Highly Accurate Numerical Simulations of Pulsating One-Dimensional Detonations

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43^{rd} AIAA Aerospace Sciences Meeting and Exhibit
Reno, Nevada

10-13 January 2005

Motivation

- Accurate and rapid solution of challenging physical problems is facilitated by both hardware and software.
- Moore’s Law hardware gains may be on the wane.
- Improved algorithms can supersede hardware gains.
- Here, we apply shock-fitting and high order discretization to dramatically increase the accuracy of classical pulsating detonation solutions and enable prediction of new physical phenomena.

General Review of Pulsating Detonations

- Erpenbeck, *Phys. Fluids*, 1962,
- Fickett and Wood, *Phys. Fluids*, 1966,
- Lee and Stewart, *JFM*, 1990,
- Bourlioux, *et al.*, *SIAM J. Appl. Math.*, 1991,
- He and Lee, *Phys. Fluids*, 1995,
- Short, *SIAM J. Appl. Math.*, 1997,
- Sharpe, *Proc. R. Soc.*, 1997.

Review of Recent Work of Special Relevance

- Kasimov and Stewart, *Phys. Fluids*, 2004: published detailed discussion of limit cycle behavior with shock-fitting; error $\sim O(\Delta x)$.
- Ng, Higgins, Kiyanda, Radulescu, Lee, Bates, and Nikiforakis, *CTM*, in press, 2005: in addition, considered transition to chaos; error $\sim O(\Delta x)$.
- Present study similar to above, but error $\sim O(\Delta x^5)$.

Model: Reactive Euler Equations

- one-dimensional,
- unsteady,
- inviscid,
- one step kinetics with finite activation energy,
- calorically perfect ideal gases with identical molecular masses and specific heats.

Model: Reactive Euler Equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \xi}(\rho u) &= 0, \\
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial \xi}\left(\rho u^2 + p\right) &= 0, \\
\frac{\partial}{\partial t}\left(\rho\left(e + \frac{1}{2}u^2\right)\right) + \frac{\partial}{\partial \xi}\left(\rho u\left(e + \frac{1}{2}u^2 + \frac{p}{\rho}\right)\right) &= 0, \\
\frac{\partial}{\partial t}(\rho\lambda) + \frac{\partial}{\partial \xi}(\rho u \lambda) &= \alpha\rho(1-\lambda)\exp\left(-\frac{\rho E}{p}\right), \\
e &= \frac{1}{\gamma - 1}\frac{p}{\rho} - \lambda q.
\end{aligned}
$$

Unsteady Shock Jump Equations

$$\begin{aligned}\rho_s(D(t)-u_s) &= \rho_o(D(t)-u_o), \\ p_s - p_o &= (\rho_o(D(t)-u_o))^2\left(\frac{1}{\rho_o}-\frac{1}{\rho_s}\right), \\ e_s - e_o &= \frac{1}{2}(p_s+p_o)\left(\frac{1}{\rho_o}-\frac{1}{\rho_s}\right), \\ \lambda_s &= \lambda_o.\end{aligned}$$

Model Refinement

- Transform to shock attached frame via

$$x = \xi - \int_0^t D(\tau)d\tau,$$

- Use jump conditions to develop shock-change equation for shock acceleration:

$$\frac{dD}{dt} = -\left(\frac{d(\rho_s u_s)}{dD}\right)^{-1}\left(\frac{\partial}{\partial x}\left(\rho u(u - D) + p\right)\right).$$

