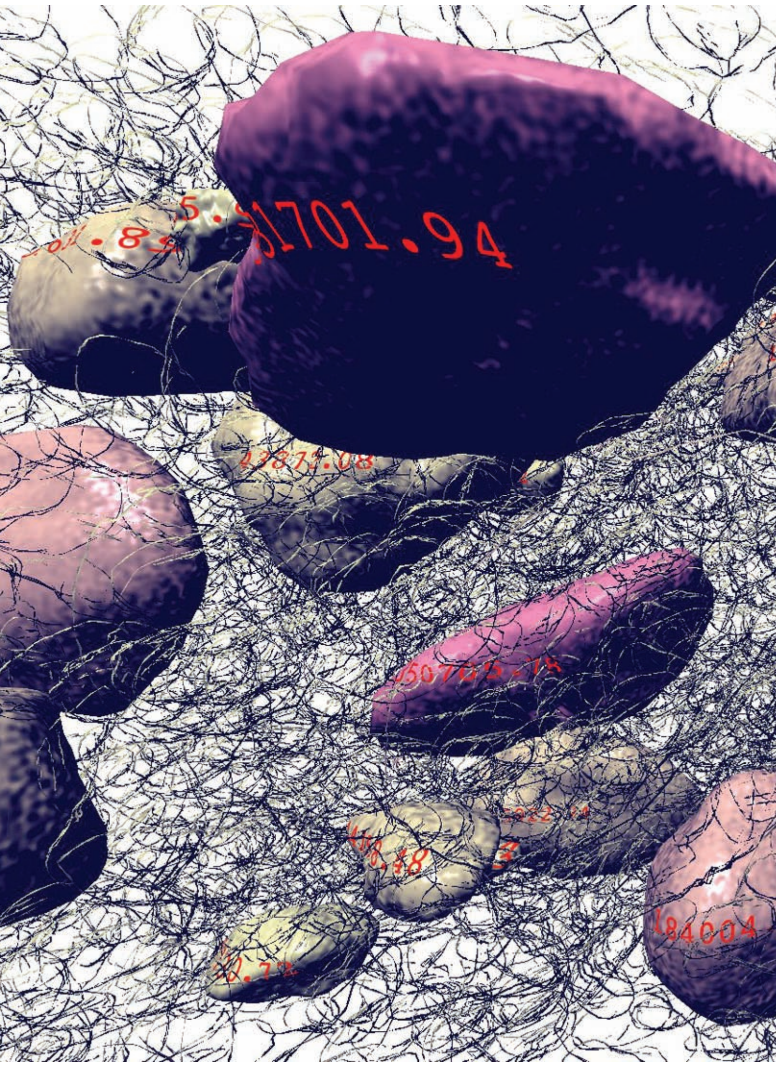
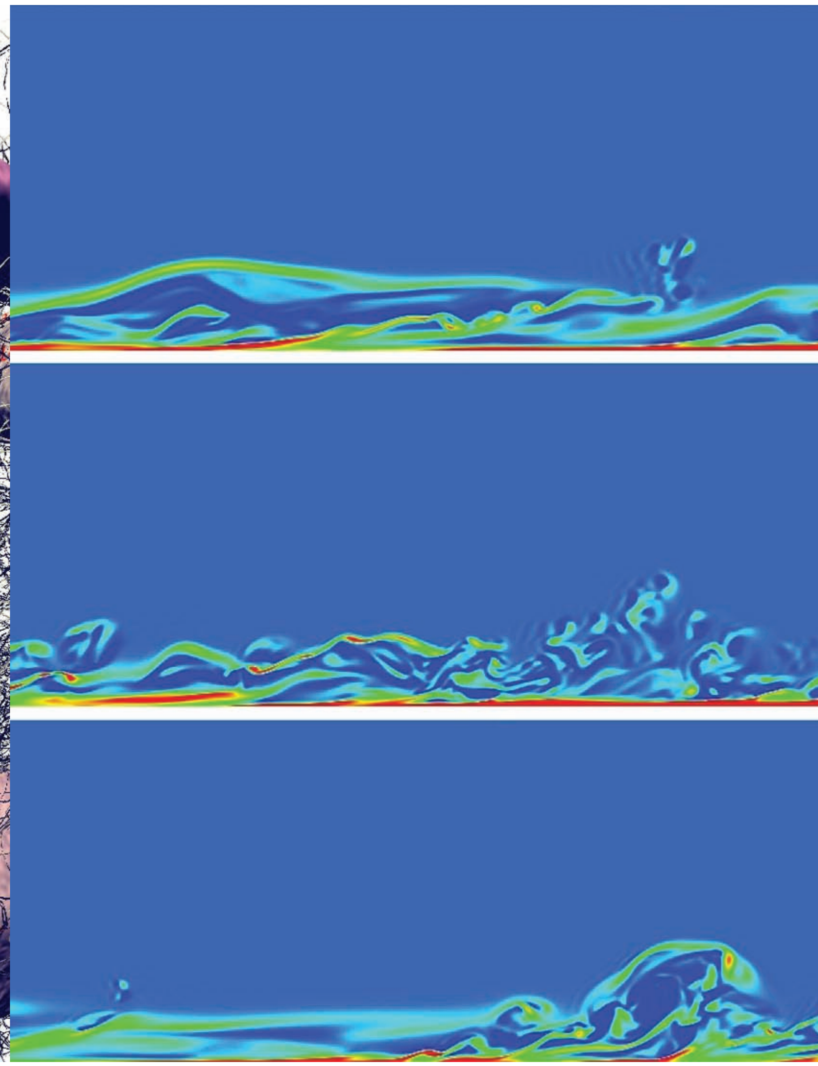
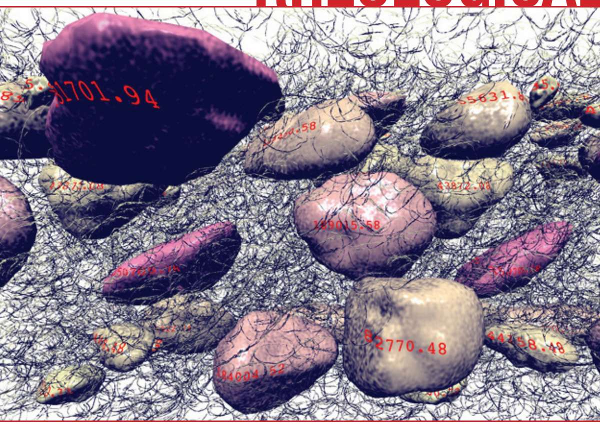




