# Stability and Stegotons

## Understanding Waves through Computation

David I. Ketcheson

CSGF Annual Meeting

July 15, 2009

DOE CSGF

APPLIED MATHEMATICS
UNIVERSITY of WASHINGTON

King Abdullah University of Science and Technology
KAUST

# Acknowledgments

- Randy LeVeque (U. Washington)

Principal funding:

- Dept. of Energy Computational Science Fellowship

Additional funding:

- Dept. of Homeland Security Graduate Fellowship
- AFOSR
- King Abdullah University of Science & Technology

King Abdullah University of Science and Technology KAUST

- A private research university made possible by a generous gift from King Abdullah

King Abdullah University of Science and Technology KAUST

- A private research university made possible by a generous gift from King Abdullah

"The World's First Computational Science University"

- One quarter of faculty devoted entirely to Mathematical and Computational Science (chaired by David Keyes)

King Abdullah University of Science and Technology KAUST

- A private research university made possible by a generous gift from King Abdullah

"The World's First Computational Science University"

- One quarter of faculty devoted entirely to Mathematical and Computational Science (chaired by David Keyes)
- World's best visualization facility

King Abdullah University of
Science and Technology

KAUST

- A private research university made possible by a generous gift from King Abdullah

"The World's First Computational Science University"

- One quarter of faculty devoted entirely to Mathematical and Computational Science (chaired by David Keyes)
- World's best visualization facility
- 14th fastest supercomputer

King Abdullah University of Science and Technology

KAUST

- A private research university made possible by a generous gift from King Abdullah

"The World's First Computational Science University"

- One quarter of faculty devoted entirely to Mathematical and Computational Science (chaired by David Keyes)
- World's best visualization facility
- 14th fastest supercomputer
- Generous research funding that is being spread around the world (Stanford, MIT, Berkeley, Caltech, UT-Austin, Cornell, UCSD, Texas A&M, Georgia Tech, Penn State, Woods Hole, ...)

King Abdullah University of Science and Technology KAUST

- A private research university made possible by a generous gift from King Abdullah

"The World's First Computational Science University"

- One quarter of faculty devoted entirely to Mathematical and Computational Science (chaired by David Keyes)
- World's best visualization facility
- 14th fastest supercomputer
- Generous research funding that is being spread around the world (Stanford, MIT, Berkeley, Caltech, UT-Austin, Cornell, UCSD, Texas A&M, Georgia Tech, Penn State, Woods Hole, ...)
- Partnerships with IBM, Boeing, Dow, GE, Schlumberger, ...

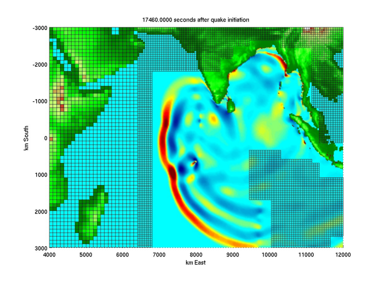
# Wave Equations

Hyperbolic PDEs describe numerous phenomena:

# Wave Equations

Hyperbolic PDEs describe numerous phenomena:

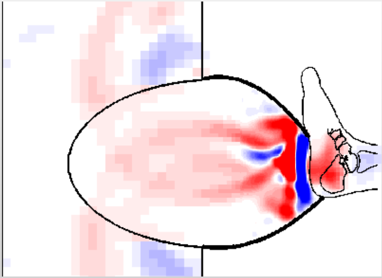
- Geophysical
  - Earthquakes
  - Tsunamis
  - Volcanic eruptions



# Wave Equations

Hyperbolic PDEs describe numerous phenomena:

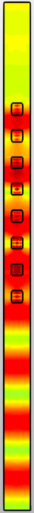
- Geophysical
  - Earthquakes
  - Tsunamis
  - Volcanic eruptions
- Biological
  - Ultrasound therapy
  - Lithotripsy/shock-wave therapy
  - Shell shock



# Wave Equations

Hyperbolic PDEs describe numerous phenomena:

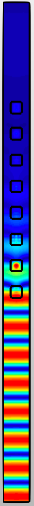
- Geophysical
  - Earthquakes
  - Tsunamis
  - Volcanic eruptions
- Biological
  - Ultrasound therapy
  - Lithotripsy/shock-wave therapy
  - Shell shock
- Engineering
  - Bandgaps
  - Lenses
  - Metamaterials



# Wave Equations

Hyperbolic PDEs describe numerous phenomena:

- Geophysical
  - Earthquakes
  - Tsunamis
  - Volcanic eruptions
- Biological
  - Ultrasound therapy
  - Lithotripsy/shock-wave therapy
  - Shell shock
- Engineering
  - Bandgaps
  - Lenses
  - Metamaterials



# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...
- higher order methods are more expensive for any fixed gridsize $h$

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...
- higher order methods are more expensive for any fixed gridsize $h$
- Tradeoff between refining grid ($h$) and increasing order ($p$)

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...
- higher order methods are more expensive for any fixed gridsize $h$
- Tradeoff between refining grid ($h$) and increasing order ($p$)
- As $h$ gets smaller, higher order pays off more

Thus high order becomes essential as

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...
- higher order methods are more expensive for any fixed gridsize $h$
- Tradeoff between refining grid ($h$) and increasing order ($p$)
- As $h$ gets smaller, higher order pays off more

Thus high order becomes essential as

- Computers get faster

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...
- higher order methods are more expensive for any fixed gridsize $h$
- Tradeoff between refining grid ($h$) and increasing order ($p$)
- As $h$ gets smaller, higher order pays off more

Thus high order becomes essential as

- Computers get faster
- Memory becomes limiting factor

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...
- higher order methods are more expensive for any fixed gridsize $h$
- Tradeoff between refining grid ($h$) and increasing order ($p$)
- As $h$ gets smaller, higher order pays off more

Thus high order becomes essential as

- Computers get faster
- Memory becomes limiting factor
- Error tolerances get smaller

# The Importance of High Order Accuracy

- Truncation error $E \approx Ch^p \qquad (h \ll 1)$
- Higher order $\implies$ smaller error, but...
- higher order methods are more expensive for any fixed gridsize $h$
- Tradeoff between refining grid ($h$) and increasing order ($p$)
- As $h$ gets smaller, higher order pays off more

Thus high order becomes essential as

- Computers get faster
- Memory becomes limiting factor
- Error tolerances get smaller
- Multiscale, 3D problems become the norm

*I think there will be always a demand for high order schemes, because you will always push the computers to the limit...*

*...In a high order scheme you can get, with fewer resources, more accurate results...*

*...The issue about high order methods is robustness. When the method is high order and sophisticated, it's less robust...*
*...if the second order scheme goes unstable once every four days, the high order scheme goes unstable once every two days, and you have to fix it.*
*I think that this is something basic that you cannot get rid of. This is the trade off. So, you have to choose.*

–David Gottlieb

# High Order Discretization: The Method of Lines

$$U_t + f(U)_x = 0$$

# High Order Discretization: The Method of Lines

$$U_t + f(U)_x = 0$$

First discretize the spatial derivatives to obtain a system of ODEs:

$$\frac{du}{dt} = F(u).$$

# High Order Discretization: The Method of Lines

$$U_t + f(U)_x = 0$$

First discretize the spatial derivatives to obtain a system of ODEs:

$$\frac{du}{dt} = F(u).$$

then apply a numerical ODE solver to obtain a fully discrete system:

$$u_i^{n+1} = G(u^n)$$

# High Order Discretization: The Method of Lines

$$U_t + f(U)_x = 0$$

First discretize the spatial derivatives to obtain a system of ODEs:

$$\frac{du}{dt} = F(u).$$

then apply a numerical ODE solver to obtain a fully discrete system:

$$u_i^{n+1} = G(u^n)$$

PDEs $\Longrightarrow$ ODEs $\Longrightarrow$ algebraic equations

# High Order Discretization: The Method of Lines

$$U_t + f(U)_x = 0$$

First discretize the spatial derivatives to obtain a system of ODEs:

