

This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

# Kelvin-Helmholtz shear instability with strong thermal nonequilibrium

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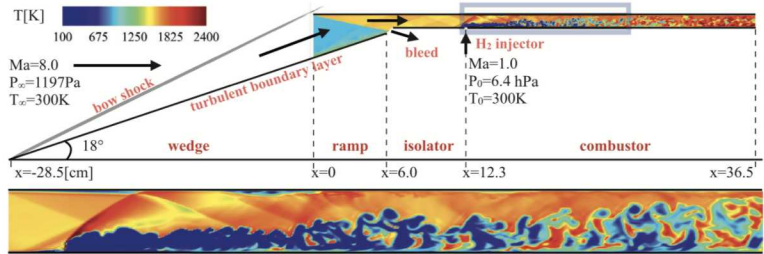
# Acknowledgment

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- Sandia National Laboratories is a multitechnology laboratory managed and operated by National Technology and 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. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.
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- Thanks to Stan Moore and Steven Plimpton

# Combustion process in extreme conditions



(Source: NASA)



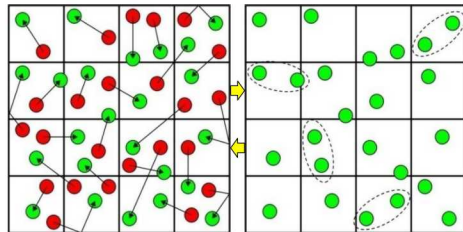
Fiévet et al., *Proc. Combustion Institute*, 2017

- Supersonic  $\rightarrow$  short mixing and reaction time
- Interactions between shock wave, cross-jet shear layer, and boundary layer
- Strong **thermal** and chemical nonequilibrium

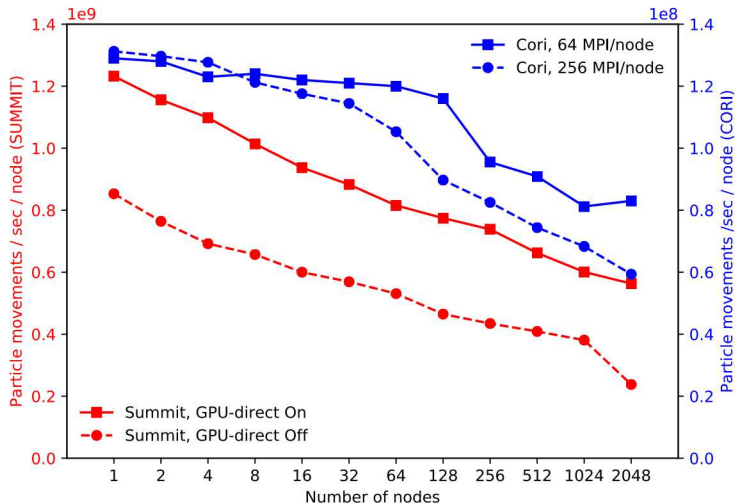
What is the effect of thermal nonequilibrium on Kelvin-Helmholtz instability?

# Direct Simulation Monte Carlo (DSMC)

- Proposed by G. A. Bird
- Solves the Boltzmann equation stochastically
- Proven to be very accurate for rarefied gas flows
- Track the motion of a large number of simulators in physical space and time
- Each simulator represents a group of particles which follows same probability distribution functions
- Collisions between simulators are computed in a stochastic manner
- SPARTA (**S**tochastic **P**arallel **R**arefied-gas **T**ime-accurate **A**nalyzer)
  - ▶ <https://sparta.sandia.gov/>



# SPARTA Performance - Weak scale

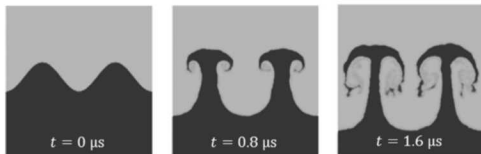


- Kokkos
- Cori, NERSC
  - ▶ Intel Xeon Phi Processor 7250
  - ▶ 68 core/node
  - ▶ 28M particle/node
  - ▶ 262144 cell/node
- Summit, OLCF, ORNL
  - ▶ Nvidia V100 GPU
  - ▶ 6 gpu/node
  - ▶ 57M particle/node
  - ▶ 442368 cell/node

