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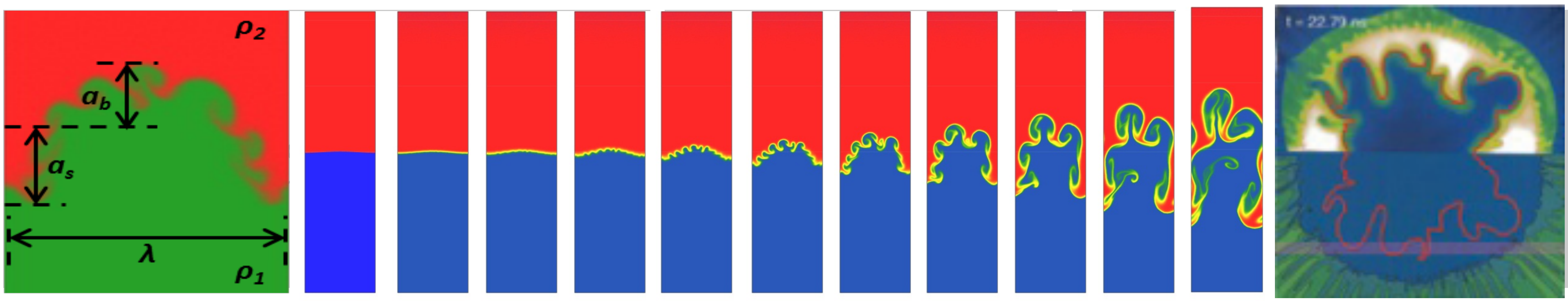

DSMC Investigation of Hydrodynamic Instabilities in Gases

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30th Rarefied Gas Dynamics Symposium
University of Victoria, Victoria B.C., Canada
July 10-15, 2016

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Instabilities: When do they occur?

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Clark et al. 2013

Infinitesimal disturbances amplify spontaneously and ultimately dominate the flows.

The growth of the instability is influenced by viscosity, compressibility, three-dimensionality, density ratio.

It is postulated that the failure to achieve ignition at NIF can be attributed to the **Rayleigh-Taylor instability (RTI).**

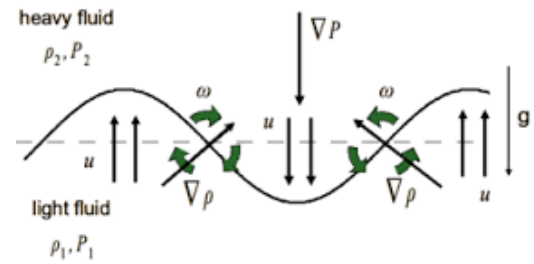
RTI can produce the Kelvin-Helmholtz instability (KHI) and has the Richtmyer-Meshkov instability (RMI) as a limiting case.

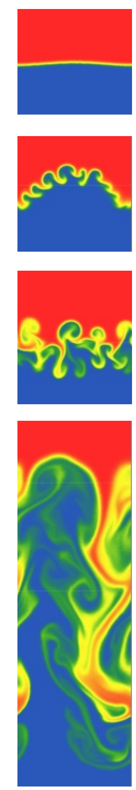
Applications range from Inertial Confinement Fusion (ICF, mm) to the formation of supernova remnants (light-years).

Molecular methods like DSMC are becoming increasingly popular for investigating the effects of viscosity and diffusivity in ICF applications, which are known as “kinetic” or “ion-kinetic” effects. (Larroche *et al.* 2016)

Rayleigh-Taylor Instability (RTI)

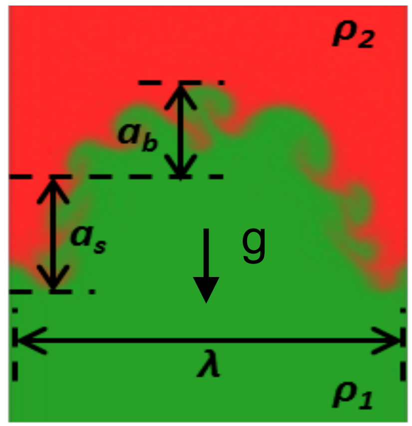
- RTI is an instability of an interface between two fluids of different densities which occurs when the lighter fluid is pushing the heavier fluid.
- Baroclinic torque at the interface creates vorticity and induces a velocity field that increases the amplitude, which in turn increases the baroclinic torque.
- RTI has four main stages:
    - Linear (linear growth of initial perturbations)
    - Nonlinear (mushroom-like structures appear)
    - Structures interact and compete (as in RMI, KHI)
    - Turbulent mixing





Characteristic & Nondimensional Quantities

Initial Interface



Bubble

Spike

$$a = a_b + a_s$$

Amplitude

$$A = \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1}$$

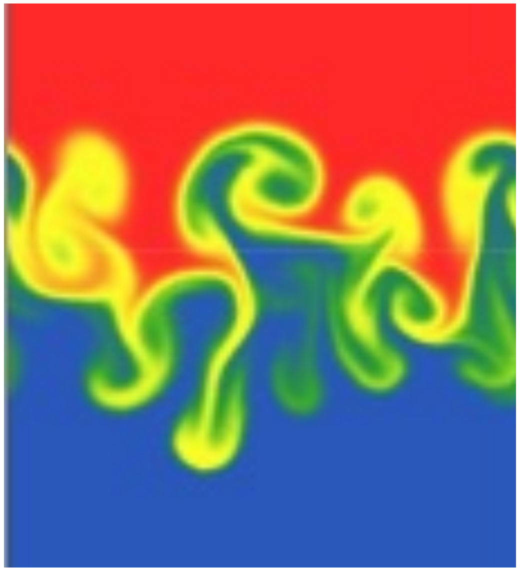
Atwood Number

$$\mathrm{Re}_p = \frac{\lambda \sqrt{\frac{A}{1+A} g \lambda}}{\nu}$$

Reynolds Number
(Wei & Livescu 2012)

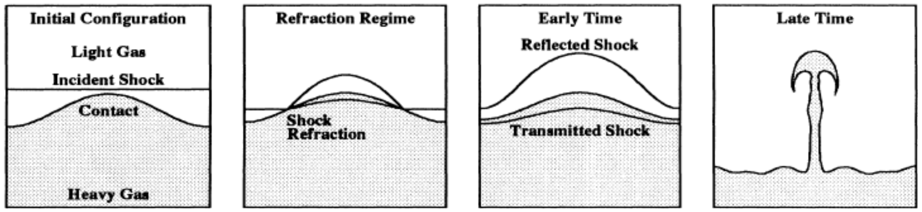
Most Unstable Wavelength

- The initial growth rates of small-amplitude perturbations are influenced by the fluid properties.
- Viscosity and diffusivity inhibit small-wavelength perturbations from growing, allowing a particular wavelength, the **most unstable wavelength**, to emerge, **outpacing** the growth of all other wavelengths:



$$\lambda_m \approx 4\pi(v^2 / Ag)^{1/3}$$

RTI Is Related to RMI



Grove et al., Phys. Rev. Lett., 71 (21), 3473 (1993).

