Numerical simulation of the Richtmyer–Meshkov instability

Candidate number: 8243V

Supervisor: Dr. Nikolaos Nikiforakis

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Abstract

The evolution of the flowfield produced by the passage of a shock wave through an inverse chevron-shaped region of dense gas (sulphur hexafluoride) is studied by experimental and numerical means. Experimental data is from the Atomic Weapons Establishment’s 20 cm × 10 cm shock tube with a Mach number of 1.26. A contemporary multicomponent Riemann-based solver is used to integrate the hyperbolic differential equations, while adaptive mesh refinement is used to efficiently capture the evolving flow features at fine scales. The development of the flow is accurately captured by the two-dimensional numerical solution, with strong qualitative agreement seen, allowing for simulated flow physics to be discussed. Quantitative comparison between experimental results and simulation is made where possible. The solver is then extended to capture flow with different materials, initially replacing the SF$_6$ chevron with water described by the stiffened gas equation of state. Motivated by the practical applications of the geometry, analysis of the flow of copper modelled by a Cochran–Chan equation of state is presented.
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Introduction

The Richtmyer–Meshkov instability (RMI) occurs when an interface between two fluids of different densities is impulsively accelerated, usually by the passage of a shock wave, which causes existing perturbations on the boundary to grow due to misalignment of the pressure and density gradients across the interface. As the instability grows, secondary instabilities such as the Kelvin–Helmholtz instability develop, ultimately leading to a region of turbulent mixing between the two originally separated fluids.

A rigorous theoretical and numerical treatment of the instability was first provided by Robert Richtmyer in 1960, which was later experimentally supported with shock-tube experiments by Evgeny Meshkov in 1969. Qualitative similarities are observed between the RMI and the instability produced by continuous acceleration of an interface between fluids, the Rayleigh–Taylor instability (RTI). As such, the RMI is sometimes referred to as the “impulsive Rayleigh–Taylor instability”.

Occurrences of the RMI are found in many areas of physics. During a supernova, the gaseous outer layers of a star are blasted away by a shock wave; the early formation of this is governed by the RMI (Arnett, 2000), while later evolution of the supernova remnant is determined by the RTI (Kane et al., 1999). The RMI is also important in studies of inertial confinement fusion (Mikaelian, 1985), where turbulent mixing can be a desirable effect, as well as in understanding the deflagration to detonation transition (Khokhlov et al., 1999).

This report begins with a brief discussion of the theoretical origin of the RMI, followed by an overview of the formulation of the governing equations of the solver and the numerical methods employed. The algorithm is validated in 2D against experimental data and the extension from an ideal gas to stiffened gas is confirmed in 1D with an analytic solution. A shock tube problem with complex geometry is then considered and compared both qualitatively and quantitatively with experimental data from the Atomic Weapons Establishment (AWE). The same geometry is then considered with different equations of state, beginning with water modelled as a stiffened gas. Finally, the solver is extended to model three-phase flow and applied to an inverse chevron consisting of copper separating regions of trinitrotoluene (TNT) and water.

Theoretical background

While the numerical scheme described in this paper is compressible, as required to capture shock waves, the origin of the instability can be understood in an incompressible context. From the dynamical equation of the vorticity field ($\omega = \nabla \times \mathbf{v}$),

$$\frac{D\omega}{Dt} = \frac{1}{\rho^2} \nabla \rho \times \nabla p + \omega \cdot \nabla \mathbf{v} - \omega \cdot \nabla \mathbf{v},$$

(1)

where $\frac{D}{Dt}$ is the convective derivative. We can see that the baroclinic term leads to a deposition of vorticity at the interface between fluids of different densities. If we consider the interaction of a shock wave with an interface perturbed by a single sinusoidal mode, as in Figure 1, this will lead to a maximal production of vorticity at points of minimal perturbation, resulting in an increase in amplitude with time. As the system evolves, this leads to a “mushrooming” effect.

In shock tube experiments, the shock wave is typically reflected by the downstream boundary, resulting in a secondary interaction with the system. As this occurs after vorticity generation has already
increased the amplitude of perturbations at any interfaces, the result of the reshock is to produce a region of turbulent mixing.

**Equations of state**

An equation of state provides a constitutive relation between thermodynamic variables. To fully determine the governing equations, we require an equation of state for each component of the flow. Each material can be described by a different equation of state, with thermodynamic variables at each cell obtained by a volume weighted average. An ideal gas has equation of state,

\[ p = \rho (1 - \gamma) e, \]  

where \( \gamma = \frac{C_p}{C_v} \) is the adiabatic index and \( e \) is the energy density. This is equivalent to the more familiar form of the ideal gas law, \( pV = nRT \), but in a more useful form.

The stiffened gas equation of state is,

\[ p + \gamma p_\infty = \rho (1 - \gamma) e, \]  

where \( p_\infty \) is a “reference pressure” which describes an effective pressure acting on the fluid due to internal interactions when zero external pressure is applied. For example, water can be modelled as a stiffened gas; the near incompressibility of water can then be understood by considering that any externally applied pressure is insignificant compared to the reference pressure.