# DSMC at low $Kn$ flows

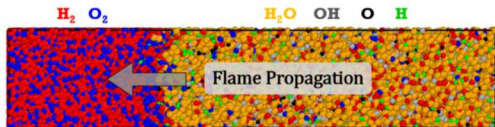
- Richtmyer-Meshkov Instability  
( $Kn = 3.5 \times 10^{-3}$ )

Gallis et al., *Physics of Fluids*, 2015



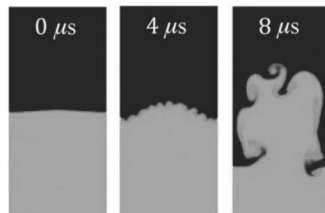
- 1D flame propagation ( $Kn = 3 \times 10^{-3}$ )

Sebastião et al, *Combustion and Flame*, 2018



- Rayleigh-Taylor Instability  
( $Kn = 2 \times 10^{-4}$ )

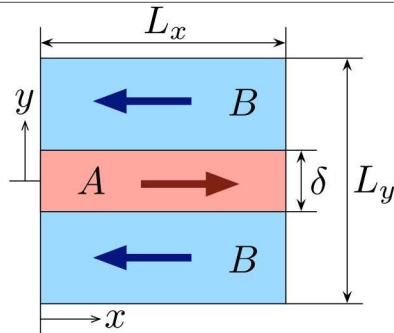
Gallis et al., *Physical Review Fluids*, 2016



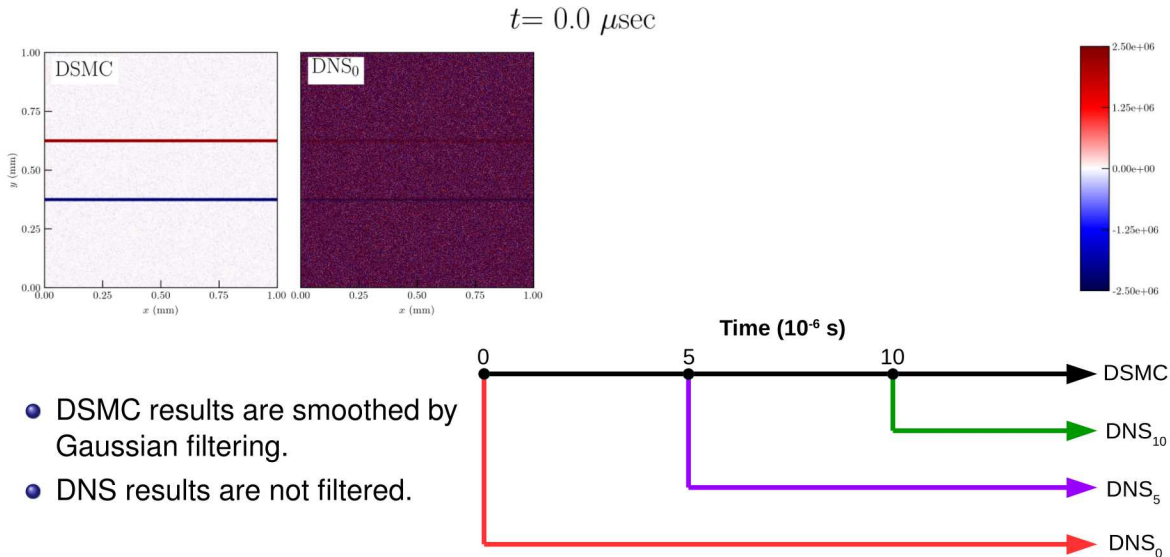
# Simulation setup

- $O_2$  gases
- 2 Dimensional, Periodic BCs
- $P = 1\text{atm}$
- $U_A = -U_B = 50\text{m/s}$
- Convective  $Ma = U_A/C \approx 0.15$
- $L_x = L_y = 1\text{ mm}$ ,  $\delta/L_y = 0.25$
- $Kn = \lambda/\delta = 2.4 \times 10^{-4}$
- DSMC - SPARTA
  - ▶ 100 particle/cell,  $\Delta t = 100\text{ ps}$
  - ▶ No. of Cells =  $20000 \times 20000$
- DNS - 2D Incompressible
  - ▶ No. of grids =  $2000 \times 2000$ ,  $\Delta t = 1\text{ ns}$

