
Chih-Hao Chang 1, Xiaolong Deng 2 and Theo G. Theofanous 3

UC Santa Barbara, Goleta, CA 93117, USA

We introduce a new numerical method for solving the compressible Navier-Stokes equations in flow domains that may be separated by any number of interfaces, fluid-to-fluid or fluid-to-solid, at arbitrarily high density ratios and acoustic-impedance mismatch, and subjected to pressure waves of arbitrarily high amplitudes and steepness. A principal aim is the ab initio prediction of interfacial instabilities under superposition of multiple active modes (Rayleigh-Taylor, Kelvin-Helmholtz, Richtmeyer-Meshkov) along with mean flow development, as found for example in rapidly-accelerated immersed-fluid bodies. We insist on a sharp-interface treatment (fluid-property and normal-stress jumps), and a unique feature of our approach is solving for motion of each element of the piecewise-curved interface as an exact Riemann problem within an overall conservative scheme that couples consistently the bulk-fluid motions to that of the interface. Sample simulations of liquid drops subjected to shock waves demonstrate for the first time the numerical prediction of the key phenomena found in recent experimental and theoretical studies of this class of problems [Theofanous, Ann. Rev. Fluid Mech. 43:661-90, 2011].

I. Introduction

Gas-liquid interfaces, when subject to accelerations and/or velocity gradients, are unstable to infinitesimal perturbations—a classical subject that is well understood, mainly via linear theory, but individually for each class of such flows (Rayleigh-Taylor, Kelvin-Helmholtz, and Richtmeyer-Meshkov). Approximate, analytical, weakly non-linear and even non-linear methods exist for some cases, but again only for the rather idealized problems that involve accelerations normal to the interface or velocity gradients in flows parallel to the interface. While these inform qualitatively about systems found in practice, absent are understanding and capability to treat superposition of mechanisms in arbitrary flows, as for example those arising in the presence of accelerating, oblique or curved interfaces. More severely, absent are such methods that can accommodate compressible and shock-wave-bearing flows. This is the subject addressed by the numerical work summarized in this paper. The canonical problem is aerobreakup of liquid drops 1 and the supporting experiments, carried out in a large-scale shock tube, include Newtonian as well as viscoelastic liquids. Applications of significant current interest include de-icing of airplane wings, internal-combustion, rocket, and pulse-detonation engines, and dissemination of liquid agents in the atmosphere. A companion paper deals with collective effects of so-produced sprays 7.

II. Numerical Methods

It has been established 3 that the sine qua non for our task is a numerical treatment that observes the exact boundary conditions at the interface. An immediate consequence is that the interface must be represented sharply, both dynamically and kinematically. This means that the singular surface that marks each elementary portion of the interface must have its own unique velocity that is computed from the balance of forces and kinematics on either side of it. The key to achieving this is an exact Riemann solution that incorporates the normal-stress jump across a curved segment.

---

1 Assistant Researcher, Center for Risk Studies and Safety, UCSB.
2 Assistant Project Scientist, Center for Risk Studies and Safety, UCSB.
3 Professor, Chemical Engineering Department; Director, Center for Risk Studies and Safety, UCSB.
We use a Level Set function to represent the interface. Rather than the usual approach of convecting it along with the flow field of the neighboring-bulk, at each time step we construct a new Level Set function that is anchored to the interface velocity. The method is fully conservative, and the order of the numerical scheme is further improved by a curved sub-cell representation of the interface.

A high-fidelity treatment also demands that the viscous and conductive fluxes are fully resolved\(^4\), and we found that even with a highly-efficient code, and with adaptive mesh refinement, the gridding requirements exceeded desirable levels of effort. Thus we have embedded a thin-layer treatment, which was further informed and verified by a conformal-mapping solution of the flow over a solid sphere. The updating of the flow and temperature fields in the vicinity of the interface are computed by exact balances of diffusive fluxes (tangential stresses, heat fluxes) across the interface, while observing equality of temperatures and tangential velocities at the interface. The overall method is summarized by the flow diagram in Figure 1.1. Details can be found in a related full publication\(^6\).

![Flow Diagram](image)

**Figure 1** The computational flow of the MuSiC\(^+\) code.

The above are implemented in an AMR infrastructure with the unstructured cut-cell grid embedded at the lower end of an adaptive hierarchy of nested Cartesian meshes that are tailored to the efficiency of the numerical scheme for this class of problems. All sharp areas, including shocks are subject to refinement, and to release when no further needed. The code has been written in a way that is convenient to parallelize.

### III. Illustrative Results

Sample results provided below address four kinds of applications: (a) validation tests on simple problems whose solutions are known, (b) prediction of Rayleigh-Taylor instability (RTI) development on a spherical-shape drop accelerated by a blast wave, (c) prediction of viscous Kelvin-Helmholtz instability (KHI) on a spherical drop subjected to high speed gas flow, and (d) simulation of a large-scale, underwater explosion.

#### A. Validation Tests

**A.1 Prediction of the Bailey-Hiatt drag-coefficient data**

A series of calculations were carried out for flow over an 1.8 mm solid sphere, varying the flow Mach number over the range \(0.3 < M < 1.3\). The solid boundary was kept isothermal, which according to our estimates was the case in
the experiments (conducted with copper or iron spheres). The results using the conformal-mesh option are summarized in Figure 2.

![Figure 2](image)

**Figure 2** Comparison of predicted drag coefficients with the Bailey-Hiatt data.

A.2 The viscous boundary layer on an inclined flat plate

Simulations were carried out for an impulsively-generated, 100 m/s flow over a flat plate at an angle of incidence 45°. The skin friction is compared with the analytical result in Figure 3.