The solver described in Shyue (2001), of which we employ an implementation, uses a general Mie–Grüneisen equation of state, described by equations for the total energy density and pressure,

\[ e(\rho, T) = e_{\text{ref}}(\rho) + e_T(\rho, T), \]  
\[ p(\rho, T) = p_{\text{ref}}(\rho) + \rho \Gamma e_T(\rho, T), \]

where the subscripts “ref” and “T” refer to “reference” and “thermal” states of the quantities \( p \) and \( e \), \( \Gamma = \gamma - 1 \) is the Grüneisen gamma, and \( T \) is the temperature. Both the ideal and stiffened gas equations of state can be cast in this form with \( p_{\text{ref}} = e_{\text{ref}} = 0 \) and \( p_{\text{ref}} = -p_\infty \gamma; e_{\text{ref}} = 0 \) respectively.

A number of empirically determined equations of state with fitted parameters can be used. For solid explosives and metals, we can use an experimentally determined equation of state as described in
Cochran and Chan (1979),

\[
\begin{align*}
\epsilon_{\text{ref}}(\rho, T) &= -\frac{A}{\rho_0 (1 - \varepsilon_1)} \left[ \left( \frac{\rho}{\rho_0} \right)^{\varepsilon_1-1} - 1 \right] + \frac{B}{\rho_0 (1 - \varepsilon_2)} \left[ \left( \frac{\rho}{\rho_0} \right)^{\varepsilon_2-1} - 1 \right], \tag{5a} \\
p_{\text{ref}}(\rho, T) &= A \left( \frac{\rho}{\rho_0} \right)^{\varepsilon_1} - B \left( \frac{\rho}{\rho_0} \right)^{\varepsilon_2}. \tag{5b}
\end{align*}
\]

<table>
<thead>
<tr>
<th>Ideal gas</th>
<th>Density / kg m(^{-3})</th>
<th>(\gamma)</th>
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</thead>
<tbody>
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<td>1.4</td>
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<table>
<thead>
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<th>Stiffened gas</th>
<th>Density / kg m(^{-3})</th>
<th>(\gamma)</th>
<th>(p_\infty) / GPa</th>
</tr>
</thead>
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<table>
<thead>
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<th>Density / kg m(^{-3})</th>
<th>(\gamma)</th>
<th>(A) / GPa</th>
<th>(B) / GPa</th>
<th>(\varepsilon_1)</th>
<th>(\varepsilon_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copper</td>
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<td>3</td>
<td>145.67</td>
<td>147.75</td>
<td>2.99</td>
<td>1.99</td>
</tr>
<tr>
<td>TNT</td>
<td>1840</td>
<td>1.93</td>
<td>12.87</td>
<td>13.42</td>
<td>4.1</td>
<td>3.1</td>
</tr>
</tbody>
</table>

Table 1: Values for the parameters of each equation of state for selected materials from Shyue (2001). Unless otherwise stated, these values should be assumed throughout this report.

Values of \(p_{\text{ref}}(\rho)\) must be specified at each point in the flow. However, because the fluids are compressible, we know only the density of the mixture, not the density of each individual component. Determination of the equation of state of the mixture is likely to be inaccurate. This problem is compounded by the fact that our equation of state can be purely empirical, with only a limited domain of applicable densities. While there exist more advanced approaches to multicomponent flow (see Saurel and Abgrall (1999), (2003), and (2007) for further details), these are beyond the scope of this project.

**Numerical method**

We employ the shock-capturing algorithm described in Shyue (2001). This allows for accurate modelling of multicomponent flows using an arbitrary Mie–Grüneisen equation of state, which describes a wide variety of dissimilar materials. Shyue considers a system consisting of the Euler equations for compressible flow augmented with a further set of equations to accurately capture mixing of fluids and evolve thermodynamic parameters of the equations of state.

While a complete description of the algorithm is beyond the scope of this project, an overview is presented here. For details of the Riemann problem, Toro (2009) is a valuable reference; for the approach of linearising the conservation laws to simplify the solution, see Roe (1981) and LeVeque (1997) for the wave propagation formalism; and for the multicomponent algorithm described herein, see Shyue (1998) and (2001).
Governing equations

We consider inviscid compressible flows described by the Euler equations,

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \]
\[ \frac{\partial \rho u_i}{\partial t} + \nabla \cdot (\rho u_i \mathbf{u}) + \frac{\partial p}{\partial x_i} = 0, \]
\[ \frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{u} (E + p)) = 0, \]

where \( \mathbf{u}, p, \rho \) and \( E = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2 \) denote the velocity, pressure, density, and total energy density respectively. The index \( i \) runs over the spatial dimensions of the problem. However, these equations are not sufficient to describe multicomponent flow. For brevity, the derivation of additional governing equations is discussed in one dimension and two fluid components, though the extension to higher dimensions does not introduce a great deal of mathematical complexity.

In order to track the volume fraction of each component, an additional equation is introduced,

\[ \frac{\partial Y}{\partial t} + \mathbf{u} \cdot \nabla Y = 0, \]

where \( Y \) is the volume fraction of one component of the flow. The volume fraction of the other component, by unitarity, is \( 1 - Y \).

