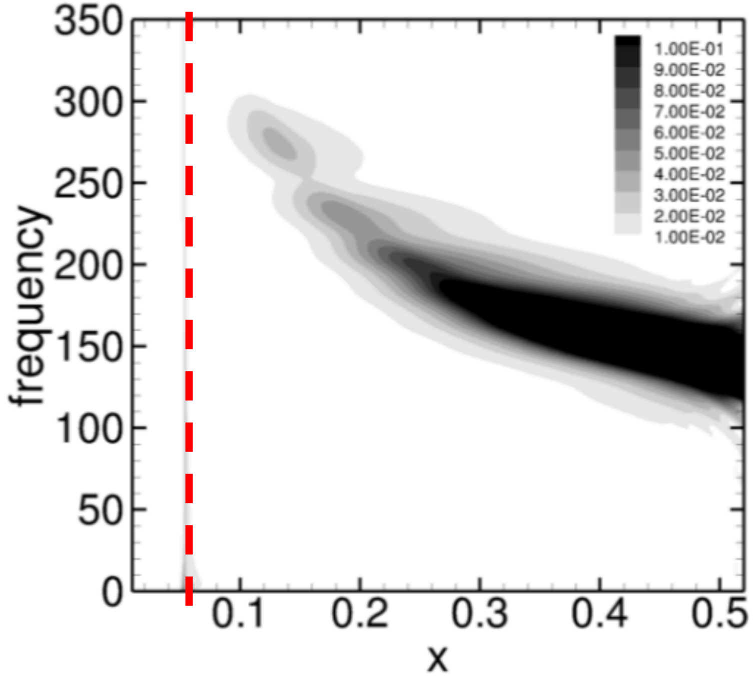
Particle collision location located upstream of neutral curve

Pulse Disturbance – trigger second mode

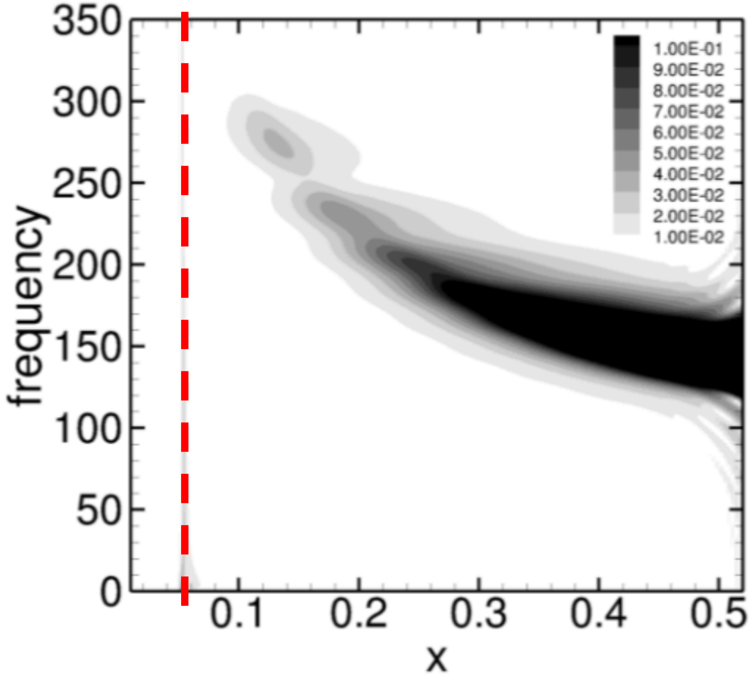


Particle Simulations

Linear



Nonlinear

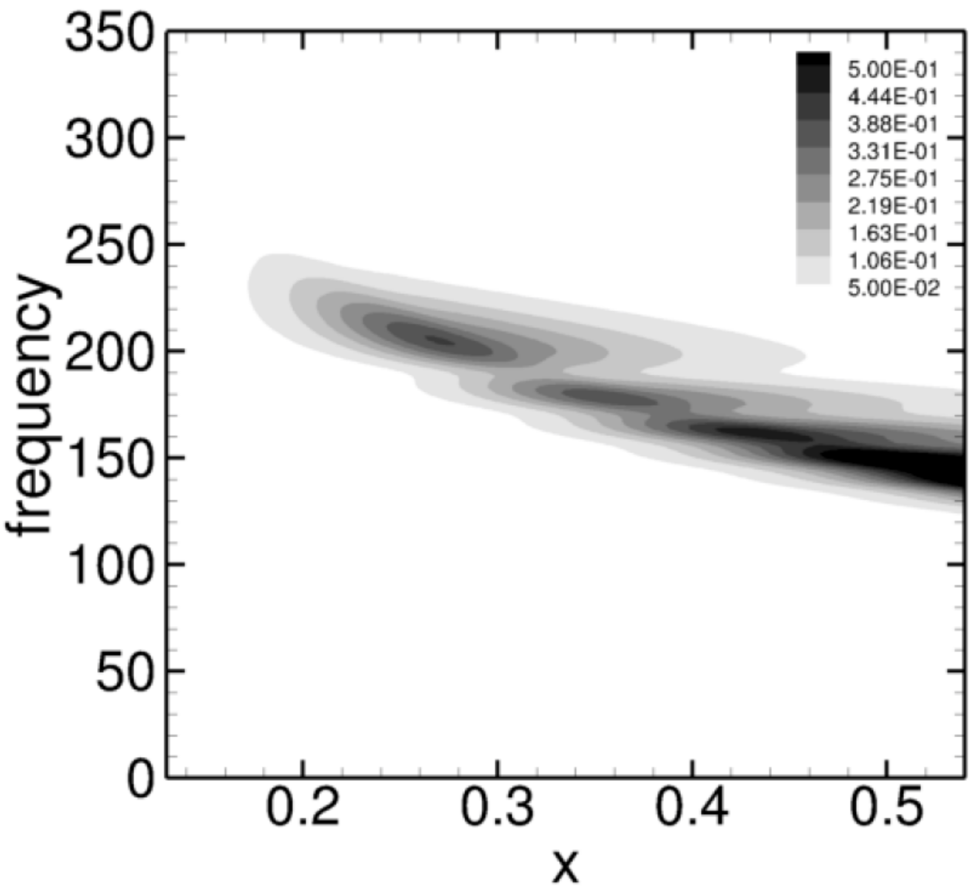


- Particles of size 10μm leads to non-dimensional pressure signature of $p_0'/p_\infty = \mathcal{O}(10^{-3} - 10^{-4})$
- Pressure signature is highly dependent on flow conditions, particle properties, impingement location, etc.

