# Finite-volume Methods and Software for Hyperbolic PDEs and Conservation Laws

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#### CLAWPACK Software: http://www.amath.washington.edu/~claw Supported in part by NSF, DOE

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#### **Outline**

- · Volcanic flows, ash plumes, pyroclastic flow
- · Finite volume methods for hyperbolic equations
- Conservation laws and source terms
- Riemann problems and Godunov's method
- Wave propagation form
- Wave limiters and high-resolution methods
- Software: CLAWPACK
- Tsunami modeling, shallow water equations
- Lithotripsy and shock wave therapy

#### Algorithms, software

Marsha Berger, NYU Donna Calhoun, UW Phil Colella, UC-Berkeley Jan Olav Langseth, Oslo

Volcanoes Marica Pelanti, UW grad student (now at Paris VI) Roger Denlinger, Dick Iverson, USGS CVO Alberto Neri, T. E. Ongaro, Pisa

Tsunamis David George, UW grad student Harry Yeh, OSU

Lithotripsy and shock wave therapy Kirsten Fagnan, UW grad student Tom Matula, Mike Bailey, UW APL

# Marica Pelanti, Donna Calhoun, Joe Dufek, and David George at Mount St. Helens



- Flow of magma in conduit
- Little dissolved gas  $\implies$  lava flows
- Dissolved gas expansion  $\implies$  phase transition, ash jet
- Atmospheric shock wave
- Ash plumes, Plinian columns
- · Collapsing columns, pyroclastic flows or surges
- Lahars (mud flows)
- Debris flows

#### Mount St. Helens



# High-pressure initial blast



### **AMR** computation



#### Blast zone at Mount St. Helens



### Trees blown down by MSH blast



http://volcanoes.usgs.gov/Hazards/Effects/MSHsurge\_effects.html



Two-phase fluid flow composed of solid particles (dust) in a gas.

Gas phase: compressible;

Dust phase: incompressible (constant microscopic density).

Dust particles are assumed to be dispersed (vol. fraction  $\alpha_d \ll 1$ ), with negligible particle-particle interaction. The solid phase is thus considered *pressureless*.

Model accounts for:

- Gravity;
- Interphase drag force;
- Interphase heat transfer.

Some of the neglected phenomena: viscous stress, turbulence.

#### Model Equations for dusty gas

Conservation of mass, momentum, and energy for gas and dust

$$\begin{split} \rho_t + \nabla \cdot (\rho \mathbf{u}_g) &= 0, \\ (\rho \mathbf{u}_g)_t + \nabla \cdot (\rho \mathbf{u}_g \otimes \mathbf{u}_g + p \mathbf{l}) &= \rho \mathbf{g} - D(\mathbf{u}_g - \mathbf{u}_d), \\ E_t + \nabla \cdot ((E + p)\mathbf{u}_g) &= \rho \mathbf{u}_g \cdot \mathbf{g} - D(\mathbf{u}_g - \mathbf{u}_d) \cdot \mathbf{u}_d - Q(T_g - T_d), \\ \beta_t + \nabla \cdot (\beta \mathbf{u}_d) &= 0, \\ (\beta \mathbf{u}_d)_t + \nabla \cdot (\beta \mathbf{u}_d \otimes \mathbf{u}_d) &= \beta \mathbf{g} + D(\mathbf{u}_g - \mathbf{u}_d), \\ \Omega_t + \nabla \cdot (\Omega \mathbf{u}_d) &= \beta \mathbf{u}_d \cdot \mathbf{g} + D(\mathbf{u}_g - \mathbf{u}_d) \cdot \mathbf{u}_d + Q(T_g - T_d). \end{split}$$

