WENO Shock-Fitted Solution to 1-D Euler Equations with Reaction

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Introduction

- Euler equations with reaction.
- Simple two species irreversible exothermic reaction.
- High order numerical method to resolve behavior.
- Shock fitting to maintain order in presence of discontinuity.
- ZND structure for f=1.8 and 1.6.

Review

- Fickett and Davis, *Detonation: Theory and Experiment*, 1979.
- LeVeque, *Numerical Methods for Cons. Laws*, 1992
- Osher and Fedkiw, *L.S.M. Dyn. Imp. Surfaces*, 2003
- Jiang and Shu, *J. Comp. Phys.*, 1996
- Short and Sharpe - 1D linear stability results
- Bdzil - Shock Change Equation

Numerical Difficulties

- PDE versus conservation at the shock.
- Shock capturing - oscillations.
- Shock tracking - evolution of shock location on fixed grid.
- Shock fitting - numerical grid aligned with shock locus.

Governing Equations in 1-D

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0$$

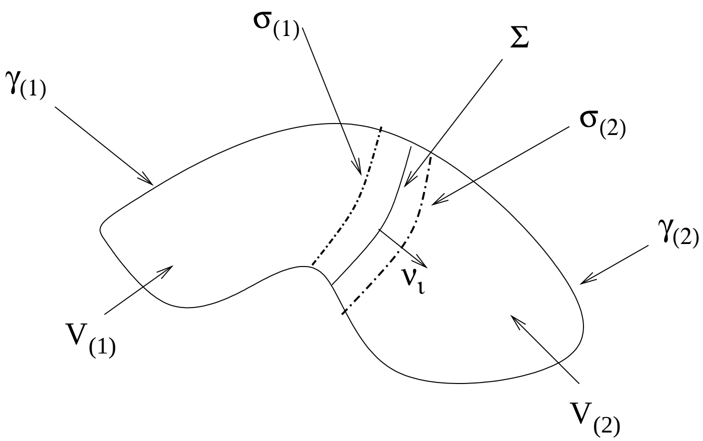
$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) = 0$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(u(\rho\left(e + \frac{u^2}{2}\right) + p)\right) = 0$$

$$\frac{\partial}{\partial t}(\rho\lambda) + \frac{\partial}{\partial x}(\rho\lambda u) = k\rho(1-\lambda)\exp\left(\frac{-E\rho}{p}\right)$$

$$p = \rho R T \quad e = \tfrac{1}{\gamma-1} p/\rho - \lambda q$$

Jump Conditions



Governing PDE's do not hold over a discontinuity - must appeal to integral formulation.

$$\frac{d}{dt}\int_{M\cancel{V}} F\,d\cancel{V} = \underbrace{\int_{M\cancel{V}} B\,d\cancel{V}}_{\text{volume forces}} + \underbrace{\int_{MS} T_i n_i\,dS}_{\text{surface forces}}$$

$$[\![F(D_i - v_i) + T_i]\!] = 0$$

$$[\![\rho(D-u)]\!] = 0$$

$$[\![\rho u(D-u) - p]\!] = 0$$

$$[\![\rho\left(e + \frac{u^2}{2}\right)(D-u) - up]\!] = 0$$

$$[\![\rho\lambda(D-u)]\!] = 0$$

This gives $\rho(D)$, $u(D)$, $p(D)$, $\lambda(D)$ given the quiescent state.

Wave Frame Transformation

$$\left.\begin{aligned}\bar{x}(x,t) &= x - s(t) \qquad -\infty < x < +\infty \\ \bar{t}(x,t) &= t \qquad\qquad\qquad \text{all } x \text{ and } t,\end{aligned}\right\}\qquad \begin{aligned}\frac{\partial f}{\partial t} &= \frac{\partial \bar{f}}{\partial \bar{x}}\frac{\partial \bar{x}}{\partial t} + \frac{\partial \bar{f}}{\partial \bar{t}}\frac{\partial \bar{t}}{\partial t} \\ &= \frac{\partial \bar{f}}{\partial \bar{x}}(-\dot{s}(t)) + \frac{\partial \bar{f}}{\partial \bar{t}} \\ &= -D\frac{\partial \bar{f}}{\partial \bar{x}} + \frac{\partial \bar{f}}{\partial \bar{t}} \\ \frac{\partial f}{\partial x} &= \frac{\partial \bar{f}}{\partial \bar{x}}\frac{\partial \bar{x}}{\partial x} + \frac{\partial \bar{f}}{\partial \bar{t}}\frac{\partial \bar{t}}{\partial x} \\ &= \frac{\partial \bar{f}}{\partial \bar{x}}\end{aligned}$$

