High-Order Shock-Capturing Methods for Study of Shock-Induced Turbulent Mixing with Adaptive Mesh Refinement Simulations

Man Long Wong
Sanjiva K. Lele

Advanced Modeling & Simulation Seminar

Jun 6th, 2019
Motivation

- **Richtmyer-Meshkov (RM) instability**, or RMI, occurs when a shock wave passes through a perturbed interface separating two fluids with different densities.

- In natural phenomena/engineering applications:
  - Supernova explosion (SNe)
  - Inertial confinement fusion (ICF)
  - Supersonic combustion in scramjet

![RMI evolution (Image Credit: B. M. Wilson, R. Mejia-Alvarez and K. P. Prestridge)](image1)

![Supernova remnant (Image Credit: NASA/ESA/HEIC and The Hubble Heritage Team (STScI/AURA))](image2)
Motivation

• A lack of understanding of turbulent mixing induced from RMI, due to:
  ○ Only simultaneous measurements of density and velocity fields in 2D\textsuperscript{1,2}
  ○ Direct numerical simulations still too expensive
  ○ Methods to save computational cost:
    ● High-order shock-capturing schemes
    ● Adaptive gridding for localized and mobile features (shocks, mixing regions, etc.)

• High-order numerical schemes with adaptive mesh refinement (AMR) still not very popular for RMI simulations:
  ○ Tritschler et al.\textsuperscript{3} used high-order schemes with uniform grid to study RMI with re-shock
  ○ Grinstein and Gowardhan\textsuperscript{4} used AMR but only second order scheme for RMI simulations
  ○ Mcfarland et al.\textsuperscript{5} also used second order scheme with AMR for inclined interface RMI


Motivation

- Goals of research:
  - Numerical framework for simulations of RMI and similar types of flows. The framework combines:
    - Improved high-order shock-capturing methods to preserve fine-scales better
    - AMR technique that only applies fine grid cells around localized features
  - Study the turbulent mixing induced by RMI through simulations:
    - Variable-density mixing effects
    - Effects of Reynolds number
    - Analyze the performance of reduced-order modeling through second-moment closures
Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows

2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability

3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock

4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability
Weighted compact nonlinear schemes (WCNS’s): governing equation

- Consider a scalar conservation law for 1D problem:
  \[
  \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0
  \]

- Semi-discretize this equation on a grid with \(N\) points:
  \[
  \frac{\partial u_j}{\partial t} + \left. \frac{\partial f(u)}{\partial x} \right|_j = 0
  \]

- Need a discrete approximation of the flux derivative:
  \[
  \left. \frac{\partial f(u)}{\partial x} \right|_j
  \]
Illustration of methodology of WCNS’s \(^6\) \(^7\)

Given the solution values at cell nodes

\(u_{j-2}\)
\(u_{j-1}\)
\(u_j\)
\(u_{j+1}\)
\(u_{j+2}\)
\(u_{j+3}\)

\(j - 2\)
\(j - 1\)
\(j\)
\(j + 1\)
\(j + 2\)
\(j + 3\)

\(j - \frac{3}{2}\)
\(j - \frac{1}{2}\)
\(j + \frac{1}{2}\)
\(j + \frac{3}{2}\)
\(j + \frac{5}{2}\)

---


Illustration of methodology of WCNS’s

Left-biased interpolation for solution value at cell midpoint $\tilde{u}_{j+\frac{1}{2}}$

---

6 Deng and Zhang, “Developing high-order weighted compact nonlinear schemes”.

7 Zhang, Jiang, and Shu, “Development of nonlinear weighted compact schemes with increasingly higher order accuracy”.

---

Given the solution values at cell nodes, left-biased interpolation for solution value at cell midpoint $\tilde{u}_{j+\frac{1}{2}}$.

Explicit/compact finite difference to approximate $\hat{f}(u_j)$ at nodes, e.g. explicit sixth order midpoint-and-node-to-node finite difference (MND):

$\hat{f}(u_j) \approx \tilde{f}_j + \frac{1}{2} \tilde{f}_{j+1} - \frac{1}{2} \tilde{f}_{j-1}$

$\hat{f}(u_j) \approx \tilde{f}_j + \frac{1}{2} \tilde{f}_{j+1} - \frac{1}{2} \tilde{f}_{j-1}$

$\hat{f}(u_j) \approx \tilde{f}_j + \frac{1}{2} \tilde{f}_{j+1} - \frac{1}{2} \tilde{f}_{j-1}$

$\hat{f}(u_j) \approx \tilde{f}_j + \frac{1}{2} \tilde{f}_{j+1} - \frac{1}{2} \tilde{f}_{j-1}$
Illustration of methodology of WCNS’s

Given the solution values at cell nodes Left-biased interpolation for solution value at cell midpoint Right-biased interpolation for solution value at cell midpoint Flux-difference splitting method to get the interface solution value and flux at midpoint from left-biased and right-biased interpolated values

