Kelvin-Helmholtz instability with thermal r

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Sandia National Laboratories

DSMC 2019

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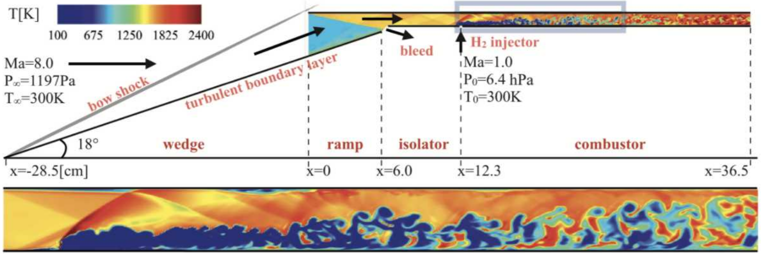
- Thanks to Stan Moore and Steven Plimpton

Combustion process in extreme conditions

(Source: NASA)

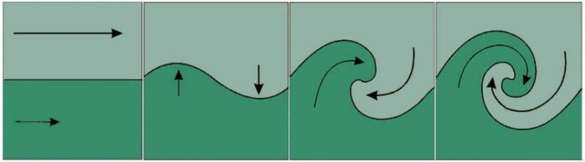


Fiévet et al., *Proc. Combustion Institute*, 2017

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

Kelvin-Helmholtz instability

(Source: Washingtonpost.com)



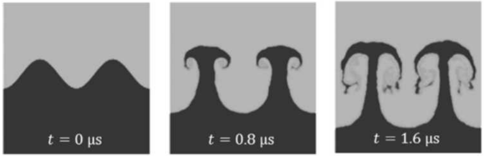
Philippi et al., *CILAMCE*, 2015

In this presentation

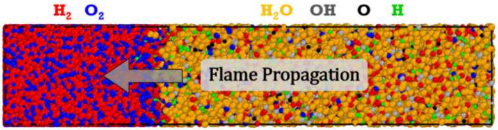
What is the effect of thermal nonequilibrium on Kelvin-Helmholtz instability?

DSMC at low Kn flows

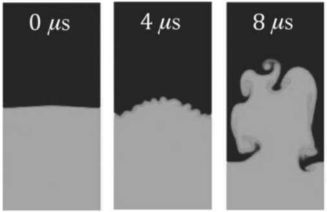
- Richtmyer-Meshkov Instability
  Gallis et al., *Physics of Fluids*, 2015



- 1D flame propagation
  Sebastião et al, *Combustion and Flame*, 2018



- Rayleigh-Taylor Instability
  Gallis et al., *Physical Review Fluids*, 2016

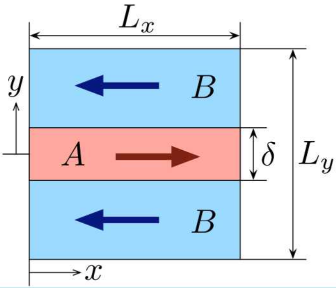


Simulation setup

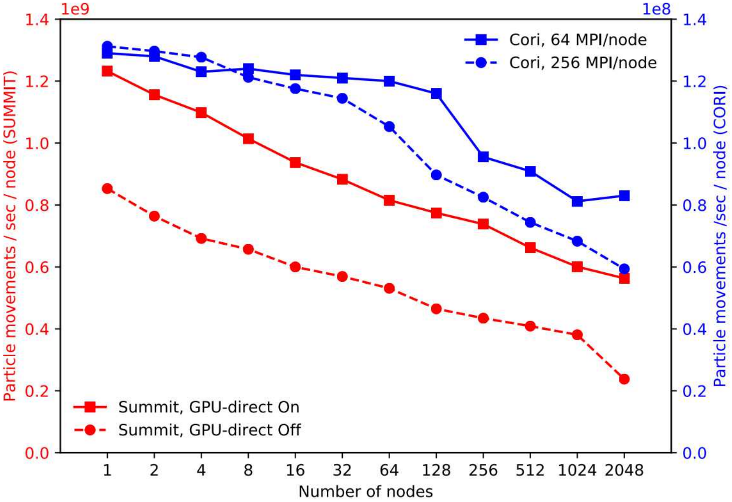
- DSMC with SPARTA
- 2 Dimensional
- Periodic BCs
- $U_A = -U_B$
- $L_x = L_y = 1$ mm, $\Delta t = 100$ ps
- VSS model
- 100 particle/cell
- No. of Cells (Simulation) $= 20000 \times 20000$
- No. of Cells (I/O) $= 2000 \times 2000$

