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.

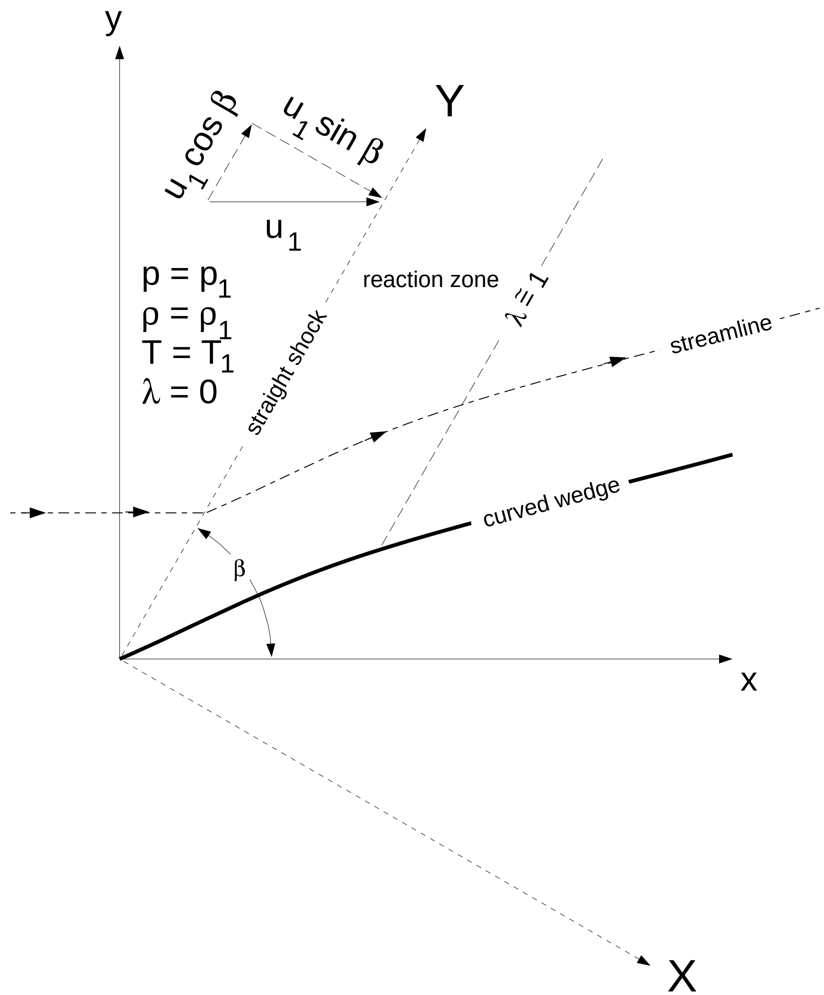
Verification and Validation

- *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

- Samaras, *Can. J. Research* , 1948.
- Gross, *AIAA J.*, 1963.
- Lee, *AIAA J.*, 1966.
- Pratt, *J. Propul. Power*, 1991.
- Powers, *et al.*, *AIAA J., Phys. Fluids, Shock Waves*, 1992-96.

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

$$\begin{aligned}
\frac{\partial}{\partial X}(\rho U) + \frac{\partial}{\partial Y}(\rho V) &= 0, \\
\frac{\partial}{\partial X}\left(\rho U^2 + p\right) + \frac{\partial}{\partial Y}(\rho U V) &= 0, \\
\frac{\partial}{\partial X}(\rho U V) + \frac{\partial}{\partial Y}\left(\rho V^2 + p\right) &= 0, \\
\frac{\partial}{\partial X}\left(\rho U\left(e + \frac{1}{2}(U^2 + V^2) + \frac{p}{\rho}\right)\right) & \\
+\frac{\partial}{\partial Y}\left(\rho V\left(e + \frac{1}{2}(U^2 + V^2) + \frac{p}{\rho}\right)\right) &= 0, \\
\frac{\partial}{\partial X}(\rho U \lambda) + \frac{\partial}{\partial Y}(\rho V \lambda) &= \alpha\rho(1-\lambda)H(T - T_i), \\
e &= \frac{1}{\gamma - 1}\frac{p}{\rho} - \lambda q, \\
p &= \rho R T.
\end{aligned}$$

Model Reductions: PDEs$\longrightarrow$ODEs

Assume no Y variation, so

$$\begin{aligned}
\frac{d}{dX}\left(\rho U\right) &= 0, \\
\frac{d}{dX}\left(\rho U^2 + p\right) &= 0, \\
\frac{d}{dX}\left(\rho U V\right) &= 0, \\
\frac{d}{dX}\left(\rho U \left(e + \frac{1}{2}(U^2 + V^2) + \frac{p}{\rho}\right)\right) &= 0, \\
\frac{d}{dX}\left(\rho U \lambda\right) &= \alpha \rho (1 - \lambda) H(T - T_i).
\end{aligned}$$

Model Reductions: ODEs⟶DAEs

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

ZND reaction zone structure ODE supplemented with extended Rankine-Hugoniot algebraic conditions.

