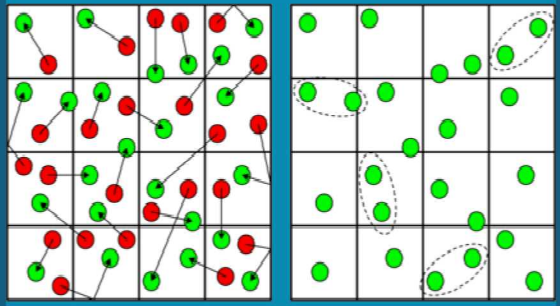
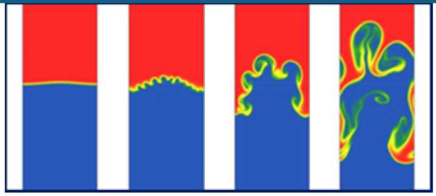
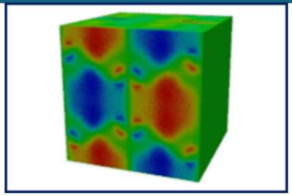
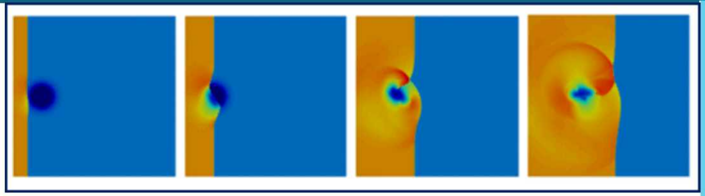
SAND2019-11265C

DSMC Simulations of Shock-Vortex Interactions







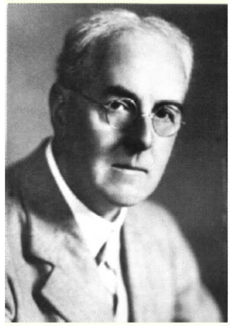


PRESENTED BY:

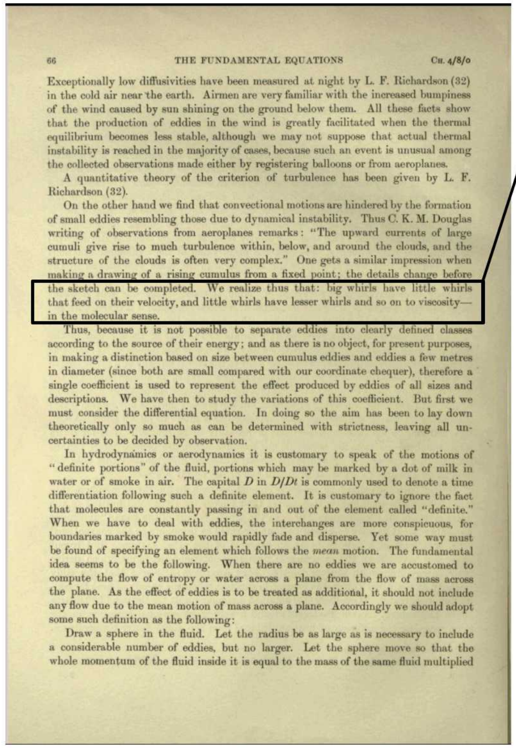
Timothy P. Koehler, M. A. Gallis, J. R. Torczynski

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Motivation and Background



L. Richardson



66 THE FUNDAMENTAL EQUATIONS CH. 4/8/0

Exceptionally low diffusivities have been measured at night by L. F. Richardson (32) in the cold air near the earth. Airmen are very familiar with the increased bumpiness of the wind caused by sun shining on the ground below them. All these facts show that the production of eddies in the wind is greatly facilitated when the thermal equilibrium becomes less stable, although we may not suppose that actual thermal instability is reached in the majority of cases, because such an event is unusual among the collected observations made either by registering balloons or from aeroplanes.

A quantitative theory of the criterion of turbulence has been given by L. F. Richardson (32).

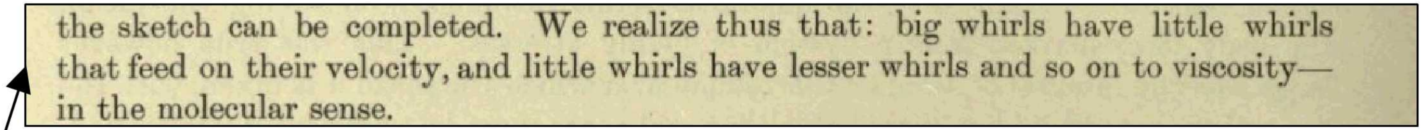
On the other hand we find that convectional motions are hindered by the formation of small eddies resembling those due to dynamical instability. Thus C. K. M. Douglas writing of observations from aeroplanes remarks: "The upward currents of large cumuli give rise to much turbulence within, below, and around the clouds, and the structure of the clouds is often very complex." One gets a similar impression when making a drawing of a rising cumulus from a fixed point; the details change before the sketch can be completed. We realize thus that: big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls and so on to viscosity—in the molecular sense.

Thus, because it is not possible to separate eddies into clearly defined classes according to the source of their energy; and as there is no object, for present purposes, in making a distinction based on size between cumulus eddies and eddies a few metres in diameter (since both are small compared with our coordinate chequer), therefore a single coefficient is used to represent the effect produced by eddies of all sizes and descriptions. We have then to study the variations of this coefficient. But first we must consider the differential equation. In doing so the aim has been to lay down theoretically only so much as can be determined with strictness, leaving all uncertainties to be decided by observation.

