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

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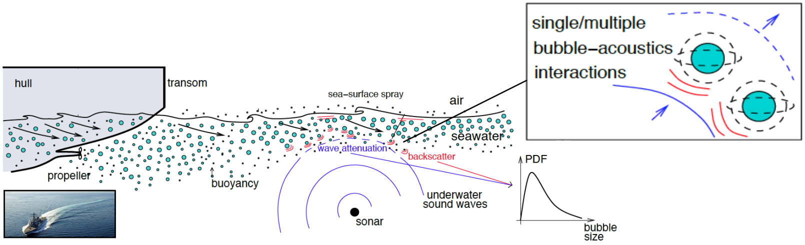
5th February 2019

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**

Five-equation model

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

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

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

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

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

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)

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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]

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***, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Proposed model

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

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

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

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

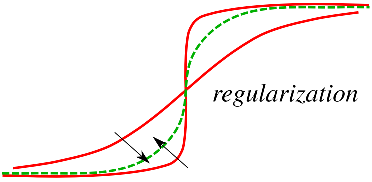
Closure:

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

[***Jain***, 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 ⇒ bounded ϕ.
5. mass balance equation ⇒ consistent with ϕ.
6. momentum equation ⇒ kinetic energy conservation.
7. energy equation ⇒ approximate entropy conservation.



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***, Mani & Moin, *CTR Annual Research Briefs*, 2018]

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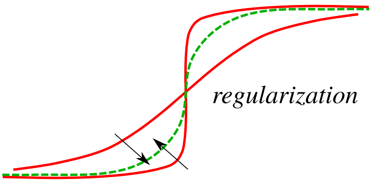

volume fraction advection equation

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

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

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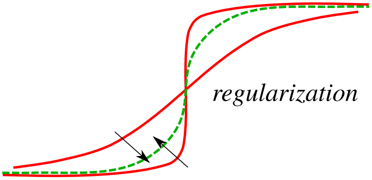

mass balance equation

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

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

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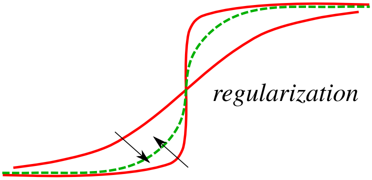

momentum equation

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

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

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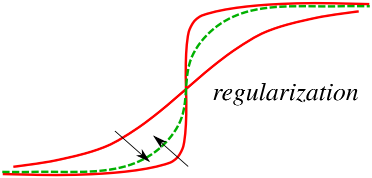


energy equation

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

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

Verification cases

Fluid properties:

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

	air	water	kerosene
ρ (kg/m^3)	1.225	997	820
μ (N/m^2)	0.0000181	0.00089	0.00164
γ	1.4	4.4	4.4
π (MPa)	0	600	326.6
c (m/s)	338.1	1627.4	1324

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:

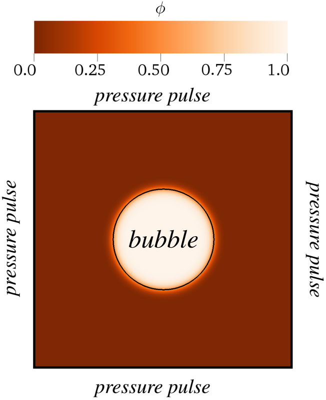
- Fluids: *air, water*
- Domain: $10\mu m \times 10\mu m$
- Bubble diameter: $4\mu m$

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*



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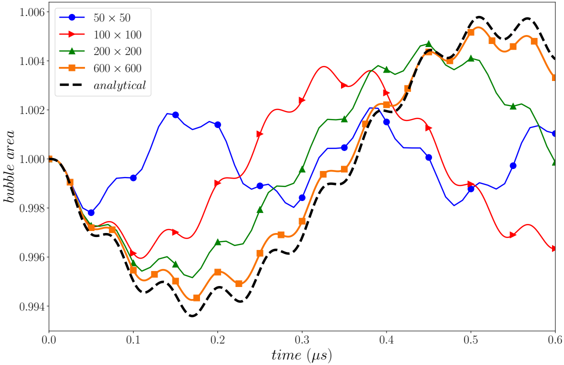
Initial transient bubble response