Explicit/compact finite difference to approximate \( \hat{f}(u) \) at nodes, e.g. explicit sixth order midpoint-and-node-to-node finite difference (MND):

\[
\tilde{u}_{R,j+\frac{1}{2}} \neq \tilde{u}_{L,j+\frac{1}{2}}
\]

\[
\tilde{u}_{R,j+\frac{1}{2}} \neq \hat{f}_{j+1} - \hat{f}_{j} = \frac{u_{j+2} - u_{j+1}}{x_{j+\frac{3}{2}} - x_{j+\frac{1}{2}}}
\]

\[
\hat{f}(u) \neq \frac{f_{j+1} - f_{j}}{x_{j+\frac{3}{2}} - x_{j+\frac{1}{2}}}
\]

\[
\tilde{u}_{R,j+\frac{1}{2}} \neq \frac{u_{j+2} - u_{j+1}}{x_{j+\frac{3}{2}} - x_{j+\frac{1}{2}}}
\]

\[
\hat{f}(u) \neq \frac{f_{j+1} - f_{j}}{x_{j+\frac{3}{2}} - x_{j+\frac{1}{2}}}
\]

\[
\tilde{u}_{R,j+\frac{1}{2}} \neq \frac{u_{j+2} - u_{j+1}}{x_{j+\frac{3}{2}} - x_{j+\frac{1}{2}}}
\]

\[
\hat{f}(u) \neq \frac{f_{j+1} - f_{j}}{x_{j+\frac{3}{2}} - x_{j+\frac{1}{2}}}
\]
Illustration of methodology of WCNS’s \(^6\) \(^7\)

Flux-difference splitting method to get the interface solution value and flux at midpoint from left-biased and right-biased interpolated values

\(^6\)Deng and Zhang, “Developing high-order weighted compact nonlinear schemes”.

\(^7\)Zhang, Jiang, and Shu, “Development of nonlinear weighted compact schemes with increasingly higher order accuracy”. 
Illustration of methodology of WCNS’s \(^6\) \(^7\)

**Explicit/compact finite difference to approximate** \(\frac{\partial f(u)}{\partial x} \bigg|_j\) at nodes, e.g.

**explicit sixth order midpoint-and-node-to-node finite difference (MND):**

\[
\frac{\partial f(u)}{\partial x} \bigg|_j \approx \frac{1}{\Delta x} \left[ \frac{3}{2} \left( \tilde{f}_{j+\frac{1}{2}} - \tilde{f}_{j-\frac{1}{2}} \right) - \frac{3}{10} \left( f_{j+1} - f_{j-1} \right) - \frac{25}{384} \left( \tilde{f}_{j+\frac{3}{2}} - \tilde{f}_{j-\frac{3}{2}} \right) \right]
\]
Left-biased explicit interpolations

\[ EI_0 : \tilde{u}^{(0)}_{j + \frac{1}{2}} = \frac{1}{8} \left( 3u_{j-2} - 10u_{j-1} + 15u_j \right) \]

\[ EI_1 : \tilde{u}^{(1)}_{j + \frac{1}{2}} = \frac{1}{8} \left( -u_{j-1} + 6u_j + 3u_{j+1} \right) \]

\[ EI_2 : \tilde{u}^{(2)}_{j + \frac{1}{2}} = \frac{1}{8} \left( 3u_j + 6u_{j+1} - u_{j+2} \right) \]

\[ EI_3 : \tilde{u}^{(3)}_{j + \frac{1}{2}} = \frac{1}{8} \left( 15u_{j+1} - 10u_{j+2} + 3u_{j+3} \right) \]

\[ EI_{\text{upwind}} = \sum_{k=0}^{2} d_k^{\text{upwind}} EI_k \quad (5^{\text{th}} \text{ order}); \quad EI_{\text{central}} = \sum_{k=0}^{3} d_k^{\text{central}} EI_k \quad (6^{\text{th}} \text{ order}) \]
Nonlinear interpolations

In weighted essentially non-oscillatory (WENO) interpolations, the linear weights $d_k$ are replaced with nonlinear weights $\omega_k$ for shock-capturing:

$$EI_{\text{upwind}} = \sum_{k=0}^{2} d_{k}^{\text{upwind}} E I_k \quad (5\text{th order}); \quad EI_{\text{central}} = \sum_{k=0}^{3} d_{k}^{\text{central}} E I_k \quad (6\text{th order})$$

$$EI_{\text{nonlinear}} = \sum_{k=0}^{2} \omega_{k}^{\text{upwind}} E I_k \quad / \quad \sum_{k=0}^{3} \omega_{k}^{\text{central}} E I_k$$

- $\omega_k^{\text{upwind}}$: traditional WENO weights by Jiang and Shu (JS)$^8$ and improved weights (Z)$^9$
- $\omega_k^{\text{central}}$: CU-M2 weights $^{10}$

---


Locally dissipative (LD) nonlinear weights

- The LD\textsuperscript{11} nonlinear weights (hybrid weights) are introduced for localized dissipation at shocks or discontinuities for regularization:

\[
\omega_k = \begin{cases} 
\sigma \omega_k^{\text{upwind}} + (1 - \sigma) \omega_k^{\text{central}}, & \text{if } R_\tau > \alpha_{RL}, \\
\omega_k^{\text{central}}, & \text{otherwise}
\end{cases}, \quad k = 0, 1, 2, 3
\]

where \(R_\tau\) is a relative smoothness indicator. \(\sigma\) is a shock sensor.

