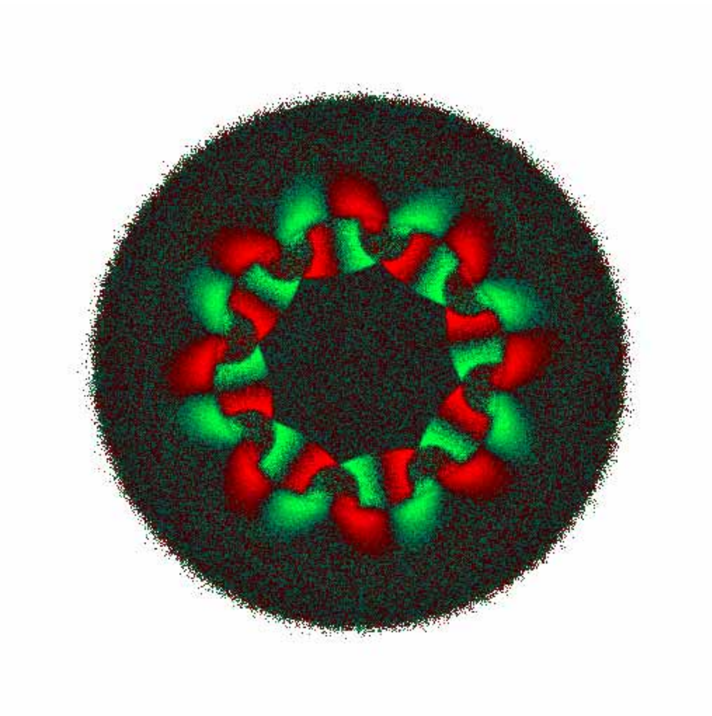
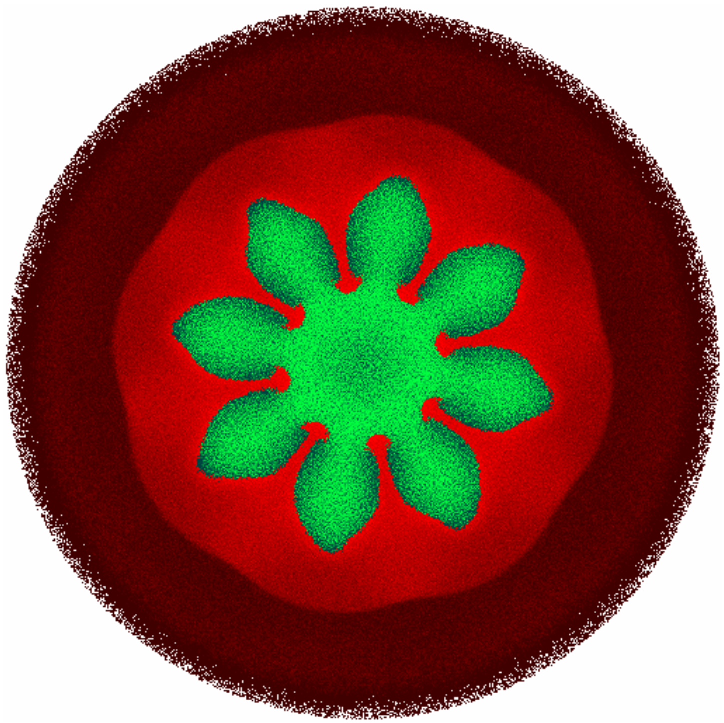
Molecular Dynamics Simulation of Shocks and Richtmyer-Meshkov Instability in Cylindrical Geometry

angular velocity at t = 30



density at t = 100



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18 IWPCTM,
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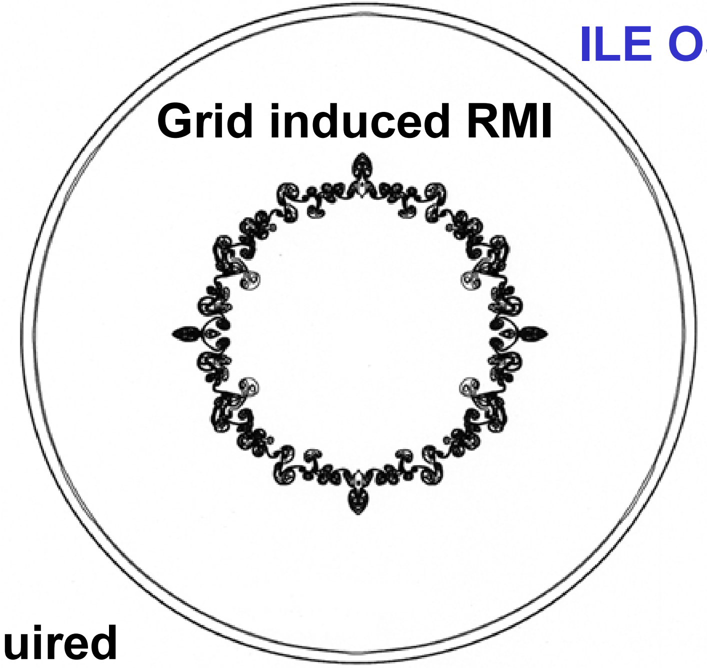
Pasadena, USA

Introduction

Difficulty in hydrodynamic simulation in converging geometry

ILE OSAKA

- Singularity at the center
- Numerical instability and viscosity depend on the grid structure



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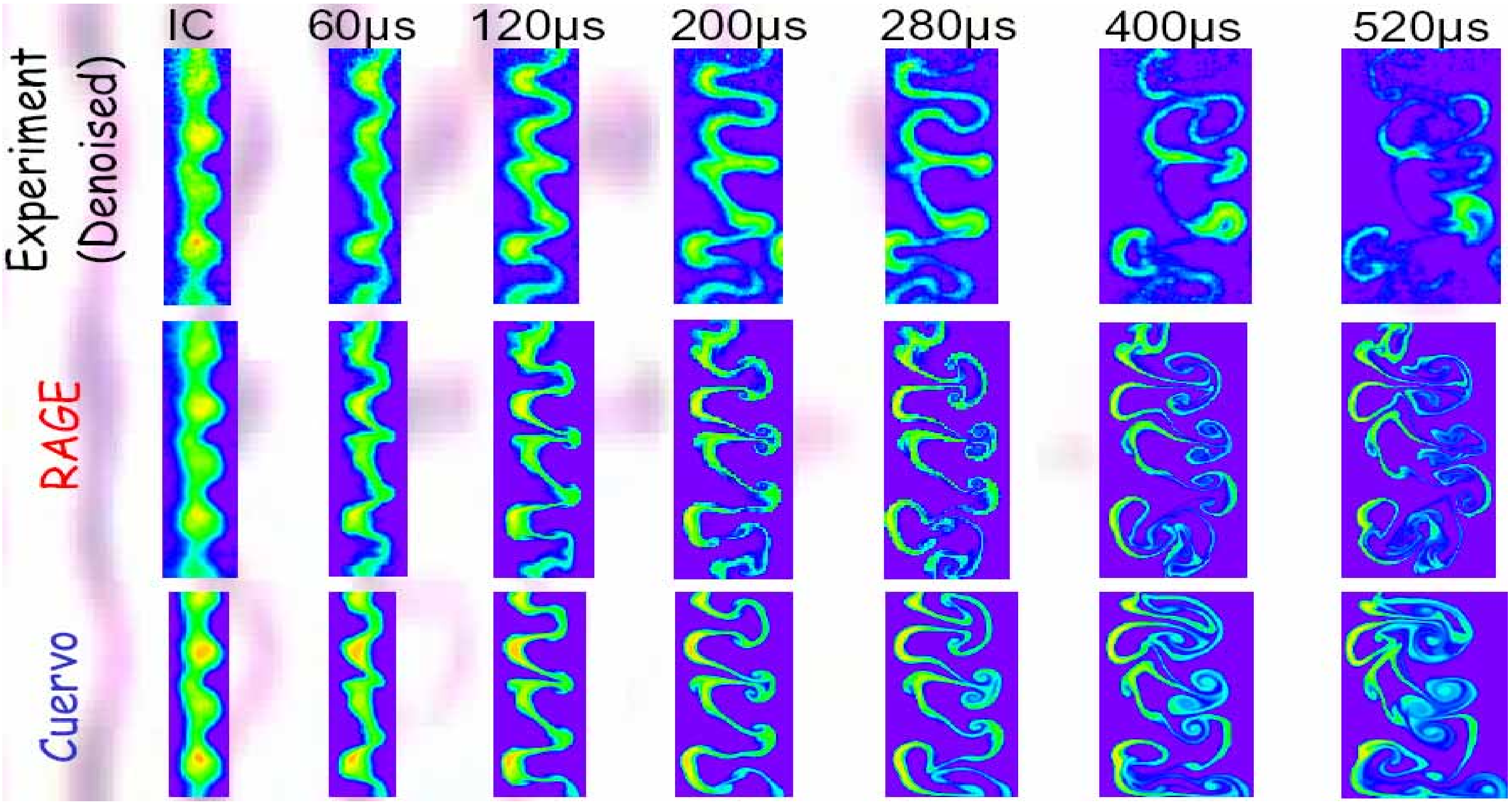
Molecular Dynamic Simulation

