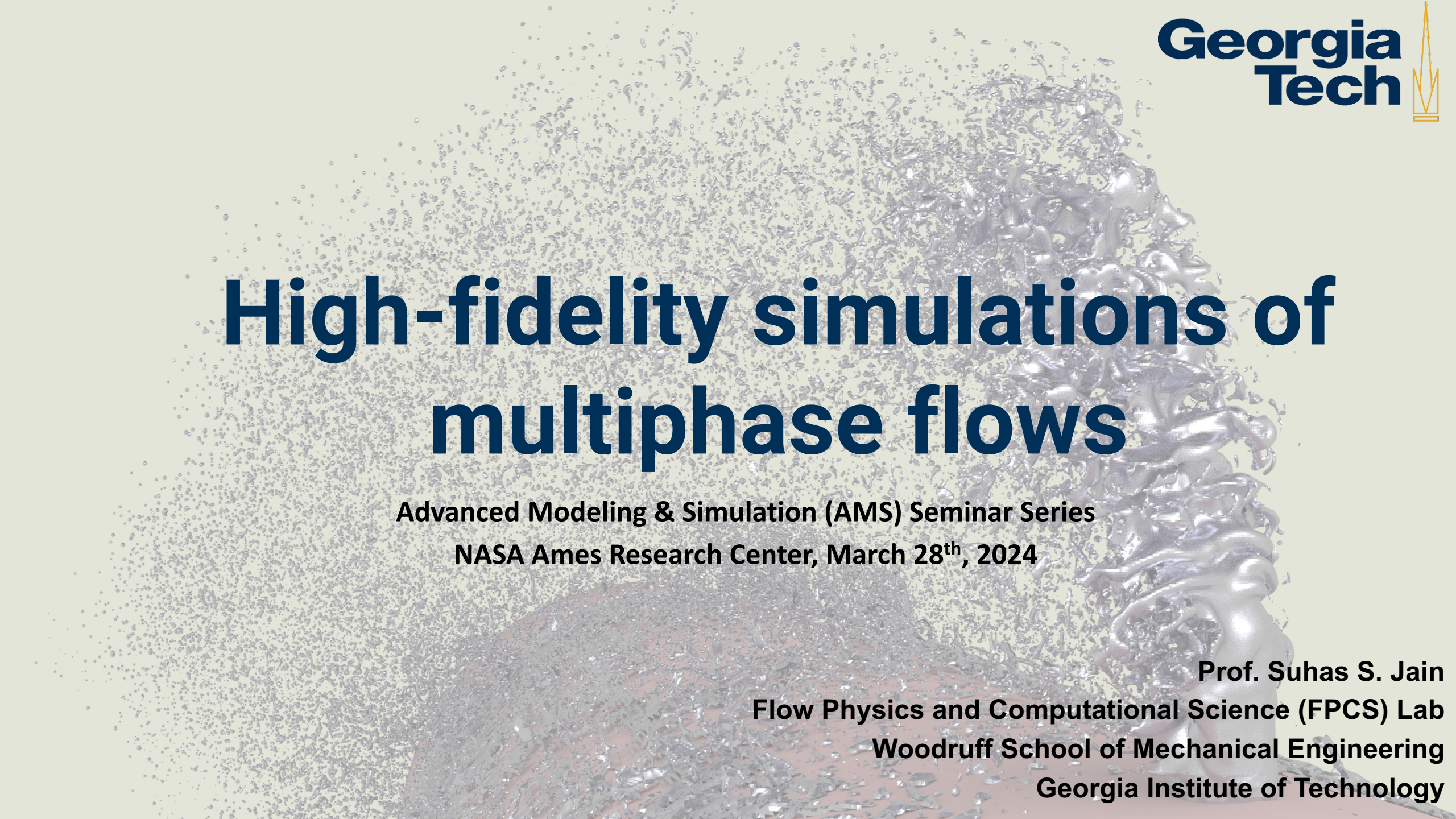


High-fidelity simulations of multiphase flows

Advanced Modeling & Simulation (AMS) Seminar Series

NASA Ames Research Center, March 28th, 2024

Prof. Suhas S. Jain

Flow Physics and Computational Science (FPCS) Lab

Woodruff School of Mechanical Engineering

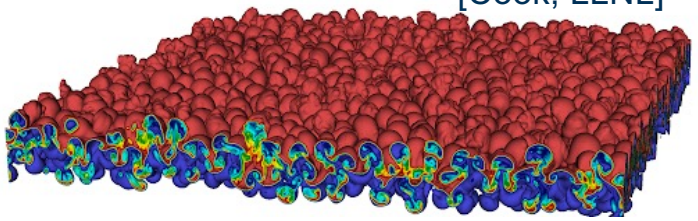
Georgia Institute of Technology

Multiphase flows



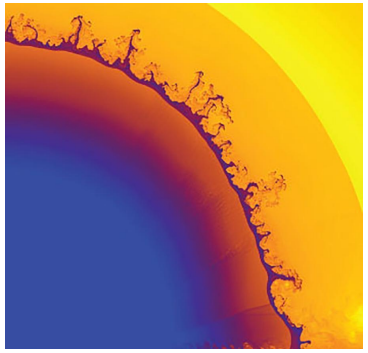
atomization
(printer, combustor, propulsion)

[Cook, LLNL]



Rayleigh-Taylor instability
(fusion)

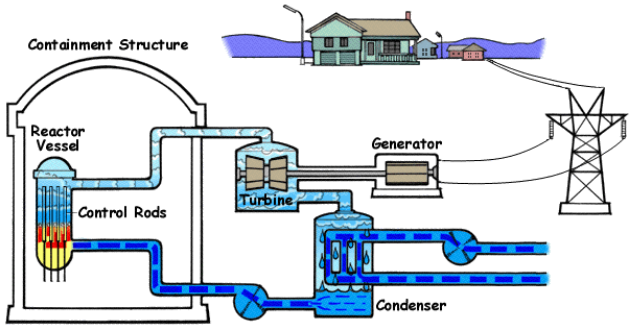
[Evangelista et al., 2016]



Richtmyer-Meshkov instability
(supernova)

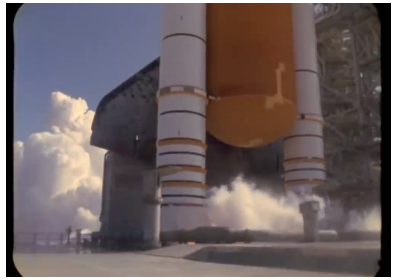


surfactant transport
(emulsion)



phase change - boiling
(nuclear reactor, energy)

[NASA Kennedy Space Center]



bubble acoustics
(sound suppression system)

[Koumoutsakos, 2013]



bubble cavitation
(marine propeller, lithotripsy)

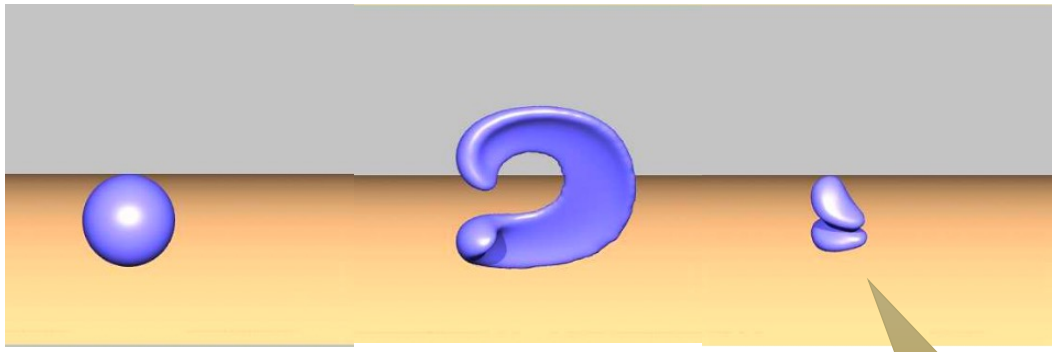


Solidification/melting
(additive manufacturing, ice accretion, solid propulsion)

Georgia Tech

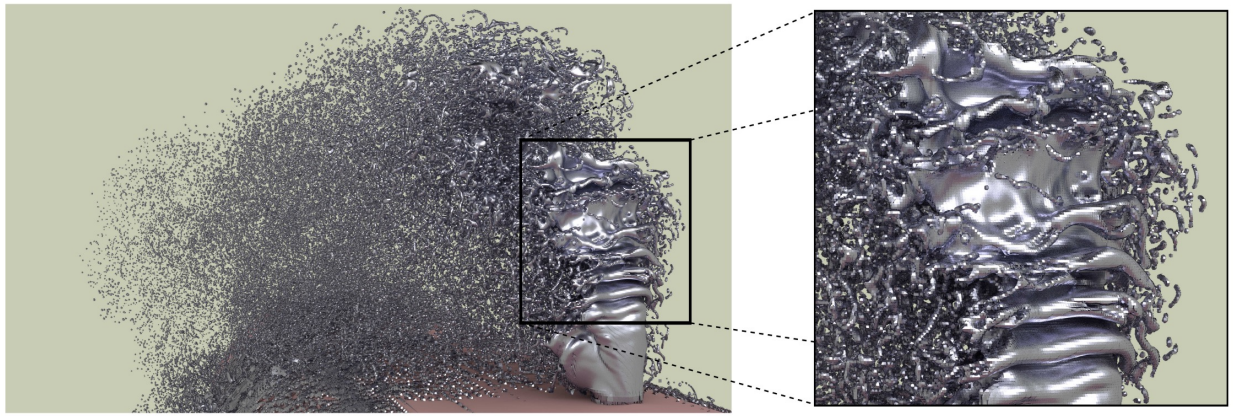
Modeling two-phase flows is challenging

1. discrete conservation of
   - mass of each fluid
   - total momentum
   - kinetic energy*
2. discontinuities in density across the interface
3. dynamic creation of interfaces and complex topological changes



drop deformation in shearing flow [1]

80% of mass is lost



liquid jet in air crossflow [2]

[1] - Enright, *Ph.D. thesis*, 2002
[2] – Prakash, **Jain,** Lovett, Raghunandan, Ravikrishna, & Tomar, *At. Sprays*, 2019

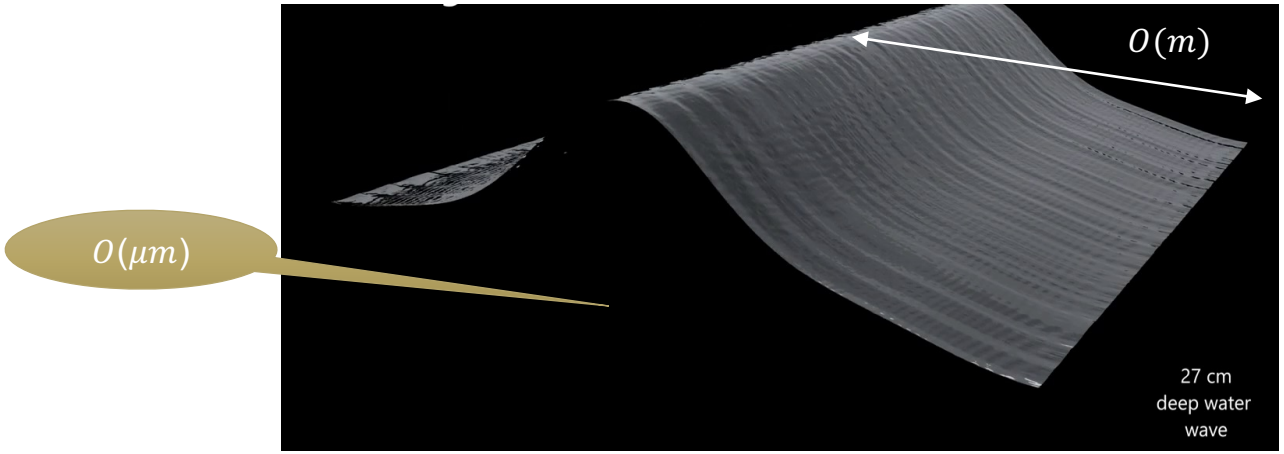
Georgia Tech

More challenges

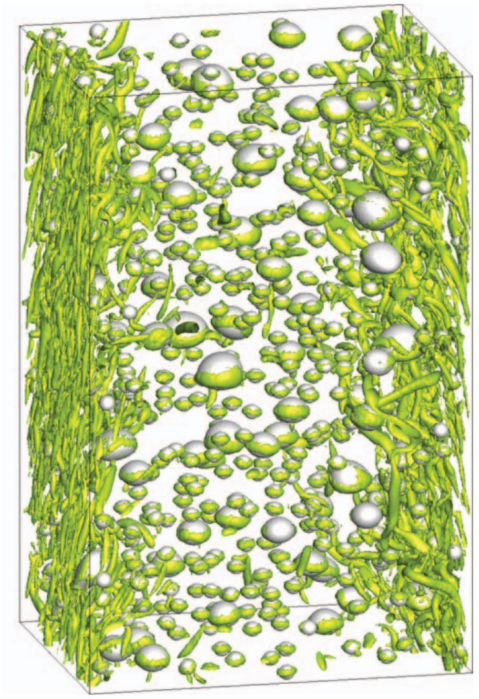
4. large separation of scales

5. robust for high-Re flows

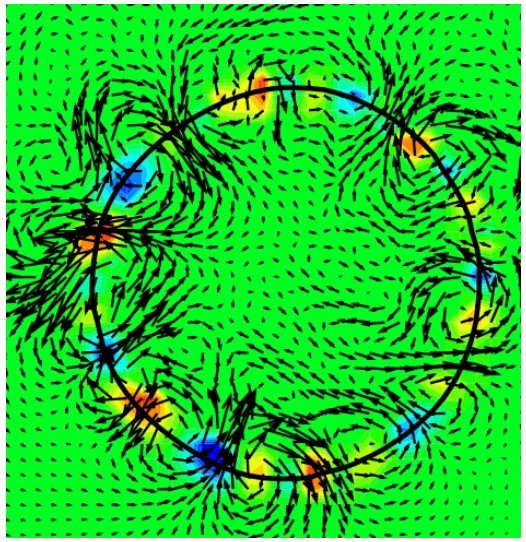
6. accurate modeling of surface tension effects



turbulent breaking wave [1]



turbulent bubble column [2]



drop advection - surface tension model [3]

[1] – Chan, Mirjalili, **Jain**, Urzay, Mani & Moin, *Phys. Rev. Fluids*, 2019
[2] - Tryggvason et al., *Phys. Fluids.*, 2013
[3] - Abadie et al., *J. Comput. Phys.*, 2015

Georgia Tech

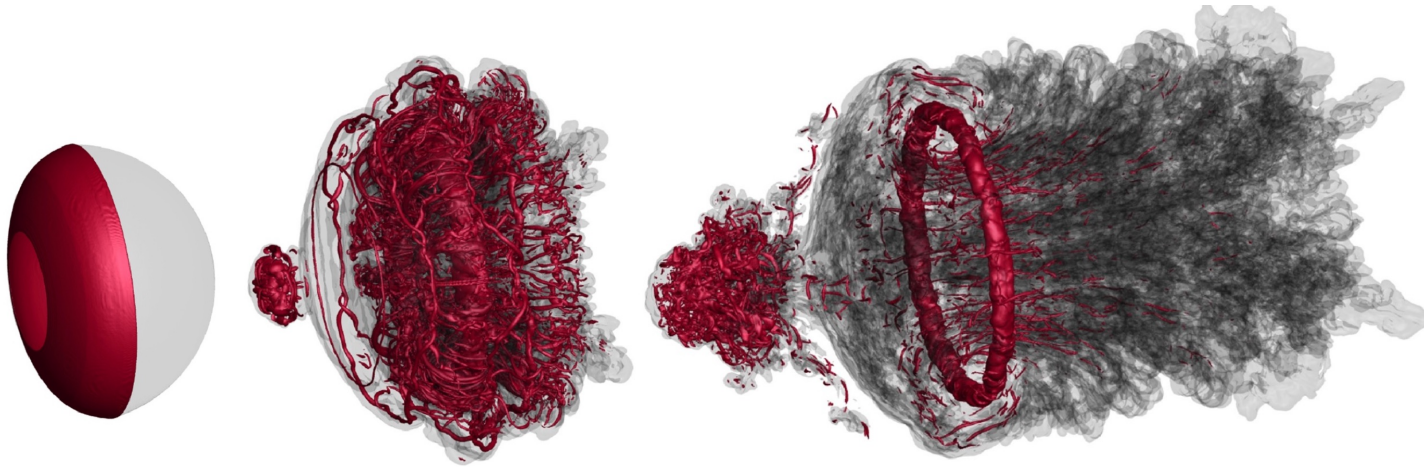
Additional challenges in compressible flows

