Harmony in High Speed Combustion

Joseph M. Powers,
Professor and Associate Chair,
Department of Aerospace and Mechanical Engineering,
Department of Applied and Computational Mathematics and Statistics
(concurrent)

University of Notre Dame, Notre Dame, Indiana

Los Alamos National Laboratory

11 March 2015
Acknowledgments

- Christopher M. Romick, Ph.D. candidate, ND-AME
- Tariq D. Aslam, Technical Staff Member, LANL
Verification and Validation Overview

- We will consider here verification and validation of a multi-scale problem using Direct Numerical Modeling, which captures both coarse and fine scales.

- One key algorithm is the Wavelet Adaptive Multiresolution Method (WAMR), one of the methods employed in the University of Notre Dame-led Center for Shock Wave Processing of Advanced Materials (C-SWARM), a NNSA-supported PSAAP II Center.

- C-SWARM is in Year 1 of a five-year project associated with exascale scientific computing of challenging multi-scale shock physics problems.
Verification and Validation Overview, cont.

• C-SWARM is a joint effort with Notre Dame, Indiana U., and Purdue U.

• Its problem is shocking mechanically pre-activated pressed metallic powders to synthesize new metallic structures.

• We will develop verified and validated predictive codes prepared for an exascale environment.

• The WAMR code, in development at Notre Dame for 20 years, will be used today on a different problem in reactive gas dynamics.
Disharmony in High Speed Combustion

https://www.youtube.com/watch?v=rYxsilgRxi4

Prof. Frank Lu, University of Texas-Arlington.

Described as “25 Hz,” but there is acoustic energy present across the frequency spectrum. Disorder.
Harmony: Organ Pipe Resonance

\[ a/\ell \sim 1000 \text{ Hz. Higher order harmonic at 2000 Hz. Order.} \]
Motivation

- Combustion dynamics are influenced by various balances of *advection*, *reaction*, and *diffusion*.

- Depending on flow conditions, one may observe simple structures, patterned harmonic structures, or chaotic structures.

- Often, the critical balance is between *advection* and *reaction*, with diffusion serving as only a small perturbation.

- Near stability thresholds, diffusion can play a determining role.

- Full non-linear dynamics can induce complex behavior.

- Extreme care *may or may not be* needed in numerical simulation to carefully capture the multi-scale physics.
Introduction

• Standard result from non-linear dynamics: small scale phenomena can influence large scale phenomena and vice versa.

• What are the risks of using models which ignore diffusion (Euler vs. Navier-Stokes)?

• Might there be risks in using standard filtering strategies: implicit time-advancement, numerical viscosity, LES, and turbulence modeling, all of which introduce *nonphysical diffusion* to filter small scale physical dynamics?
Powers & Paolucci (AIAA J., 2005) studied the reaction length scales of inviscid \( \text{H}_2 - \text{O}_2 \) detonations and found the finest length scales on the order of microns and the largest on the order of centimeters for atmospheric ambient pressure.

This range of scales must be resolved to capture the dynamics.

In a one-step kinetic model only a single reaction length scale is induced compared to the multiple length scales of detailed kinetics.

We examine i) a simple one-step model and ii) a detailed model appropriate for hydrogen.
One-Step Reaction Kinetics Model
One-Dimensional Unsteady Compressible Reactive Navier-Stokes Equations

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0, \\
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} \left( \rho u^2 + P - \tau \right) = 0, \\
\frac{\partial}{\partial t} \left( \rho \left( e + \frac{u^2}{2} \right) \right) + \frac{\partial}{\partial x} \left( \rho u \left( e + \frac{u^2}{2} \right) + j^q + (P - \tau) u \right) = 0, \\
\frac{\partial}{\partial t} (\rho Y_B) + \frac{\partial}{\partial x} (\rho u Y_B + j_B^m) = \rho r.
\]

