

High fidelity simulations on the development of shock-induced hydrodynamic instability

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Outlines of the talk

- ***** Research exposure and interest
- Introduction and motivation
- Mathematical formulation
- High-order numerical method
- Numerical results and discussion
- Concluding remarks and future study

Research exposures



Research Interests

- High-order numerical methods discontinuous Galerkin
- Kinetic theory for continuum-rarefied gas flows
- Physics of multi-components gas flows
- Shock-induced hydrodynamic instability
- Patter formations in biological process
- Heat and mass transfer
- Turbulent flows
- Maximum-Entropy moment methods for Vlasov system

Introduction

- Hydrodynamic instability research determines whether a flow is stable or unstable, and if so, how these instabilities develop the turbulent mixing.
- There are three primary hydrodynamic instabilities in fluid dynamics.



Richtmyer-Meshkov instability (RMI)



Kelvin-Helmholtz instability (KHI)



Rayleigh-Taylor instability (RTI)

- RMI is a shock-induced hydrodynamic instability that occurs in combination with the KHI when an initially perturbed interface separating by distinct fluid properties is accelerated by an incident shock wave.
- RMI can be considered as the impulsive limit of RTI, where primary perturbations expand across the interface and ultimately emerge into a turbulent fluid mixing as the uniform gravitational acceleration increases.

Introduction

In RMI, when an incident shock wave strikes on a bubble interface of density inhomogeneity, various complex wave patterns occur, and subsequent turbulent mixing generates along the gas interface due to the baroclinic mechanism *i.e. misalignment between the density and pressure gradients*.



- Supersonic combustion in scramjet engines
- Explosive detonation
- Supernova explosions
- Inertial confinement fusion
- Medical shock wave Lithotripsy, and many more......

Applications

Motivation

- Shock-bubble interaction is a basic and fundamental configuration in the studies of shock-induced hydrodynamic instability.
- For the development of shock-induced hydrodynamic instability on gas bubbles:
 - ✓ Mathematical Modeling for multi-component gas flows
 - ✓ Numerical method for simulations of multi-component gas flows
 - ✓ Validation of numerical solver
 - ✓ Physics of flow field etc.
- Few studies are available on the shock-induced gas bubbles having polygonal interfaces that provide good conditions for shock refraction physical phenomena.
- The thermal non-equilibrium effects, including bulk viscosity of diatomic and polyatomic gases on the flow morphology of shock-induced polygonal bubbles will be investigated.
- The effects of shock Mach number and aspect ratio on the shock-accelerated polygonal bubbles will be investigated.
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Mathematical formulation for shockinduced hydrodynamics instability

Model 1: 2D compressible Euler equations for two-component gas flows

The shock-induced hydrodynamic instability are basically simulated by solving the compressible multi-species flow model with a gas mixture.

 ϕ_1

 ρ : mass density

u,*v* : components of velocity vector

- p : pressure
- E : total energy
- ϕ : mass fraction

: mass fraction for first component

 $\phi_2 = 1 - \phi_1$: mass fraction for second component

Total energy is calculated as

$$\rho E = \frac{p}{\gamma_{mix} - 1} + \frac{1}{2} \rho \left(u^2 + v^2 \right)$$
$$\gamma_{mix} = \frac{C_{p_1} \phi_1 + C_{p_2} \phi_2}{C_{v_1} \phi_1 + C_{v_2} \phi_2}$$

where

Shankar et al., Physics of Fluids, 23, 024102 (2011)

- Interestingly, it has been found in the previous research works of Picone and Boris (JFM,1988) Samtaney and Zabusky (JFM, 1994), Quirk and Karni (JFM, 1996) that *the different values of specific heat capacities values for each gas do not affect the details of the vorticity generation qualitatively, particularly the creation of large-scale structures.*
- This model can be configured as an unsteady compressible laminar flow that assumes a singlecomponent perfect gas with a specific heat ratio.

Compressible Navier-Stokes-Fourier (NSF) equations

- locity vector
- cous stress
- at flux

NSF equation is considered as *de facto* mathematical equation for all possible flow

Stokes' hypothesis (1845):

$$\mu_b \approx \lambda + \frac{2}{3}\mu = 0$$
, equivalently, $\lambda = -\frac{2}{3}\mu$,

- μ_{h} : bulk visocsity
- : first coefficient of visocsity (shear viscosity)
- : second coefficient of visocsity

This assumption is valid only for monatomic gas and at thermal equilibrium condition.

