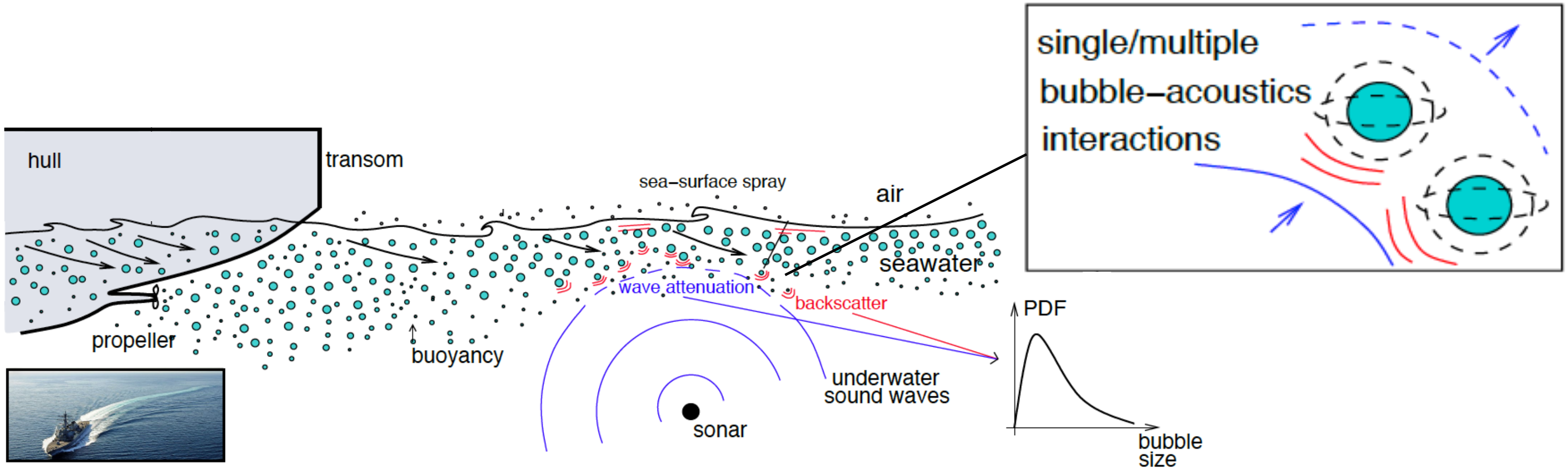
A conservative diffuse-interface method for simulation of two-phase compressible flows with acoustics

Suhas S Jain, Ali Mani & Parviz Moin

Center for Turbulence Research, Stanford University

20th November 2018

Introduction and Motivation



(courtesy: Dr. J. Urzay)

applications

- bubble acoustics
- high pressure liquid fuel injection

challenges

- Need to **maintain thermodynamic consistency** at the interface.
- Numerical study of turbulence and acoustics require
  - **a stable method for long-time integrations**
  - **a non-dissipative method**
  - **a conservative method**

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

Five-equation model

$$\frac{\partial \phi_1}{\partial t} + \vec{u} \cdot \vec{\nabla} \phi_1 = 0,$$

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

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

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

$$\frac{\partial \rho (e+k)}{\partial t} + \vec{\nabla} \cdot (\rho H \vec{u}) = 0,$$

Closure:

$$p = f(\rho_1 \phi_1, \rho_2 \phi_2, \rho e, \phi_1)$$

[Allaire et al., *JCP*, 2002]

diffuse-interface (DI) vs sharp-interface methods (SI)

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

sharp-interface methods

- Hermann, *CTR Summer Proc.*, 2016 - geometric volume of fluid (VoF)
- Huber et al., *JCP*, 2015 - level set
- He et al., *JCP*, 2015 - algebraic VoF

advantages of DI methods over SI methods

- less expensive
- easy load balancing and parallel scalability
- conserves mass of each phase discretely

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

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

State-of-the-art methods

five-equation model

- Perigaud & Saurel, *JCP*, 2005 → capillary and viscous effects
- Shukla et al., *JCP*, 2010 & Tiwari et al., *JCP*, 2013 → interface regularization
- Chiapolino et al., *JCP*, 2017 → unstructured grids

Other models

- Abgrall, *JCP*, 1996 → four-equation model
- Saurel & Abgrall, *JCP*, 1999 → seven-equation model

Summary

- five-equation model is the most preferred choice
- no previous implementation using non-dissipative schemes
- all interface regularization (sharpening) terms are in non-conservative form
- no previous study of bubble acoustics in turbulent environment