7. maintaining thermodynamic consistency at the interface

8. conservation of
   - total energy
   - entropy*

9. accurate modeling of shock interaction with interface

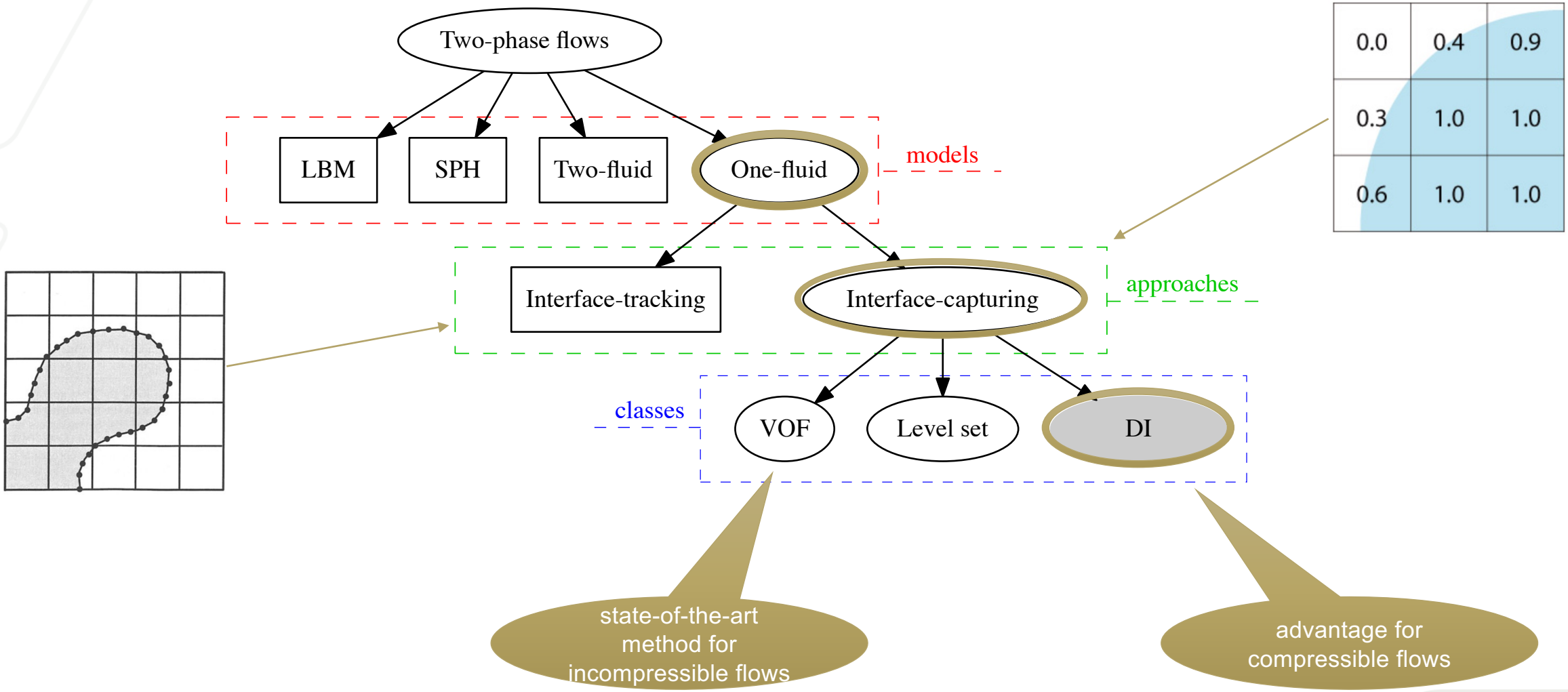
*absence of dissipative mechanisms



shock-bubble interaction [1]

[1] - Diegelmann et al., *Combust. Flame*, 2017

Classification of methods



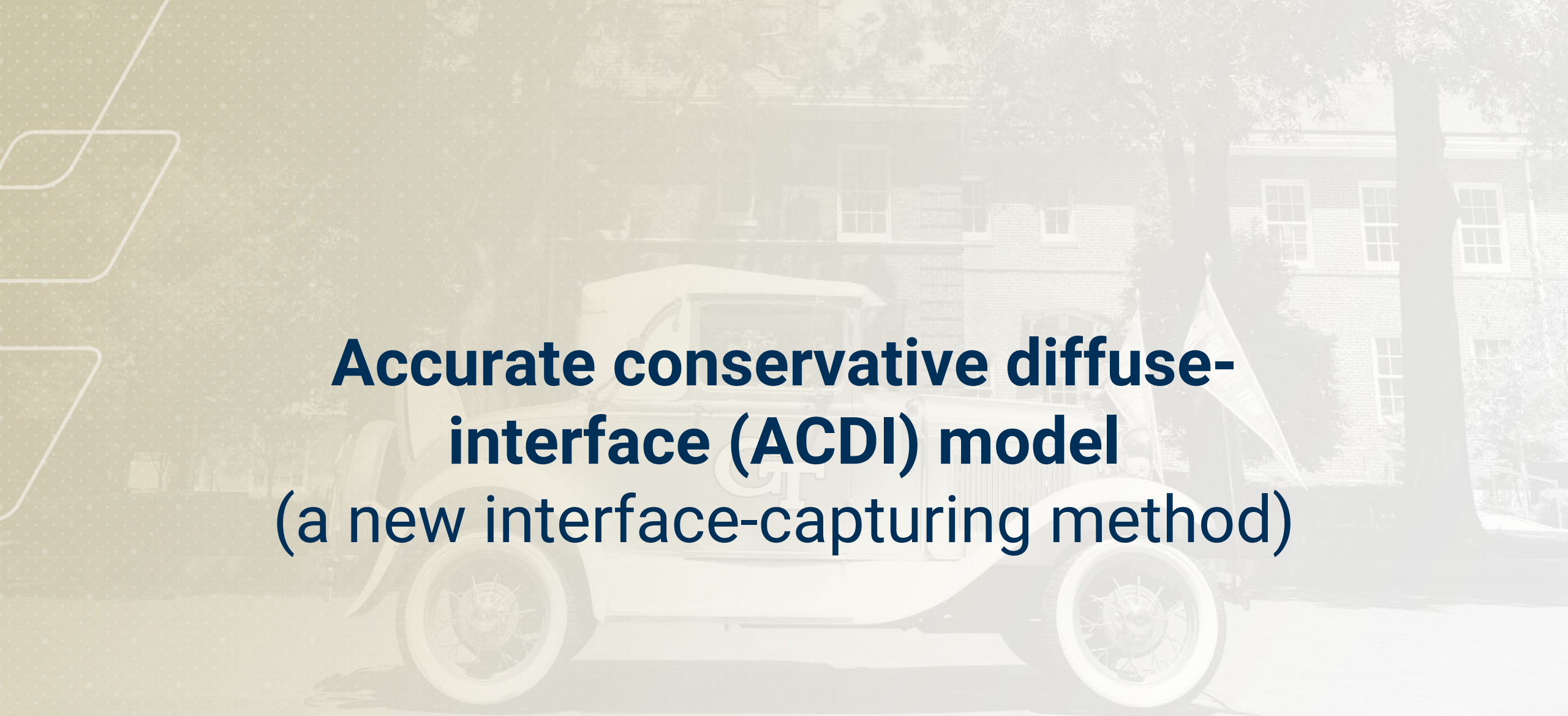
Mirjalili, **Jain**, & Dodd, *CTR Annual Research Briefs*, 2017

Contents

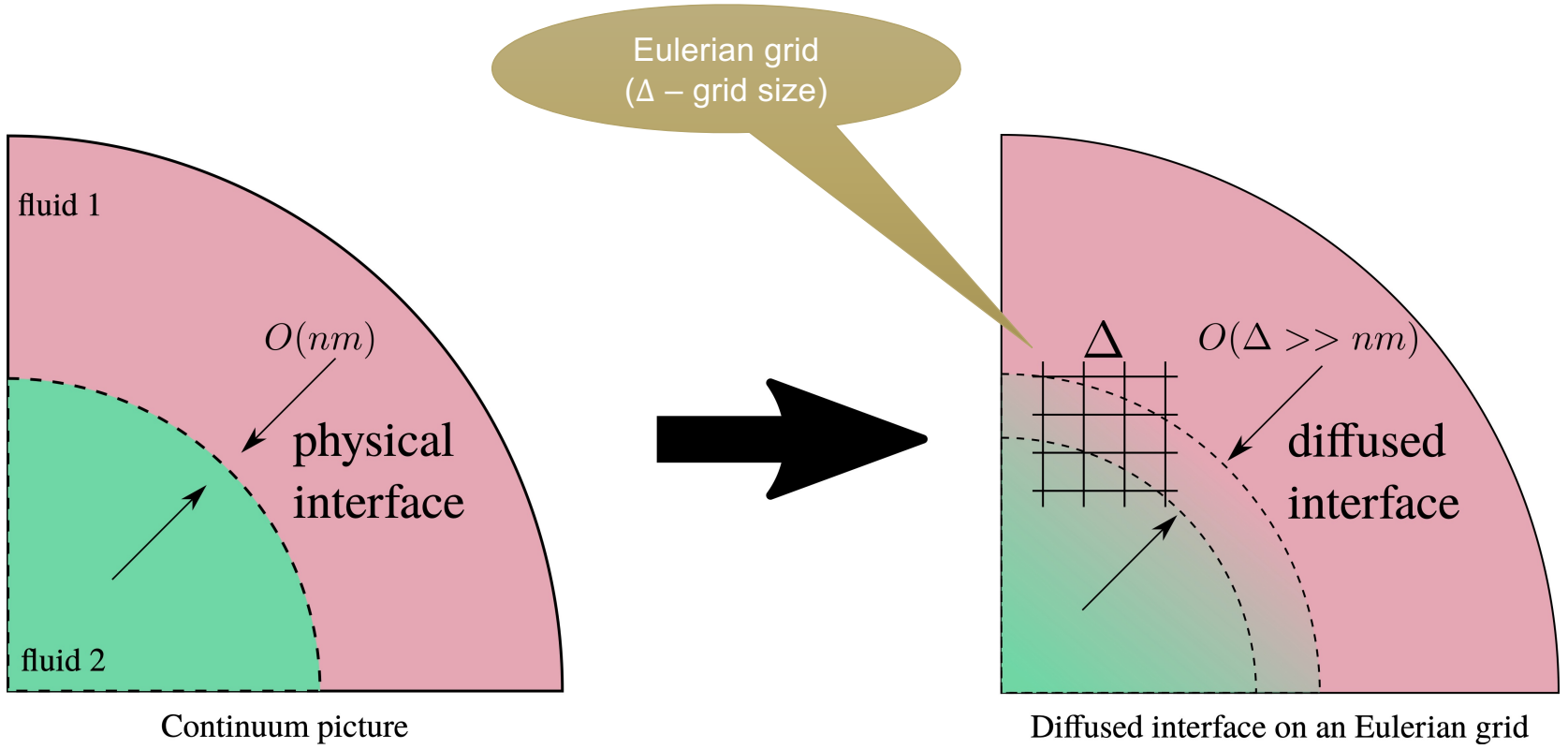
- Accurate conservative diffuse-interface/phase-field method
- Complex geometries
- Compressible flows
- Kinetic energy and entropy preserving formulation
- Other relevant work

Georgia Tech

Accurate conservative diffuse-interface (ACDI) model
(a new interface-capturing method)



Diffuse-interface formalism



Jain, Mani, & Moin, *J. Comput. Phys.*, **418**, 2020

Conservative diffuse-interface/phase-field (CDI) model

velocity scale

interface thickness scale

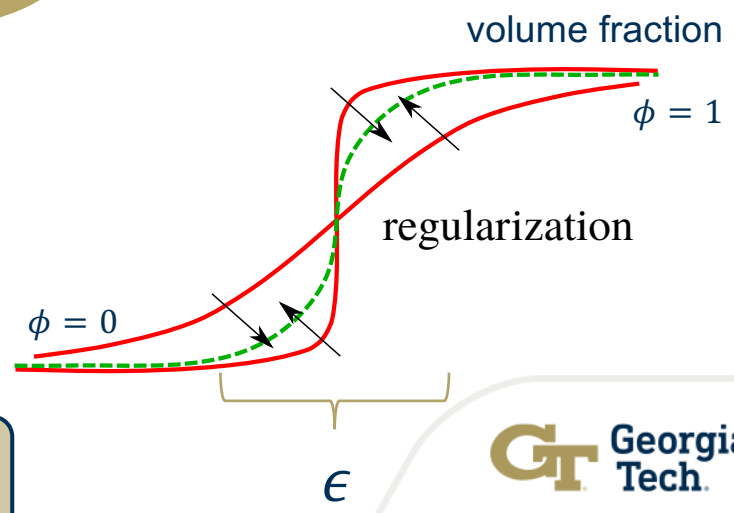
$$\frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi) = \vec{\nabla} \cdot \left[\Gamma \left\{ \epsilon \vec{\nabla}\phi - \phi(1-\phi) \frac{\vec{\nabla}\phi}{|\vec{\nabla}\phi|} \right\} \right]$$

regularization term
(diffusion-sharpening)

- Equilibrium solution:

spatial coordinate
normal to interface

$$\phi \rightarrow \frac{1}{2}\left\{1 + \tanh\left(\frac{s}{2\epsilon}\right)\right\}$$



Other models

- Cahn-Hilliard models – 4th order PDE
- Allen-Cahn models – non conservative

Chiu, & Lin, *J. Comput. Phys.*, 2011

Georgia Tech

new model development

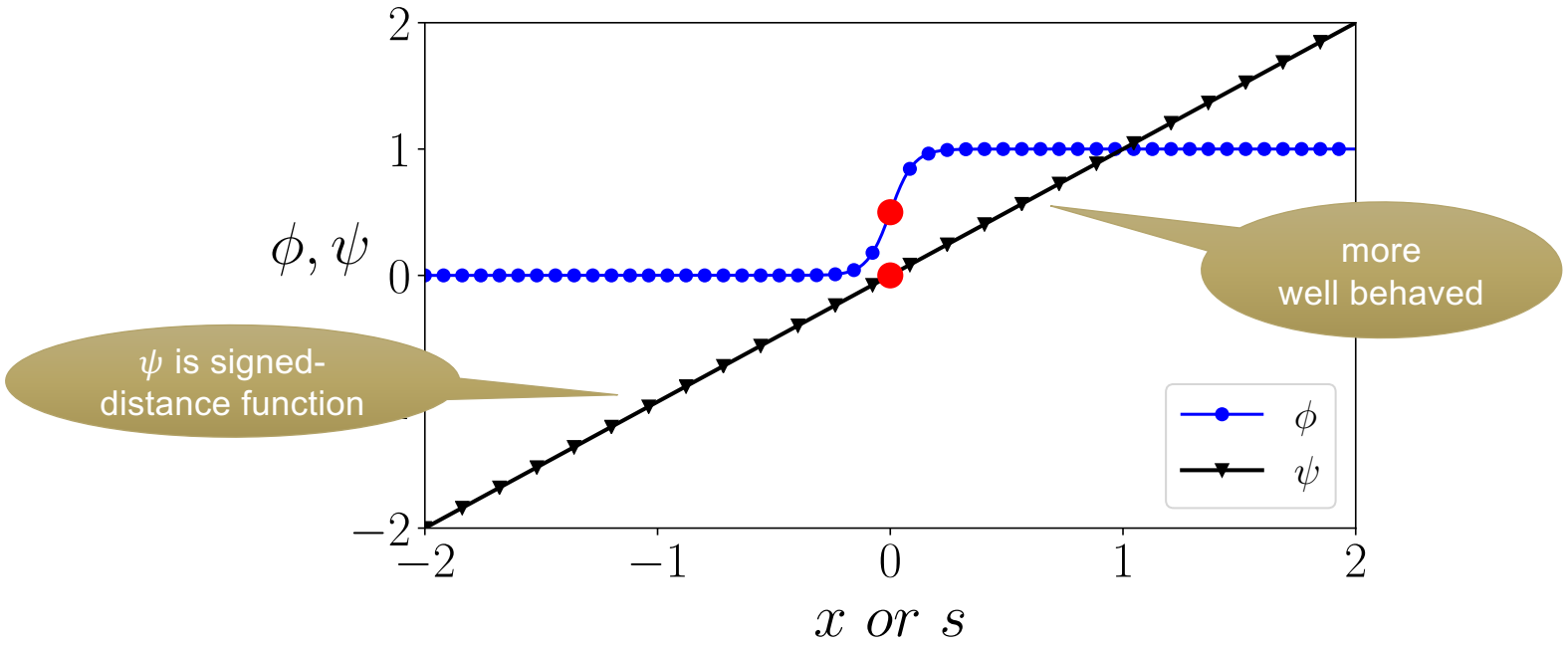
$\vec{n} = \vec{\nabla}\phi/|\vec{\nabla}\phi|$

assuming RHS is the stiffest term:

$$\phi \to \frac{1}{2}\left\{1 + \tanh\left(\frac{s}{2\epsilon}\right)\right\}$$

inverting

$$\psi = \epsilon \log\left(\frac{\phi}{1-\phi}\right)$$



reformulate the model

idea

regularization in transformed coordinate!