In non-monatomic gases,

- Rotational and vibrational modes are closely related to thermal non-equilibrium.
- ✤ Rotational nonequilibrium effects are easily excited at room temperature.
- Vibrational non-equilibrium effects become relevant when the temperature is greater than 1000 K

In this study,

- Considered room temperature (~ 300 K)
- Neglecting Vibrational non-equilibrium effects
- Rotational thermal non-equilibrium effects are accounted by introducing with excess normal stress

$$\Delta = -\mu_b \nabla \cdot \mathbf{u}$$

where
$$\mu_b = \text{bulk visocsity} = f_b \cdot \mu$$

 $\mu = \text{first coefficient of visocsity (shear viscosity)}$
 $\nabla \cdot \mathbf{u} = \text{dilatational term}$

In monatomic gases,

 $\Delta = 0 \text{ equivalently, } \nabla \cdot \mathbf{u} = 0$

For non-monatomic gases -- nitrogen (air), methane and CO_2 ,

dilatational term, $\nabla \cdot \mathbf{u}$ plays a significant role in compressible flow.





 $\mu_{\rm bulk} \approx 2000\,\mu$ Hypersonic entry into Mars and Venus atmosphere

Argon gas: $\mu_b \approx 0$,
Nitrogen gas: $\mu_b \approx 0.8 \mu$,
Methane gas: $\mu_b \approx 1.33 \mu$,
Carbon dioxide gas: $\mu_b \approx 2000 \mu$.

For non-monatomic gases, compressible Navier-Fourier (NF) equations

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + p \mathbf{I} \\ (\rho E + p) \mathbf{u} \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \Pi + \Delta \mathbf{I} \\ (\Pi + \Delta \mathbf{I}) \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

 Π : viscous stress,

- Δ : excess normal stress,
- **Q**: heat flux.

where

$$\mathbf{\Pi} = 2\mu \left[\nabla \mathbf{u} \right]^{(2)}, \quad \mathbf{\Delta} = -\mu_b \nabla \cdot \mathbf{u}, \qquad \mathbf{Q} = k \nabla T$$

Chapman-Enskog linear transport coefficients

$$\mu = \left(\frac{T}{T_{ref}}\right)^{s+1}, \quad \mu_b = f_b \mu, \quad k = \left(\frac{T}{T_{ref}}\right)^s$$

 $s \rightarrow$ the index of the inverse power laws of gas molecules

$$s = \frac{1}{2} + \frac{1}{\upsilon - 1}$$

v: exponent of the inverse power laws

for the gas-particle interaction potentials

High-order numerical method



High-order Numerical Method for Modern CFD

Which kind of numerical approach can be suitable for solving highly non-linear system ?



High-order Numerical Method for Modern CFD

Finite Difference Methods

Advantages

- ➢ Easy to implement
- Easy to make high-order

Disadvantages

Applicable only for structured meshes



Finite Volume Methods

Advantages

- Naturally conservative (captures discontinuity in the flow field)
- Applicable on any type of meshes – structured, unstructured

Disadvantages

 Difficult to devise stable higher order scheme (need ENO-WENO schemes etc.)



Finite Element Methods

Advantages

- Can be any order of accuracy
- Applicable on any type of meshes – structured, unstructured

Disadvantages

Not naturally conservative



High-order Discontinuous Galerkin Method

DG method = FV method + FE method

Advantages

- Strong mathematical supports
- *hp*–adaptivity (geometric and order-accuracy flexibility)
- Provide high-order accurate solution
- Easy to handle arbitrary grid (structured and unstructured)
- Highly parallel efficiency due to local nature
- Possible to solve any PDE system (Hyperbolics, Parabolic, Elliptic)

Drawbacks

- High order methods are not necessary, for most of the engineering applications.
- Extra efforts are needed for solving viscous dominant flows and elliptic PDEs
- Extra efforts are needed for simulation of the complex geometries with curve boundaries
- Extra efforts for limiters in case of discontinuous problems
- Too expensive

~	FVM	FDM	FEM	DG
High-order/Low dispersion	X	1	1	1
Unstructured meshes	1	X	1	1
Stability for convervation laws	1	1	X	1

Mixed-type discontinuous Galerkin formulation



Source : J.N. Reddy, An Introduction of the Finite Element Method, Tata McGraw-Hill, 2012

Computational domain: decomposition and transformation

Computational domain is tessellated into a collection of non-overlapping elements