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Proposed model

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

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

$$\frac{\partial \rho_l \phi_l}{\partial t} + \vec{\nabla}\cdot(\rho_l\vec{u}\phi_l) = \boxed{\vec{\nabla}\cdot R_l} \qquad l = 1, 2$$

$$\frac{\partial \rho\vec{u}}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}\otimes\vec{u} + p\mathbb{1}) = \vec{\nabla}\cdot\underline{\underline{\tau}} + \boxed{\vec{\nabla}\cdot(\vec{f}\otimes\vec{u})}$$

$$\frac{\partial E}{\partial t} + \vec{\nabla}\cdot(\vec{u}E) + \vec{\nabla}\cdot(p\vec{u}) = \boxed{\vec{\nabla}\cdot(\vec{f}k)} + \vec{\nabla}\cdot(\underline{\underline{\tau}}\cdot\vec{u}) + \boxed{\sum_{l=1}^{2}\vec{\nabla}\cdot(\rho_l h_l \vec{a}_l)}$$

Closure:

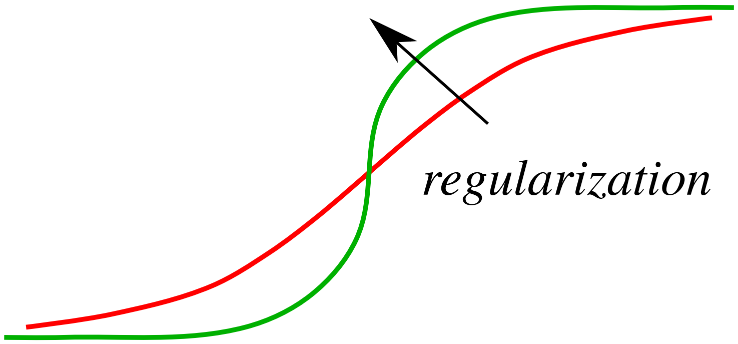
$$p = \frac{\rho e + \left(\frac{\phi\beta_1}{\alpha_1} + \frac{(1-\phi)\beta_2}{\alpha_2}\right)}{\left(\frac{\phi}{\alpha_1} + \frac{1-\phi}{\alpha_2}\right)}$$

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Improvements over the state-of-the-art methods

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

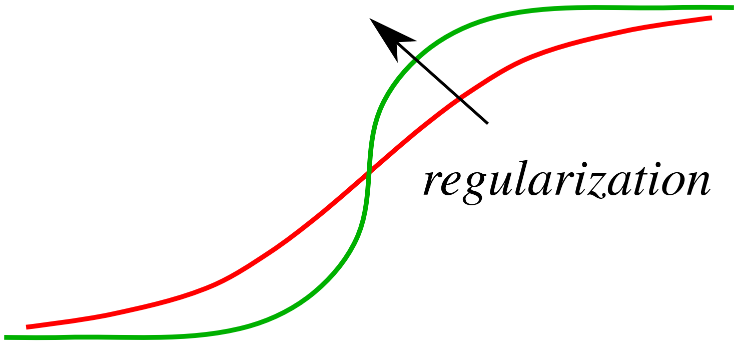
1. conservative form of regularization terms.
   - mass of each phase, momentum and energy is discretely conserved.



[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Improvements over the state-of-the-art methods

1. conservative form of regularization terms.
   - mass of each phase, momentum and energy is discretely conserved.
2. satisfies interface equilibrium condition.



interface equilibrium condition

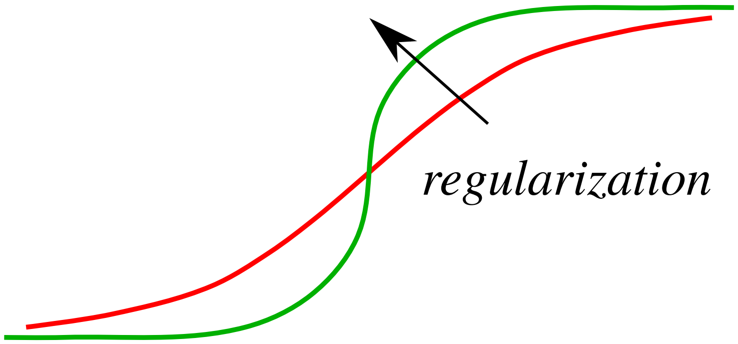
If $u_i^k = u_0$ and $p_i^k = p_0$ then, $u_i^{k+1} = u_0$ and $p_i^{k+1} = p_0$ should be satisfied. (Abgrall, *JCP*, 1996)

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Improvements over the state-of-the-art methods

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

1. conservative form of regularization terms.
   - mass of each phase, momentum and energy is discretely conserved.
2. satisfies interface equilibrium condition.
3. central-difference scheme (non-dissipative).

