Wave Propagation Software, Computational Science, and Reproducible Research

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- Hyperbolic PDEs and Riemann problems
- Wave propagation and shock formation
- Applications to many practical problems
- Finite volume methods: Godunov and high-resolution
- General formulation based on Riemann solvers
- Implementation in CLAWPACK software
- Some extensions: adaptive mesh refinement, manifolds
- Example: Shallow water on the sphere
- Shallow water equations over bathymetry with innundation
- f-wave formulation, well-balanced schemes
- TsunamiClaw and tsunami simulations

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 - Aerodynamics shocks near transonic or supersonic aircraft
 - Detonation waves coupled with combustion
 - Astrophysics stellar dynamics, supernova explosions, ...
- Magnetohydrodynamics:
 - magnetic storms, stellar dynamics
 - plasma physics, fusion reactors
- Relativistic flows:
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Elastic waves

- Seismology earthquakes, imaging
- Shock waves in tissue and bone lithotripsy and shock wave therapy
- Shock induced phase transitions
- Volcanic flows
 - Dusty gas jets and pyroclastic flows
 - Lava flows
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First order hyperbolic PDE in 1 space dimension

Linear:
$$q_t + Aq_x = 0$$
, $q(x,t) \in \mathbb{R}^m$, $A \in \mathbb{R}^{m \times m}$

Conservation law: $q_t + f(q)_x = 0$, $f: \mathbb{R}^m \to \mathbb{R}^m$ (flux)

Quasilinear form: $q_t + f'(q)q_x = 0$

Hyperbolic if A or f'(q) is diagonalizable with real eigenvalues.

Models wave motion ar advective transport.

Eigenvalues are wave speeds.

Example: Linear acoustics in a 1d tube

$$q = \left[egin{array}{c} p \\ u \end{array}
ight] \quad \begin{array}{c} p(x,t) = {
m pressure \ perturbation} \\ u(x,t) = {
m velocity} \end{array}$$

Equations:

or

$$\left[\begin{array}{c}p\\u\end{array}\right]_t+\left[\begin{array}{cc}0&\kappa\\1/\rho&0\end{array}\right]\left[\begin{array}{c}p\\u\end{array}\right]_x=0.$$

Eigenvalues: $\lambda = \pm c$, where $c = \sqrt{\kappa/\rho} =$ sound speed

Second order form: Can combine equations to obtain

$$p_{tt} = c^2 p_{xx}$$

Special initial data:

$$q(x,0) = \begin{cases} q_l & \text{if } x < 0\\ q_r & \text{if } x > 0 \end{cases}$$

Example: Acoustics with bursting diaphram

$$P_{l}$$
 P_{r} P_{r} v_{r}

Pressure:



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Waves propagating in x-t space:



Left-going wave $W^1 = q_m - q_l$ and right-going wave $W^2 = q_r - q_m$ are eigenvectors of A.

Nonlinear compressible flow — Euler equations

Conservation of mass, momentum, energy: $q_t + f(q)_x = 0$ with

$$q = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix}, \qquad f(q) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(E+p) \end{bmatrix}$$

where

$$p = \text{pressure} = p(\rho, E)$$
 (Equation of state)

The Jacobian f'(q) has eigenvalues u - c, u, u + c where

$$c = \sqrt{rac{dp}{d
ho}}$$
 at constant entropy

Eigenvalues vary with $q \implies$ shocks, rarefactions.

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Example: Shock tube problem in gas dynamics



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$$\left(\begin{array}{ccc} \rho_{I} & \rho_{I} & u_{I} \end{array} \right) \left(\begin{array}{ccc} \rho_{r} & \rho_{r} & u_{r} \end{array} \right)$$



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Riemann Problem for gas dynamics

Waves propagating in x-t space:



Similarity solution (function of x/t alone).

Waves can be approximated by discontinuties: Approximate Riemann solvers

Waves can steepen up and form shocks



Waves can steepen up and form shocks



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Waves can steepen up and form shocks

 \implies even smooth data can lead to discontinuous solutions.



Computational challenges!

Need to capture sharp discontinuities.

PDE breaks down, standard finite difference approximation to $q_t + f(q)_x = 0$ can fail badly: nonphysical oscillations, convergence to wrong weak solution.

