Uncertainty quantification for hyperbolic PDEs

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Lituya Bay Mega Tsunami, Alaska, 1958

- Earthquake induced rockslide tsunami.
- Highest recorded wave run-up: 524 m !!!
- Widely studied.
- Simulation of Asuncion, Castro, SM, Sukys, Sanchez, 2014:

What is needed I: The model

- Two-layer Savage-Hutter (Shallow water) model.

$$
\begin{cases}
\frac{\partial h_1}{\partial t} + \frac{\partial q_1}{\partial x} = 0 \\
\frac{\partial q_1}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q_1^2}{h_1} + \frac{g}{2} h_1^2\right) + g h_1 \frac{\partial h_2}{\partial x} = g h_1 \frac{dH}{dx} + S_f + S_{b_1} \\
\frac{\partial h_2}{\partial t} + \frac{\partial q_2}{\partial x} = 0 \\
\frac{\partial q_2}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q_2^2}{h_2} + \frac{g}{2} h_2^2\right) + r g h_2 \frac{\partial h_1}{\partial x} = g h_2 \frac{dH}{dx} - r S_f + S_{b_2} + \tau.
\end{cases}
\tag{1}
$$

- With
  - Coulomb friction: $\tau = -g(1-r)h_2 \frac{q_2}{|q_2|} \tan(\delta_0)$,
  - Interlayer friction: $S_f = c_f \frac{h_1 h_2}{h_2 + r h_1}(u_2 - u_1)|u_2 - u_1|$

What is needed II: The numerical scheme

- Savage-Hutter equations are Non-conservative hyperbolic system

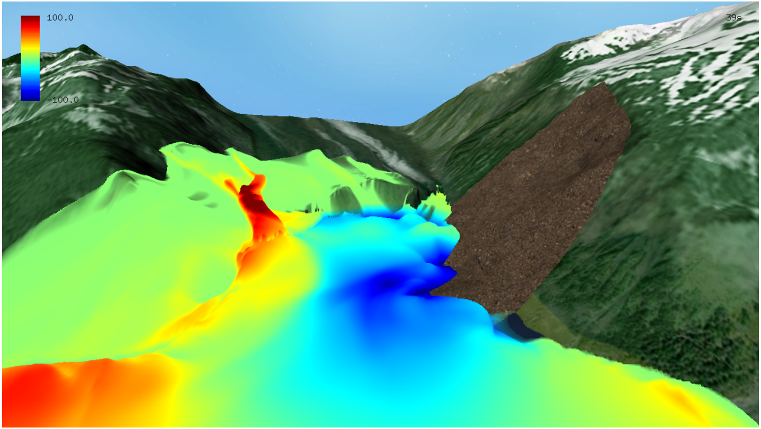
$$\mathbf{U}_t + \mathbf{A}(\mathbf{U})\mathbf{U}_x = 0.$$

- Specially designed Path conservative finite volume scheme
- Need to discretize Non-conservative product carefully.
- Optimized GPU implementation.

What is needed III: Inputs

- Initial data.
- Boundary conditions.
- Model parameters:
  - Acceleration due to gravity g.
  - Interlayer density ratio r
  - Bottom friction parameters $S_{b_{1,2}}$
  - Coulomb friction angle δ_0
  - Interlayer friction parameter c_f

Run-up at $T = 39s$



Critique of the simulation

- Sources of Errors
  - Modeling error

    Savage-Hutter is a good model (checked in the lab).
  - Numerical (discretization) error.
    - Good numerical scheme (Discretization error can be made as small as possible).
  - Measurement (Data) errors:
    - Rather low for initial data and boundary conditions.
    - Unacceptably high for r, c_f, δ_0 (even in the lab !!!)
    - Standard deviation is about 50 percent of mean !!!
- High measurement error $\Rightarrow$ low trust in simulation ?