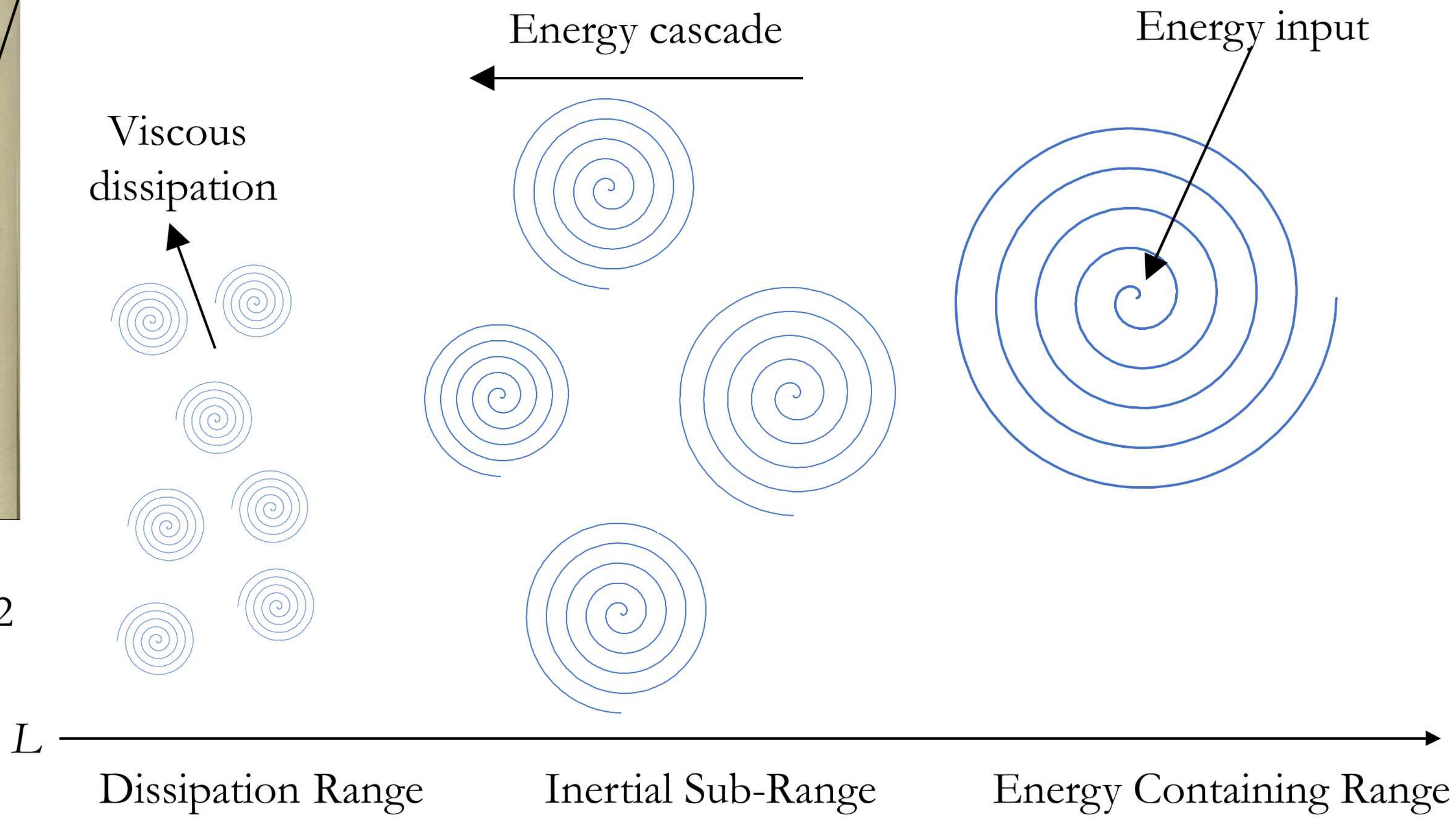
In hydrodynamics or aerodynamics it is customary to speak of the motions of "definite portions" of the fluid, portions which may be marked by a dot of milk in water or of smoke in air. The capital D in D/Dt is commonly used to denote a time differentiation following such a definite element. It is customary to ignore the fact that molecules are constantly passing in and out of the element called "definite." When we have to deal with eddies, the interchanges are more conspicuous, for boundaries marked by smoke would rapidly fade and disperse. Yet some way must be found of specifying an element which follows the *mean* motion. The fundamental idea seems to be the following. When there are no eddies we are accustomed to compute the flow of entropy or water across a plane from the flow of mass across the plane. As the effect of eddies is to be treated as additional, it should not include any flow due to the mean motion of mass across a plane. Accordingly we should adopt some such definition as the following:

Draw a sphere in the fluid. Let the radius be as large as is necessary to include a considerable number of eddies, but no larger. Let the sphere move so that the whole momentum of the fluid inside it is equal to the mass of the same fluid multiplied

Weather Prediction by Numerical Processes, 1922



the sketch can be completed. We realize thus that: big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls and so on to viscosity—in the molecular sense.



Motivation and Background

Turbulence is usually studied at the continuum limit:

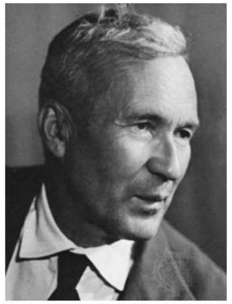
$$Kn = M/Re$$

For example: $Re \sim 10^7$ and $M \sim 1 \rightarrow Kn = 10^{-7}$

For a gas flow with a turbulent Mach number M and a turbulent Reynolds number Re the ratio of the Kolmogorov length scale to the mean free path scales as:

$$Re^{1/4}/M$$

- Consider a hypothetical flow with Re=10,000 and M=0.3. This ratio is ~30 → $Kn \sim O(0.01)$
  - Smallest scale of turbulence (Kolmogorov scale) becomes comparable to the smallest scale of motion (thermal fluctuations)
  - Kolmogorov scale **no longer a continuum medium.**



A. Kolmogorov

- The question whether turbulent energy dissipation is correlated to molecular fluctuations was originally posed by von Neumann in 1950:
  - Gases have a finite mean free path (MFP)
  - CFD is correct to the limit of cell volume tending to zero
  - Eventually, the cell size becomes comparable to the MFP

Are the hydrodynamic equations still valid?