Advantage
- spatial mesh and EOS are not required
- non LTE system can be treated
- viscosity, heat conduction are automatically taken into account
- conservation laws are automatically satisfied

Disadvantage
- system size limited by computer power
- limited temperature

Today's hydrodynamic codes looks well but they are still inaccurate

RM gas curtain experiments and simulations



Pictures from W.Rider and J.Kamm, LANL

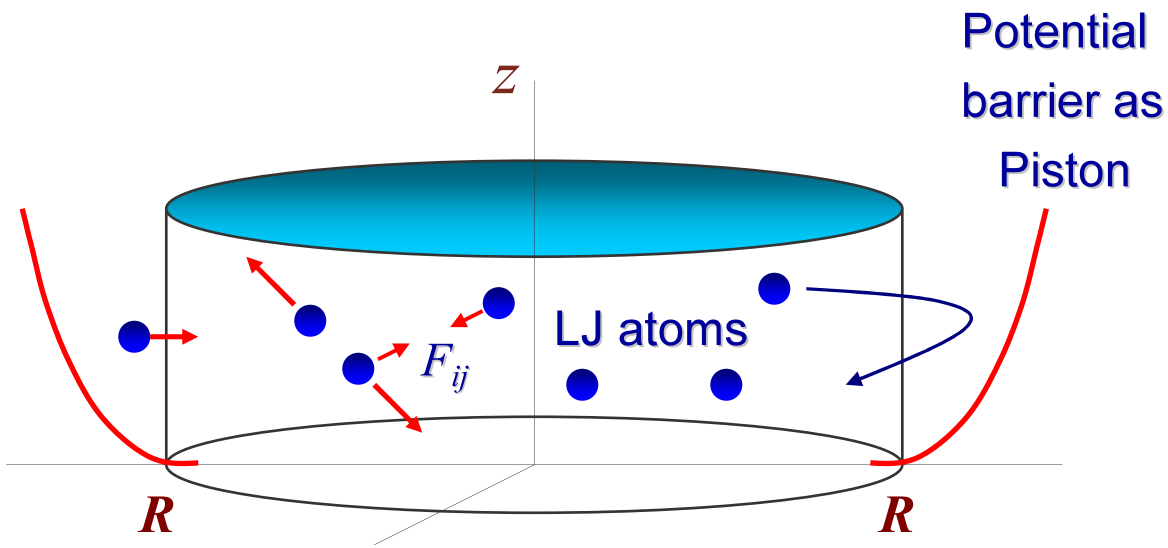
executive summary

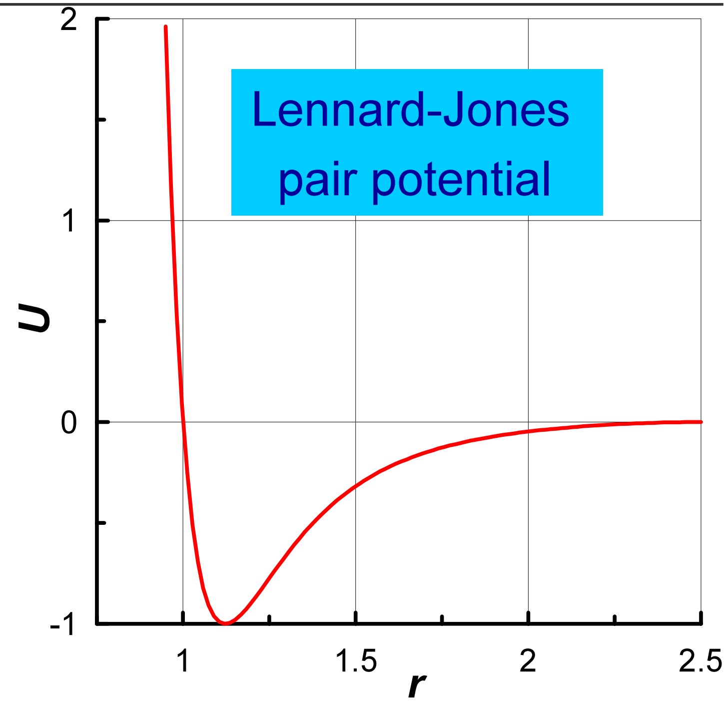
- **MD simulation provides a new tool for a study of hydrodynamic instabilities, when CFD fails.**
- **Mode dependence of nonlinear growth is investigated for cylindrical RMI. Higher mode decays slower.**
- **Growth of mixing zone in cylindrical RMI is much larger than that in planar RMT (shocks hit interface repeatedly).**
- **In a shell case (two interfaces), many higher modes appear on its inner surface, and thickness of mixing zone is thinner than that on single interface.**

Outline of Talk

- **Introduction of Molecular Dynamic simulation**
- **Shock wave in cylindrical geometry**
  - **structure and stability of rippled front**
- **Richtmyer-Meshkov instability in cylindrical geometry**
  - **nonlinear dynamics of RMI**
  - **dependence of nonlinear growth on mode number**
  - **comparison with planar geometry**
  - **shell structure**
  - **(animation)**