- Simulation cases and initial conditions

Case	A	B	$U_A - U_B$ (m/s)	T_A^{trans} (K)	T_A^{rot} (K)	T_A^{vib} (K)	T_B^{trans} (K)	T_B^{rot} (K)	T_B^{vib} (K)	δ/L_y
I	O_2	O_2	100	300	300	300	300	300	300	0.25
II	O_2	O_2	100	300	300	1800	300	300	300	0.25
III	N_2	O_2	100	1500	1500	1500	300	300	300	0.25

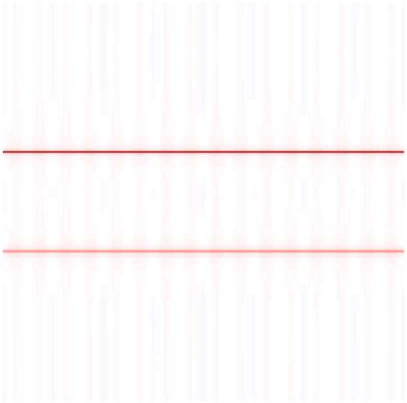


SPARTA Performance - Weak scale

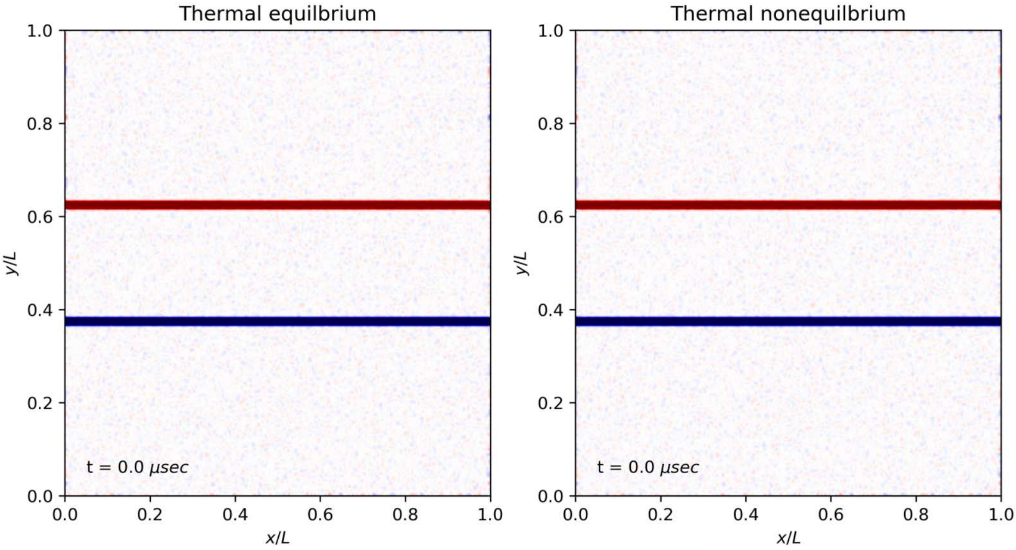


- Kokkos
- Cori, NERSC
  - Intel Xeon Phi Processor 7250
  - 68 core/node
  - 28M particle/node
  - 262144 cell/node
- Summit, OLCF, ORNL
  - Nvidia V100 GPU
  - 6 gpu/node
  - 57M particle/node
  - 442368 cell/node

Vorticity evolution - Direct Numerical Simulation



Vorticity evolution, DSMC



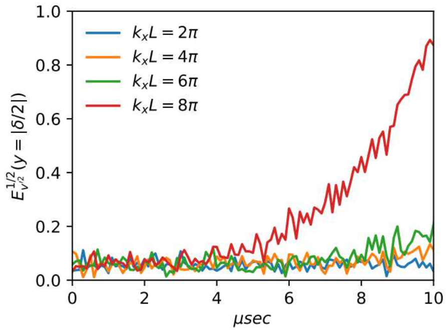
Growth Rate, Perturbation at shear boundaries