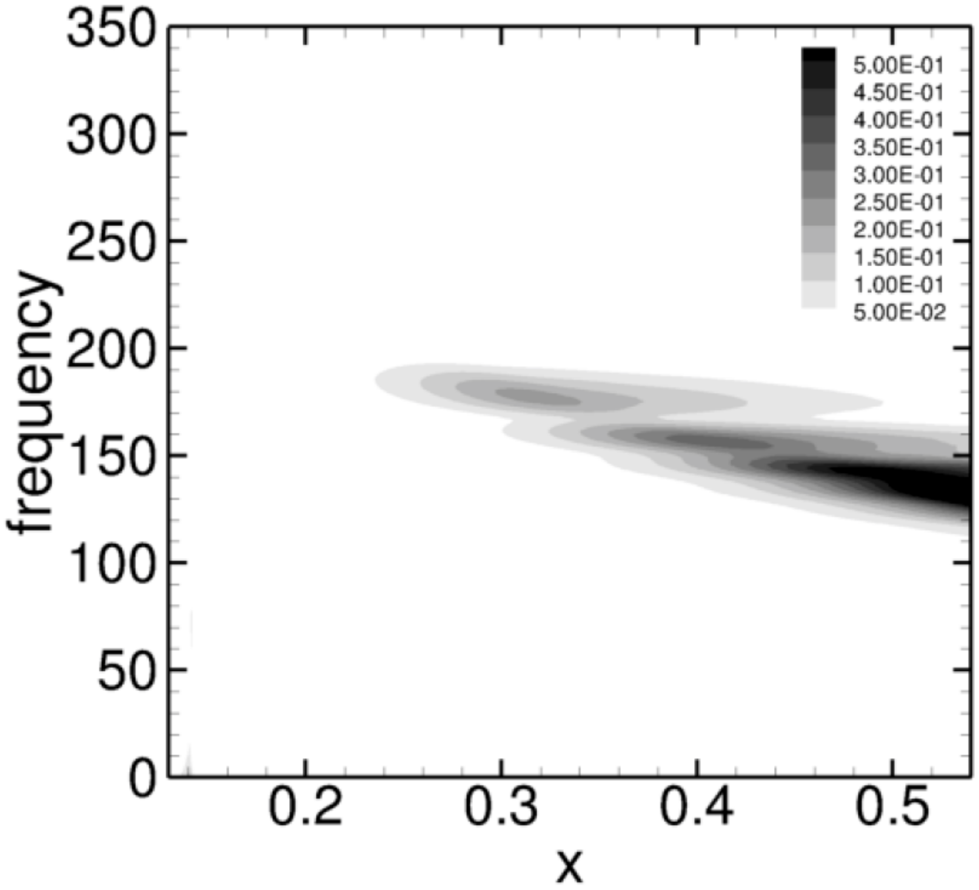
Pressure Signature

Particle collision location located downstream of neutral curve

Pulse Disturbance



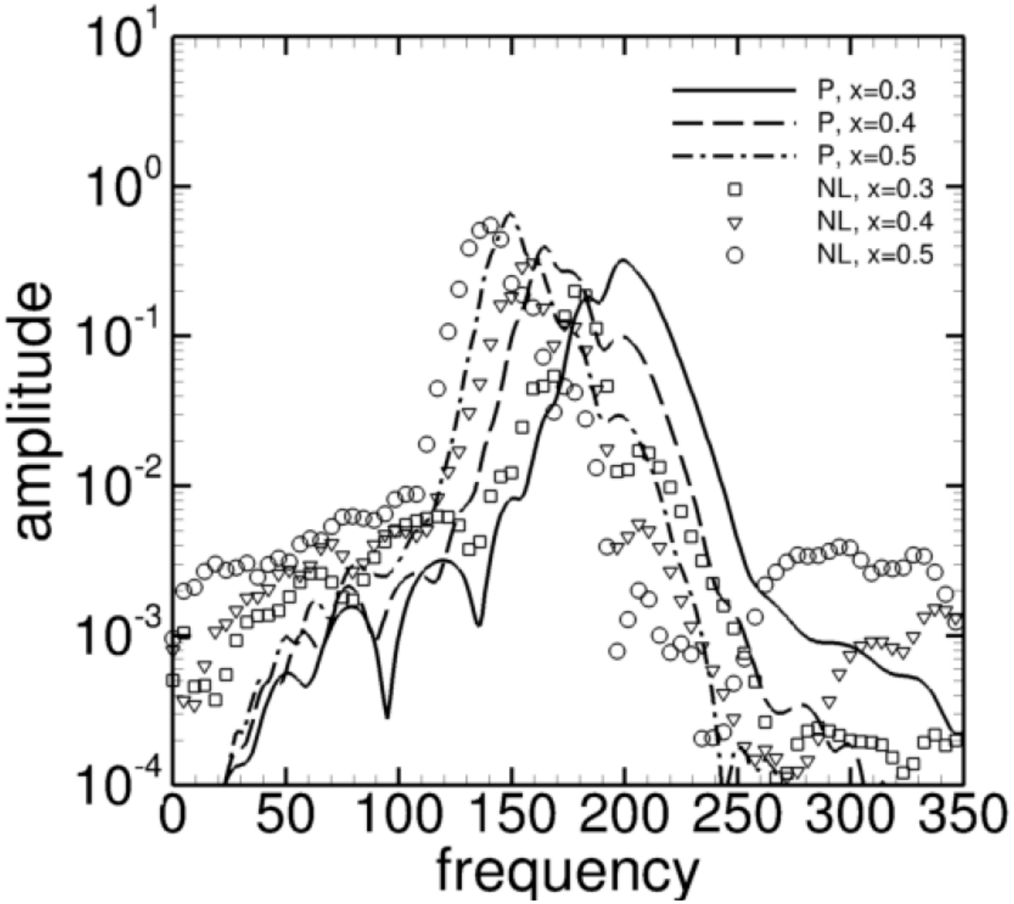
Particle Simulations



- Particle impingement at downstream location inside neutral curve for relevant frequencies
- Results for pulse and particle simulations are very different (due to initial disturbance level and receptivity)

Pressure Signature

Pulse Disturbance



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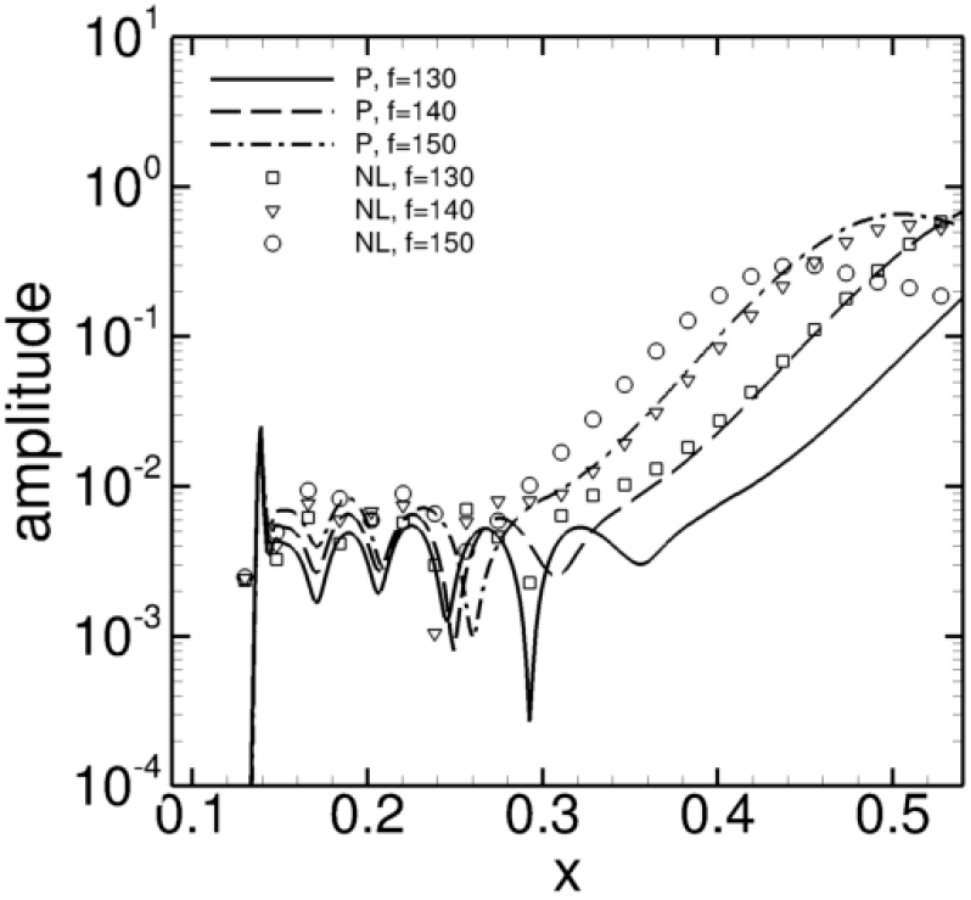

