Shock-Fitted Numerical Solutions for Two-Dimensional Detonations

with Periodic Boundary Conditions

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2-D Euler equations with reaction
2 species chemical kinetics
Calorically perfect ideal gas mixture
High-order convergence
Background

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\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0,
\]
\[
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} + \frac{\partial (\rho uv)}{\partial y} = 0,
\]
\[
\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho vu)}{\partial x} + \frac{\partial (\rho v^2 + p)}{\partial y} = 0,
\]
\[
\frac{\partial}{\partial t} \left( \rho \left( e + \frac{1}{2} (u^2 + v^2) \right) \right) + \\
\frac{\partial}{\partial x} \left( \rho u \left( e + \frac{1}{2} (u^2 + v^2) + \frac{p}{\rho} \right) \right) + \\
\frac{\partial}{\partial y} \left( \rho v \left( e + \frac{1}{2} (u^2 + v^2) + \frac{p}{\rho} \right) \right) = 0.
\]
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\[
A \rightarrow B
\]

Let \( \lambda \) denote mass fraction of \( B \)

\[
\frac{\partial}{\partial t} (\rho \lambda) + \frac{\partial}{\partial x} (\rho u \lambda) = a \rho (1 - \lambda) \exp \left( \frac{-E \rho}{p} \right)
\]
Background

- 2-D shock geometry
- 2-D Euler equations with reaction
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\[ e = \frac{1}{\gamma - 1} \frac{p}{\rho} - q\lambda \]
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Motivation

What are the state-of-the-art numerical techniques used for discontinuous problems?

- **Shock capturing**
  - Robust
  - Numerical viscosity reduces convergence to $O(\Delta x)$

- **Shock tracking**
  - Robust
  - Description of discontinuous motion varies
  - Converges at $O(\Delta x)$
Accuracy loss due to differentiation across discontinuities. High order convergence can be achieved through shock-fitting

- Governing equations are posed in fitted coordinates
- Solution is smooth within each domain
- Analytic jump conditions used to compute shock speed
- Restricted to embedded shocks
Accuracy loss due to differentiation across discontinuities. High order convergence can be achieved through shock-fitting

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Motivation

Accuracy loss due to differentiation across discontinuities.
High order convergence can be achieved through shock-fitting

- Governing equations are posed in fitted coordinates
  - Shock location is fixed
- Solution is smooth within each domain
  - Regular finite differencing is adequate
- Analytic jump conditions used to compute shock speed
- Restricted to embedded shocks
Consider transform

\[ \xi = \xi(x, y, t), \quad \eta = \eta(x, y, t), \quad \tau = t \]

applied to

\[ \frac{\partial F}{\partial t} + \frac{\partial f_i}{\partial y^i} = B \]

\[ D_n = \left[ \begin{array}{c} f_i \\ \left[ F \right] \end{array} \right] \nu_i \]

where only derivatives are transformed.
Shock-Fit Transformation

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applied to

\[ \frac{\partial F}{\partial t} + \frac{\partial f^i}{\partial y^i} = B \quad D_n = \left[ \frac{f^i}{[F]} \right] \nu_i \]

where only derivatives are transformed.
Consider transform
\[
\xi = \xi(x, y, t), \quad \eta = \eta(x, y, t), \quad \tau = t
\]
applied to
\[
\frac{\partial F}{\partial t} + \frac{\partial f_i}{\partial y^i} = B \quad D_n = \left[ \begin{bmatrix} f^i \end{bmatrix} \right] \nu_i
\]
where only derivatives are transformed.

\( x \) and \( y \) momentum are still solved.
Transformed Equations

The resulting fitted equations are

\[
\frac{\partial}{\partial \tau} \left( \sqrt{gF} \right) + \frac{\partial}{\partial \eta^j} \left( \sqrt{gF} \frac{\partial \eta^j}{\partial t} + \sqrt{g} f^i \frac{\partial \eta^j}{\partial y^i} \right) = \sqrt{g} B
\]

- Conservation form with proper shock speed

\[
\bar{D}_n = \left[ \frac{\sqrt{gF} \frac{\partial \eta^j}{\partial t} + \sqrt{g} f^i \frac{\partial \eta^j}{\partial y^i}}{\sqrt{gF}} \right] \bar{v}_j
\]