Shock propagation

- Incident shock travels down in upper gas
- Transmitted shock travels down in lower gas
- Reflected shock travels upward in upper gas

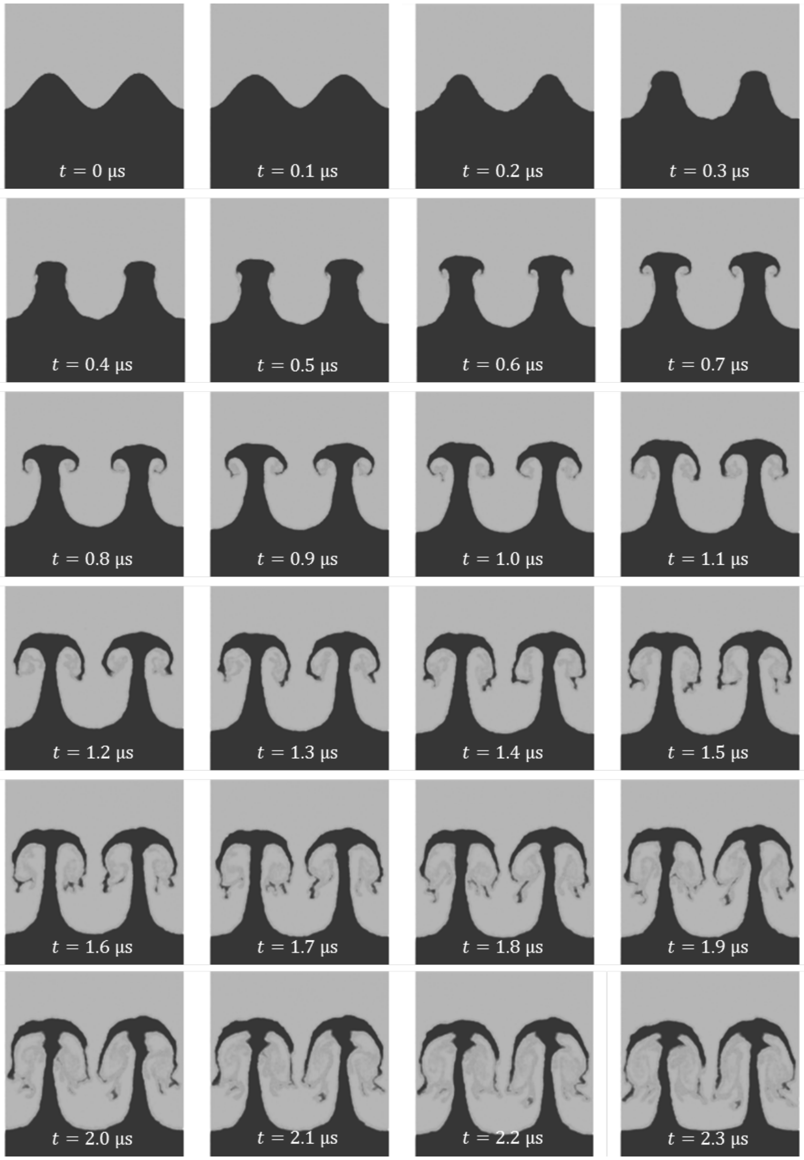
Interface motion

- Interface is accelerated to constant velocity
  - Travels in same direction as shock
- Vorticity generated baroclinically at interface
  - Density & pressure gradients misaligned

Perturbation growth

- Initially, amplitude growth is linear with time
- Later, amplitude growth becomes nonlinear
  - When amplitude is similar to wavelength
- Bubbles, spikes, roll-up, more instabilities

Gallis et al. Physics of Fluids (2015)

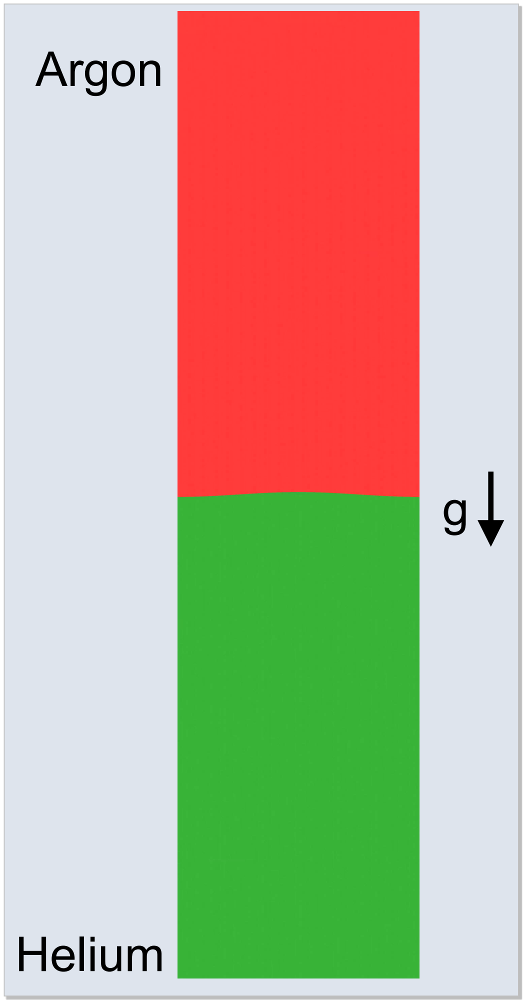


Why DSMC for Rayleigh-Taylor Instability?

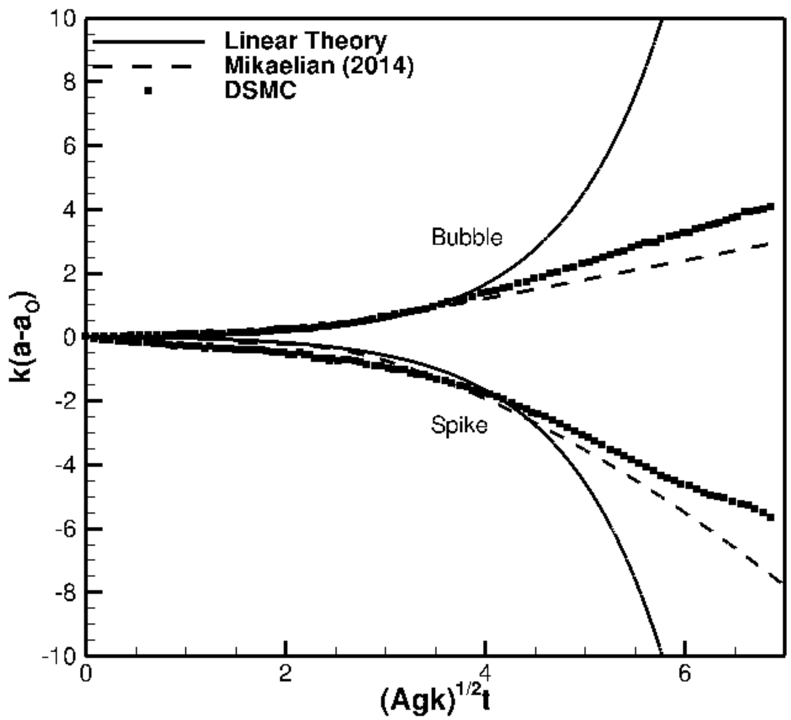
- DSMC provides a molecular-level description of the hydrodynamic processes that may be physically more realistic for **large accelerations and chemically reacting flows and the representation of naturally occurring thermal fluctuations**
- DSMC inherently accounts for transport properties
- The DSMC method offers the potential to identify the impact of molecular level effects (e.g., rotational and vibrational energy exchange, gas-phase chemical reactions, and gas-surface interactions) on hydrodynamic instabilities.
- Typical 2D DSMC simulation characteristics:
  - Physical Domain: 1 mm x 4 mm (ICF-pellet-size domain)
  - # Cells: 4 billion
  - # Particles: 400 billion
  - # Cores: ¼-½ million
  - Run time: 30 hrs (= 900, 1800 CPU years)
  - Time steps: 200,000 × 0.1 ns = 20 μs