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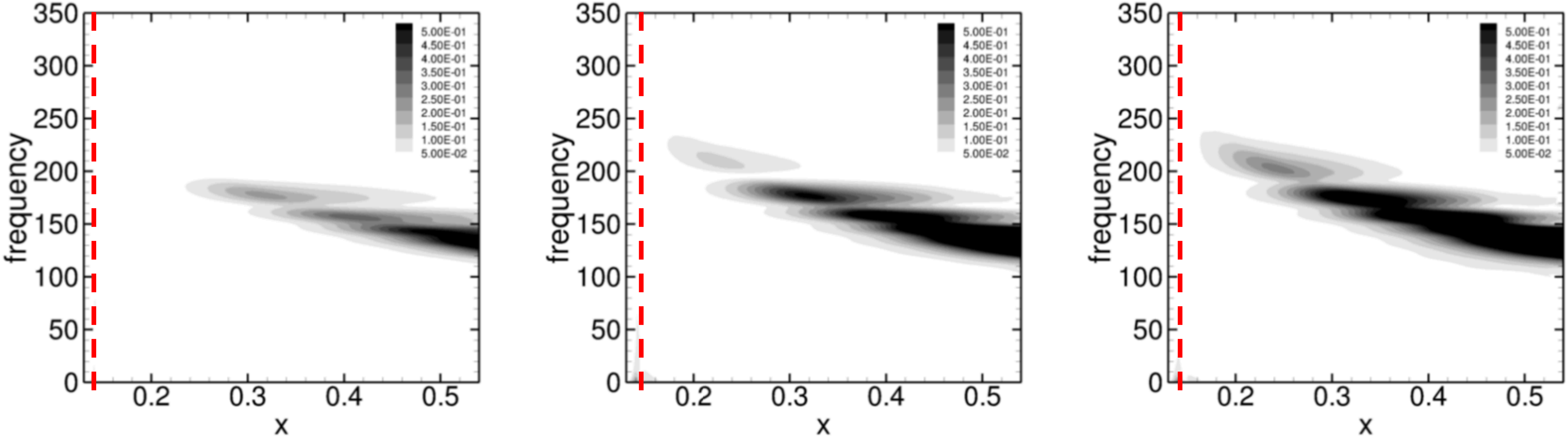
Effects of Particle Size

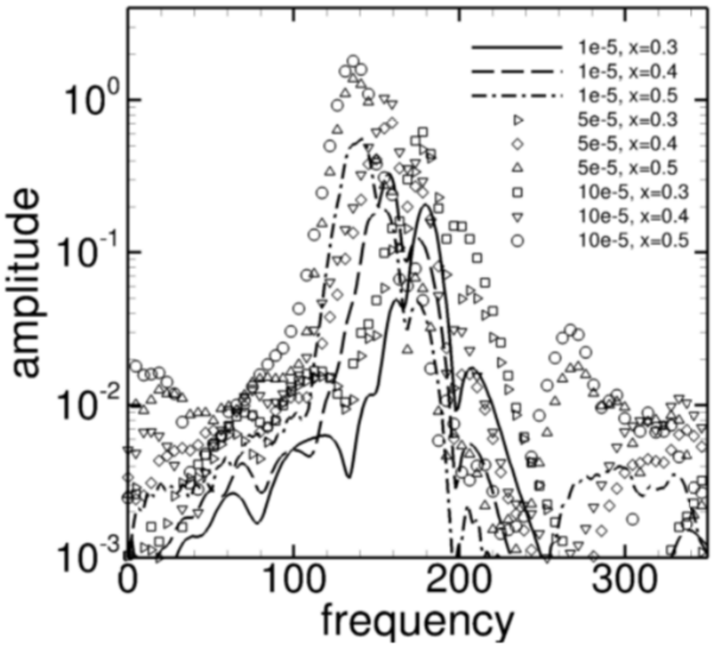
Particle with D_p=10μm *Particle with D_p=50μm* *Particle with D_p=100μm*

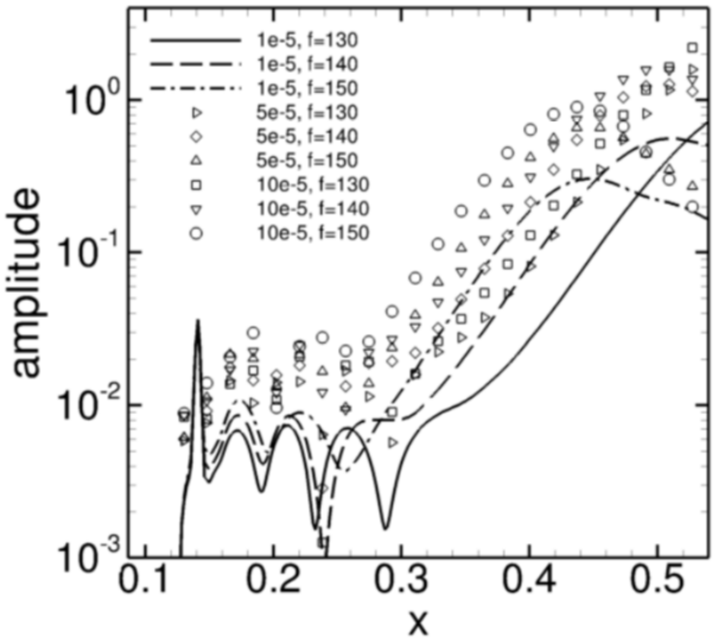


- Broad frequency spectrum introduced by particle collision (with low frequency peak)
- Particle collision location downstream of neutral curve,