Equations are transformed to a steady moving reference frame.
Constitutive Relations

\[ P = \rho RT, \]
\[ e = \frac{p}{\rho (\gamma - 1)} - qY_B, \]
\[ r = H(P - P_s)a(1 - Y_B)e^{-\frac{\tilde{E}}{\gamma/\rho}}, \]
\[ j_B^m = -\rho D \frac{\partial Y_B}{\partial x}, \]
\[ \tau = \frac{4}{3} \mu \frac{\partial u}{\partial x}, \]
\[ j_q^a = -k \frac{\partial T}{\partial x} + \rho D q \frac{\partial Y_B}{\partial x}. \]

with \( D = 10^{-4} \frac{m^2}{s}, k = 10^{-1} \frac{W}{mK}, \) and \( \mu = 10^{-4} \frac{Ns}{m^2}, \) so for \( \rho_o = 1 \frac{kg}{m^3}, \)

\( Le = Sc = Pr = 1. \)
Case Examined

Let us examine this one-step kinetic model with:

- a fixed reaction length, $L_{1/2} = 10^{-6}$ m, which is similar to that of the finest H$_2$-O$_2$ scale.
- a fixed diffusion length, $L_\mu = 10^{-7}$ m; mass, momentum, and energy diffusing at the same rate.
- an ambient pressure, $P_o = 101325$ Pa, ambient density, $\rho_o = 1$ kg/m$^3$, heat release $q = 5066250$ m$^2$/s$^2$, and $\gamma = 6/5$. 
Numerical Method

- Finite difference, uniform grid
  \[ \Delta x = 2.50 \times 10^{-8} \text{ m}, \ N = 8001, \ L = 0.2 \text{ mm} \].

- Computation time = 192 hours for 10 \( \mu \text{s} \) on an AMD 2.4 GHz with 512 kB cache.

- A point-wise method of lines approach was used.

- Advective terms were calculated using a combination of fifth order WENO and Lax-Friedrichs.

- Sixth order central differences were used for the diffusive terms.

- Temporal integration was accomplished using a third order Runge-Kutta scheme.
Physical Piston Problem

- Initialized with inviscid ZND solution.
- Moving frame travels at the CJ velocity.
- Integrated in time for long time behavior.
Below a Critical Activation Energy, the Detonation is Stable
At Higher Activation Energy, Fundamental Harmonic Due to Balance Between Reaction and Advection Between Lead Shock and End of Reaction Zone: An Organ Pipe Resonance
Diffusion Delays Transition to Instability

- Lee and Stewart revealed for $E < 25.26$ the steady ZND wave is linearly stable.
- For the inviscid case Henrick et al. found the stability limit at $E_0 = 25.265 \pm 0.005$.
- In the viscous case $E = 26.647$ is still stable; however, above $E_0 \approx 27.1404$ a period-1 limit cycle can be realized.
Period-Doubling Phenomena Predicted

- As in the inviscid limit, the viscous case goes through a period-doubling phase.
- For the inviscid case, the period-doubling began at $E_1 \approx 27.2$.
- In the viscous case, the beginning of this period doubling is delayed to $E_1 \approx 29.3116$. 

Viscous Detonations:
Chaos and Order

Viscous Detonations:

Period-5

Period-6

Chaotic

Period-3
Diffusion Delays Transition to Chaos

- In the inviscid limit, the point where bifurcation points accumulate is found to be $E_\infty \approx 27.8324$.

- For the viscous case, $L_\mu / L_{1/2} = 1/10$, the accumulation point is delayed until $E_\infty \approx 30.0411$.