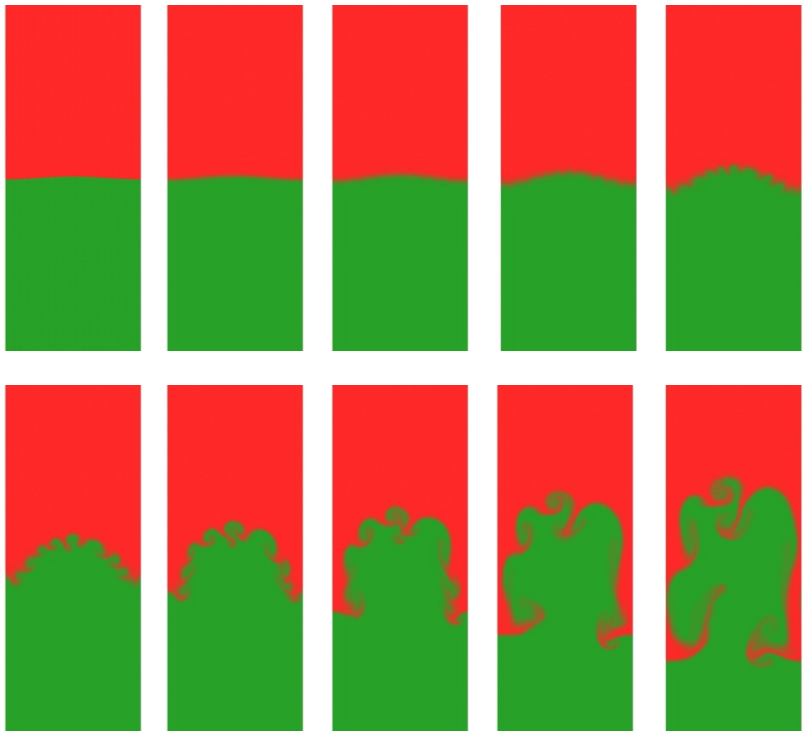
DSMC Simulations of the Rayleigh-Taylor Instability in Gases

- The interface between argon (red) and helium (green) gases is slightly perturbed: $\lambda = 0.001m,\ a = 10\mu m,\ A = 0.81$
- Initial state hydrostatic equilibrium
- Acceleration of the system excites the RTI
  - Initially, thermal fluctuations and diffusion perturb the interface
  - The initial perturbation amplitude grows exponentially
  - A second growth stage occurs at the most unstable wavelength, which forms "**bubbles**" and "**spikes**"
  - Additional instabilities break up the larger structures, resulting in turbulent mixing of the gases



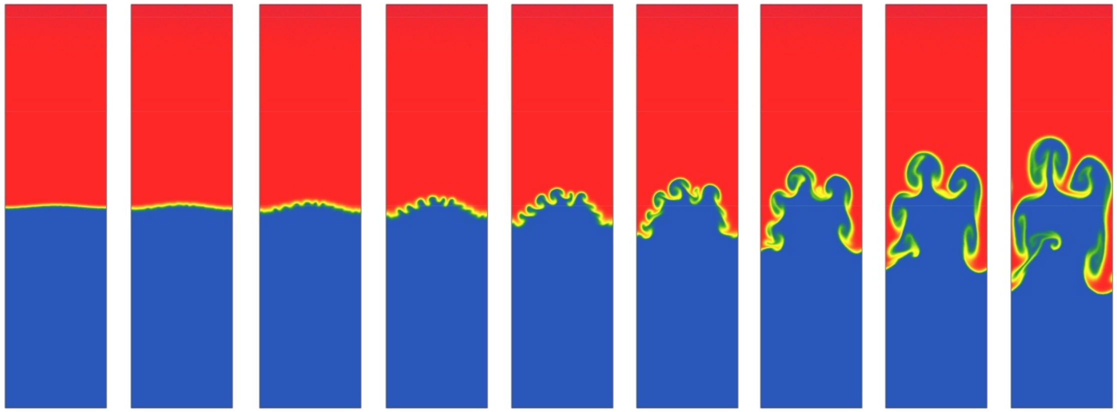
Development of 1-mm Wavelength Perturbation for Gravity 10^8 m/s^2



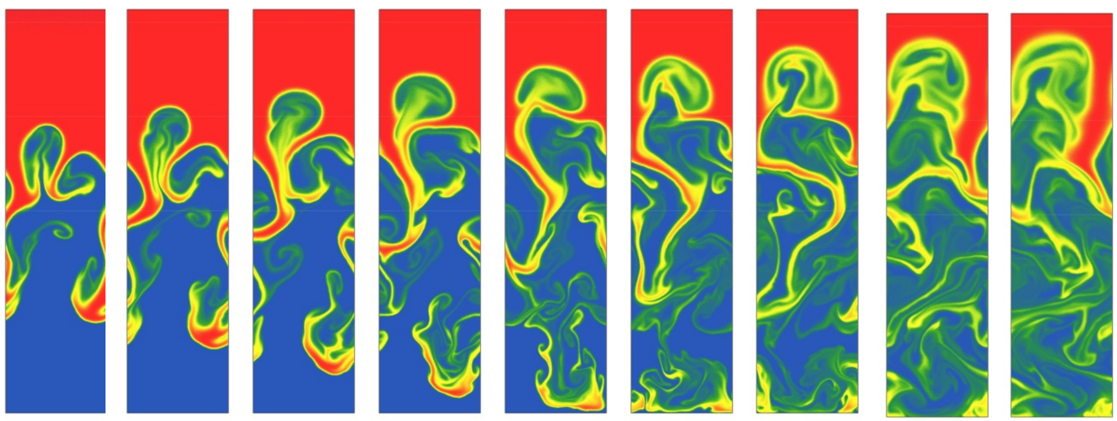


- Initial perturbations of a small wavelength develop and grow exponentially.
- Smaller structures, corresponding to the most unstable wavelength, appear.
  - Their number is independent of the molecular simulation ratio and the random number seed.
- Larger structures emerge as the smaller disturbances interact and combine.

Density Profiles for 1-mm Wavelength Perturbation for Gravity 10^8 m/s^2



Images progress at 10,000 time step increments

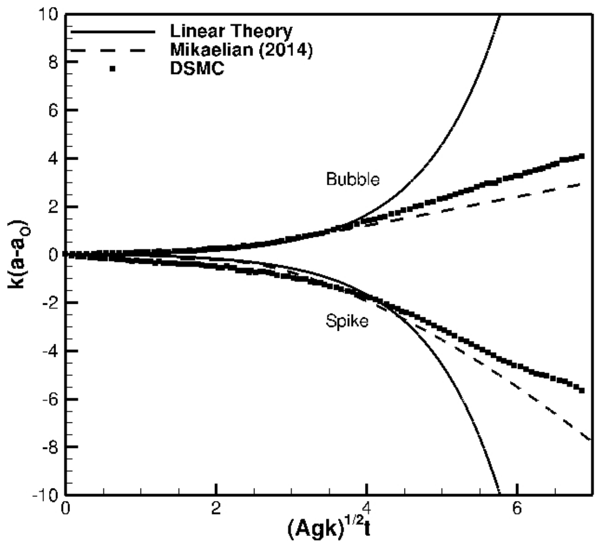


Initially, diffusion thickens the interface. Subsequently, bubbles and spikes appear.