 $\begin{array}{l} \alpha_g, \alpha_d = \text{volume fractions} \ (\alpha_g + \alpha_d = 1, \alpha_d \ll 1); \\ \rho_g, \rho_d = \text{material mass densities} \ (\rho_d = \text{const.}); \ \rho = \alpha_g \rho_g, \ \beta = \alpha_d \rho_d = \text{macroscopic densities}; \\ \mathbf{u}_g, \mathbf{u}_d = \text{velocities}; \ p_g = \text{gas pressure}, \ p = \alpha_g p_g; \\ e_g, e_d = \text{specific total energies}, \ E = \alpha_g \rho_g e_g, \ \Omega = \alpha_d \rho_d e_d; \\ e_g = \epsilon_g + \frac{1}{2} ||\mathbf{u}_g||^2, \ e_d = \epsilon_d + \frac{1}{2} ||\mathbf{u}_d||^2; \ e_g, \ e_d = \text{specific internal energies}; \ T_g, \ T_d = \text{temperatures}; \\ \mathbf{g} = (0, 0, -g) = \text{gravity acceleration} \ (z \ \text{direction}), \ g = 9.8 \ \text{m/s}^2; \end{array}$ 

D =drag function; Q = heat transfer function.

#### **Closure Relations**

Gas equation of state:

$$p_g = (\gamma - 1)\rho_g \epsilon_g$$
,  $\gamma = c_{pg}/c_{vg}$  = const.;

Dust energy relation:

$$\epsilon_d = c_{vd}T_d$$
,  $c_{vd} = \text{const.}$ ;

Drag

$$D = \frac{3}{4} C_{\mathrm{d}} \frac{\beta \rho}{\rho_d d} || \mathbf{u}_g - \mathbf{u}_d ||,$$

 $d = dust particle diameter, C_d = drag coefficient,$ 

$$C_{\rm d} = \begin{cases} \frac{24}{Re} \left( 1 + 0.15 R e^{0.687} \right) & \text{if } Re < 1000 \,, \\ 0.44 & \text{if } Re \ge 1000 \,, \end{cases}$$

 $Re = \text{Reynolds number} = \frac{\rho d||\mathbf{u}_g - \mathbf{u}_d||}{\mu}, \ \mu = \text{dynamic viscosity of the gas.}$ 

#### Heat transfer

$$Q = \frac{N u \, 6 \kappa_g \beta}{\rho_d d^2} \,,$$

Nu = Nusselt number = 2 + 0.65 $Re^{1/2}Pr^{1/3}$ , Pr = Prandtl number =  $\frac{c_{Pg\mu}}{\kappa_g}$ ,  $\kappa_g$  = gas thermal conductivity.

Influence of the diameter  $D_v$  and the exit velocity  $v_v$ 



Regions of different types of eruption columns (Neri–Dobran, 1994).



#### Vent conditions and physical properties [Neri-Dobran, 1994]:

$p_v$	$T_v$	$\alpha_{dv}$	d	$ ho_d$
[MPa]	[K]		$[\mu m]$	$[kg/m^3]$
0.1	1200	0.01	10	2300

Gas and dust in thermal and mechanical equilibrium at the vent.

Test 1.  $D_v = 100 \text{ m}, v_v = 80 \text{ m/s}$ .  $\rightarrow$  Collapsing volcanic column

Test 2.  $D_v = 100 \text{ m}, v_v = 200 \text{ m/s}. \rightarrow Transitional/Plinian column$ 

Injection of a hot supersonic particle-laden gas from a volcanic vent into a cooler atmosphere.

- *Initially:* Standard atmosphere vertically stratified in pressure and temperature all over the domain;
- At the vent: Gas pressure, velocities, temperatures, volumetric fractions of gas and dust assumed to be fixed and constant;
- Ground boundary: modeled as a free-slip reflector;
- Other boundaries:

2D experiments: Axisymmetric configuration. Symmetry axis: free-slip reflector; Upper and right-hand edges of the domain: free flow boundaries (all the variables gradients set to zero).

*Fully 3D experiments:* Upper and lateral sides: free-flow boundaries.

# Collapsing column. $D_v = 100 \,\mathrm{m}, v_v = 80 \,\mathrm{m/s}.$



Dust density (axisymmetric). Uniform grid,  $200 \times 100$  cells. Cell size = 10 m. CFL = 0.9.