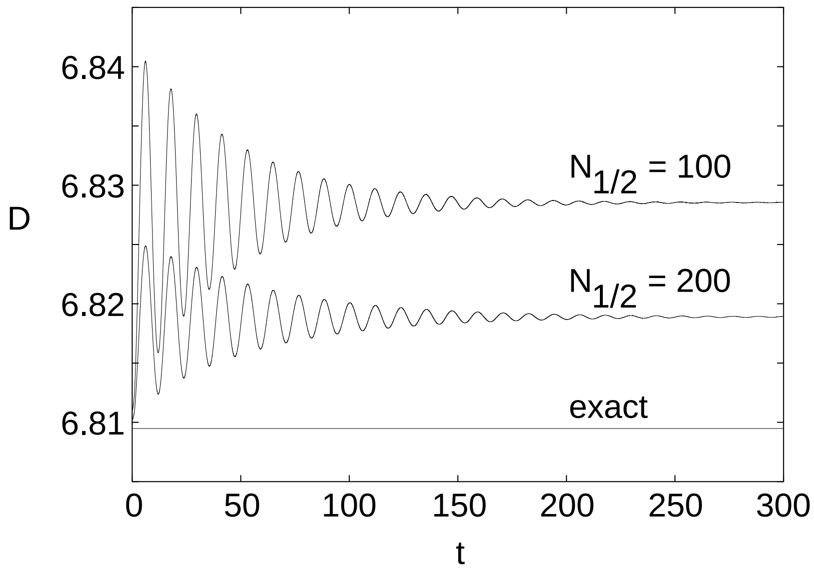
Numerical Method

- point-wise method of lines,
- uniform spatial grid,
- fifth order spatial discretization (WENO5M) takes PDEs into ODEs in time only,
- fifth order explicit Runge-Kutta temporal discretization to solve ODEs.
- details in Henrick, Aslam, Powers, *JCP*, in review.

Numerical Simulations

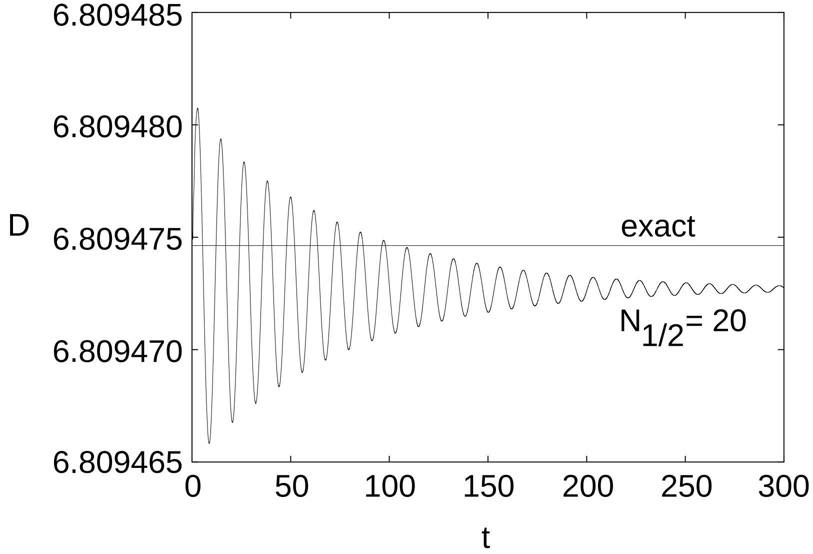
- $\rho_o = 1, p_o = 1, L_{1/2} = 1, q = 50, \gamma = 1.2$,
- Activation energy, E, a variable bifurcation parameter, $25 \leq E \leq 28.4$,
- CJ velocity: $D_{CJ} = \sqrt{11} + \sqrt{\frac{61}{5}} \approx 6.80947463$,
- from 10 to 200 points in $L_{1/2}$,
- initial steady CJ state perturbed by truncation error,
- integrated in time until limit cycle behavior realized.