$$\frac{du}{dt} = F(u).$$

then apply a numerical ODE solver to obtain a fully discrete system:

$$u_i^{n+1} = G(u^n)$$

PDEs $\implies$ ODEs $\implies$ algebraic equations

**Decouples spatial and temporal accuracy**

# High Order Discretization: The Method of Lines

$$U_t + f(U)_x = 0$$

First discretize the spatial derivatives to obtain a system of ODEs:

$$\frac{du}{dt} = F(u).$$

then apply a numerical ODE solver to obtain a fully discrete system:

$$u_i^{n+1} = G(u^n)$$

PDEs $\Longrightarrow$ ODEs $\Longrightarrow$ algebraic equations

**Decouples spatial and temporal accuracy**

Alternative: Cauchy-Kovalevskaya generalization of Lax-Wendroff

# Shocks lead to Oscillations

- Nonlinear wave equations naturally develop discontinuities ('shocks')
- Godunov's Theorem: even for the advection equation, any linear numerical method that is more than first order accurate will develop oscillations when approximating a shock.
- Higher order methods are even more prone to oscillations

# Shocks lead to Oscillations

- Nonlinear wave equations naturally develop discontinuities ('shocks')
- Godunov's Theorem: even for the advection equation, any linear numerical method that is more than first order accurate will develop oscillations when approximating a shock.
- Higher order methods are even more prone to oscillations

Burger's equation: $u_t + \left(\frac{1}{2}u^2\right)_x = 0$

# Avoiding Oscillations

## Total Variation Diminishing

The total variation semi-norm:

$$||u||_{\mathrm{TV}} = \int |u_x| dx$$

**TVD**: $||u(t+\Delta t)||_{\mathrm{TV}} \leq ||u(t)||_{\mathrm{TV}}$.

$$\text{TVD} \implies \text{no spurious oscillations}$$
$$\text{TVD} \implies \text{compact space} \implies \text{convergence}$$

**BUT**

TVD methods are at most 2nd order accurate
(1st order accurate in 2D)

Hence much focus has shifted to **non-oscillatory** methods

# Other constraints: Positivity

Consider the equations of inviscid, compressible flow:

$$\begin{aligned} \rho_t + (\rho u)_x &= 0 \\ (\rho u)_t + (\rho u^2 + p)_x &= 0 \\ E_t + (u(E+p))_x &= 0. \end{aligned}$$

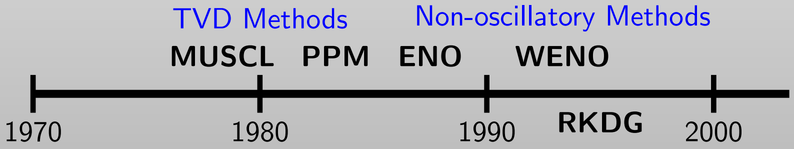
Physics says:

- $\rho \geq 0$
- $p \geq 0$
- $E \geq 0$

$\Longrightarrow$ Violation leads to unphysical states

# Dodging Godunov's Theorem

- **The Challenge:** Develop high-order numerical methods that avoid oscillations and/or preserve positivity.
- **The Solution:** Use methods that are nonlinear, even when applied to linear equations.
- **The Difficulty:** Very hard to directly analyze high-order full discretizations.
- Note that one must still sacrifice either formal high order or strict non-oscillatory property (or both) to go beyond 2nd order and 1D.



# The Method of Lines: Stability

Rather than analyze the full discretization directly, design a spatial discretization that satisfies the required bound with Forward Euler integration *under an appropriate timestep restriction.*

$$||u^n + \Delta t F(u^n)||_{\mathsf{TV}} \leq ||u^n||_{\mathsf{TV}} \quad 0 \leq \Delta t \leq \Delta t_{\mathsf{FE}} \qquad (*)$$

Then if $(*)$ is integrated by a strong stability preserving (SSP) time integrator, the numerical solution satisfies

$$||u^{n+1}||_{\mathsf{TV}} \leq ||u^n||_{\mathsf{TV}}$$

when applied to any system satisfying $(*)$ *under an appropriate timestep restriction.*

Decouples spatial and temporal stability analysis

# Wave Propagation Methods

Traditional flux-differencing methods for hyperbolic PDEs are tailored to the conservation law:

$$\mathbf{q}_t + f(\mathbf{q})_x = 0.$$

# Wave Propagation Methods

Traditional flux-differencing methods for hyperbolic PDEs are tailored to the conservation law:

$$\mathbf{q}_t + f(\mathbf{q})_x = 0.$$

Wave propagation methods are more general and easily handle non-traditional problems...