- Ensure minimal numerical dissipation in smooth regions (central interpolation) and one-sided interpolation at discontinuities

- \(\omega_k^{\text{upwind}}\) is the Z nonlinear weights and \(\omega_k^{\text{central}}\) is improved from CU-M2 nonlinear weights for localized numerical dissipation

---

Approximate dispersion relation (ADR) technique\textsuperscript{12}

- For linear schemes, analytical dispersion and dissipation characteristics can be obtained from Fourier analysis.
- ADR used to compute the characteristics of the nonlinear schemes numerically:

\begin{itemize}
  \item (a) Dispersion characteristics
  \item (b) Dissipation characteristics
\end{itemize}

Numerical tests: 1D shock tube problems

1. Shu-Osher problem\textsuperscript{13} [200 points]: Mach 3 shock interacting with a sinusoidal density field

2. Multi-species shock tube\textsuperscript{14} [100 points]:


Numerical test: 2D double Mach reflection\textsuperscript{15}

- A Mach 10 shock impinges on the wall, and a complex shock reflection structure evolves
- Kelvin-Helmholtz instability along the slip line is only damped by numerical dissipation
- The smaller the numerical dissipation, the more the rolled up vortices along the slip line

Numerical test: 2D double Mach reflection (cont.)

- Density contours [Full domain grid size: $960 \times 240$):

(a) WCNS5-JS
(b) WCNS5-Z
(c) WCNS6-CU-M2
(d) WCNS6-LD

- WCNS5-JS and WCNS5-Z too dissipative to produce rolled-up vortices along the slip line.
- WCNS6-CU-M2 and WCNS6-LD can capture much more fine-scale vortical structures along the slip line.
Numerical test: 3D Taylor-Green vortex

- An essentially incompressible periodic problem
- As time evolves, the inviscid vortex stretches and produces features at smaller scales
- Zero Q-criterion at $t = 8$ with $64^3$ grid:

(a) WCNS5-JS  
(b) WCNS5-Z  
(c) WCNS6-CU-M2  
(d) WCNS6 – LD

- Finer features are captured with WCNS6-CU-M2 and WCNS6-LD
Numerical test: 3D Taylor-Green vortex (cont.)

- **WCNS6-LD** preserves more KE over times
- Both WCNS6’s outperform WCNS5’s in predicting growth of enstrophy
- Both WCNS6’s can better capture features up to high wavenumber
Summary

• Improved nonlinear interpolation developed for a type of nonlinear schemes for problems with shocks and material interfaces
• The interpolation adaptively switches between one-sided interpolation around discontinuities and non-dissipative central interpolation in smooth regions
• The improved scheme WCNS-LD:
  ○ robust at shocks and discontinuities through the regularization
  ○ good resolution and low dissipation properties that are more suited for vortical features
Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows

2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability

3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock

4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability
Overview of patch-based adaptive mesh refinement (AMR)

- Patch-based AMR\textsuperscript{16}\textsuperscript{17} designed for uniform structured Cartesian grids
- A hierarchy of nested "patches" of levels of varying grid resolution
- **Multi-time stepping** with Runge-Kutta schemes:
  \[
  \frac{\Delta t_l}{\Delta x_l} = \frac{\Delta t_{l-1}}{\Delta x_{l-1}} = \ldots = \frac{\Delta t_0}{\Delta x_0}
  \]
- Requires numerical scheme in **conservative** form for treatment at coarse-fine AMR grid boundaries to ensure **discrete conservation**:
  \[
  \frac{\partial u_{i,j}}{\partial t} + \frac{\hat{F}_{i+\frac{1}{2},j} - \hat{F}_{i-\frac{1}{2},j}}{\Delta x} + \frac{\hat{G}_{i,j+\frac{1}{2}} - \hat{G}_{i,j-\frac{1}{2}}}{\Delta y} = 0
  \]


Relation between finite difference schemes and flux difference form

- For a central finite difference scheme (compact or explicit) for flux derivative:

\[
\alpha \hat{F}'_{j-\frac{1}{2}} + \beta \hat{F}'_{j+\frac{1}{2}} + \alpha \hat{F}'_{j+\frac{3}{2}} = \frac{1}{\Delta x} \left( -a_{\frac{5}{2}} F_{j-2} - a_{2} F_{j-\frac{3}{2}} - a_{\frac{3}{2}} F_{j-1} - a_{1} F_{j-\frac{1}{2}} + a_{1} F_{j+\frac{1}{2}} + a_{\frac{3}{2}} F_{j+1} + a_{2} F_{j+\frac{3}{2}} + a_{\frac{5}{2}} F_{j+2} \right)
\]

- Can be rewritten into flux difference form:

\[
\alpha \hat{F}'_{j-\frac{1}{2}} + \beta \hat{F}'_{j+\frac{1}{2}} + \alpha \hat{F}'_{j+\frac{3}{2}} = a_{\frac{5}{2}} F_{j-1} + a_{2} F_{j-\frac{1}{2}} + \left( a_{\frac{3}{2}} + a_{\frac{5}{2}} \right) F_{j} + (a_{1} + a_{2}) F_{j+\frac{1}{2}} + \left( a_{\frac{3}{2}} + a_{\frac{5}{2}} \right) F_{j+1} + a_{2} F_{j+\frac{3}{2}} + a_{\frac{5}{2}} F_{j+2}
\]

s.t.

\[
\hat{F}'_{j} = \frac{1}{\Delta x} \left( \hat{F}_{j+\frac{1}{2}} - \hat{F}_{j-\frac{1}{2}} \right)
\]
Hydrodynamics Adaptive Mesh Refinement Simulator (HAMeRS)\textsuperscript{19}