Elemental transformation according to numerical integration rule





Mixed-type discontinuous Galerkin formulation



Multiplying by a test function q(x) and integrate over element

$$\begin{cases} \int_{E} \Theta q(\mathbf{x}) d\Omega - \int_{E} \nabla \mathbf{U} \cdot q(\mathbf{x}) d\Omega = 0, \\ \int_{E} \frac{\partial \mathbf{U}}{\partial t} q(\mathbf{x}) d\Omega + \int_{E} \left(\nabla \mathbf{F}_{inv}(\mathbf{U}) + \nabla \mathbf{F}_{vis}(\mathbf{U}, \Theta) \right) \cdot q(\mathbf{x}) d\Omega = 0 \end{cases}$$

Using integration by parts and Green-Gauss divergence theorem:

$$\begin{cases} \int_{E} \Theta q \, \mathrm{d}\Omega + \int_{E} \nabla q \, \mathrm{U} \, \mathrm{d}\Omega - \prod_{\partial E} \mathbf{U} \cdot \hat{\mathbf{n}} \cdot q \, \mathrm{d}\sigma = 0, \\ \int_{E} \frac{\partial \mathbf{U}}{\partial t} q \, \mathrm{d}\Omega + \int_{E} \left(\mathbf{F}_{\mathrm{inv}}(\mathbf{U}) + \mathbf{F}_{\mathrm{vis}}(\mathbf{U}, \mathbf{S}) \right) \nabla q \, \mathrm{d}\Omega - \prod_{\partial E} \left(\mathbf{F}_{\mathrm{inv}}(\mathbf{U}) + \mathbf{F}_{\mathrm{vis}}(\mathbf{U}, \mathbf{S}) \right) \cdot \hat{\mathbf{n}} \cdot q \, \mathrm{d}\sigma = 0. \end{cases}$$

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Mixed-type discontinuous Galerkin formulation

test function : $q(\mathbf{x}) = \varphi_l(\boldsymbol{\xi}(\mathbf{x}))$ conservative variables: $\mathbf{U} \approx U_h = \sum_{l=1}^{N_k} \hat{u}_l(t) \varphi_l(\boldsymbol{\xi}(\mathbf{x}))$ **FEM approach : Galerkin formulation** auxiliary variable: $\Theta \approx \Theta_h = \sum_{l=1}^{N_k} \hat{s}_l(t) \varphi_l(\boldsymbol{\xi}(\mathbf{x}))$ (high-order flexibility) N_{k} = number of basis function for the polynomial function P^{k} , where $\varphi_{I}(\boldsymbol{\xi}(\mathbf{x})) =$ basis function $\mathbf{U} \cdot \hat{\mathbf{n}} \approx \hat{\mathbf{H}}_{aux} \left(\mathbf{U}^+, \mathbf{U}^- \right)$ $\mathbf{F}_{inv}(\mathbf{U}) \cdot \hat{\mathbf{n}} \approx \hat{\mathbf{H}}_{inv}(\mathbf{U}^+, \mathbf{U}^-)$ **FVM approach: flux reconstruction** $\mathbf{F}_{vic}(\mathbf{U},\mathbf{S})\cdot\hat{\mathbf{n}}\approx\hat{\mathbf{H}}_{vic}(\mathbf{U}^+,\mathbf{S}^-,\mathbf{U}^-,\mathbf{S}^-)$ (Numerical fluxes) **Consistency condition** : H(u, u) = f(u)**Continuity condition** : $H(u_1, u_R)$ is Lipschitz continuous for u_1 and u_R **Monotonicity condition**: $H(u_1, u_p)$ is $H(\uparrow, \downarrow)$ non-dereasing function of u_1 , and non-increasing function of u_R . 22

Weak formulation of mixed-type DG spatial discretization

Temporal discretization

Semi-discrete form of ordinary differential equation

$$\mathbf{M}\frac{\partial U_h}{\partial t} = \mathbf{L}(U_h)$$

M = orthogonal mass matrix $\mathbf{L}(U_h) =$ residual function

Explicit third-order TVD Runge-Kutta scheme

$$U_{h}^{(1)} = U_{h}^{n} + \Delta t \,\mathbf{M}^{-1}\mathbf{L}\left(U_{h}^{n}\right)$$
$$U_{h}^{(2)} = \frac{3}{4}U_{h}^{n} + \frac{1}{4}U_{h}^{(1)} + \frac{1}{4}\Delta t \,\mathbf{M}^{-1}\mathbf{L}\left(U_{h}^{(1)}\right)$$
$$U_{h}^{n+1} = \frac{1}{3}U_{h}^{n} + \frac{2}{3}U_{h}^{(2)} + \frac{2}{3}\Delta t \,\mathbf{M}^{-1}\mathbf{L}\left(U_{h}^{(2)}\right),$$

