Shock-Fitted Numerical Solutions for Two-Dimensional Detonations

with Periodic Boundary Conditions

Andrew Henrick, Tariq D. Aslam, Joseph M. Powers

11^{th} SIAM International Conference on Numerical Combustion

Granada, Spain

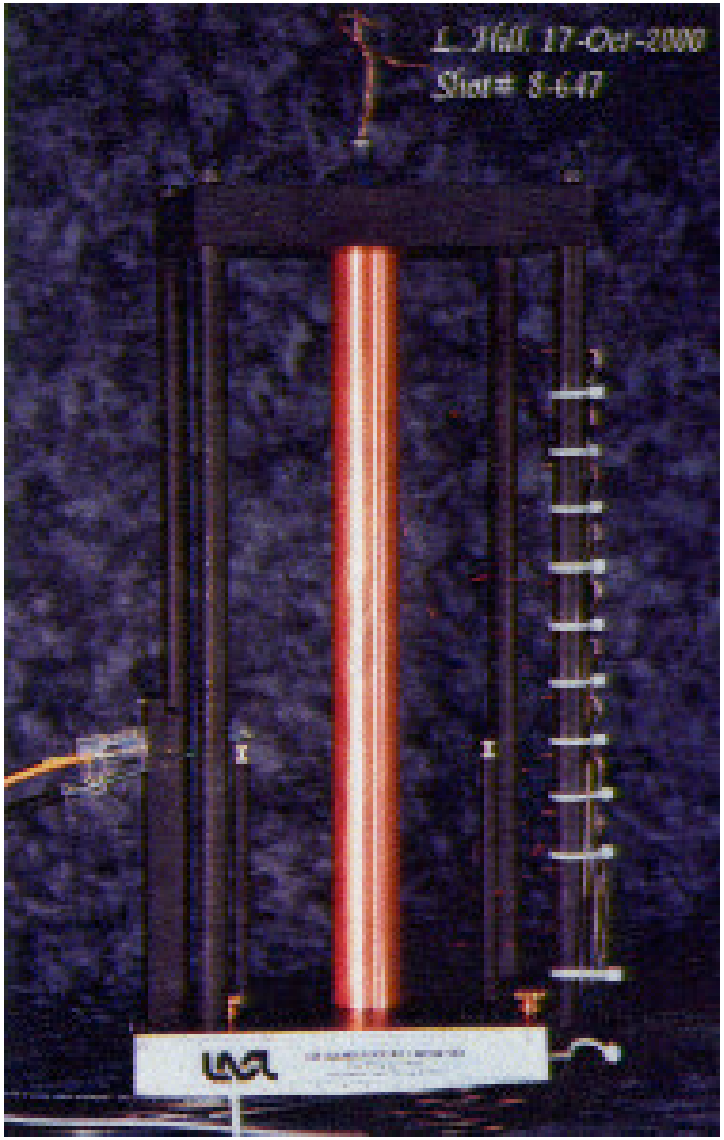
Los Alamos National Laboratory

University of Notre Dame

April 23, 2006

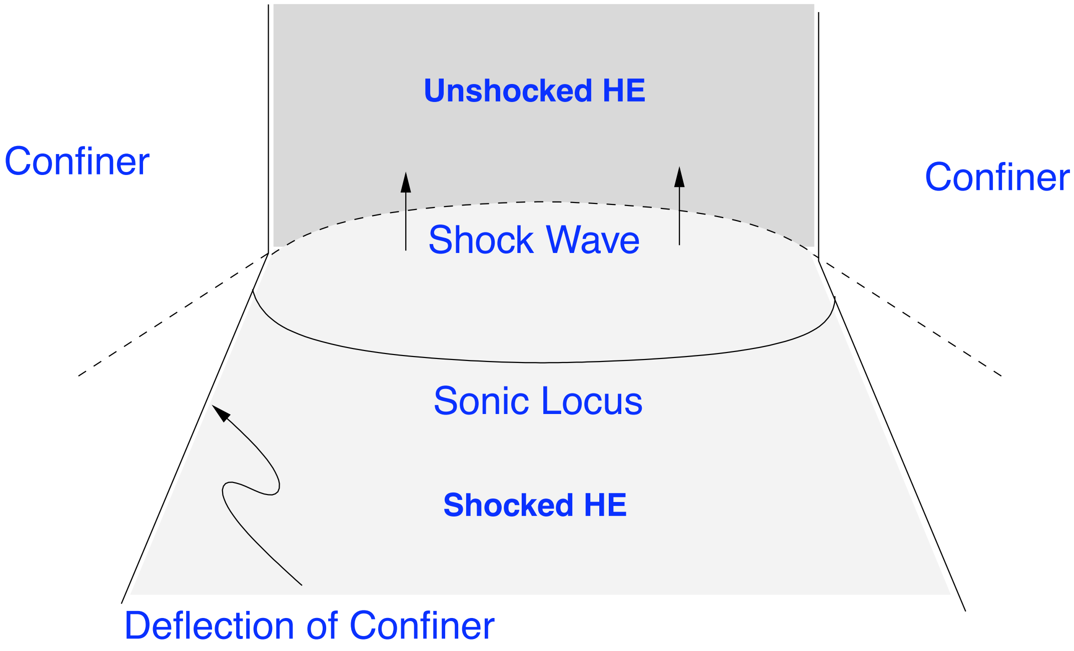
Presentation Outline

- Introduction
- Motivation & Background
- General Formulation
  - Shock-Fitted Transformation
  - Numerical Method
- 1-D Limiting Case
  - Comparison with Linear Stability Theory
  - Pulsating Detonation
- 2-D Results



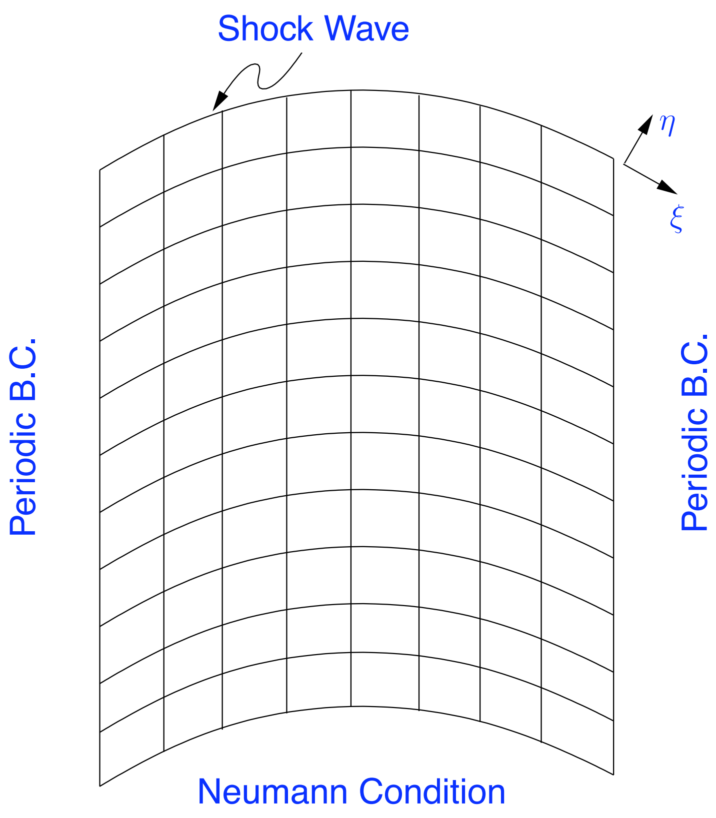
Background

- 2-D shock geometry
- 2-D Euler equations with reaction
- 2 species chemical kinetics
- Calorically perfect ideal gas mixture
- High-order convergence



Background

- 2-D shock geometry
- 2-D Euler equations with reaction
- 2 species chemical kinetics
- Calorically perfect ideal gas mixture
- High-order convergence