In-house flow solver built on parallel SAMRAI library from LLNL to simulate compressible single-species and multi-species flows with adaptive mesh refinement (AMR) and high-order shock-capturing methods:

\textbf{Application}

\textbf{Navier-Stokes}
\textbf{Euler}

\textbf{Refinement Tagger}

\textbf{Value Tagger}
\textbf{Gradient Tagger}
\textbf{Multiresolution Tagger}

\textbf{Euler Initial Conditions}
\textbf{Euler Boundary Conditions}

\textbf{Convective Flux Scheme}
\textbf{Diffusive Flux Scheme}

\textbf{N.-S. Initial Conditions}
\textbf{N.-S. Boundary Conditions}

\textbf{Sixth-Order FD in Non-Conservative Form}
\textbf{Sixth-Order FD in Conservative Form}

\textbf{Ideal Gas Equation of State}

\textbf{Flow Model}
\textbf{Single-Species}
\textbf{Multi-Species (Isothermal and Isobaric Equilibrium)}
\textbf{Multi-Species (Isobaric Equilibrium)}

\textbf{Sensors}
\textbf{Numerical Schemes}
\textbf{Physical Models}

Numerical test: 2D inviscid shock-vortex interaction

- Isentropic vortex interacts with Mach 1.2 stationary shock
- Distorted vortex produces reflected shocks
- Multiple sound waves generated from reflected shock-vortex interaction

Sound pressure, \( \frac{(p - p_{\infty})}{\rho_{\infty} c_{\infty}^2} \), of reference solution with grid resolution 4096 \( \times \) 4096:

\[ \text{(a) } t = 4 \quad \text{(b) } t = 8 \quad \text{(c) } t = 16 \]

Numerical test: 2D inviscid shock-vortex interaction (cont.)

Refined regions of AMR simulation with base grid resolution $128 \times 128$ and $1 : 2$ refinement ratio (green: level 1; red: level 2):

Comparison with $512 \times 512$ uniform grid simulation:

(a) Global sound pressure  
(b) Local sound pressure
Numerical test: 2D inviscid shock-vortex interaction (cont.)

- Weighted number of cells:
  \[ \sum_{l=0}^{l_{\text{max}}} \omega_l N_l, \quad \omega_l = \frac{\Delta x_{l_{\text{max}}}}{\Delta x_l} \]

- In this test problem:
  \[ \omega_0 = 1/4, \quad \omega_1 = 1/2, \quad \omega_2 = 1 \]

Weighted number of cells of AMR simulation \( \approx 30\% \) of number of cells of uniform grid (262144 cells) simulation at the end
Numerical test: 3D viscous shock-bubble interaction

- $Ma_s = 1.68$, $R = 1.016$ mm
- Material interface with characteristic length scale $\epsilon_i = 0.125$ mm
- A quadrant of the domain is simulated

- Different grids settings:

<table>
<thead>
<tr>
<th>Grid</th>
<th>Base grid resolution</th>
<th>Refinement ratios</th>
<th>Finest grid spacing ($\mu$m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$384 \times 128 \times 128$</td>
<td>1:2, 1:2</td>
<td>7.94</td>
</tr>
<tr>
<td>B</td>
<td>$768 \times 256 \times 256$</td>
<td>1:2, 1:2</td>
<td>3.97</td>
</tr>
<tr>
<td>C</td>
<td>$1536 \times 512 \times 512$</td>
<td>1:2, 1:2</td>
<td>1.98</td>
</tr>
</tbody>
</table>

- Gradient sensor on pressure, multiresolution sensor on density, and sensor on mass fraction used for refinement
Numerical test: 3D viscous shock-bubble interaction (cont.)

- Conservative multi-component Navier-Stokes equations for ideal fluid mixture are solved:

\[
\begin{align*}
\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho u Y_i) + \nabla \cdot J_i &= 0 \\
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu + p\delta - \tau) &= 0 \\
\frac{\partial E}{\partial t} + \nabla \cdot [(E + p) u] - \nabla \cdot (\tau \cdot u - q_c - q_d) &= 0
\end{align*}
\]

where \(\rho, u, p\) and \(E\) are the density, velocity vector, pressure and total energy of the fluid mixture respectively. \(Y_i\) is the mass fraction of species \(i = 1, 2, \ldots, N\), with \(N\) the total number of species.

- \(J_i\) is diffusive mass flux for each species. \(\tau, q_c\) and \(q_d\) are viscous stress tensor, conductive heat flux and inter-species diffusional enthalpy flux respectively of the mixture.

- Sixth order finite differences for viscous and diffusive fluxes
Numerical test: 3D viscous shock-bubble interaction (cont.)

- Density fields in $xy$ plane at $z = 0$ of AMR simulation with grid C:

(a) $t = 2.8 \mu s$

(b) $t = 8.8 \mu s$

(c) $t = 17.6 \mu s$
Numerical test: 3D viscous shock-bubble interaction (cont.)

- Refined regions (green: level 1; red: level 2):

(a) $t = 2.8\ \mu s$

(b) $t = 8.8\ \mu s$

(c) $t = 17.6\ \mu s$
Numerical test: 3D viscous shock-bubble interaction (cont.)