$$\frac{\partial \rho}{\partial \bar{t}} + \frac{\partial}{\partial \bar{x}}\left(\rho u - D\rho\right) = 0$$

$$\frac{\partial}{\partial \bar{t}}\left(\rho u\right) + \frac{\partial}{\partial \bar{x}}\left(\rho u^2 + p - D\rho u\right) = 0$$

$$\frac{\partial}{\partial \bar{t}}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial \bar{x}}\left(u\left(\rho\left(e + \frac{u^2}{2}\right) + p\right) - D\rho\left(e + \frac{u^2}{2}\right)\right) = 0$$

$$\frac{\partial}{\partial \bar{t}}\left(\rho\lambda\right) + \frac{\partial}{\partial \bar{x}}\left(\rho\lambda u - D\rho\lambda\right) = M\dot{\omega}$$

Shock Change Equation

At the shock, $\rho u = f(D)$ according to the jump conditions.

$$\begin{aligned} \frac{d}{dt}(\rho u)\Big|_{x=s} &= \frac{dD}{dt}\ \frac{d}{dD}(\rho u)\Big|_{x=s} \\ &= \frac{\partial}{\partial t}(\rho u)\Big|_{x=s} + D\ \frac{\partial}{\partial x}(\rho u)\Big|_{x=s} . \end{aligned}$$

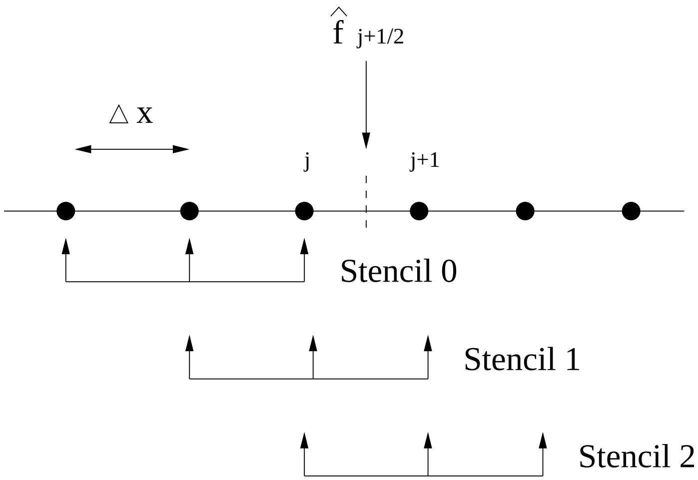
Also the momentum equation gives

$$\frac{\partial}{\partial t}(\rho u)\Bigg|_{x=s} = -\ \frac{\partial}{\partial x}(\rho u^2 + p)\Bigg|_{x=s} .$$

Combining the two gives

$$\frac{dD}{dt} = \left(\frac{d}{dD}(\rho u)\right)^{-1} \left(\frac{\partial}{\partial x}\left(D\rho u - \rho u^2 - p\right)\right)\Bigg|_{x=s} .$$

Numerics: WENO5 Mapped



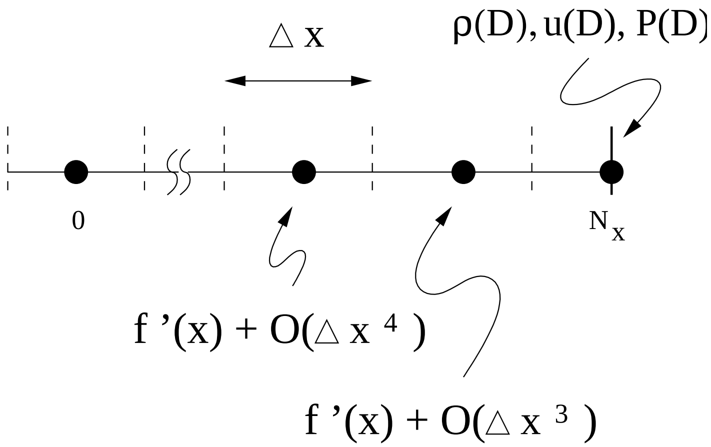
$$\left.\frac{df}{dx}\right|_{x_j} = \frac{\hat{f}_{j+1/2} - \hat{f}_{j-1/2}}{\Delta x}$$ and