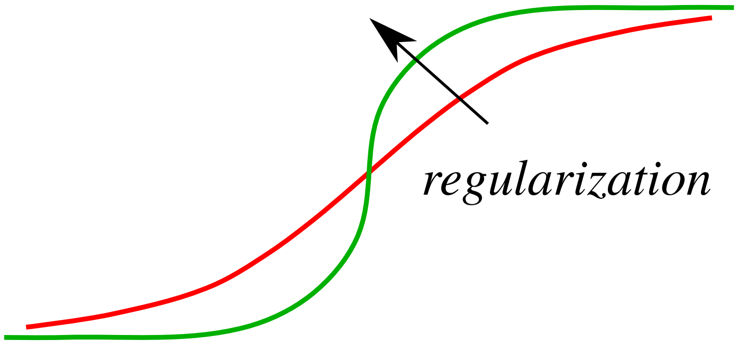


[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Improvements over the state-of-the-art methods

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

1. conservative form of regularization terms.
   - mass of each phase, momentum and energy is discretely conserved.
2. satisfies interface equilibrium condition.
3. central-difference scheme (non-dissipative).
4. volume fraction equation $\Rightarrow$ bounded ϕ.



volume fraction advection equation

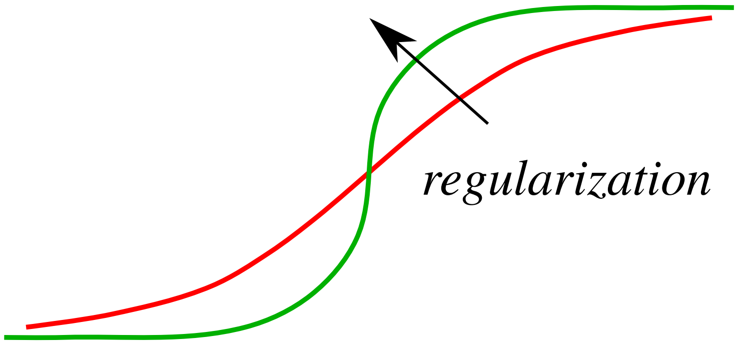
$$\frac{\partial \phi_1}{\partial t} + \vec{\nabla} \cdot (\vec{u}\phi_1) = \phi_1(\vec{\nabla} \cdot \vec{u}) + \vec{\nabla} \cdot \vec{a}$$

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

Improvements over the state-of-the-art methods

1. conservative form of regularization terms.
   - mass of each phase, momentum and energy is discretely conserved.
2. satisfies interface equilibrium condition.
3. central-difference scheme (non-dissipative).
4. volume fraction equation $\Rightarrow$ bounded ϕ.
5. mass balance equation $\Rightarrow$ consistent with ϕ.



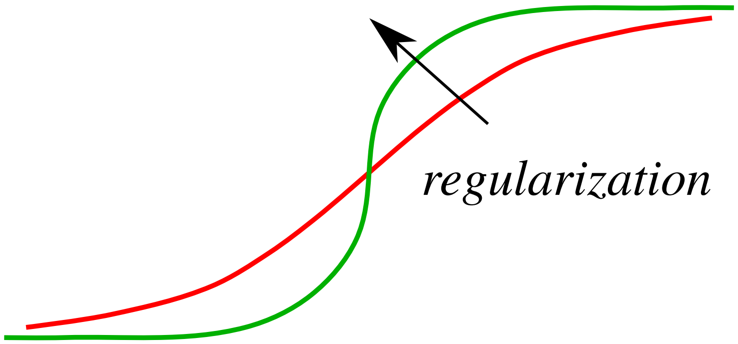
mass balance equation

$$\frac{\partial \rho_l \phi_l}{\partial t} + \vec{\nabla} \cdot (\rho_l \vec{u} \phi_l) = \vec{\nabla} \cdot R_l \qquad l = 1, 2$$

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Improvements over the state-of-the-art methods

1. conservative form of regularization terms.
   - mass of each phase, momentum and energy is discretely conserved.
2. satisfies interface equilibrium condition.
3. central-difference scheme (non-dissipative).
4. volume fraction equation $\Rightarrow$ bounded ϕ.
5. mass balance equation $\Rightarrow$ consistent with ϕ.
6. momentum equation $\Rightarrow$ kinetic energy conservation.



momentum equation

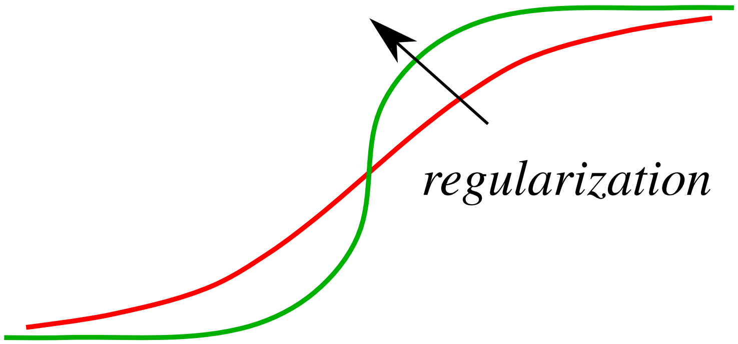
$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u} + p \mathbb{1}) = \vec{\nabla} \cdot \underline{\underline{\tau}} + \vec{\nabla} \cdot (\vec{f} \otimes \vec{u})$$

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Improvements over the state-of-the-art methods

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

1. conservative form of regularization terms.
   - mass of each phase, momentum and energy is discretely conserved.
2. satisfies interface equilibrium condition.
3. central-difference scheme (non-dissipative).
4. volume fraction equation $\Rightarrow$ bounded ϕ.
5. mass balance equation $\Rightarrow$ consistent with ϕ.
6. momentum equation $\Rightarrow$ kinetic energy conservation.
7. energy equation $\Rightarrow$ approximate entropy conservation.