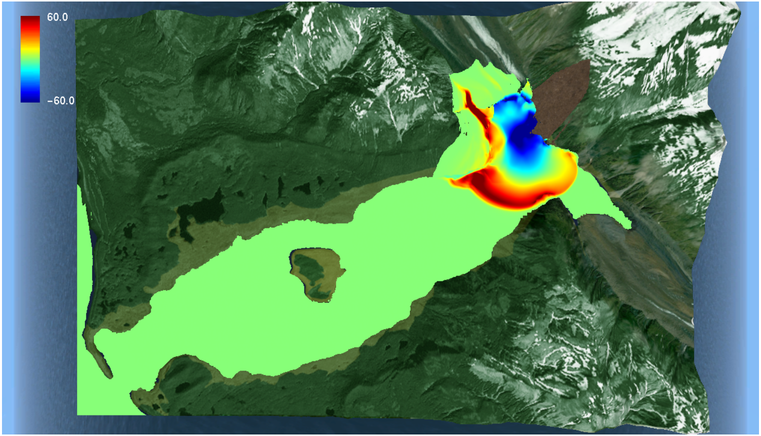
Generic situation in Science and Engineering

- Mathematical modeling of any physical/chemical/biological phenomena:
- Model inputs: are obtained by Measurements:
  - Initial conditions.
  - Boundary data.
  - Coefficients.
  - Parameters.
- Measurements are Uncertain.
- Uncertain Inputs $\Rightarrow$ Uncertain Solutions (Outputs).
- $+$ Many models based on Uncertain Dynamics (high Model $+$ Numerical error).

What is UQ

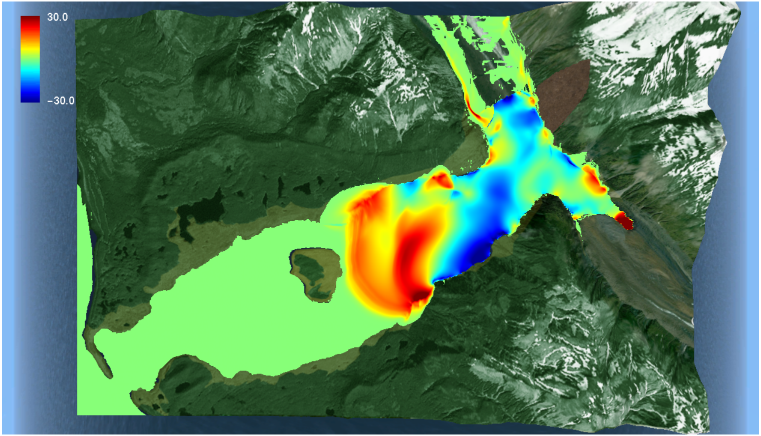
- Uncertainty quantification includes:
  - Modeling of uncertain inputs and dynamics.
  - Efficient Computation of the resulting output uncertainty.
  - Interpretation of the uncertain output.
  - Possible Risk assessment of the process.

Run-up Mean at $T = 39s$

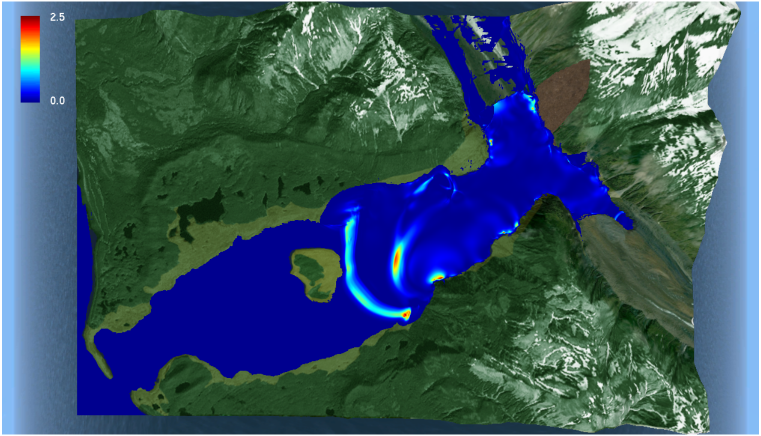


Run-up Variance at $T = 39s$

Run-up Mean at $T = 120s$



Run-up Variance at $T = 120s$



Aims and outline of mini course

- AIM: *To provide a brief overview of UQ for a specific class of PDEs (hyperbolic conservation laws) with a specific class of methods (Statistical sampling (Monte Carlo) methods)*.
- Outline:
  - Brief introduction to Conservation laws.
  - High-resolution finite volume schemes
  - Modeling with Random fields
  - (Multi-level) Monte Carlo methods
  - Measure valued and statistical solutions
  - Massively parallel HPC implementation ?