3D visualization of mass fraction with grid C at end of simulation $t = 17.6 \mu s$
Numerical test: 3D viscous shock-bubble interaction (cont.)

- $y_{\text{max}}$ is the $y$ coordinate of the upper point with SF$_6$ concentration equals $0.01 \max(Y_{\text{SF6}})$
  
  $l_x = x_d - x_u$
  
  $l_{yz} = y_{\text{max}} + z_{\text{max}}$

- All statistical quantities of interests are grid converged

**Graphs:**

(a) Centroid

(b) $l_x/l_y$

(c) Circulation

(d) Integrated scalar dissipation rate

Man Long Wong
AMS Seminar
Jun 6th, 2019 30 / 62
Summary

- AMR framework developed for multi-species CFD applications
- Physics-based sensors such as gradient and multiresolution sensors implemented to detect features for refinement
- Framework successfully tested with simulations that consist of interactions between shocks, material interfaces, and vortices
- The sensors for mesh refinement can successfully identify:
  - Shock wave and acoustic waves
  - Vortical features
  - Mixing regions

---

21 One more 2D viscous shock-cylinder interaction problem is presented in thesis
Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows

2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability

3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock

4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability
Problem setup

- Compressible 2D and 3D multi-species Navier-Stokes simulations set up to study shock-induced mixing between SF$_6$ and air due to RM instability:

  - $Ma_s = 1.45$
  - $At = \frac{\rho_{SF_6} - \rho_{air}}{\rho_{SF_6} + \rho_{air}} = 0.68$
  - 2D domain is cross-section of the 3D domain
  - Mixing region shocked **twice** (first shock and re-shock)
Perturbations

Perturbation modes seeded on the interfaces:

- **2D:**
  \[ S(y) = A \sum_{m} \cos \left( \frac{2\pi m}{L_y} y + \phi_m \right) \]

- **3D:**
  \[ S(y, z) = A \sum_{m} \cos \left( \frac{2\pi m}{L_{yz}} y + \phi_m \right) \cos \left( \frac{2\pi m}{L_{yz}} z + \psi_m \right) \]

- 11 modes in total: \( 0.833 \text{ mm} \leq \lambda_m \leq 1.25 \text{ mm} \)
- \( A = 0.0141 \text{ mm} \)

- Estimated with impulsive theory, 2D and 3D problems have same:
  - linear growth rates \( \dot{\eta}_{imp} \)
  - time scales \( \tau_c \)
Configurations of 2D and 3D adaptive mesh refinement (AMR) simulations

- Simulated with the AMR solver (HAMeRS)
- Sixth order WCNS-LD for convective flux
- Sixth order finite differences for diffusive and viscous fluxes
- Three levels of adaptive meshes (two levels of AMR)
- Gradient and multiresolution sensors; also sensor on mass fraction field
- Grid resolutions used for convergence test:

<table>
<thead>
<tr>
<th>2D Grid</th>
<th>Base Grid Resolution</th>
<th>Refinement Ratio</th>
<th>Finest Grid Spacing (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>2560 × 128</td>
<td>1:2, 1:4</td>
<td>0.0244</td>
</tr>
<tr>
<td>E</td>
<td>5120 × 256</td>
<td>1:2, 1:4</td>
<td>0.0122</td>
</tr>
<tr>
<td>F</td>
<td>10240 × 512</td>
<td>1:2, 1:4</td>
<td>0.0061</td>
</tr>
<tr>
<td>G</td>
<td>20480 × 1024</td>
<td>1:2, 1:4</td>
<td>0.0031</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3D Grid</th>
<th>Base Grid Resolution</th>
<th>Refinement Ratio</th>
<th>Finest Grid Spacing (mm)</th>
<th>Maximum Weighted Grid Spacing (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>640 × 32 × 32</td>
<td>1:2, 1:4</td>
<td>0.0977</td>
<td>30M</td>
</tr>
<tr>
<td>C</td>
<td>1280 × 64 × 64</td>
<td>1:2, 1:4</td>
<td>0.0488</td>
<td>144M</td>
</tr>
<tr>
<td>D</td>
<td>2560 × 128 × 128</td>
<td>1:2, 1:4</td>
<td>0.0244</td>
<td>778M</td>
</tr>
</tbody>
</table>

- ~34 points across smallest initial wavelength for grid D
Visualizations of mole fraction (3D, grid D)

(a) $t = 0.05$ ms (after first shock)  
(b) $t = 0.40$ ms  
(c) $t = 1.10$ ms (before re-shock)  
(d) $t = 1.20$ ms (after re-shock)  
(e) $t = 1.40$ ms  
(f) $t = 1.75$ ms
2D grid convergence study (over 24 realizations)

Mixing width \( W = \int 4\bar{X}_{SF_6} (1 - \bar{X}_{SF_6}) dx \);
Mixedness \( \Theta = \frac{\int X_{SF_6} (1 - X_{SF_6}) dx}{\int \bar{X}_{SF_6} (1 - \bar{X}_{SF_6}) dx} \);
TKE = \frac{1}{2} \rho u'' \cdot u''

(a) Mixing width
(b) Mixedness
(c) TKE (integrated)
(d) Scalar dissipation rate (integrated)
(e) Enstrophy (integrated)
3D grid convergence study