Movie: collapsing column .... Movie: rising column

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# High resolution finite volume methods

Hyperbolic conservation law:

 $1D: q_t + f(q)_x = 0 2D: q_t + f(q)_x + g(q)_y = 0$  $1D: q_t + f'(q)q_x = 0 2D: q_t + f'(q)q_x + g'(q)q_y = 0$ 

Variable coefficient linear hyperbolic system:

$$1D: q_t + A(x)q_x = 0 \qquad 2D: q_t + A(x,y)q_x + B(x,y)q_y = 0$$

Def: Hyperbolic if eigenvalues of Jacobian f'(q) in 1D or  $\alpha f'(q) + \beta g'(q)$  in 2D are real and there exists a complete set of eigenvectors.

Eigenvalues are wave speeds, eigenvectors yield decomposition of data into waves.

#### Finite-difference Methods

- Pointwise values  $Q_i^n \approx q(x_i, t_n)$
- Approximate derivatives by finite differences
- Assumes smoothness

#### Finite-volume Methods

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

$$\frac{\partial}{\partial t} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x,t) \, dx = f(q(x_{i-1/2},t)) - f(q(x_{i+1/2},t))$$

leads to conservation law  $q_t + f_x = 0$  but also directly to numerical method.



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.



#### Then either:

1. Compute new cell averages by integrating over cell at time  $t_{n+1}$ ,

or ...



#### Then either:

- 1. Compute new cell averages by integrating over cell at time  $t_{n+1}$ , or...
- 2. Compute fluxes at interfaces and flux-difference,

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



#### or ...

3. Update old cell averages by contributions from all waves entering the cell.

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

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

$$q(x,0) = \begin{cases} q_l & \text{if } x < x_{i-1/2} \\ q_r & \text{if } x > x_{i-1/2} \end{cases}$$



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# Riemann solution for the SW equations



The Roe solver uses the solution to a linear system

$$q_t + \hat{A}_{i-1/2} q_x = 0, \qquad \hat{A}_{i-1/2} = f'(q_{\text{ave}}).$$

All waves are simply discontinuities.

Typically a fine approximation if jumps are approximately correct.

# 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.)

# **CLAWPACK**

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

#### Some applications

- Acoustics, ultrasound, seismology, lithotripsy
- Elasticity, plasticity, nonlinear elasticity
- Electromagnetic waves, photonic crystals
- Flow in porous media, groundwater contamination
- Oil reservoir simulation
- Geophysical flow on the sphere
- Hyperbolic equations on general curved manifolds (CLAWMAN)
- Chemotaxis and pattern formation
- Semiconductor modeling
- Traffic flow
- Multi-fluid, multi-phase flows, bubbly flow
- Incompressible flow (projection methods or streamfunction vorticity)
- Combustion, detonation waves
- Astrophysics: binary stars, planetary nebulae, jets
- Magnetohydrodynamics, plasmas
- Relativistic flow, black hole accretion
- Numerical relativity --- gravitational waves, cosmology

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#### Generated by

- Earthquakes,
- Landslides,
- Submarine landslides,
- Volcanoes,
- · Meteorite or asteroid impact

There were 97 significant tsunamis during the 1990's, causing 16,000 casualties.

- 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

#### Sumatra event of December 26, 2004

Magnitude 9.1 quake

Rupture along subduction zone  $\approx$  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.



(Similar to Cascadia subduction zone off WA coast)

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# **Tsunami simulations**

#### Movies:

- Fault area
- Bay of Bengal
- Sri Lanka
- Indian Ocean



#### 424.0000 seconds after quake initiation

#### Cross section of Indian Ocean & tsunami

Surface elevation on scale of 10 meters:



Cross-section on scale of kilometers:



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



### Local modeling near Madras





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3rd Int'l workshop on long-wave runup models

Benchmark Problem 2: Scale model of part of coastline of Okushiri Island, site of 1993 tsunami.



Movie of water surface

# Tide gauge 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)

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# 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	$\lambda$	$\mu$	$c_p$	$c_s$
water brass bone "air"	$1000 \\ 8560 \\ 1850 \\ 100$	2190.4 6624.1 9305.5 3 9	0.0 4528.2 3126.5	1.48 1.36 2.9	$0.0 \\ 0.73 \\ 1.3 \\ 0.0$

Cartesian grid cells cut be interface contain averaged values.



# Shock wave therapy simulations



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

- 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
- Papers and simulations:

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