Stable Case, $E = 25$: Kasimov's Shock-Fitting



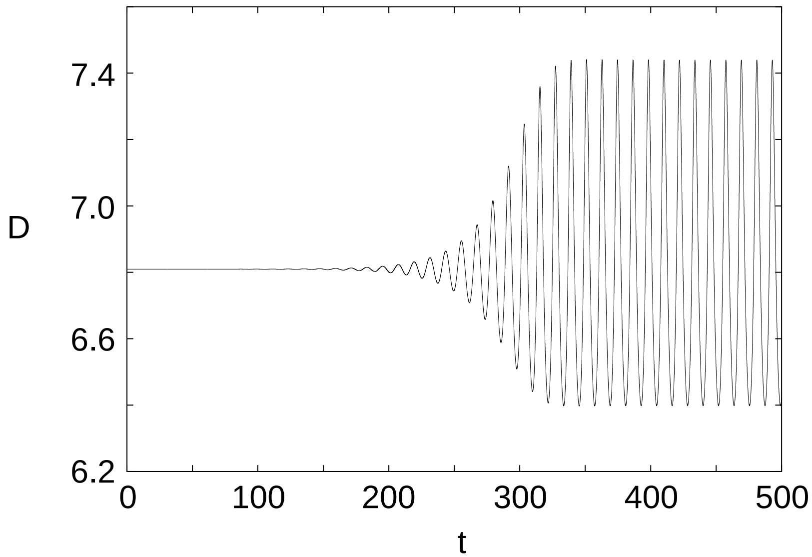
- $N_{1/2} = 100,\ 200,$
- minimum error in D: $\sim 9.40 \times 10^{-3}$,
- Error in D converges at $O(\Delta x^{1.01})$.

Stable Case, $E = 25$: Improved Shock-Fitting



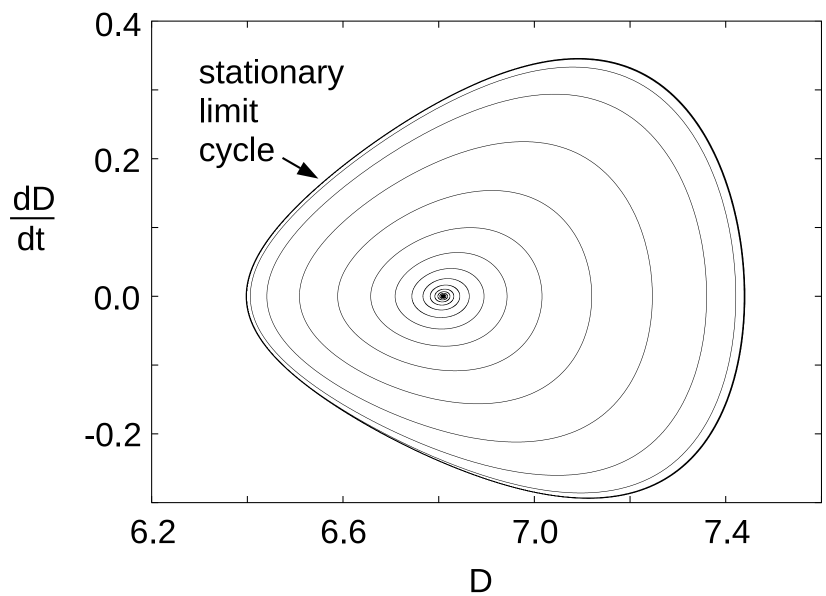
- $N_{1/2} = 20,\ 40,$
- minimum error in D: $\sim\ 6.00 \times 10^{-8}$, for $N_{1/2} = 40$.
- Error in D converges at $O(\Delta x^{5.01})$.