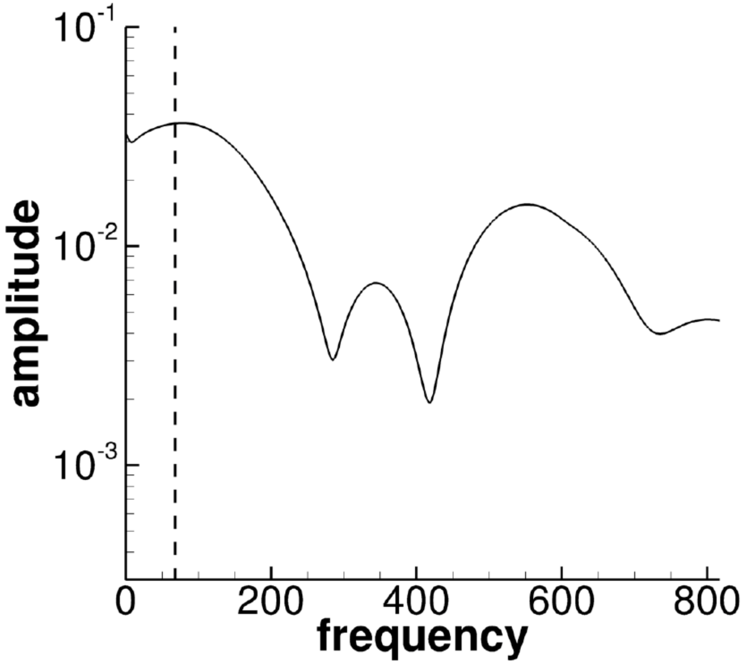
Effects of Particle Size

Pressure amplitude versus frequency for different particle sizes



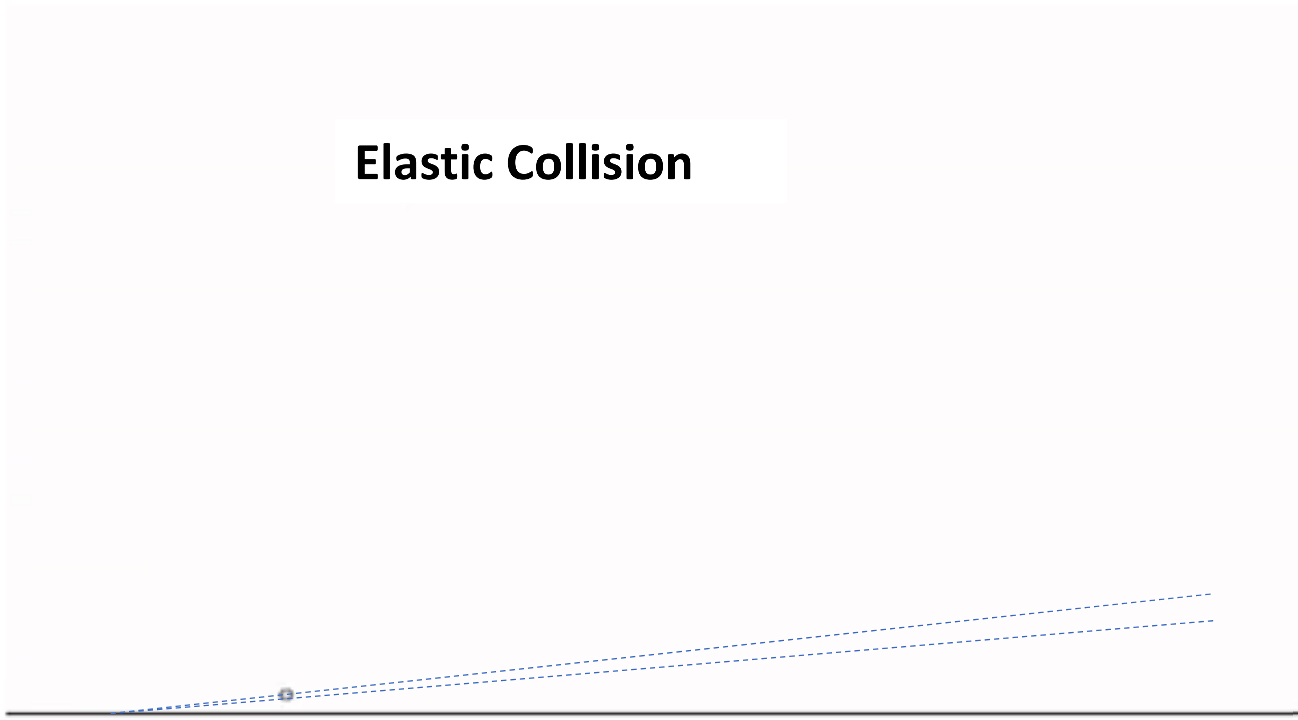


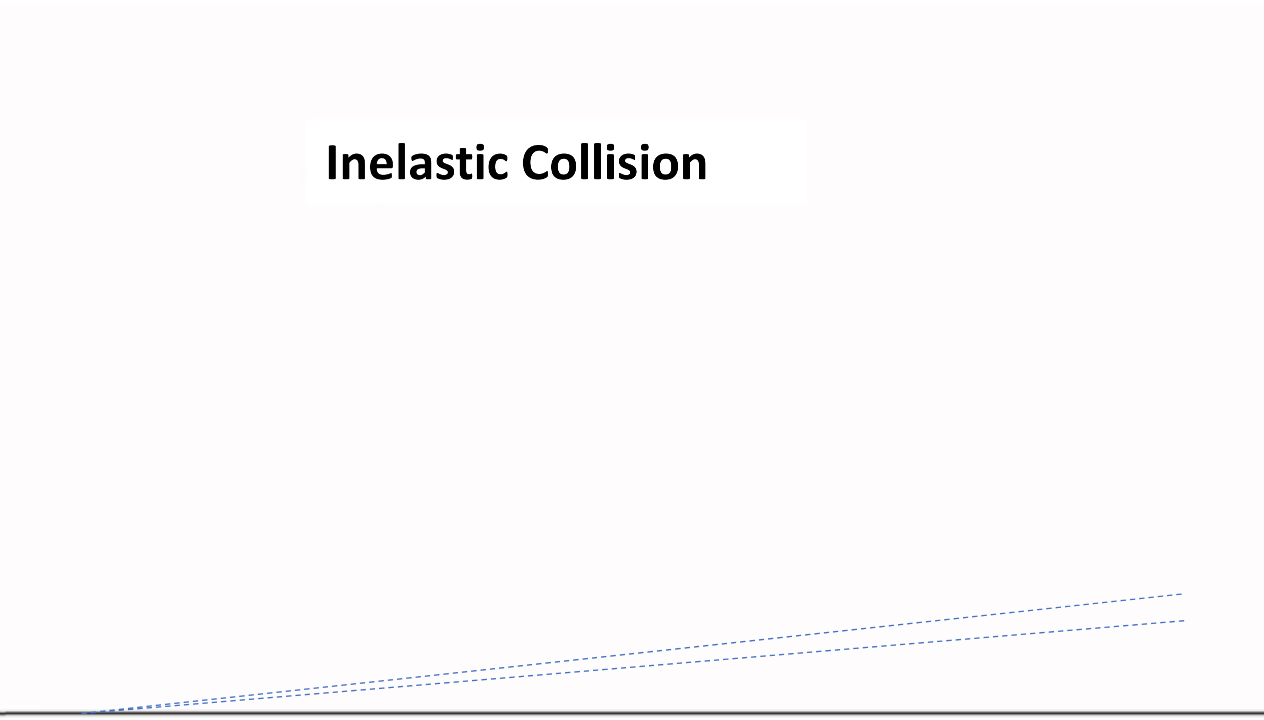
Estimate of excitation frequency



- As expected, larger particle size lead to vertical shift in amplitude curves
- In addition to higher disturbance amplitudes, a change in spectrum is observed
- Rough estimate for excitation frequency captures first peak in the spectrum ($f \sim v_p/2\delta_{99}$)