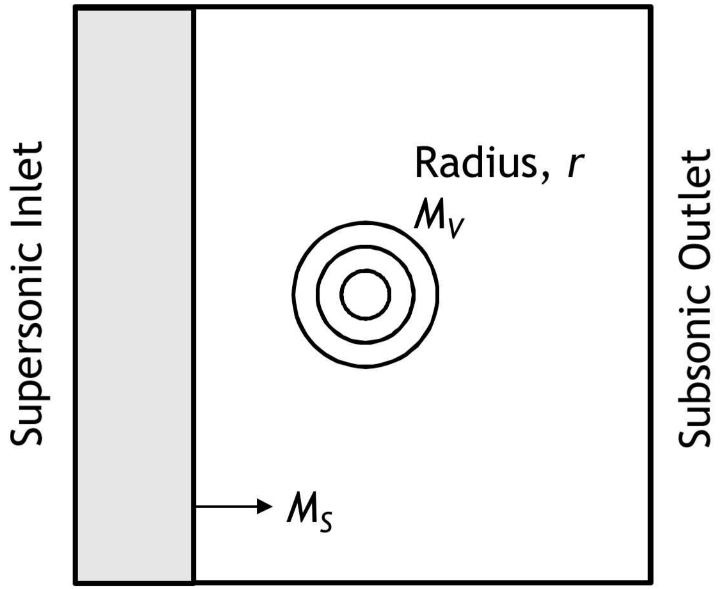
J. von Neumann

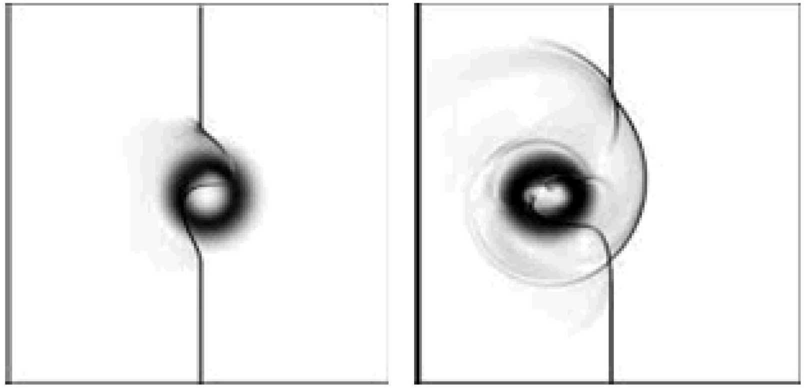
Problem Statement and Modeling Approach

- **Problem:** Study shock interaction with a vortex at the molecular level, to include non-continuum physics (thermal fluctuations, finite mean free path)
  - Extensive work exists at continuum experimentally, analytically, and numerically

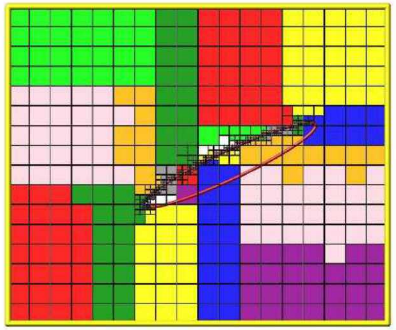
- **Approach:** Use DSMC via SPARTA to study shock/vortex interactions
  - Parametrics: shock strength and vortex size

- **Goal:** Assess the feasibility of DSMC studies of turbulent processes to provide additional physical insight



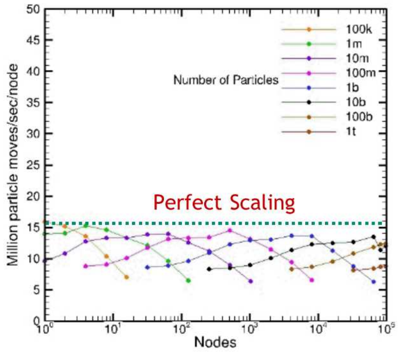


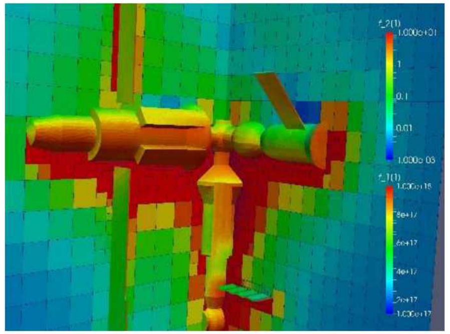
SPARTA: Sandia's Highly Scalable DSMC Code

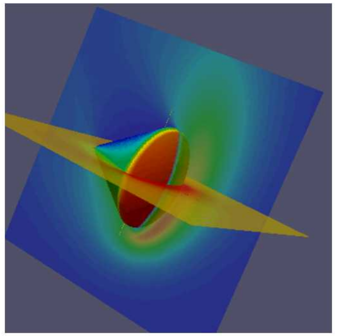


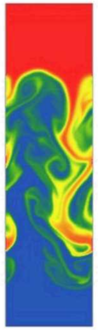
SPARTA = Stochastic PArallel Rarefied-gas Time-accurate Analyzer

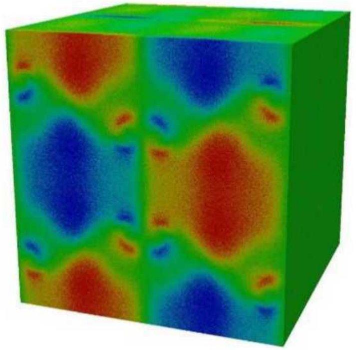
- 1D, 2D, 2D-Axisymmetric or 3D; Serial or Parallel
- Cartesian, hierarchical grid.
  - Octree (up to 16 levels in 64-bit cell ID).
  - Load balancing, automatic grid adaptation, *in situ* visualization.
- Next-gen performance portability through Kokkos Abstractions.
  - GPUs, Xeon Phis, ...
  - Sequoia (1.57 million cores).
  - 100% Trinity utilization (heterogenous run).
- Open source.
  - 3000+ downloads, 100+ users worldwide.
  - Collaborators: ORNL, LANL, ANL, LBNL, NASA, ESA, Academia.
- Hydrodynamic simulations.
  - Taylor-Green Vortex and Minimal Couette Flow.
  - Richtmyer-Meshkov & Rayleigh-Taylor Instabilities.