Background

- 2-D shock geometry
- 2-D Euler equations with reaction
- 2 species chemical kinetics
- Calorically perfect ideal gas mixture
- High-order convergence

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

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) + \frac{\partial}{\partial y}(\rho u v) = 0,$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v u) + \frac{\partial}{\partial y}(\rho v^2 + p) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{1}{2}(u^2 + v^2)\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{1}{2}(u^2 + v^2) + \frac{p}{\rho}\right)\right) + \frac{\partial}{\partial y}\left(\rho v\left(e + \frac{1}{2}(u^2 + v^2) + \frac{p}{\rho}\right)\right) = 0.$$

Background

- 2-D shock geometry
- 2-D Euler equations with reaction
- 2 species chemical kinetics
- Calorically perfect ideal gas mixture
- High-order convergence

$$A \rightarrow B$$

Let λ denote mass fraction of B

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

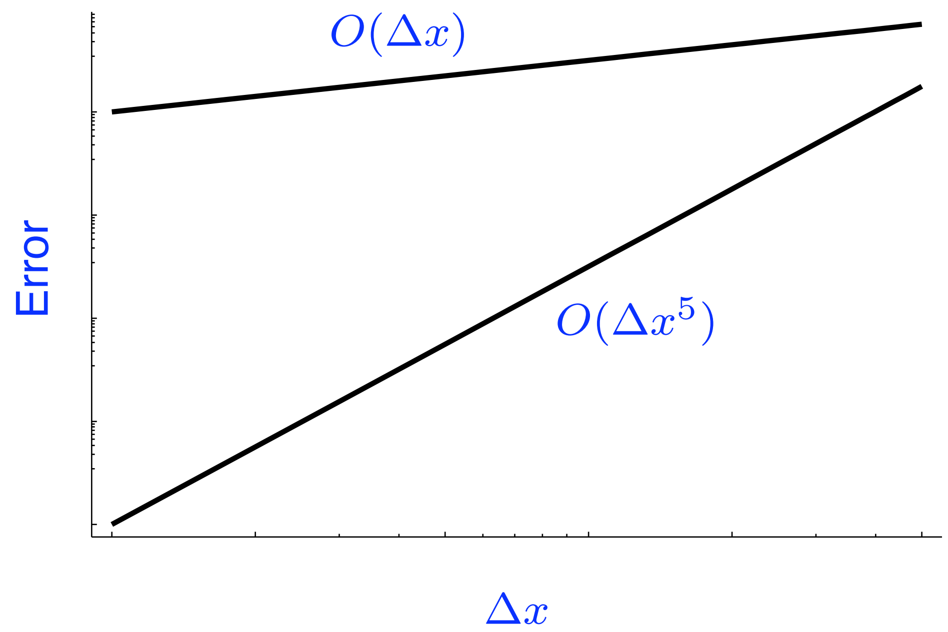
Background

- 2-D shock geometry
- 2-D Euler equations with reaction
- 2 species chemical kinetics
- Calorically perfect ideal gas mixture
- High-order convergence

$$e = \frac{1}{\gamma - 1}\frac{p}{\rho} - q\lambda$$

Background

- 2-D shock geometry
- 2-D Euler equations with reaction
- 2 species chemical kinetics
- Calorically perfect ideal gas mixture
- High-order convergence



Motivation

What are the state-of-the-art numerical techniques used for discontinuous problems?

- Shock capturing
  - Robust
  - Numerical viscosity reduces convergence to $O(\Delta x)$
- Shock tracking
  - Robust
  - Description of discontinuous motion varies
  - Converges at $O(\Delta x)$

Motivation

Accuracy loss due to differentiation across discontinuities. High order convergence can be achieved through shock-fitting

- Governing equations are posed in fitted coordinates
- Solution is smooth within each domain
- Analytic jump conditions used to compute shock speed
- Restricted to embedded shocks

Motivation

Accuracy loss due to differentiation across discontinuities. High order convergence can be achieved through shock-fitting

- Governing equations are posed in fitted coordinates
  - Shock location is fixed
- Solution is smooth within each domain
- Analytic jump conditions used to compute shock speed
- Restricted to embedded shocks

Motivation

Accuracy loss due to differentiation across discontinuities. High order convergence can be achieved through shock-fitting

- Governing equations are posed in fitted coordinates
  - Shock location is fixed
- Solution is smooth within each domain
  - Regular finite differencing is adequate
- Analytic jump conditions used to compute shock speed
- Restricted to embedded shocks

Shock-Fit Transformation

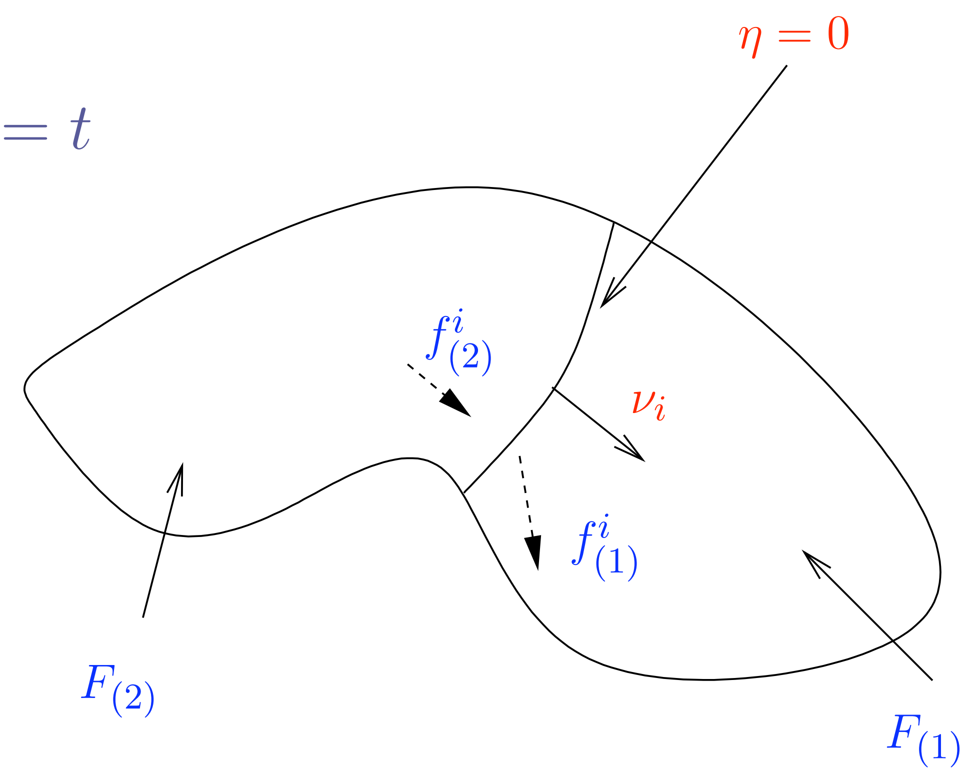
Consider transform

$$\xi = \xi(x, y, t), \quad \eta = \eta(x, y, t), \quad \tau = t$$

applied to

$$\frac{\partial F}{\partial t} + \frac{\partial f^i}{\partial y^i} = B \qquad D_n = \frac{[\![f^i]\!]}{[\![F]\!]}\nu_i$$

where only derivatives are transformed.