NATIONAL LEADERSHIP COMPUTING SYSTEM

NASA's National Leadership Computing System (NLCS) initiative provides access to the Agency's largest supercomputers to selected non-NASA researchers doing cutting-edge, computationally intensive science and engineering of national interest. NLCS demonstrates the Agency's support for important national priorities, and its commitment to continued U.S. leadership in high-end scientific and technical computing and computational modeling. By inviting industry and academia participation, NASA can help advance U.S. technology and education, and assist U.S. competitiveness. In return for NLCS awards, much of the resulting knowledge will be made publicly available.

MODELING THE RHEOLOGICAL PROPERTIES OF CONCRETE



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WILLIAM GEORGE
National Institute of Standards and Technology
(301) 975-4943
wgeorge@nist.gov

Figure 1: Snapshot of a flowing suspension of rocks in a mortar matrix (concrete). The mortar matrix is not visible in this image. Graphical processing unit programming was used within the application to place the stress value on the surface of each rock. Rocks with a stress value below a specified threshold are shown only as silhouettes.

Project Description: Modeling and predicting physical properties of concrete remains a great challenge, as it involves phenomena taking place over many length and time scales. For example, concrete is typically composed of cement (micrometer scale with interactions at the nanometer scale), sand (millimeter scale), and aggregates (centimeter scale). Even at each representative length scale, there can be considerable variation and other factors to consider, such as the addition of chemical admixtures in the cement paste, sand diameter variation of over a factor of 100, or shape variation of aggregates (rounded or crushed).

The rheological properties of complex fluids, specifically viscosity and yield stress (the applied stress when flow begins), play an important role in a wide variety of technological and environmental processes. Understanding how a fluid yields under stress is a subject of great interest and remains an outstanding problem in the field of fluid physics.

In this project, we study the flow of dense suspensions composed of rigid bodies having a wide range of sizes and shapes, under a variety of flow conditions (shear and around obstacles). Our goal is to advance the general understanding of the flow properties of these complex fluids. While this research is applicable to many areas, the focus of our study is to understand, and ultimately to predict, the rheological properties of cement-based materials.

Relevance of Work to NASA: This research focuses on advancing our understanding of fundamental mechanisms that control the flow of suspensions. It is important to understand how these materials start to flow and to tune their physiochemical properties in order to control their movement as the material is applied. This knowledge will be useful in the development of materials and techniques for the building and repair of structures under various conditions such as low- and high-gravity environments. Further, suspensions are utilized in a wide variety of technological processes and, because this study is largely parametric in nature, results are transferable to other fields.

Computational Approach: Recently, a new computational fluid dynamics (CFD) method called Dissipative Particle Dynamics (DPD) has been developed, which holds promise for modeling complex fluids. Indeed, DPD may have some advantages over other CFD methods because DPD can naturally accommodate many boundary conditions and does not require meshing (or re-meshing) of the computational domain. On the surface, DPD looks very much like a molecular dynamics algorithm where particles, subject to inter-atomic forces, move according to Newton's laws. However, the particles in DPD are not atomistic, but a mesoscopic-scale (between the macroscopic- and atomic- scale ranges) representation of the fluid. We have adopted this approach due to its potential for modeling rigid bodies with a wide variety of shapes. Custom visualization software is used to explore the results of the simulations in detail. Representative snapshots of this software in use are shown in Figures 1 and 2.

Results: Results from recent simulations have advanced our understanding of suspensions in two particular areas: yield stress and the formation of stress chains in dense suspensions. Our studies have helped provide fundamental insights into the physical mechanisms that control yield stress. These simulations indicate that current theoretical models are inadequate for describing the yielding behavior of dense colloidal suspensions [1, 3]. We have also successfully modeled and visualized the formation of stress chains in dense suspensions. These stress chains are accompanied by giant stress fluctuations and have been seen in recent physical experiments [2].

Role of High-End Computing: Our ability to simulate dense suspensions has been enabled by access to NASA's computational resources. Simulations of the size and duration needed to reveal the characteristics of these dense suspensions are only possible on large parallel supercomputers such as Columbia. We have typically utilized 500–1,000 processors for each simulation—some of which still required over 100 hours of continuous compute time to complete. Results from these simulations, some exceeding 20 gigabytes, have been transferred from the NASA Advanced Supercomputing (NAS) facility in California to the National Institute of Standards and Technologies (NIST) in Maryland via a high-speed Internet2 connection facilitated by NAS network administrators in collaboration with their NIST counterparts.

Future: We are in the process of completing an analysis of the localized stress transmission in dense colloidal suspensions, which is expected to provide greater insight into the fundamental mechanisms that control yield stress. The next goal is to study the dependence of yield stress and viscosity on the strength of inter-particle interactions. We will also explore the role of aggregate shape and size distribution on rheological properties of suspensions, comparing results with currently available experimental data. We are interested in studying the structural rearrangements that occur in very dense colloidal suspensions. These systems serve as idealized models of molecular glasses, which are difficult to visualize because the length and time scales are too small. Finally, we have recently modified our code to model suspensions with a non-Newtonian fluid matrix in order to expand the types of suspensions that we can study. Such suspensions are very realistic and representative of many building materials, such as mortars and concrete. We intend to apply for additional compute time on NASA's computational resources for advancing this research and to expand the research to include the study of the chemical properties of cement as it cures.