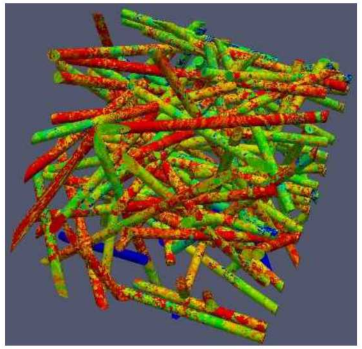






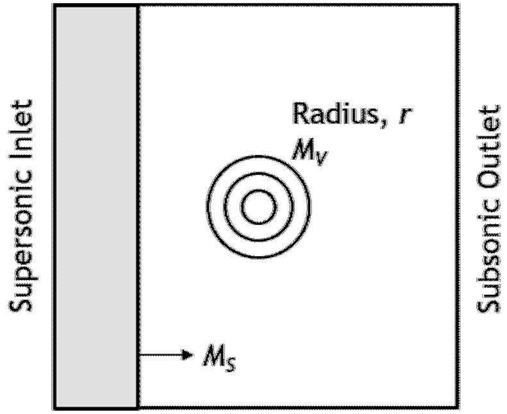






Model Description and Computational Specifics

Initial vortex description:



$$u_\theta = \begin{cases} u_m\, r/r_1 & r < r_1 \\ u_m \frac{r_1}{r_1^2 - r_2^2} & r_1 \geq r \geq r_2 \\ 0 & r \geq r_2 \end{cases}$$

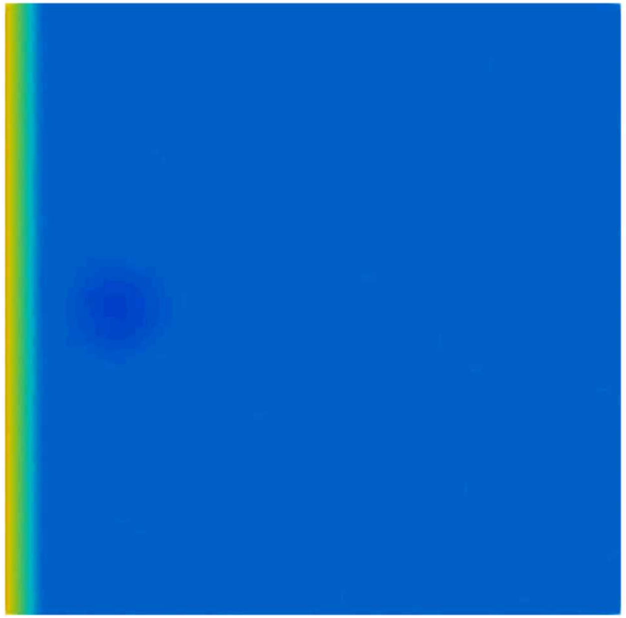
Case	M_s	M_v	r_1 (mfp)	r_2 (mfp)	$Kn=\lambda/r_1$
1	1.1	0.14	900	2000	0.001
2	1.5	1.00	900	2000	0.001
3	1.5	0.63	900	2000	0.001
4	2	1.13	900	2000	0.001
5	1.1	0.14	90	200	0.01
6	1.5	1.00	90	200	0.01
7	1.5	0.63	90	200	0.01
8	2	1.13	90	200	0.01

Numerics and Computational Specifics:

- Required 5000 simulators per cell
- Simulations were run for 24 – 48 hours using:
  - 32k nodes (524,288 cores with 4 threads/core) on LLNL Sequoia
  - 5k nodes (320,000 cores with 4 threads/core) on LLNL Trinity
- Load balancing challenges:
  - Temporal density changes in this flow required regular load balancing
  - Memory efficient load balancer was developed

Effect of Relative Shock Strength (Kn = 0.01)