Shock-Fit Transformation

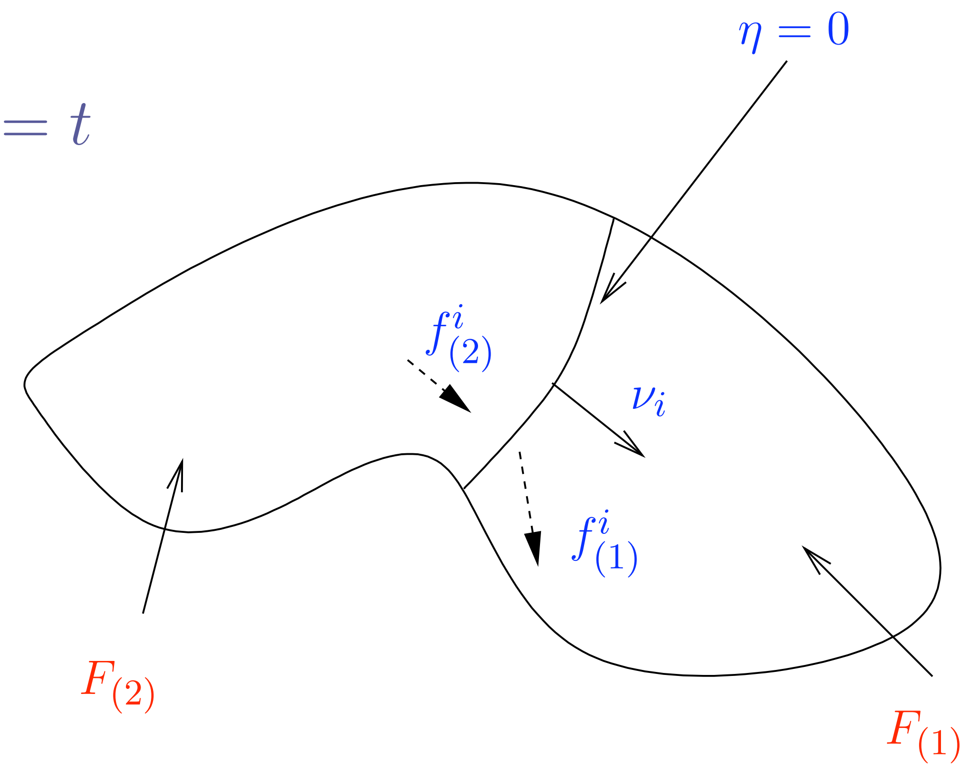
Consider transform

$$\xi = \xi(x, y, t), \quad \eta = \eta(x, y, t), \quad \tau = t$$

applied to

$$\frac{\partial F}{\partial t} + \frac{\partial f^i}{\partial y^i} = B \quad D_n = \frac{[\![f^i]\!]}{[\![F]\!]} \nu_i$$

where only derivatives are transformed.



Shock-Fit Transformation

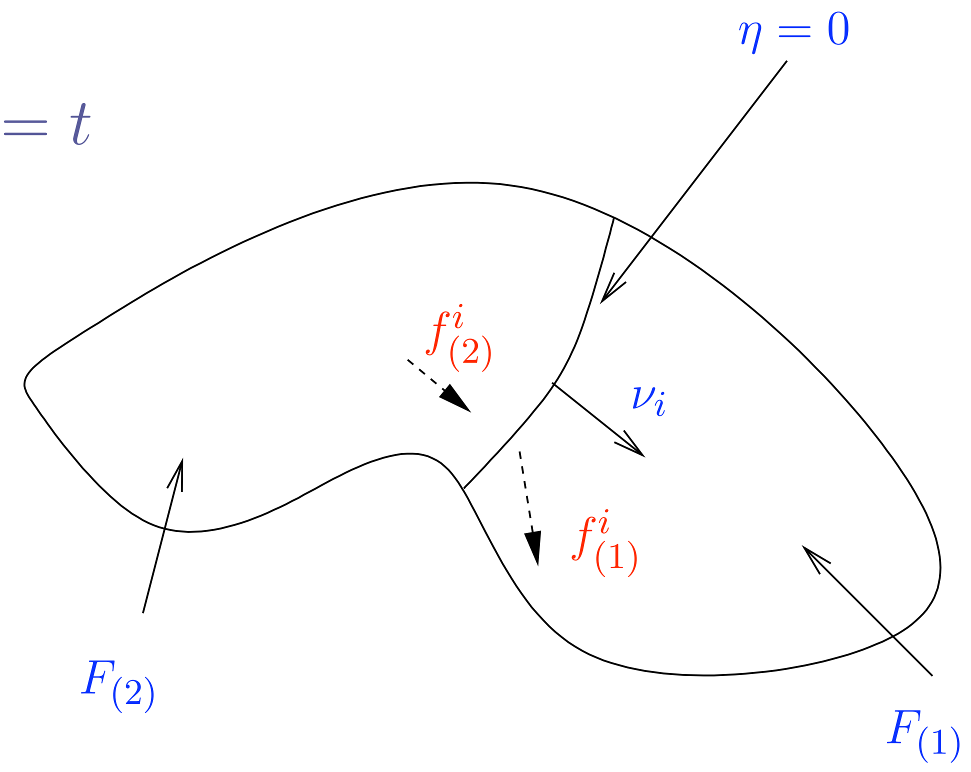
Consider transform

$$\xi = \xi(x, y, t), \quad \eta = \eta(x, y, t), \quad \tau = t$$

applied to

$$\frac{\partial F}{\partial t} + \frac{\partial f^i}{\partial y^i} = B \quad D_n = \frac{[\![f^i]\!]}{[\![F]\!]}\nu_i$$

where only derivatives are transformed.



Shock-Fit Transformation

Consider transform

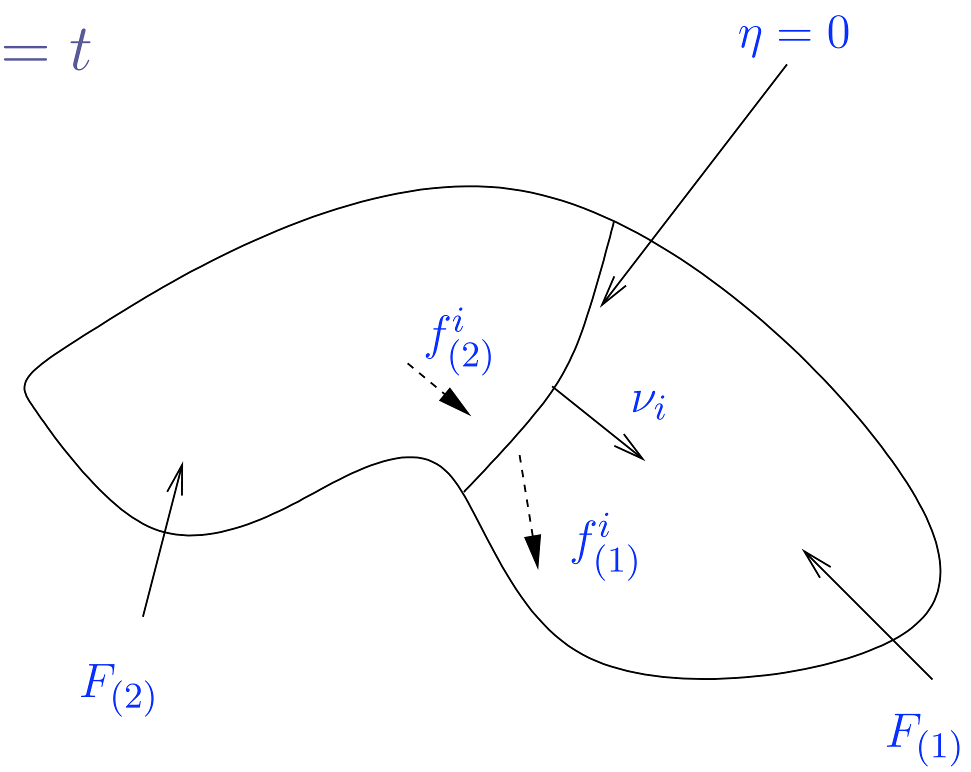
$$\xi = \xi(x, y, t), \quad \eta = \eta(x, y, t), \quad \tau = t$$

applied to

$$\frac{\partial F}{\partial t} + \frac{\partial f^i}{\partial y^i} = B \quad D_n = \frac{[\![f^i]\!]}{[\![F]\!]} \nu_i$$

where only derivatives are transformed.