Integral form of conservation law

$$\frac{d}{dt} \int_{x_1}^{x_2} q(x,t) \, dx = f(q(x_1,t)) - f(q(x_2,t))$$

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For smooth q:
$$-\int_{x_1}^{x_2} \frac{\partial}{\partial x} f(q(x,t)) dx$$

$$\implies \qquad \int_{x_1}^{x_2} q_t + f(q)_x \, dx = 0 \qquad \forall x_1, \ x_2$$

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$$\implies \qquad \int_{x_1}^{x_2} q_t + f(q)_x \, dx = 0 \qquad \forall x_1, \ x_2$$

Integral form holds for discontinuous q.

Integrating in t gives

$$\int_{x_1}^{x_2} q(x,t_2) \, dx = \int_{x_1}^{x_2} q(x,t_1) \, dx - \int_{t_1}^{t_2} [f(q(x_2,t)) - f(q(x_1,t))] \, dt$$
Finite volume methods

Approximate cell averages:
$$Q_i^n \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x, t_n) dx$$

Updating formula (conservation form):

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} [F_{i+1/2}^n - F_{i-1/2}^n]$$

where the numerical flux is

$$F_{i-1/2}^n \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2}, t)) \, dt.$$

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Note: can rewrite as

$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} + \frac{F_{i+1/2}^n - F_{i-1/2}^n}{\Delta x} = 0.$$

Looks like finite difference approximation to $q_t + f_x = 0$, but $F_{i-1/2}^n$ is properly viewed as average flux through cell edge.



1. Solve Riemann problems at all interfaces, yielding waves $\mathcal{W}^p_{i-1/2}$ and speeds $s^p_{i-1/2}$, for $p=1,\ 2,\ \ldots,\ m$.

Riemann problem: Original equation with piecewise constant data.



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3. Update cell averages by contributions from all waves entering cell:

$$\begin{split} Q_i^{n+1} &= Q_i^n - \frac{\Delta t}{\Delta x} [\mathcal{A}^+ \Delta Q_{i-1/2} + \mathcal{A}^- \Delta Q_{i+1/2}] \\ \text{where } \mathcal{A}^\pm \Delta Q_{i-1/2} &= \sum_{i=1}^m (s_{i-1/2}^p)^\pm \mathcal{W}_{i-1/2}^p. \end{split}$$

Upwind wave-propagation algorithm

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left[\sum_{p=1}^m (s_{i-1/2}^p)^+ \mathcal{W}_{i-1/2}^p + \sum_{p=1}^m (s_{i+1/2}^p)^- \mathcal{W}_{i+1/2}^p \right]$$

where

$$s^+ = \max(s, 0), \qquad s^- = \min(s, 0).$$

Note: Requires only waves and speeds.

Applicable also to hyperbolic problems not in conservation form.

For $q_t + f(q)_x = 0$, conservative if waves chosen properly, e.g. using Roe-average of Jacobians.

Great for general software, but only first-order accurate (upwind method for linear systems).

Wave-propagation form of high-resolution method

$$Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{\Delta x} \left[\sum_{p=1}^{m} (s_{i-1/2}^{p})^{+} \mathcal{W}_{i-1/2}^{p} + \sum_{p=1}^{m} (s_{i+1/2}^{p})^{-} \mathcal{W}_{i+1/2}^{p} \right] - \frac{\Delta t}{\Delta x} (\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2})$$

Correction flux:

$$\tilde{F}_{i-1/2} = \frac{1}{2} \sum_{p=1}^{M_w} |s_{i-1/2}^p| \left(1 - \frac{\Delta t}{\Delta x} |s_{i-1/2}^p| \right) \widetilde{\mathcal{W}}_{i-1/2}^p$$

where $\widetilde{W}_{i-1/2}^p$ is a limited version of $W_{i-1/2}^p$ to avoid oscillations. (Unlimited waves $\widetilde{W}^p = W^p \implies$ Lax-Wendroff for a linear system \implies nonphysical oscillations near shocks.)

Limiter methods

Differencing $W_{i+1/2}^p - W_{i-1/2}^p$ approximates q_{xx} . Gives second order terms in Taylor series (Lax-Wendroff) This improves solution only if q is sufficiently smooth.

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Host of high-resolution methods developed since late 70's: flux corrected transport, TVD methods, flux limiters, slope limiters, PPM, ENO, WENO, ...

Developed by: Boris, Book, Harten, Zwas, van Leer, Roe, Osher, Zalesak, Sweby, Colella, Woodward, Engquist, Chakravarthy, Shu, ...