Solution converges to the analytical solution

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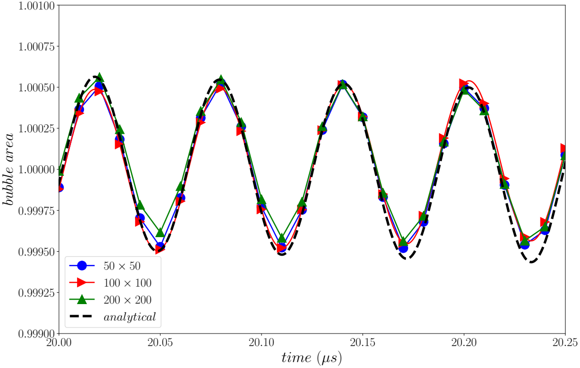
Bubble response at later times



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

Plane acoustic wave incident on an air-water interface

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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:

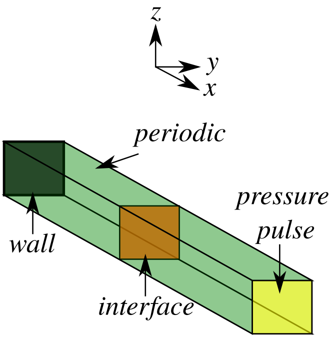
- Grid: $1000 \times 10 \times 10$
- Time step: $\Delta t = 1ps$
- Total time: $1\mu s$
- Interface: $\Gamma = 1$, $\epsilon = \Delta x$

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

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

Oblique acoustic wave incident on an water-kerosene interface

Snell's law:

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

$$\theta_i = \theta_r$$

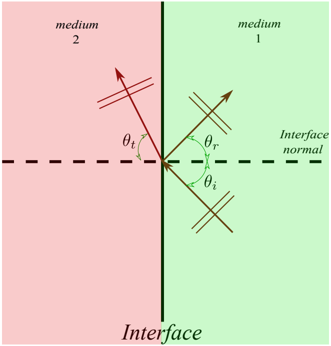
Total internal reflection:

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

For,
$c_2 > c_1 \Rightarrow \theta_t > \theta_i$.
$\therefore \exists\ \theta_c \mid \forall \theta_i > \theta_c \nexists\ \theta_t$
$\Rightarrow$ Total internal reflection

Critical angle:

$$sin(\theta_c) = \frac{c_1}{c_2}$$



Continued

Physical parameters:

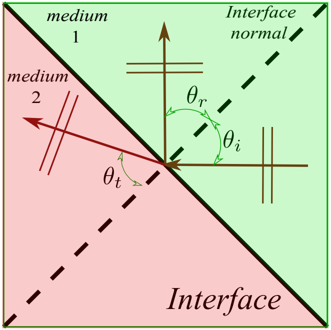
- Fluids: *water,kerosene*
- Domain: $10\mu m \times 10\mu m$

Simulation parameters:

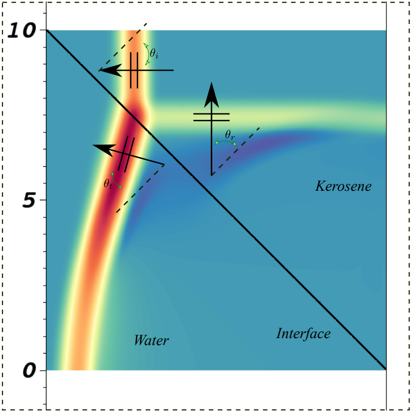
- Grid: 1000×1000
- Interface: $\Gamma = 1$, $\epsilon = \Delta x$

Case:

$\theta_i = 45^0$
$\theta_r = 45^0$
$\theta_t = 60.358^0$
$\theta_c = 54.5^0$



Reflection and transmission at the interface



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

ongoing and future work

- compressible Rayleigh-Taylor simulation
- extension to acoustics in turbulent environments
- detection of bubble size distribution using acoustic signals