- x and y momentum are still solved



Transformed Equations

The resulting fitted equations are

$$\frac{\partial}{\partial \tau}\left(\sqrt{g}F\right) + \frac{\partial}{\partial \eta^j}\left(\sqrt{g}F\frac{\partial \eta^j}{\partial t} + \sqrt{g}f^i\frac{\partial \eta^j}{\partial y^i}\right) = \sqrt{g}B$$

- Conservation form with proper shock speed

$$\bar{D}_n = \frac{\left[\!\left[\sqrt{g}F\frac{\partial \eta^j}{\partial t} + \sqrt{g}f^i\frac{\partial \eta^j}{\partial y^i}\right]\!\right]}{\left[\!\left[\sqrt{g}F\right]\!\right]}\bar{\nu}_j$$

- $\sqrt{g} = \left|\left|\frac{\partial y}{\partial \eta}\right|\right|$ is the determinant of the metric tensor
- $-\frac{\partial \eta^i}{\partial t} = \frac{\partial \eta^i}{\partial y^j}\frac{\partial y^j}{\partial \tau} \rightarrow \bar{U}^i = \frac{\partial \eta^i}{\partial y^j}U^j$

Formulation: Conserved Quantities

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

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) + \frac{\partial}{\partial y}(\rho u v) = 0,$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v u) + \frac{\partial}{\partial y}(\rho v^2 + p) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{1}{2}(u^2 + v^2)\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{1}{2}(u^2 + v^2) + \frac{p}{\rho}\right)\right) + \frac{\partial}{\partial y}\left(\rho v\left(e + \frac{1}{2}(u^2 + v^2) + \frac{p}{\rho}\right)\right) = 0,$$

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

$$e = \frac{1}{\gamma - 1}\frac{p}{\rho} - q\lambda.$$

$$\begin{pmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \end{pmatrix} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho\left(e + \frac{1}{2}(u^2 + v^2)\right) \\ \rho\lambda \end{pmatrix}$$

Formulation: Shock-Fitted Eqns.

$$\frac{\partial}{\partial \tau}\begin{bmatrix}F_1'\\F_2'\\F_3'\\F_4'\\F_5'\end{bmatrix} + \frac{\partial}{\partial \xi}\left(\frac{\partial \xi}{\partial t}\begin{bmatrix}F_1'\\F_2'\\F_3'\\F_4'\\F_5'\end{bmatrix} + \frac{1}{\sqrt{g}}\frac{\partial y}{\partial \eta}\begin{bmatrix}F_2'\\ \frac{F_2'^2}{F_1'}+\sqrt{g}p\\ \frac{F_2'F_3'}{F_1'}\\ \frac{F_2'F_4'}{F_1'}+\sqrt{g}\frac{F_2'}{F_1'}p\\ \frac{F_2'F_5'}{F_1'}\end{bmatrix} - \frac{1}{\sqrt{g}}\frac{\partial x}{\partial \eta}\begin{bmatrix}F_3'\\ \frac{F_2'F_3'}{F_1'}\\ \frac{F_3'^2}{F_1'}+\sqrt{g}p\\ \frac{F_3'F_4'}{F_1'}+\sqrt{g}\frac{F_3'}{F_1'}p\\ \frac{F_3'F_5'}{F_1'}\end{bmatrix}\right)$$

$$+\frac{\partial}{\partial \eta}\left(\frac{\partial \eta}{\partial t}\begin{bmatrix}F_1'\\F_2'\\F_3'\\F_4'\\F_5'\end{bmatrix} - \frac{1}{\sqrt{g}}\frac{\partial y}{\partial \xi}\begin{bmatrix}F_2'\\ \frac{F_2'^2}{F_1'}+\sqrt{g}p\\ \frac{F_2'F_3'}{F_1'}\\ \frac{F_2'F_4'}{F_1'}+\sqrt{g}\frac{F_2'}{F_1'}p\\ \frac{F_2'F_5'}{F_1'}\end{bmatrix} + \frac{1}{\sqrt{g}}\frac{\partial x}{\partial \xi}\begin{bmatrix}F_3'\\ \frac{F_2'F_3'}{F_1'}\\ \frac{F_3'^2}{F_1'}+\sqrt{g}p\\ \frac{F_3'F_4'}{F_1'}+\sqrt{g}\frac{F_3'}{F_1'}p\\ \frac{F_3'F_5'}{F_1'}\end{bmatrix}\right) = \begin{bmatrix}0\\0\\0\\0\\ \zeta\end{bmatrix}$$

$$p = \frac{(\gamma-1)}{\sqrt{g}}\left(F_4' - \frac{(F_2')^2+(F_3')^2}{2F_1'} + qF_5'\right), \quad \zeta = \frac{a}{\sqrt{g}}(F_1'-F_5')\exp\left(\frac{-EF_1'}{\sqrt{g}p}\right)$$

Formulation: Shock Change Eqn.

At the shock, $E = \rho(e + \frac{1}{2}(u^2 + v^2)) = f(D_n)$.

$$\frac{\partial D_n}{\partial \tau} = \left(\left. \frac{\partial E}{\partial D_n} \right|_{\mathcal{S}} \right)^{-1} \left. \frac{\partial E}{\partial \tau} \right|_{\mathcal{S}}$$

Formulation: Shock Change Eqn.

At the shock, $E = \rho(e + \frac{1}{2}(u^2 + v^2)) = f(D_n)$.

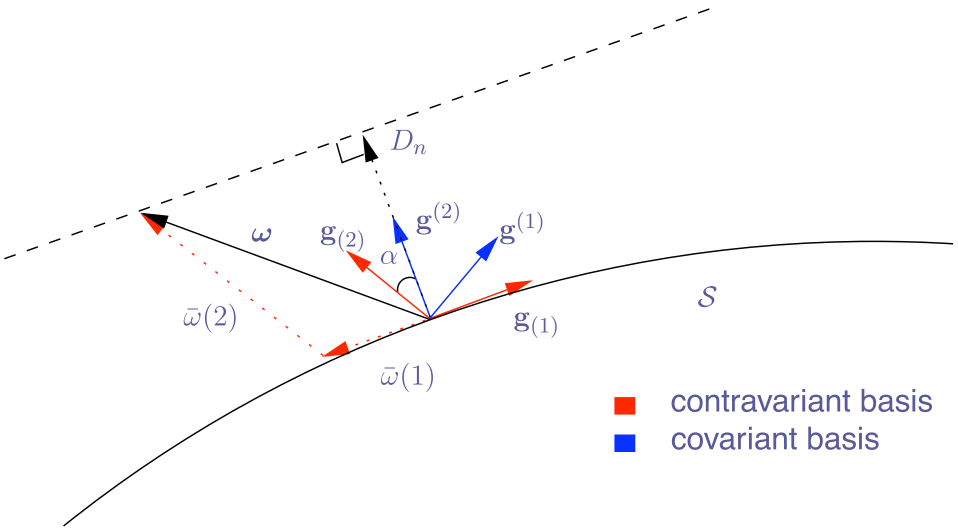
- $|\mathbf{v}| = v^i v_j = u^2 + v^2$ is invariant.

$$\frac{\partial D_n}{\partial \tau} = \left(\left. \frac{\partial E}{\partial D_n} \right|_{\mathcal{S}} \right)^{-1} \left. \frac{\partial E}{\partial \tau} \right|_{\mathcal{S}}$$

- $\left. \frac{\partial E}{\partial \tau} \right|_{\mathcal{S}}$ is already calculated in the flow field.

Thus system is closed.