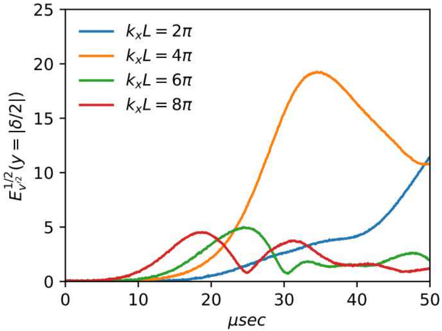
- Stability theory

$$v = V_o(y)\exp(-\mathbf{i}k_x x + st)$$

where k_x is wavenumber and $s = |k_x(U_A - U_B)|$

- Thermal equilibrium case





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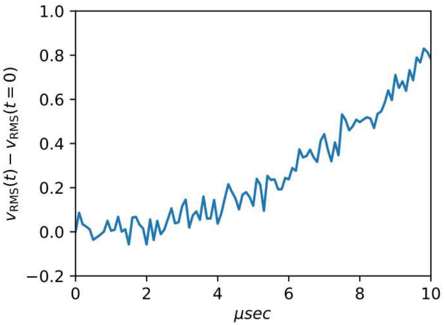
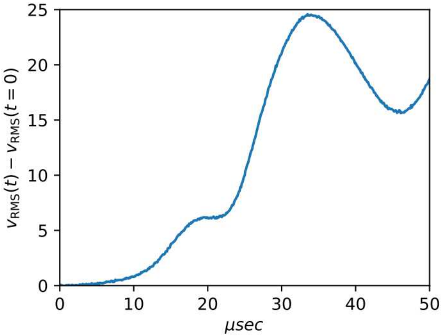
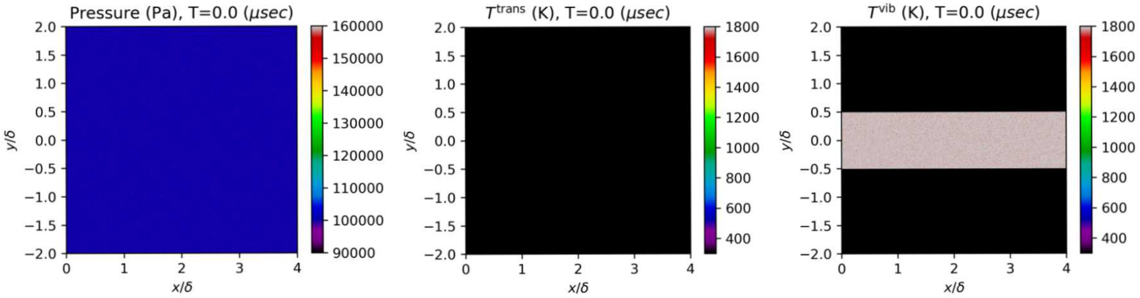


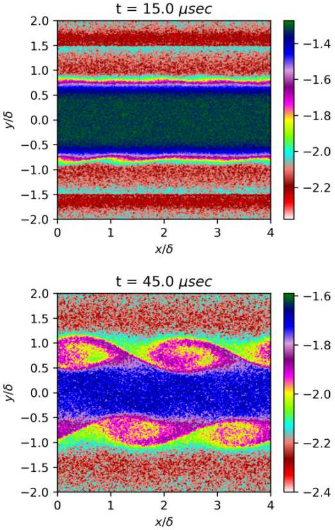


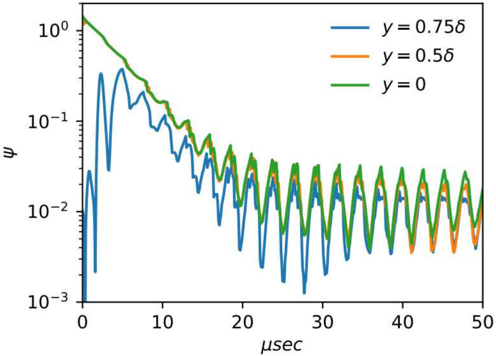
Pressure and temperatures, SEIZURE ALERT!!

