Exact Solutions for Two-Dimensional Reactive Flow
for Verification of Numerical Algorithms

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Motivation

- Computational tools are critical in design of aerospace vehicles which employ high speed reactive flow.
- Comparing computational predictions with those of exact solutions in grid resolution studies is a robust verification.
- We develop a new exact solution and employ it to verify a modern shock-capturing reactive flow algorithm for flows with an immersed boundary.
Verification and Validation

- **verification**: solving the equations right.

- **validation**: solving the right equations.

- Focus here is exclusively on verification.

- Limiting assumptions necessary for exact solution preclude meaningful validation exercise.

- Verification and validation always necessary but never sufficient: finite uncertainty must be tolerated.
Partial Review of Oblique Detonations

Oblique Detonation Schematic

- Straight shock.
- Curved wedge.
- Orthogonal coordinate system aligned with shock.
Model: Reactive Euler Equations

- two-dimensional,
- steady,
- inviscid,
- irrotational,
- one step kinetics with zero activation energy,
- calorically perfect ideal gases with identical molecular masses and specific heats.
Model: Reactive Euler PDEs

\[
\frac{\partial}{\partial X} (\rho U) + \frac{\partial}{\partial Y} (\rho V) = 0, \\
\frac{\partial}{\partial X} (\rho U^2 + p) + \frac{\partial}{\partial Y} (\rho UV) = 0, \\
\frac{\partial}{\partial X} (\rho UV) + \frac{\partial}{\partial Y} (\rho V^2 + p) = 0, \\
\frac{\partial}{\partial X} \left( \rho U \left( e + \frac{1}{2}(U^2 + V^2) + \frac{p}{\rho} \right) \right) + \frac{\partial}{\partial Y} \left( \rho V \left( e + \frac{1}{2}(U^2 + V^2) + \frac{p}{\rho} \right) \right) = 0, \\
\left( \frac{\partial}{\partial X} (\rho U \lambda) + \frac{\partial}{\partial Y} (\rho V \lambda) \right) = \alpha \rho (1 - \lambda) H(T - T_i), \\
e = \frac{1}{\gamma - 1} \frac{p}{\rho} - \lambda q, \\
p = \rho RT.
\]
Model Reductions: PDEs → ODEs

Assume no $Y$ variation, so

\[
\frac{d}{dX} (\rho U) = 0,
\]
\[
\frac{d}{dX} (\rho U^2 + p) = 0,
\]
\[
\frac{d}{dX} (\rho U V) = 0,
\]
\[
\frac{d}{dX} \left( \rho U \left( e + \frac{1}{2}(U^2 + V^2) + \frac{p}{\rho} \right) \right) = 0,
\]
\[
\frac{d}{dX} (\rho U \lambda) = \alpha \rho (1 - \lambda) H(T - T_i).
\]
Model Reductions: ODEs $\rightarrow$ DAEs

\[
\begin{align*}
\rho U &= \rho_1 u_1 \sin \beta, \\
\rho U^2 + p &= \rho_1 u_1^2 \sin^2 \beta + p_1, \\
V &= u_1 \cos \beta, \\
\frac{\gamma}{\gamma - 1} \frac{p}{\rho} - \lambda q + \frac{1}{2} (U^2 + u_1^2 \cos^2 \beta) &= \frac{\gamma}{\gamma - 1} \frac{p_1}{\rho_1} + \frac{1}{2} u_1^2, \\
\frac{d\lambda}{dX} &= \alpha \frac{1 - \lambda}{U} H(T - T_i).
\end{align*}
\]

ZND reaction zone structure ODE supplemented with extended Rankine-Hugoniot algebraic conditions.
Model Reductions: Inversion of Algebraic Relations

with $\mathcal{M}_1 \equiv M_1 \sin \beta$,

$$\rho(\lambda) = \frac{\rho_1 (\gamma + 1) \mathcal{M}_1^2}{1 + \gamma \mathcal{M}_1^2 \pm \sqrt{(1 + \gamma \mathcal{M}_1^2)^2 - (\gamma + 1) \mathcal{M}_1^2 \left(2 + \frac{\gamma - 1}{\gamma} \frac{2 \lambda q}{R T_1} + (\gamma - 1) \mathcal{M}_1^2\right)}}$$

$$U(\lambda) = \frac{\rho_1 u_1 \sin \beta}{\rho(\lambda)}$$

$$p(\lambda) = p_1 + \rho_1^2 u_1^2 \sin^2 \beta \left(\frac{1}{\rho_1} - \frac{1}{\rho(\lambda)}\right)$$

$$T(\lambda) = \frac{p_1}{\rho(\lambda) R} + \frac{\rho_1^2 u_1^2 \sin^2 \beta}{\rho(\lambda) R} \left(\frac{1}{\rho_1} - \frac{1}{\rho(\lambda)}\right)$$

$$q \leq \frac{\gamma R T_1 (\mathcal{M}_1^2 - 1)^2}{2(\gamma^2 - 1) \mathcal{M}_1^2}, \quad \text{CJ limitation.}$$