- Spatially varying flux:

$$\mathbf{q}_t + f(\mathbf{q}, x)_x = 0$$

# Wave Propagation Methods

Traditional flux-differencing methods for hyperbolic PDEs are tailored to the conservation law:

$$\mathbf{q}_t + f(\mathbf{q})_x = 0.$$

Wave propagation methods are more general and easily handle non-traditional problems...

- Spatially varying flux:

$$\mathbf{q}_t + f(\mathbf{q}, x)_x = 0$$

- Near-equilibrium systems:

$$\mathbf{q}_t + f(\mathbf{q})_x = S(\mathbf{q}) \text{ with } f(\mathbf{q})_x \approx S(\mathbf{q})$$

# Wave Propagation Methods

Traditional flux-differencing methods for hyperbolic PDEs are tailored to the conservation law:

$$\mathbf{q}_t + f(\mathbf{q})_x = 0.$$

Wave propagation methods are more general and easily handle non-traditional problems...

- Spatially varying flux:

$$\mathbf{q}_t + f(\mathbf{q}, x)_x = 0$$

- Near-equilibrium systems:

$$\mathbf{q}_t + f(\mathbf{q})_x = S(\mathbf{q}) \text{ with } f(\mathbf{q})_x \approx S(\mathbf{q})$$

- Quasilinear systems not in conservation form:

$$\kappa(x)\mathbf{q}_t + A(\mathbf{q}, x)\mathbf{q}_x = 0$$

# Wave Propagation Methods

Traditional flux-differencing methods for hyperbolic PDEs are tailored to the conservation law:

$$\mathbf{q}_t + f(\mathbf{q})_x = 0.$$

Wave propagation methods are more general and easily handle non-traditional problems. . .

- Spatially varying flux:

$$\mathbf{q}_t + f(\mathbf{q}, x)_x = 0$$

- Near-equilibrium systems:

$$\mathbf{q}_t + f(\mathbf{q})_x = S(\mathbf{q}) \text{ with } f(\mathbf{q})_x \approx S(\mathbf{q})$$

- Quasilinear systems not in conservation form:

$$\kappa(x)\mathbf{q}_t + A(\mathbf{q}, x)\mathbf{q}_x = 0$$

- Any combination of the above

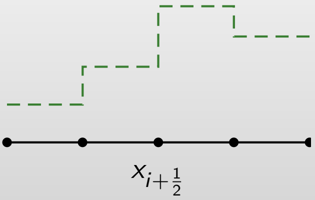
# Finite Volume Godunov-type Methods

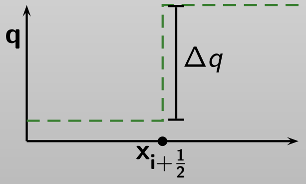
- Solution represented by cell averages $Q_i$
- Each cell interface represents a *Riemann problem*
- Flux-differencing:

$$Q_i^{n+1} = Q_i^n + \frac{\Delta t}{\Delta x}\left(F(x_{i-\frac{1}{2}}) - F(x_{i+\frac{1}{2}})\right)$$