Jain, *J. Comput. Phys.*, **469**, 2022

Georgia Tech

Accurate conservative diffuse-interface model

CDI model:

$$\frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi) = \vec{\nabla} \cdot \left[\Gamma \left\{ \epsilon \vec{\nabla}\phi - \phi(1-\phi) \frac{\vec{\nabla}\phi}{|\vec{\nabla}\phi|} \right\} \right]$$

revised (new) *ACDI* model:

new conservative regularization term

$$\frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi) = \vec{\nabla} \cdot \left[\Gamma \left\{ \epsilon \vec{\nabla}\phi - \frac{1}{4} \left\{ 1 - \tanh^2 \left(\frac{\psi}{2\epsilon} \right) \right\} \frac{\vec{\nabla}\psi}{|\vec{\nabla}\psi|} \right\} \right]$$

maintains boundedness of ϕ if $\Gamma \geq |u|_{max}$; $\epsilon > 0.5\Delta x$ with central scheme

Jain, *J. Comput. Phys.*, **469**, 2022

Georgia Tech

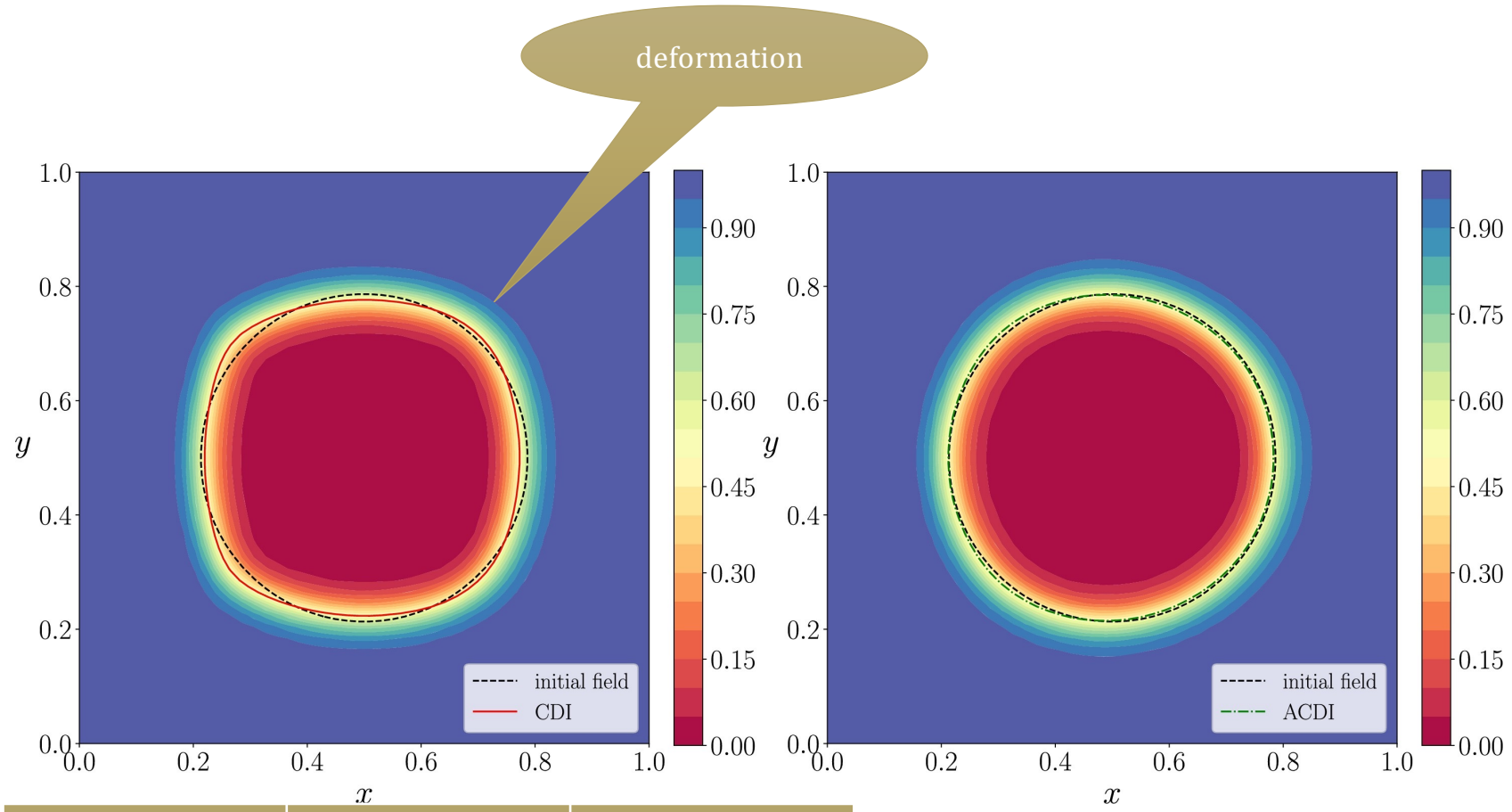
Advection of a bubble/drop

50×50 grid points

$\vec{u} = 5i$

1×1

$t = 1$,



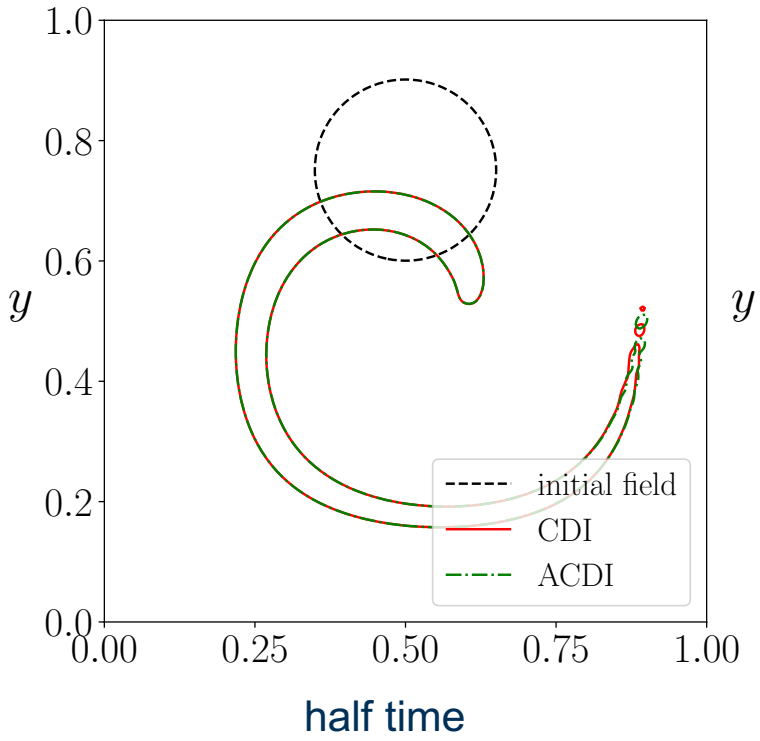
$$E = \int_{\Omega} |\phi - \phi_o| dV$$

$$= \sum_{m} |\phi_m - \phi_{mo}| dV$$

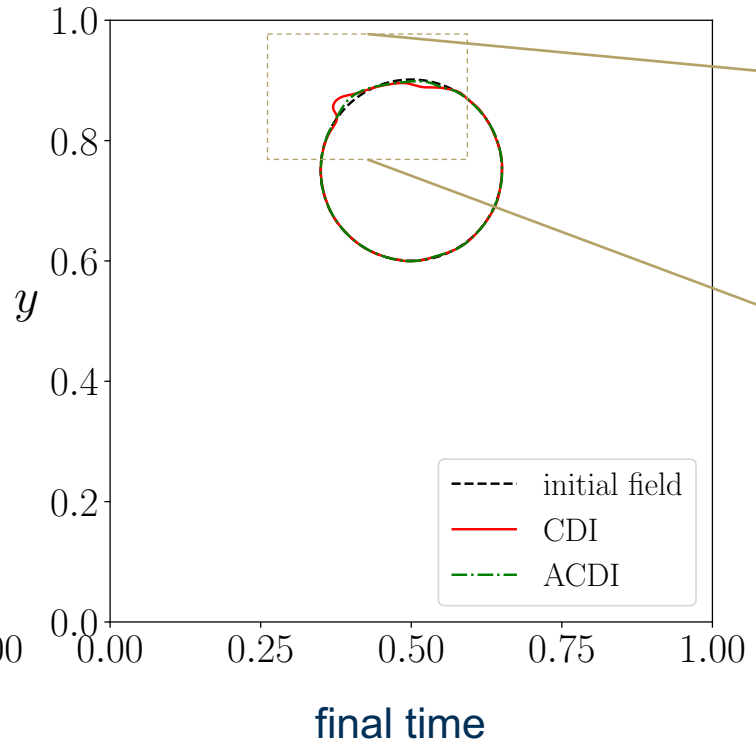
	CDI	ACDI
$Error\ (E)$	0.01352	0.00576

Jain, *J. Comput. Phys.*, **469**, 2022

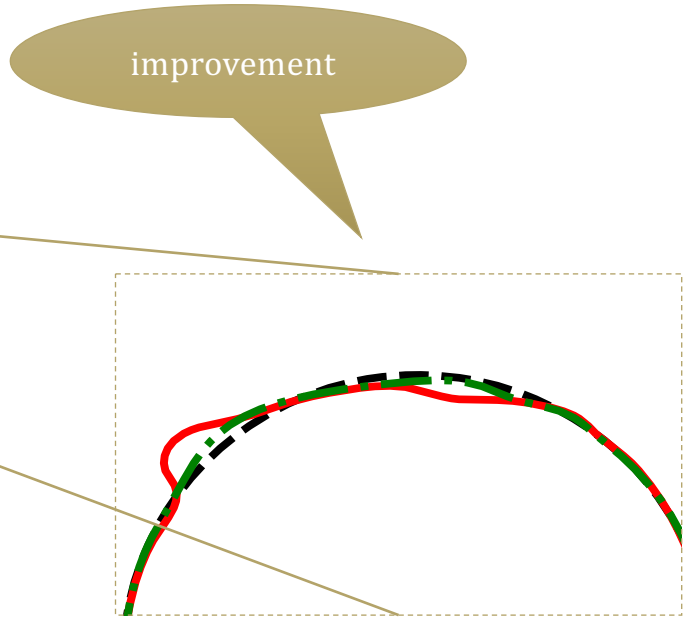
Drop in shear flow



half time



final time



shearing velocity field

$$u = -\sin^2(\pi x)\sin(2\pi y)\cos\left(\frac{\pi t}{T}\right)$$

$$v = -\sin(2\pi x)\sin^2(\pi y)\cos\left(\frac{\pi t}{T}\right)$$

$$E = \int_\Omega |\phi - \phi_o| dV$$

$$= \sum_m |\phi_m - \phi_{mo}| dV$$

	CDI	ACDI
$Error\ (E)$	1.95×10^{-3}	8.66×10^{-4}

Jain, *J. Comput. Phys.*, **469**, 2022

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Improvement in computation of surface tension force

- Continuum Surface Force formulation [1]:

$$\vec{F} = \sigma\kappa\vec{\nabla}\phi$$

CDI model (classical CSF):

$$\kappa = -\vec{\nabla}\cdot\vec{n} = -\vec{\nabla}\cdot\left(\frac{\vec{\nabla}\phi}{|\vec{\nabla}\phi|}\right)$$

ACDI model (Improved CSF):

$$\kappa = -\vec{\nabla}\cdot\vec{n} = -\vec{\nabla}\cdot\left(\frac{\vec{\nabla}\psi}{|\vec{\nabla}\psi|}\right)$$

more accurate curvature calculation

[1] – Brackbill et al., *J. Comput. Phys.*, 1992
Jain, *J. Comput. Phys.*, **469**, 2022

Georgia Tech

Reduction in spurious currents

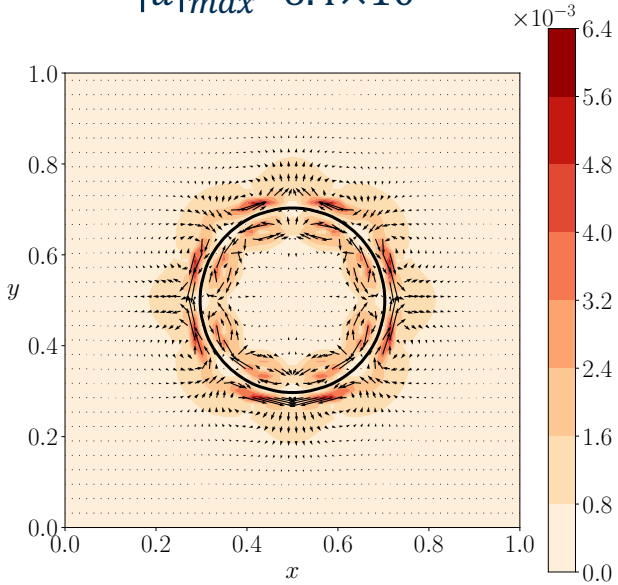
inaccuracies in curvature calculation → spurious currents/velocity field