Considering the conservation of the quantity \( \rho e \) from the Euler equations (Equation 6c), combined with the Mie–Grüneisen equation of state (Equation 4b) leads to further equations,

\[ \frac{\partial}{\partial t} \left( \frac{1}{\Gamma} \right) + u \frac{\partial}{\partial x} \left( \frac{1}{\Gamma} \right) = 0, \]
\[ \frac{\partial}{\partial t} \left( -\frac{p_{\text{ref}}}{\Gamma} + \rho e_{\text{ref}} \right) + u \frac{\partial}{\partial x} \left( -\frac{p_{\text{ref}}}{\Gamma} + \rho e_{\text{ref}} \right) = 0. \]

This has been split into two equations in order to allow accurate computation of the pressure (note that each bracketed term is a member of the overall state vector Equation 11),

\[ p = \left[ (\rho E) - \frac{(\rho u)^2}{2 (\rho)} + (p_{\text{ref}}) - (\rho e_{\text{ref}}) \right] / \left( \frac{1}{\Gamma} \right). \]

In summary, the total state vector is,

\[ \mathbf{q} = [\rho \quad \rho \mathbf{u} \quad \rho E \quad \frac{p_{\text{ref}}}{\Gamma} \quad \rho e_{\text{ref}} \quad Y]^T, \]

which obeys the governing equations, in quasilinear form,

\[ \frac{\partial \mathbf{q}}{\partial t} + \mathbf{A} (\mathbf{q}) \frac{\partial \mathbf{q}}{\partial x} = 0, \]

with,

\[ \mathbf{A} (\mathbf{q}) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{K - u^2}{u} & \frac{u (2 - \Gamma)}{\Gamma} & -\rho \Gamma & -\Gamma & \Gamma & 0 \\ \frac{u (K - H)}{u} & \frac{H - u^2 \Gamma}{u} & \frac{u (\Gamma + 1)}{u} & -u p \Gamma & u \Gamma & -u \Gamma & 0 \\ -\phi & \phi & 0 & 0 & 0 & 0 & 0 \\ -\chi & \chi & 0 & 0 & u & 0 & 0 \\ -\psi & \psi & 0 & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & u \end{bmatrix}. \]
where \( K = \Gamma u^2 \), \( H = E + p/\rho \), \( \phi = -\Gamma'/\Gamma^2 \), \( \chi = (\Gamma'p'_{\text{ref}} - \Gamma'p_{\text{ref}})/\Gamma^2 \), and \( \psi = e_{\text{ref}} + \rho e'_{\text{ref}} \).

In order to solve these equations numerically, it is useful to find the eigendecomposition of the matrix \( \Lambda (q) \). This is achieved with a diagonal matrix of eigenvalues,

\[
\Lambda = K^{-1} A K = \text{diag} (u - c, u, u + c, u, u, u),
\]

(14)

where \( K \) is a matrix whose columns are the corresponding right eigenvectors of \( A \),

\[
K = \begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 \\
\phi & 0 & \phi & 1 & 0 & 0 & 0 \\
\chi & 0 & \chi & 0 & 1 & 0 & 0 \\
\psi & 0 & \psi & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 
\end{bmatrix}.
\]

(15)

The projection of the state vector \( q \) onto the basis formed by the eigenvectors is given by \( w = K^{-1} q \). By direct substitution of \( q = K w \) into Equation 12, and then using Equation 14, we can recast the governing equations as,

\[
\frac{\partial w_i}{\partial t} + \Lambda \frac{\partial w_i}{\partial x} = 0.
\]

(16)

This provides a substantial simplification over the original formulation, as we have obtained completely decoupled equations of motion for each characteristic variable \( w_i \),

\[
\frac{\partial w_i}{\partial t} + \lambda_i \frac{\partial w_i}{\partial x} = 0.
\]

(17)

### The Riemann problem

The Riemann problem deals with the solution for \( t > 0 \) of a set of hyperbolic conservation laws with initial conditions which consist of a single jump discontinuity,

\[
q(t = 0, x) = \begin{cases}
q_L & x < 0 \\
q_R & x > 0
\end{cases}.
\]

(18)

By solving the Riemann problem at each cell boundary in a numerical grid, we can integrate the governing equations over the domain (Equation 16) to progress the solution forward in time. This approach for solving hyperbolic systems of conservation laws was proposed in Godunov (1959). In Roe (1981), the quasilinear problem (Equation 12) is replaced with an approximate linear problem,

\[
\frac{\partial q}{\partial t} + \hat{A}(q_L, q_R) \frac{\partial q}{\partial x} = 0,
\]

(19)