Wave-propagation form of high-resolution method

$$Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{\Delta x} \left[\sum_{p=1}^{m} (s_{i-1/2}^{p})^{+} \mathcal{W}_{i-1/2}^{p} + \sum_{p=1}^{m} (s_{i+1/2}^{p})^{-} \mathcal{W}_{i+1/2}^{p} \right] - \frac{\Delta t}{\Delta x} (\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2})$$

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CLAWPACK — Conservation LAWs PACKage

http://www.amath.washington.edu/~claw/

- Fortran codes with Matlab graphics routines.
- Many examples and applications to run or modify.
- 1d, 2d, and 3d.
- Adaptive mesh refinement, MPI for parallel computing.

User supplies:

- Riemann solver, splitting data into waves and speeds (Need not be in conservation form)
- Boundary condition routine to extend data to ghost cells Standard bc1.f routine includes many standard BC's
- Initial conditions qinit.f
- Source terms srcl.f

Software goals

- General framework for broad application.
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Research:

- Application to new scientific/engineering problems.
- Extensions of methods to more challenging problems.
- Compare different methods on standard test problems.

Reproducible research!

Some extensions and related software

- AMRCLAW adaptive mesh refinement (Marsha Berger)
- CLAWMAN on 2d manifolds (James Rossmanith, Derek Bale)
- BEARCLAW f90 version (Sorin Mitran)
- AstroBEAR including MHD (Adam Frank, Alexei Poludenko)
- ChomboClaw interface to C++ (Donna Calhoun, Phil Colella et.al.)
- AMROC C++ AMR code (Ralf Deiterding)
- TsunamiClaw SW over bathymetry (David George)

Recent work with Donna Calhoun and Christiane Helzel:

Mapping of Cartesian grid in rectangle $[-3,1] \times [-1,1]$ to sphere.



Ratio of largest to smallest cell is < 2.

Grid is highly non-orthogonal at a few points near equator.

Movie of mapping

Numerical results on the sphere

Direct application of CLAWPACK — wave-propagation finite volume method

AMRCLAW can also be used.

Movie — shallow water on the sphere

Movie — depth vs. "latitude" compared to 1d solution

Movie — with adaptive mesh refinement

Movie — in computational plane

- Shallow water equations over bathymetry with dry states
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But first ...

- Wave propagation algorithms for spatially varying fluxes
- Source terms and well balanced schemes
- Implementation via change in Riemann solver

Riemann problem for spatially-varying flux

$$q_t + f(q, x)_x = 0$$

Applications:

- Wave propagation in heterogeneous nonlinear media
- Flow in heterogeneous porous media
- Traffic flow with varying road conditions
- Solving conservation laws on curved manifolds

Riemann problem for spatially-varying flux

$$q_t + f(q, x)_x = 0$$

Cell-centered discretization: Flux $f_i(q)$ defined in *i*th cell.



Need $f_{i-1}(Q_{i-1/2}^*) = f_i(Q_{i-1/2}^*) \implies m$ propagating waves plus jump in q (= m waves for the m components of q).

Flux-based wave decomposition (f-waves)

Choose waveforms r^p (e.g. eigenvectors of Jacobian on each side).

Then decompose flux difference:

$$f_i(Q_i) - f_{i-1}(Q_{i-1}) = \sum_{p=1}^m \beta^p r^p \equiv \sum_{p=1}^m \mathcal{Z}^p$$



Wave-propagation algorithm using f-waves

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} [\mathcal{A}^+ \Delta Q_{i-1/2} + \mathcal{A}^- \Delta Q_{i+1/2}] - \frac{\Delta t}{\Delta x} [\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2}]$$

Standard version: $Q_i - Q_{i-1} = \sum_{p=1}^m W_{i-1/2}^p$

$$\begin{aligned} \mathcal{A}^{-} \Delta Q_{i+1/2} &= \sum_{p=1}^{m} (s_{i+1/2}^{p})^{-} \mathcal{W}_{i+1/2}^{p} \\ \mathcal{A}^{+} \Delta Q_{i-1/2} &= \sum_{p=1}^{m} (s_{i-1/2}^{p})^{+} \mathcal{W}_{i-1/2}^{p} \\ \tilde{F}_{i-1/2} &= \frac{1}{2} \sum_{p=1}^{m} |s_{i-1/2}^{p}| \left(1 - \frac{\Delta t}{\Delta x} |s_{i-1/2}^{p}| \right) \widetilde{\mathcal{W}}_{i-1/2}^{p}. \end{aligned}$$