- Nonequilibrium case



Reaching equilibrium





Speed of sound

$V_{O_2,s} \approx 330 ms^{-1}$

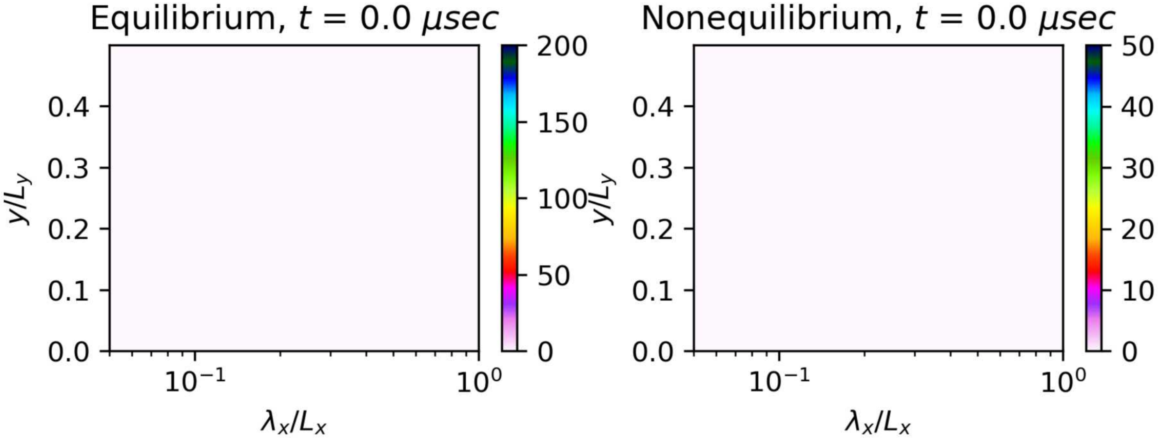
$(300K,\ 1\ atm)$

$$f = V_{O_2,s}/Ly$$
$$\approx 3.3 \times 10^5 s^{-1}$$

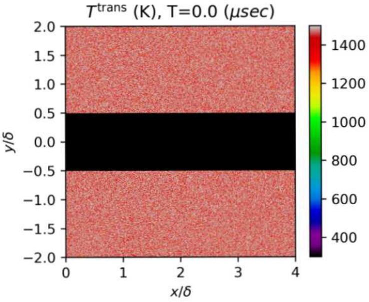
$$\psi = \frac{|T_y^{\text{vib}} - T_y^{\text{trans}}|}{(T_y^{\text{vib}} + T_y^{\text{trans}})/2}, \quad T_y = \frac{\int \rho T \,\mathrm{d}x}{\int \rho \,\mathrm{d}x}$$

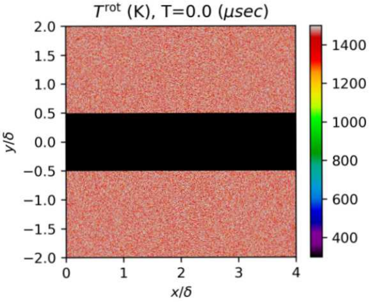
Turbulent kinetic energy spectra

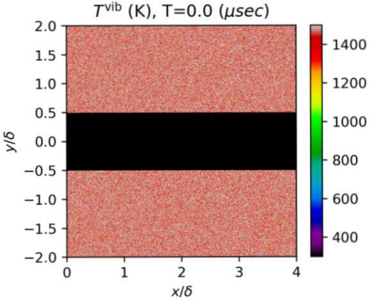
$$\frac{1}{2}\langle \rho u_i'' u_i'' \rangle_x(y) = \int E(k_x, y)\, \mathrm{d}k_x \approx \int k_x E(k_x, y)\, \mathrm{d}\log k_x$$



N_2 (1500K) and O_2 (300K)







Conclusion

- K-H instability simulation with DSMC
- Equilibrium process $\rightarrow$ Acoustic wave
- Traveling acoustic wave $\rightarrow$ Slow growth of K-H roll-ups

Discussion and future work

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

Thank you!!
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