- \( \sqrt{g} = \left| \frac{\partial y}{\partial \eta} \right| \) is the determinant of the metric tensor

\[
- \frac{\partial \eta^i}{\partial t} = \frac{\partial \eta^i}{\partial y^j} \frac{\partial y^j}{\partial \tau} \rightarrow \bar{U}^i = \frac{\partial \eta^i}{\partial y^j} U^j
\]
Formulation: Conserved Quantities

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) = 0,
\]
\[
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2 + p) + \frac{\partial}{\partial y} (\rho u v) = 0,
\]
\[
\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (\rho v u) + \frac{\partial}{\partial y} (\rho v^2 + p) = 0,
\]
\[
\frac{\partial}{\partial t} \left( \rho \left( e + \frac{1}{2} (u^2 + v^2) \right) \right) +
\frac{\partial}{\partial x} \left( \rho u \left( e + \frac{1}{2} (u^2 + v^2) + \frac{p}{\rho} \right) \right) +
\frac{\partial}{\partial y} \left( \rho v \left( e + \frac{1}{2} (u^2 + v^2) + \frac{p}{\rho} \right) \right) = 0,
\]
\[
\frac{\partial}{\partial t} (\rho \lambda) + \frac{\partial}{\partial x} (\rho u \lambda) = a \rho (1 - \lambda) \exp \left( \frac{-E \rho}{p} \right),
\]
\[e = \frac{1}{\gamma - 1} \frac{p}{\rho} - q \lambda.\]
Formulation: Shock-Fitted Eqns.

\[ \frac{\partial}{\partial \tau} \begin{bmatrix} F_1' \\ F_2' \\ F_3' \\ F_4' \\ F_5' \end{bmatrix} + \frac{\partial}{\partial \xi} \begin{bmatrix} F_1' \\ F_2' \\ F_3' \\ F_4' \\ F_5' \end{bmatrix} + \frac{1}{\sqrt{g}} \frac{\partial y}{\partial \eta} \begin{bmatrix} F_2' \\ F_2' F_3' + \sqrt{g} P \\ F_2' F_4' + \sqrt{g} \frac{F_3'}{F_1'} P \\ F_2' F_5' + \sqrt{g} \frac{F_3'}{F_1'} P \\ \end{bmatrix} - \frac{1}{\sqrt{g}} \frac{\partial x}{\partial \eta} \begin{bmatrix} F_3' \\ F_3' F_4' + \sqrt{g} P \\ F_3' F_5' + \sqrt{g} \frac{F_3'}{F_1'} P \\ \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \]

\[ p = \frac{(\gamma - 1)}{\sqrt{g}} \left( F_4' - \frac{(F_2')^2 + (F_3')^2}{2F_1'} + qF_5' \right), \quad \zeta = \frac{a}{\sqrt{g}} \left( F_1' - F_5' \right) \exp \left( \frac{-EF_1'}{\sqrt{g}p} \right) \]
At the shock, \( E = \rho(e + \frac{1}{2}(u^2 + v^2)) = f(D_n). \)

\[
\frac{\partial D_n}{\partial \tau} = \left( \frac{\partial E}{\partial D_n} \bigg|_S \right)^{-1} \frac{\partial E}{\partial \tau} \bigg|_S
\]
At the shock, \( E = \rho(e + \frac{1}{2}(u^2 + v^2)) = f(D_n) \).

\[ |v| = v^i v_j = u^2 + v^2 \text{ is invariant.} \]

\[
\frac{\partial D_n}{\partial \tau} = \left( \frac{\partial E}{\partial D_n} \right)_S^{-1} \frac{\partial E}{\partial \tau} \bigg|_S
\]

\[ \frac{\partial E}{\partial \tau} \bigg|_S \text{ is already calculated in the flow field.} \]

Thus system is closed.
Shock-Fitted Geometry

Since $S : \eta^2 = 0$

- $g^{(1)}$ is embedded in the shock
- $g^{(2)} \parallel \nu$

Note that $\eta^1$ in general contributes artificial tangential shock velocity.