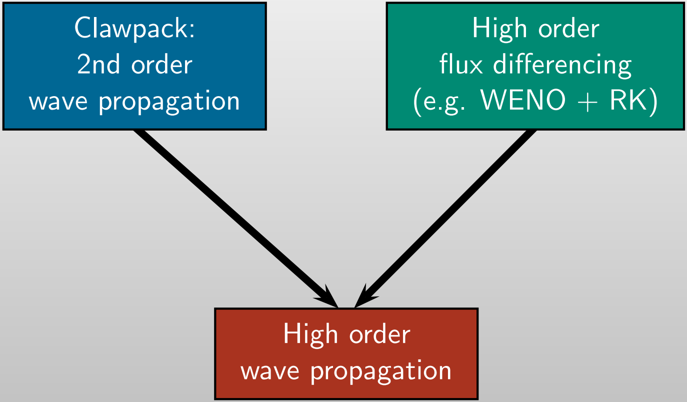
- Wave propagation:

$$Q_i^{n+1} = Q_i^n + \frac{\Delta t}{\Delta x}\left(\mathcal{W}^+_{i-\frac{1}{2}} + \mathcal{W}^-_{i+\frac{1}{2}}\right)$$



# The Best of Both Worlds




Implemented in the **SharpClaw** software package at
`www.clawpack.org`

# Elasticity in 1 Dimension

$$\begin{aligned} \epsilon_t - u_x &= 0 \\ \rho(x)u_t - \sigma(\epsilon, x)_x &= 0 \end{aligned}$$

$\epsilon(x,t)$ : Strain $\quad$ $u(x,t)$ : Velocity

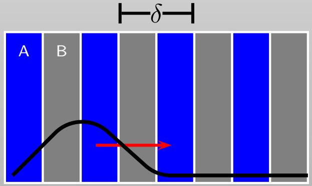
$\sigma(\epsilon, x)$ : Stress $\quad$ $\rho(x)$ : Density

# Elasticity in 1 Dimension

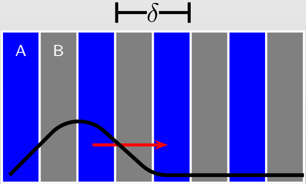
$$\begin{aligned} \epsilon_t - u_x &= 0 \\ \rho(x) u_t - \sigma(\epsilon, x)_x &= 0 \end{aligned}$$

$\epsilon(x,t)$ : Strain    $u(x,t)$ : Velocity

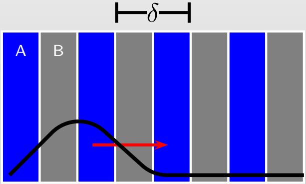
$\sigma(\epsilon, x)$ : Stress    $\rho(x)$ : Density



# Stegotons

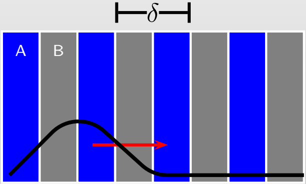


# Stegotons




Linear elasticity: $\sigma = K\epsilon$

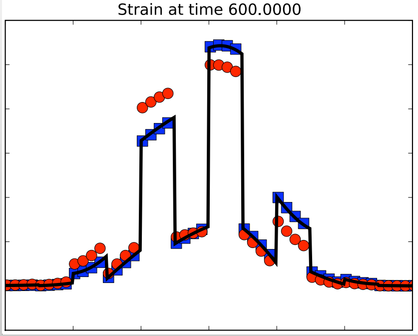
# Stegotons

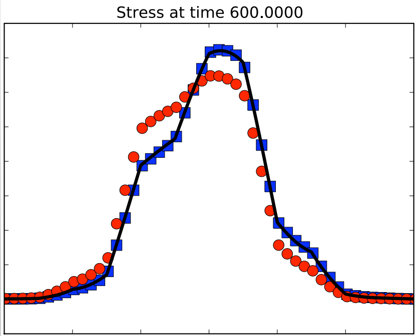



Linear elasticity: $\sigma = K\epsilon$

Nonlinearity: $\sigma = e^{K\epsilon} - 1$

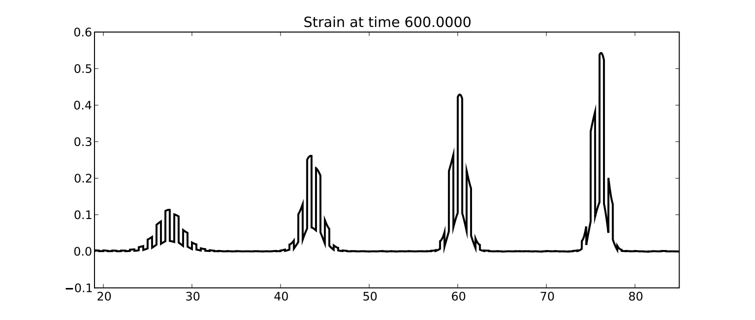
# A comparison of high and low order accuracy