Model Reductions: Inversion of Algebraic Relations

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

$$\rho(\lambda) = \frac{\rho_1(\gamma+1)\mathcal{M}_1^2}{1+\gamma\mathcal{M}_1^2 \pm \sqrt{\left(1+\gamma\mathcal{M}_1^2\right)^2 - (\gamma+1)\mathcal{M}_1^2\left(2+\frac{\gamma-1}{\gamma}\frac{2\lambda q}{RT_1}+(\gamma-1)\mathcal{M}_1^2\right)}},$$

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

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

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

$$q \leq \frac{\gamma RT_1(\mathcal{M}_1^2-1)^2}{2(\gamma^2-1)\mathcal{M}_1^2},$$ CJ limitation.

$+$ shocked; $-$ unshocked. Take the shocked branch.

Reaction Zone Structure Solution

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

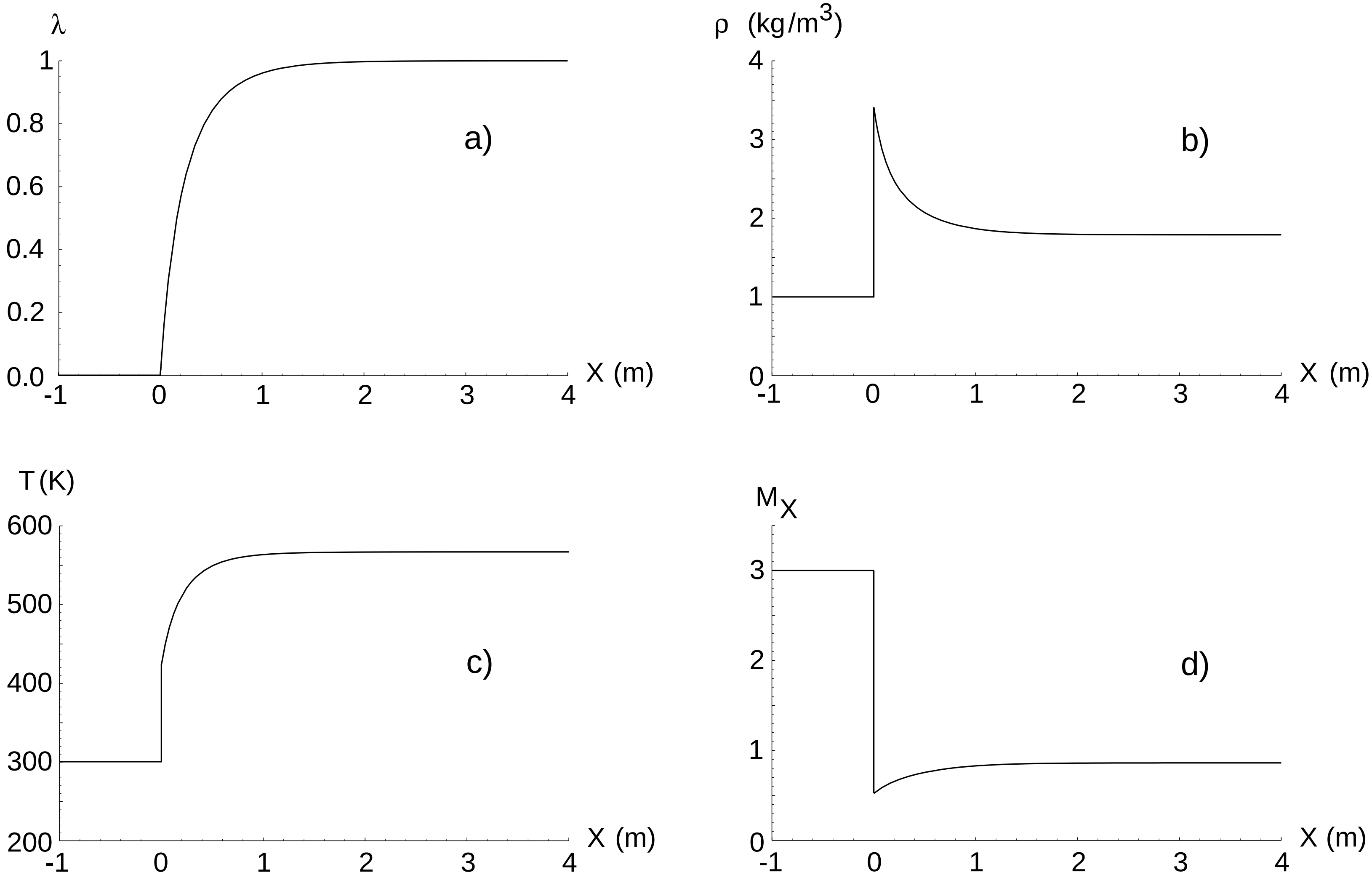
$$X(\lambda) = a_1\left(2a_3\left(\sqrt{1-a_4\lambda}-1\right) + \ln\left(\left(\frac{1}{1-\lambda}\right)^{a_2}\left(\frac{\left(1-\sqrt{\frac{1-a_4\lambda}{1-a_4}}\right)\left(1+\sqrt{\frac{1}{1-a_4}}\right)}{\left(1+\sqrt{\frac{1-a_4\lambda}{1-a_4}}\right)\left(1-\sqrt{\frac{1}{1-a_4}}\right)}\right)^{a_3\sqrt{1-a_4}}\right)\right).$$