Co-Investigators

- Nicos S. Martys, Edward J. Garboczi, John G. Hagedorn, Judith E. Terrill, all of the National Institute of Standards and Technology

Publications

[1] Martys, N., Lootens, D., George, W., Satterfield, S., and Hebraud, P., "Spatial-Temporal Correlations at the Onset of Flow in Concentrated Suspensions," The XVth International Congress On Rheology, Ed. A. Co, L.G. Leal, R. H. Colby, A.J. Giacomin, *AIP Conf Proc. Vol. 1027*, Monterey, CA, pp. 207–209, 2008.

[2] Lootens, D., Martys, N., George, W., Satterfield, S., and Hebraud, P., "Stress Chains Formation under Shear of Concentrated Suspension," The XVth International Congress On Rheology, Ed. A. Co, L. G. Leal, R. H. Colby, A. J. Giacomin, *AIP Conf Proc. Vol. 1027*, Monterey, CA, pp. 677–679, 2008.

[3] Martys, N., Lootens, D., George, W., and Hebraud, P., "Spatial-Temporal Correlations of Colloids in Start-up Flows," (submitted to *Physical Review Letters*).

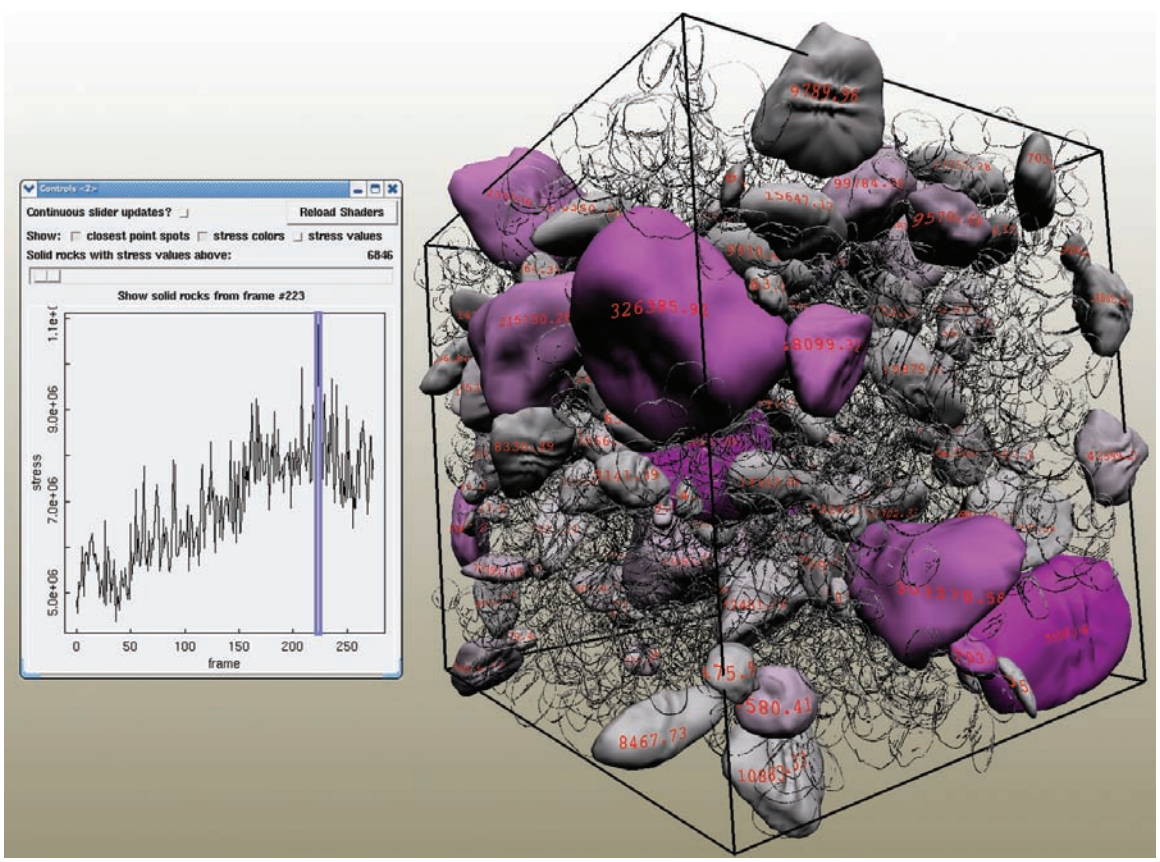
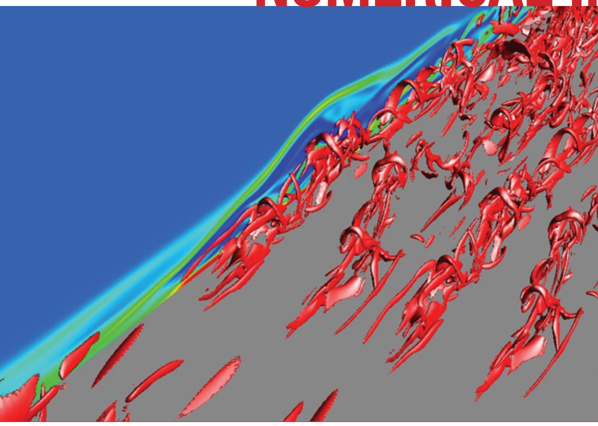