- stationary drop
- finite surface tension

2 orders of magnitude lower

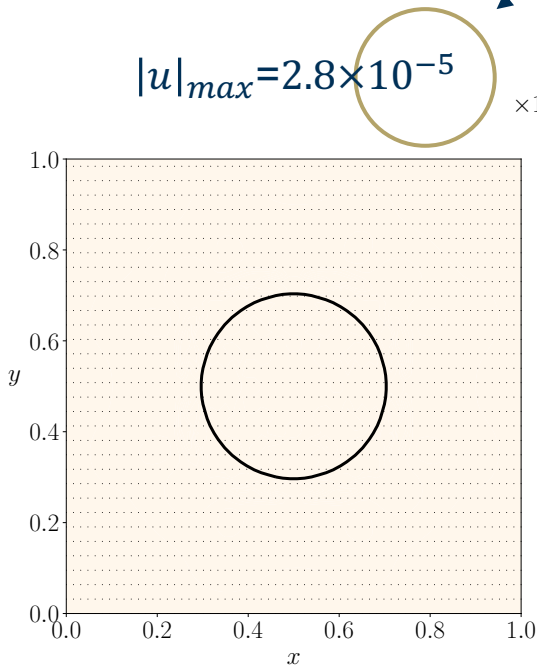
spurious velocity field at final time

$|u|_{max}=6.4\times10^{-3}$



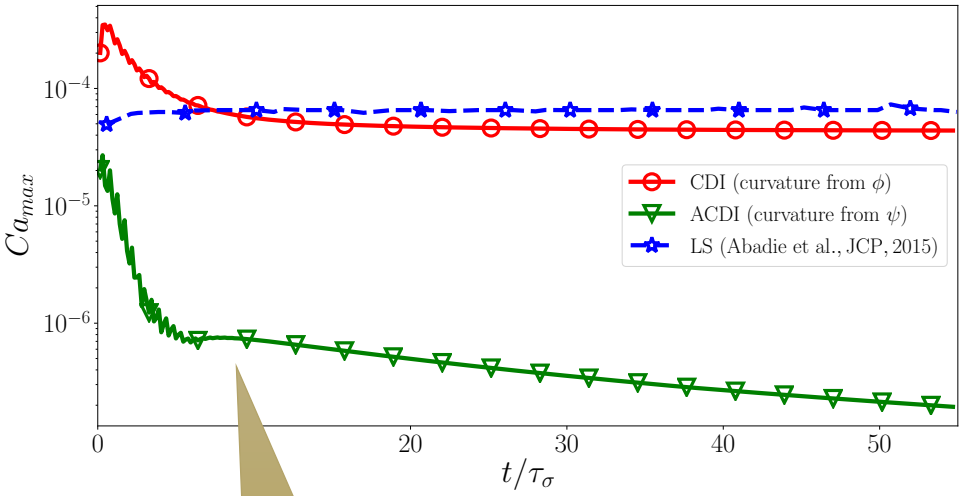
CDI

$|u|_{max}=2.8\times10^{-5}$



ACDI

max spurious velocity



more accurate than CDI and level − set method

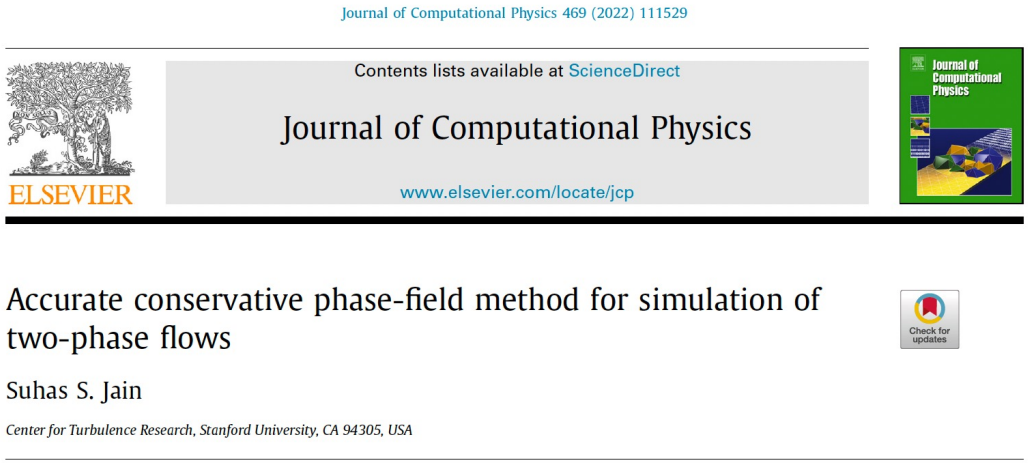
$$Ca_{max} = \frac{\mu|u|_{max}}{\sigma}$$

$$\tau_\sigma = \sqrt{\frac{\rho D^3}{\sigma}}$$

Jain, *J. Comput. Phys.*, **469**, 2022

Summary of this section

- A new *phase-field (ACDI) model* for two-phase flows
  - conservative, bounded
  - more accurate interface shape
  - more accurate curvature
    - improves surface tension force calculation
  - cost effective (PDE-only model) compared to geometric-based sharp-interface methods



Journal of Computational Physics 469 (2022) 111529

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Accurate conservative phase-field method for simulation of two-phase flows

Suhas S. Jain

Center for Turbulence Research, Stanford University, CA 94305, USA

Complex geometries

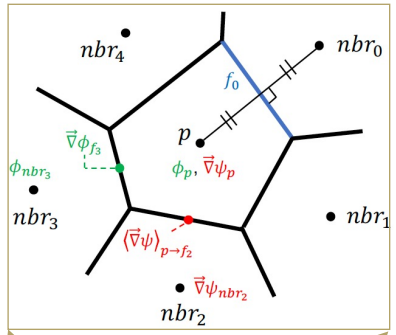


Collaborator: Hanul Hwang

Georgia Tech

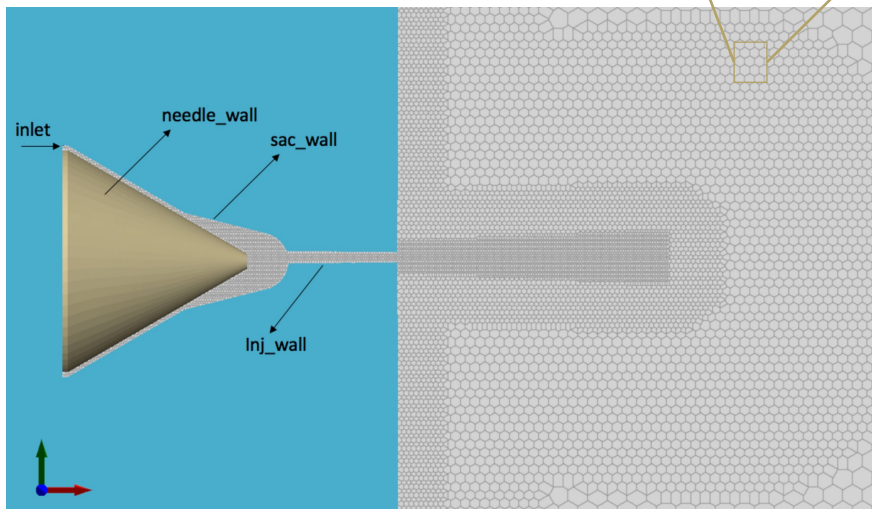
Unstructured grid formulation – complex geometries

- accurate unstructured grid formulation [1]
- Voronoi grid
- Energy stability proved on collocated grids [1]
  - Important for high density ratio multiphase flows
- new robust multiphase solver – charLES-M

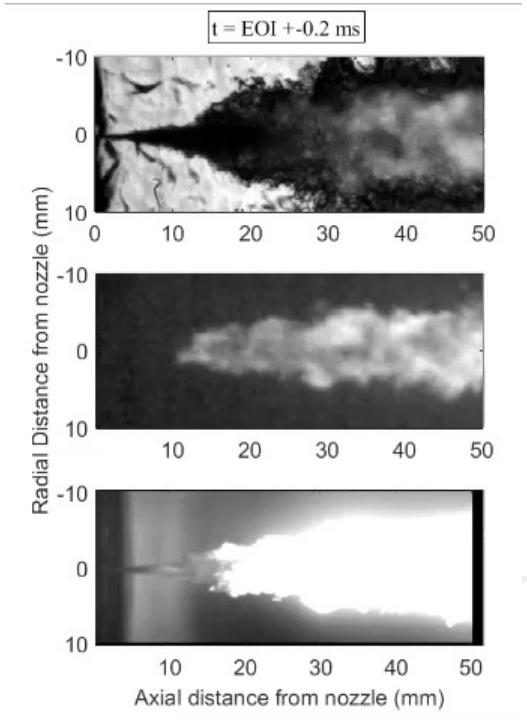


ECN Spray A conditions:

Fuel	n-Dodecane
Fuel Density	713 kg/m^3
Ambient Gas	100% N_2
Gas Density	22.8 kg/m^3
Injection Pressure	150 MPa
Ambient Pressure	2MPa
Ambient Temperature	303K



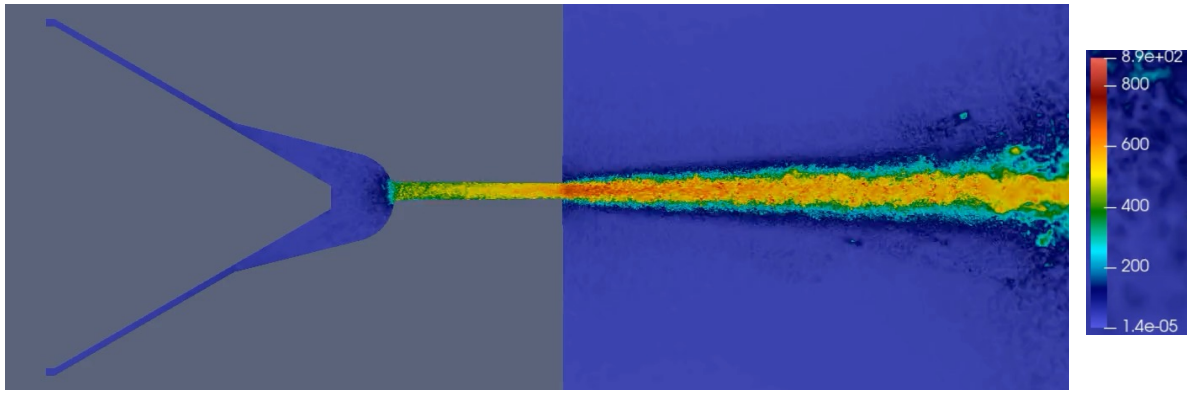
Exp: SPhERe Lab at GT



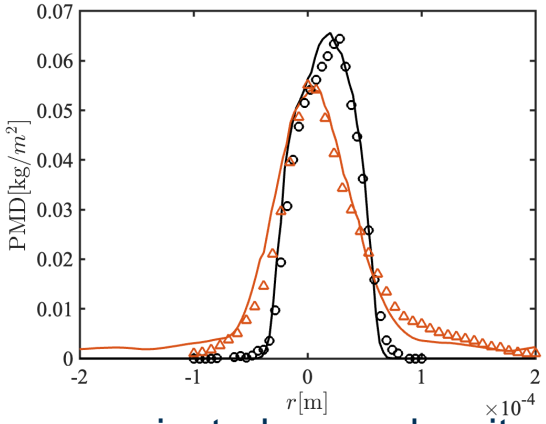
[1] - Hwang & **Jain**, *J. Comput. Phys.*, 2024 (accepted; in press)

O - exp (0.1 mm)
Δ - exp (2.0 mm)

Spray A



velocity



projected mass density

Grid: 46M CVs

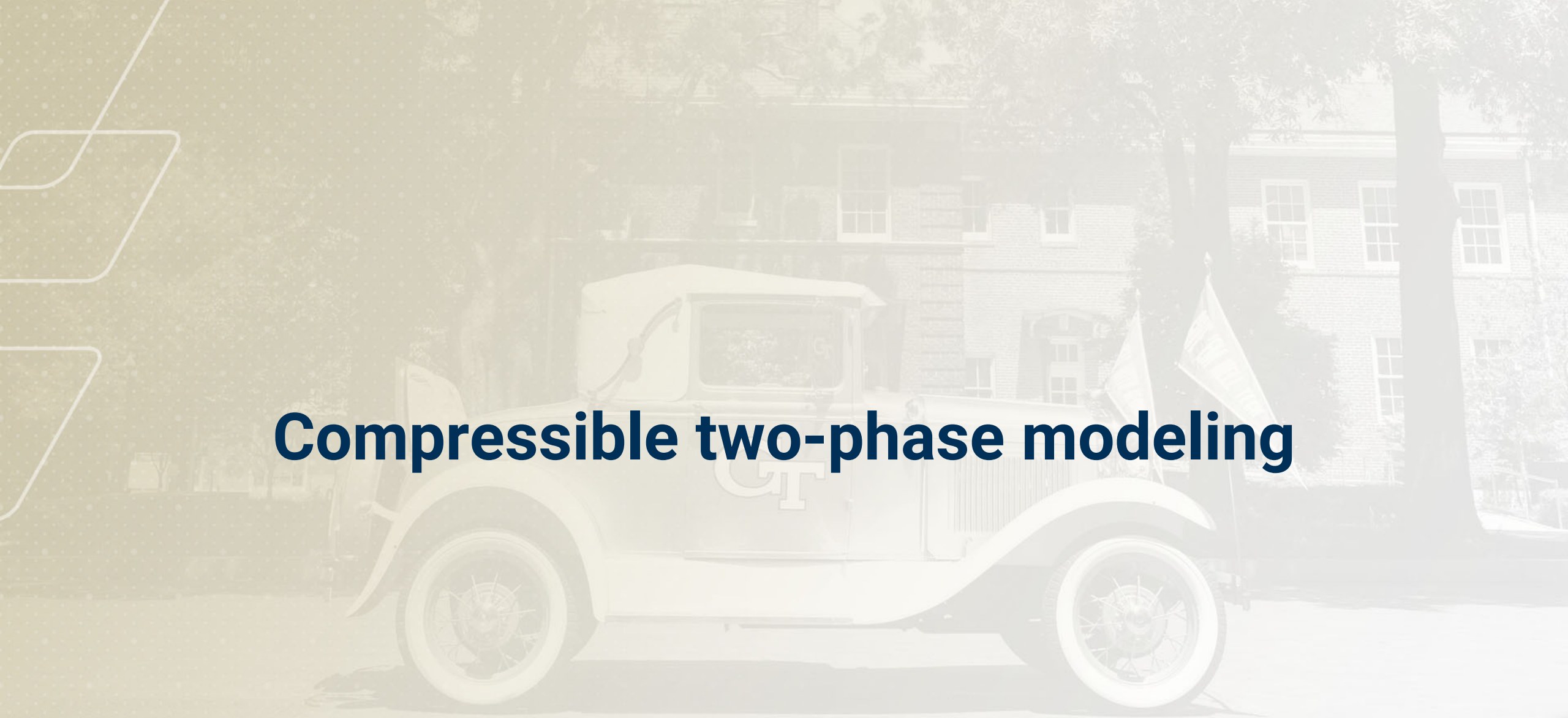


rendered using Blender

Hwang & **Jain**, *J. Comput. Phys.*, 2024 (accepted; in press)

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Compressible two-phase modeling



Baseline five-equation model

volume fraction:
$$\frac{\partial \phi_1}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi_1) = \phi_1(\vec{\nabla} \cdot \vec{u})$$

species mass:
$$\frac{\partial \rho_1 \phi_1}{\partial t} + \vec{\nabla} \cdot (\rho_1 \vec{u} \phi_1) = 0$$
$$\frac{\partial \rho_2 \phi_2}{\partial t} + \vec{\nabla} \cdot (\rho_2 \vec{u} \phi_2) = 0$$

momentum:
$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u} + p\mathbb{1}) = 0$$

total energy:
$$\frac{\partial E}{\partial t} + \vec{\nabla} \cdot (\vec{u}E) + \vec{\nabla} \cdot (\vec{u}p) = 0$$

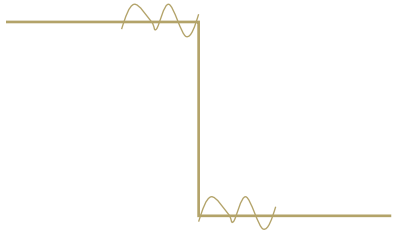
Isobaric closure law: $p = p_1 = p_2$

Mixture EOS: $p = f(\rho e, \phi_1, \alpha_1, \alpha_2, \beta_1, \beta_2, \ldots)$

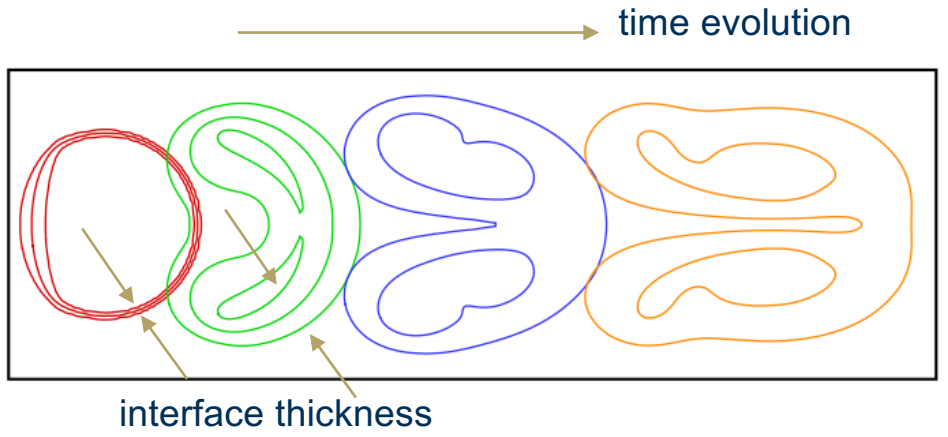
Kapila, *J. Comput. Phys.*, 2001; Allaire, *J. Comput. Phys.*, 2002

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- Cons:
  - cannot be used with a non-dissipative scheme

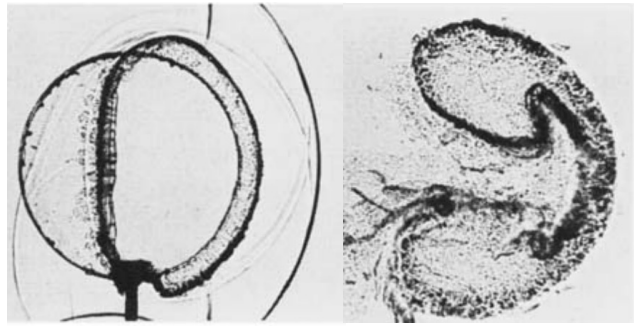


  - dissipative scheme: interface diffuses over time – poor accuracy



Mach 1.22 shock interaction with helium bubble in air [1]