Elastic vs. Inelastic Collision

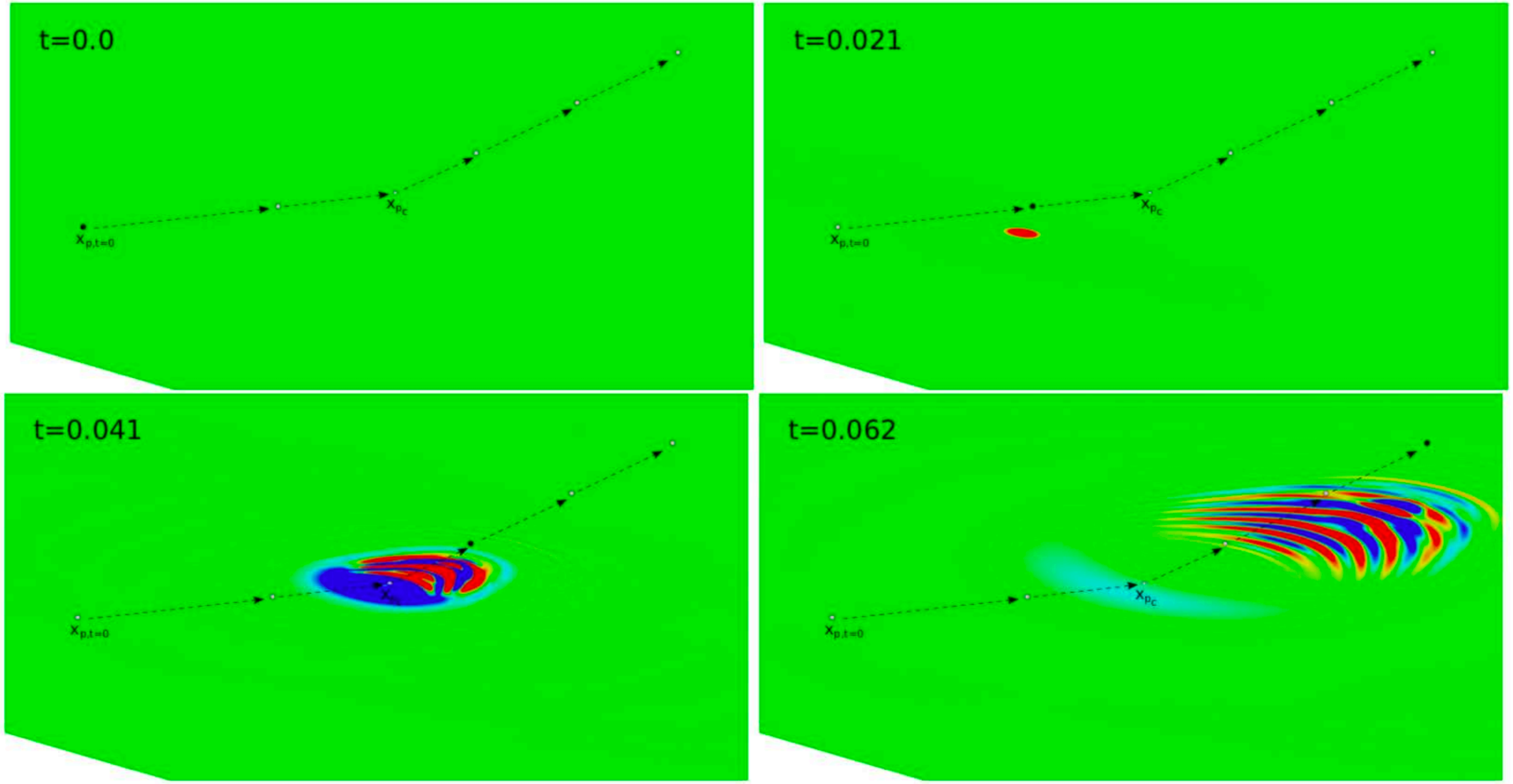




Note: Dashed lines mark approximate path of particle.

3D Flat Plate BL Particle Flow Simulation

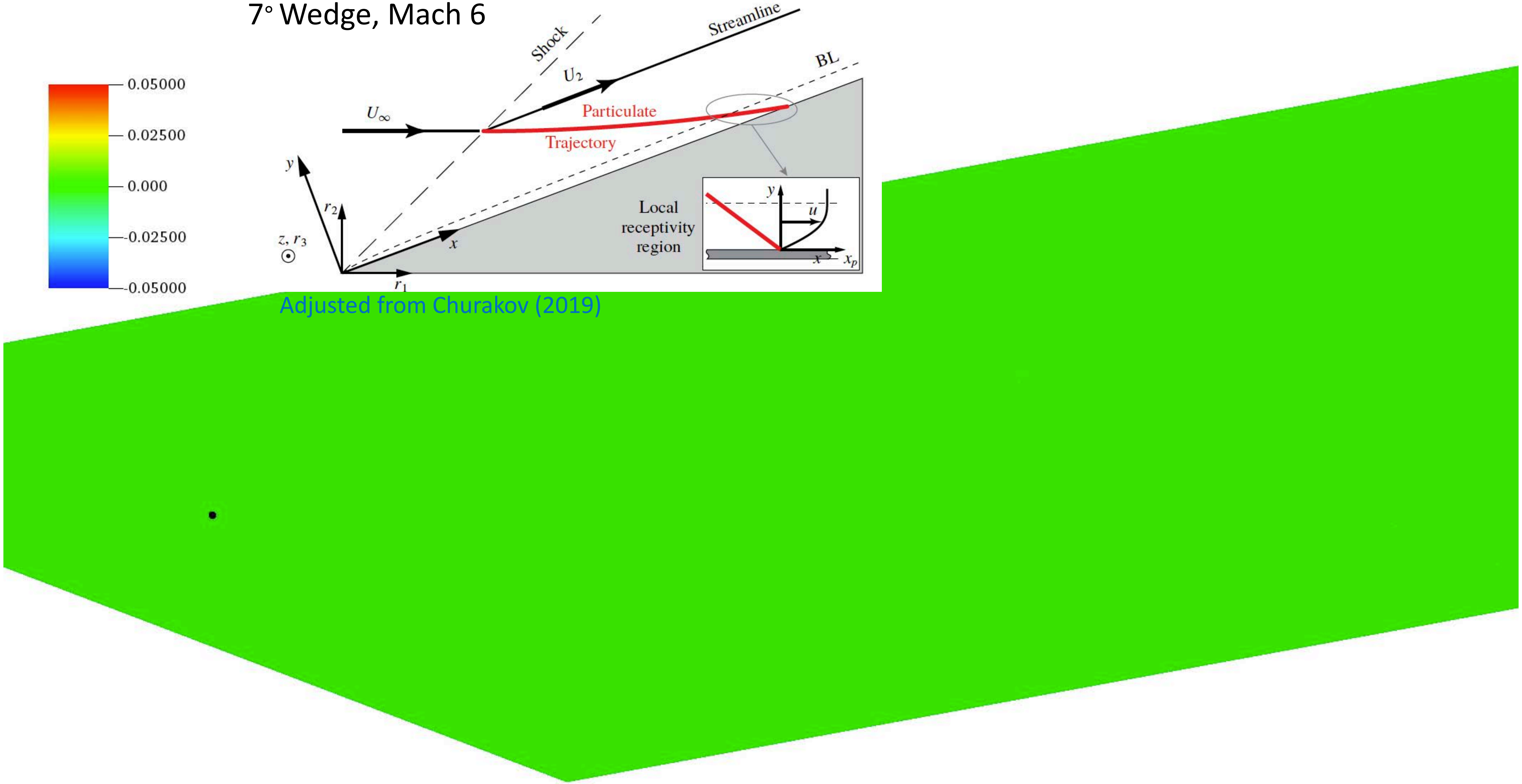
3D Mach 5.35 Flat Plate Boundary Layer Flow



- AMR is ideal candidate for particulate induced transition simulations due to different scales that need to be resolved,
- Greater resolution needed for computing particle trajectory than for resolving downstream wavepacket development,
- Grid levels can be removed after particle collision detected.