Molecular dynamics simulation technique



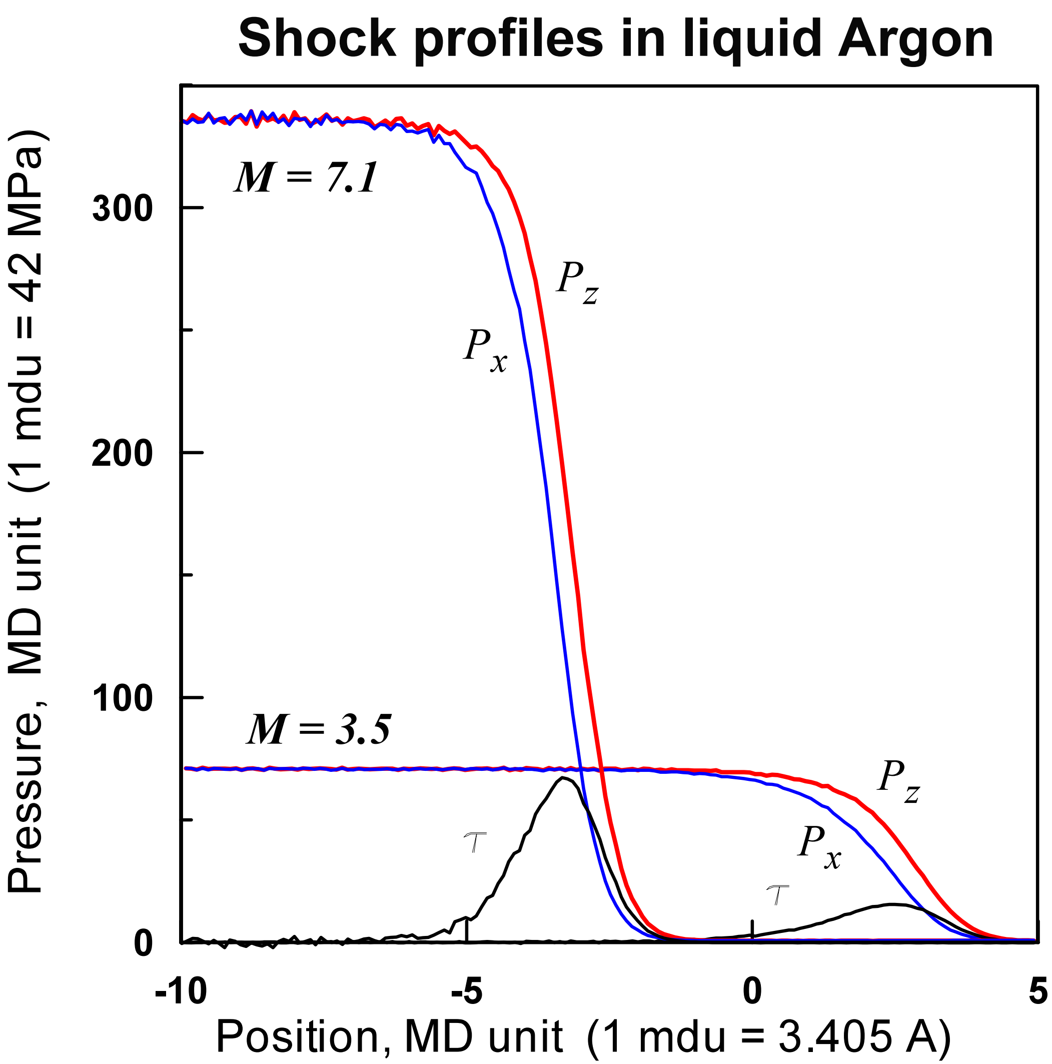


- **Periodical boundary conditions are imposed on the system along z-axis**
- **The atoms interact via Lennard-Jones (LJ) pair potential with cutoff at r_c**

$$\phi_{LJ}(r) = 4\varepsilon[(\sigma / r)^{12} - (\sigma / r)^{6}] \quad \text{if} \quad 0 < r < r_c = 2.5\sigma$$

- **The piston is simulated by an external potential $\sim[r_i - R(\phi_i, t)]^2$ and its position may depend on angles in case of perturbed boundary as well as on time to generate shock waves.**

Shock R-H relations are satisfied within accuracy of 10^{-5}



V. Zhakhovskii, K. Nishihara, S.I. Anisimov, and S. Zybin

JETP Lett., v.65, 755 (1997)

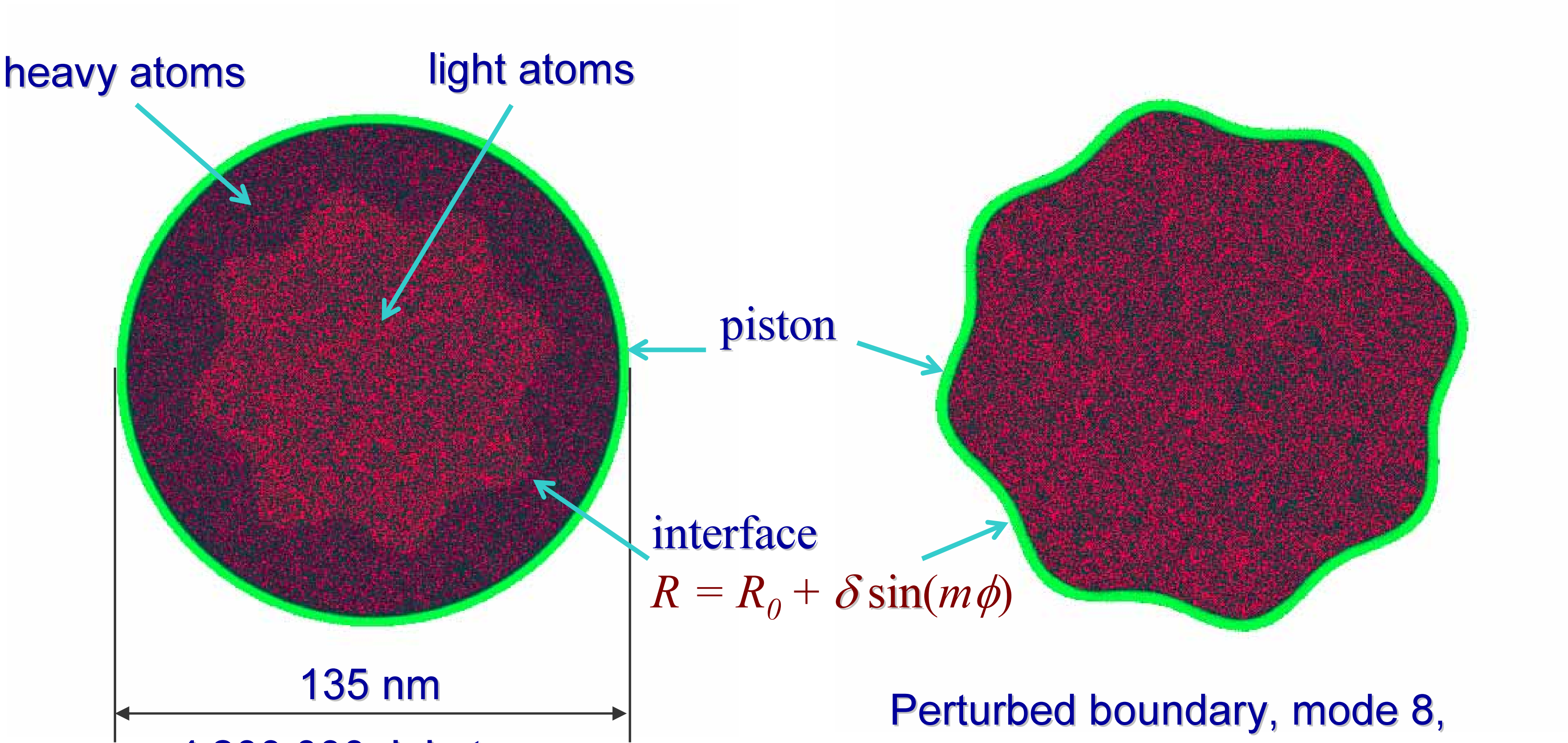
JETP Lett., v.66, 99 (1997)