energy equation

$$\frac{\partial E}{\partial t} + \vec{\nabla}\cdot(\vec{u}E) + \vec{\nabla}\cdot(p\vec{u}) = \vec{\nabla}\cdot(\vec{f}k) + \vec{\nabla}\cdot(\underline{\underline{\tau}}\cdot\vec{u}) + \sum_{l=1}^{2}\vec{\nabla}\cdot(\rho_l h_l \vec{a}_l)$$

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

Verification cases

Fluid properties:

Stiffened gas equation of state: $p = (\gamma - 1)\rho e - \pi$

	air	water
ρ (kg/m^3)	1.225	997
μ (N/m^2)	0.0000181	0.00089
γ	1.4	4.4
π (MPa)	0	600

Analytical solution:

Rayleigh-Plesset equation in 2D bounded domain

$$\frac{P_B(t) - P_S(t)}{\rho_L} = ln\left(\frac{S}{R}\right)\left\{R\ddot{R} + (\dot{R})^2\right\} + \left(\frac{R^2 - S^2}{2S^2}\right) + \frac{2\nu_L \dot{R}}{R} + \frac{\sigma}{\rho_L R}$$

Pressure driven bubble oscillation

Physical parameters:

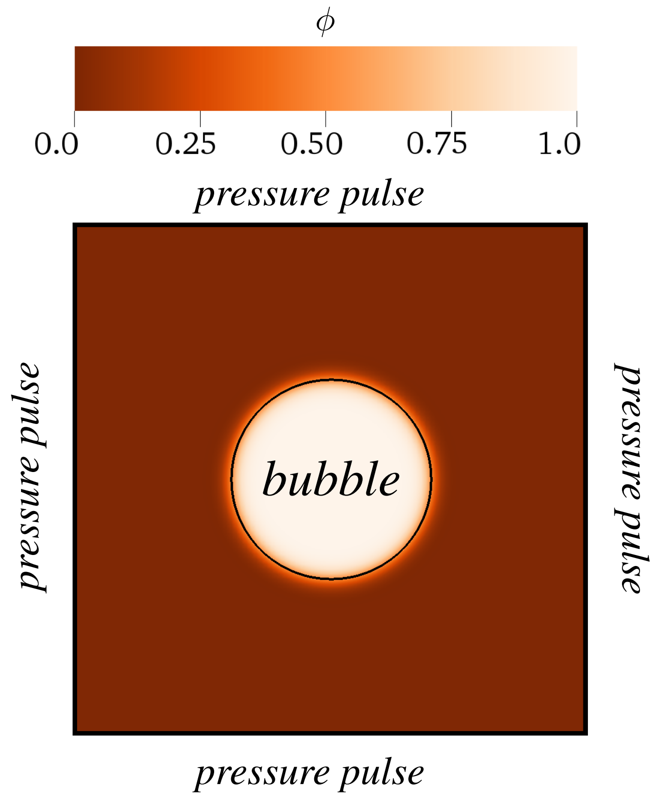
- Fluids: *air, water*
- Domain: $10\mu\text{m} \times 10\mu\text{m}$
- Bubble diameter: $4\mu\text{m}$

Simulation parameters:

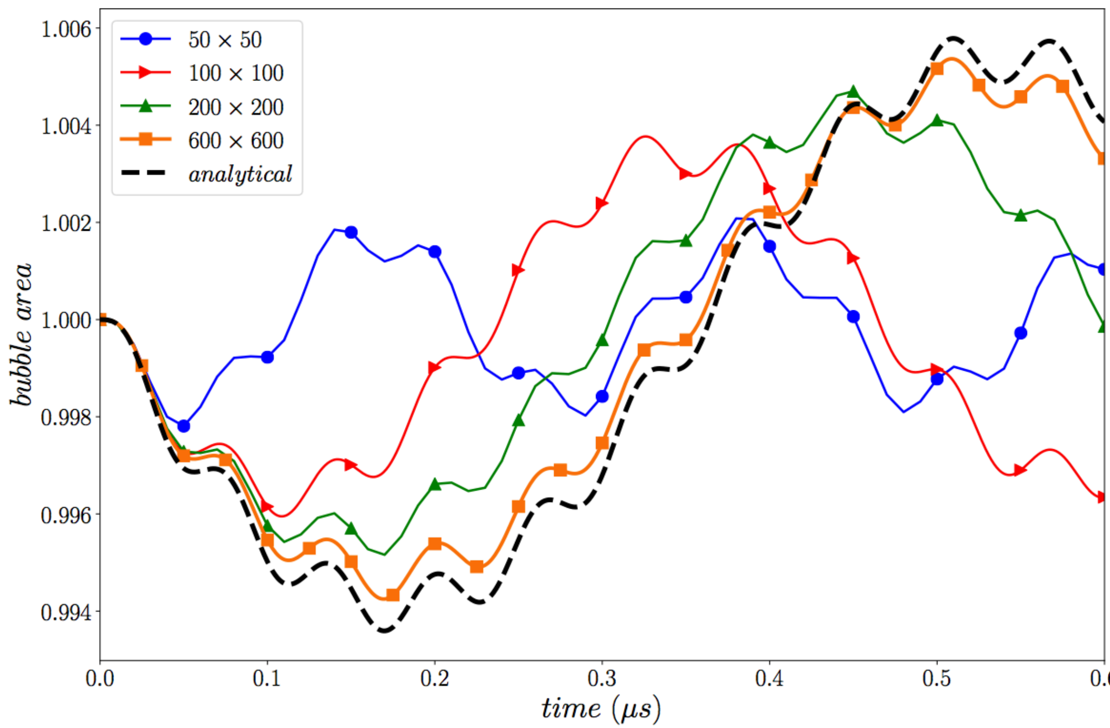
- Grid: 50×50, 100×100, 200×200 and 600×600
- Total time: $50\mu s$
- Interface: $\Gamma = 1$, $\epsilon = \Delta x$