Conservation laws

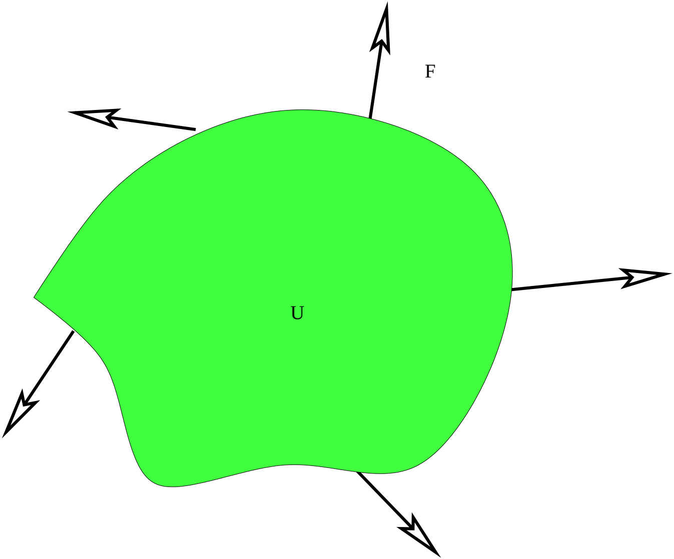
- Let D be a domain.
- Let $\mathbf{U}$ be a quantity of interest.
- $\mathbf{F}$ is flux across the boundary, then

$$\frac{d}{dt}\int_D \mathbf{U} dx = -\int_{\partial D} \mathbf{F}\cdot\mathbf{n} ds.$$

- Using divergence theorem gives,

$$\mathbf{U}_t + \mathrm{div}(\mathbf{F}(\mathbf{U})) = 0,$$

Conservation law



Example: Fluid dynamics

- Euler equations of Compressible fluid dynamics.
- Conservation of mass:

$$\rho_t + \mathrm{div}(\rho \mathbf{u}) = 0.$$

- Conservation of momentum:

$$(\rho \mathbf{u})_t + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u} + p\mathcal{I}) = 0,$$

- Conservation of energy:

$$E_t + \mathrm{div}((E + p)\mathbf{u}) = 0.$$

- Equation of state (Ideal gas):

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho \mathbf{u}^2,$$

Euler equations

- Are a system of conservation laws:

$$
\begin{aligned}
\rho_t + \mathrm{div}(\rho \mathbf{u}) &= 0, \\
(\rho \mathbf{u})_t + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u} + p\mathcal{I}) &= 0, \\
E_t + \mathrm{div}((E + p)\mathbf{u}) &= 0.
\end{aligned}
$$

- Other examples are
  - Shallow water equations (Meterology).
  - MHD equations (Plasma physics).
  - Flows in porous media (Oil reservoirs).
  - Einstein equations (Relativity).
  - Many, many other applications.

Simplest Example: scalar conservation law

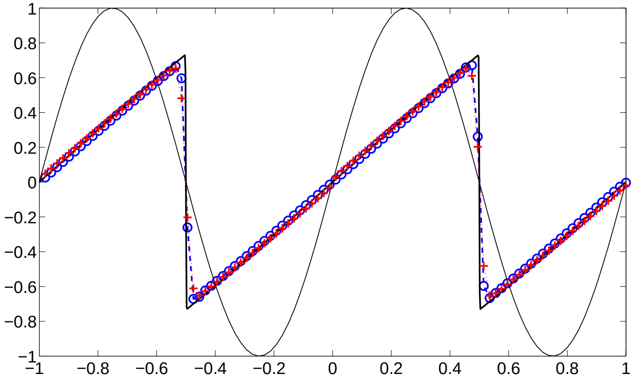
- In one dimension, equation of the form

$$u_t + (f(u))_x = 0,$$

- Solutions: Discontinuities for smooth initial data.
- Shock formation
- Weak solutions: for all test functions φ,

$$\int_D \int_{\mathbb{R}_+} (u\varphi_t + f(u)\varphi_x) dxdt + \int_d u_0(x)\varphi(x,0)dx = 0.$$