Case 5

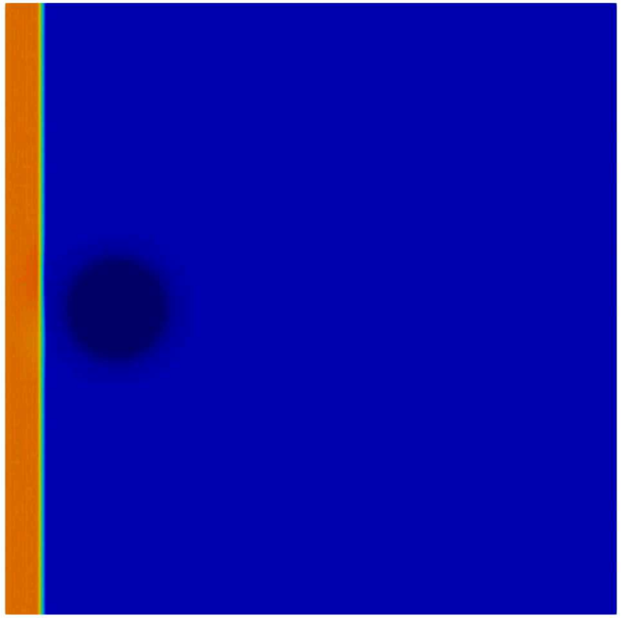


$M_S = 1.1$, $M_V = 0.14$

Case 7

$M_S = 1.5$, $M_V = 1.0$

Case 8



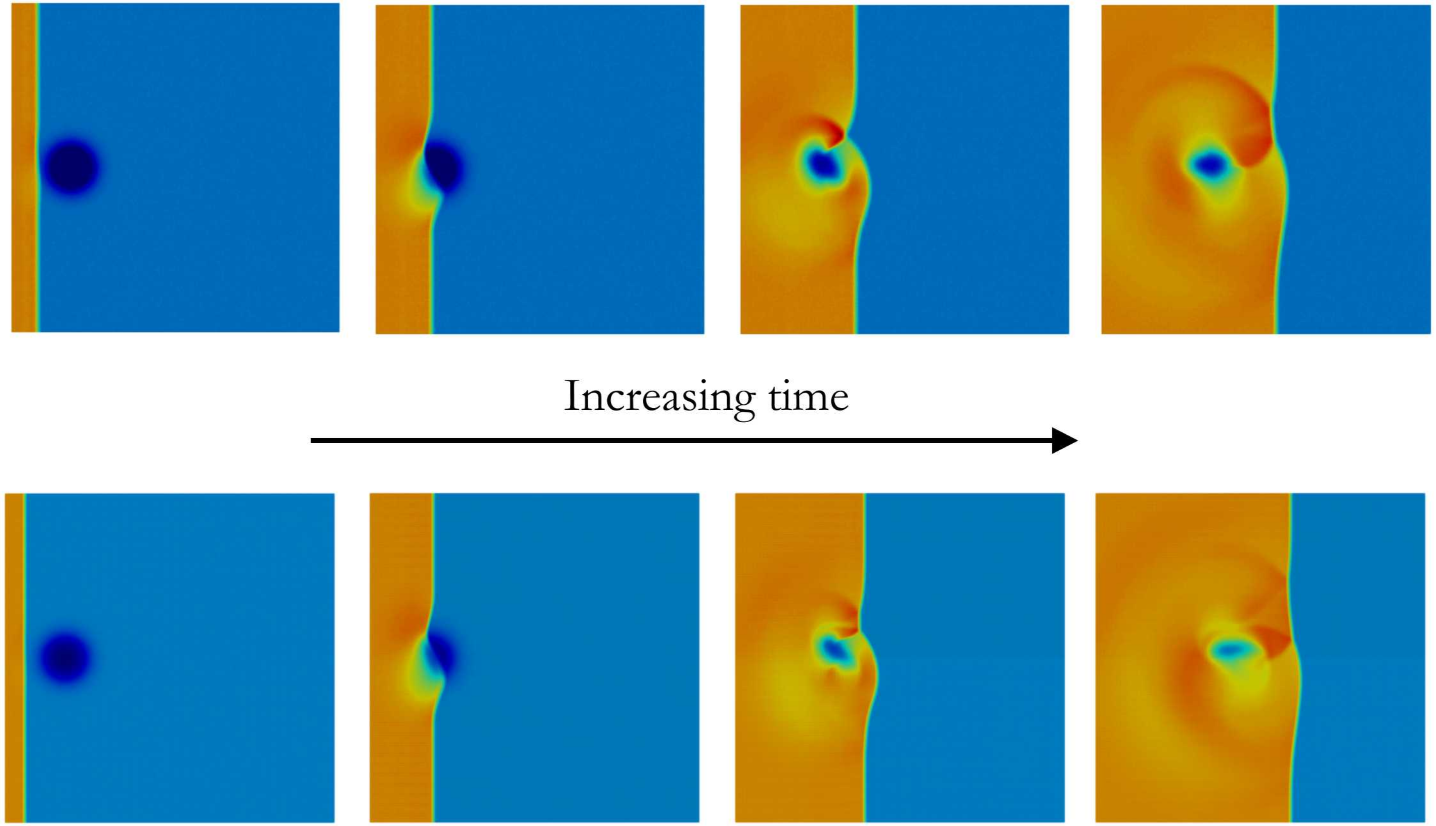
$M_S = 2.0$, $M_V = 1.13$

Characteristic observations:

- Weak vortex does not significantly change shock
- Shock is distorted by a stronger vortex
- Refracted and reflected shocks occur and propagate at differing velocities

Effect of Relative Shock Strength (Kn = 0.01) on Density

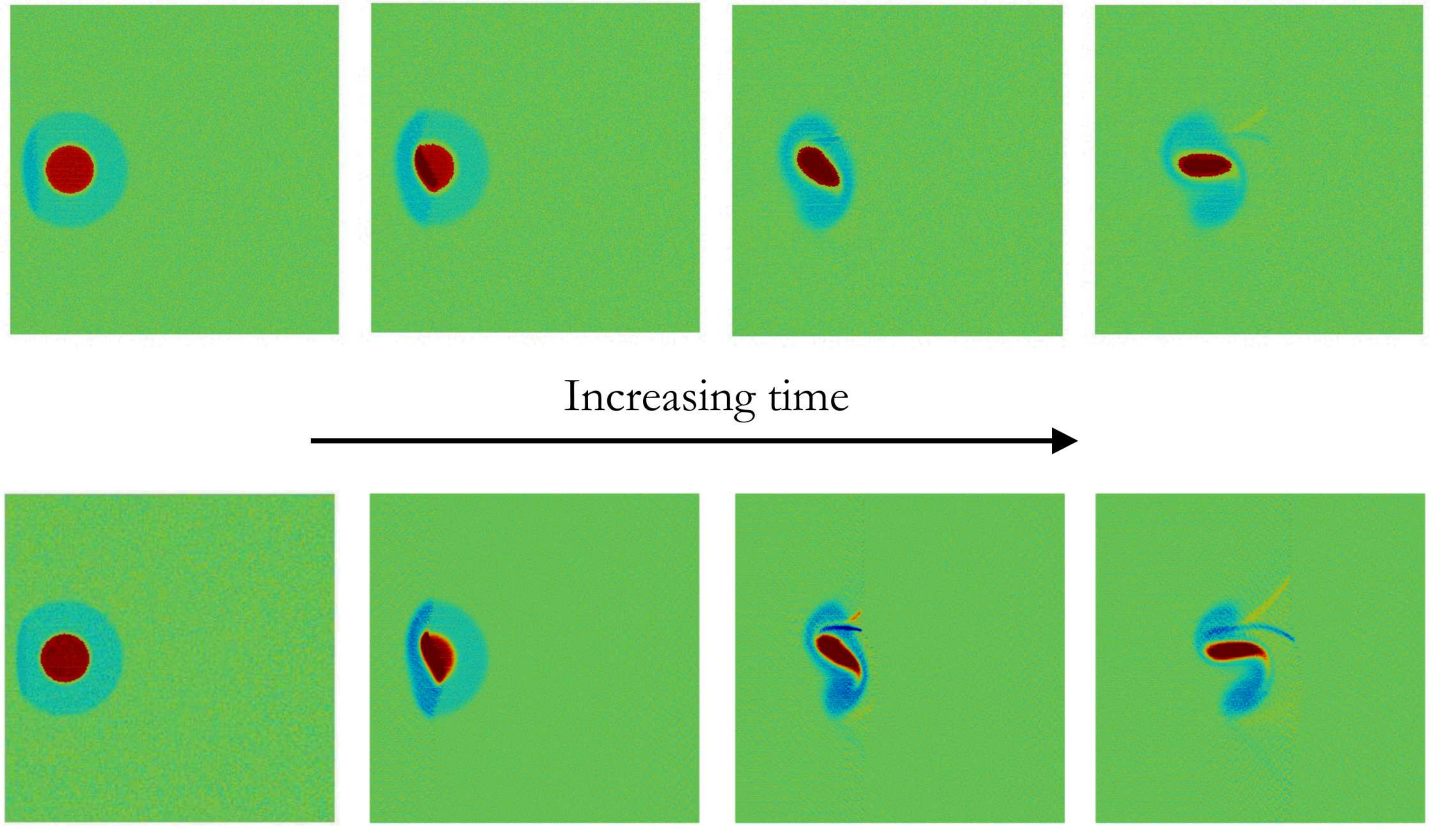
$M_S = 1.5$, $M_V = 1.0$ (Case 6)