$$\mathbf{M} = \begin{cases} \int_{I_n} \varphi_i \, \varphi_j dk = C_{ij}, & \text{if } i = j \\ \int_{I_n} \varphi_i \, \varphi_j dk = 0, & \text{if } i \neq j \end{cases}$$



Basis (polynomial) functions



Summary of present numerical scheme

- Computational domain decomposition with uniform rectangular meshes
- Hierarchical basis function based on Legendre polynomials
- ✤ Lax-Friedriches, Roe and HLLC schemes for inviscid flux term
- ✤ Alternating (Local DG) scheme for viscous and auxiliary flux terms
- ✤ Gauss-Legendre quadrature rule for surface and volume numerical integrations
- ✤ 3rd-order TVD Runge-Kutta scheme for temporal integration
- * A high-order moment limiter proposed by Krivodonova is used for controlling artificial oscillations

Numerical Results

Order accuracy test of present DG scheme

A smooth 1D density wave propagation problem with initial condition:

$$u(x,0) = 1.0 \rho(x,0) = 1.0 + 0.2 \sin(\pi x) p(x,0) = 1.0$$
 $\forall x \in [0,6],$



1D-Riemann problem: Sod shock tube



Singh and Torrilhon, Physics of Fluids, 35, 012117 (2023)

1D stiff shock structure problem



Singh et al., Journal of Computational Physics, 457, 111052 (2022)

2D shock-cylindrical bubble interaction



Singh et al., Physics of Fluids, 33, 066103 (2021)

2D shock-cylindrical bubble interaction

Experimental results (Ding et al., 2015)



Singh, Physics of Fluids, 32, 126112 (2020)

Ding et al., J. Fluid Mech. 828, 289 (2017).³²

2D shock-square heavy bubble interaction



Singh, Physics of Fluids, 32, 126112 (2020)

Flow morphology of shock-induced light square bubble



- ✓ Shock Mach number =1.21
- ✓ Bubble filled with helium gas
- ✓ Rankine-Hugoniot condition for initialization
- ✓ Third-order DG method
- ✓ Mesh of 1200x600 grid points



Singh and Torrilhon, Physics of Fluids, 35, 012117 (2023)

Flow morphology of shock-induced heavy square bubble



- ✓ Shock Mach number =1.21
- ✓ Bubble filled with SF6 gas
- ✓ Rankine-Hugoniot condition for initialization
- ✓ Third-order DG method
- ✓ Mesh of 1200x600 grid points



Singh and Battiato, Computer & Fluids, 242, 105502 (2022)

Flow parameters on shock-induced hydrodynamics instability

- ✓ Atwood number
- ✓ Bubble (interface) shape
- ✓ Incident shock Mach number

Atwood number is defined by

$$At = \frac{\rho_b - \rho_g}{\rho_b + \rho_g}$$

- $\rho_b = \text{bubble gas density}$ $\rho_g = \text{ambient gas density}$
- At > 0: convergent configuration (light-heavy-configuration) At < 0: divergent configuration (heavy-light-configuration)



(a) Light interface



(b) Heavy interface

Atwood number effects on shock-induced square bubble





Singh, Physics of Fluids, 32, 126112 (2020)

Interface shape effects on shock-induced bubble



(a) Shock-accelerated SF₆ square bubble

---- DS

t = 10

 $\tau = 8.4$

 $\tau = 3.5$

-RS

IS



T = 15 T = 3.5 T = 3.5 T = 8.4 T = 8.4 T = 8.4

(b) Shock-accelerated SF₆ cylindrical bubble





(b) Shock-accelerated SF₆ cylindrical bubble



(a) Shock-accelerated He square bubble



(b) Shock-accelerated He cylindrical bubble



(a) Shock-accelerated He square bubble



(b) Shock-accelerated He cylindrical bubble

Singh, Physics of Fluids, 32, 126112 (2020)

Shock Mach number effects on shock-induced heavy square bubble



Singh and Battiato, accepted in Physica D: Nonlinear Phenomena (2023)