Figure 2: Graph of the average system stress, that is, applied force per unit area over time, is shown to the left of a visualization of the dense suspension. Interactive controls allow for the detailed exploration of the simulation results. This custom exploration software is supported on both desktop systems and an immersive visualization environment.

TRANSITION IN HIGH-SPEED BOUNDARY LAYERS: NUMERICAL INVESTIGATIONS USING DNS



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FRANK HUSMEIER
Greenberg Traurig, LLP
(520) 621-4424
husmeierf@gtlaw.com
http://cfdlab.web.arizona.edu

◄ Detail of Figure 1.

Project Description: Flight vehicles, cruising faster than the speed of sound, experience high heating rates at their surface. In a high-density environment, these aero-thermal loads are even further increased due to the transition process of a laminar high-speed boundary layer to turbulence. In the past, engineers used a relatively conservative approach for the design of thermal protection systems (TPS). In this approach, the turbulent boundary layer was assumed to be present over the entire TPS. For the design of future high-speed vehicles, however, design margins will need to be reduced to enhance payload capabilities. To reach this goal, the transition process of a high-speed boundary layer must be better understood to provide the design community with accurate physical models for prediction of the transition point.

The transition process of a laminar high-speed boundary layer to turbulence is studied using direct numerical simulations (DNS). In this approach, the Navier-Stokes equations governing the flow are solved directly using very efficient and accurate numerical methods that scale well with large parallel computers such as NASA's Columbia supercomputer. Understanding the transition physics is mandatory for finding advanced methods to: control the transition process; provide a numerical database for an in-depth validation of engineering predictions (for example, turbulence models) of the various transition stages; and provide the design community with accurate physical models for prediction of the transition point.

Relevance of Work to NASA: This project is partially funded by NASA's Aeronautics Research Mission Directorate and is an important part of NASA's quest to understand the transition process of high-speed boundary layers. Reliable transition predictions are critically important for the design and safe operation of any high-speed, advanced flight vehicle. Examples include the Hyper-X Program as well as the Constellation Program with both the Orion Crew Exploration Vehicle and the Ares Crew Launch Vehicle. The large increase in wall heat transfer due to transition to turbulence in high-speed boundary layers is one of the major difficulties in the design and operation of high-speed flight vehicles. In addition to these aero-thermal loads, transition to turbulence has a large impact on the aerodynamic performance and flight characteristics of these vehicles as skin friction is drastically increased. This fact is especially important for flight vehicles that have only a lifting body, such as the X-43. Accurate transition prediction can, in some cases, increase its range or, in others, result in a reduction of size and weight with comparable performance.