$M_S = 2.0$, $M_V = 1.13$ (Case 8)

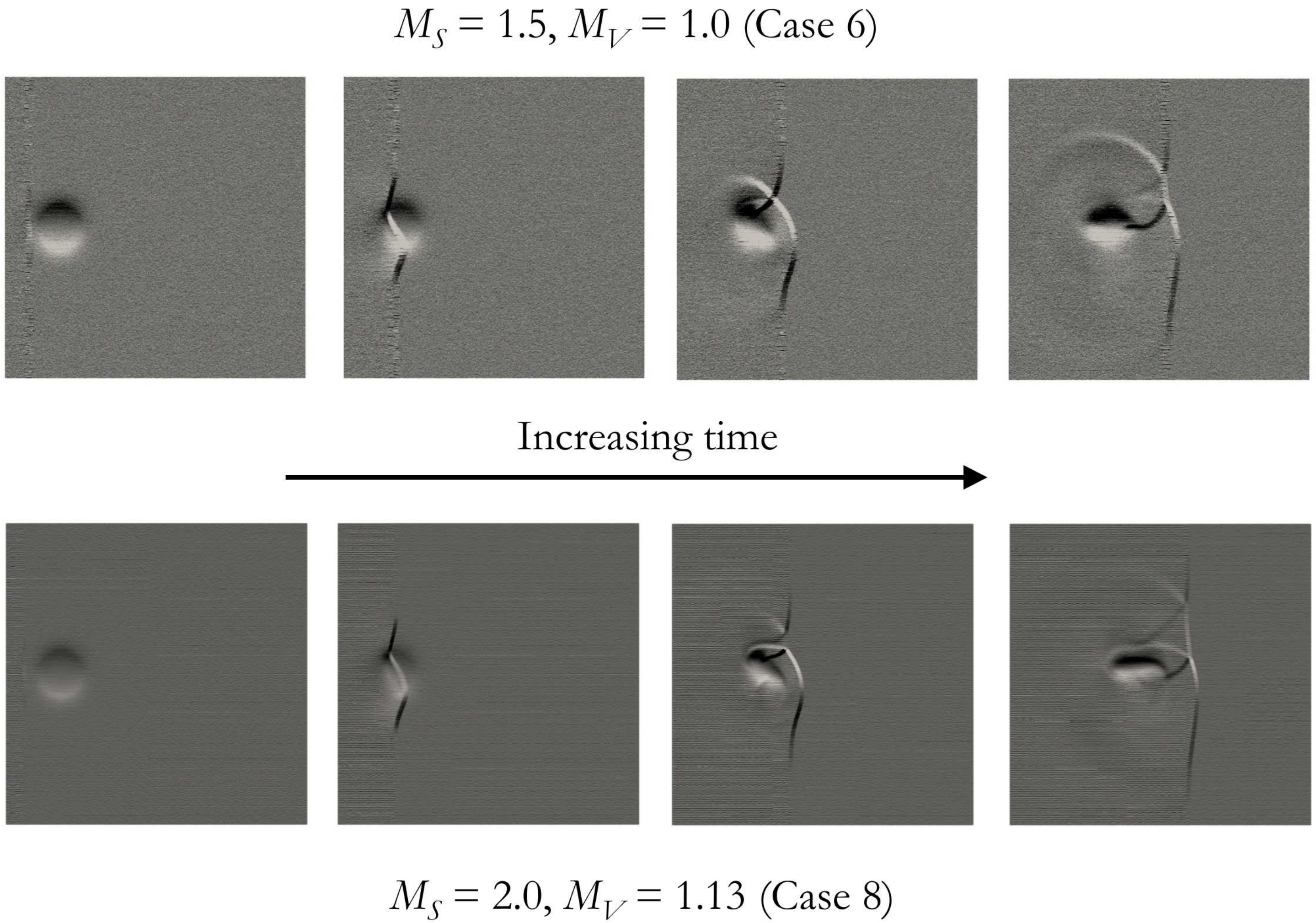
Effect of Relative Shock Strength (Kn = 0.01) on Vorticity

$M_S = 1.5$, $M_V = 1.0$ (Case 6)