Haas & Sturtevant, *J. Fluid Mech.*, 1987



[1] - Shukla et al., *J. Comput. Phys.*, 2010

Georgia Tech

Corrections to baseline five-equation model

volume fraction: $\frac{\partial \phi_1}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi_1) = \phi_1(\vec{\nabla} \cdot \vec{u})$

$\longrightarrow$ $\frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi) = \phi(\vec{\nabla} \cdot \vec{u}) + \vec{\nabla} \cdot \left[\Gamma \left\{ \epsilon \vec{\nabla}\phi - \frac{1}{4} \left\{ 1 - \tanh^2 \left(\frac{\psi}{2\epsilon} \right) \right\} \frac{\vec{\nabla}\psi}{|\vec{\nabla}\psi|} \right\} \right]$

species mass:

$$\frac{\partial \rho_1 \phi_1}{\partial t} + \vec{\nabla} \cdot (\rho_1 \vec{u} \phi_1) = 0$$

$$\frac{\partial \rho_2 \phi_2}{\partial t} + \vec{\nabla} \cdot (\rho_2 \vec{u} \phi_2) = 0$$

momentum: $\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u} + p\mathbb{1}) = 0$

total energy: $\frac{\partial E}{\partial t} + \vec{\nabla} \cdot (\vec{u}E) + \vec{\nabla} \cdot (\vec{u}p) = 0$

$\longrightarrow$?

global conservation of kinetic energy

conservation of entropy & interface equilibrium/thermodynamic consistency condition [1]

[1] - Abgrall, *J. Comput. Phys.*, 1996
Jain, Mani, & Moin, *J. Comput. Phys.*, **418**, 2020

Georgia Tech

Final conservative and consistent model

volume fraction:

$$\frac{\partial \phi_1}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi_1) = \phi_1(\vec{\nabla} \cdot \vec{u}) + \vec{\nabla} \cdot \vec{a}_1$$

species mass:

$$\frac{\partial \rho_1 \phi_1}{\partial t} + \vec{\nabla} \cdot (\rho_1 \vec{u} \phi_1) = \vec{\nabla} \cdot (\rho_1 \vec{a}_1)$$

$$\frac{\partial \rho_2 \phi_2}{\partial t} + \vec{\nabla} \cdot (\rho_2 \vec{u} \phi_2) = \vec{\nabla} \cdot (\rho_2 \vec{a}_2)$$

momentum:

$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u} + p\mathbb{1}) = \vec{\nabla} \cdot \left(\vec{u} \otimes \sum_{l=1}^{2} \rho_l \vec{a}_l \right) + \vec{\nabla} \cdot \underline{\underline{\tau}} + \sigma\kappa\vec{\nabla}\phi + \rho\vec{g}$$

total energy:

$$\frac{\partial E}{\partial t} + \vec{\nabla} \cdot (\vec{u}E) + \vec{\nabla} \cdot (\vec{u}p) = \vec{\nabla} \cdot \left(k \sum_{l=1}^{2} \rho_l \vec{a}_l \right) + \vec{\nabla} \cdot \left(\sum_{l=1}^{2} \rho_l h_l \vec{a}_l \right) + \vec{\nabla} \cdot (\underline{\underline{\tau}} \cdot \vec{u}) + \sigma\kappa\vec{u} \cdot \vec{\nabla}\phi + \rho\vec{g} \cdot \vec{u}$$

highlighted terms are the newly derived consistent regularization terms

viscous, surface tension, and gravity terms

general mixture EOS:

$$p = f(\rho e, \phi_1, \alpha_1, \alpha_2, \beta_1, \beta_2, ...)$$

discretized with a central scheme → low dissipative

Jain, Mani, & Moin, *J. Comput. Phys.*, **418**, 2020

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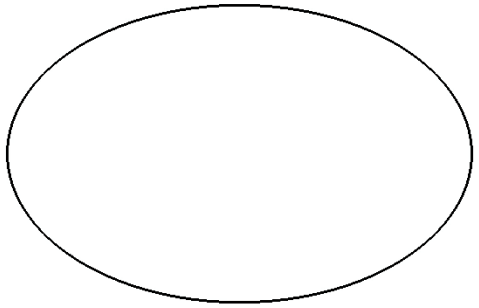
$$La = \frac{\rho d \sigma}{\mu^2}$$

Oscillating drop

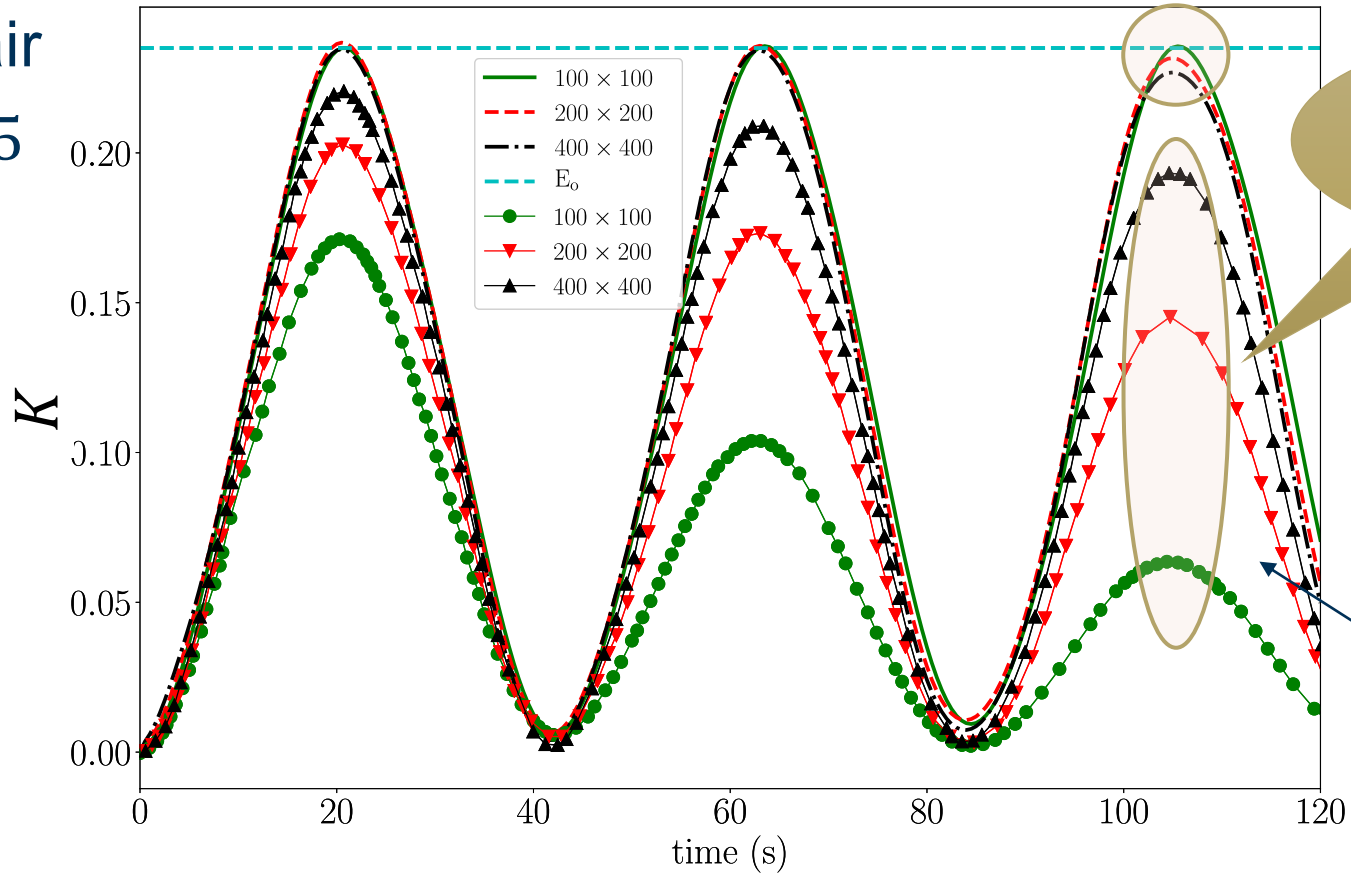
water droplet in air

$a = 0.625,\ b = 0.5$

$La = 1.4 \times 10^9$



Our results



due to numerical dissipation added to stabilize the flow

Garrick et al., *J. Comput. Phys.*, 2017

kinetic energy + surface energy $\approx E_o$ (constant) *

Jain, Mani, & Moin, *J. Comput. Phys.*, **418**, 2020

*when viscous effects are negligible

Georgia Tech

Acoustic-interface interaction: oblique incidence

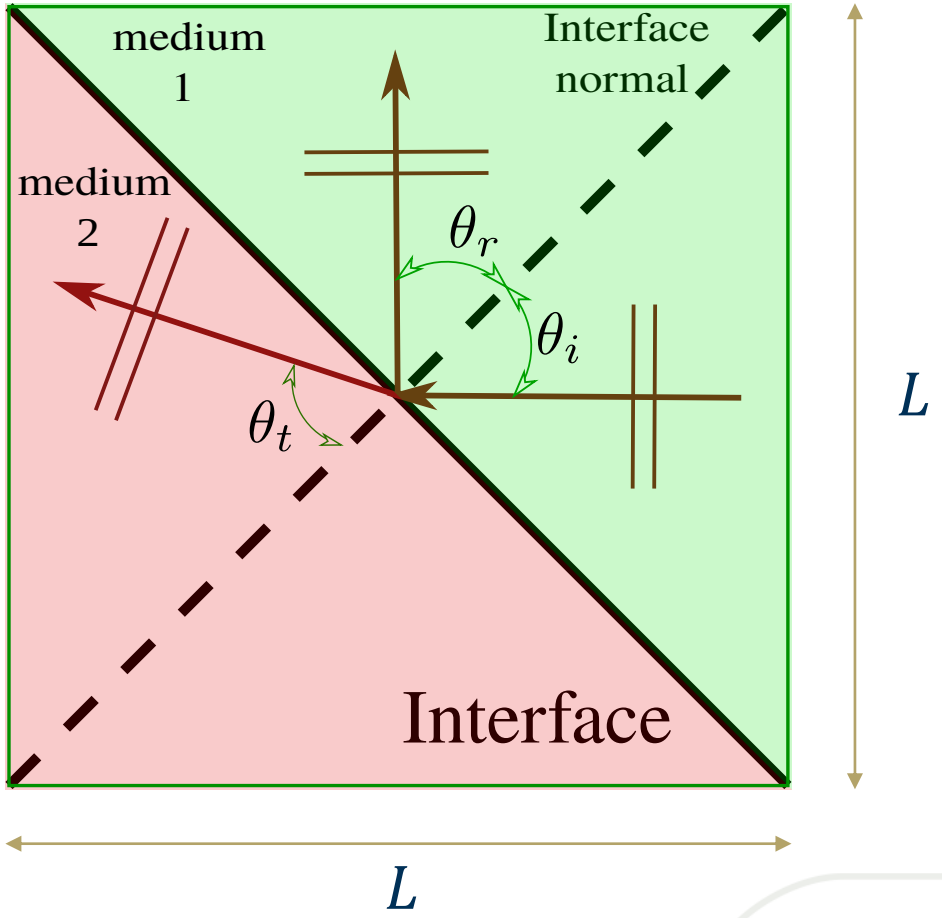
Setup:

- $2D$ domain
- medium 1: kerosene
- medium 2: water
- L=10μm

Snell's law:

$$\frac{\sin(\theta_i)}{c_1} = \frac{\sin(\theta_t)}{c_2}$$

$$\theta_r = \theta_i$$



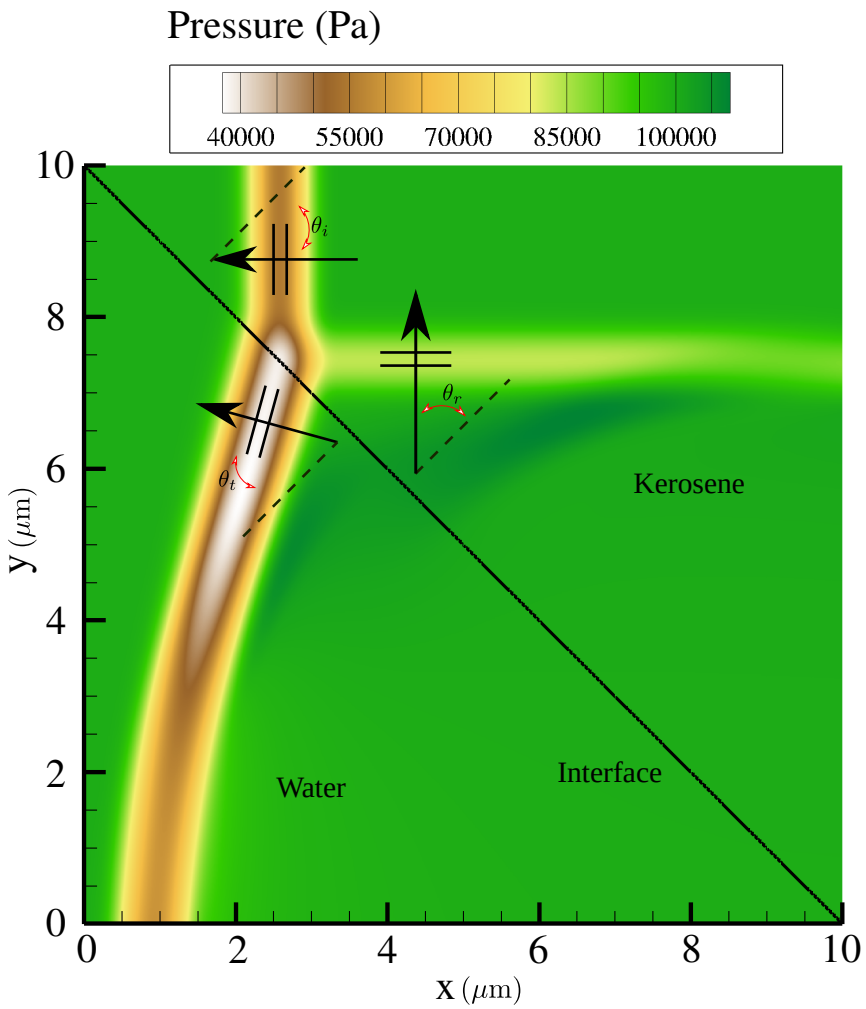
Jain, Mani, & Moin, *J. Comput. Phys.*, **418**, 2020

Georgia Tech

Acoustic-interface interaction: oblique incidence

$$\theta_i = 45°$$
$$\theta_r = 45°$$
$$\theta_t = 60.36°$$

	theory	simulation
$\mathbb{R}$	0.36238	0.36366
$\mathbb{T}$	1.36238	1.36452

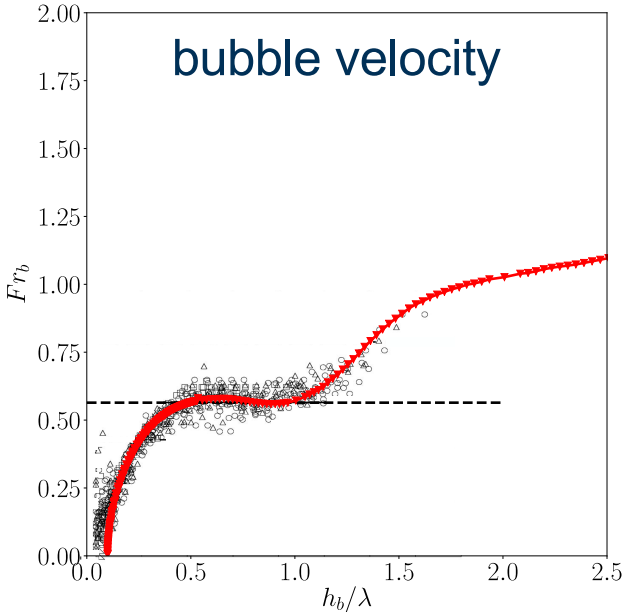


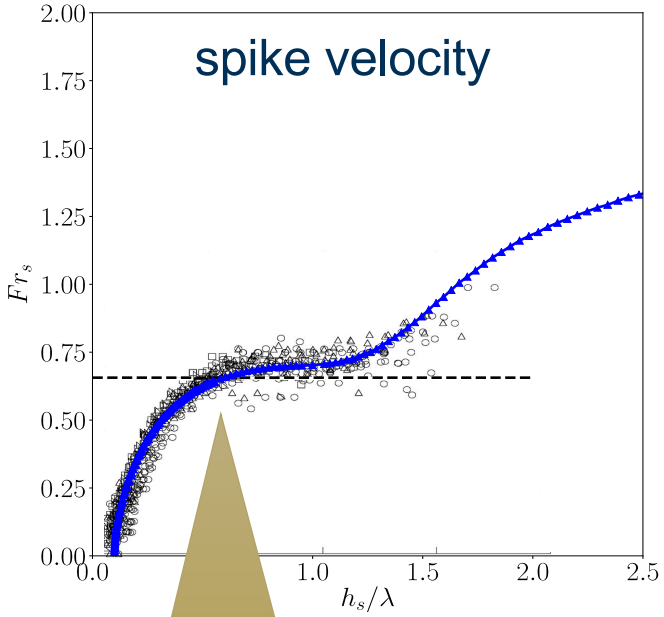
Jain, Mani, & Moin, *J. Comput. Phys.*, **418**, 2020