RTI for Ar/He with Different Wavelengths

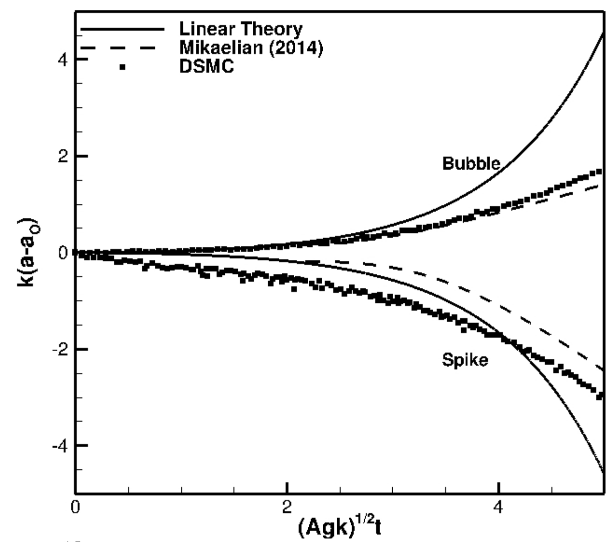
$\lambda = 1\,mm$

$\mathrm{Re}_p = 7500$



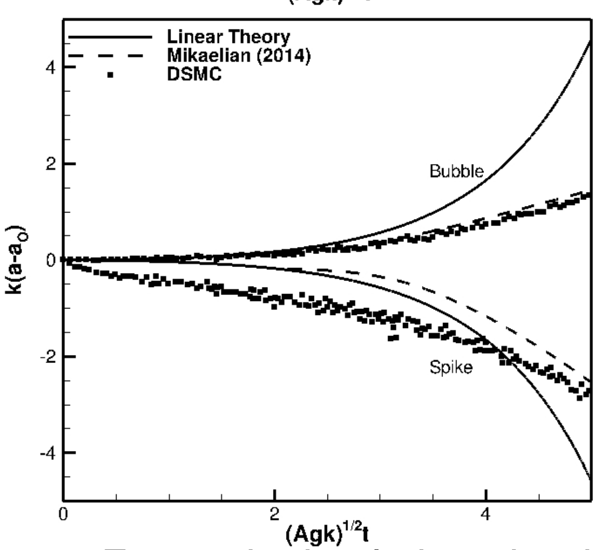
$\lambda = 0.5\,mm$

$\mathrm{Re}_p = 2600$



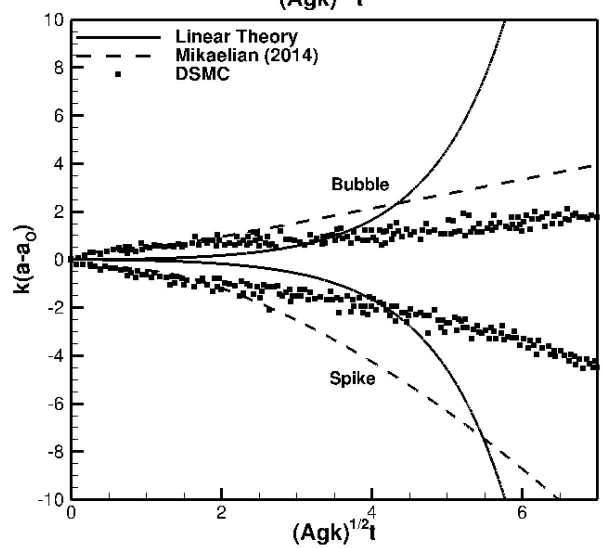
$\lambda = 0.25\,mm$

$\mathrm{Re}_p = 936$



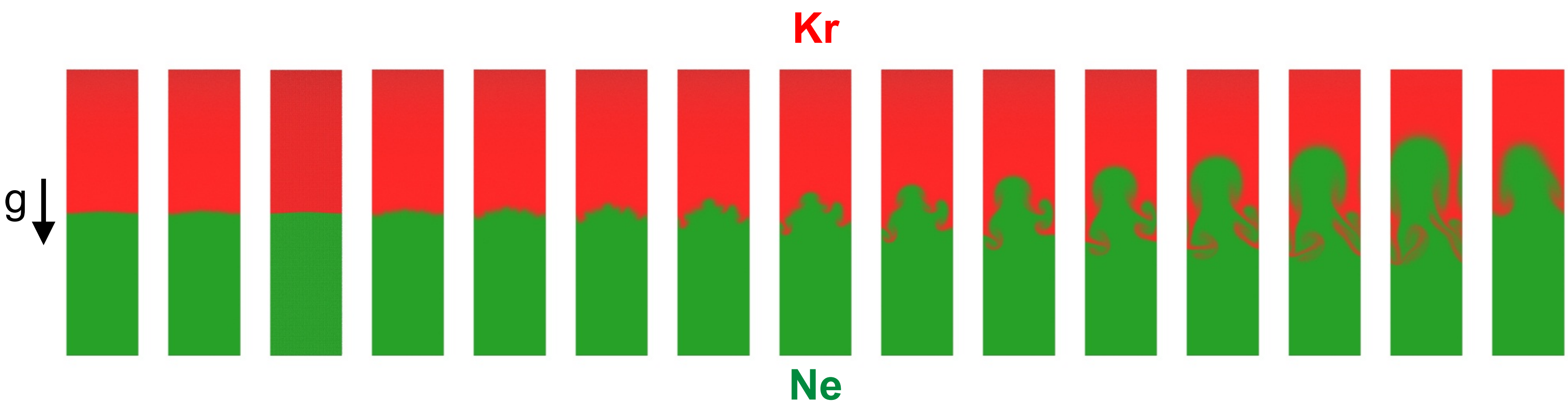
$\lambda = 0.1\,mm$

$\mathrm{Re}_p = 237$

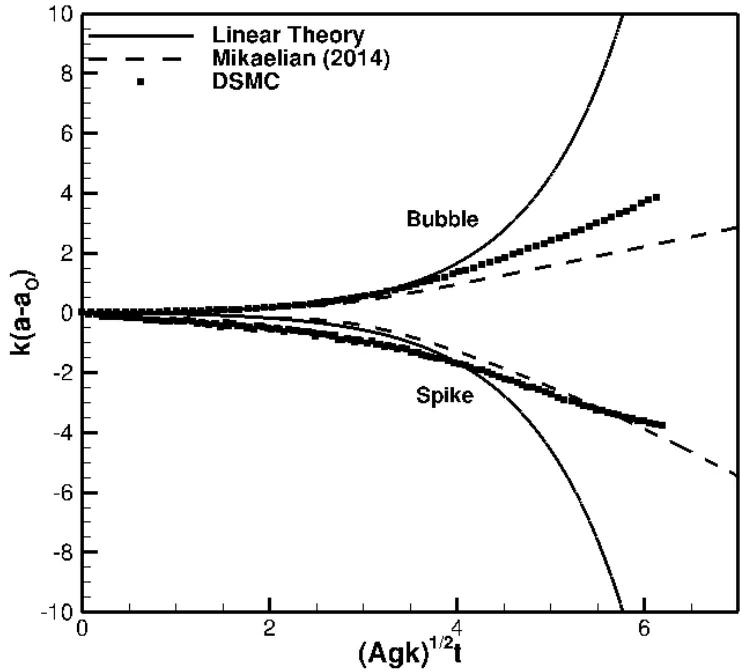


For each simulation, the domain width is one wavelength, and the amplitude is 1% of the wavelength.