Computational Approach: The Navier-Stokes equations are integrated in time by employing a fourth-order Runge-Kutta scheme. The spatial derivatives are discretized using fourth-order split-finite differences in the streamwise and wall-normal direction. Assuming that the spanwise direction is periodic, integration variables are transformed into spectral space using Fast Fourier Transforms. Furthermore, the spanwise discretization is pseudo-spectral; that is, all nonlinear terms in the governing equations are computed in physical space [1, 2]. The use of an explicit time integration scheme and a standard finite difference method for discretization of the spatial derivatives allows the simulation code to scale very well on large parallel computers such as Columbia.

Results: The project was divided in two subprojects. One part focused on the transition process of a hypersonic cone and flat-plate boundary layer at Mach 8, whereas the second subproject concentrated on the transition process of a supersonic flat-plate boundary layer at Mach 3. For the first subproject, the following milestones were achieved:

- Two strong transition mechanisms (so-called "oblique breakdown" and "oblique fundamental resonance") were identified, which may lead to a fully developed turbulent boundary layer at Mach 8.
- For these mechanisms, highly resolved direct numerical simulations were performed—the first simulations of this kind at hypersonic speeds.

- The influence of the nose tip radius of a cone on the transition process for a hypersonic boundary layer was studied intensively.

For the second project, key results are summarized as follows:

- The entire path of laminar-turbulent transition for a supersonic boundary layer via oblique breakdown was studied.
- It was demonstrated that oblique breakdown indeed breaks down to turbulence since a turbulent stage was reached near the outflow.
- This is one of the first highly resolved direct numerical simulations that captures the entire transition path for a supersonic, flat-plate boundary layer.

Role of High-End Computing: Numerical study of high-speed boundary-layer transition is crucial for understanding the transition process and underlying physical mechanisms since experimental investigations in high-speed wind tunnels are very difficult to perform. Only a few experimental studies that provide high-quality datasets exist. Hence, accurate simulations of the entire transition process—from the linear stage to breakdown to turbulence, including the turbulent regime—are mandatory for understanding high-speed boundary-layer transition. These simulations pose a formidable computational challenge, requiring grid sizes approaching half a billion grid points and more. Even with the current high-end supercomputing systems (for example, Columbia), such calculations still take several weeks to complete on 256 processors.

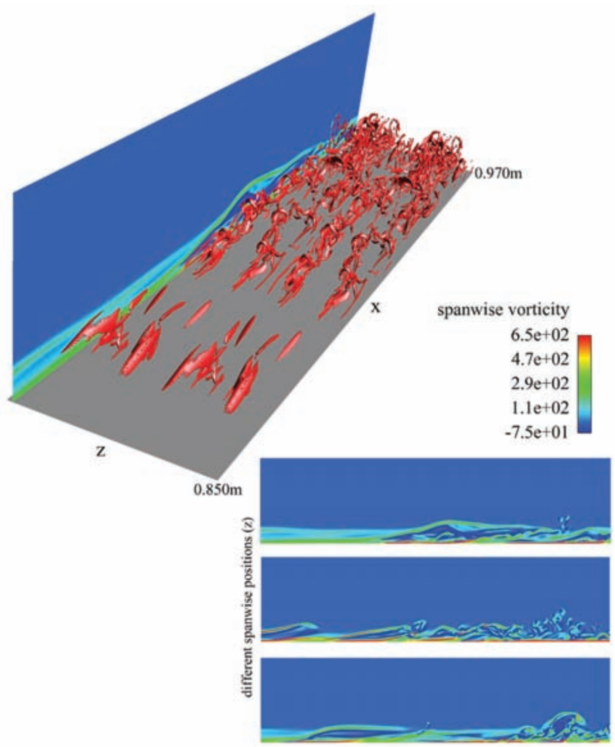

Figure 1: Transition to turbulence initiated by "oblique breakdown" for a supersonic flow over a flat plate. Ma=3, T=103.6 K, Re=2.181E6 1/m, f=6.36 kHz, forcing location x=0.452 m. Isosurfaces of Q=30000 [3].