Three-dimensional Rayleigh-Taylor instability

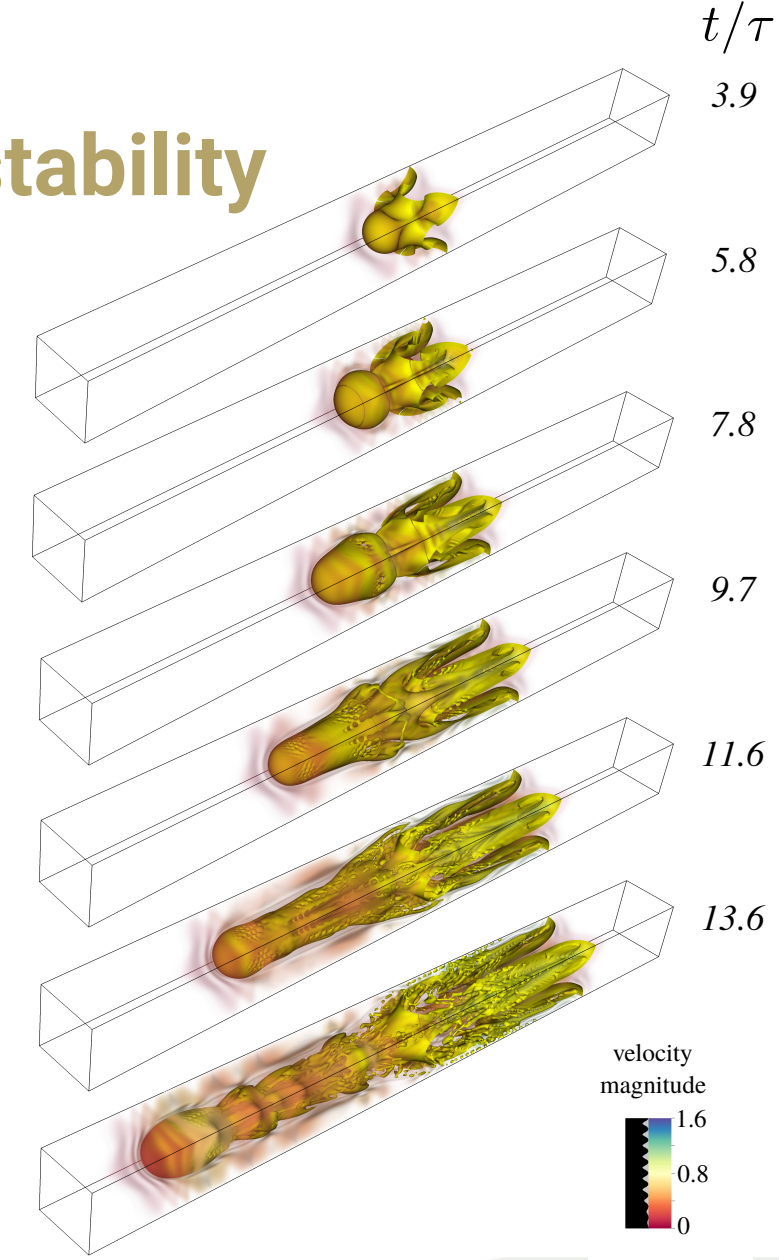
Setup:

- $12\lambda \times \lambda \times \lambda$
- $1200 \times 100 \times 100$
- $At = (\rho_1 - \rho_2)/(\rho_1 + \rho_2) = 0.15$
- $Re = \frac{U\lambda}{\nu} = 1000$





experimental results by Wilkinson and Jacobs, 2007



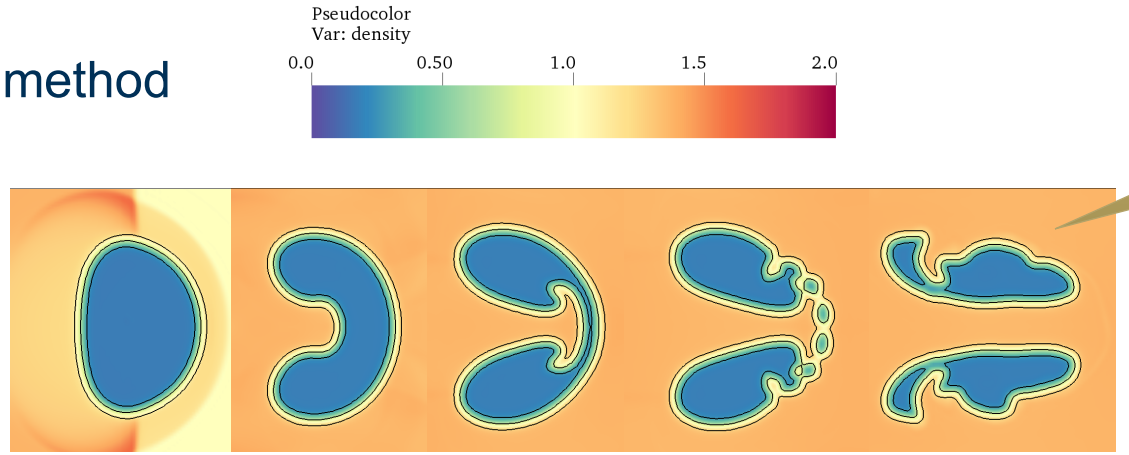
Jain, Mani, & Moin, *J. Comput. Phys.*, **418**, 2020

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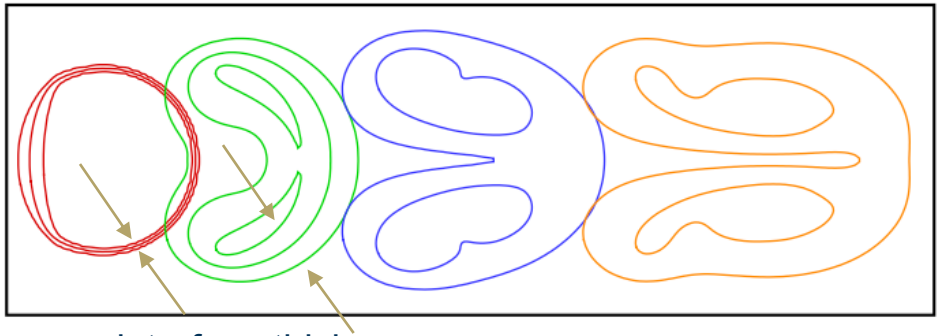
Shock-bubble interaction

Setup:

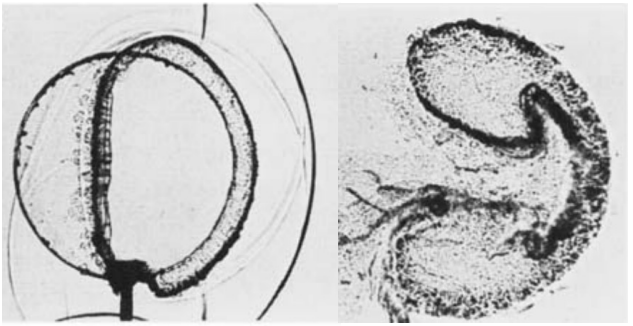
- LAD shock-capturing method
- $M = 1.22$ shock
- bubble: helium
- medium: air



interface thickness is preserved



Haas & Sturtevant, *J. Fluid Mech.*, 1987



Jain, Adler, West, Mani, Moin, & Lele, *J. Comput. Phys.*, **475**, 2023

Georgia Tech

Summary of this section

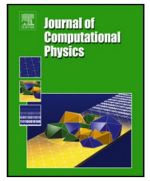
- A model for compressible two-phase flows
  - conservative and consistent model – robust simulations
  - low-dissipative method – cost effective
  - acoustic-interface interaction simulations
  - shock-interface interaction simulations

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A conservative diffuse-interface method for compressible two-phase flows

Suhas S. Jain *, Ali Mani, Parviz Moin

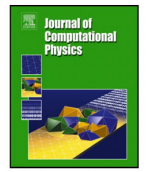
Center for Turbulence Research, Stanford University, CA, 94305, USA

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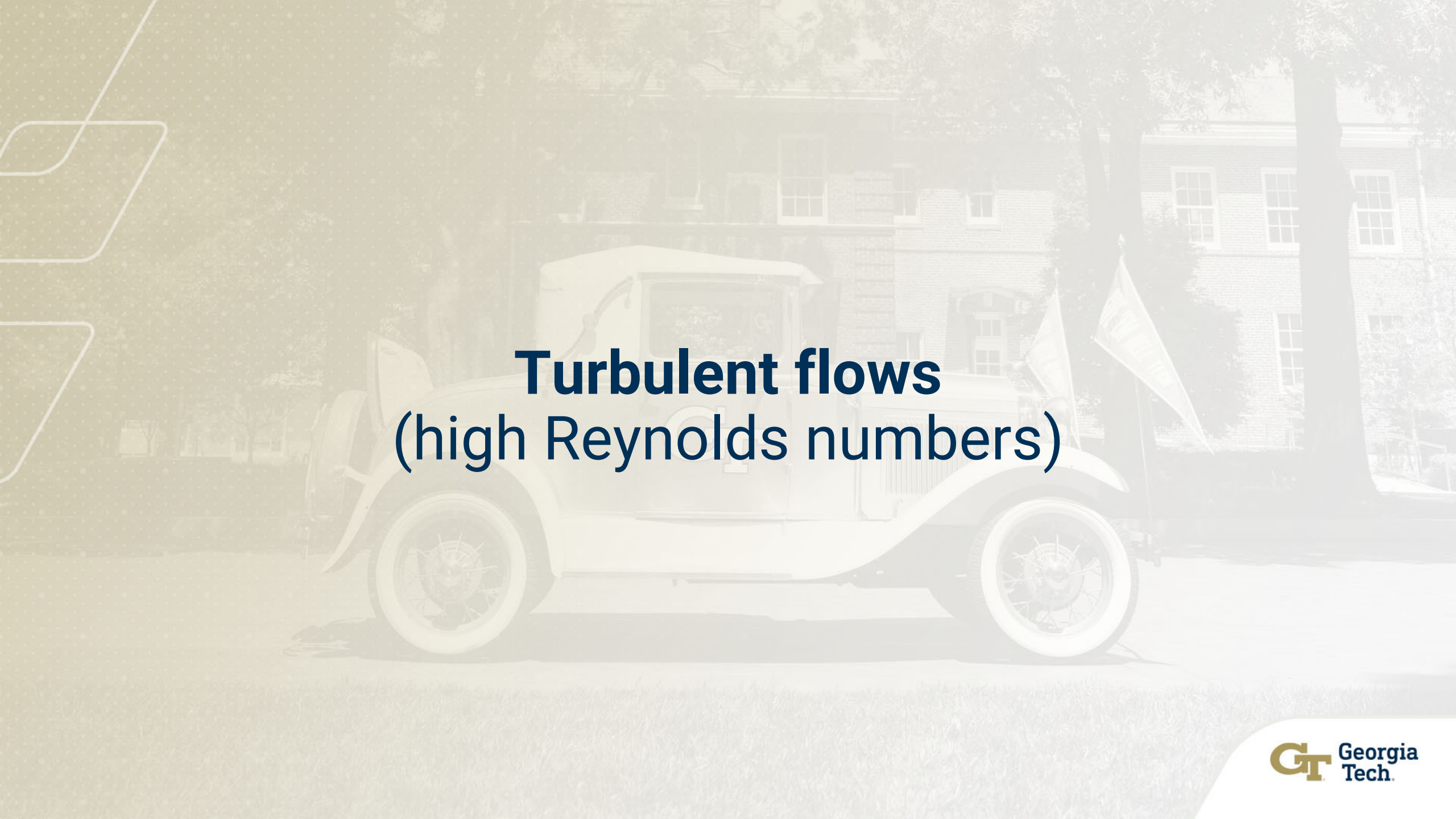
journal homepage: www.elsevier.com/locate/jcp



Assessment of diffuse-interface methods for compressible multiphase fluid flows and elastic-plastic deformation in solids

Suhas S. Jain *,[1], Michael C. Adler [1], Jacob R. West [1], Ali Mani, Parviz Moin, Sanjiva K. Lele

Center for Turbulence Research, Stanford University, CA 94305, USA

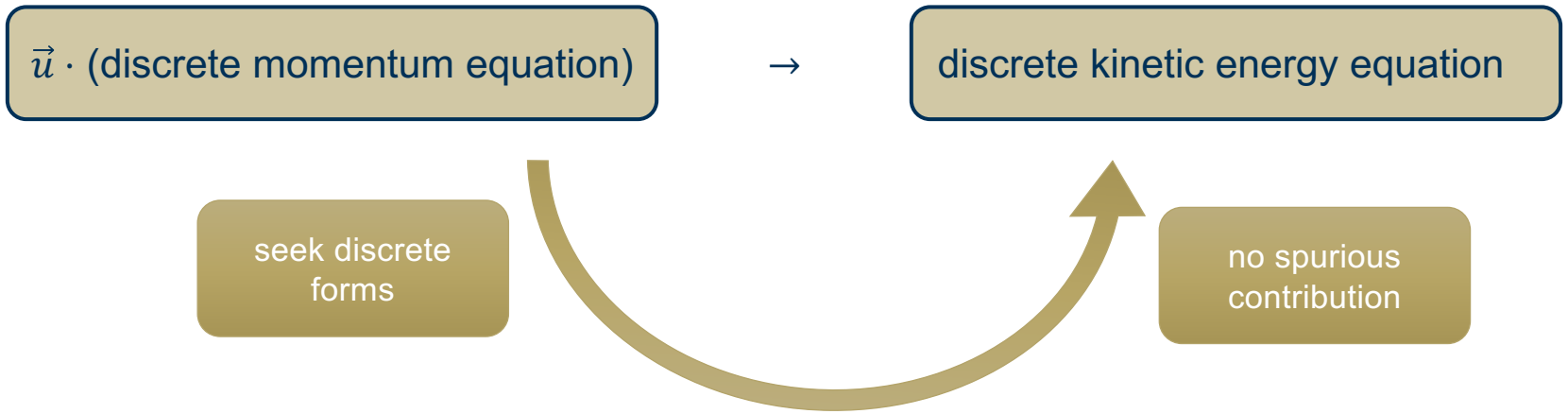


Turbulent flows
(high Reynolds numbers)

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Kinetic energy preserving (KEP) scheme

- Discrete conservation of kinetic energy:
  - improves numerical stability
  - approach:



  - sufficient condition for numerical stability → incompressible flows [1]

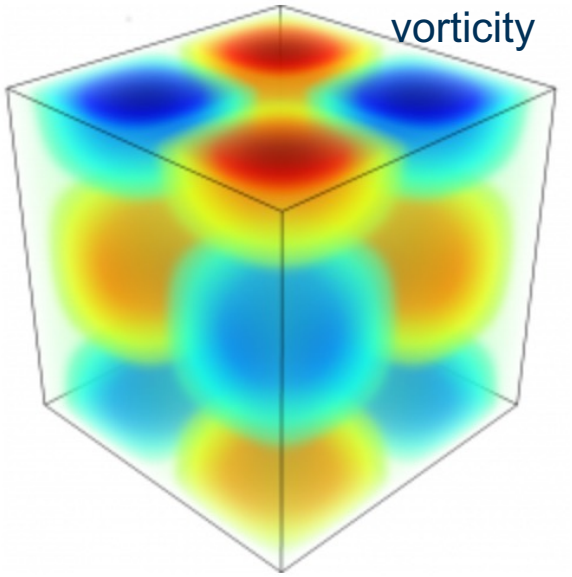
[1] – Morinishi et al., *J. Comput. Phys.*, 1998