- For $E > 30.0411$, a region exists with many relative maxima in the detonation pressure; it is likely the system is in the chaotic regime.
Approximations to Feigenbaum’s Constant

\[ \delta_\infty = \lim_{n \to \infty} \delta_n = \lim_{n \to \infty} \frac{E_n - E_{n-1}}{E_{n+1} - E_n} \]

Feigenbaum predicted \( \delta_\infty \approx 4.669201 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( E_n )</th>
<th>( \delta_n )</th>
<th>( E_n )</th>
<th>( \delta_n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>25.2650</td>
<td>-</td>
<td>27.1404</td>
<td>-</td>
</tr>
<tr>
<td>1</td>
<td>27.1875</td>
<td>3.86</td>
<td>29.3116</td>
<td>3.793</td>
</tr>
<tr>
<td>2</td>
<td>27.6850</td>
<td>4.26</td>
<td>29.8840</td>
<td>4.639</td>
</tr>
<tr>
<td>3</td>
<td>27.8017</td>
<td>4.66</td>
<td>30.0074</td>
<td>4.657</td>
</tr>
<tr>
<td>4</td>
<td>27.82675</td>
<td>-</td>
<td>30.0339</td>
<td>-</td>
</tr>
</tbody>
</table>
Similar Behavior to Logistics Map:

\[ x_{n+1} = r x_n (1 - x_n) \]

- The period-doubling behavior and transition to chaos predicted in both the viscous and inviscid limit have striking similarities to that of the logistic map.

- Within the chaotic region, there exist pockets of order.

- Periods of 5, 6, and 3 are found within this region.
Diffusion Delays Instability: Bifurcation Diagram

(a) no diffusion  
(b) diffusion
Diminishing Diffusion De-Stabiliizes \( (E = 27.6339) \)

- The system undergoes transition from a stable detonation to a period-1 limit cycle, to a period-2 limit cycle.
- The amplitude of pulsations increases.
- The frequency decreases.
Harmonic Analysis - PSD

- Harmonic analysis can be used to extract the multiple frequencies of a signal.
- The discrete one-sided mean-squared amplitude Power Spectral Density (PSD) for the pressure was used:

$$\Phi_d(0) = \frac{1}{N^2} |P_o|^2, $$

$$\Phi_d(\tilde{f}_k) = \frac{2}{N^2} |P_k|^2, \quad k = 1, 2, \ldots, (N/2 - 1),$$

$$\Phi_d(N/2) = \frac{1}{N^2} |P_{N/2}|^2,$$

where $P_k$ is the standard discrete Fourier Transform of $p$,

$$P_k = \sum_{n=0}^{N-1} p_n \exp \left( -\frac{2\pi ink}{N} \right), \quad k = 0, 1, 2, \ldots, N/2.$$
Higher Order Harmonics Predicted as Activation Energy Increases

\[ \Phi_d (\overline{T}) \text{ [dB]} \]

- \( f_x \)
- \( \frac{f_x}{2} \)
- \( \frac{3 f_x}{2} \)
- \( 2 f_x \)

\[ E_a = 26.0 \]
\[ E_a = 27.5 \]
\[ E_a = 27.7 \]
Diffusion Modulates the Amplitude and Shifts the Frequency

\[ E_\alpha = 27.7 \]
Bifurcation of Oscillatory Modes: Baroque Harmonies!
Simple One-Step Model: Conclusions

- Dynamics of one-dimensional detonations are influenced by mass, momentum, energy diffusion, especially so in the region of high frequency instability.

- In general, the effect of diffusion is stabilizing.

- Bifurcation and transition to chaos show similarities to the logistic map.

- The structures are deterministic and often harmonious, but with possible baroque complexity.
Detailed Reaction Kinetics Model
Unsteady, Compressible, Reactive Navier-Stokes Equations

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,
\]
\[
\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I} - \mathbf{\tau}) = 0,
\]
\[
\frac{\partial}{\partial t} \left( \rho \left( e + \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) \right) + \nabla \cdot \left( \rho \mathbf{u} \left( e + \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) + (p \mathbf{I} - \mathbf{\tau}) \cdot \mathbf{u} + \mathbf{q} \right) = 0,
\]
\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i + \mathbf{j}_i) = \overline{M_i} \dot{\omega}_i,
\]
\[
\begin{align*}
p &= \mathcal{R}T \sum_{i=1}^{N} \frac{Y_i}{M_i}, & e &= e(T, Y_i), & \dot{\omega}_i &= \dot{\omega}_i(T, Y_i), \\
\mathbf{j}_i &= \rho \sum_{k=1}^{N} \frac{M_k D_{ik} Y_k}{M} \left( \frac{\nabla y_k}{y_k} + \left( 1 - \frac{M_k}{M} \right) \frac{\nabla p}{p} \right) - \frac{D_{i}^T \nabla T}{T}, \\
\mathbf{\tau} &= \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right), \\
\mathbf{q} &= -k \nabla T + \sum_{i=1}^{N} \mathbf{j}_i h_i - \mathcal{R}T \sum_{i=1}^{N} \frac{D_{i}^T}{M_i} \left( \frac{\nabla y_i}{y_i} + \left( 1 - \frac{M_i}{M} \right) \frac{\nabla p}{p} \right).
\end{align*}
\]
Computational Methods