DSMC Simulations of the RTI for Kr/Ne

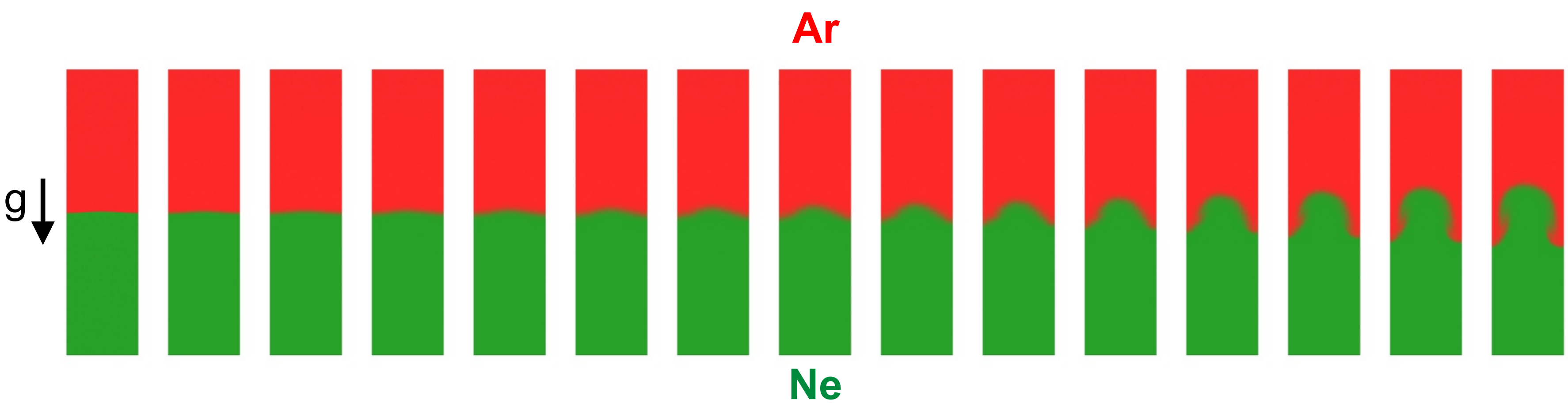


A = 0.61
Gravity = 10^8 m/s^2

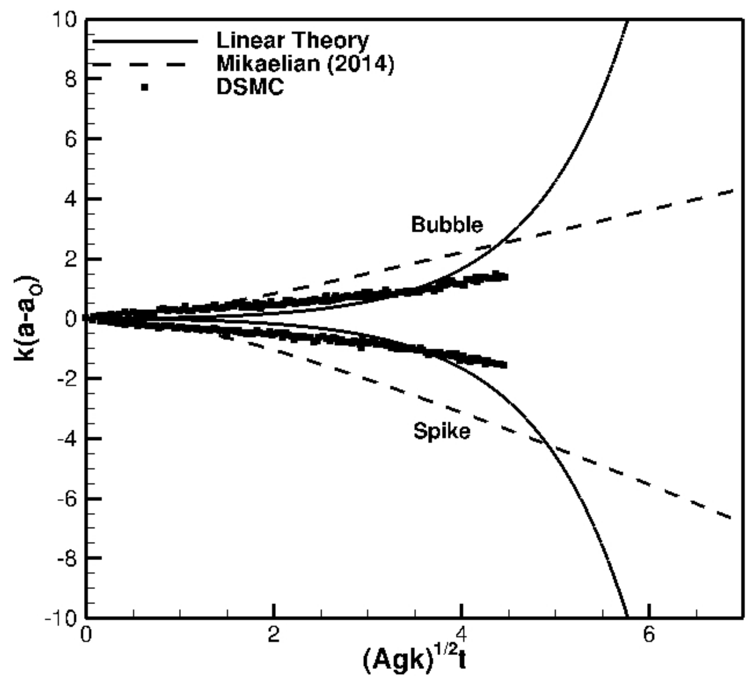


$$Re_p = 12800$$

DSMC Simulations of the RTI for Ar/Ne



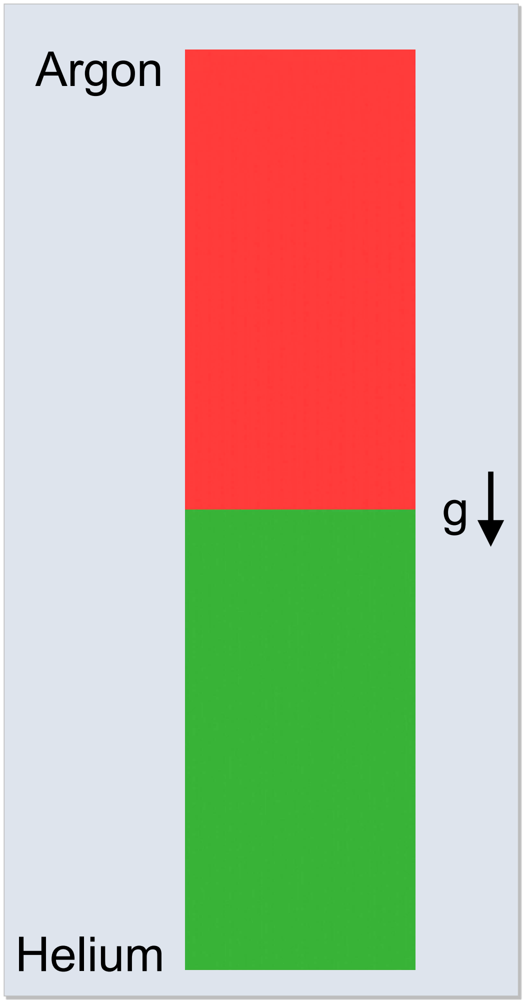
A = 0.32
Gravity = 10^8 m/s^2



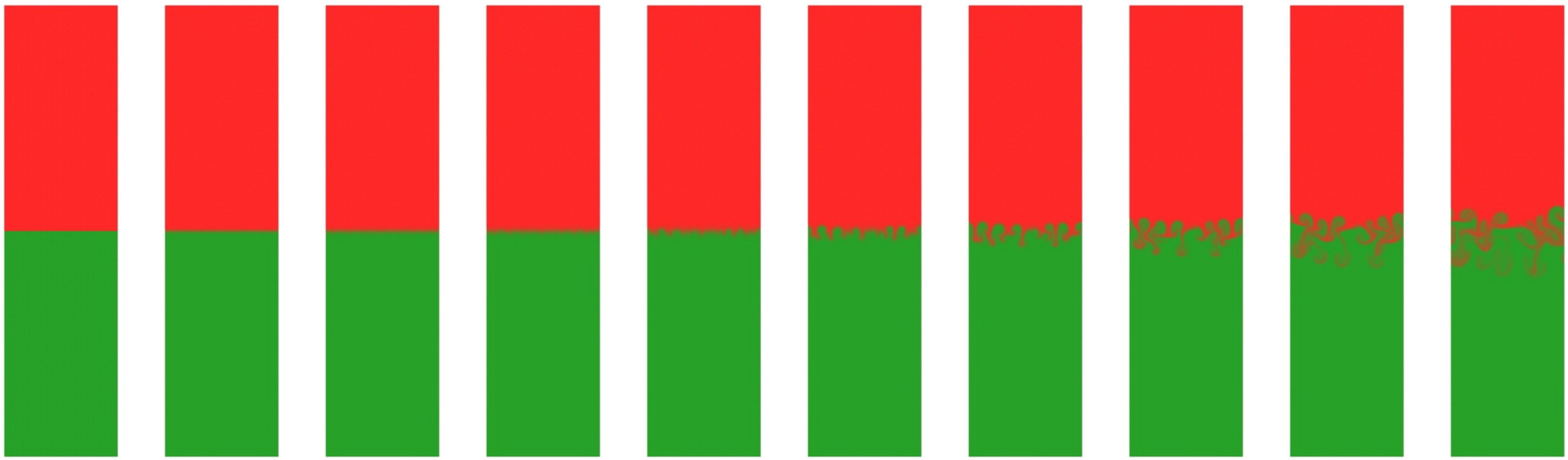
$$Re_p = 6000$$

RTI from an Initially Molecularly Flat Interface

- The interface between argon (red) and helium (green) gases is initially flat
- Acceleration of the system excites the RTI
  - Initially, thermal fluctuations and diffusion perturb the interface
  - The amplitude of thermal fluctuations grows exponentially
  - Gases penetrate each other differently, forming "**bubbles**" and "**spikes**"