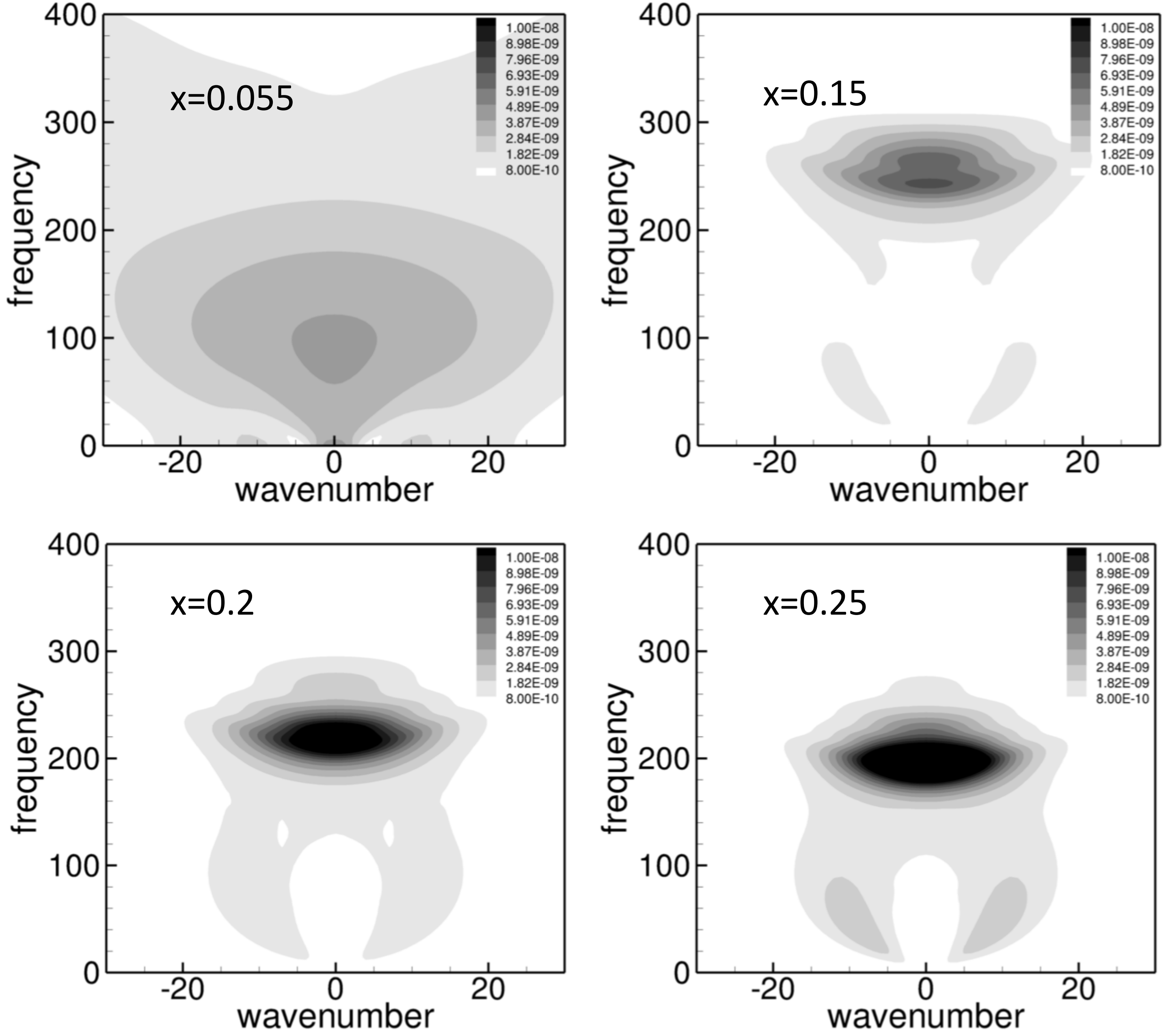
3D Flat Plate BL Particle Flow Simulation

Simulation Setup:
7° Wedge, Mach 6



Adjusted from Churakov (2019)

3D Flat Plate B-L Particle Flow Simulation

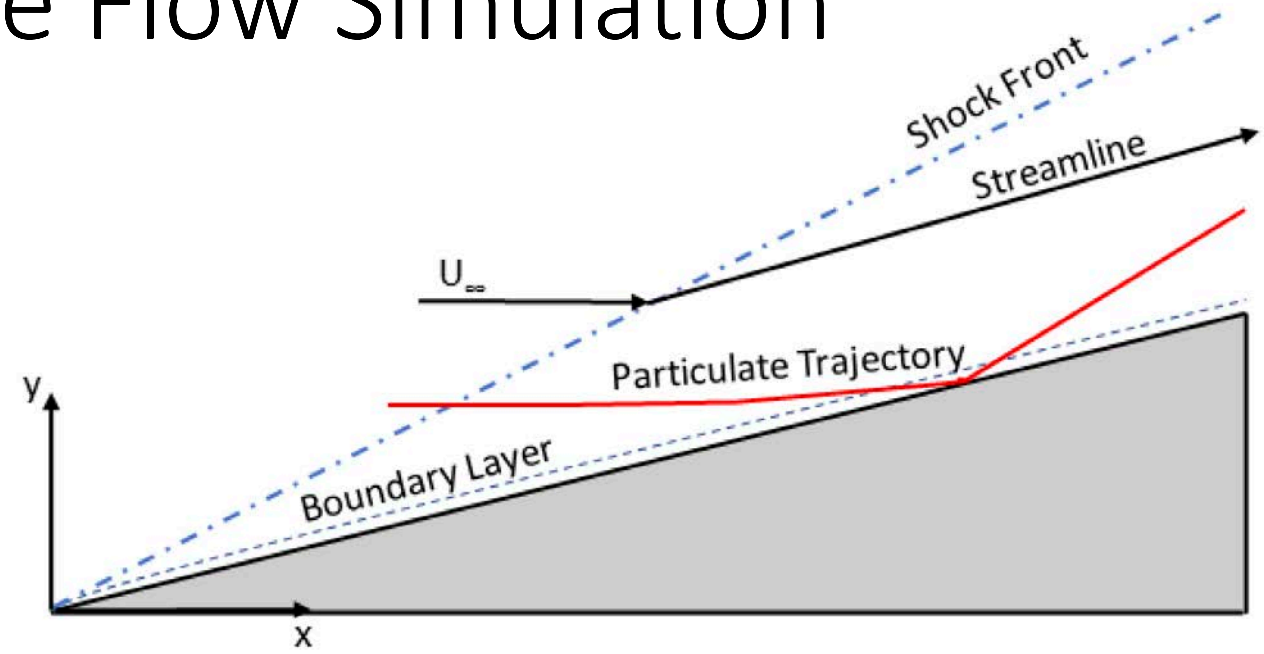


- Particulate collision with boundary-layer upstream of neutral curve,
- Frequency-wavenumber plots for various downstream locations,
- Wavepacket dominated by second mode 2D instability,
- Validated against wall-forcing simulations,