Linearly Unstable, Non-linearly Stable Case: $E = 26$



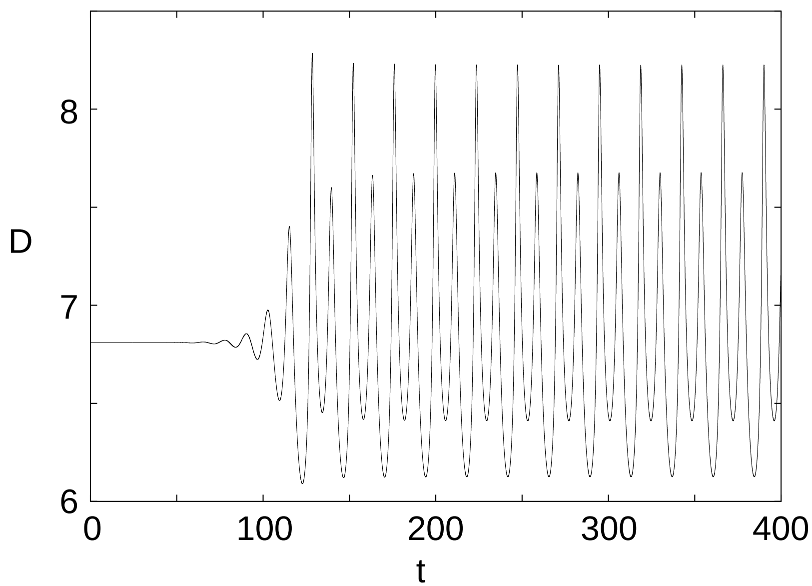
- One linearly unstable mode, stabilized by non-linear effects,
- Growth rate and frequency match linear theory to five decimal places.

$D, \ \frac{dD}{dt}$ **Phase Plane:** $E = 26$



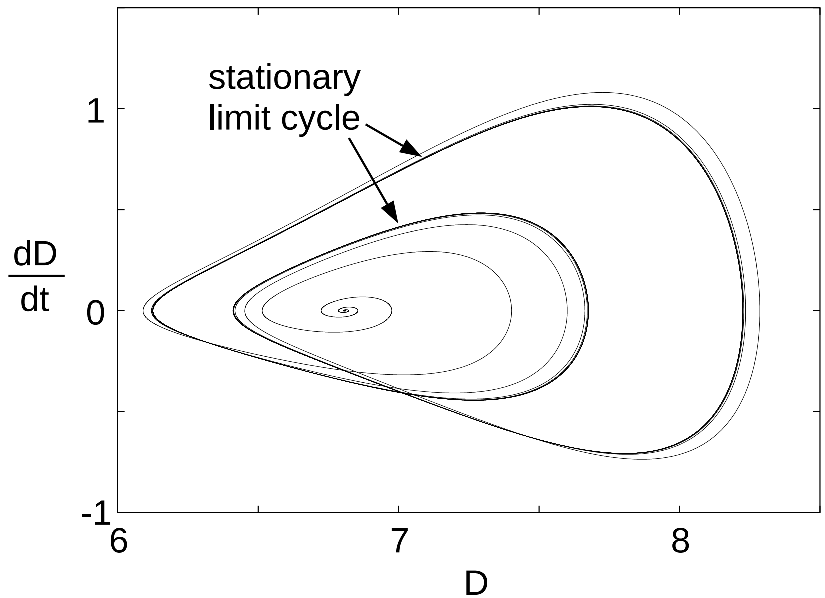
- Unstable spiral at early time, stable period-1 limit cycle at late time,
- Bifurcation point of $E = 25.265 \pm 0.005$ agrees with linear stability theory.

Period Doubling: $E = 27.35$



- $N_{1/2} = 20$,
- Bifurcation to period-2 oscillation at $E = 27.1875 \pm 0.0025$.