Method	$T_A^{\text{trans}} = T_A^{\text{rot}} = T_B^{\text{trans}} = T_B^{\text{rot}}$	$T_A^{\text{vib}}$	$T_B^{\text{vib}}$
DNS	300K	300K	300K
DSMC (Eq)	300K	300K	300K
DSMC (Non-Eq)	300K	<b>1800K</b>	300K

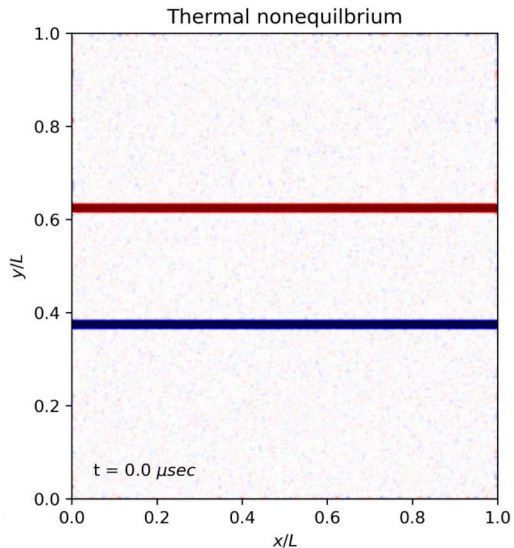
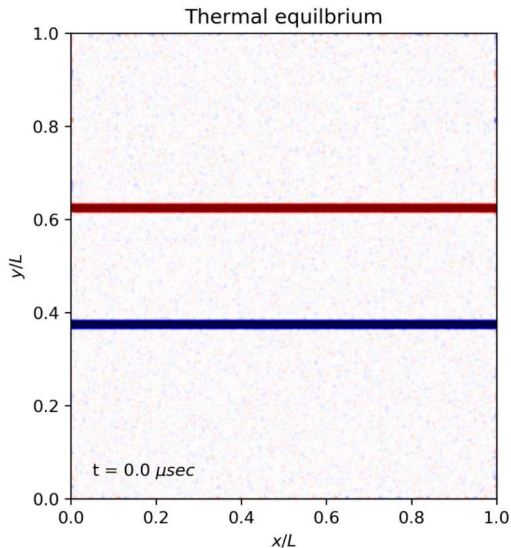


# DSMC vs DNS - Vorticity evolution



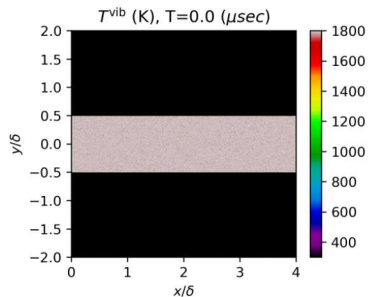
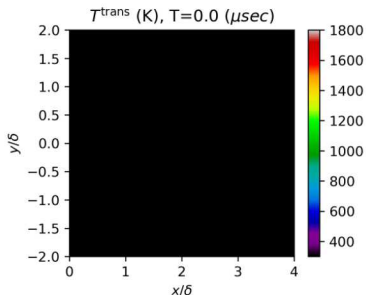
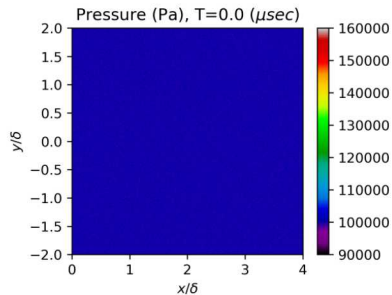


# Vorticity evolution, DSMC

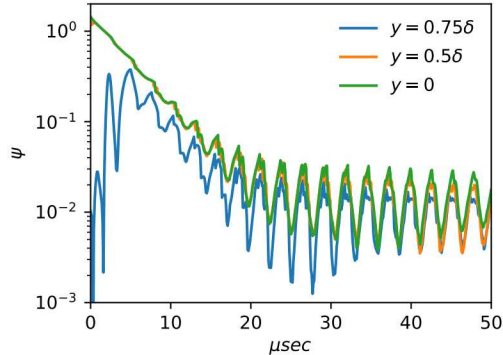
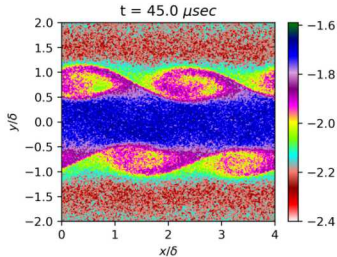
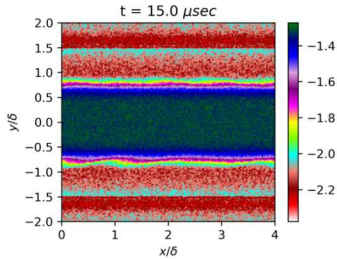