Non-linearity ⇒ Shocks



Entropy Solutions

- Weak solutions not necessarily unique.
- Have to be augmented by incorporating Physics – entropy criteria.
- Entropy shouldnot decrease – 2nd law of thermodynamics.
- Entropy solution: For all $\varphi \geq 0 \in C_c^\infty(\mathbb{R} \times \mathbb{R}_+)$, we have

$$\int_D \int_{\mathbb{R}_+} (S(u)\varphi_t + Q(u)\varphi_x) dxdt + \int_D S(u_0)\varphi(x,0)dx \geq 0$$

- Where the pair (S, Q) is the entropy-entropy flux pair satisfying,
  - S, Q are smooth with S convex.
  - $Q' = S'f'$
- Infinitely many entropies for scalar equations !!!
- Entropy solutions exist, are unique and stable in $L^1(D)$.

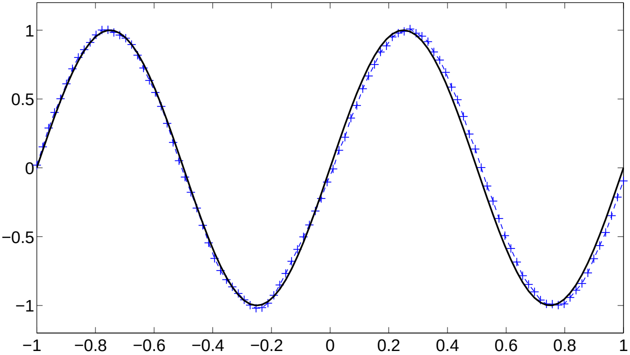
Numerical schemes: Linear advection

- Simplest example of scalar conservation law: $u_t + au_x = 0$
- Simplest Finite difference numerical scheme:
  - Forward Euler in time.
  - Central difference in space.
- Scheme is

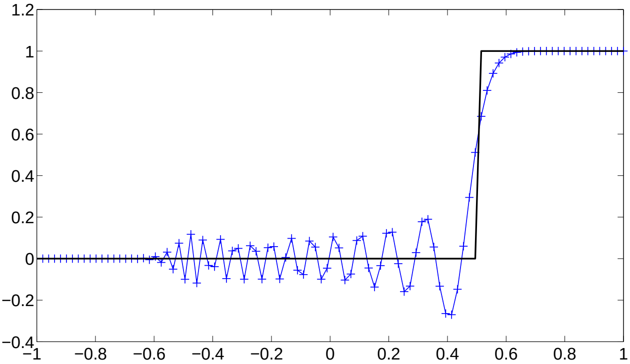
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0.$$

- Unconditionally unstable. Solutions blow up.
- Use Runge-Kutta (RK3) time integrator.

Linear Advection $a = 1$: Smooth solution



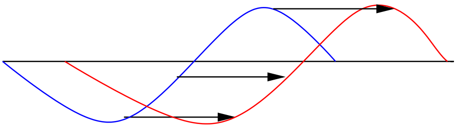
Linear Advection $a = 1$: Discontinuous solution



What goes wrong ?

- Exact solution (constant along Characteristics):

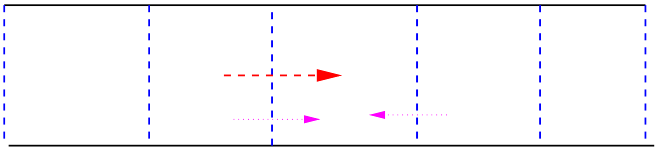
$$u(x,t) = u_0(x - at),$$



- Hyperbolicity:
  - Finite speed of information propagation.
  - Preferred directions of information propagation.
- Generalized to systems by considering real eigenvalues of Jacobian matrix

What goes wrong ?