Mixing width \( W = \int 4\bar{X}_{SF_6} (1 - \bar{X}_{SF_6}) dx \); Mixedness \( \Theta = \frac{\int X_{SF_6} (1 - X_{SF_6}) dx}{\int \bar{X}_{SF_6} (1 - \bar{X}_{SF_6}) dx} \); TKE = \( \frac{1}{2} \rho \bar{u}_i' u_i'' \)

(a) Mixing width  
(b) Mixedness  
(c) TKE (integrated)  
(d) Scalar dissipation rate (integrated)  
(e) Enstrophy (integrated)
Mole fraction fields $t^* = t/\tau_c$

**2D, grid G**

(a) $t^* = 7.5 \ (t = 0.40 \ ms)$  
(b) $t^* = 20.7 \ (t = 1.10 \ ms)$  
(c) $t^* = 22.6 \ (t = 1.20 \ ms)$  
(d) $t^* = 32.9 \ (t = 1.75 \ ms)$

**3D, grid D**

(a) $t^* = 7.5 \ (t = 0.40 \ ms)$  
(b) $t^* = 20.7 \ (t = 1.10 \ ms)$  
(c) $t^* = 22.6 \ (t = 1.20 \ ms)$  
(d) $t^* = 32.9 \ (t = 1.75 \ ms)$
Reduced Reynolds number 3D simulations

- Reynolds number $Re_W$ is reduced by increasing physical transport coefficients (TC’s) by factors of 2 & 4 ($\mu$, $\mu_v$, $D$, and $\kappa$). This is as same as cases with reduced $Re_W$, while $Sc$ and $Pr$ unchanged.

\[
Re_W = \frac{\bar{\rho} u_{rms} W}{\mu}, \quad \text{where} \quad u_{rms} = \sqrt{\frac{u''u''}{3}}
\]

- $\langle \cdot \rangle$ is additional averaging in central part of mixing layer: $4 \bar{X}_{SF_6} (1 - \bar{X}_{SF_6}) > 0.9$
Mole fraction fields

(a) $t^* = 7.5 \ (t = 0.40 \text{ ms})$
(b) $t^* = 20.7 \ (t = 1.10 \text{ ms})$
(c) $t^* = 22.6 \ (t = 1.20 \text{ ms})$
(d) $t^* = 32.9 \ (t = 1.75 \text{ ms})$

Physical transport coefficients, grid D

(a) $t^* = 7.5 \ (t = 0.40 \text{ ms})$
(b) $t^* = 20.7 \ (t = 1.10 \text{ ms})$
(c) $t^* = 22.6 \ (t = 1.20 \text{ ms})$
(d) $t^* = 32.9 \ (t = 1.75 \text{ ms})$

$4\times$ physical transport coefficients, grid D
Flow compressibility and effective Atwood number

- Turbulent Mach number $Ma_t$ and effective Atwood number $At_e$:

$$Ma_t = \frac{\sqrt{3}u_{rms}}{c}, \quad At_e = \frac{\sqrt{\rho' \rho}}{\rho}$$

- Flows are weakly compressible
- $At_e \approx 0$ due to initially diffuse interface, but flows become non-Boussinesq ($At_e > 0.05$) as the interfaces become sharper after first shock and re-shock
Mixing: mixing width

- The mixing width is normalized by $\dot{\eta}_{imp}$ and $\tau_c$:
  \[ W^* = \frac{W - W|_{t=0}}{\dot{\eta}_{imp}\tau_c} \]

- With physical TC’s, $W^*$ of 2D case grows at a faster rate compared to that of 3D case after first shock initially but growth rates are similar at late times.

- After re-shock, the 2D mixing width grows at a much faster rate.

- 3D case with reduced Reynolds number has slower growth rate in mixing width before re-shock but growth rates are similar after re-shock.
Mixing: mixedness

- The mixedness is defined as:

\[ \Theta = \frac{\int X_{\text{SF}_6} (1 - X_{\text{SF}_6}) \, dx}{\int \bar{X}_{\text{SF}_6} (1 - \bar{X}_{\text{SF}_6}) \, dx} \]

- Mixedness quantifies the amount of fluids molecularly mixed within the mixing region.

- The 2D and 3D mixedness values are converging to 0.7 and 0.8 respectively [0.85 for 3D RMI from Tritschler et al.\textsuperscript{22}, 0.8 for 3D RMI from Mohaghar et al.\textsuperscript{23}]

\textsuperscript{22} Tritschler et al., “On the Richtmyer–Meshkov instability evolving from a deterministic multimode planar interface”.

\textsuperscript{23} Mohaghar et al., “Evaluation of turbulent mixing transition in a shock-driven variable-density flow”.
Mixing: mole fraction profiles

(a) After first shock, before reshock, 3D

(b) After reshock, 3D

- The normalized position is defined as: \( x^* = \frac{x - x_i}{W(t)} \)

- Asymmetric, spikes penetrate more than bubbles

- Profiles collapse quite well at late times, similar to planar Rayleigh-Taylor instability\textsuperscript{24}

Mixing: mole fraction variance profiles

\[ \Theta = \frac{\int X_{SF_6} (1 - X_{SF_6}) \, dx}{\int \bar{X}_{SF_6} (1 - \bar{X}_{SF_6}) \, dx} = 1 - 4 \int \bar{X}^{12}_{SF_6} \, dx^* \]

(a) After first shock, before reshock, 3D

(b) After reshock, 3D

- Fluids harder to mix in the heavier fluid side indicated by larger variance
- Approaching self-similarity near end of simulations
TKE time evolution

• TKE is defined as:

\[ TKE = \frac{1}{2} \rho \left( u'' \right)^2 \]

• TKE decays at faster rate for 3D problem compared to 2D
• Among 3D cases, TKE decays at faster rate before re-shock for case with smaller Reynolds number
• After re-shock, all 3D cases have similar TKE decay rates
Turbulent kinetic energy (TKE) profiles

- The TKE is normalized as: 
  \[ TKE^* = \frac{(TKE)W}{\int TKE \, dx} \]

- Peak of TKE is biased towards the lighter fluid side, especially before reshock.