with the matrix \( \hat{A} \) obeying requirements of a) strict hyperbolicity (a set of real eigenvalues and linearly independent eigenvectors) b) consistency with the exact Jacobian matrix, \( \hat{A}(q, q) = \Lambda (q) \) c) conservation across discontinuities \( F(q_R) - F(q_L) = \hat{A}(q_R - q_L) \). Conservation is guaranteed by criterion (c), while (b) is necessary if we hope to recover the exact Jacobian from the approximation.
An explicit construction of \( \hat{A} \) is provided by “Roe averaging” each variable in \( A \) such that,
\[
\hat{A} = \frac{\sqrt{\rho_L} \hat{A}_L + \sqrt{\rho_R} \hat{A}_R}{\sqrt{\rho_L} + \sqrt{\rho_R}},
\]
(20)
Following the approach in LeVeque (1997), the jump in \( q \) can be written as a sum of weighted Roe-averaged eigenvalues (where \( 7 \) is the dimension of the state vector),
\[
\Delta q = q_R - q_L = \sum_{i=1}^{7} \hat{\alpha}_i \hat{k}_i = \sum_{i=1}^{7} \mathcal{W}_i,
\]
(21)
where \( \mathcal{W}_i \) are the wave strengths of each characteristic across the boundary. With the grid discretised in a standard finite-volume formulation, where \( Q^n_j \) represents the cell average of the state vector over the interval \([x_j, x_{j+1}]\),
\[
Q^n_j = \frac{1}{\Delta x} \int_{x_j}^{x_{j+1}} q(x, t_n) \, dx,
\]
(22)
we can use a standard first-order upwind scheme to progress the solution to \( t + \Delta t \), with \( \lambda_i^- = \min(\lambda_i, 0) \) and \( \lambda_i^+ = \max(\lambda_i, 0) \),
\[
Q^{n+1}_j = Q^n_j - \frac{\Delta t}{\Delta x} \sum_{i=1}^{7} \left[ (\lambda_i^- \mathcal{W}_i)_{j+1} + (\lambda_i^+ \mathcal{W}_i)_j \right].
\]
(23)
In practice, we wish to improve accuracy with a higher order solver. However, direct application of a higher order upwind scheme will give rise to spurious oscillations at discontinuities in the problem. As such, this first order scheme is combined with a higher order correction weighted by a flux limiter. Defining the Courant–Friedrichs–Lewy (CFL) number as (Courant et al., 1928),
\[
C = \frac{\Delta t}{\Delta x} \max(\lambda),
\]
(24)
where \( \max(\lambda) \) denotes the fastest travelling characteristic on the grid, we require \( C < 1 \) for stability. Heuristically, this can be justified by arguing that information must not travel more than one grid length during a single time step. A target CFL number of 0.95 is used throughout this work.

**Adaptive Mesh Refinement**

As the Richtmyer–Meshkov instability deals with turbulent mixing at the interfaces of two fluids, in addition to simulating the bulk motion of the fluid, we are also concerned with fine detail at the sub-millimetre scale. If we attempted an accurate solution by increasing the resolution of a uniform grid, the simulation would quickly become prohibitively time consuming, as the computational time for a simulation on a 2D grid will scale as approximately \( O(\Delta x^{-3}) \). The number of cells scales as \( O(\Delta x^{-2}) \), while the CFL condition (Equation 24) imposes an additional factor of \( \Delta x^{-1} \).

A solution to this problem is provided by Adaptive Mesh Refinement (AMR), first proposed in Berger and Colella (1989). This scheme is implemented by discretising the domain as a hierarchy of subgrids of increasing resolution. Each subgrid is a regular Cartesian grid, so optimised high-order solvers can be used, but the domain can be dynamically refined after each step where necessary to capture evolving features of the flow. Conservation laws are imposed by matching fluxes at the boundaries of subgrids. Subgrids are refined in time as well as space in order to progress each at an optimal CFL number. The criterion for refinement is \( |\nabla \rho| > \epsilon \), where \( \epsilon \) is taken to be \( 4 \times 10^{-4} \) kg m\(^{-4} \) throughout the air–SF\(_6\) simulations. \( \nabla \rho \) is computed numerically by a second order derivative.
Figure 2: Refinement level of the domain at late time for a simulation of an air–SF$_6$ chevron simulation. Red, yellow, green and blue correspond to total refinement levels of $\times 1$, $\times 2$, $\times 8$ and $\times 16$ respectively. Interfaces between the two materials are the most refined, with the location of transmitted and reflected waves also visible due to local refinement around them.

**Experimental method**

Experiments mentioned in this report were conducted in AWE’s 20 cm $\times$ 10 cm shock tube with a Mach number of 1.26 (70 kPa overpressure, parameters for the shock wave in Table 2). SF$_6$ seeded with an olive oil aerosol tracer is used as the dense gas (Atwood number 0.67), separated from air by microfilm membranes supported on a fine wire grid of 25 $\mu$m diameter and 4 mm spacing. Interfaces along the direction of flow are not separated by membranes. Upon impact by the shock wave, the microfilm membrane fragments, allowing the two gases to mix.

Laser sheet images are produced by using a laser pulsed every 80 $\mu$s to illuminate a planar slice of the shock tube. Mie scattered light is captured by a rotating drum camera on black and white film (see Holder et al. (2003) for more information about the experimental configuration). Under the assumption that the amount of scattered light is proportional to the density of the tracer, the laser sheet images are imitated with density plots. Mock-schlieren images prove useful to visualise propagation of shocks as well as material interfaces, and are modelled by the formula,

$$\phi = \exp \left( -k \frac{|\nabla \rho|}{\max (|\nabla \rho|)} \right),$$  \hspace{1cm} (25)

where $k$ is a factor to amplify small gradients.

**Validation**

**Stiffened gas equation of state**

An exact model solution from Chinnayya et al. (2004) was used to validate the numerical solution for an air–water interface. The water is modelled by the stiffened gas equation of state (Equation 3), and air as an ideal gas, both with parameters as described in Table 1, with the exception of the $\rho_{\text{air}} = 50 $ kg m$^{-3}$. The interface separating the water (left portion of the domain) and gas (right) is initially at $x = 0.7$ m. The water has pressure $10^8$ Pa, and the air $10^5$ Pa.
Figure 3 shows plots of the density and pressure at \( t = 237.44 \mu s \). These data show that the shock has been accurately captured without spurious oscillation at the fluid interface, and good agreement with the exact solution is observed.