- Taylor expansion no longer valid near discontinuities
- Direction of propagation is incorrect !!!.



- We need Upwinding.

Upwind finite difference scheme

- Form of the scheme,

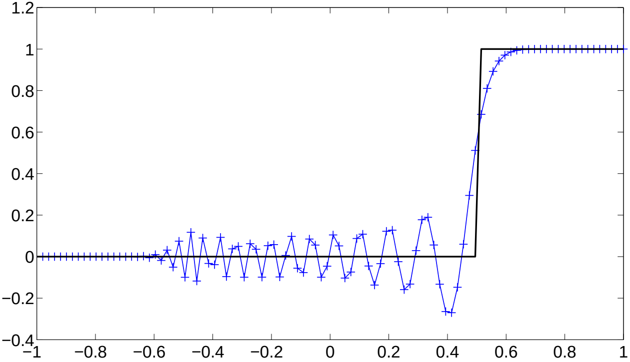
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0.$$

- First order in space and time.
- Proved to converge as $\Delta x \to 0$ if CFL condition is satisfied,

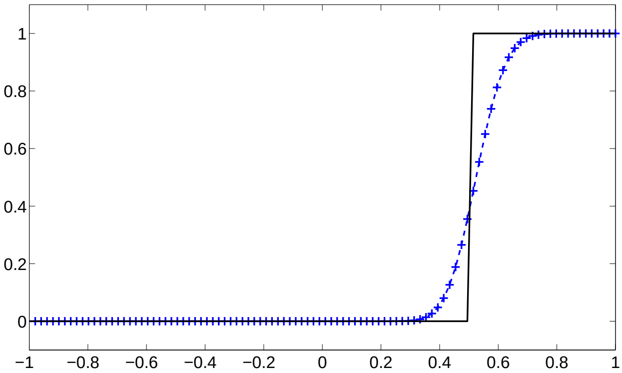
$$a\frac{\Delta t}{\Delta x} \leq 1.$$

- How to upwind for nonlinear equations ?

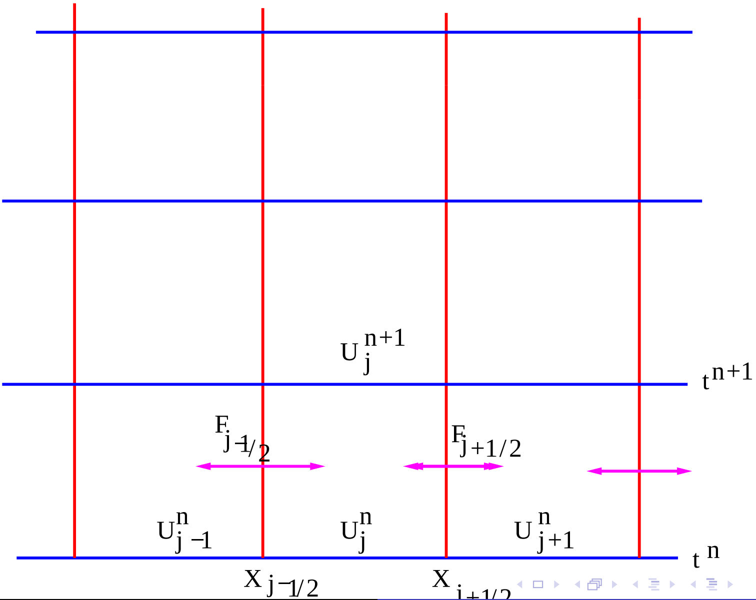
Linear Advection: Discontinuous solution



Linear Advection: Discontinuous solution



The grid



Finite Volume Schemes

- The domain is divided into cells (control volumes).
- Solutions may be discontinuous – methods based on cell averages:

$$u_j^0 = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u(0,x)dx$$

- Cell Average is evolved for each time step.
- Based on conservation inside each volume i.e

$$\frac{d}{dt} \int_{x_{j-1/2}}^{x_{j+1/2}} u^h(x,t) + \frac{1}{\Delta x} f(u^h(x_{j+1/2}+) - f(u^h(x_{j-1/2}-))) = 0$$