Wave-propagation algorithm using f-waves

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} [\mathcal{A}^+ \Delta Q_{i-1/2} + \mathcal{A}^- \Delta Q_{i+1/2}] - \frac{\Delta t}{\Delta x} [\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2}]$$

Using *f*-waves:
$$f_i(Q_i) - f_{i-1}(Q_{i-1}) = \sum_{p=1}^m \mathcal{Z}_{i-1/2}^p$$

$$\mathcal{A}^{-}\Delta Q_{i-1/2} = \sum_{p:s_{i-1/2}^{p} < 0} \mathcal{Z}_{i-1/2}^{p}$$

$$\mathcal{A}^+ \Delta Q_{i-1/2} = \sum_{p:s_{i-1/2}^p > 0} \mathcal{Z}_{i-1/2}^p,$$

$$\tilde{F}_{i-1/2} = \frac{1}{2} \sum_{p=1}^{m} \operatorname{sgn}(s_{i-1/2}^{p}) \left(1 - \frac{\Delta t}{\Delta x} |s_{i-1/2}^{p}| \right) \widetilde{\mathcal{Z}}_{i-1/2}^{p}$$

Source terms and quasi-steady solutions

$$q_t + f(q)_x = \psi(q)$$

Steady-state solution:

$$q_t = 0 \implies f(q)_x = \psi(q)$$

Balance between flux gradient and source.

Quasi-Steady solution:

Small perturbation propagating against steady-state background.

 $q_t \ll f(q)_x \approx \psi(q)$

Want accurate calculation of perturbation.

Examples:

- Shallow water equations with bottom topography and flat surface
- Stationary atmosphere where pressure gradient balances gravity

Fractional steps for a quasisteady problem

Alternate between solving homogeneous conservation law

$$q_t + f(q)_x = 0 \tag{1}$$

and source term

$$q_t = \psi(q). \tag{2}$$

When $q_t \ll f(q)_x \approx \psi(q)$:

- Solving (1) gives large change in q
- Solving (2) should essentially cancel this change.

Numerical difficulties:

- (1) and (2) are solved by very different methods. Generally will not have proper cancellation.
- Nonlinear limiters are applied to $f(q)_x$ term, not to small-perturbation waves. Large variation in steady state hides structure of waves.

Incorporating source term in f-waves

$$q_t + f(q)_x = \psi$$
 with $f(q)_x \approx \psi$.

Concentrate source at interfaces: $\Psi_{i-1/2} \,\delta(x - x_{i-1/2})$

Split $f(Q_i) - f(Q_{i-1}) - \Delta x \Psi_{i-1/2} = \sum_p Z_{i-1/2}^p$

Use these waves in wave-propagation algorithm.



Incorporating source term in f-waves

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Split
$$f(Q_i) - f(Q_{i-1}) - \Delta x \Psi_{i-1/2} = \sum_p Z_{i-1/2}^p$$

Use these waves in wave-propagation algorithm.

Steady state maintained:

If
$$\frac{f(Q_i)-f(Q_{i-1})}{\Delta x} = \Psi_{i-1/2}$$
 then $\mathcal{Z}^p \equiv 0$

Near steady state:

Deviation from steady state is split into waves and limited.

- Small amplitude in ocean (< 1 meter) but can grow to 10s of meters at shore.
- Run-up along shore can inundate 100s of meters inland
- Long wavelength (as much as 200 km)
- Propagation speed \sqrt{gh} (bunching up at shore)
- Average depth of Pacific or Indian Ocean is 4km \implies average speed 200 m/s \approx 450 mph

Cross section of Indian Ocean & tsunami

Surface elevation on scale of 10 meters:



Cross-section on scale of kilometers:



Shallow water equations with topography B(x)

$$h_t + (hu)_x = 0$$

$$(hu)_t + \left(hu^2 + \frac{1}{2}gh^2\right)_x = -ghB_x(x)$$

h(x,t) = depth of water u(x,t) = horizontal velocity

This has the form of a conservation law with a source term:

$$q_t + f(q)_x = \psi(q, x),$$

where

$$q = \begin{bmatrix} h \\ hu \end{bmatrix}, \quad f(q) = \begin{bmatrix} hu \\ hu^2 + gh^2/2 \end{bmatrix}, \quad \psi(q, x) = \begin{bmatrix} 0 \\ -ghB'(x) \end{bmatrix}$$

Shallow water equations with topography B(x, y)

$$h_t + (hu)_x + (hv)_y = 0$$

$$(hu)_t + \left(hu^2 + \frac{1}{2}gh^2\right)_x + (huv)_y = -ghB_x(x,y)$$

$$(hv)_t + (huv)_x + \left(hv^2 + \frac{1}{2}gh^2\right)_y = -ghB_y(x,y)$$

Applications:

- Tsunamis
- Estuaries
- River flooding, dam breaks
- Debris flows from volocanic eruptions

Methods to be discussed all extend to 2d (and 3d)

The Riemann problem

The Riemann problem for $q_t + f(q)_x = 0$ has special initial data

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Dam break problem for shallow water equations



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One-dimensional example:



Solved on uniform grid with h = 0 in dry cells.