Future: We are planning to extend our computational efforts by using our recently developed high-order accurate Navier-Stokes code to investigate boundary-layer transition for a cone at Mach 3.5 (in close cooperation with experimental efforts at NASA Langley Research Center). This code will enable us to submit our future simulations on NASA's Pleiades supercomputer since it utilizes Message Passing Interface for its parallelization routines. Furthermore, we will be able to efficiently allocate a larger number of processors for these simulations (beyond 1,000). To meet this challenge, we will work closely with NASA's high-end computing experts to optimize our new Navier-Stokes code.

Co-Investigators

- Christian Mayer, Andreas Laible, The University of Arizona

Publications

[1] Husmeier, F. and Fasel, H.,"Numerical Investigations of Hypersonic Boundary Layer Transition over Circular Cones," *AIAA Paper 2007-3843*, 2007.

[2] Laible, A., Mayer, C., and Fasel, H., "Numerical Investigation of Supersonic Transition for a Circular Cone at Mach 3.5," *AIAA 2008-4397,* 2008.

[3] Mayer, C.S.J., von Terzi, D.A., and Fasel, H., "DNS of Complete Transition to Turbulence Via Oblique Breakdown at Mach 3," *AIAA Paper 2008-4398*, 2008.

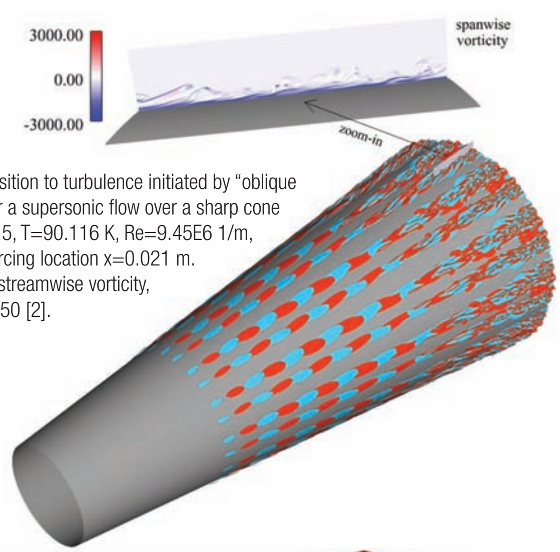

Figure 2: Transition to turbulence initiated by "oblique breakdown" for a supersonic flow over a sharp cone (7 deg). Ma=3.5, T=90.116 K, Re=9.45E6 1/m, f=45.2 kHz, forcing location x=0.021 m. Isosurfaces of streamwise vorticity, blue: -50, red: 50 [2].

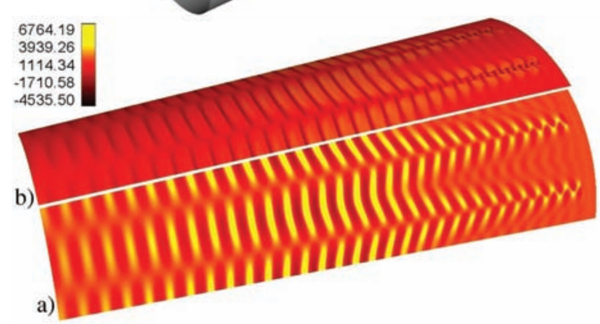

Figure 3: Transition to turbulence initiated by "oblique breakdown" for a hypersonic flow over a sharp cone (7 deg). Ma=8, T=53.35 K, Re=3333333, f=88 kHz. Wall-normal heat flux at a) the wall, and b) boundary layer edge [1].