**Air–SF\(_6\) block experiment**

Previous work within the Laboratory for Scientific Computing saw the development of a viscid shock-capturing multicomponent solver which was then used to investigate the interaction of a shock wave with a rectangular block of SF\(_6\) in air (Bates et al., 2007). This simulation was repeated with the current solver to confirm its accuracy in two dimensions with an ideal gas equation of state. Figure 4 shows the configuration and dimensions of the simulation; material parameters were as in Table 1, with additional parameters for the shock wave shown in Table 2. Per Holder and Barton (2004), a perturbation of root mean square amplitude 0.01 cm with wavelengths 0.5 cm to 5 cm was applied to both interfaces. The simulation was performed with a base grid of 110 \( \times \) 40 and refinement levels \( \times 2, \times 4, \times 2 \) leading to an effective resolution of 1760 \( \times \) 640.

A comparison of experimental data to simulation is shown in Figure 5. Strong agreement is seen with both the overall extent and details of the flow captured accurately by the solver. Significant errors are introduced at late time due to a) small random fluctuations present in the initial conditions not captured by the perturbation applied, and b) the drainage hole upstream of the SF\(_6\) block not being modelled; this is shown to have a significant effect at later times in Bates et al. (2007).
Figure 5: Validation of the model in 2D against experimental data. Left: laser-sheet images from Bates et al. (2007), middle: simulated density, right: simulated mock-schlieren. Frames are taken at (a) 206 $\mu$s, (b) 446 $\mu$s, (c) 926 $\mu$s, (d) 1726 $\mu$s, (e) 2046 $\mu$s, (f) 2846 $\mu$s, (g) 4046 $\mu$s measured from initial shock–SF$_6$ contact.
Results and discussion

Chevron shock tube experiment with air–SF$_6$ interface

Holder and Barton (2004) presents further shock tube results. Figure 6 shows the initial conditions for an experiment investigating the interaction of a shock wave with a block of SF$_6$ in the shape of an inverse chevron. Material parameters are as in Table 1, with shock overpressure as in Table 2 leading to a Mach 1.26 shock. The simulation was performed with the same refinement levels as in the SF$_6$ block validation.

![Figure 6: Configuration for the SF$_6$ inverse chevron simulation.](image)

Figure 6: Configuration for the SF$_6$ inverse chevron simulation. The lengths in the diagram have values $h = 20\,\text{cm}$, $L = 35\,\text{cm}$, $L_{\text{chevron}} = 15\,\text{cm}$, $\theta = 157^\circ$. The chevron has a total amplitude of 2 cm.

Samples of experimental laser-sheet images, and simulated density and mock-schlieren plots are shown in Figure 7. Times for the images are measured from shock arrival at the left interface. As such, Figure 7(a) shows the initial conditions, with the membrane separating the upstream air from the SF$_6$ chevron clearly visible. Initial perturbations in the experimental data are too small to be distinguishable.

By Figure 7(b), the shock wave has passed the upstream interface and compressed the chevron by approximately a third. Increased SF$_6$ density leads to a higher concentration of tracer and therefore more scattered light. In both the laser-sheet images and simulation data, we can see the perturbations on the interfaces begin to develop to comparable amplitudes. In Figure 7(c), the shock has exited the chevron and has reached the end of the shock tube. Refraction of the shock at the right boundary, resulting in a force directed perpendicular to it, has lead to the formation of a “jet” of SF$_6$ in the centre of the chevron, as well as formation of vortices near the walls of the shock tube.

Fragments of the membranes used to initially separate the fluids can be seen being ejected in Figure 7(d). The shock wave is visible in the middle of the SF$_6$ region having been reflected by the head of the shock tube. Development of the instability at the upstream boundary is visible in the form of air intrusions to the chevron.

By Figure 7(e), reshock of the right interface has lead to large instabilities forming, as well as a distinct blunting of the jet. Reshock of the left interface has reduced the amplitude of the instability present. The initially planar shock wave has been bowed due to the differing travel times across its length. Reflected waves within the block can be seen in the mock-schlieren images. Development
Figure 7: Comparison of simulation to experiment for the SF$_6$ chevron case. *Left:* laser sheet frames, *middle:* simulated density, *right:* simulated mock-schlieren. Times displayed are (a) 0.0 ms, (b) 0.5 ms, (c) 1.3 ms, (d) 1.9 ms, (e) 2.2 ms, (f) 2.7 ms, (g) 3.3 ms.
of the vortices at the edges of the shock tube has caused further upstream propagation of air by Figure 7(f). In the simulation images, the large-scale instabilities at the left boundary have evolved into a region of fine-scale turbulent mixing, which has been well-captured by AMR.

The position of the left and right edges of the SF$_6$ region were tracked in the simulation, with results shown in Figure 8. Times at which salient events take place are labelled and described in the caption. Having been shocked at time (b), the jet undergoes a period of linear growth until reshock by the reflected shock wave at time (c), at which point propagation of the jet slows. Similar results are seen for the left interface, which moves at constant velocity until the block is reshocked at time (c). When the left interface is reshocked at time (d), the velocity of the interface reverses and perturbations travel upstream.

As the problem possesses symmetry about the $x = 0.1$ m plane, vorticity in the upper half will, barring numerical errors and the effects of initial perturbations, exactly cancel that in the lower half. Therefore, the definition of total circulation, $\Gamma = \int \omega \cdot dA$, must be modified to give the total positive circulation,

$$\Gamma^+ = \int_S \min(0, \omega) \, dA,$$

(26)

where $\omega$ is a scalar quantity as the simulation is performed in 2D. This is equivalent to the total circulation for the region $0 \text{ cm} \leq x \leq 0.1 \text{ cm}$.