Cells can change between wet and dry.

Riemann problems may have one side dry or generate dry state in solution.

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Sumatra event of December 26, 2004

Magnitude 9.1 quake near Sumatra, where Indian tectonic plate is being subducted under the Burma platelet.

Rupture along subduction zone

pprox 1200 km long, 150 km wide

Propagating at \approx 2 km/sec (for \approx 10 minutes)

Fault slip up to 15 m, uplift of several meters. (Fault model from Caltech Seismolab.)





Tsunami simulations

- 2D shallow water + bathymetry
- Finite volume method
- Cartesian grid
- Cells can be dry (h = 0)
- Cells become wet/dry as wave moves on shore
- Mesh refinement on rectangular patches
- Adaptive follows wave, more levels near shore



Tsunami simulations



424.0000 seconds after quake initiation

For movies, see

http://www.amath.washington.edu/~dgeorge/research.html

- Wave propagation problems are generally formulated as hyperbolic systems.
- Many practical applications in science and engineering.
- General software for high-resolution methods, AMR: http://www.amath.washington.edu/~claw
- This talk, paper and codes:

http://www.amath.washington.edu/~rjl/pubs/icm06

• Other papers and simulations:

http://www.amath.washington.edu/~rjl/research.html

R. J. LeVeque International Congress of Mathematicians, Madrid, 2006

Jason-1 Satellite passed over the Indian Ocean during the tsunami event.

Surface height on two passes (one a week before)

Disparity shows tsunami:





Comparison of simulation with satellite data



Shock Wave Therapy and Lithotripsy

Setup:

Pressure pulse:



- Shock wave lithotripsy is a well-established procedure for noninvasive destruction of kidney stones.
- Typically several thousand shocks applied at rate of 1 to 4 pulses per second.

Lithotripter at the UW Applied Physics Lab



Tom Matula (APL researcher) and Kirsten Fagnan (AMath grad student)

R. J. LeVeque International Congress of Mathematicians, Madrid, 2006

Stresses in lithotripsy

Kidney stone



Idealized cylinder





movie

- 2D elastic wave equations (+ axisymmetry)
- Preliminary results in 3D
- Models compression and shear waves
- Heterogeneous material
- Nonlinearity in compression waves

Equations of linear elasticity

$$\sigma_t^{11} - (\lambda + 2\mu)u_x - \lambda v_y = 0$$

$$\sigma_t^{22} - \lambda u_x - (\lambda + 2\mu)v_y = 0$$

$$\sigma_t^{12} - \mu(v_x + u_y) = 0$$

$$\rho u_t - \sigma_x^{11} - \sigma_y^{12} = 0$$

$$\rho v_t - \sigma_x^{12} - \sigma_y^{22} = 0$$

where $\lambda(x, y)$ and $\mu(x, y)$ are Lamé parameters.

This has the form $q_t + Aq_x + Bq_y = 0$. The matrix $(A\cos\theta + B\sin\theta)$ has eigenvalues $-c_p$, $-c_s$, 0, c_s , c_p where the P-wave speed and S-wave speed are $c_p = \sqrt{\frac{\lambda+2\mu}{\rho}}$, $c_s = \sqrt{\frac{\mu}{\rho}}$

Extracorporeal Shock Wave Therapy (ESWT)

New uses are currently being tested





Ankle bone data



	ρ	λ	μ	c_p	c_s
water brass bone "air"	$1000 \\ 8560 \\ 1850 \\ 100$	2190.4 6624.1 9305.5 3.9	$0.0 \\ 4528.2 \\ 3126.5 \\ 0.0$	$1.48 \\ 1.36 \\ 2.9 \\ 0.2$	$0.0 \\ 0.73 \\ 1.3 \\ 0.0$

Cartesian grid cells cut be interface contain averaged values.



Shock wave therapy simulations



Movie: With good acoustic coupling Movie: With poor acoustic coupling