Shock-Fitted Geometry



- $\mathrm{g}_{(i)}$ lie along fitted coords.
- $\mathrm{g}^{(i)}$ are reciprocal basis
- $\boldsymbol{\omega} = \mathrm{U}|_{\mathcal{S}}$ is the shock velocity

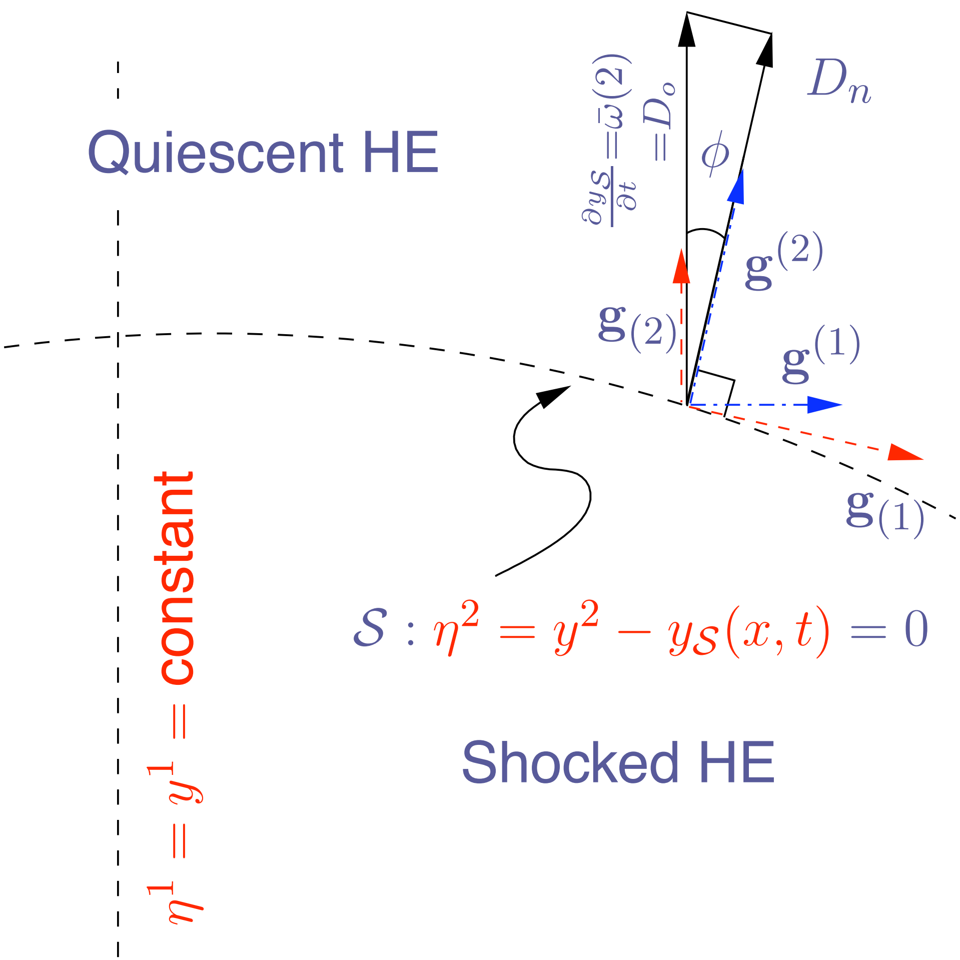
Since $\mathcal{S} : \eta^2 = 0$

- $\mathrm{g}_{(1)}$ is embedded in the shock
- $\mathrm{g}^{(2)} || \boldsymbol{\nu}$

Note that η^1 in general contributes artificial tangential shock velocity.

Thus, $D_n = \cos(\alpha)\omega(2) \leq |\boldsymbol{\omega}|$, in general.

Shock-Fitted Geometry: $x \equiv \xi$



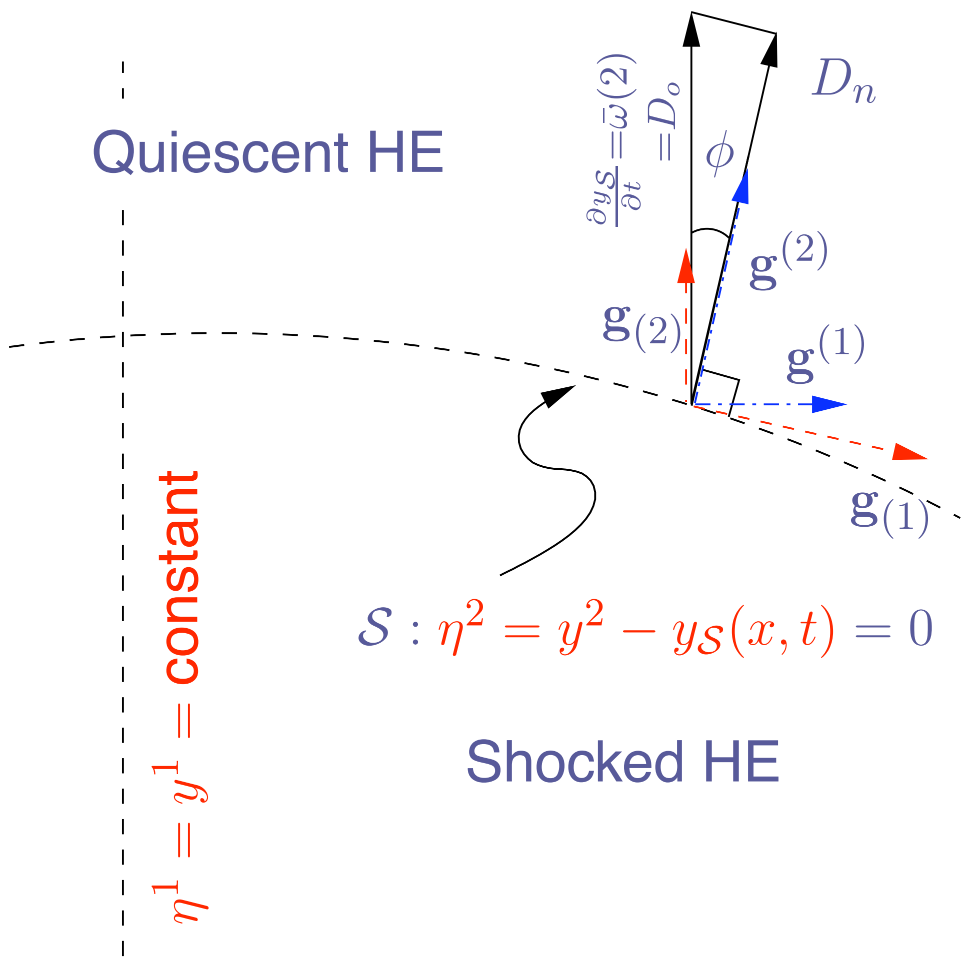
$$\mathbf{g}_{(1)} = \begin{pmatrix} 1 \\ \frac{\partial y_{\mathcal{S}}}{\partial \eta^1} \end{pmatrix}, \qquad \mathbf{g}_{(2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

$$\mathbf{g}^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \mathbf{g}^{(2)} = \begin{pmatrix} -\frac{\partial y_{\mathcal{S}}}{\partial y^1} \\ 1 \end{pmatrix},$$

and the grid velocity components are

$$\frac{\partial \xi}{\partial t} = 0 \qquad \frac{\partial \eta}{\partial t} = -\frac{\partial y_{\mathcal{S}}}{\partial t}$$

Shock-Fitted Geometry: $x \equiv \xi$



In this case

- $\sqrt{g} = 1$
- $\alpha = \phi$, the shock angle
- $D_o = \frac{\partial y_S}{\partial t} = D_n \sqrt{1 + \left(\frac{\partial y_S}{\partial y^1}\right)^2}$