(a) After first shock, before reshock, 3D
(b) After reshock, 3D
Anisotropy

- The Reynolds stress anisotropy tensor $b_{ij}$ for 2D and 3D flows defined as:

$$
b_{ij}^{2D} = \frac{\tilde{R}_{ij}}{\tilde{R}_{kk}} - \frac{1}{2} \delta_{ij}, \quad b_{ij}^{3D} = \frac{\tilde{R}_{ij}}{\tilde{R}_{kk}} - \frac{1}{3} \delta_{ij}, \quad \text{where} \quad \tilde{R}_{ij} = \frac{\rho u_i' u_j'}{\bar{\rho}}$$

- 2D Reynolds normal stresses becoming isotropic at a faster rate than 3D stresses before re-shock
- After re-shock, 2D Reynolds normal stresses become isotropic
Summary

- 2D and 3D RMI have very different time evolution for mixing width and TKE and final mixedness values.
- Reynolds stresses of 2D flow approaching isotropy quickly after both shocks; Reynolds stresses of 3D flows remain anisotropic at the end of simulations.
- Fluids are more difficult to mix in 2D configuration.

- Reducing $Re_W$ has significant effect before re-shock:
  - smaller growth rate of $W$
  - larger $\Theta$
  - larger decay rate of TKE

- Reynolds number has much smaller effect on the growth of mixing width/decay of TKE after re-shock.

More analysis on probability density functions and spectra can be found in manuscript submitted to Physical Review Fluids\textsuperscript{25}

Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows

2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability

3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock

4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability
Favre-averaged momentum equation

- Direct numerical simulation (DNS) or large eddy simulation (LES) still very expensive
- Reynolds-averaged / Favre-averaged Navier-Stokes (RANS/FANS) simulation with turbulence modeling is an interim tool
- Most turbulent mixing models only tested with experimental results for RM turbulence
- High-fidelity simulation data also important for model validation
- Favre-averaged momentum equation (\(\tilde{\cdot} = \overline{\rho(\cdot)}/\bar{\rho}\)):

\[
\frac{\partial (\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial (\bar{\rho}\tilde{u}_k\tilde{u}_i)}{\partial x_k} = -\frac{\partial (\bar{p}\tilde{\delta}_{ki})}{\partial x_k} + \frac{\partial \tilde{\tau}_{ki}}{\partial x_k} - \frac{\partial (\bar{\rho}\tilde{R}_{ki})}{\partial x_k}
\]

- \(\tilde{R}_{ij} = \bar{\rho}u_i''u_j''/\bar{\rho}\): Favre-averaged Reynolds stress
Reynolds stress

- Algebaric closure model based on turbulent kinetic energy is not good:

\[
\tilde{R}_{ij} \approx \frac{2}{3} k \delta_{ij} - 2C_{\mu} S \sqrt{k} \tilde{S}_{ij}, \quad \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij},
\]

- To improve, transport equation of \( \tilde{R}_{ij} \) is considered:

\[
\frac{\partial \tilde{R}_{ij}}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_k \tilde{R}_{ij})}{\partial x_k} = a_i \left( \frac{\partial \bar{\rho}}{\partial x_j} - \frac{\partial \tilde{u}_k}{\partial x_k} \right) + a_j \left( \frac{\partial \bar{\rho}}{\partial x_i} - \frac{\partial \tilde{u}_k}{\partial x_k} \right) - \bar{\rho} \tilde{R}_{ik} \frac{\partial \tilde{u}_j}{\partial x_k} - \bar{\rho} \tilde{R}_{jk} \frac{\partial \tilde{u}_i}{\partial x_k}
\]

+ turbulent transport (unclosed) + pressure strain redistribution (unclosed) + dissipation (unclosed)
Turbulent mass flux for RM instability

- $a_i = \frac{\rho' u'_i}{\bar{\rho}}$: velocity associated with turbulent mass flux
- To close $\bar{\rho} a_i$, BHR model by Besnard et al.\textsuperscript{26} suggests to model transport of $\bar{\rho} a_i$:

$$\frac{\partial (\bar{\rho} a_i)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_k a_i)}{\partial x_k} = b \left( \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \bar{\tau}_{ki}}{\partial x_k} \right) - \bar{R}_{ik} \frac{\partial \bar{\rho}}{\partial x_k} + \text{redistribution} + \text{turbulent transport (unclosed)} + \text{destruction (unclosed)}$$

- $b = -\rho' (1/\rho)'$: density-specific-volume covariance
- BHR-3 model by Schwarzkopf et al.\textsuperscript{27} recommends to model transport of $\bar{\rho} b$:

$$\frac{\partial \bar{\rho} b}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_k b)}{\partial x_k} = -2 (b + 1) a_k \frac{\partial \bar{\rho}}{\partial x_k} + \text{redistribution} + \text{turbulent transport (unclosed)} + \text{destruction (unclosed)}$$