$$\begin{aligned}
a_1 &= \frac{1}{(\gamma+1)\mathcal{M}_1}\frac{\sqrt{\gamma R T_1}}{\alpha}, \\
a_2 &= 1+\gamma\mathcal{M}_1^2, \\
a_3 &= \mathcal{M}_1^2 - 1, \\
a_4 &= 2\frac{\mathcal{M}_1^2}{(\mathcal{M}_1^2-1)^2}\frac{\gamma^2-1}{\gamma}\frac{q}{RT_1}.
\end{aligned}$$

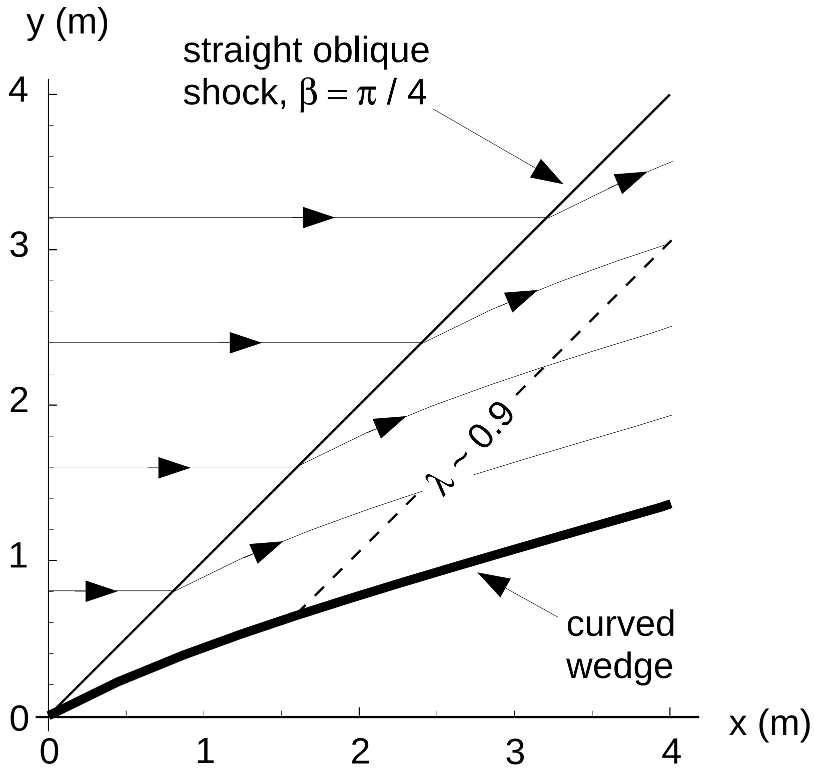
Parametric Values

Independent Parameter	Units	Value
R	$J/kg/K$	287
α	$1/s$	1000
β	rad	$\pi/4$
γ	-	$6/5$
T_1	K	300
M_1	-	3
ρ_1	kg/m^3	1
q	J/kg	300000
T_i	K	$131300/363$

Reaction Zone Structure Normal to Shock



Exact Solution: Streamlines



- Curved streamlines identical to wedge contour.
- Streamline curvature approaches zero as reaction completes.