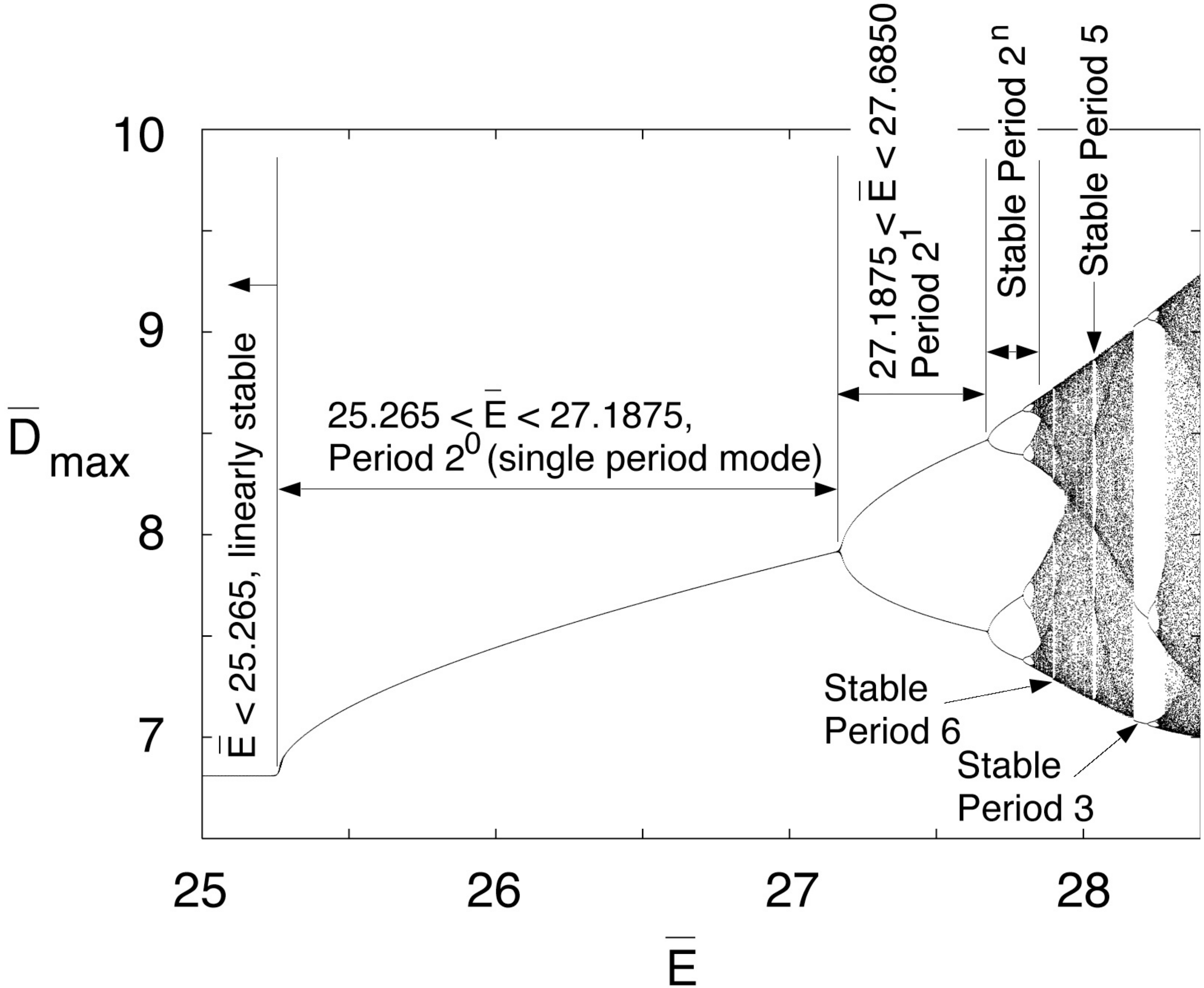
relating the phase speed, the shock surface, the normal shock speed, and the shock slope.

Numerical Method

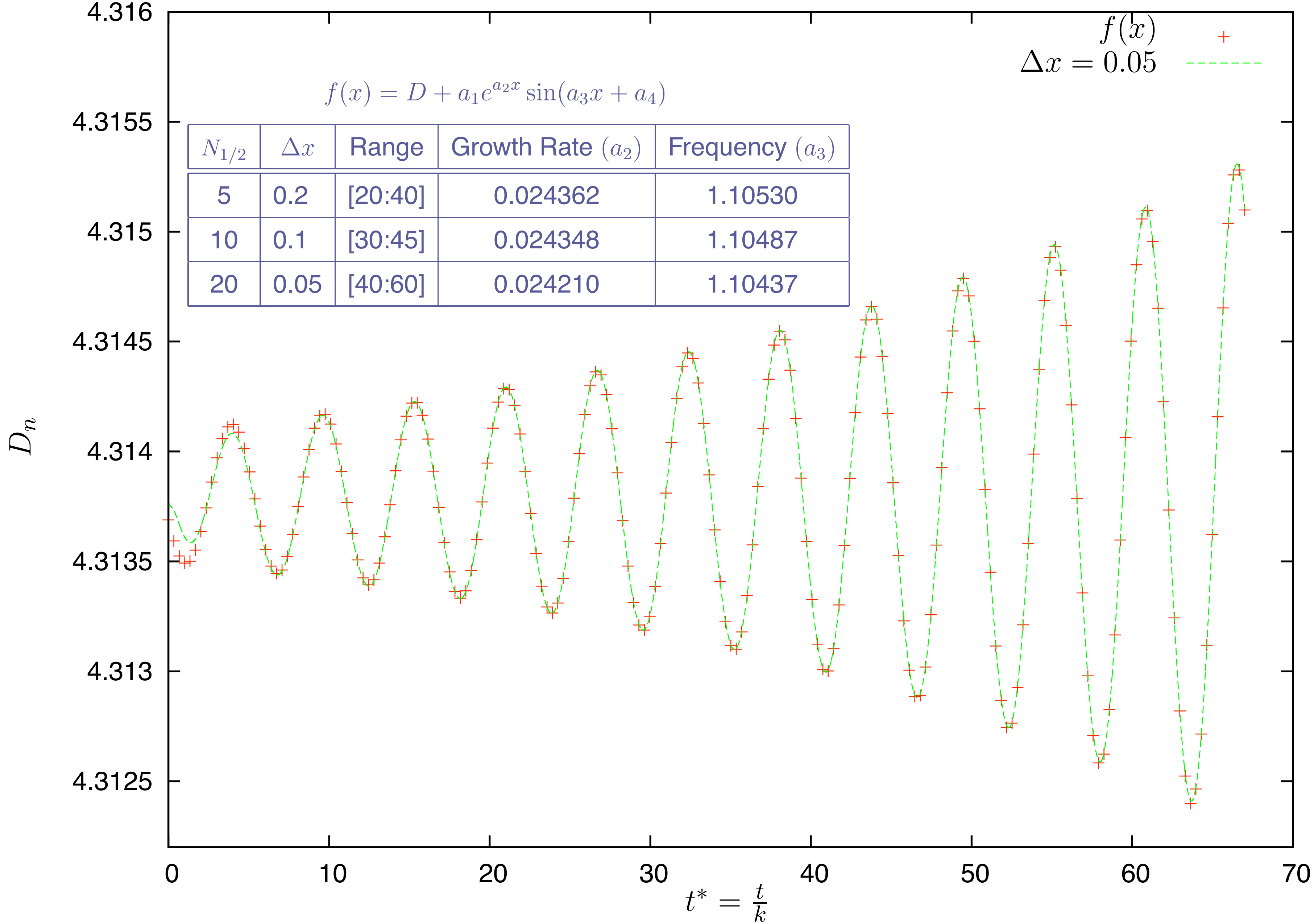
The method of lines is used to separate spatial and temporal integration

- $O(\Delta t^5)$ Runge-Kutta integration in time
- $O(\Delta x^5)$ or $O(\Delta y^5)$ WENO5M with Lax-Friedrich's flux splitting to differentiate in space
- At the shock
  - Rankine-Hugoniot jump conditions used directly
  - One-sided finite differencing used
  - Shock-change equation gives evolution of D_n