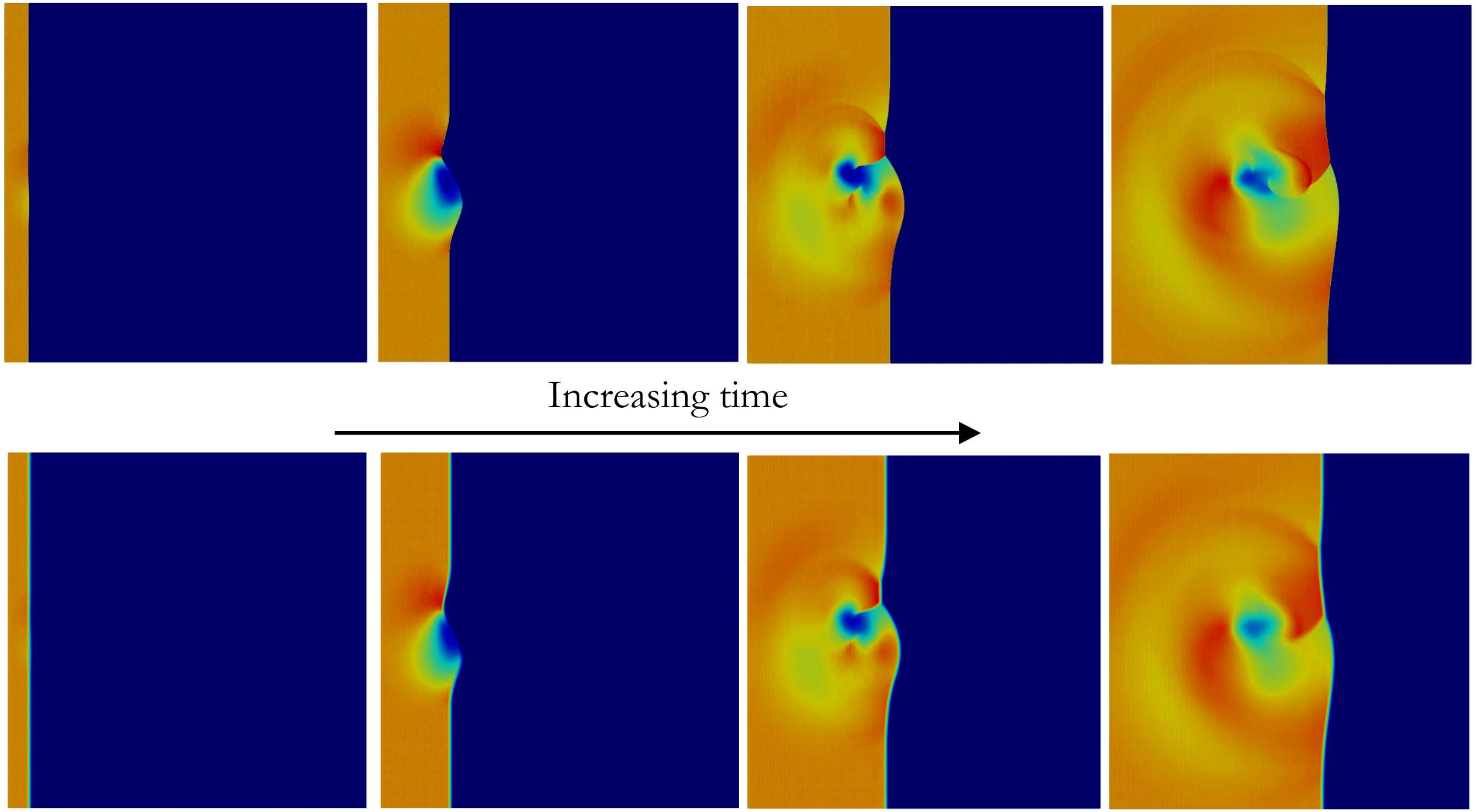
$M_S = 2.0$, $M_V = 1.13$ (Case 8)

Effect of Relative Shock Strength (*Kn* = 0.01) on Schlieren



Effect of Knudsen Number on Pressure

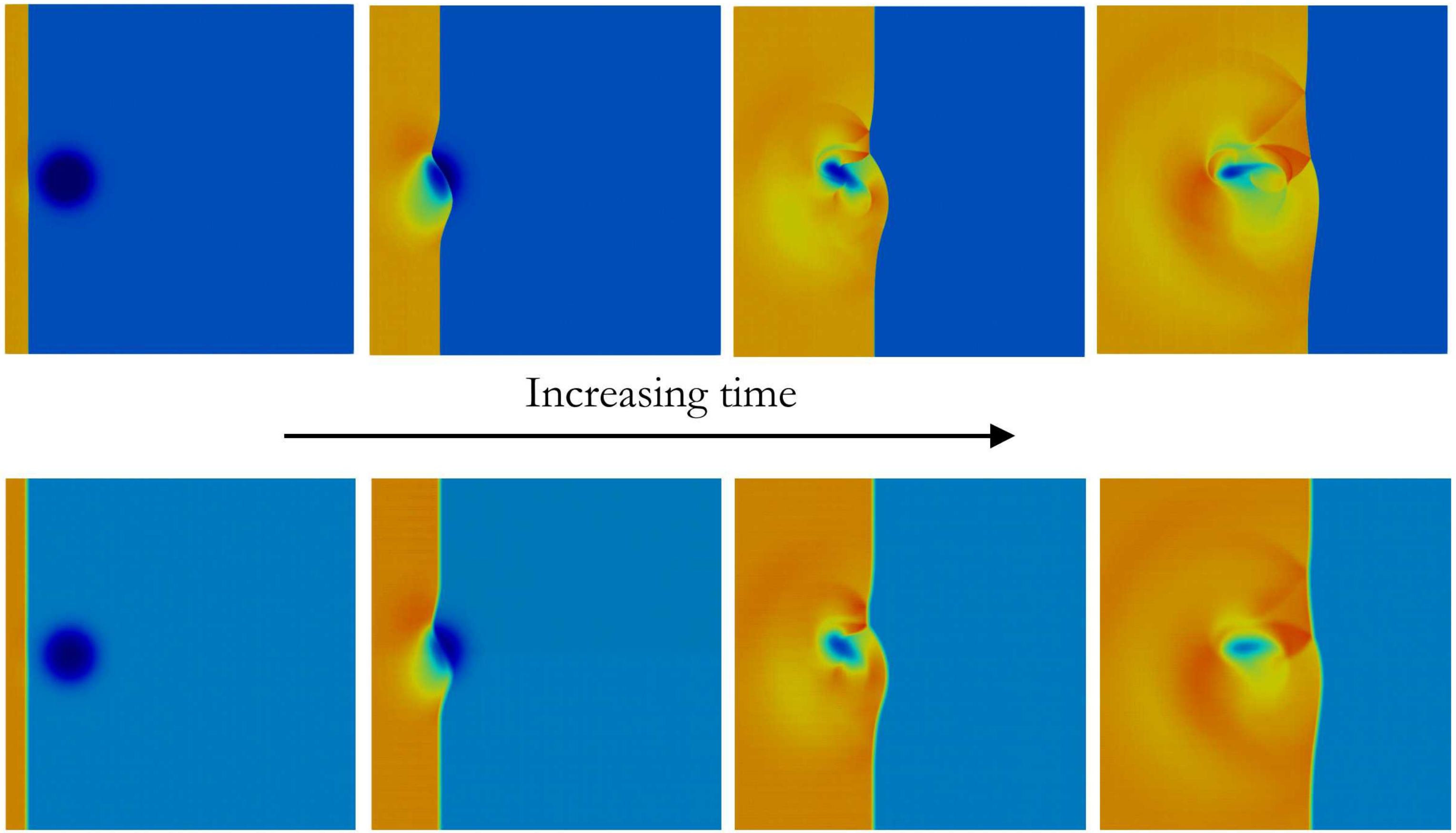
Near continuum *Kn*=0.001 (Case 4)