$$\hat{f}_{j\pm 1/2} = \sum_{k=0}^{2} \omega_k^{(M)} \hat{f}^k_{j\pm 1/2},$$

where $\omega_k^{(M)}$ approximates the ideal weights to high order in smooth region of the flow.

- Conservative numerical scheme.
- Fifth order even near critical points of order one.
- Points near shock must still be considered.

Numerics: Boundary Points



- Third and fourth order one-sided derivatives at boundary points.
- Spatial order of the scheme is at best third order globally.

- At the shock, conserved variables are functions of D and the quiescent state.
- $\frac{\partial}{\partial x}$ at $x = s$ for shock change equation calculated to third order.

Numerics: Lax-Friedrichs Flux

To properly discretize this system which involves both left and right traveling waves, use the Local Lax-Friedrichs flux:

$$f^{\pm} = f \pm \alpha u \qquad \text{where} \qquad \alpha = |u - D| + c,$$

the maximum wave speed magnitude. The numerical flux $\hat{f}$ is then found using WENO5M for both the f^+ and f^- LLF:

$$\hat{f} = \frac{1}{2}(\hat{f}^+ + \hat{f}^-)$$

Numerics: Runge-Kutta Time Integration

Integration in time using third-order TVD Runge-Kutta:

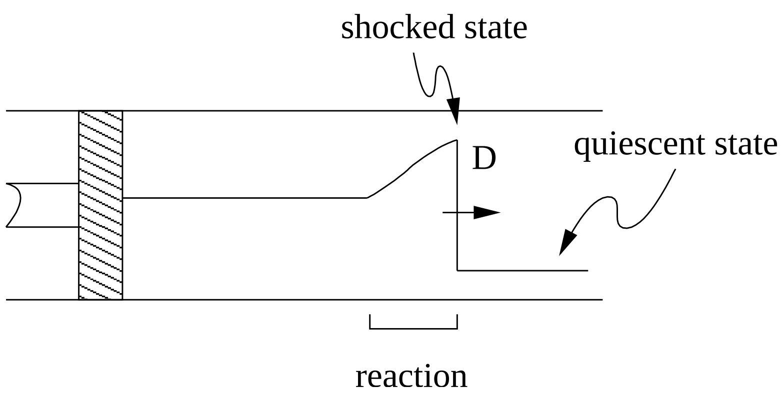
$$u^* = u^n + \Delta t \mathcal{L}(u^n),$$

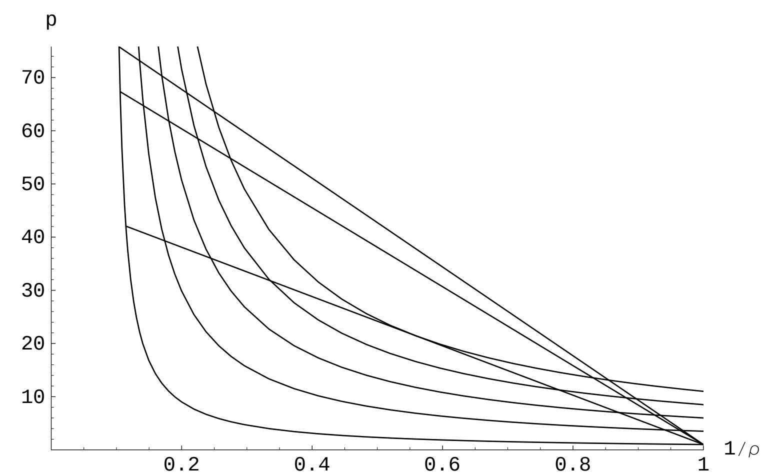
$$u^{**} = \frac{3}{4}u^n + \frac{1}{4}u^* + \frac{1}{4}\Delta t \mathcal{L}(u^*),$$

$$u^{n+1} = \frac{1}{3}u^n + \frac{2}{3}u^{**} + \frac{2}{3}\Delta t \mathcal{L}(u^{**}),$$

where $\mathcal{L} = -\frac{\hat{f}_{j+1/2} - \hat{f}_{j+1/2}}{\Delta x}$.