- **Inviscid**
  - Shock-fitting: Fifth order algorithm adapted from Henrick et al., *JCP*.
  - Shock-capturing: Second order min-mod algorithm

- **Viscous**
  - Wavelet method (WAMR), developed by Vasilyev and Paolucci, *JCP*
  - User-defined threshold parameter $\epsilon$ controls error: *automatic verification!*

\[
\begin{align*}
  u^J(x) &= \sum_k u_{0,k} \Phi_0,k(x) + \sum_{j=0}^{J-1} \sum_{\lambda} d_{j,\lambda} \Psi_j(x) \\
  &\quad \left\{ \lambda : |d_{j,\lambda}| \geq \epsilon \right\} \\
  &\quad \left\{ \lambda : |d_{j,\lambda}| < \epsilon \right\} \\
  &= u^J_\epsilon + R^J_\epsilon
\end{align*}
\]

- All methods used a fifth order explicit Runge-Kutta scheme for time integration
Automatic Verification with WAMR

- Sod shock tube result from Brill, Grenga, Powers, and Paolucci, 11th World Congress on Computational Mechanics, 2014.
- The error is controlled by WAMR.
Cases Examined

- Overdriven detonations with ambient conditions of 0.421 atm and 293.15 K
- Initial stoichiometric mixture of $2\text{H}_2 + \text{O}_2 + 3.76\text{N}_2$
- $D_{CJ} \sim 1972$ m/s
- Overdrive is defined as $f = D_o^2/D_{CJ}^2$
- Overdrives of $1.018 < f < 1.150$ were examined
Typical Stable Steady Wave Profile

\[ f = 1.15 \]
Stable Detonation at High Overdrive

For high enough overdrives, the detonation relaxes to a steady propagating wave in the inviscid case as well as in the diffusive case.
Lower Overdrive: High Frequency Instability, No Diffusion

\[ f = 1.10 \]

A single fundamental frequency oscillation occurs at a frequency of 0.97 MHz. This frequency agrees with the experimental observations of Lehr (Astro. Acta, 1972).

**Organ pipe oscillation between shock and end of reaction zone:** \( \nu \sim \frac{a}{\ell} = \frac{(1000 \text{ m/s})}{(0.0001 \text{ m})} \approx 10 \text{ MHz.} \)
Validation with Lehr’s High Frequency Instability

- Stoichiometric mixture of $2\text{H}_2 + \text{O}_2 + 3.76\text{N}_2$ at 0.421 atm
- Observed 1.04 MHz frequency for projectile velocity corresponding to $f \approx 1.10$
- For $f = 1.10$, the predicted frequency of 0.97 MHz agrees with observed frequency and the prediction by Yungster and Radhakrishan of 1.06 MHz

(Astro. Acta, 1972)
The addition of viscosity has a stabilizing effect, decreasing the amplitude of the oscillations. The pulsation frequency relaxes to 0.97 MHz.
As the overdrive is lowered, multiple frequencies appear, and the amplitude of the oscillations continues to grow. These multiple frequencies persist at long time.
Low Frequency Mode Appearance - Viscous vs. Inviscid

\[ f = 1.035 \]

Viscosity still decreases the amplitude of oscillation, though the effect is reduced compared to higher overdrives.
Viscous H$_2$-Air Harmonics: Effect of Overdrive