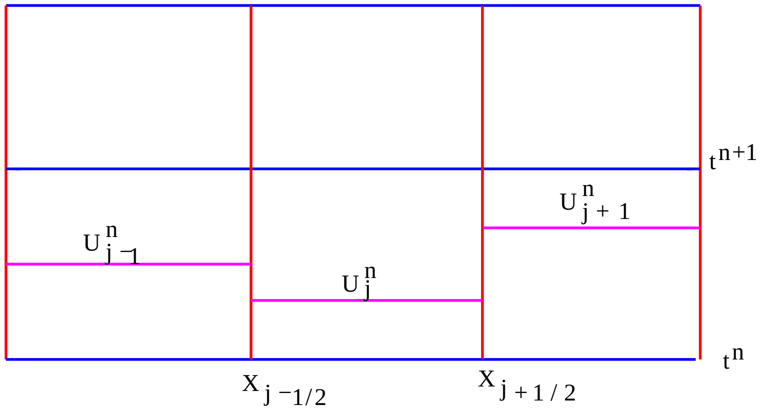
Riemann Solvers a la Godunov

- How to define interface fluxes ?
- At the nth time level and each interface, we have Riemann problems with data,

$$u^h(x,t) = \begin{cases} u_j^n & x < x_{j+1/2} \\ u_{j+1} & x > x_{j+1/2} \end{cases}$$

- Evolve the solution exactly .
- Stop the evolution before neighboring waves interact.
- Average over each cell to obtain u_j^{n+1}.

Riemann Problems



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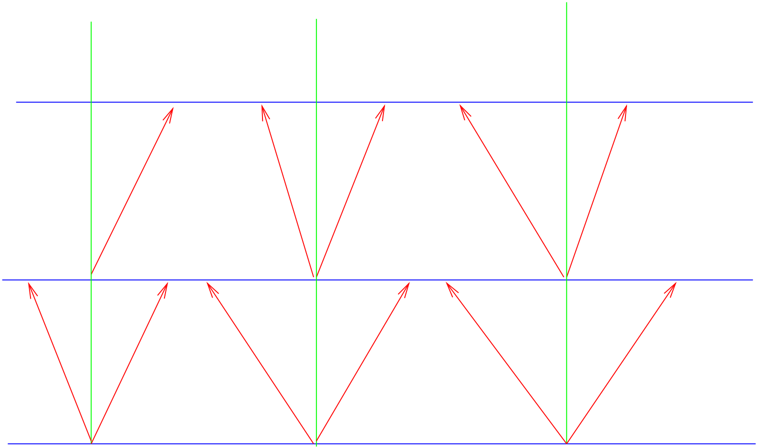

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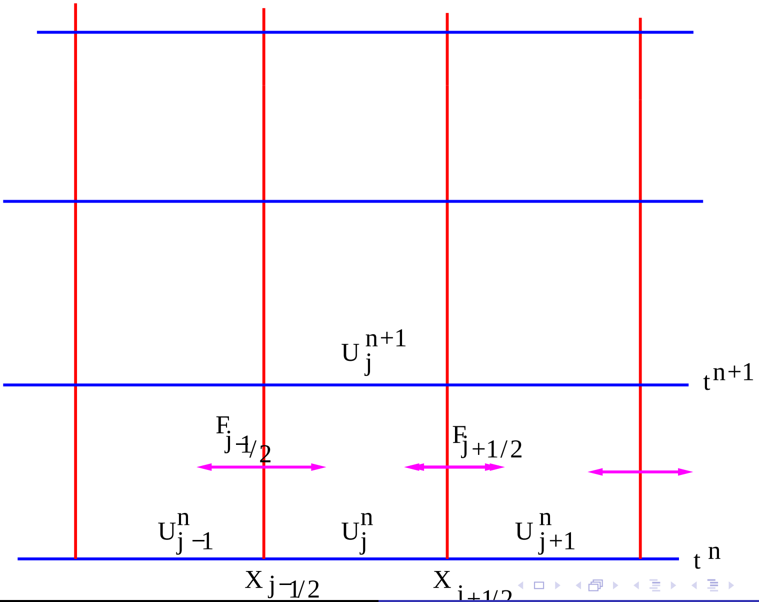
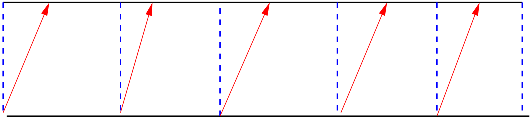