ZND Structure Problem

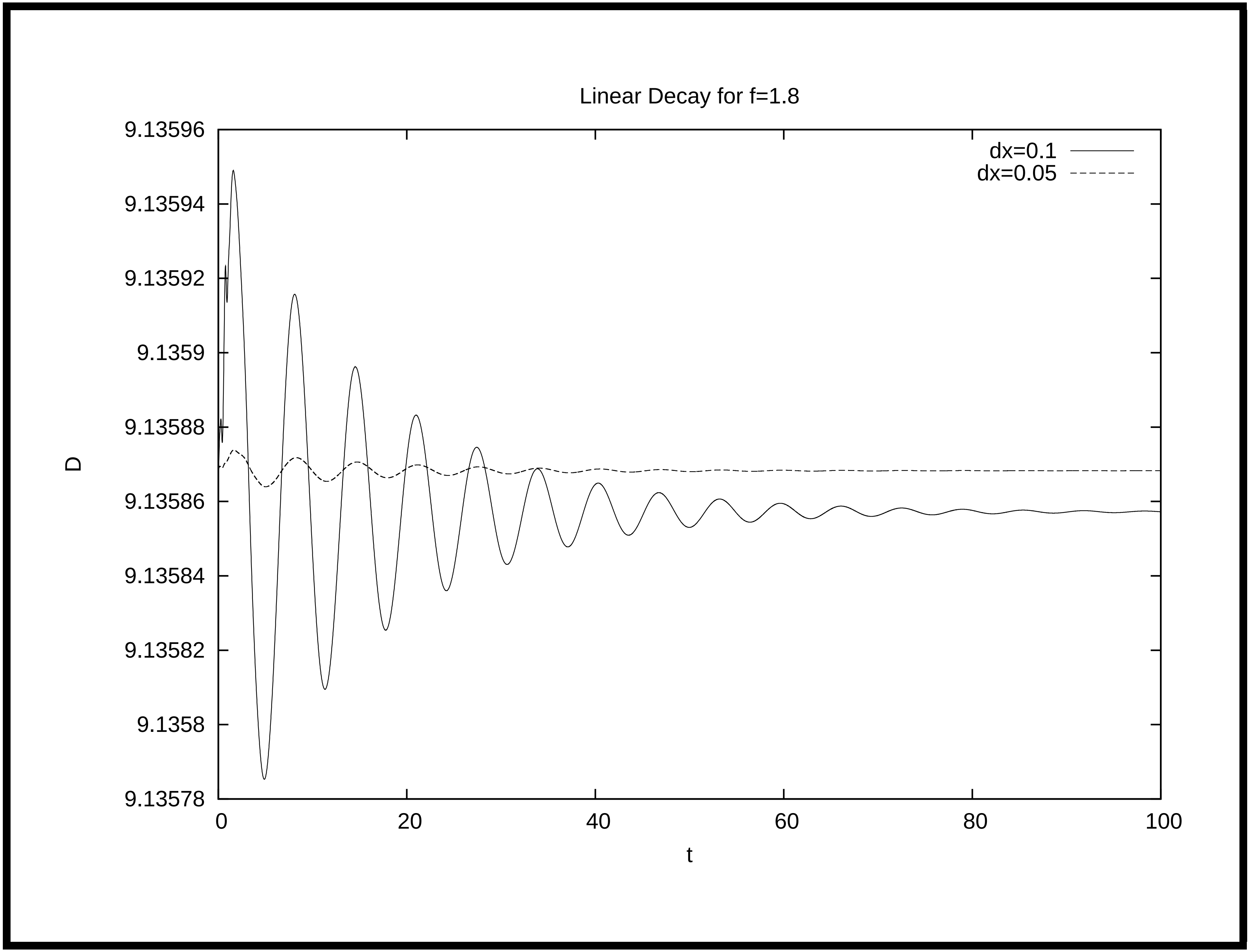