  - Finally, additional instabilities break up the larger structures resulting in turbulent and chaotic mixing of the gases



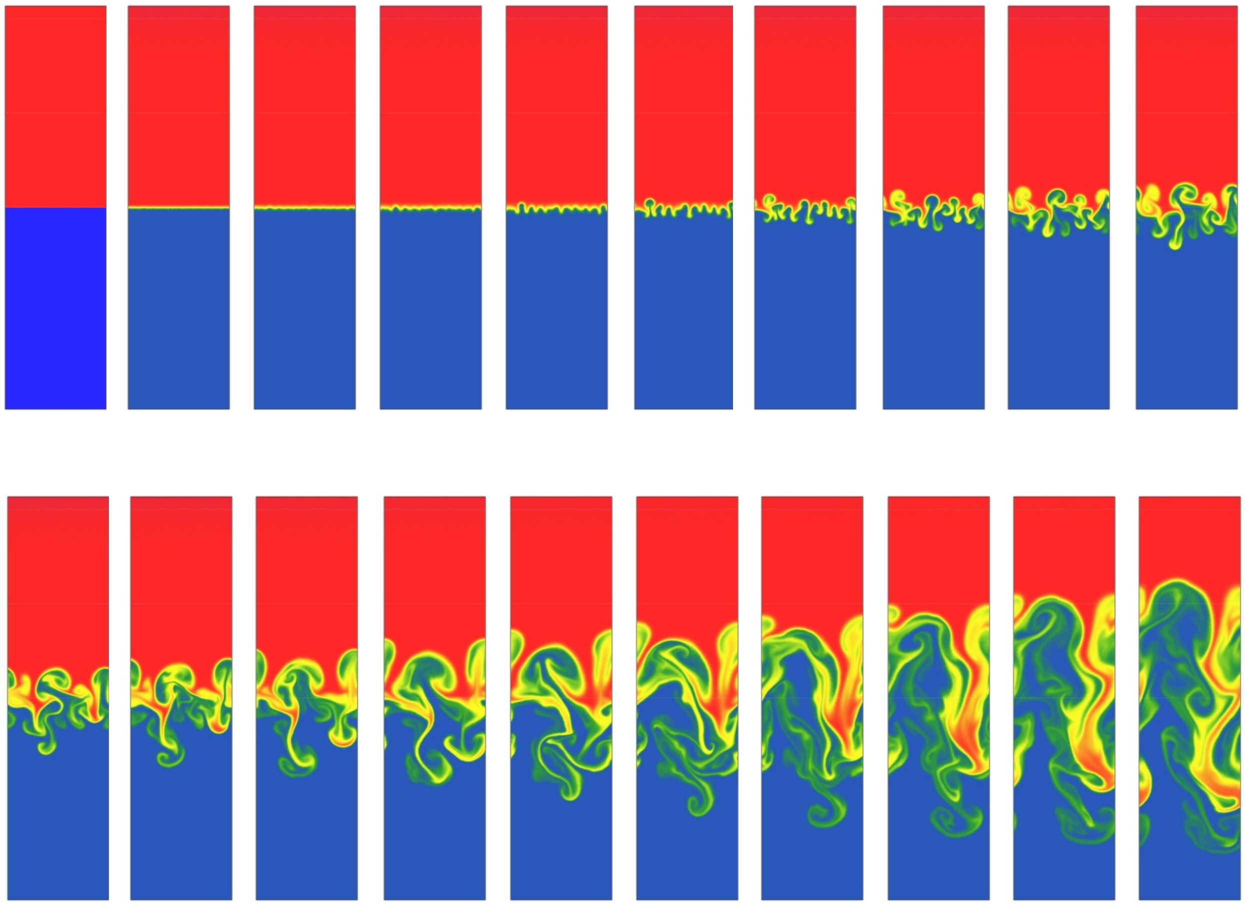
RTI from an Initially Flat Interface



Images progress at 10,000 time step increments

The numbers of bubbles and spikes correspond to the most unstable wavelength.

Density Profiles for an Initially Flat Interface

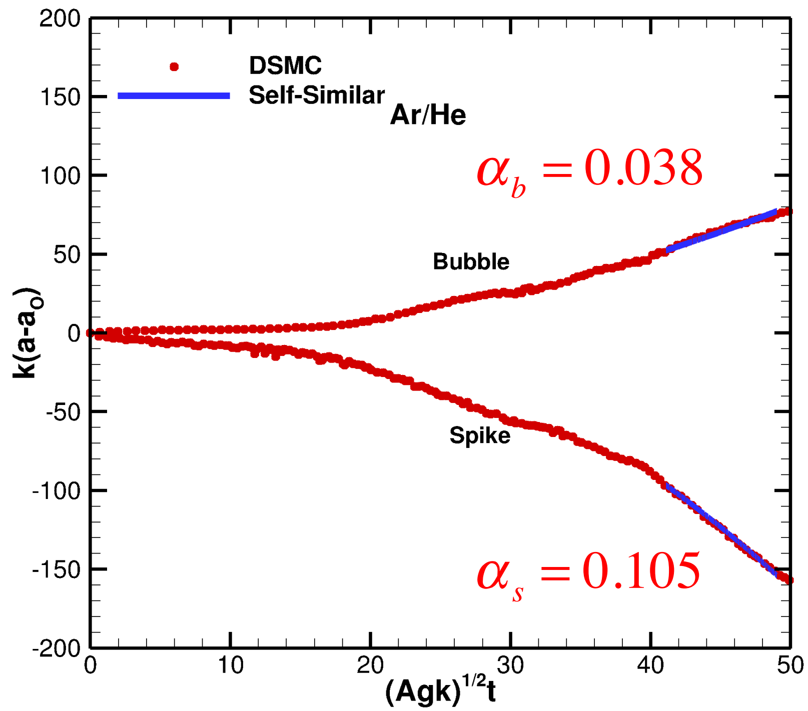


Images progress at 10,000 time step increments

Late-Time Behavior: Self-Similarity

At late times, under certain idealized conditions, the flow can forget its initial conditions and enter a self-similar growth phase (Fermi and von Neumann 1953) described by the following equation:

$$a_{b,s} = \alpha_{b,s} A g t^2$$



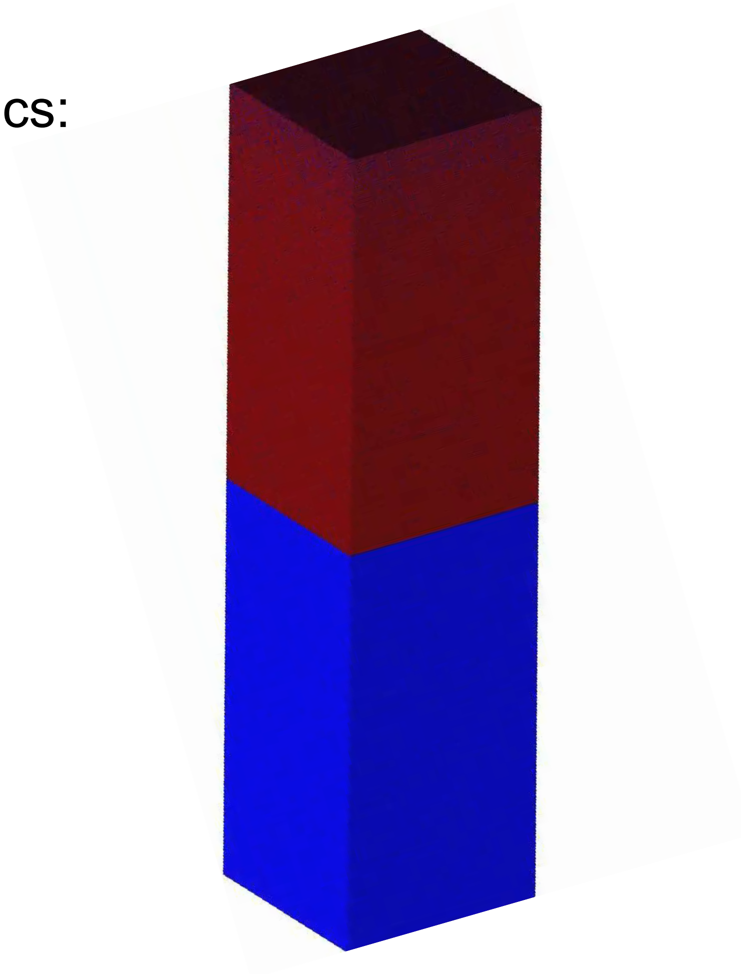
Self-similar behavior is observed for long times.
Waviness is due to competition between bubbles and spikes.

RTI in 3D: Density Profile

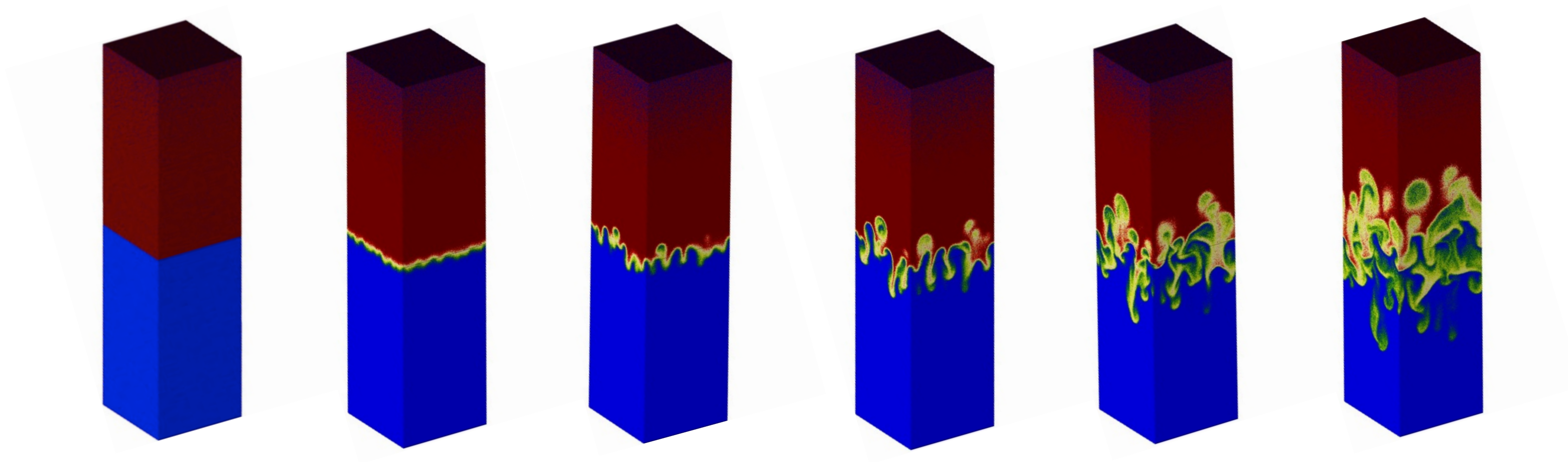
Typical 3D DSMC simulation characteristics:
Physical Domain: 1 mm x 1 mm x 4 mm