![Figure 8: Position of the left and right limits of the SF$_6$ region throughout the simulation, determined by the extremal cells with at least 10% volume fraction of SF$_6$. Experimental measurements are shown with estimated errors. Marked times correspond to: (a) at 0 ms, shock impacting SF$_6$; (b) at 0.85 ms, shock leaving SF$_6$; (c) at 1.57 ms, reshock of the jet; (d) at 2.10 ms, shock leaving SF$_6$; (e) at 2.90 ms, jet hitting the end of the shock tube.](image-url)

Circulation is shown in Figure 9, with marked times corresponding to Figure 8. The vorticity field immediately after each marked time is shown in Figure 10 for comparison. Many of the pertinent events are clearly displayed as abrupt changes in positive circulation. The impact of the shock wave with the left interface at time (a) leads to a small amount of circulation due to perturbations (not
Figure 9: Total and positive circulation for the air–SF$_6$ chevron case. $t = 0$ corresponds to the time of impact of the shock wave on the left side of the chevron. Markers (a)–(e) are as in Figure 8.

Figure 10: Vorticity fields for the SF$_6$ chevron case. (a)–(e) are taken soon after each corresponding point in Figure 9.

visible in the vorticity field), with significantly more produced when interacting with the chevron profile at time (b). The latter interaction is non-instantaneous due to the finite overall width of the chevron. Circulation then increases, more so when the jet is reshocked at time (c). Reshock of the left interface, with its perturbations now given approximately 2 ms to increase in amplitude due the RMI, leads to the circulation more than doubling, indicating the development of turbulent mixing of air and SF$_6$. The impact of the jet with the end of the shock tube at time (e) has no visible effect on the positive circulation.
**Convergence and computational time**

We might reasonably be concerned that AMR might introduce numerical errors to the solution. The dynamic creation and destruction of subgrids, if not performed carefully, could lead to the introduction of spurious waves. To confirm that AMR did not introduce errors, the simulation was performed at multiple resolutions with the circulation shown in Figure 11. No initial perturbations were applied. Two conclusions can be drawn from these data:

1. Circulation is seen to increase with the effective resolution of the simulation. The development of the Richtmyer–Meshkov instability leads to a region of turbulent mixing, and as turbulence occurs at all length scales, by increasing the resolution we capture details which will exist at shorter scales (see Sytine et al. (2000) for further consideration of this effect). However, the overall structure, including maxima and minima, is represented well over different resolutions.

2. Differences are primarily due to the effective resolution, not the base resolution. Very little difference is seen between simulations performed at the same effective resolution (for example, $110 \times 40 \times 2, \times 2$ compared to $440 \times 160$).

![Figure 11: Total positive circulation for various base resolutions and refinement levels.](image)

Relative computation times for various base resolution and refinement levels are shown in Table 3. Substantial speed improvements are seen by reaching an effective resolution with a lower base resolution combined with several refinement levels. Computational time increases by a factor of approximately 12 when doubling the resolution of the base grid without AMR, so by extrapolation the execution time for the maximum effective resolution without AMR would have been approximately nine days. From this, coupled with the second point above, we conclude that AMR is a useful approach to reduce computation time without sacrificing the accuracy of the numerical solution.
Table 3: Comparative run times for various base grid resolutions and refinement levels. Computational time is normalised to the longest run, approximately 17 hours.

<table>
<thead>
<tr>
<th>Base grid resolution</th>
<th>AMR levels</th>
<th>Effective resolution</th>
<th>Relative computation time</th>
</tr>
</thead>
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<td>1.000</td>
</tr>
</tbody>
</table>

Effect of perturbation amplitude

Figure 12: Comparison of flowfield for different initial perturbations at 2.7 ms. Top: schlieren field, bottom: vorticity field. Columns correspond to 0 cm, 0.01 cm, and 0.1 cm initial perturbation amplitude respectively.

Density and schlieren fields for different amplitudes of initial perturbation are shown in Figure 12. Both the schlieren and vorticity field plots show that the region of mixing between the two fluids is strongly dependent on the amplitude of the initial perturbations. Negligible vorticity is seen at the left interface when no initial perturbation is applied, while by comparison an approximately 7 cm region of turbulent mixing is shown for the 0.1 cm perturbation case. Again, the mock-schlieren images show that AMR has effectively captured the fine structure of the flow.

Figure 13 shows the positive circulation over time for three different initial perturbation amplitudes. Differences between the 0.01 cm and 0.1 cm cases are seen to be small until the shock wave interacts with the chevron interface, at which point the larger perturbations lead to substantial development of vorticity along the interface. In all cases, larger initial perturbation leads to a more substantial change in circulation at reshock, as well as a uniformly more intense circulation throughout the simulation.
Chevron shock tube simulation with air–water interface

Simulation of the inverse chevron geometry is extended to a configuration in which the dense gas is replaced with water modelled by a stiffened gas equation of state. Material parameters are as defined in Table 1, with the exception of the density of air, $\rho_{\text{air}} = 50 \text{ kg m}^{-3}$. Shock speed is chosen to be Mach 2.5 (implementation details in Appendix A). The simulation is performed with a base grid of $110 \times 40$ and refinement levels of $\times 2, \times 2$. An initial perturbation of amplitude 0.01 cm is applied to both interfaces.