PRL, v.83, 1175 (1999)

Shock front thickness is enough thin compared with perturbation amplitude

Molecular dynamics simulation technique

Typical snapshots of MD systems at the beginning of compression



4 200 000 LJ atoms

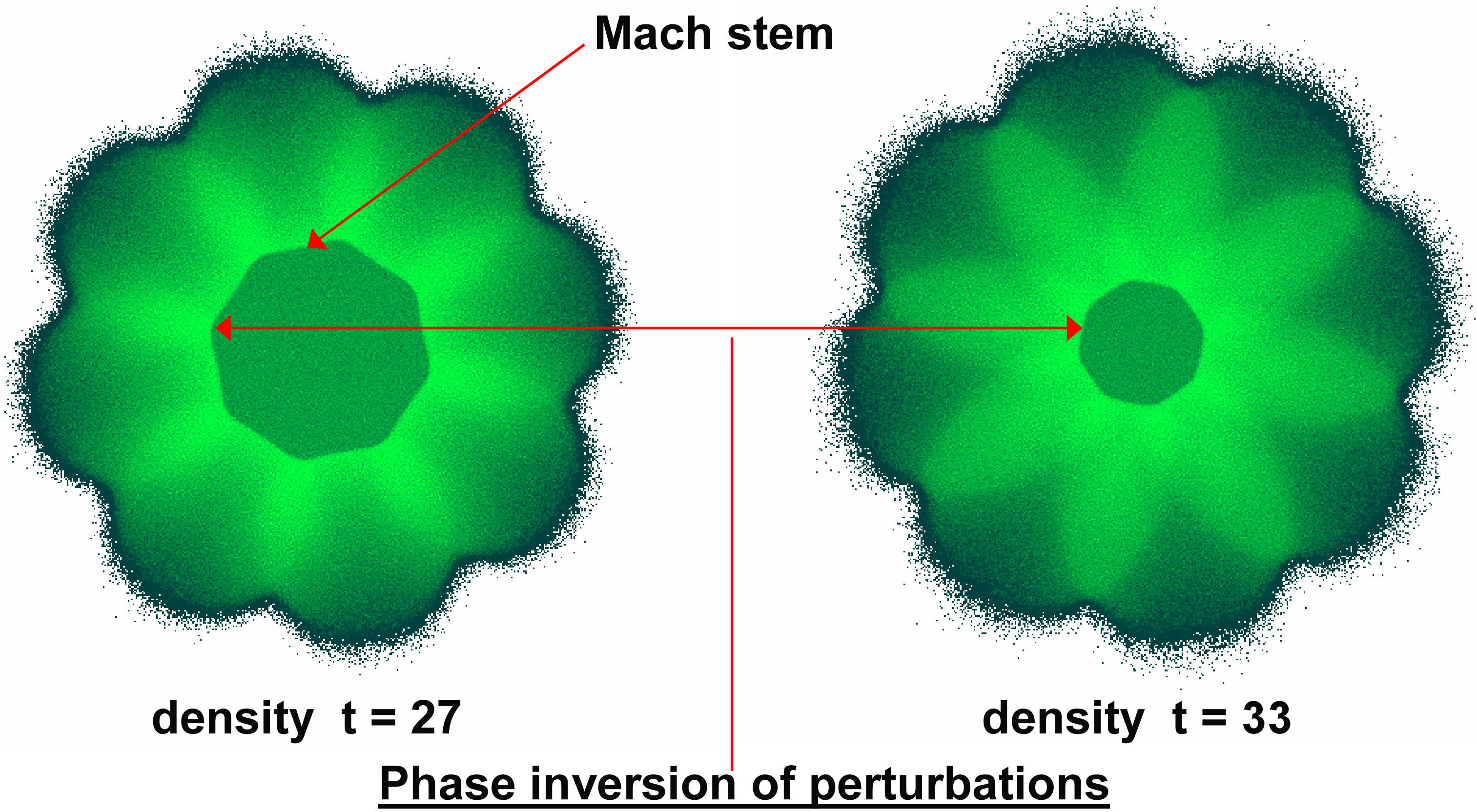
Perturbed boundary, mode 8,
only light atoms in the system

- Each pixel represents a small domain, which is occupied approximately 30 atoms
- Green colors correspond negative radial velocity of a domain, red colors mean positive velocity. *Brightness* is proportional to absolute values and balances according maximal amplitude.

MD simulation of perturbed shock front, of which ripples oscillate in time.

First generation of Mach stems appears at very early stage of SW converging

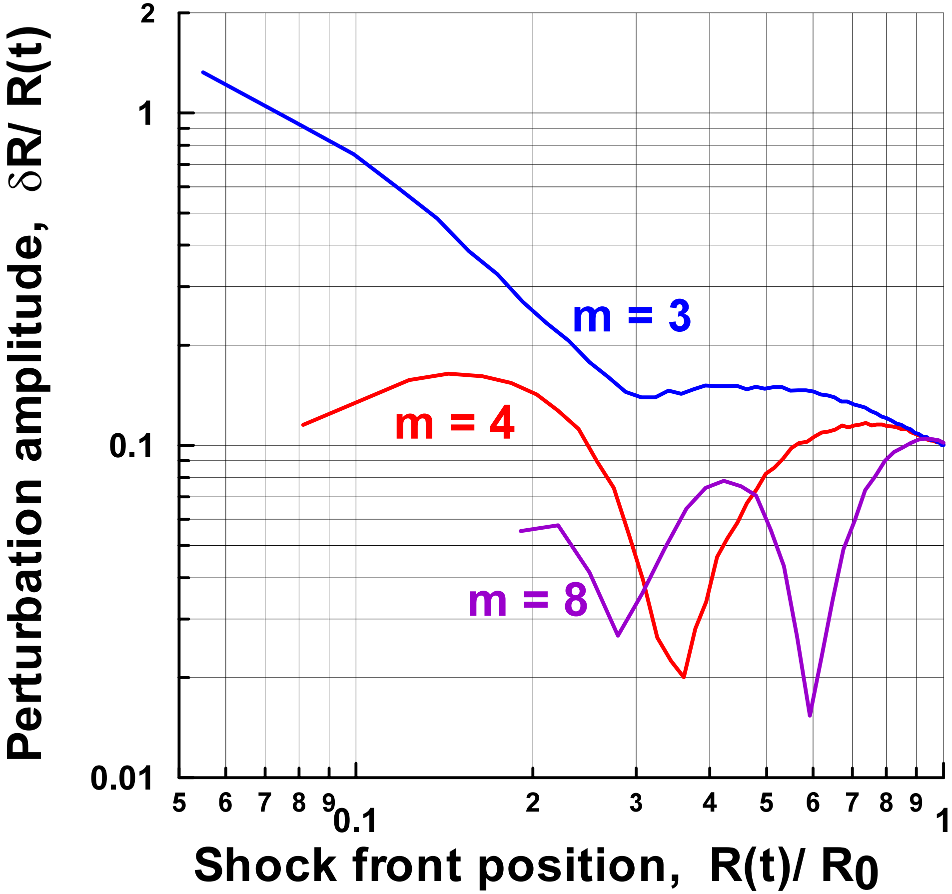
Brightness is proportional to density.