High Mach Number Limit Solution

$$
\begin{aligned}
\frac{\rho(\lambda)}{\rho_1} &= \frac{\gamma+1}{\gamma-1}\left(1-\frac{1}{\mathcal{M}_1^2}\frac{\gamma+1}{\gamma}\left(\frac{2\gamma}{\gamma^2-1}+\frac{\lambda q}{RT_1}\right)+O\left(\frac{1}{\mathcal{M}_1^4}\right)\right), \\
\frac{U(\lambda)}{u_1\sin\beta} &= \frac{\gamma-1}{\gamma+1}\left(1+\frac{1}{\mathcal{M}_1^2}\frac{\gamma+1}{\gamma}\left(\frac{2\gamma}{\gamma^2-1}+\frac{\lambda q}{RT_1}\right)+O\left(\frac{1}{\mathcal{M}_1^4}\right)\right), \\
\frac{p(\lambda)}{p_1} &= \mathcal{M}_1^2\frac{2\gamma}{\gamma+1}\left(1-\frac{1}{\mathcal{M}_1^2}\frac{\gamma^2-1}{2\gamma}\left(\frac{1}{\gamma+1}+\frac{\lambda q}{RT_1}\right)+O\left(\frac{1}{\mathcal{M}_1^4}\right)\right).
\end{aligned}
$$

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

$$
X_r \sim \frac{\gamma-1}{\gamma+1}\frac{u_1\sin\beta}{\alpha}.
$$

Reaction zone thickness

Low Heat Release Limit

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

$$X(\lambda) = a_1 \left(a_5 \ln(1-\lambda) - \frac{a_3 a_4}{2}\lambda \right).$$

Invert to form

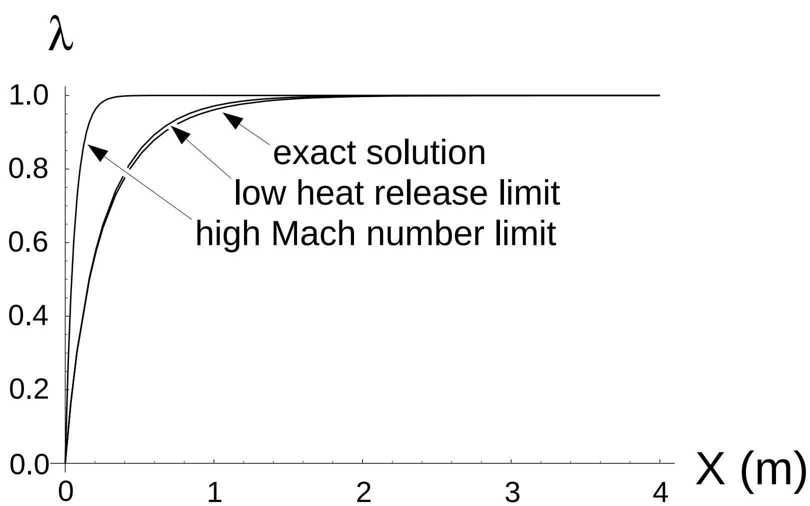
$$\lambda(X) = 1 - \frac{2a_5}{a_3 a_4} W_0 \left[\frac{a_3 a_4}{2a_5} \exp\left(\frac{X}{a_1 a_5} + \frac{a_3 a_4}{2a_5} \right) \right].$$

$$X_r \sim \frac{\gamma - 1}{\gamma + 1} \frac{u_1 \sin\beta}{\alpha} \left(1 + \frac{2}{(\gamma - 1)\mathcal{M}_1^2} + \frac{\gamma + 1}{\gamma(\mathcal{M}_1^2 - 1)} \frac{q}{RT_1} \right).$$

Lambert W_0 function utilized:

$$W_0(we^w) = w.$$

Exact versus Asymptotic Solutions

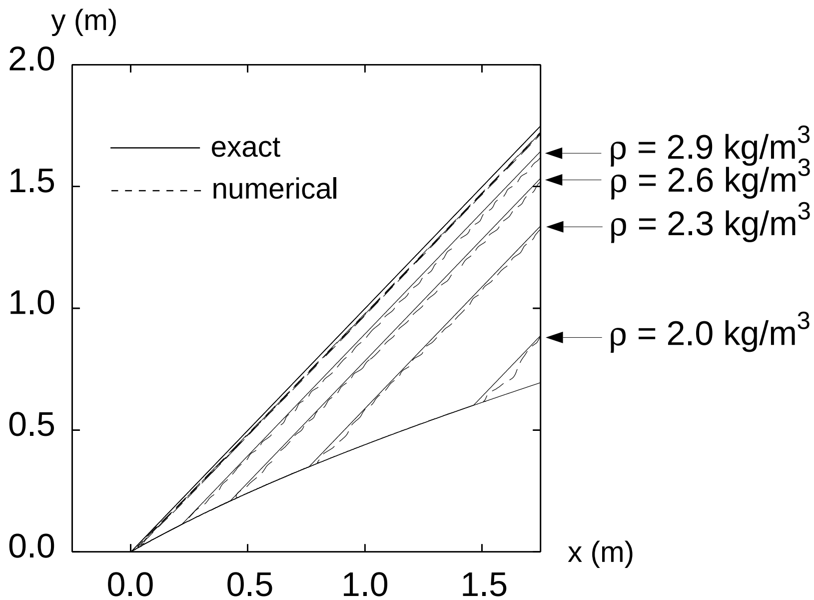


- High Mach number limit solution agrees poorly.
- Low heat release limit solution agrees well.

Verification of Modern Shock Capturing Algorithm

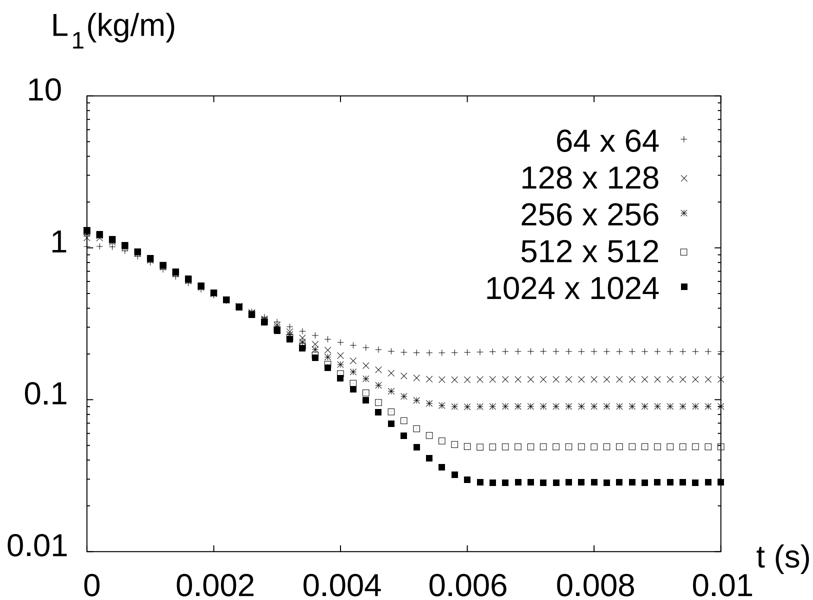
- Algorithm of Xu, Aslam, and Stewart, 1997, *CTM*.
- Uniform Cartesian grid.
- Embedded internal boundary with level set representation.
- Nominally fifth order weighted essentially non-oscillatory (WENO) discretization.
- Non-decomposition based Lax-Friedrichs solver.
- Third order Runge-Kutta time integration.

Exact versus Numerical Solutions



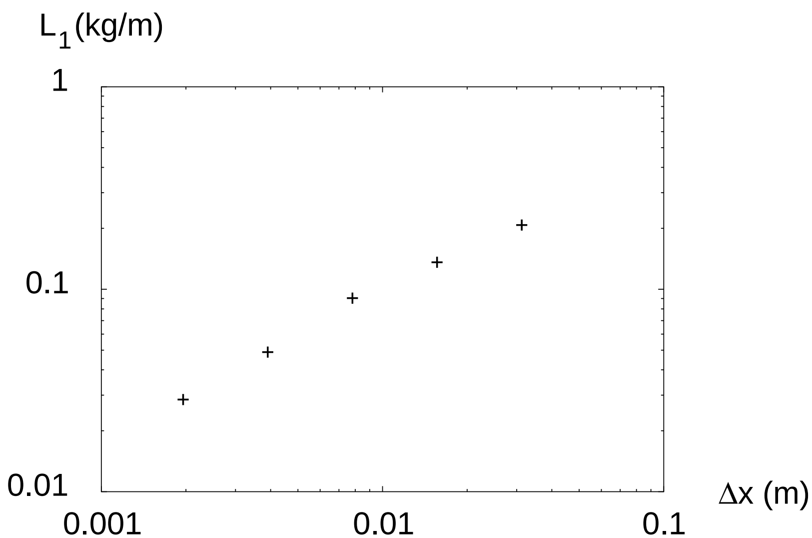
- 256×256 uniform numerical grid.
- good agreement in picture norm.
- numerical solution stable.

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.

Grid Convergence



- Convergence rate: $O\left(\Delta x^{0.779}\right)$.
- 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.