Profiles of $\bar{\rho}a_1$ (in moving frame of interface)

- Using highest Reynolds number 3D case in previous section
- $\tilde{x} = x - x_i$, where $x_i$ is location of interface
- After both first shock and re-shock, $\bar{\rho}a_1$ spreads and the peak decreases over time
Budget of turbulent mass flux, $\bar{\rho}a_1$ (in moving frame of interface)

(a) $t = 1.10$ ms (before re-shock)  
(b) $t = 1.20$ ms (after re-shock)  
(c) $t = 1.75$ ms

- The **production** and **destruction** (unclosed) terms are dominant terms in the budget.
- The net LHS (rate of change + convection) is negative in the middle part of mixing layer, causing $\bar{\rho}a_1$ to decrease in magnitude after first shock and re-shock.
- **Turbulent transport** (unclosed) term spreads the profile.
- **Redistribution** and **convection** terms are small over time.
Budget of turbulent mass flux, $\bar{\rho}a_1$

- **Destruction** consists of three unclosed components: $\bar{\rho}(1/\rho)'p_{,1}'$, $-\bar{\rho}(1/\rho)'\tau_{1,i,i}'$,

$$\bar{\rho}\epsilon_{a_1} = -\bar{\rho}u_i' \frac{\partial u_k'}{\partial x_k}$$

- $\bar{\rho}(1/\rho)'p_{,1}'$ is the only important term after re-shock

![Graphs showing turbulent mass flux over time](image)

(a) $t = 0.40$ ms  
(b) $t = 1.10$ ms  
(c) $t = 1.20$ ms (after re-shock)  
(d) $t = 1.75$ ms
Assessment of BHR-3$^{29}$ model: unclosed terms of transport equation of $\bar{\rho}a_1$

- Turbulent mass flux, $\bar{\rho}a_1$:

<table>
<thead>
<tr>
<th>Unclosed Term</th>
<th>Exact Form</th>
<th>Modeled Form $^{28}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulent transport</td>
<td>$\bar{\rho}\frac{\partial}{\partial x}(\rho'u'u'/\bar{\rho})$</td>
<td>$2C_a\bar{\rho}\frac{\partial}{\partial x}\left[\left(\bar{S}\hat{R}<em>{11}/\sqrt{k}\right)</em>{a_1,a_1}\right]$</td>
</tr>
<tr>
<td>Destruction</td>
<td>$\bar{\rho}\left(\frac{1}{\rho}\right)'\frac{\partial \rho'}{\partial x}$</td>
<td>$-C_a\bar{\rho}\sqrt{\frac{k}{S}}a_1$</td>
</tr>
</tbody>
</table>

- $C_a$ and $C_{a1}$ are model coefficients; $S$ is a turbulent length scale

- Assuming $S$ uniform inside mixing region (ignoring $S'$), cancelling common terms and operators for analyzing validity of model after re-shock (after mixing transition has occurred)

$^{28}k = \hat{R}_{ii}/2$ is turbulent kinetic energy per unit mass

$^{29}$Schwarzkopf et al., “Application of a second-moment closure model to mixing processes involving multicomponent-miscible fluids”
BHR-3 assessment: unclosed terms of $\bar{\rho}a_1$ transport equation (after re-shock)

- Turbulent transport:

  \[
  \begin{align*}
  (a) & \ t = 1.20 \text{ ms} \\
  (b) & \ t = 1.75 \text{ ms}
  \end{align*}
  \]

- Destruction:

  \[
  \begin{align*}
  (a) & \ t = 1.20 \text{ ms} \\
  (b) & \ t = 1.75 \text{ ms}
  \end{align*}
  \]
BHR-3 assessment: turbulent length scales $S$ (after re-shock)

- $W$: integral mixing width
- Least square fit within mixing region to estimate $S$’s required for turbulent transport and destruction terms of $\bar{\rho}a_1$
- Two length scale turbulence model BHR3.1 [Schwarzkopf et al., 2015] seems unnecessary for $a_1$
Summary

- $\bar{\rho} a_i$ plays an important role for modeling of $\tilde{R}_{ij}$ in BHR-3 model
- $\bar{\rho} a_1$ transport equation was analyzed
- Destruction term in budget of $\bar{\rho} a_1$ has different composition before and after re-shock (after mixing transition)
- BHR-3 model captures shapes of unclosed terms of $\bar{\rho} a_1$ transport equation well
- $S$'s required for modeling unclosed terms of $\bar{\rho} a_1$ transport equation dependent on each other

Analysis of budgets and closures for $\tilde{R}_{ij}$ and $b$ discussed in thesis
Conclusions

- High-resolution and localized dissipation schemes improved for shock problems that involve flow instabilities and turbulence
- AMR framework was developed and shown to be robust for problems that involve shocks and multi-species
- Asymmetric variable-density mixing effects examined
- Reynolds number has large effect on the flows before re-shock (before mixing transition)
- The BHR-3 model has good modeling assumptions for the $\bar{\rho}a_1$ transport equation for post-transition flows
The PhD research was partially supported by Los Alamos National Laboratory, under grant number 431679.