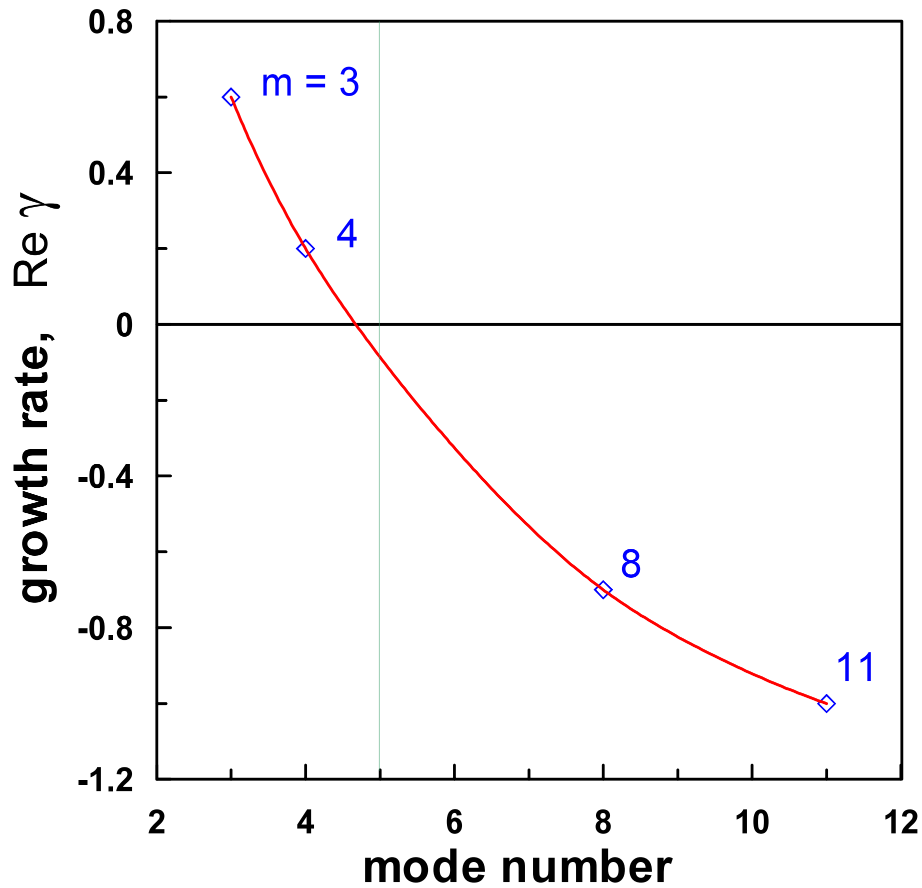
instead of circle the <u>polygons</u> (8 or 16 sides for mode 8) converge to center

Converging shock wave is unstable for low mode number

initial Mach number M = 3.1



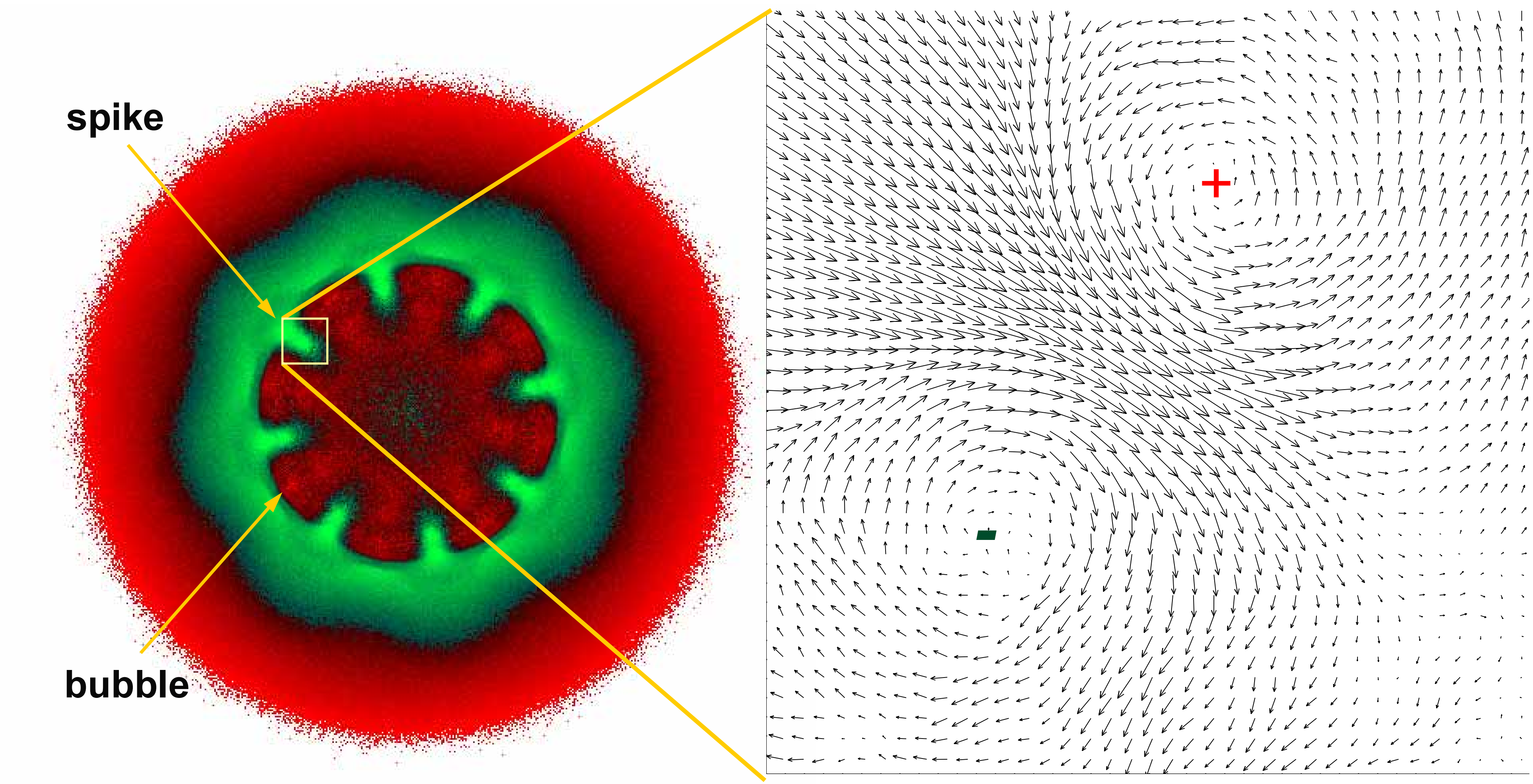
$$\frac{\delta R(t)}{R(t)} = a\left(\frac{R(t)}{R_0}\right)^{\gamma}$$