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THANK YOU

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PSAAP-II Center at Stanford (DoE Grant #107908)

References:

Jain, S, S; 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).*

Model derivation

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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***, Mani & Moin, *CTR Annual Research Briefs*, 2018]

Continued

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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

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

in the inviscid limit is

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

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

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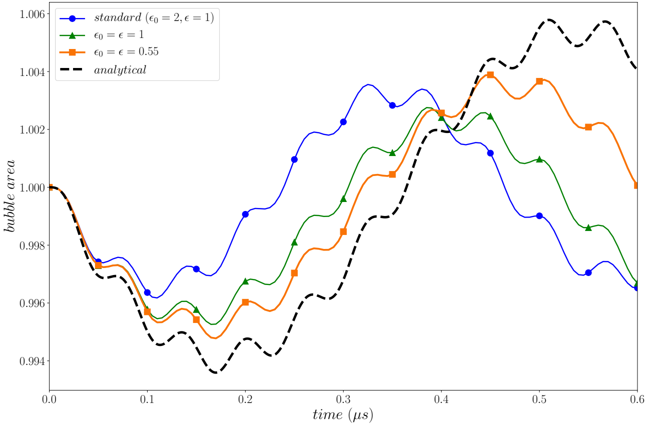
Effect of ϵ



Plane acoustic wave in water

Physical parameters:

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

Simulation parameters:

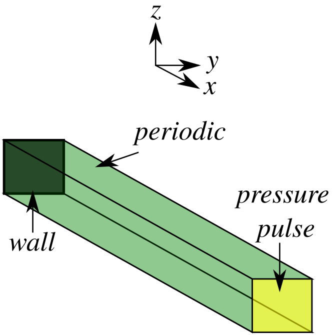
- Grid: $1000 \times 10 \times 10$
- Time step: $\Delta t = 1ps$
- Total time: $1\mu\text{s}$
- Interface: $\Gamma = 1$, $\epsilon = \Delta x$

Pressure pulse boundary condition:
$t < 614.5\text{ps}$:

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

$t > 614.5\text{ps}$:

- Wall BC.



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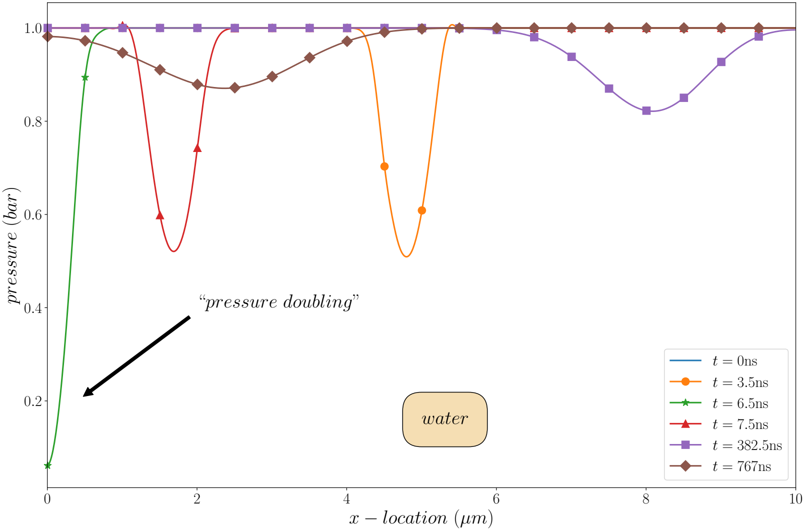

1.0
0.8
0.6
0.4
0.2
pressure (bar)
"pressure doubling"
water
$t = 0$ns
$t = 3.5$ns
$t = 6.5$ns
$t = 7.5$ns
$t = 382.5$ns
$t = 767$ns
0
2
4
6
8
10
$x - location$ (μm)

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Plane acoustic wave incident on an air-water interface