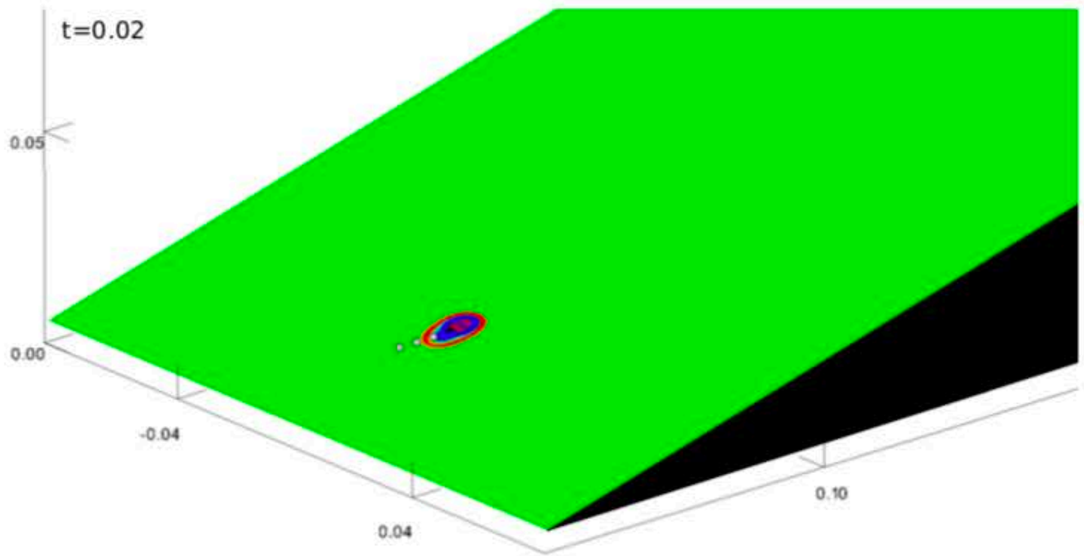
3D 14^o Wedge Particle Flow Simulation

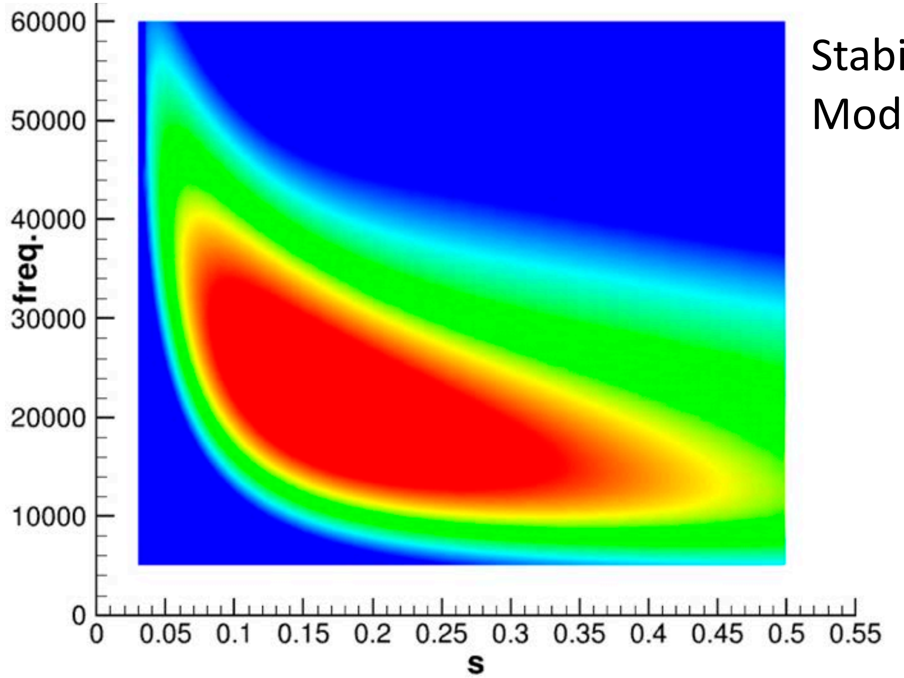
Flow conditions:

	14^o Straight Wedge
M_∞	4
$Re_\infty(1/m)$	7.381×10^6
$p_\infty(N/m^2)$	5530
$T_\infty(K)$	216.7
$U_\infty(m/s)$	1180.305



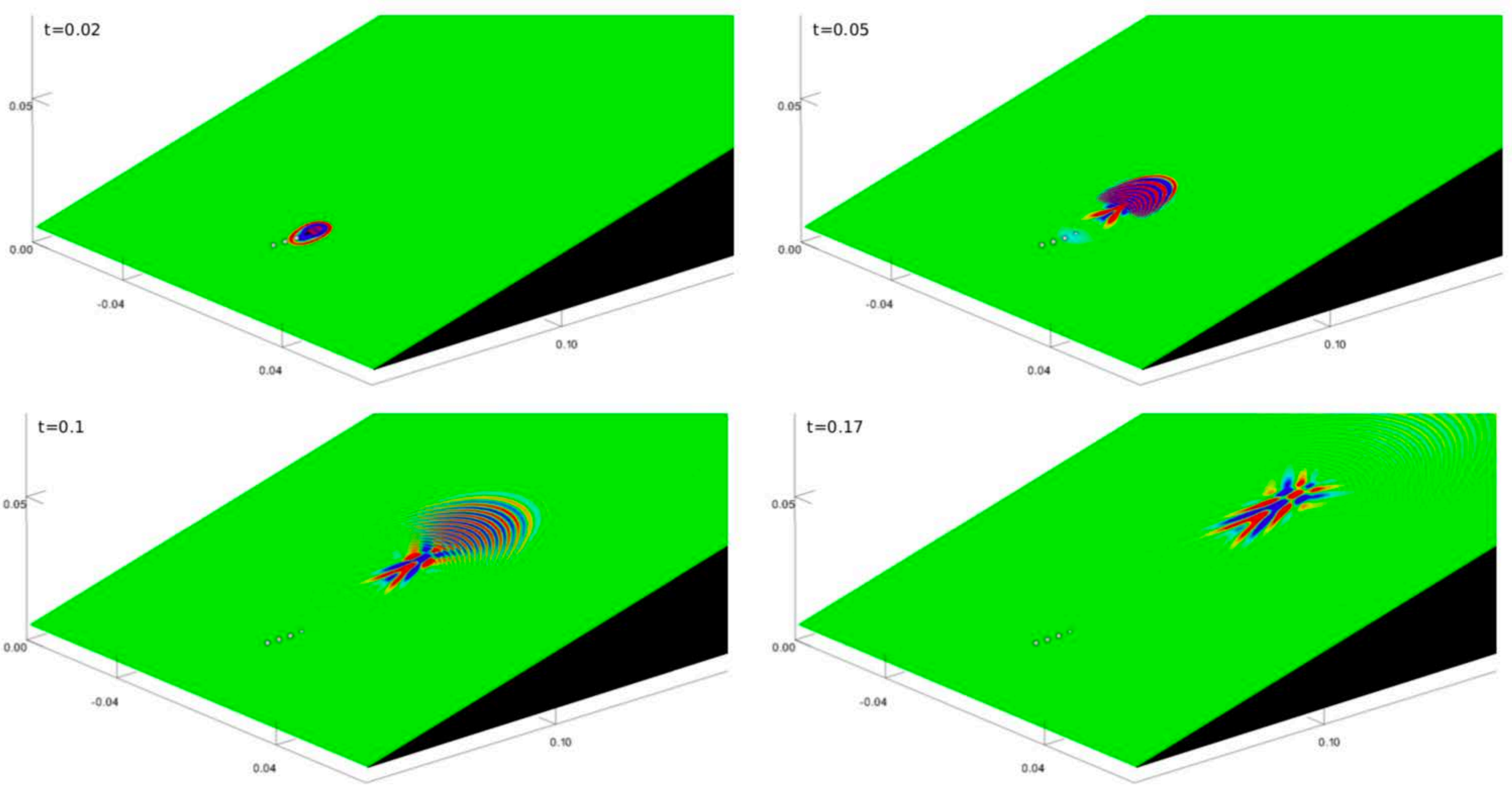
- M 4 wedge flow is first mode dominated
- Comparison with Chuvakhov (JFM 2019)