Transition regime *Kn*=0.01 (Case 8)

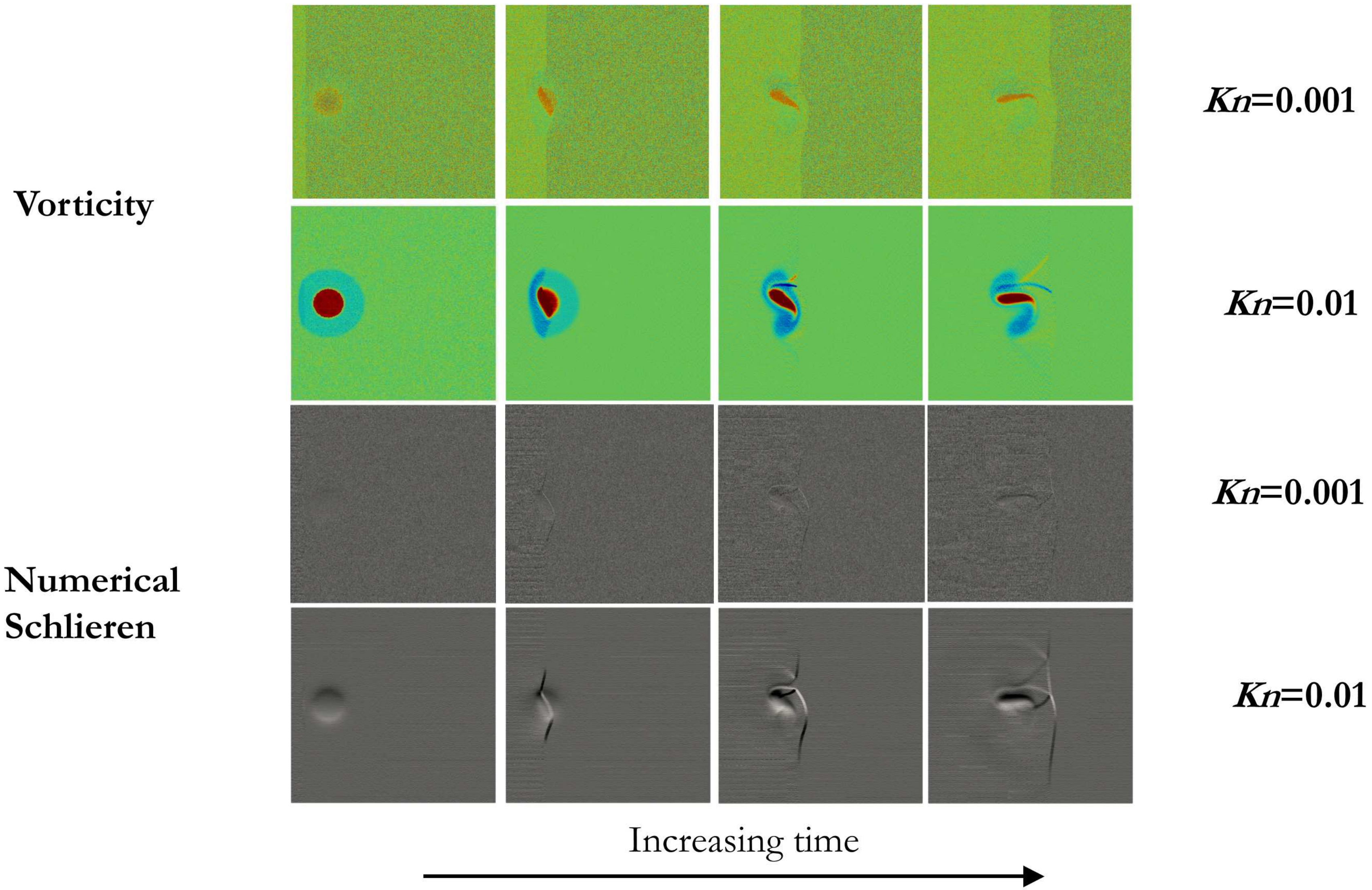
Effect of Knudsen Number on Density

Near Continuum *Kn*=0.001 (Case 4)



Transition regime *Kn*=0.01 (Case 8)

Effect of Knudsen Number on Vorticity and Schlieren



Summary

The smallest scales of turbulence responsible for the dissipation of energy may not be continuum → molecular methods may be required to understand the physics at these scales

- Shock/vortex interaction simulations show differences at the smallest scales

Computing advances have made these simulations possible

- The limits of supercomputing are challenged

Next steps:

- Perform quantitative analysis of these results
- Include additional non-equilibrium effects (internal energy relaxation, chemical reactions)
- Perform matching CFD simulations
- Expand the range of Mach numbers