Perturbations grows if the mode number m < 5

MD simulation of RM instability

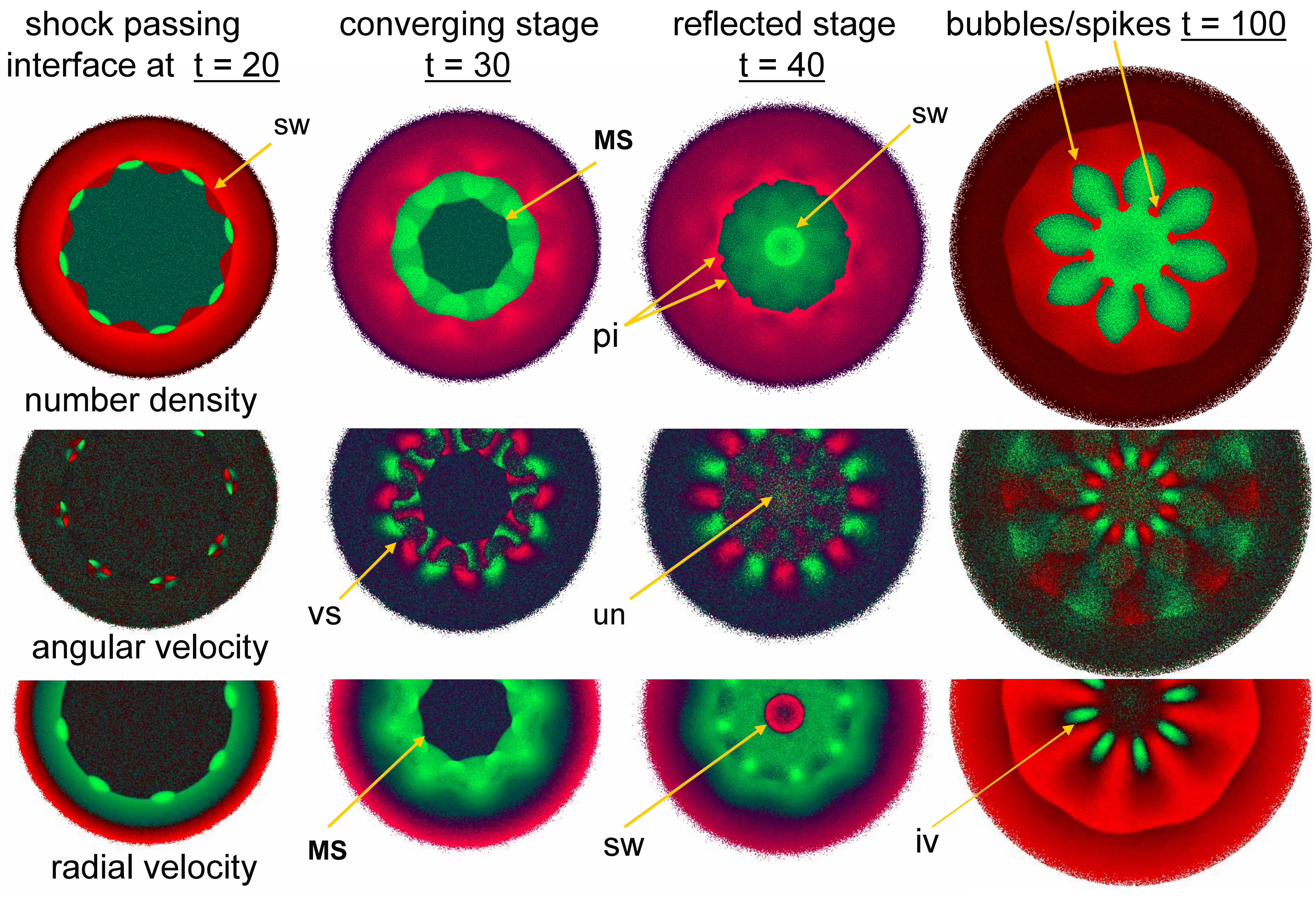
Vorticity at the interface causes RM instability



Radial velocity map,
green means negative value (to origin)

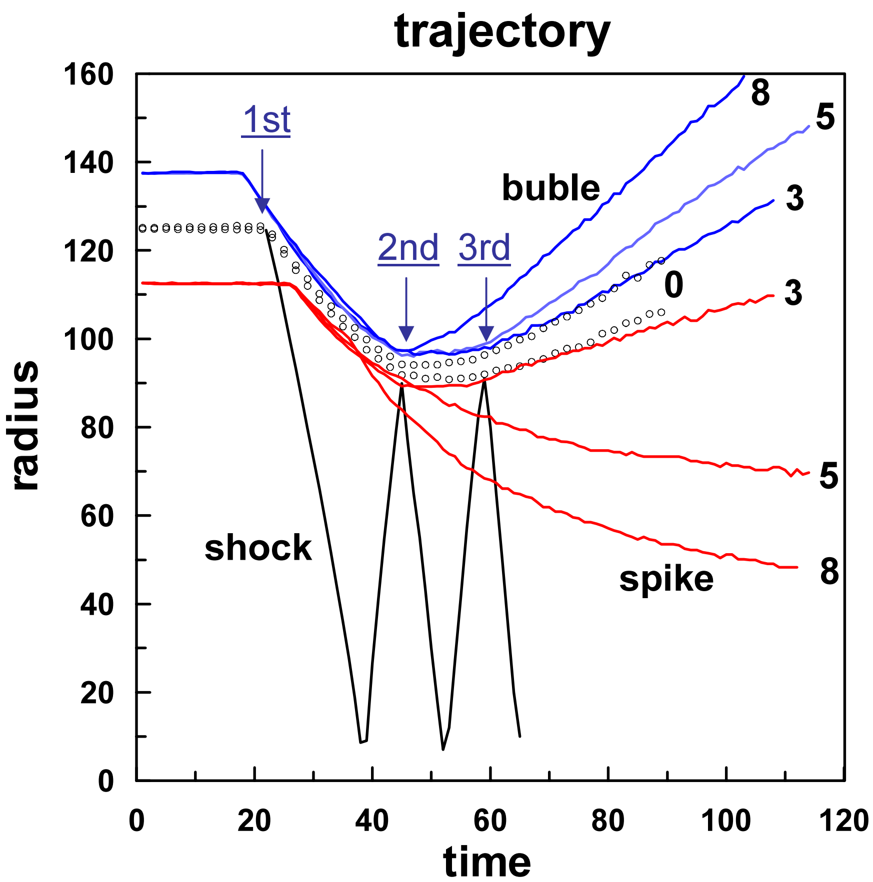
Velocity field, each arrow indicates
average velocity of about 100 atoms

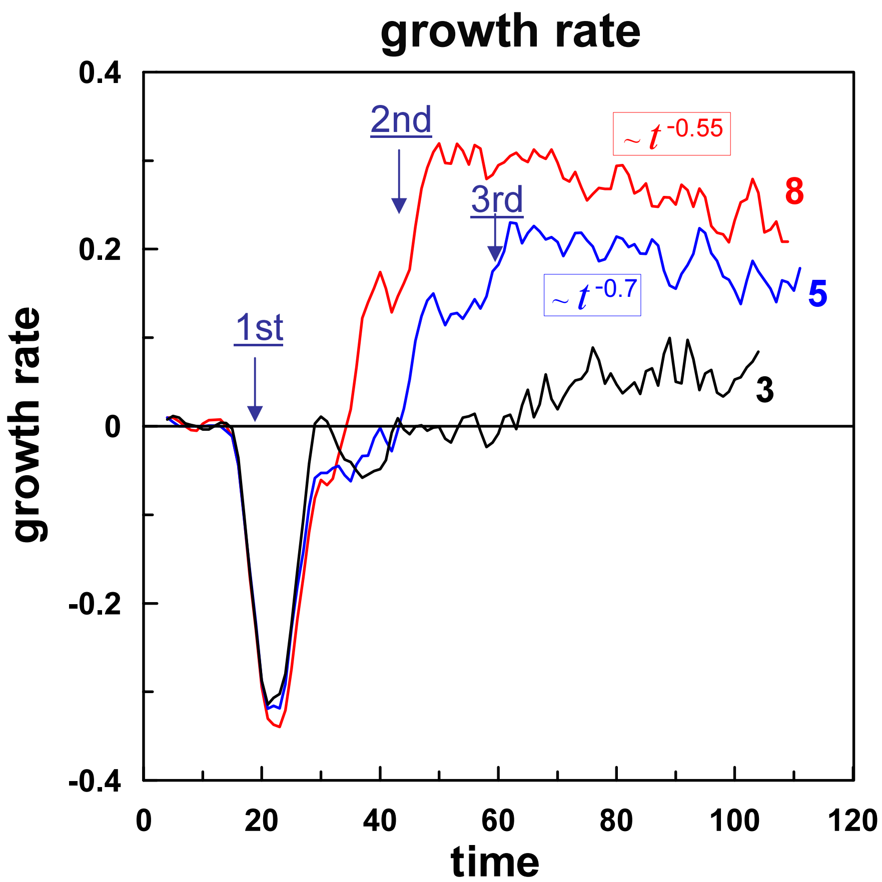
Richtmyer-Meshkov instability in cylindrical geometry



Molecular dynamics simulations show RM growth driven by multiple shocks for different mode numbers.