$D, \ \frac{dD}{dt}$ **Phase Plane:** $E = 27.35$



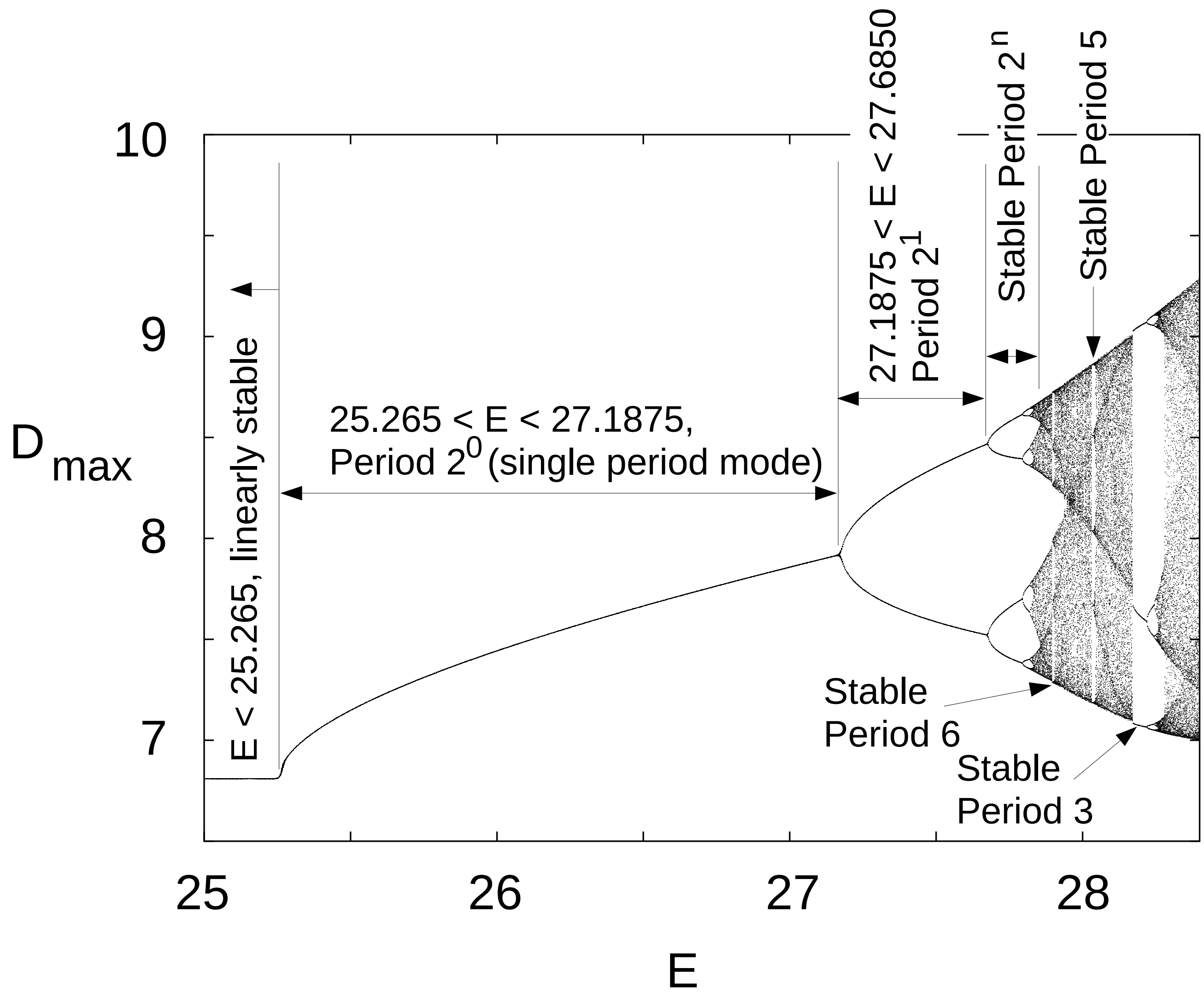
- Long time period-2 limit cycle,
- Similar to independent results of Sharpe and Ng.