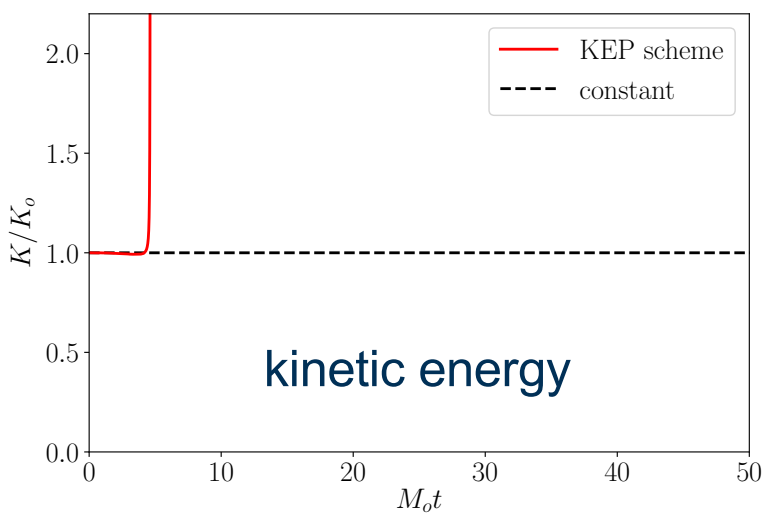
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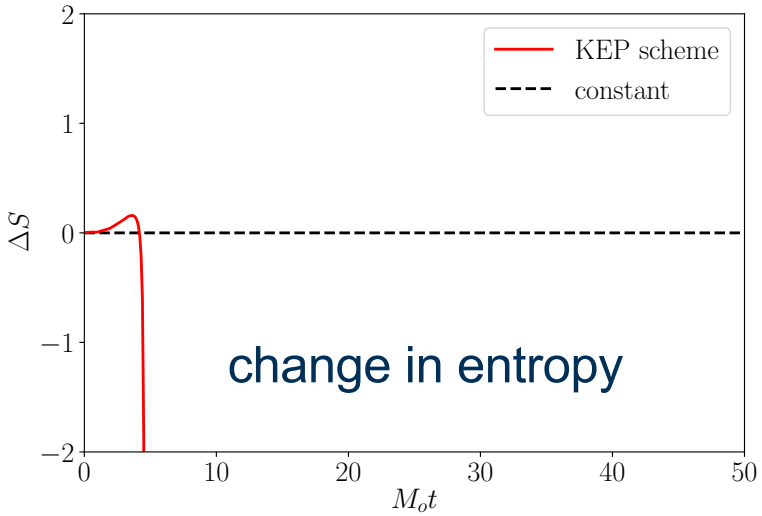
Taylor-Green vortex at infinite Re with KEP

- coarse-grid simulation – test of robustness

single phase compressible flow







$M_o = 0.05$

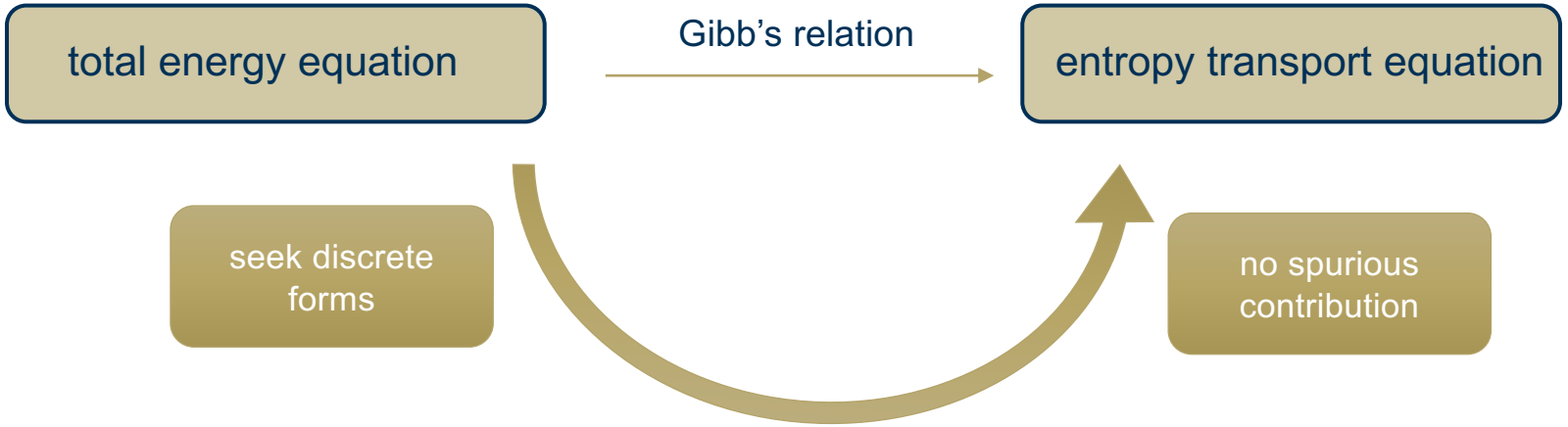
- Kinetic energy preserving (KEP) scheme [1]
  - not a sufficient condition for numerical stability → compressible flows

[1] – Feireisen, *PhD thesis*, 1983

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Kinetic energy-and entropy-preserving (KEEP) scheme

- Solve total energy equation
- approximate conservation of entropy



Other methods* fail to satisfy thermodynamic equilibrium

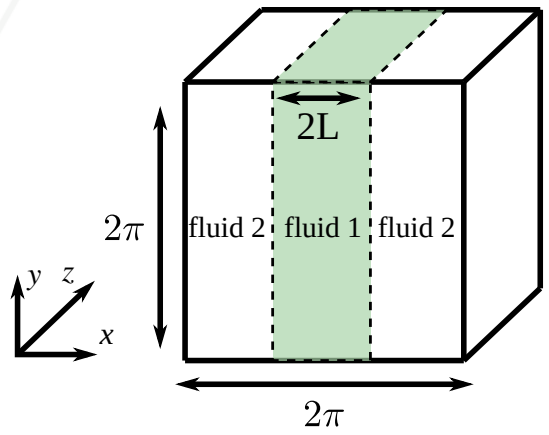
* Kennedy & Gruber, J. *Comput. Phys.*, 2008
Chandrashekar, *Comm. Comput. Phys.*, 2013
Kuya et al., *J. Comput. Phys.*, 2018

Jain & Moin, *J. Comput. Phys.*, **464**, 2022

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Taylor-Green vortex at $Re = \infty$

grid size: 64^3
$\rho_2/\rho_1 = 10$
$L = 1$

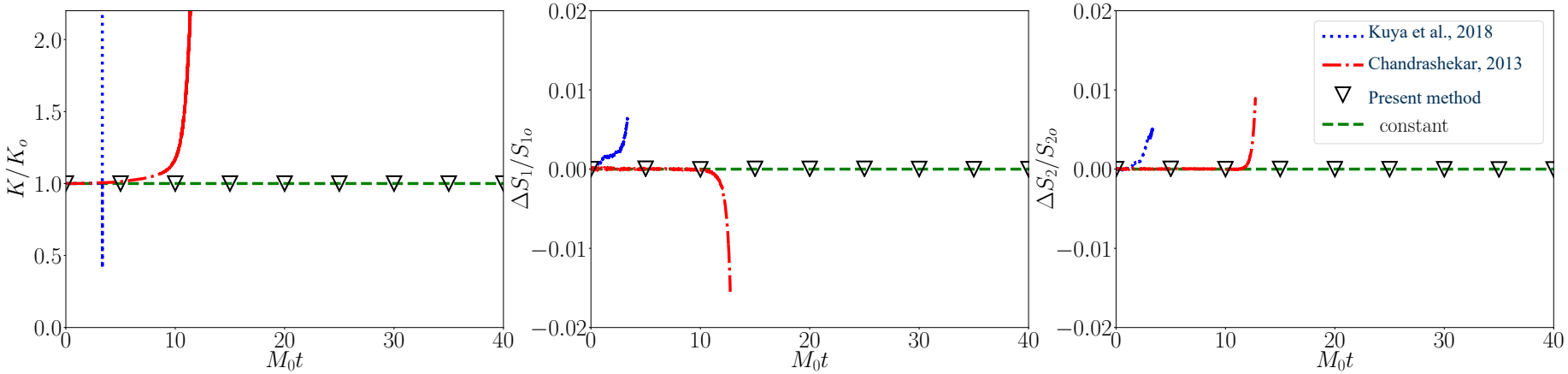


similar behavior with isotropic turbulence at $Re = \infty$

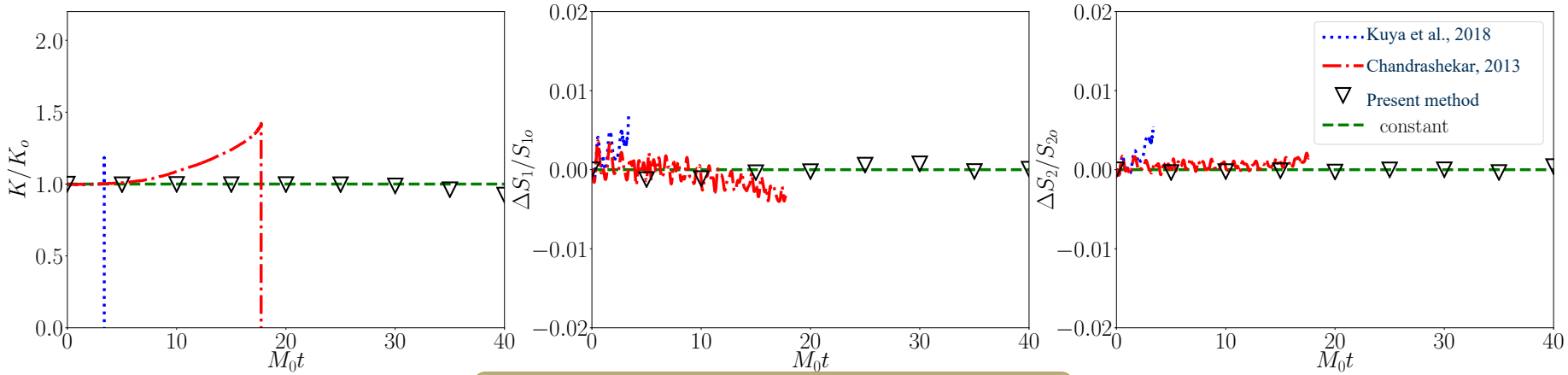
Kinetic energy

Change in entropy of fluid 1

Change in entropy of fluid 2



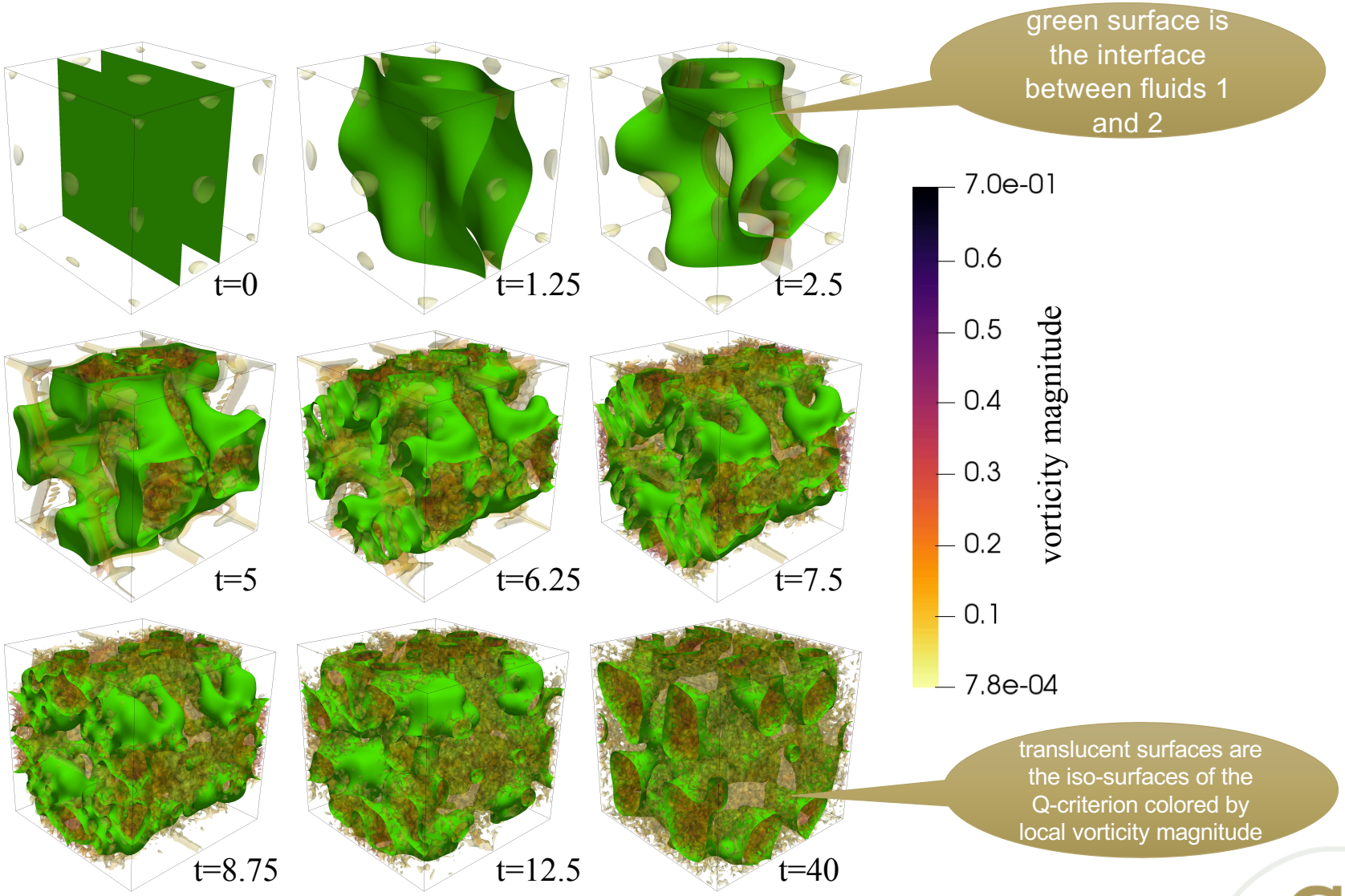
$M_o = 0.05$



$M_o = 0.2$

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Snapshots

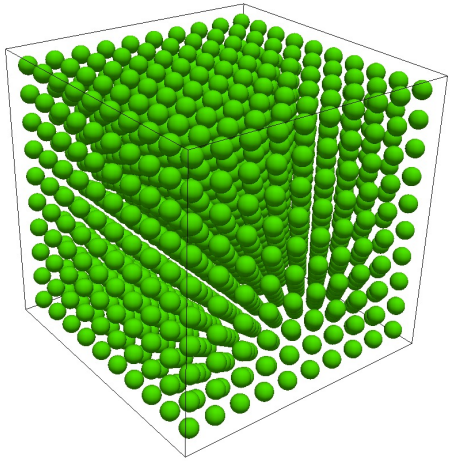


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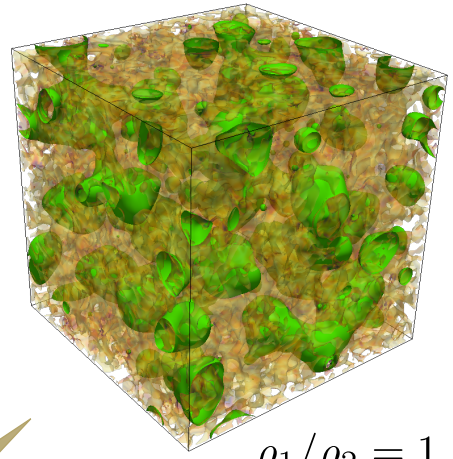
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Droplet-laden compressible isotropic turbulence