Figure 14 shows sample frames from the simulation. By Figure 14(a), the shock wave has impacted the interface, and a jet has begun to emerge. Transmission of the shock through the water is substantially lower due to the large difference in density. The most striking difference between the air–water case and the air–SF$_6$ case is the transfer of momentum to the bulk of the chevron. By Figure 14(c), we can see that the overall motion of the water dwarfs the speed of growth of the jet, leading, in Figure 14(d), to the chevron compressing the upstream air significantly and rebounding.

Also significant in Figure 14(d) is the presence of a shock produced by the impact of the water with the upstream boundary of the shock tube. This secondary shock serves to shock the jet, and reshock the left interface. By Figure 14(e), the secondary shock has caused the water to recede at the boundaries of the shock tube, leading to significant vorticity at the edges of the jet. Late evolution of the flow is shown in Figure 14(f), in which we can see substantial development of the RMI at the left interface, leading to significant intrusions into the bulk of the water. Canonical “mushrooming” of several intrusions is visible. Fine scale mixing does not seem to have developed at this point.

Circulation is shown in Figure 15. Shock of the left perturbed interface takes place at $t = 0$, leading to small amounts of circulation. Beyond this point, the behaviour is dissimilar to previous simulations, as the shock is not strongly transmitted through the dense fluid. A significant increase
Figure 14: Sample data from the water chevron simulation. *Left:* density, *middle:* mock-schlieren, *right:* vorticity. Frames are taken at (a) 1.85 ms, (b) 3.35 ms, (c) 4.85 ms, (d) 6.35 ms, (e) 7.35 ms, (f) 9.35 ms.
in circulation occurs around 5 ms, when the water impacts the end of the shock tube, leading to shock wave production.

![Graph showing circulation throughout the water chevron simulation.](image)

**Figure 15:** Circulation throughout the water chevron simulation.

**Chevron shock tube simulation with TNT–copper–water interfaces**

Motivated by the explosive applications of a chevron profile, the solver was extended to three material phases by the addition of a further advection equation for volume fraction, leading to equations similar to Equation 7 for mass fractions of components 1 and 2, \( Y^{(1)} \) and \( Y^{(2)} \) (the third following from \( Y^{(3)} = 1 - Y^{(1)} - Y^{(2)} \)). Appropriate changes were made to the eigenvalues (Equation 15) in order to correctly advect the additional quantity with a characteristic velocity of \( u \).

![Diagram showing configuration for the TNT–copper–water inverse chevron simulation.](image)

**Figure 16:** Configuration for the TNT–copper–water inverse chevron simulation. The lengths in the diagram have values \( h = 20 \text{ cm}, \ L = 35 \text{ cm}, \ L_{\text{chevron}} = 15 \text{ cm}, \ \theta = 157^\circ \).

As shown in Figure 16, the same geometry as in the SF\(_6\) chevron case is considered, but with copper replacing the SF\(_6\), TNT upstream of the chevron, and water downstream. The copper and TNT are
Figure 17: Sample data from the copper chevron simulation. *Left:* density, *middle:* mock-schlieren, *right:* vorticity. Frames are taken at: (a) 0 µs, (b) 80 µs, (c) 145 µs, (d) 215 µs, (e) 410 µs, (f) 540 µs, (g) 650 µs.
modelled by the Cochran–Chan equation of state (Equation 5), while water is modelled as a stiffened gas (Equation 3). All material parameters are as in Table 1. A shock overpressure of $10^9$ Pa is used in the TNT region, leading to a shock speed of $4 \text{km s}^{-1}$ (comparable to the detonation speed of TNT). No perturbation was applied to either interface.

Density, mock-schlieren, and vorticity plots for the simulated flow are shown in Figure 17. Figure 17(a) is captured after the left edge has been shocked, while Figure 17(b) shows the emergence of a jet and vorticity created at the right interface soon after the shock has passed. In Figure 17(c), an overdense region of copper is visible in the upstream direction, and development of the jet has progressed. Counter vortices have developed at the top and bottom of the shock tube as in the SF$_6$ case.

By Figure 17(e), vorticity at the shock tube boundaries has caused the copper to “snake” along these edges and strong vortices further into the copper have drawn material away from the edge. The jet has developed into a narrow tube of copper with an emerging instability at its end due to reshock. Collision of the jet with the end of the shock tube is shown in Figure 17(f), with the jet still forming a narrow directed tube.

![Figure 18: Circulation for the copper chevron case. Times marked are: (a) 0µs, first shock of the left interface; (b) 30µs, first shock of right interface; (c) 330µs, reshock of the jet; (d) 520µs, jet impacting the end of the shock tube.](image)

Circulation of the copper simulation is shown in Figure 18. Some qualitative similarities can be seen to Figure 9, with most marked events noticeable as changes in circulation. The most distinct difference is the presence of fluctuations between transitional regions over shorter timescales. This may be due to stronger reflections within the copper chevron region, some of which are visible in Figures 17(d)–(e).
Conclusions

The Richtmyer–Meshkov instability produced by the interaction of a shock wave with an inverse chevron of SF₆ has been accurately captured by a 2D inviscid, fully conservative hydrocode. Experimental data agrees with the simulation in bulk quantities such as the overall extent of the flow, allowing for an analysis of the flow features in quantities which cannot be experimentally measured. Initial perturbations present on the air–SF₆ interfaces are shown to have a significant effect on the late-time evolution of the flow, justifying the initial choice. AMR has been used to provide more than an order of magnitude speed improvement, and has been shown not to introduce errors into the solution.