1-D Results: Pulsating Detonations



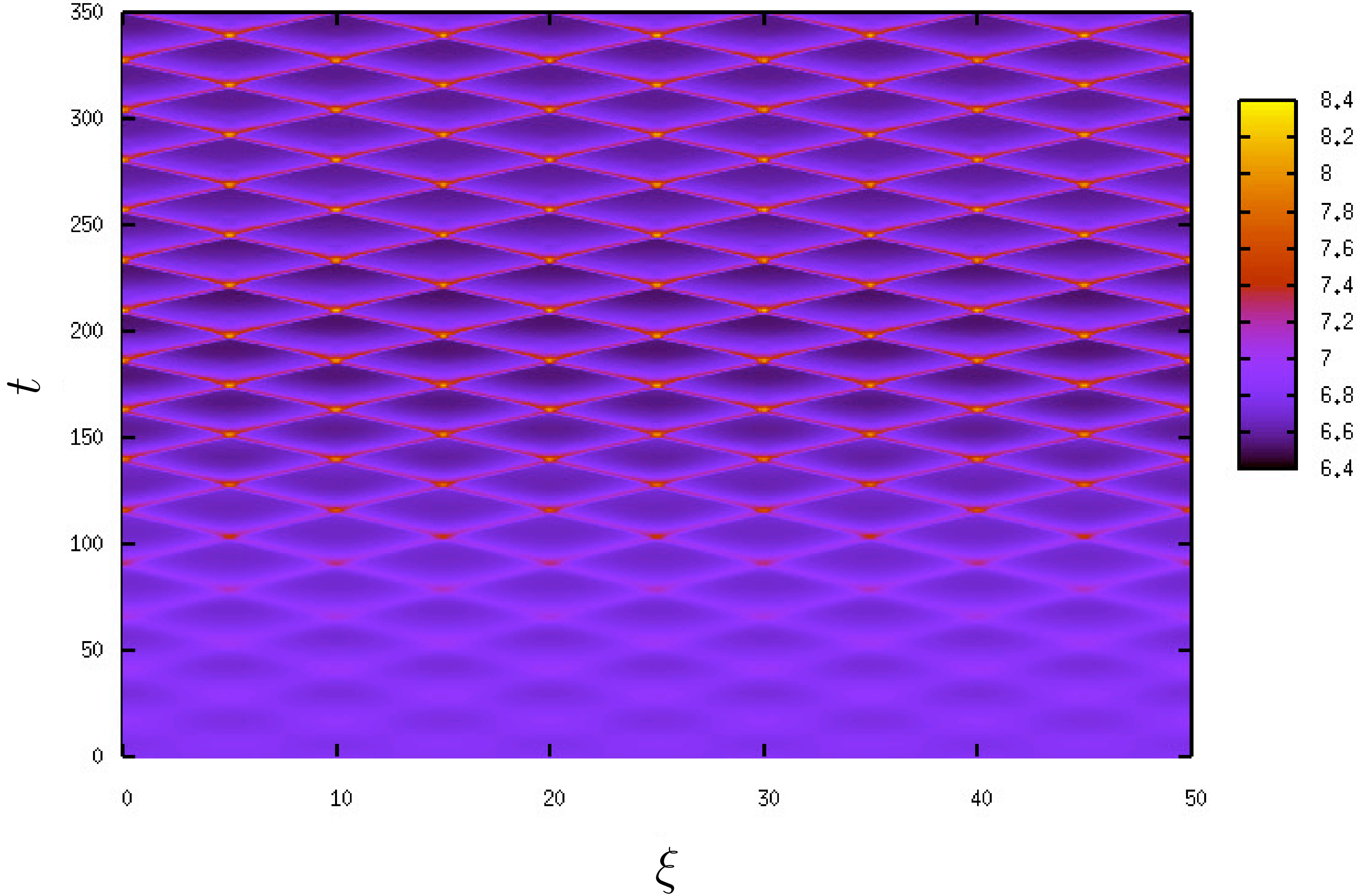
2-D Results: $E = 0, q = 15$



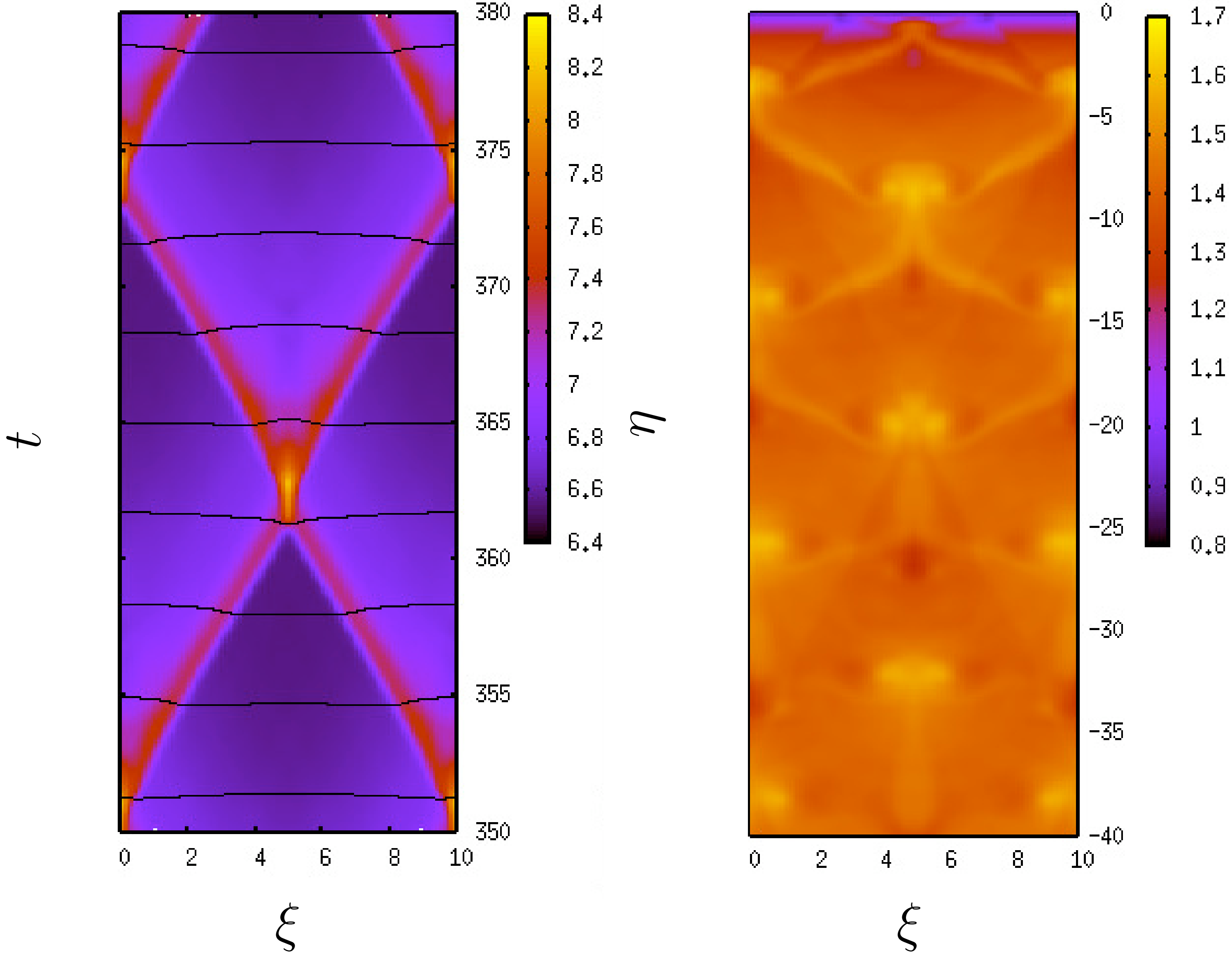
$$f(x) = D + a_1 e^{a_2 x} \sin(a_3 x + a_4)$$

$N_{1/2}$	Δx	Range	Growth Rate (a_2)	Frequency (a_3)
5	0.2	[20:40]	0.024362	1.10530
10	0.1	[30:45]	0.024348	1.10487
20	0.05	[40:60]	0.024210	1.10437