Pressure pulse boundary condition:

- Pressure: *Dirichlet*: $10^5\{1 + 0.1sin(10\omega_c t)\}$
- Velocity: *Neumann*



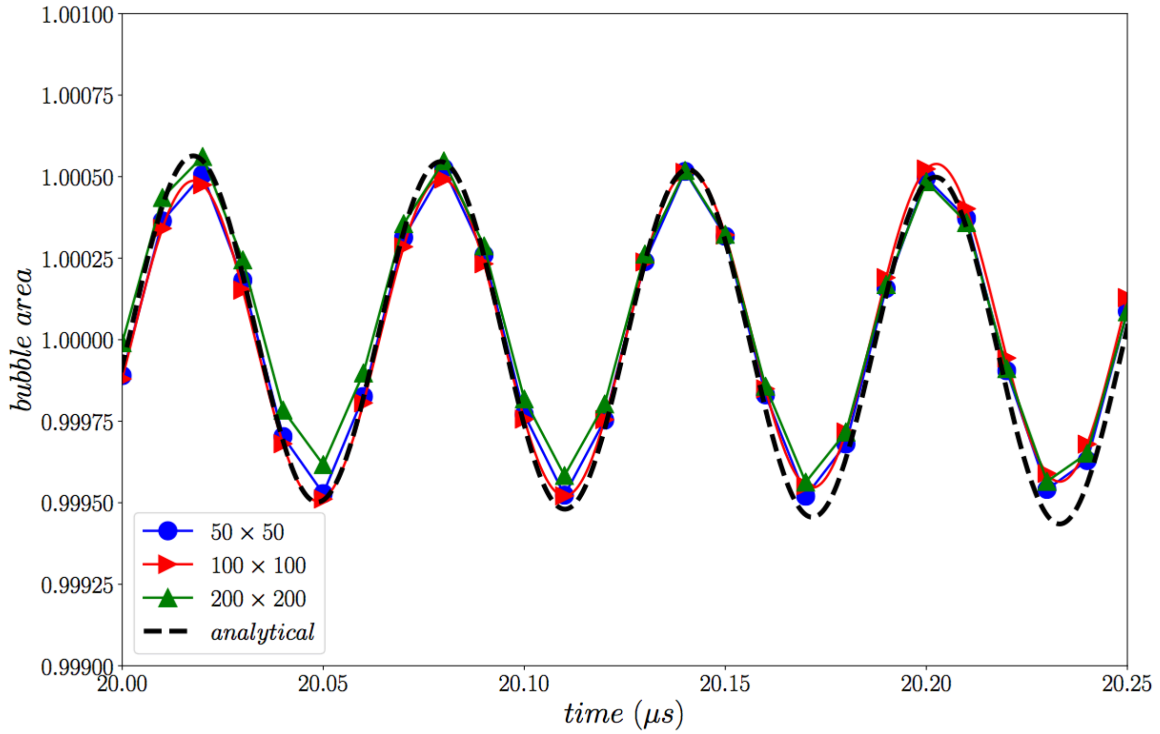
Initial transient bubble response



Solution converges to the analytical solution

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

Bubble response at later times



Long time solution is very accurate even on a coarse grid!