Transition to Chaos and Feigenbaum's Number

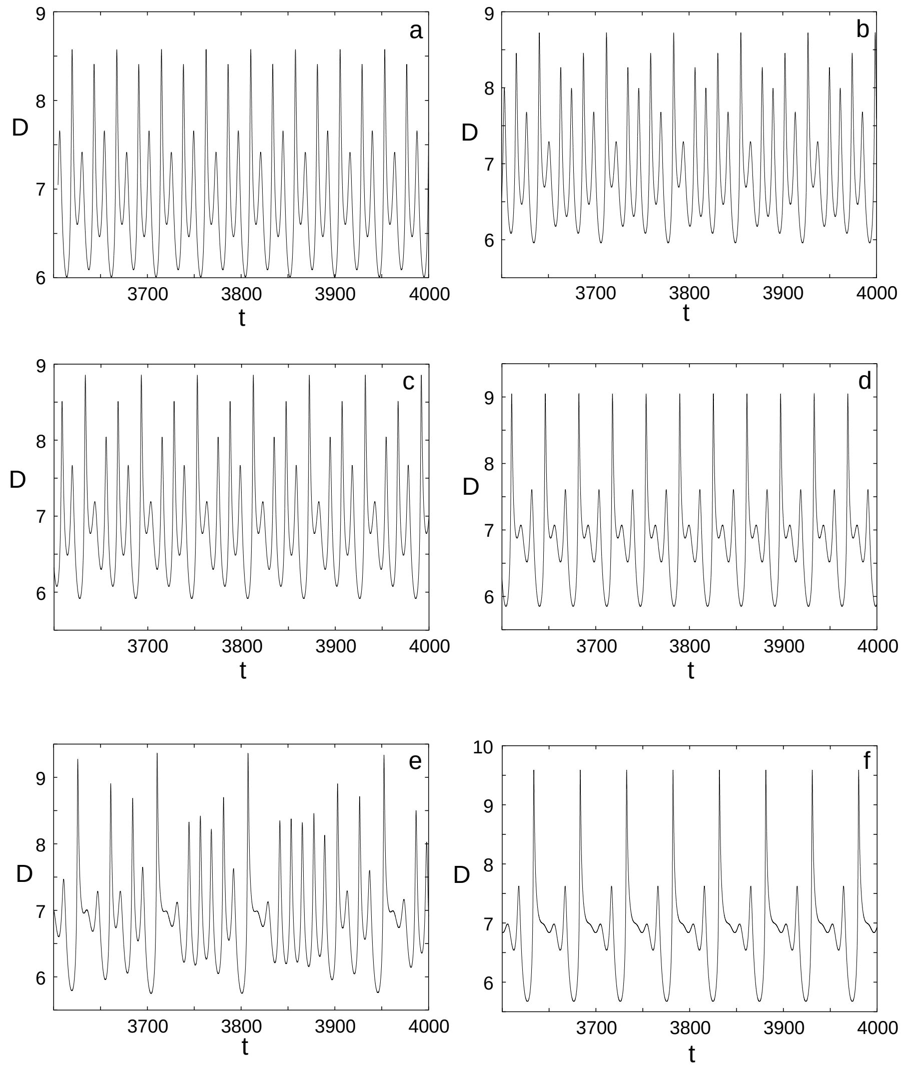
$$\lim_{n\to\infty} \delta_n = \frac{E_n - E_{n-1}}{E_{n+1} - E_n} = 4.669201\ldots.$$

n	E_n	$E_{n+1} - E_i$	δ_n
0	25.265 ± 0.005	-	-
1	27.1875 ± 0.0025	1.9225 ± 0.0075	3.86 ± 0.05
2	27.6850 ± 0.001	0.4975 ± 0.0325	4.26 ± 0.08
3	27.8017 ± 0.0002	0.1167 ± 0.0012	4.66 ± 0.09
4	27.82675 ± 0.00005	0.02505 ± 0.00025	-
$\vdots$	$\vdots$	$\vdots$	$\vdots$
∞			$4.669201\ldots$

Bifurcation Diagram



D versus t for Increasing E



Discussion

- Models which include more physics have all challenges of present study as well as many more length scales; we are years away from accurate unsteady solutions with detailed kinetics, even for one dimension.
- Algorithm craftsmanship can clearly trump hardware improvements on certain problems.
- Reliance on hardware alone to achieve the gains described here would require many decades, even assuming the empirical Moore's Law continues to hold.