Thermal non-equilibrium effects of diatomic and polyatomic gases



Singh, International Journal of Heat and Mass Transfer 179, 121708 (2021)

Degree of thermal non-equilibrium

- In irreversible thermodynamics theory, the degree of thermal nonequilibrium based on Rayleigh– Onsager theory is a vital component and is directly related to entropy production in nonequilibrium processes.
- □ To demonstrate the degree of thermal nonequilibrium, the Rayleigh–Onsager dissipation function is defined as follows

$$R^{*} = \frac{\gamma M}{\text{Re}} \frac{1}{p^{*}} \left[\Pi^{*} : \Pi^{*} + 2\gamma' f_{b} \Delta^{*2} + \frac{2}{Ec \operatorname{Pr}} \frac{Q^{*} \cdot Q^{*}}{T^{*}} \right]^{L}$$



□ The degree of nonequilibrium is **much higher** for diatomic and polyatomic gases than for monatomic gases.

Effect of bulk viscosity ratio



Spatially integrated values of degree of thermal non-equilibrium and dissipation rate

Aspect ratio effects on shock-induced rectangular bubbles



Type of bubble	Case	L_a	L_b	Aspect ratio
Square	Ι	а	а	$AR_s = 1.0$
Horizontal-aligned rectangular	II	а	0.8 <i>a</i>	$AR_{h} = 1.25$
	III	а	0.5 <i>a</i>	$AR_h = 2.0$
	IV	а	0.2 <i>a</i>	$AR_h = 5.0$
Vertical-aligned rectangular	V	0.8 <i>a</i>	а	$AR_{\nu} = 1.25$
	VI	0.5 <i>a</i>	а	$AR_{\nu} = 2.0$
	VII	0.2 <i>a</i>	а	$AR_{\nu} = 5.0$

Aspect ratio effects on shock-induced rectangular bubbles





aligned

bubbles

(c) AR_h = 5.0







Verticalaligned rectangular bubbles

Singh and Torrilhon, Physics of Fluids, 35, 012117 (2023)

Concluding remarks and future study

- The flow physics for shock-induced hydrodynamic instabilities on various gas bubbles with different shapes is investigated numerically.
- High fidelity simulations are performed with inhouse discontinuous Galerkin solver based on rectangular meshes
- ✤ Numerical results are validated with the existing experimental and computational results.
- Effects of various flow parameters Shock Mach number, Atwood number, bubble shapes, thermal non-equilibrium – on the shock-induced bubbles are investigated.
- This study will be extended for shock-gas-liquid interaction-based problems.
- Reactive shock-induced hydrodynamic instabilities will be investigated with the applications of

combustion and flame.

Selected Articles on shock-induced hydrodynamic instabilities

- S. Singh, M. Torrilhon (2023), "On the shock-driven hydrodynamic instability in square and rectangular light gas bubbles: a comparative study from numerical simulations", *Physics of Fluids*, 35, 012117 (2023)
- S. Singh, M. Battiato (2022), "Numerical simulations of Richtmyer-Meshkov instability of SF6 square bubble in diatomic and polyatomic gases", Computers & Fluids, 242, 105502 (2022)
- □ S. Singh (2021), "Contribution of Mach number to the evolution of Richtmyer-Meshkov instability induced by a shock-accelerated square light bubble", *Physical Review Fluids*, 6, 104001.
- S. Singh (2021), "Numerical investigation of thermal non-equilibrium effects of diatomic and polyatomic gases on the shock-accelerated light square bubble using a mixed-type modal discontinuous Galerkin method", International Journal of Heat and Mass Transfer, 179, 121708
- S. Singh, M. Battiato, R. S. Myong (2021), "Impact of bulk viscosity on flow morphology of shock-accelerated cylindrical light bubble in diatomic and polyatomic gases", *Physics of Fluids*, 33, 066103
- S. Singh, M. Battiato (2021), "Behavior of a shock-accelerated heavy cylindrical bubble under non-equilibrium conditions of diatomic and polyatomic gases", *Physical Review Fluids*, 6, 044001
- S. Singh (2020), "Role of Atwood number on flow morphology of a planar shock-accelerated square bubble: A numerical study", *Physics of Fluids*, 32, 126112

If you are interested in my research work, you may visit/write me:

https://www.researchgate.net/profile/Satyvir_Singh https://www.acom.rwth-aachen.de/5people/singh/start https://scholar.google.com.sg/citations?user=sQT89LYAAAAJ&hl=en

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