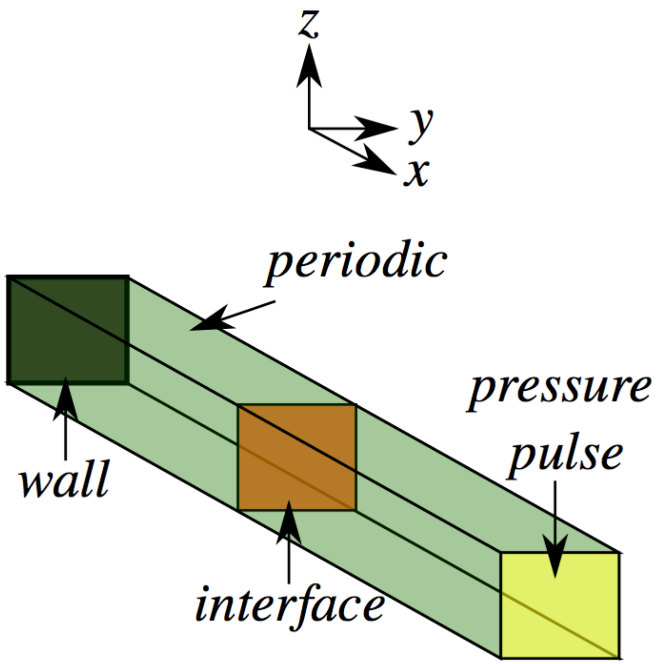
Plane acoustic wave incident on an air-water interface

Physical parameters:

- Fluids: *air, water*
- Domain: $10\mu m \times 0.1\mu m \times 0.1\mu m$
- Interface location: $5\mu m$

Simulation parameters:

- Grid: $1000 \times 10 \times 10$
- Time step: $\Delta t = 1ps$
- Total time: $1\mu s$
- Interface: $\Gamma = 1$, $\epsilon = \Delta x$



Pressure pulse boundary condition:

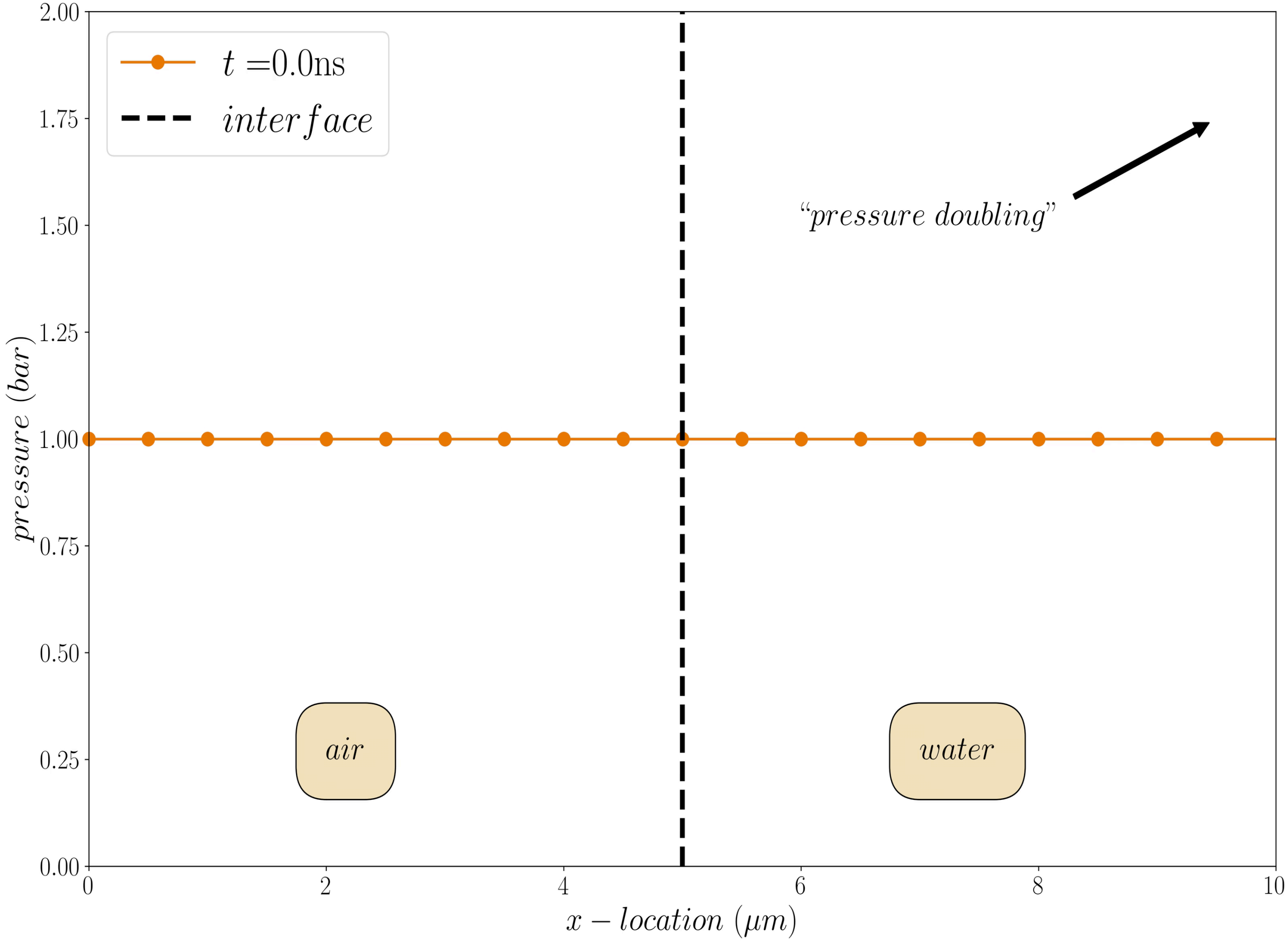
$t < 614.5$ps:

- Pressure: *Dirichlet:* $10^5\{1 - 0.5sin(c\frac{2\pi}{\lambda}t)\}$
- Velocity: *Neumann*

$t > 614.5$ps: *wall BC*

Reflection and transmission at the flat interface

$$\mathbb{R} = \frac{Z_a - Z_w}{Z_a + Z_w} = -0.999516 \qquad \mathbb{T} = \frac{2Z_a}{Z_a + Z_w} = 4.8 \times 10^{-3}$$



Conclusion

summary

- A conservative diffuse-interface method for simulation of compressible two-phase flows with acoustics.
- Improvements to the state-of-the-art methods:
    - discrete mass, momentum and energy conservation
    - central-difference scheme (non-dissipative)
    - stable method for long-time integrations
    - thermodynamic consistency at the interface
    - kinetic energy and entropy conservation

future work

- extension to acoustics in turbulent environments

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

THANK YOU

Acknowledgements:

Franklin P. and Caroline M. Johnson Fellowship

Dr. Javier Urzay & Mr. Shahab Mirjalili

ONR, Grant #N00014-15-1-2726 and 119675.
PSAAP-II Center at Stanford (DoE Grant #107908)

References:

Jain, S, S; Urzay, J; Mani, A & Moin, P, 'A conservative diffuse-interface method for the simulation of compressible two-phase flows with turbulence and acoustics', *Center for Turbulence Research, Annual Research Briefs (December 2018).*

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

Model derivation

volume fraction advection equation

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

boundedness theorem

If $0 \leq \phi_i^k \leq 1$ is satisfied for $k = 0$, then $0 \leq \phi_i^k \leq 1$ holds $\forall k > 0$ provided

$$\frac{\epsilon}{\Delta x} \geq \frac{\left(\frac{|u|_{max}}{\Gamma} + 1\right)}{2},$$

and

$$\Delta t \leq \frac{1}{\left(\frac{2\Gamma\epsilon}{\Delta x^2}\right) - \left(\frac{u_{i+1}^k - u_{i-1}^k}{2\Delta x}\right)},$$

are satisfied on a uniform one-dimensional grid, where k is the time step index and i is the grid index.
(motivated from Mirjalili et al., *JCP*, 2018)

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Continued

CTR Stanford University CENTER FOR TURBULENCE RESEARCH

mass balance equation

$$\frac{\partial \rho_1 \phi}{\partial t} + \vec{\nabla} \cdot (\rho_1 \vec{u} \phi) = \vec{\nabla} \cdot \left[\rho_{01} \Gamma \left\{ \epsilon \vec{\nabla} \phi - \phi(1-\phi) \vec{n} \right\} \right]$$

In the incompressible limit, it reduces to the volume fraction advection equation.

- Modified momentum equation ⇒ conservative kinetic energy.
- Modified energy equation ⇒ approximate conservation of entropy.

entropy conservation lemma

Let s_l be the physical entropy and T_l be the temperature of phase l, then the form of internal energy equation that satisfies

$$\sum_{l=1}^{2} \left[\rho_l \phi_l T_l \frac{D s_l}{D t} \right] = 0 \tag{1}$$

in the inviscid limit is

$$\frac{\partial \rho e}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} e) + \vec{\nabla} \cdot (p \vec{u}) - \vec{u} \cdot \vec{\nabla} p = \sum_{l=1}^{2} \left\{ h_l \vec{\nabla} \cdot (\rho_l \vec{a}_l) \right\} \tag{2}$$

[***Jain***, Urzay, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Plane acoustic wave in water

Physical parameters:

- Fluid: *water*
- Domain: $10\mu m \times 0.1\mu m \times 0.1\mu m$

Simulation parameters:

- Grid: $1000 \times 10 \times 10$
- Time step: $\Delta t = 1ps$
- Total time: $1\mu s$
- Interface: $\Gamma = 1$, $\epsilon = \Delta x$

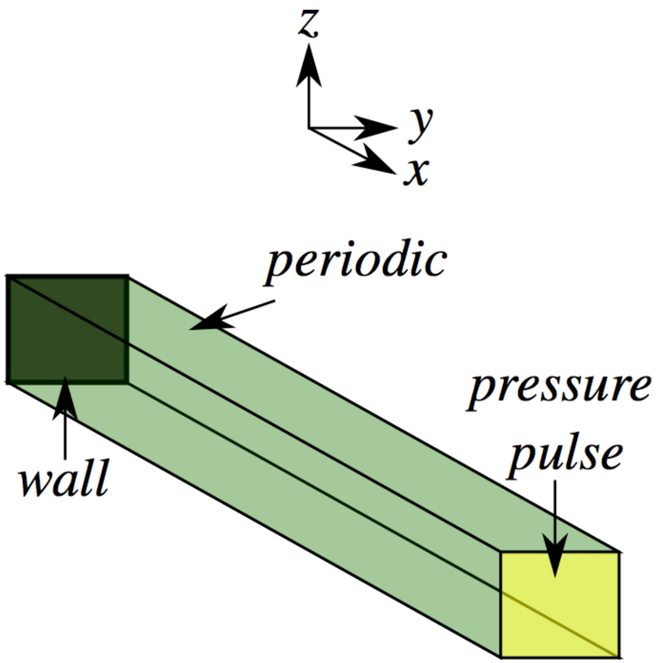
Pressure pulse boundary condition:

$t < 614.5$ps:

- Pressure: Dirichlet: $10^5(1 - 0.5sin(5112583866t))$
- Velocity: Neumann

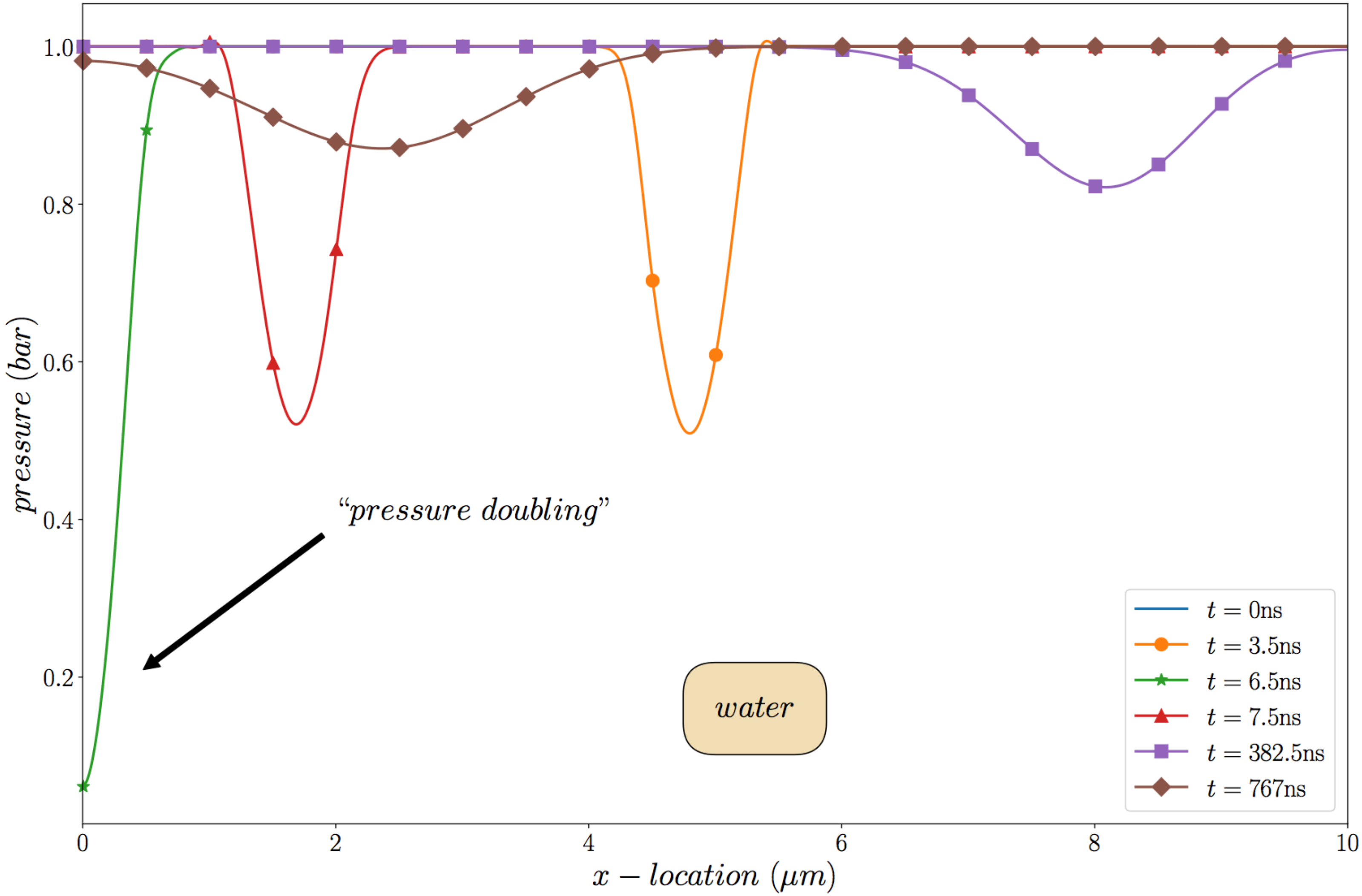
$t > 614.5$ps:

- Wall BC.



Continued

CTR Stanford University CENTER FOR TURBULENCE RESEARCH



Plane acoustic wave incident on an air-water interface

CTR Stanford University CENTER FOR TURBULENCE RESEARCH