Cells: 62.5 billion
Particles: 1.2 trillion
Cores: ½ million

Run time: 90 hrs (5400 CPU years)
Time steps: 200,000 × 0.1 ns = 20 μs



RTI from a Flat Interface in 3D

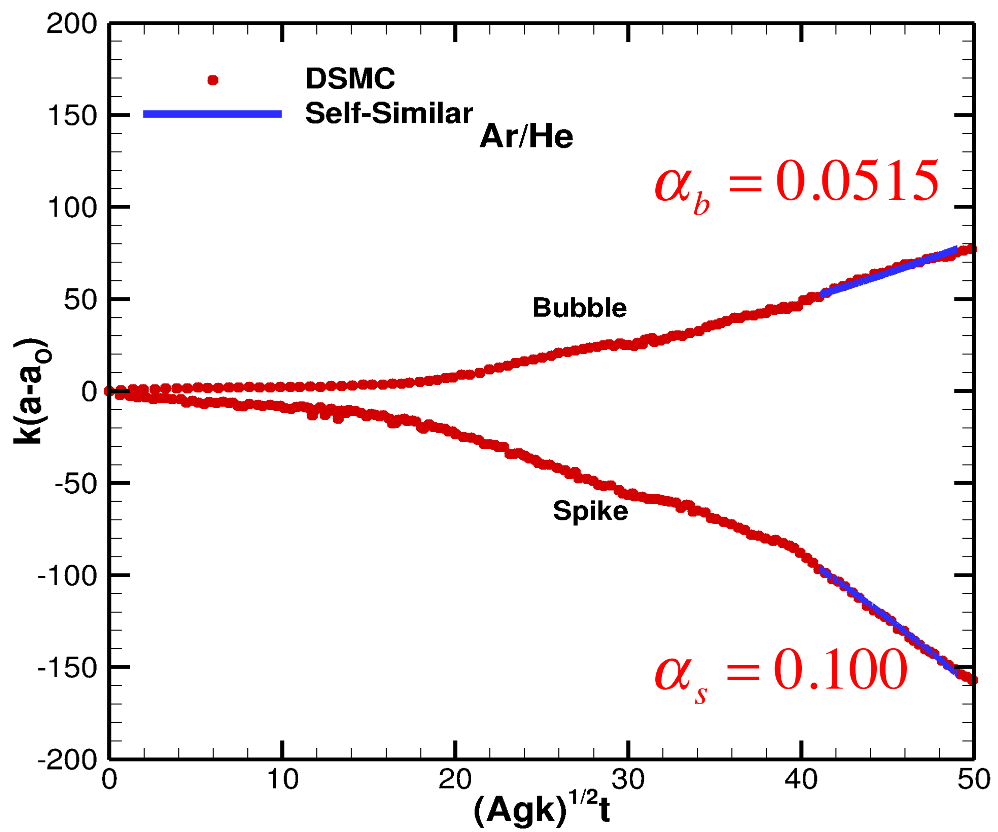


0 4 8 10 12 14

Images progress at **multiples** of 10,000 time step increments

3D Late-Time Behavior: Self-Similarity

Condition for Self-Similarity: $a_{b,s} = \alpha_{b,s} A g t^2$



Self-similar behavior is observed at late times.
Waviness is due to competition between bubbles and spikes

Conclusions

The Direct Simulation Monte Carlo (DSMC) method can simulate the Rayleigh-Taylor and Richtmyer-Meshkov instabilities.

- Structures are like those in other approaches
- Amplitude growth rates are also similar
- The growth rate in the self-similar regime is within experimental observations

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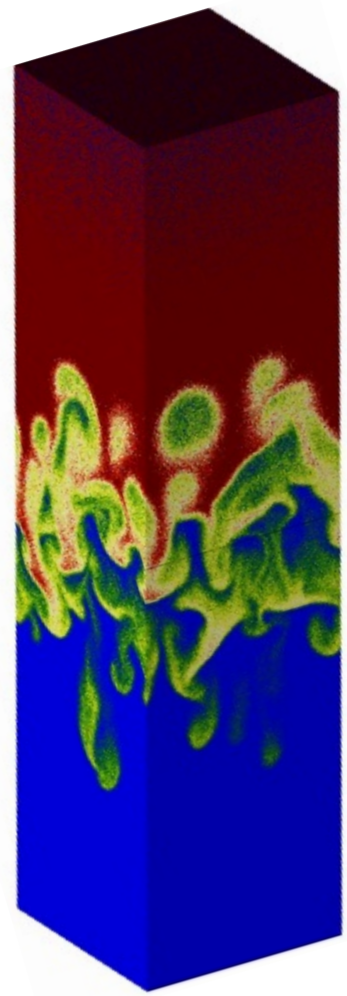
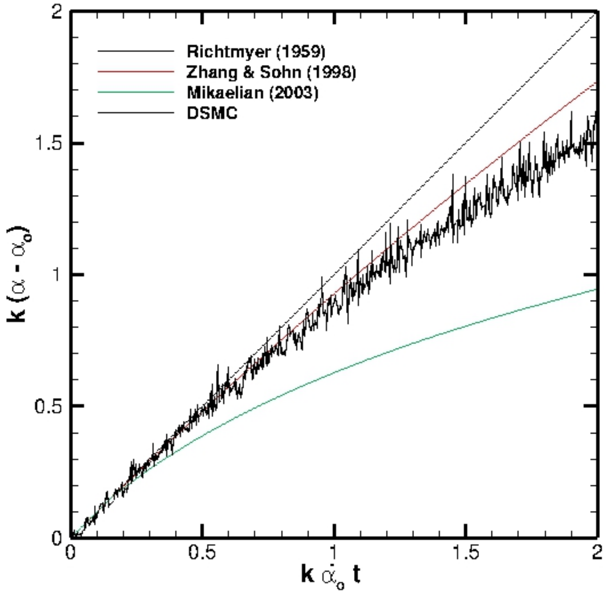
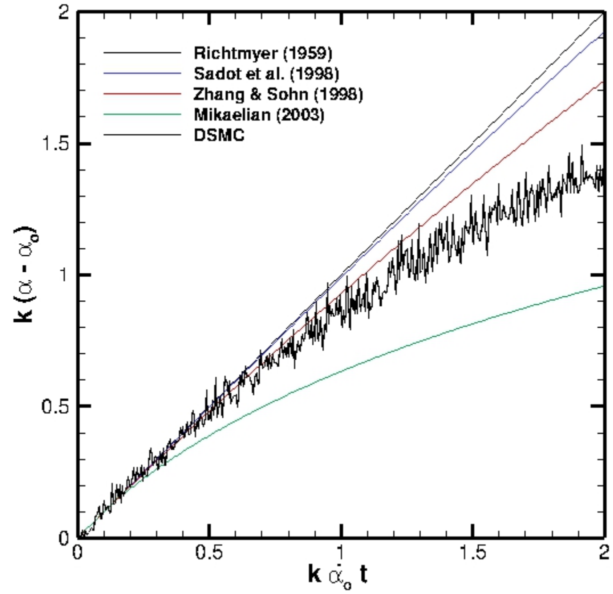


Comparing DSMC to Theoretical Models

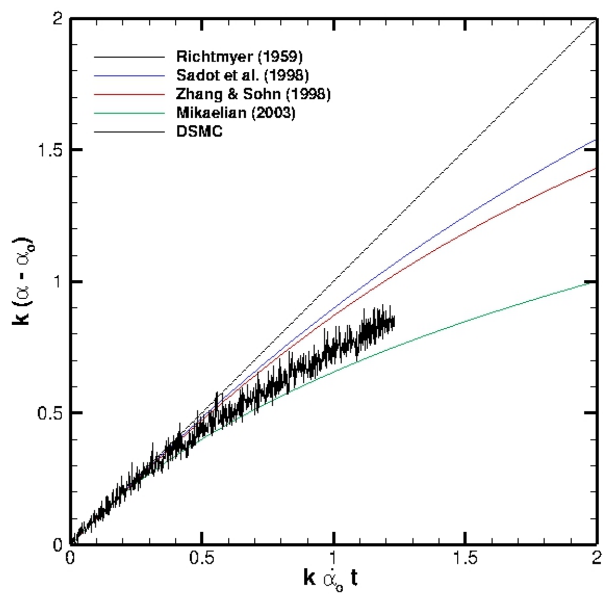
Xe/He
A=0.94



Ar/He
A=0.82



Xe/Ar
A=0.53



Ar/Ne
A=0.33