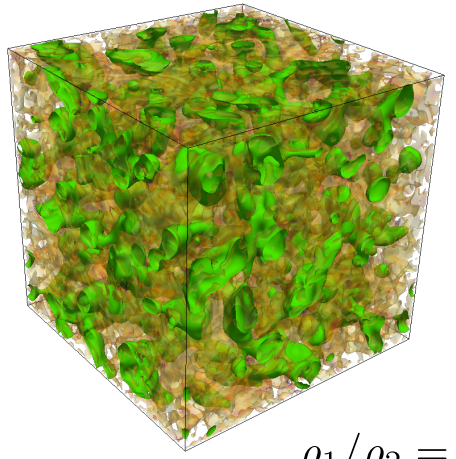
$(t = 0)$



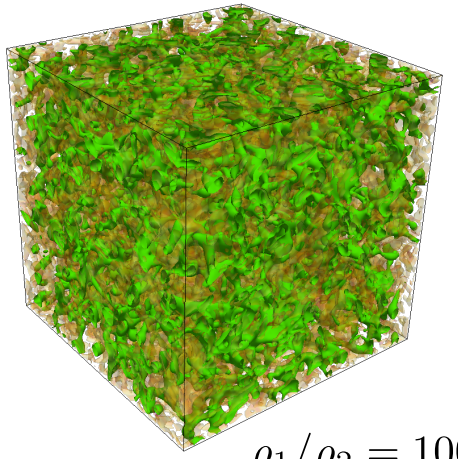
$(t = 20)$



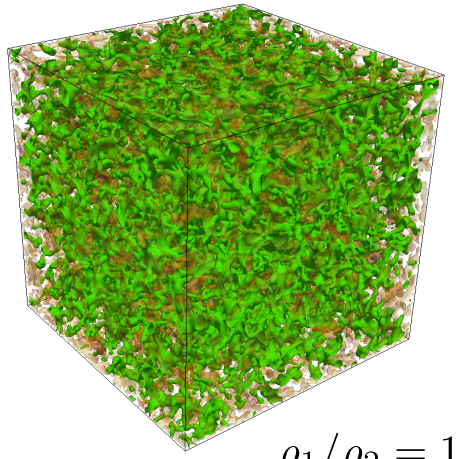
$\rho_1/\rho_2 = 1$



$\rho_1/\rho_2 = 10$



$\rho_1/\rho_2 = 100$



$\rho_1/\rho_2 = 1000$

Setup:

- $\rho_{2o} = 1$
- $\rho_{1o} = 1, 10, 100, 1000$
- $Re_{\lambda 2o} = 75$
- $M_{t1o} = M_{t2o} = 0.07$
- $We_{rms} = 1$
- uniformly spaced 1000 droplets

increased drop size

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Summary of this section

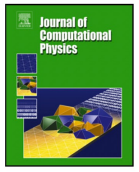
- A robust KEEP scheme for compressible two-phase flows
  - stable method for high-Re simulations
  - droplet-laden compressible isotropic turbulence

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A kinetic energy–and entropy-preserving scheme for compressible two-phase flows

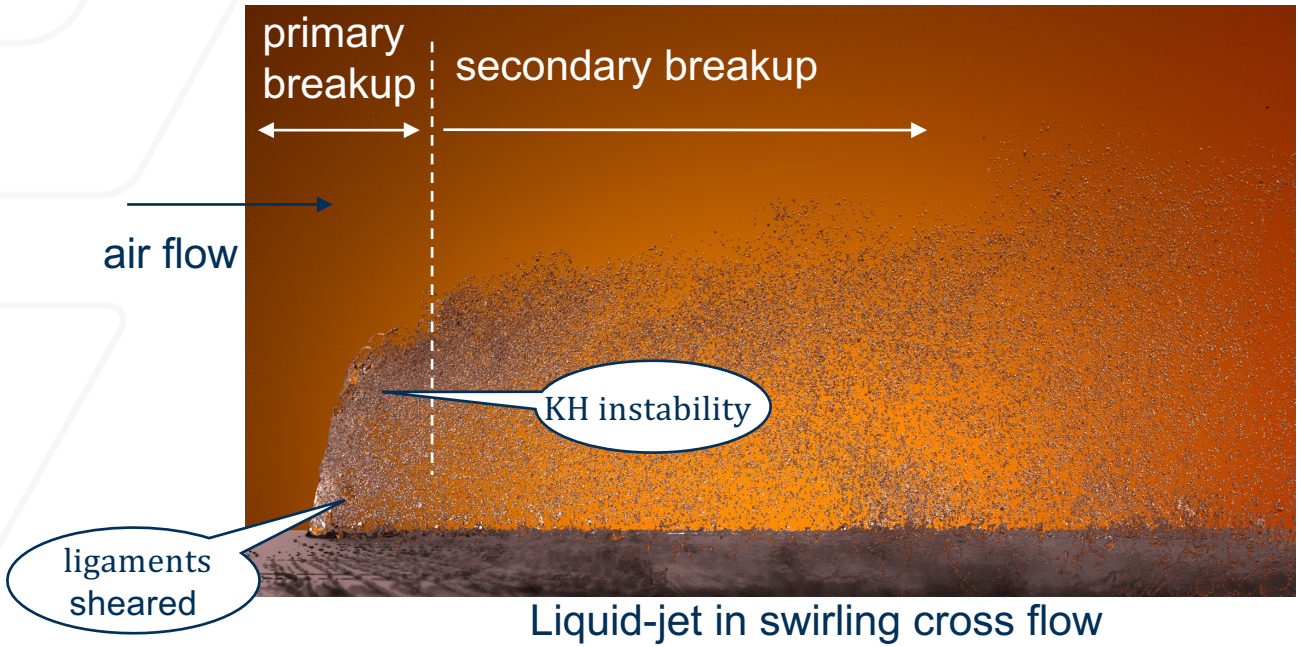
Suhas S. Jain*, Parviz Moin

Center for Turbulence Research, Stanford University, California, 94305, USA

Related past and ongoing work

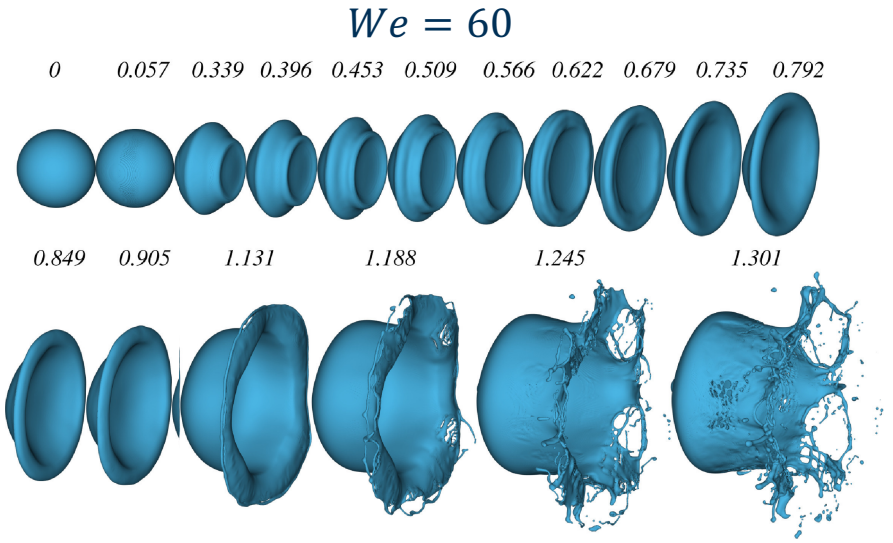


Primary and secondary atomization, phase change



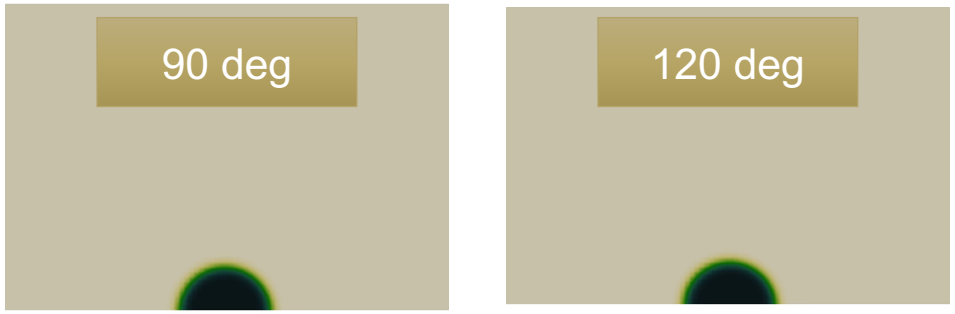
Liquid-jet in swirling cross flow

Prakash, **Jain,** Lovett, Raghunandan, Ravikrishna, & Tomar, *At. Sprays*, 2019



Effect of density on secondary breakup

Jain, Tyagi, Prakash, Ravikrishna, & Tomar, *Int. J. Multiph. Flow*, 2019



Bubble detaching from superheated wall

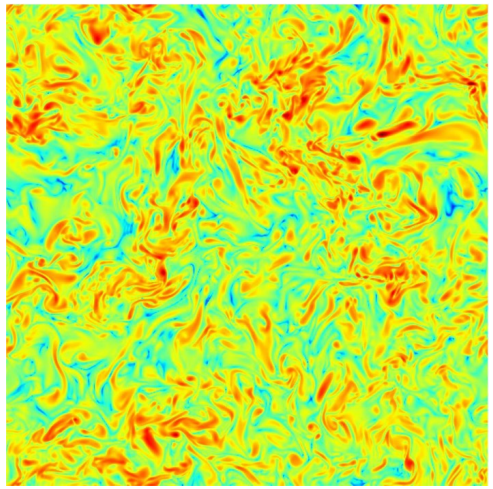
Scapin, et al., 2023

(collaboration with Luca Brandt)

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Particle-laden flows & data-driven methods

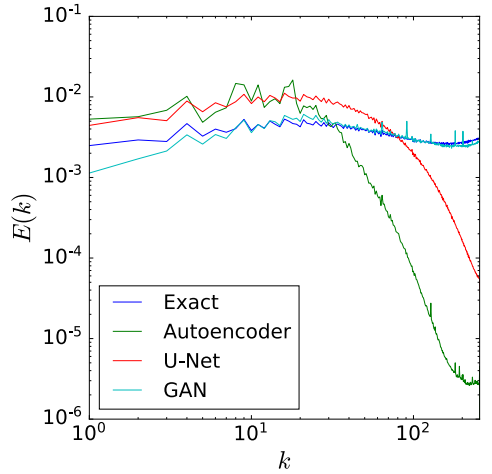
enstrophy



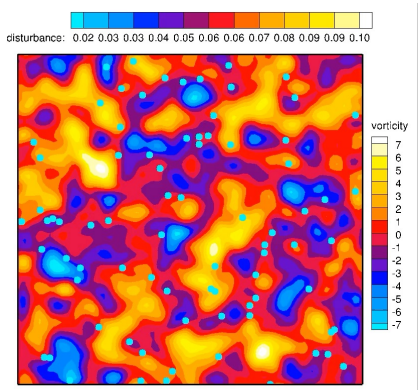
particle density



particle density spectrum



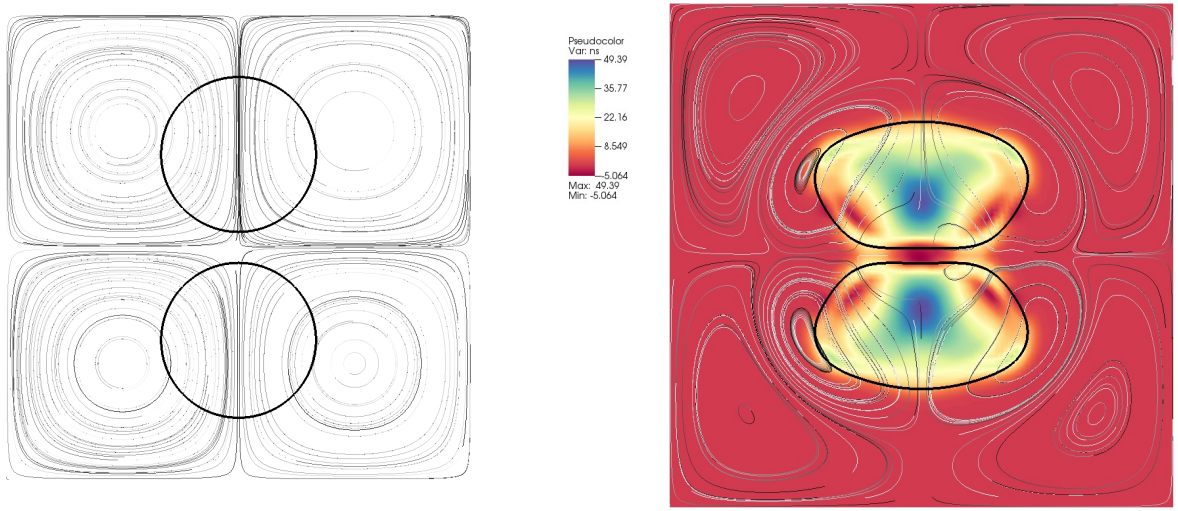
Modeling particle clustering and flow reconstruction using neural networks
Oujia & **Jain** et al., 2023 (collaboration with Kai Schneider)

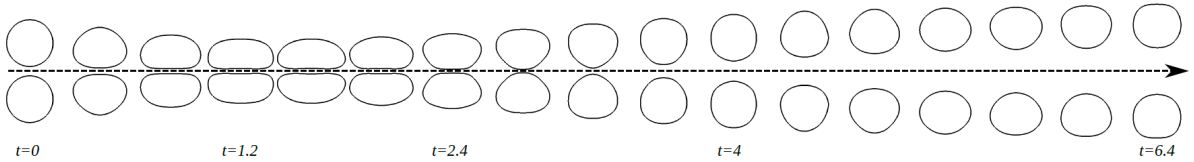


Self-induced disturbance of particles in HIT
Keane, Apte, **Jain**, Khanwale, *IJMF*, 2023
(collaboration with Sourabh Apte)

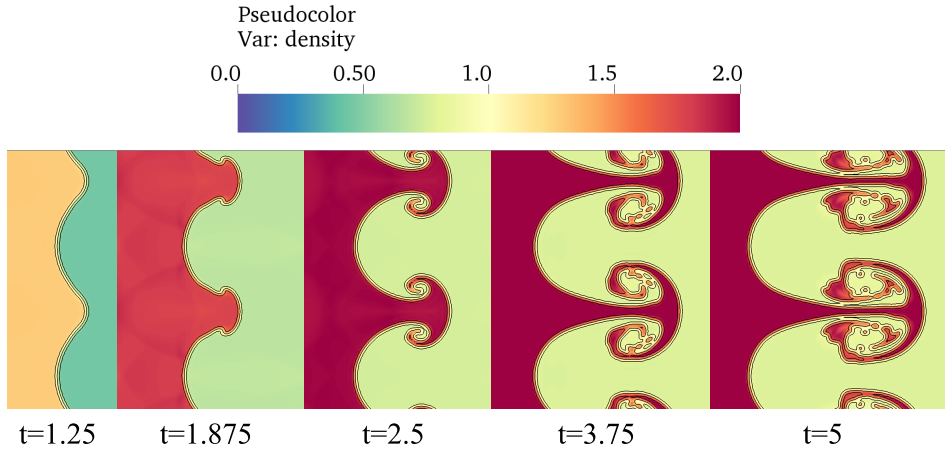
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Fluid-solid & solid-solid interactions





Reference map technique for incompressible hyperelastic solids in fluids
Jain et al., *J. Comput. Phys.*, 2019
(collaboration with Ken Kamrin)



Elastic-plastic deformation of Cu-Al shock-interface interaction
Jain, Adler, West, Mani, Moin, & Lele, *J. Comput. Phys.*, **475**, 2023

Georgia Tech

Conclusions

- A new *phase-field (ACDI) model* for two-phase flows
  - more accurate and sharper interface
    - low-cost simulations
  - mo
    -
    -
  - nat
    -
  - natural extension to compressible flows
  - kinetic-energy and entropy preserving formulation
    - robust for high-Re and high-density ratio turbulent flows

A promising interface-capturing method for efficient simulations of two-phase turbulent flows with complex geometries

Georgia Tech

Thank you

•*Acknowledgments:*

- *Prof. Parviz Moin, colleagues, and collaborators*

•*Funding support:*

- *Franklin P. and Caroline M. Johnson Stanford Graduate Fellowship*
- *National Overseas Scholarship*

Questions?