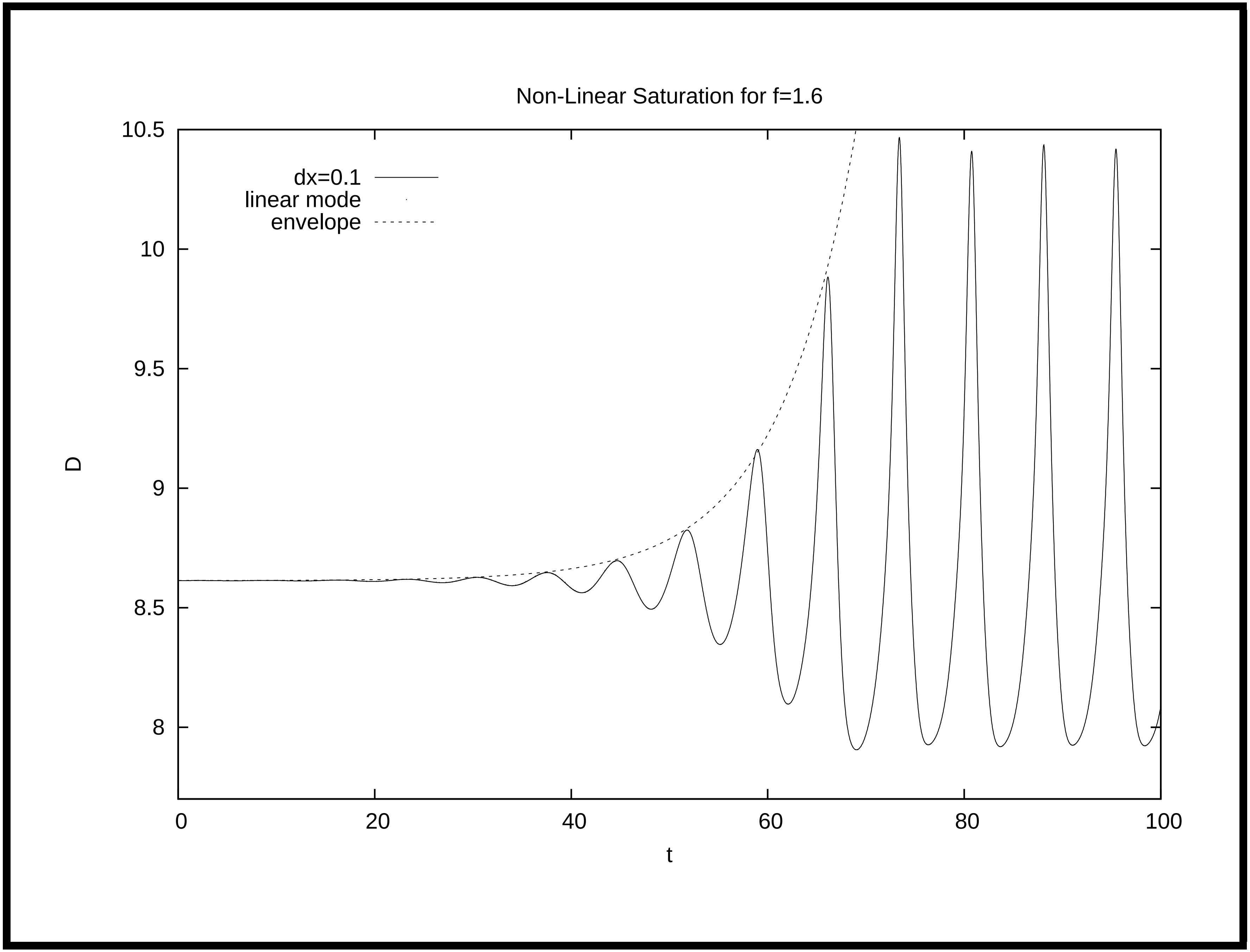