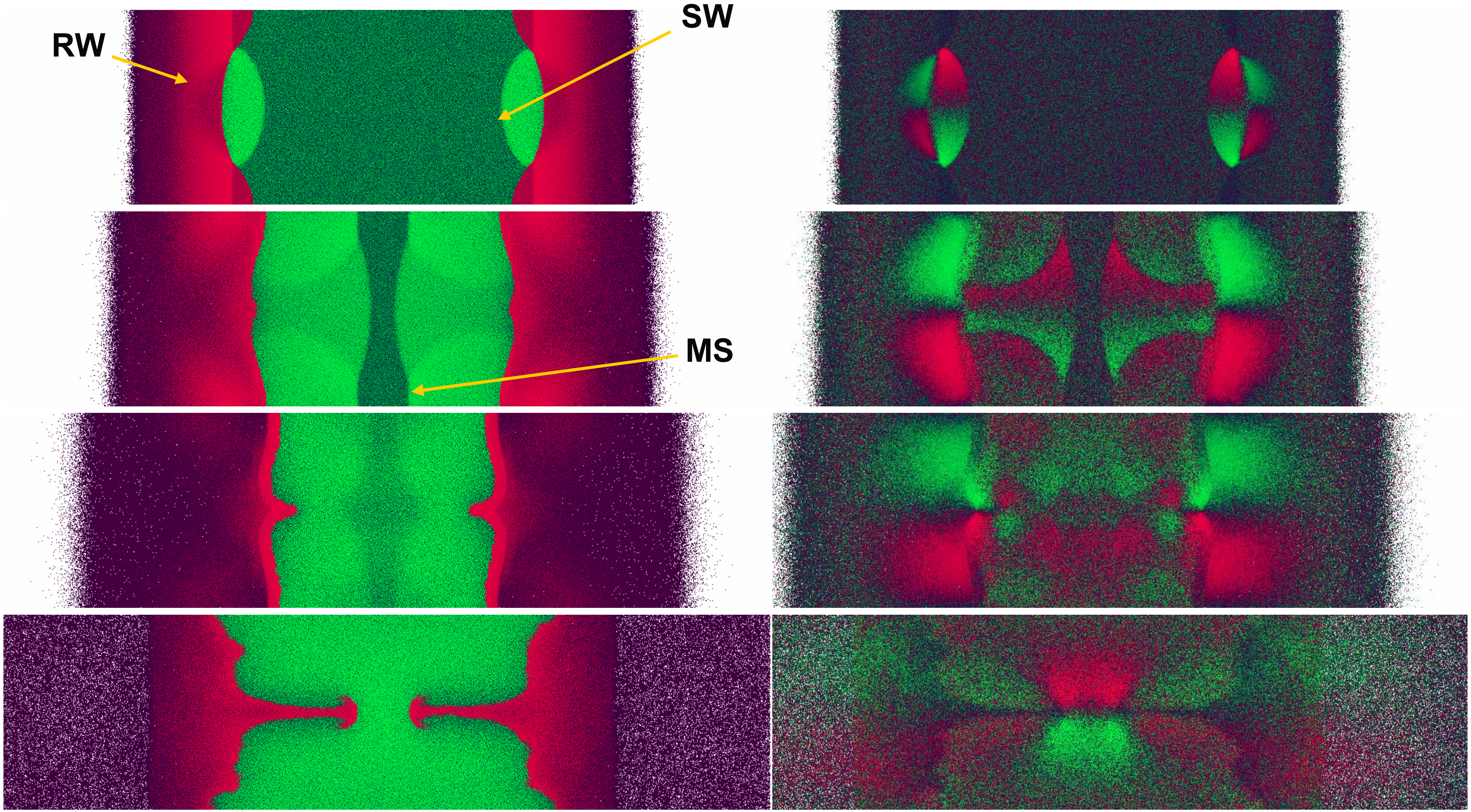
Decay of nonlinear growth is mode dependent and higher mode decays slower





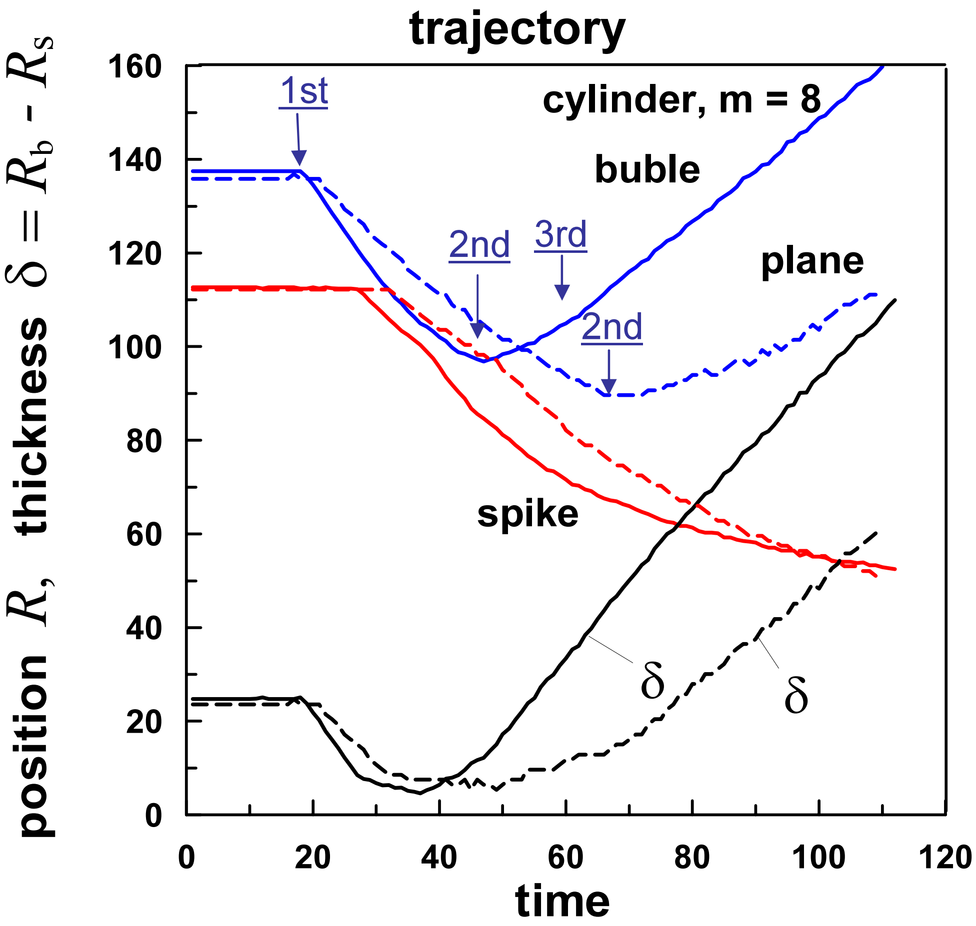
Richtmyer-Meshkov instability in planar geometry