(a) 

(b) 

(c) 

(d)

\( v \) (MHz)

\( \Phi_d (v) \) (dB)

\( \Phi_d (v) \) (dB)

\( \Phi_d (v) \) (dB)

\( \Phi_d (v) \) (dB)
Viscous H₂-Air Harmonics: Effect of Overdrive

(a) 
\[ \Phi_d(\nu) \] (dB) 
\[ \nu_l \] \[ \nu_h \] \[ 2\nu_l \] \[ \nu_h - 2\nu_l \] \[ \nu_h - \nu_l \] \[ \nu_h \] \[ \nu_h + \nu_l \]

(b) 
\[ \Phi_d(\nu) \] (dB) 
\[ \nu_o \] \[ 2\nu_o \] \[ 3\nu_o \] \[ 4\nu_o \]

(c) 
\[ \Phi_d(\nu) \] (dB) 
\[ \frac{1}{2}\nu_o \] \[ \frac{3}{2}\nu_o \] \[ 2\nu_o \] \[ 3\nu_o \] \[ 4\nu_o \] \[ 5\nu_o \]

(d) 
\[ \Phi_d(\nu) \] (dB) 
\[ \frac{1}{2}\nu_o \] \[ 2\nu_o \] \[ 3\nu_o \]
H₂-Air: Near Neutral Stability

\[ \Phi_d(\bar{f}) \ [\text{dB}] \]

\[ \begin{align*}
-100 & \quad -80 & \quad -60 & \quad -40 & \quad -20 & \quad 0 \\
0 & \quad 1 & \quad 2 & \quad 3 & \quad 4 & \quad 5
\end{align*} \]

\[ \bar{f} \ [\text{MHz}] \]

Graph showing the phase difference \( \Phi_d(\bar{f}) \) in dB as a function of \( \bar{f} \) in MHz. The graph includes frequency labels such as \( \bar{f}, 2\bar{f}, 3\bar{f} \) at specific points.
The amplitude of the oscillations continues grow as the overdrive is lowered. There appears to be a near power-law decay in the amount of energy carried by the higher harmonics.
Fine Grids Required for Accurate Shock-Capturing

\[ f = 1.10 \]

Using the same grid size as shock-fitting (\( \Delta x = 4 \mu m \)), shock-capturing misses the essential dynamics.
Fine Grids Required for Accurate Shock-Capturing

\[ f = 1.023 \]

Only when \( \Delta x = 1/2 \mu m \) is used does the PSD of shock-capturing become nearly indistinguishable with that of shock-fitting.
Near the Neutral Stability Boundary, Diffusion Damps the Small Oscillations

\[ \Phi_d(f) \text{ [dB]} \]

\( f = 1.120 \) MHz

- Inviscid
- Viscous
Diffusion Reduces the Magnitude of the First and Second Harmonics
Bifurcation Diagram for Hydrogen-Air Detonation

(a) $P_{\text{peak}}/P_{\text{avg}}$ vs. $\overline{u}/p$ (cm/s)

(b) $\nu$ (MHz) vs. $\overline{u}/p$ (cm/s)
Conclusions

- Predictions of complex hydrogen-air detonations can be verified and validated.

- WAMR gives automatic verification; other methods have been verified by selection of sufficiently fine grids.

- Long time behavior of a hydrogen-air detonation becomes more complex as the overdrive is decreased.

- Advection and reaction effects *usually* dominate those of diffusion.

- Physical diffusion causes an amplitude reduction and phase shift; it is more important near bifurcation points.

- Filtering (shock-capturing, numerical viscosity, WENO, and by inference LES, implicit time-stepping, kinetic reduction, etc.) alters detonation dynamics.

- Like Bach’s baroque harmonies, those of real detonations are complex; a Mozartian classicism is still needed to strip away the intricate excess and capture, in a validated way, the essential character of detonation.
A New Book

- Foundation of AME 60611, taught for over twenty-five years.