Results for the water chevron show that the term “stiffened gas” is appropriate and accurately describes the behaviour of the flow; in contrast to an ideal gas, the fluid does not flow as readily, but acquires a bulk velocity, leading to the production of a far broader jet, and a large-scale interaction with the downstream end of the shock tube. Shock tube simulations with a copper chevron lead to a significantly more narrow jet of material, defending the use of copper in shaped charges.

Acknowledgements

The author would like to thank Dr. Nikolaos Nikiforakis for his suggestion of the project and tutelage, Ms. Louisa Michael for invaluable advice, and Dr. Philip Blakely for technical assistance.
References


**Appendices**

**A Rankine–Hugoniot conditions**

Across a shock wave, there is a jump discontinuity in the material parameters of the flow. The Rankine–Hugoniot conditions relate the jump conditions required to the speed of propagation of the shock. Given the material parameters downstream of the shock, and the speed of the shock, this allows for full computation of the state vector of shocked gas.

Beginning with a conservation law of the form,

\[ \frac{\partial q}{\partial t} + \frac{\partial}{\partial x} f(q) = 0, \]  

(A.1)

by considering the existence of a shock at \( x_s(x) \) and integrating over a domain \((x_L, x_R)\) which encompasses the shock we obtain,

\[ \int_{x_L}^{x_R} \frac{\partial q}{\partial t} \, dx + \int_{x_L}^{x_R} \frac{\partial}{\partial x} f(q) \, dx = 0. \]  

(A.2)

If we then split the integral at the position of the shock \( x_s(t) \) and differentiate under the integral
sign,
\[ (q_L - q_R) \frac{dx_s}{dt} + \int_{x_L}^{x(t)} \frac{\partial q}{\partial t} \, dx + \int_{x_s(t)}^{x_R} \frac{\partial q}{\partial t} \, dx = f(q_L) - f(q_R), \] (A.3)

which, by letting \( x_L \to x_s(t) \) and \( x_R \to x_s(t) \) leads to the Rankine–Hugoniot jump condition,
\[ s (w_L - w_R) = f(w_L) - f(w_R) \] (A.4)

where \( s \) is the speed of propagation of the discontinuity,
\[ s = \frac{dx_s}{dt}. \] (A.5)

Applying this formalism to the 1D Euler equations in conservative form, combined with an equation of state, gives a method to fully determine the conditions upstream of a shock wave, given the speed of the shock, and the downstream parameters. For the case of an ideal gas, we obtain,
\[ p_{up} = \frac{(1 - \gamma) p_{down} + 2 s^2 \rho_{down}}{1 + \gamma}, \] (A.6a)
\[ \rho_{up} = \frac{s^2 (1 + \gamma) \rho_{down}^2}{2 p_{down} \gamma - s^2 \rho_{down} (1 - \gamma)}, \] (A.6b)
\[ u_{up} = 2 \frac{s^2 \rho_{down} - p_{down} \gamma}{s \rho_{down} (1 + \gamma)}, \] (A.6c)

where the subscripts “up” and “down” denote quantities upstream and downstream of the shock.

For constant \( p_{ref} \)

The same analysis can be applied when \( p_{ref} \) is nonzero but constant, and the same on both sides of the shock. This situation yields,
\[ p_{up} = \frac{(1 - \gamma) p_{down} + 2 p_{ref} + 2 s^2 \rho_{down}}{1 + \gamma}, \] (A.7a)
\[ \rho_{up} = \frac{s^2 (1 + \gamma) \rho_{down}^2}{2 p_{down} \gamma - 2 p_{ref} - s^2 \rho_{down} (1 - \gamma)}, \] (A.7b)
\[ u_{up} = 2 \frac{s^2 \rho_{down} - p_{down} \gamma + p_{ref}}{s \rho_{down} (1 + \gamma)}. \] (A.7c)

For varying \( p_{ref} \)

For complex equations of state with \( p_{ref} \) explicitly a function of \( \rho \), an analytic solution is generally unavailable. Fortunately, the parameters for a shock wave can be easily obtained by empirical means. Advecting a volume of the material under consideration towards a reflective boundary will result in a shock wave counterpropagating from the interface, from which the state variables can then be read. This approach was used to determine the parameters of a shock in TNT.

**B Interface noise**

For the experiments at AWE, perturbations on the interfaces arise due to both inherent background noise and the wire meshes used to segregate the fluids before the passage of the shock. According to
Holder et al. (2003), these can be modelled as noise of amplitude 0.1 m with wavelength 5 m to 50 m. A brownian spectrum was chosen, with a uniform number generator used to sample 50 frequencies, \( \nu_i \), each weighted as \( \alpha_i \propto \nu_i^{-2} \), and normalised such that,

\[
\sum_{i=1}^{50} \alpha_i^2 = A^2, \tag{B.1}
\]

where \( A \) is the desired amplitude of the perturbation.

## C Program listings

All code used for this project is attached on a DVD. The following files are entirely the work of the author:

- `render`
- `render_child`
- `grid`
- `/CAMR/projects/Shyue3D/Noise.hpp`
- `/CAMR/projects/Shyue3D/Noise2D.hpp`

The following were substantially modified by the author:

- `/CAMR/projects/Shyue3D/Driver.cpp` (primarily function `analysis`)
- `/CAMR/projects/Shyue3D/SimGrid.cpp` (`set_initial_data`, functions for calculating vorticity, and output functions).