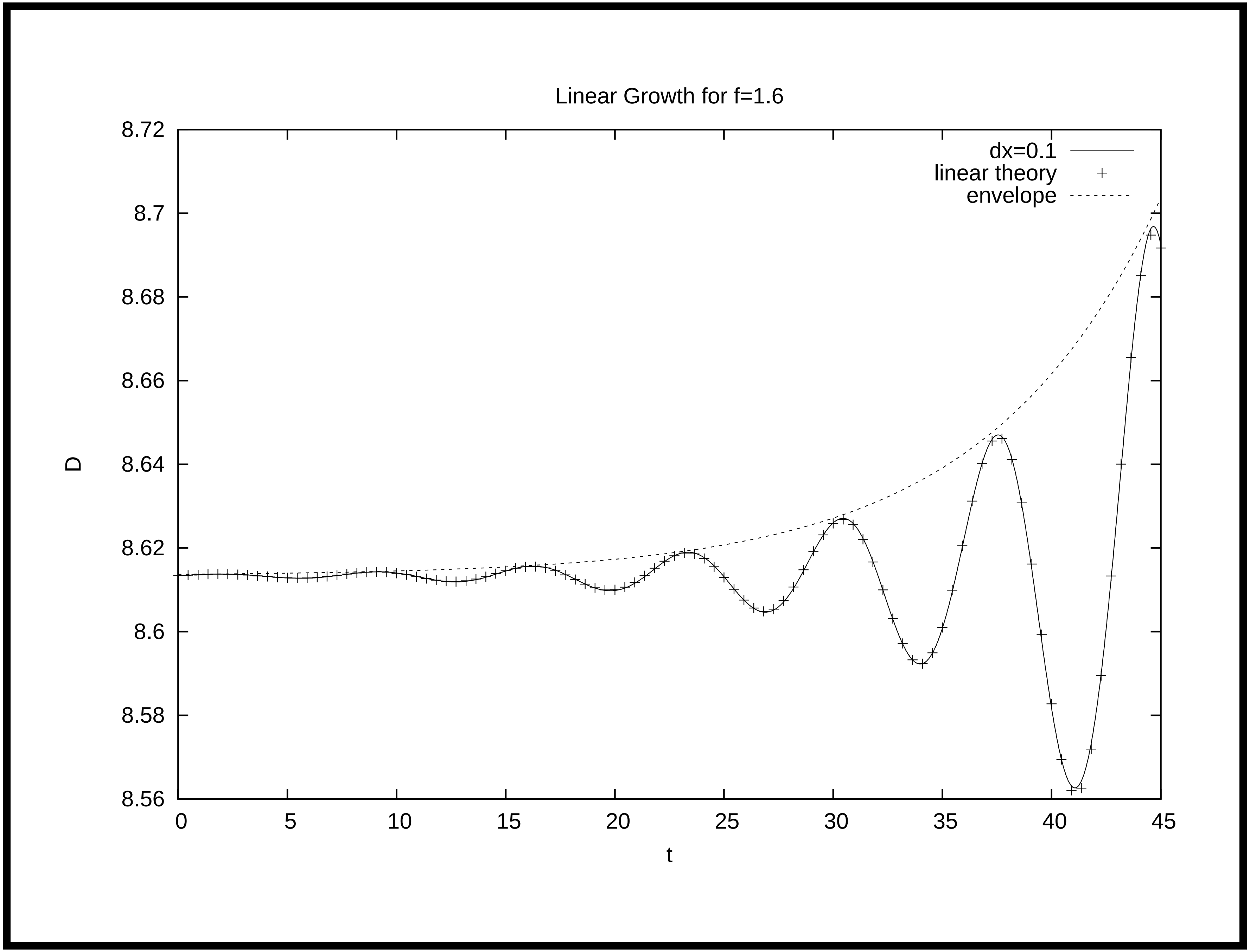
- parameters:

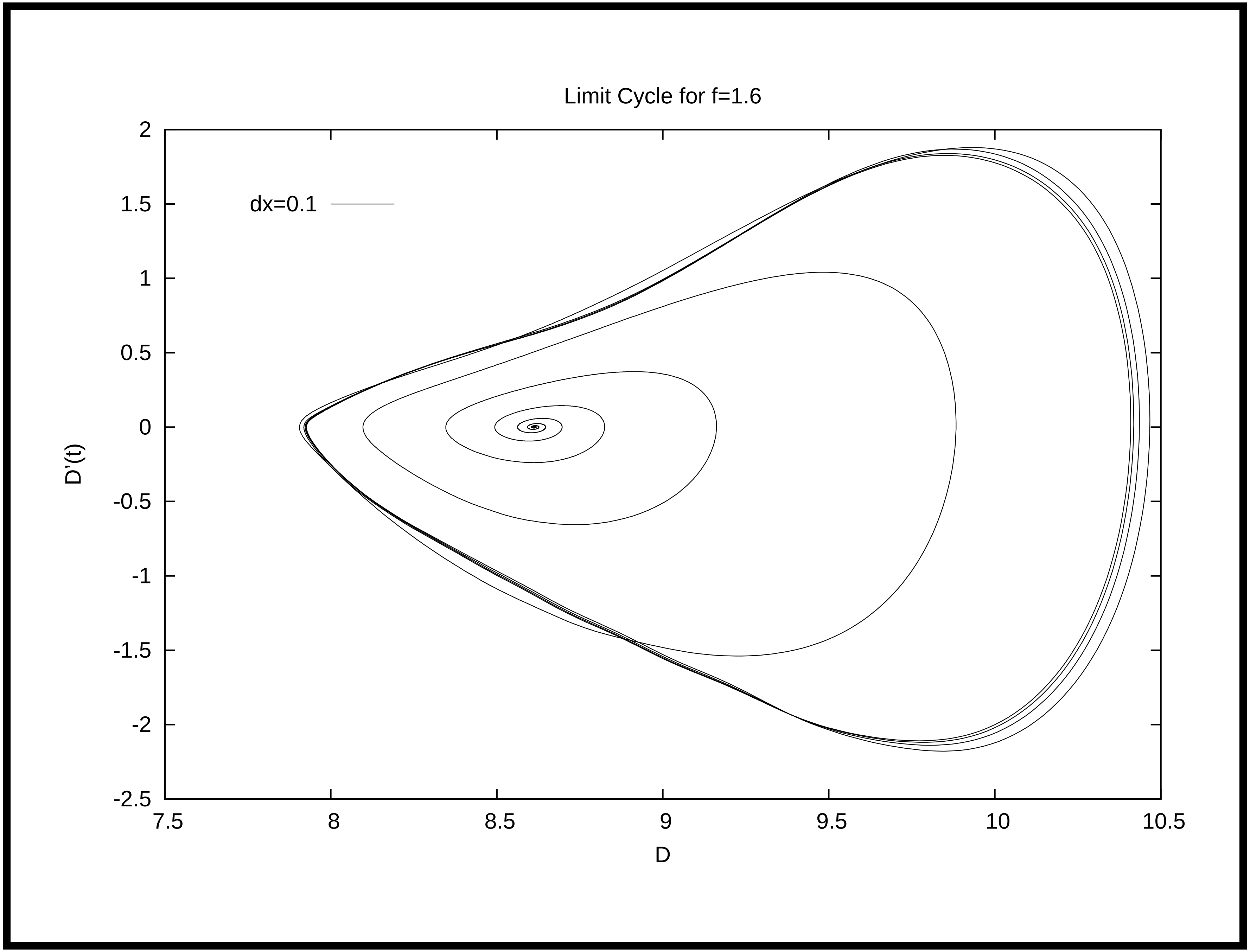
  $$E = 50, q = 50, \gamma = 1.2, D_{cj} = 6.80947$$

- quiescent state: $\rho = 1, u = 0, p = 1, \lambda = 0$
- consider $f = (D/D_{cj})^2 = 1.8$ and 1.6


Linear Decay for f=1.8
dx=0.1
dx=0.05
D
t
9.13596
9.13594
9.13592
9.1359
9.13588
9.13586
9.13584
9.13582
9.1358
9.13578
0
20
40
60
80
100


Non-Linear Saturation for f=1.6
dx=0.1
linear mode
envelope
D
t
10.5
10
9.5
9
8.5
8
0
20
40
60
80
100


Linear Growth for f=1.6
dx=0.1
linear theory
envelope
D
t
8.72
8.7
8.68
8.66
8.64
8.62
8.6
8.58
8.56
0
5
10
15
20
25
30
35
40
45



Limit Cycle for f=1.6
dx=0.1
D'(t)
D
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
7.5
8
8.5
9
9.5
10
10.5

Conclusions

- Shock fitting allows for highly accurate solutions containing a discontinuity.
- Validation of unstable mode for ZND problem from linear theory.
- Explicit stability bounds and convergence study presently lacking.
- 2-D extension needed for future work.