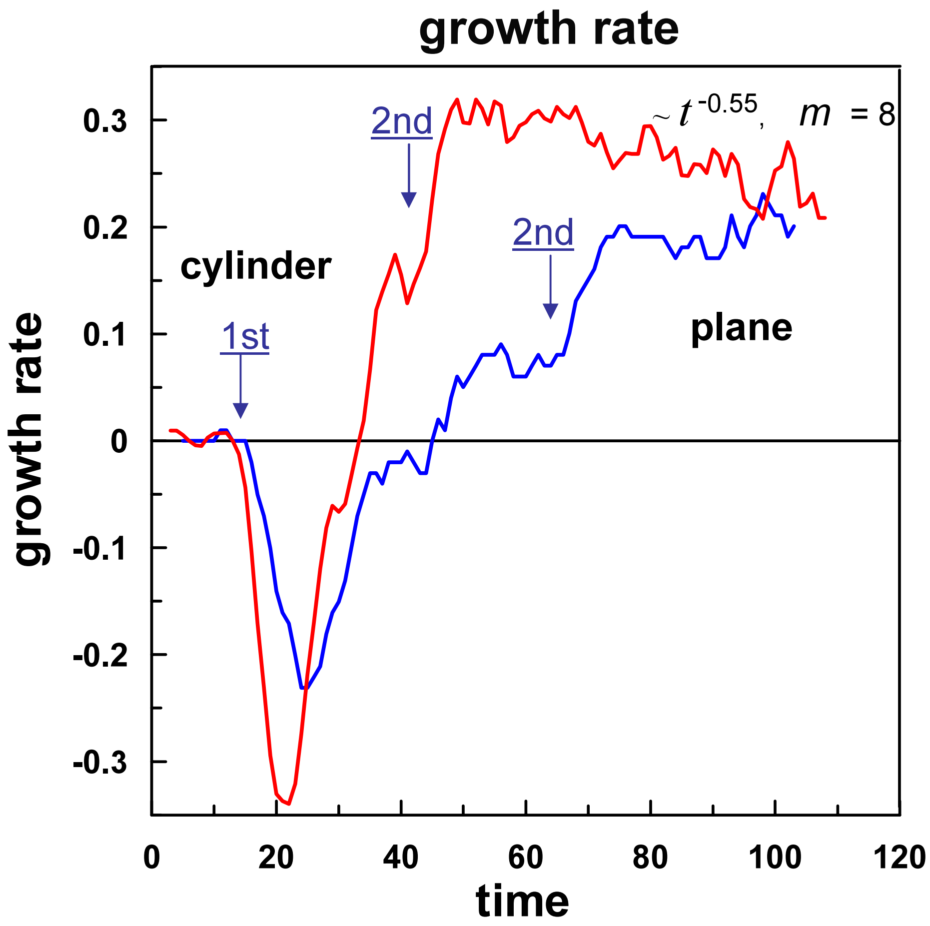
number density | y-component of velocity



Growth of mixing zone in cylindrical RMI is much larger than in planar RMI

In both cases shocks hit interface repeatedly and growth rate increases

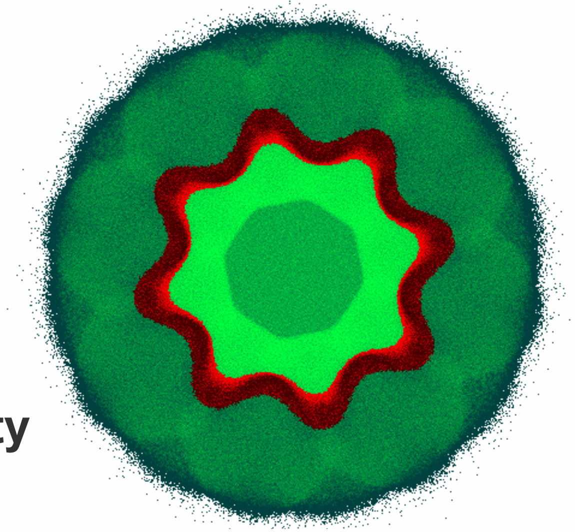




Richtmyer-Meshkov instability at shell surfaces

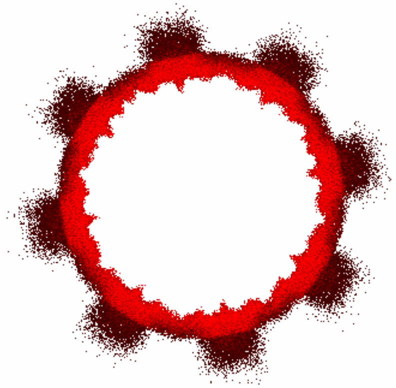
Many higher mode appear on inner surface.

Thickness of mixing zone is thinner than that on single interface.

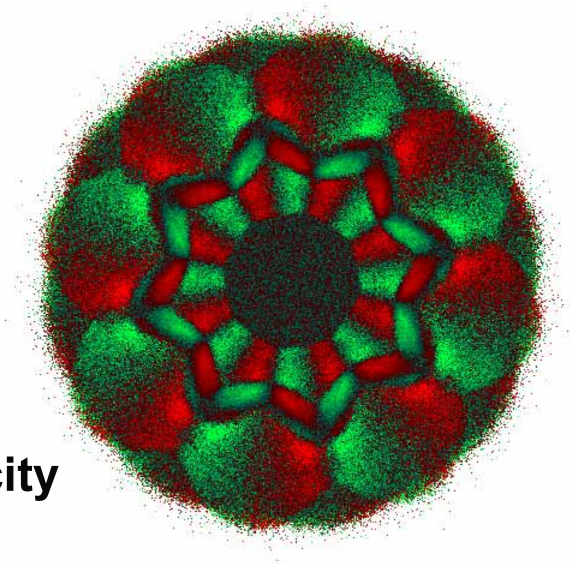


number density

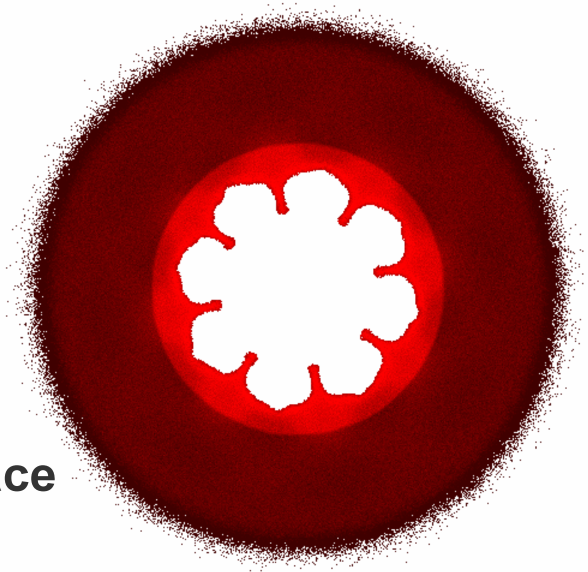
number density of heavy fluid



shell



angular velocity



single interface

Conclusion

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