![Figure 3](image)

**Figure 3** Resolving the viscous boundary layer on flat plate at an angle of incidence 45° with the flow.

A.3 Resolving the viscous boundary layer on a sphere at high Reynolds numbers

Using the conformal mesh solution as a standard, we evaluate improvements made by the thin-layer treatment as illustrated in Figure 4. The flow Mach number is 1.1 which yields $Re_\delta = 1.1 \times 10^5$. While the calculation is significantly stabilized by the thin layer, accuracy still suffers from inadequate resolution of the AMR mesh. Successively refined AMR meshes, along with the thin-layer treatment, lead to convergence to the conformal-mesh result.
B. Rayleigh-Taylor instability on a spherically-shape interface

It has been shown that the first criticality of aerobreakup (liquid drops in high-speed gas flow) is by Rayleigh-Taylor piercing (RTP)\(^1\). Here we show that our simulations can provide \textit{ab initio} predictions of this phenomenon (Figure 5). Notably, unless the fastest growing R-T wave can fit on the deformed (aerodynamically flattened) drop, the penetration process cannot proceed—this is the condition that defines the first criticality.

---

Figure 4 (a) Contribution of the thin-layer treatment in resolving viscous stresses for a Mach 1.1 flow past a sphere. (b) Detail of pressure and flow fields shows that the AMR is still limiting the resolution of the thin-layer (right) as seen by comparison to the conformal-mesh solution (left).
Figure 5 Development of Rayleigh-Taylor instability on a spherically-shaped drop subjected to the gas flow behind a Mach 1.2 shock [$M = 0.29$, $We=520$, $Oh=1.82$, $Re_g=1.57 \times 10^4$]. (a) The flow-and-deformation history. (b) Comparison of advanced stages of deformation (at 400 µs) with experiments in straight (left), oblique (right) views.

C. Kelvin-Helmholtz instability on a spherical shape

It has been shown$^{1,5}$ that the second criticality in aerobreakup is established due to dominance of Kelvin-Helmholtz waves, so that rather than deformation and penetration by RTP seen above we have shear-induced entrainment (SIE). Here we provide the first demonstration that this transition in phenomena is captured a priori by direct numerical simulation (Figure 6). The linear stability analysis result in this figure was obtained with the AROS code$^4$, with boundary layer parameters derived from the MuSiC$^+$ simulation.
Figure 6  Development of Kelvin-Helmholtz instability on a spherically-shaped drop subjected to the gas flow behind a Mach 1.2 shock. [TBP, M= 0.3, Re₉ =1.6 × 10⁴, We=1,600, Oh=0.0178]. (a) Comparison of the simulation result (40 𝜇s) to experimental image taken at 59 𝜇s following shock impact, (b) Detail of the flow field inside the thin viscous boundary layer. (c) Interfacial displacements and extraction of the growth factor in the linear regime of growth. (d) Comparison numerical simulation result with exact linear stability analysis (AROS code) and the wave number seen in the experiment. Based on the boundary layer thickness the Reynolds and Weber numbers are 124 and 15 respectively. This last result also shows that, just as in the experiment, the near-peak-growth wave is favored.

D. Large-scale underwater explosion

An explosive is located 15 m underwater and 12 m above the center of a rigid spherical target. The bottom of the domain is rigid, and so is assumed the side boundary of the axisymmetric domain. At the end of the burn the pressure is 2.12 × 10⁷ atm, and the calculation begins by releasing this pressure over the explosive zone indicated in Figure 7. To illustrate robustness of the simulation the water is assumed capable to withstand large tensile stresses.
IV. Conclusions

(a) We can predict interfacial instabilities in high-speed gas liquid flows without the aid of initializing the simulation by linear stability results. This allows simulation of curved interfaces where multiple modes are in competition, and in any case the dominant wave numbers are not known a priori.

(b) Even though shear is small compared to normal stresses, resolving the viscous boundary layer is critical to properly reflecting the gas dynamics, and therefore to the fidelity of the interfacial phenomena that emerge.

(c) In numerical simulations of drops subjected to the action of shock waves we find the two criticalities observed in experiments, and likewise the simulation reveals the dominant wave numbers. The calculated growth rates are in perfect agreement with exact linear stability analysis results.
V. NOMENCLATURE

\[ We = \frac{\rho u_s^2 d_0}{\sigma} \] Weber number;

\[ Re_g = \frac{\rho u_s d_0}{\mu_g} \] Reynolds number;

\[ Oh = \frac{\mu}{(\rho \sigma d_0)^{1/2}} \] Ohnesorge number;

\[ M_s = \frac{C_s}{C_g} \] Shock-speed Mach number;

\[ C_f = \frac{1}{\frac{1}{2} \rho_s u_s^2} \] Friction coefficient.

Where: \( d \) is drop diameter, \( C_s \) shock speed, \( C_g \) speed of sound in gas upstream the shock, \( u_s \) free-stream gas velocity, \( \mu_s / \mu_g \) gas/liquid dynamic viscosity, \( \rho_s / \rho_g \) gas/liquid density, \( \sigma \) surface tension coefficient.

VI. ACKNOWLEDGMENTS

This work was supported by the Joint Science and Technology Office, Defense Threat Reduction Agency (JSTO/DTRA), and the National Ground Intelligence Center (NGIC). We are grateful to Dr. Richard Babarsky (NGIC) for his encouragement, cooperation, and support all through this work from the very beginning. The experimental data were contributed by Dr. V. Mitkin, and the AROS calculations were provided by Dr. S. Sushchikh, both of CRSS.

VII. Reference