# Pressure and temperatures, SEIZURE ALERT!!

- Nonequilibrium case



# Reaching equilibrium



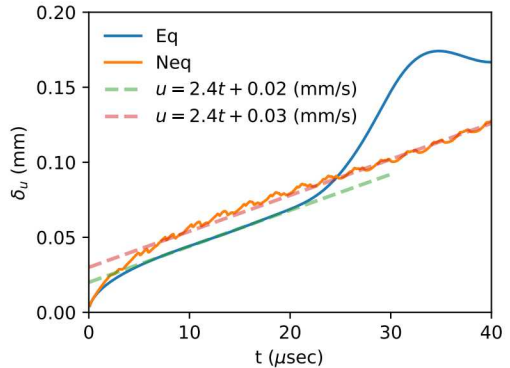
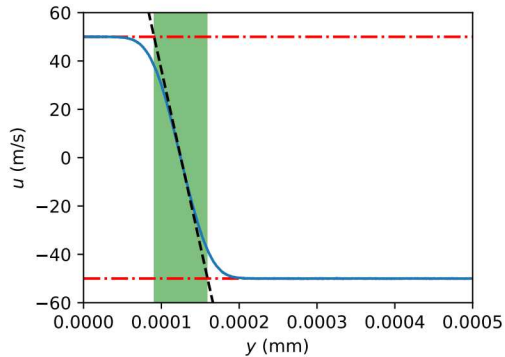
Speed of sound  
 $V_{\text{O}_2, \text{s}} \approx 330 \text{ms}^{-1}$   
 (300K, 1 atm)

$$f = V_{\text{O}_2, \text{s}} / L_y$$

$$\approx 3.3 \times 10^5 \text{s}^{-1}$$

$$\psi = \frac{|T_y^{\text{vib}} - T_y^{\text{trans}}|}{(T_y^{\text{vib}} + T_y^{\text{trans}})/2}, \quad T_y = \frac{\int \rho T \, dx}{\int \rho \, dx}$$

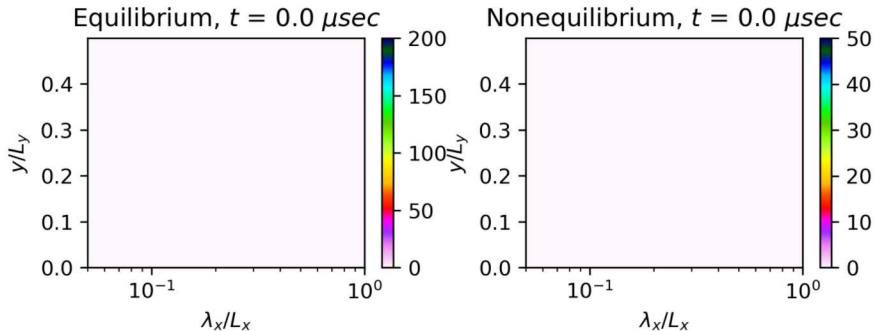
# Growth Rate, vorticity thickness



$$\delta_u \equiv \frac{1}{(\int |\omega| dx)_{\max}} \iint |\omega| dx dy$$

# Turbulent kinetic energy spectra

$$\begin{aligned} & \frac{1}{2} \langle \rho u_i'' u_i'' \rangle_x(y) \\ &= \int E(k_x, y) \, dk_x \\ &\approx \int k_x E(k_x, y) \, d \log k_x \end{aligned}$$



## With thermal nonequilibrium

- Growth of shear layer is delayed
- Instability initiates in larger-scale motions

## Conclusion

- K-H instability simulation with DSMC and DNS
- Equilibrium process  $\rightarrow$  Acoustic wave

## Discussion and future work

- Adding chemical reaction
- 3D flow?
- Interaction with shock

Thank you!!  
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