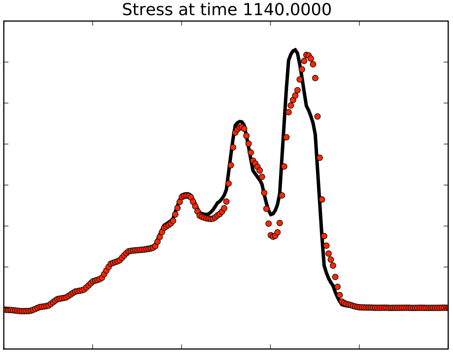

Black - "exact" solution
Red - 2nd order solution
Blue - 5th order solution

# Time Reversal Test

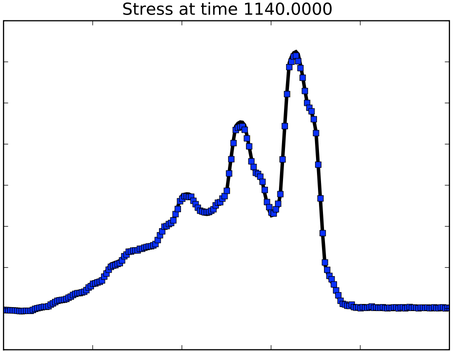



This is a unique test problem because we can expect high order convergence even after long-distance wave propagation.

# Time Reversal Test

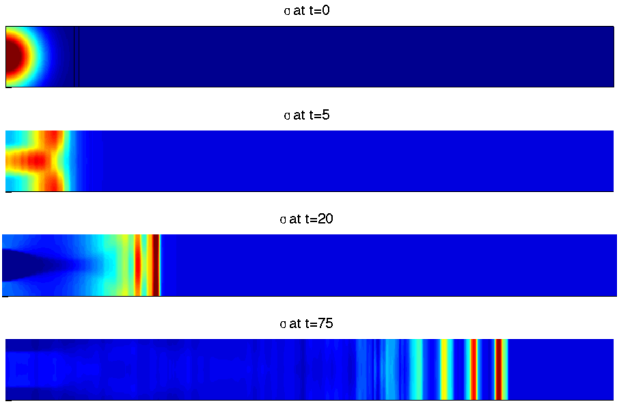



2nd order solution

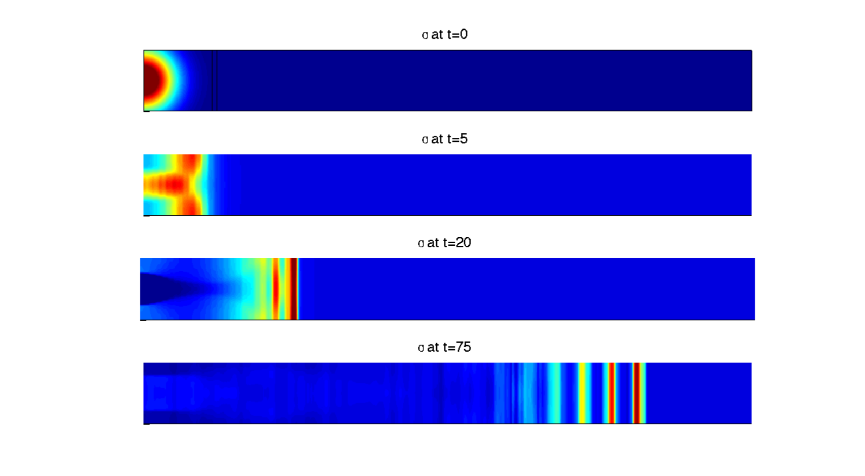



5th order solution

# Stability of 2D Stegotons



# Stability of 2D Stegotons




A partial experimental realization: Berezovski et. al., 2006