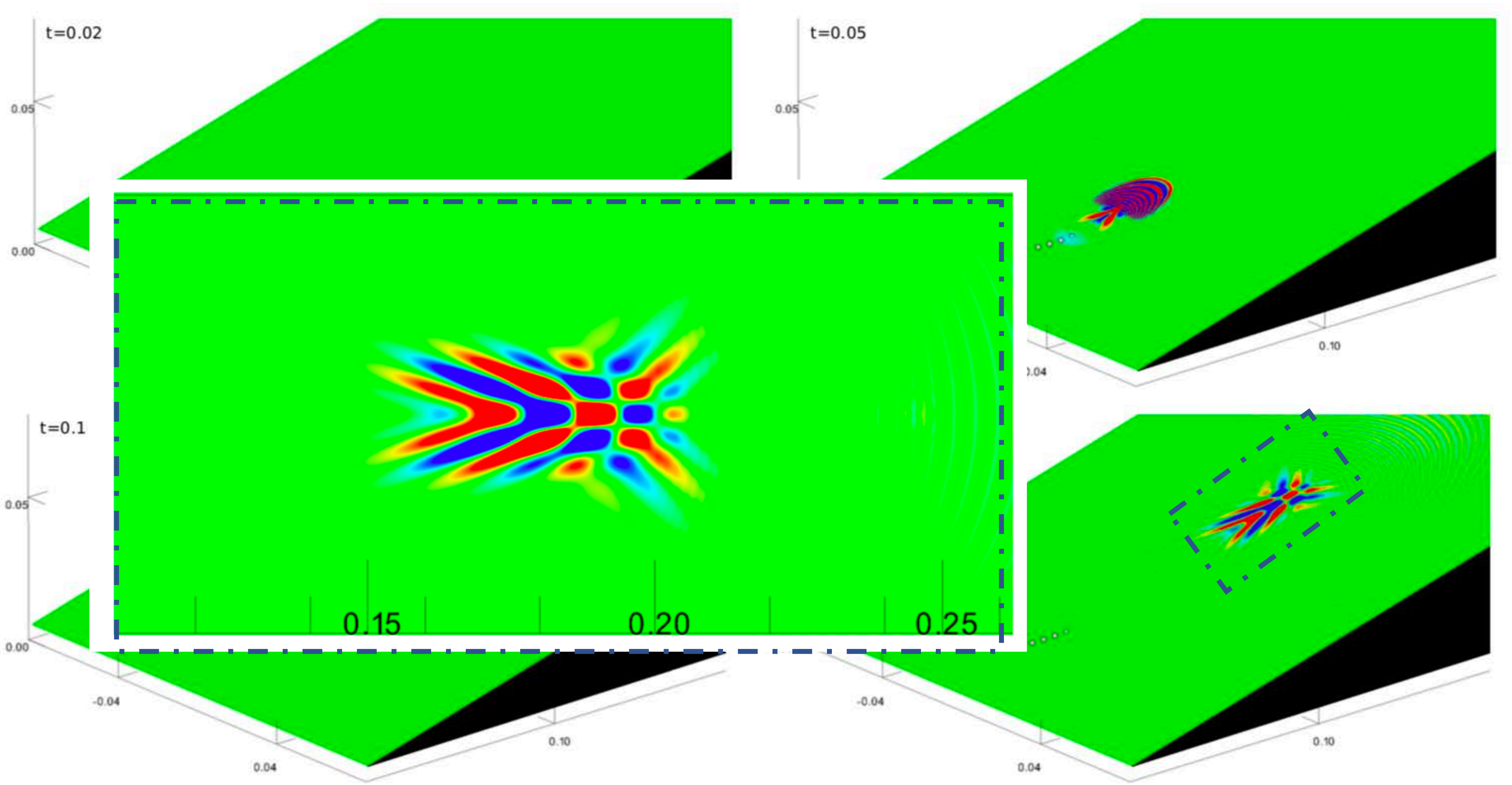


Stability Diagram for 1st Mode (β=474)

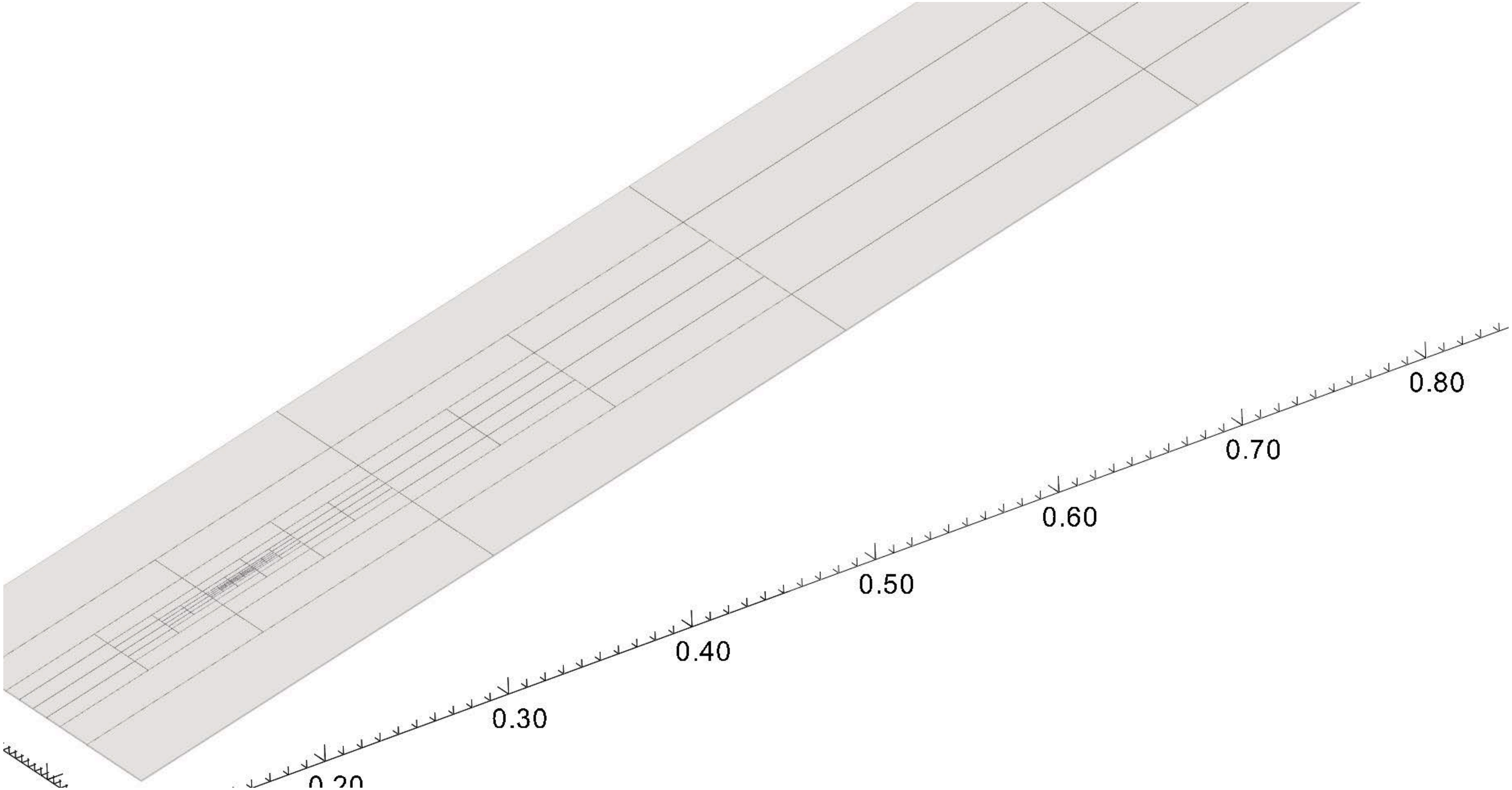
3D 14° Wedge Particle Flow Simulation



3D 14° Wedge Particle Flow Simulation



3D 14 deg Wedge Particle Flow Simulation



Why Blue Waters HPC

- Transition simulations require a high grid resolution (both spatially and temporally), not tractable on smaller computing clusters such as at UKy,
- Resources on Blue Waters enabled us to validate the AMR-WPT methodology,
- It also enabled us to extend the method to studying particle induced transition with AMR-WPT method,
- AMR refinement criteria,
- Running on 512-8191 procs, ramping up no. of procs, short queue times,
- Speed-up vs DNS,

Summary, Outlook & Research Interests

Summary and Outlook

- Efficient high-fidelity approach for particle-flow simulations has been presented,
- Particle flow interactions are highly dependent on flow conditions, etc.
- Effects of particle properties (size, weight, and composition) will be further investigated,
- Further analysis of particle flow simulations will be presented at the AIAA Aviation,

Summary, Outlook & Research Interests

Thank you to everyone at Blue Waters for your help with my research and for hosting me at Sunriver, Oregon. Special mention for Brett!

Any questions or comments?