+ shocked; − unshocked. Take the shocked branch.
Reaction Zone Structure Solution

\[
\frac{d\lambda}{dX} = \frac{\alpha}{\rho_1 u_1 \sin \beta} \rho(\lambda)(1 - \lambda), \quad \lambda(0) = 0,
\]

\[
X(\lambda) = a_1 \left( 2a_3 \left( \sqrt{1 - a_4 \lambda} - 1 \right) \right) + \ln \left( \left( \frac{1}{1 - \lambda} \right)^{a_2} \left( \frac{1 - \sqrt{1 - a_4 \lambda}}{1 + \sqrt{1 - a_4 \lambda}} \right)^{a_3} \sqrt{1 - a_4} \right)
\]

\[
a_1 = \frac{1}{(\gamma + 1) M_1} \frac{\sqrt{\gamma R T_1}}{\alpha},
\]

\[
a_2 = 1 + \gamma M_1^2,
\]

\[
a_3 = M_1^2 - 1,
\]

\[
a_4 = 2 \frac{M_1^2}{(M_1^2 - 1)^2} \frac{\gamma^2 - 1}{\gamma} \frac{q}{R T_1}.
\]
## Parametric Values

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<th>Units</th>
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Reaction Zone Structure Normal to Shock

- 

- 

- 

- 

a) 

b) 

c) 

d)
Exact Solution: Streamlines

- Curved streamlines identical to wedge contour.
- Streamline curvature approaches zero as reaction completes.
High Mach Number Limit Solution

\[
\frac{\rho(\lambda)}{\rho_1} = \frac{\gamma + 1}{\gamma - 1} \left( 1 - \frac{1}{\mathcal{M}_1^2} \frac{\gamma + 1}{\gamma} \left( \frac{2\gamma}{\gamma^2 - 1} + \frac{\lambda q}{RT_1} \right) + O \left( \frac{1}{\mathcal{M}_1^4} \right) \right),
\]

\[
\frac{U(\lambda)}{u_1 \sin \beta} = \frac{\gamma - 1}{\gamma + 1} \left( 1 + \frac{1}{\mathcal{M}_1^2} \frac{\gamma + 1}{\gamma} \left( \frac{2\gamma}{\gamma^2 - 1} + \frac{\lambda q}{RT_1} \right) + O \left( \frac{1}{\mathcal{M}_1^4} \right) \right),
\]

\[
\frac{p(\lambda)}{p_1} = \mathcal{M}_1^2 \frac{2\gamma}{\gamma + 1} \left( 1 - \frac{1}{\mathcal{M}_1^2} \frac{\gamma^2 - 1}{2\gamma} \left( \frac{1}{\gamma + 1} + \frac{\lambda q}{RT_1} \right) + O \left( \frac{1}{\mathcal{M}_1^4} \right) \right).
\]

\[
\lambda(X) = 1 - \exp \left( -\frac{(\gamma + 1)\alpha}{(\gamma - 1)u_1 \sin \beta} X \right),
\]

\[
X_r \sim \frac{\gamma - 1}{\gamma + 1} \frac{u_1 \sin \beta}{\alpha}. \quad \text{Reaction zone thickness}
\]
Low Heat Release Limit

Effects of heat release are better represented following a detailed asymptotic analysis, which yields

\[ X(\lambda) = a_1 \left( a_5 \ln(1 - \lambda) - \frac{a_3a_4}{2} \lambda \right). \]

Invert to form

\[ \lambda(X) = 1 - \frac{2a_5}{a_3a_4} W_0 \left[ \frac{a_3a_4}{2a_5} \exp \left( \frac{X}{a_1a_5} + \frac{a_3a_4}{2a_5} \right) \right]. \]

\[ X_r \sim \frac{\gamma - 1}{\gamma + 1} \frac{u_1 \sin \beta}{\alpha} \left( 1 + \frac{2}{\gamma - 1} M_1^2 + \frac{\gamma + 1}{\gamma(M_1^2 - 1)} \frac{q}{RT_1} \right). \]

Lambert \( W_0 \) function utilized:

\[ W_0(we^w) = w. \]
Exact versus Asymptotic Solutions

- High Mach number limit solution agrees poorly.
- Low heat release limit solution agrees well.
Verification of Modern Shock Capturing Algorithm

- Uniform Cartesian grid.
- Embedded internal boundary with level set representation.
- Nominally fifth order weighted essentially non-oscillatory (WENO) discretization.
- Non-decomposition based Lax-Friedrichs solver.
- Third order Runge-Kutta time integration.
Exact versus Numerical Solutions

- $256 \times 256$ uniform numerical grid.
- Good agreement in picture norm.
- Numerical solution stable.
Iterative Convergence to Steady State: Various Grids

- Coarse grids relax quickly; fine grids relax slowly.
- All grids iteratively converge to steady state.
- Iterative convergence is distinct from grid convergence.
Convergence rate: $O(\Delta x^{0.779})$.

Both shock capturing and embedded boundary induce the low convergence rate.
Conclusions

- New exact solution for two-dimensional steady detonation found.
- Excellent verification tool for computational methods.
- Numerical solutions are stable.
- Shock capturing and embedded boundary induce low order convergence rates even for high order discretizations.
- Common practice of claiming high order convergence rates without verification should be stopped.