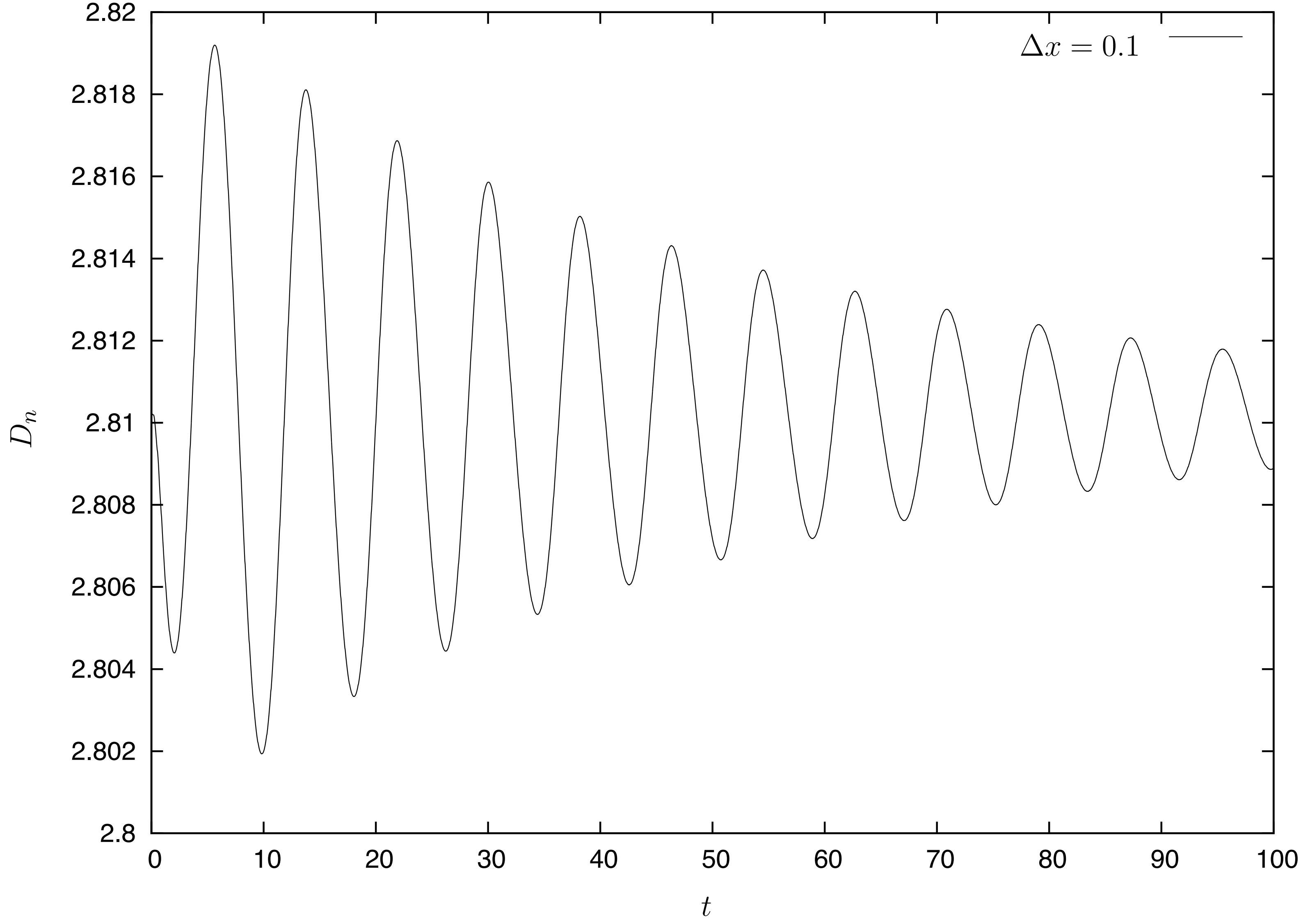
2-D Results: Detonation Cells



2-D Results: Detonation Cells



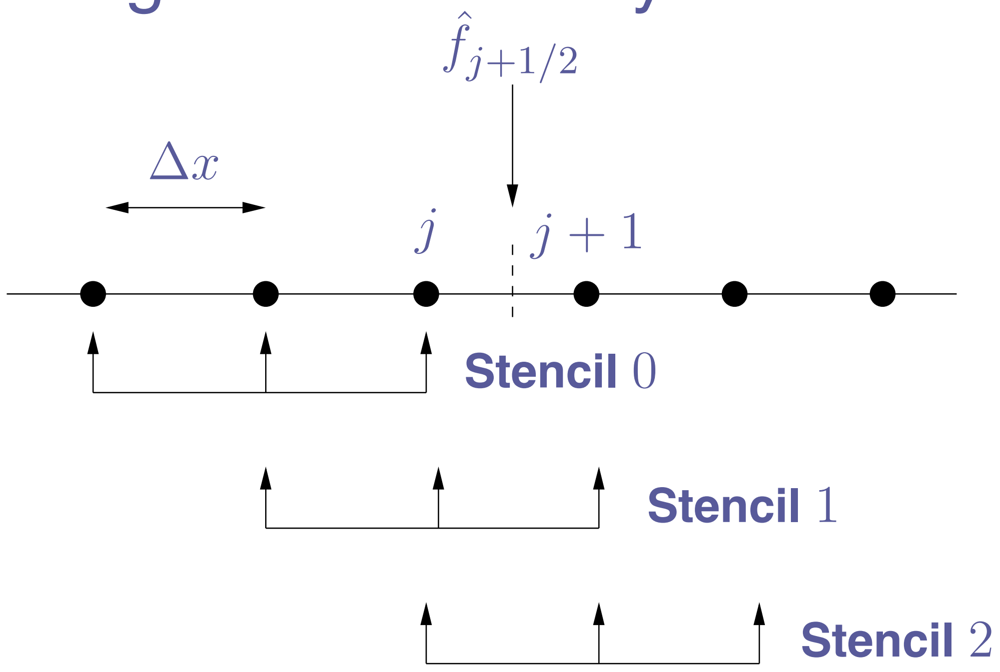
2-D Results: Linear Stability



Conclusions

- Need for highly resolved solutions to sandwich test
- Shock-fitting is a viable high order solution technique for problems involving a single embedded shock
- Conservative 2-D shock-fitted equations derived and implemented
- WENO5M combined with LLF splitting
  - allows for high order convergence
  - gives discrete conservation away from the shock
  - correctly captures shocks (degrade to $\approx O(\Delta x)$)
- Areas of current research
  - Validation from linear stability theory in progress
  - Extension to more complicated geometries

Weighted Essentially Non-Oscillatory (WENO) Schemes



- Fifth order scheme overall
- $\hat{f}^k = h + O(\Delta x^3)$
- $\hat{f}_{j\pm 1/2} = \sum_{k=0}^{2} \omega_k^{(M)} \hat{f}^k_{j\pm 1/2}$
- Schemes differ through formulation of $\omega_k^{(M)}$

Ideal weights:

$$\bar{\omega}_0 = 1/10, \qquad \bar{\omega}_1 = 6/10, \qquad \bar{\omega}_2 = 3/10.$$

WENO5 Modified (Mapped)

$$\omega_k^{(M)} = \frac{\alpha_k^*}{\sum_{i=0}^{2} \alpha_i^*} \quad \text{where} \quad \alpha_k^* = g_k(\omega_k^{(JS)})$$

$$g_k(\omega) = \frac{\omega(\bar{\omega}_k + \bar{\omega}_k^2 - 3\bar{\omega}_k\omega + \omega^2)}{\bar{\omega}_k^2 + (1 - 2\bar{\omega}_k)\omega}, \quad \omega \in [0, 1]$$

where $\omega_k^{(JS)}$ are those used by Jiang and Shu (1996)