Thus, $D_n = \cos(\alpha) \omega(2) \leq |\omega|$, in general.
Shock-Fitted Geometry: $x \equiv \xi$

\[ S : \eta^2 = y^2 - y_S(x, t) = 0 \]

\[ g(1) = \begin{pmatrix} 1 \\ \frac{\partial y_S}{\partial \eta^1} \end{pmatrix}, \quad g(2) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \]

and the grid velocity components are

\[ \frac{\partial \xi}{\partial t} = 0 \quad \frac{\partial \eta}{\partial t} = -\frac{\partial y_S}{\partial t} \]
Shock-Fitted Geometry: \( x \equiv \xi \)

In this case:

- \( \sqrt{g} = 1 \)
- \( \alpha = \phi \), the shock angle
- \( D_o = \frac{\partial y_S}{\partial t} = D_n \sqrt{1 + \left( \frac{\partial y_S}{\partial y^1} \right)^2} \)

relating the phase speed, the shock surface, the normal shock speed, and the shock slope.
Numerical Method

The method of lines is used to separate spatial and temporal integration

- $O(\Delta t^5)$ Runge-Kutta integration in time
- $O(\Delta x^5)$ or $O(\Delta y^5)$ WENO5M with Lax-Friedrich’s flux splitting to differentiate in space

At the shock

- Rankine-Hugoniot jump conditions used directly
- One-sided finite differencing used
- Shock-change equation gives evolution of $D_n$
1-D Results: Pulsating Detonations

- $D_{\text{max}}$
- $E < 25.265$, linearly stable
- $25.265 < \bar{E} < 27.1875$, Period $2^0$ (single period mode)
- $27.1875 < \bar{E} < 27.6850$, Period $2^n$
- Stable Period 2
- Stable Period 3
- Stable Period 6
- Stable Period 5
2-D Results: $E = 0$, $q = 15$

\[ f(x) = D + a_1 e^{a_2 x} \sin(a_3 x + a_4) \]

<table>
<thead>
<tr>
<th>$N_{1/2}$</th>
<th>$\Delta x$</th>
<th>Range</th>
<th>Growth Rate ($a_2$)</th>
<th>Frequency ($a_3$)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.10530</td>
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<td>[40:60]</td>
<td>0.024210</td>
<td>1.10437</td>
</tr>
</tbody>
</table>

$\Delta x = 0.05$
2-D Results: Detonation Cells
2-D Results: Detonation Cells

![Graphs showing 2-D results of detonation cells.](image)
2-D Results: Linear Stability

\[ \Delta x = 0.1 \]

\[ t \]

\[ D_n \]
Conclusions

- Need for highly resolved solutions to sandwich test
- Shock-fitting is a viable high order solution technique for problems involving a single embedded shock
- Conservative 2-D shock-fitted equations derived and implemented
- WENO5M combined with LLF splitting
  - allows for high order convergence
  - gives discrete conservation away from the shock
  - correctly captures shocks (degrade to $\approx O(\Delta x)$)
- Areas of current research
  - Validation from linear stability theory in progress
  - Extension to more complicated geometries
Weighted Essentially Non-Oscillatory (WENO) Schemes

- Fifth order scheme overall
- \( \hat{f}_j^{k+1/2} = h + O(\Delta x^3) \)
- \( \hat{f}_j^{k+1/2} = \sum_{k=0}^{2} \omega_k^{(M)} \hat{f}_j^{k+1/2} \)
- Schemes differ through formulation of \( \omega_k^{(M)} \)

Ideal weights:

\[ \bar{\omega}_0 = 1/10, \quad \bar{\omega}_1 = 6/10, \quad \bar{\omega}_2 = 3/10. \]
\[ \omega_k^{(M)} = \frac{\alpha_k^*}{\sum_{i=0}^{2} \alpha_i^*} \text{ where } \alpha_k^* = g_k(\omega_k^{(JS)}) \]

\[ g_k(\omega) = \frac{\omega(\bar{\omega}_k + \bar{\omega}_k^2 - 3\bar{\omega}_k\omega + \omega^2)}{\bar{\omega}_k^2 + (1 - 2\bar{\omega}_k)\omega}, \quad \omega \in [0, 1] \]

where \( \omega_k^{(JS)} \) are those used by Jiang and Shu (1996)