Linear Advection: Riemann solutions



- Form of the resulting scheme (Upwind scheme):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0.$$

Non-linear Equations: Explicit Formula for Godunov scheme

- The final scheme is of the form,

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}(F(u_j^n, u_{j+1}^n) - F(u_{j-1}^n, u_j^n))$$

- Where the interface flux is given by,

$$F_{j+1/2} = F(u_j^n, u_{j+1}^n) = f(u^h(x_{j+1/2}))$$

- Even more explicit formula is given by,

$$F(a,b) = \begin{cases} \min_{\theta \in [a,b]} f(\theta), & \text{if } a \leq b \\ \max_{\theta \in [b,a]} f(\theta), & \text{if } a > b \end{cases}$$

Riemann Solvers (Contd..)

- Use Approximate Riemann solvers instead of full solution of the Riemann problem.
- Example: Roe's scheme based on local linearization.
- Flux given by

$$F^R(a,b) = \begin{cases} f(a) & \text{if} f'(av(a,b)) > 0 \\ f(b) & \text{if} f'(av(a,b)) < 0 \end{cases}$$

- Needs an entropy fix.
- Another Example: Engquist-Osher flux given by,

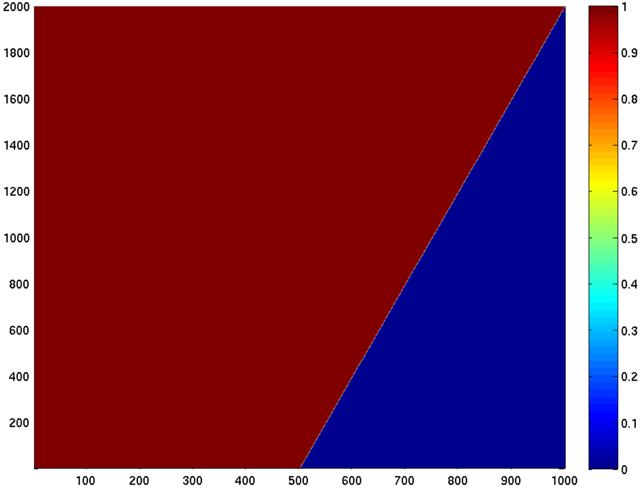
$$F^{EO}(a,b) = 0.5(f(a) + f(b) - \int_a^b |f'(\xi)| d\xi)$$

Convergence analysis

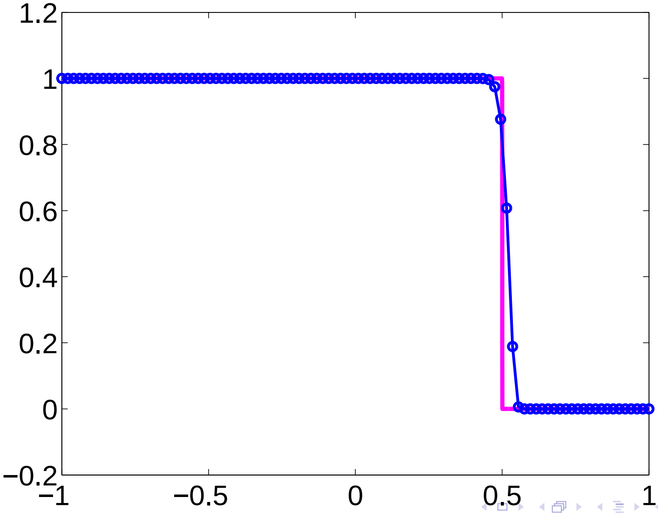
- Schemes are:
  - Formally First-order accurate.
  - Conservative: $\sum_j u_j^{n+1} = \sum_j u_j^n$.
  - Consistent: $F(a,a) = f(a)$
  - Monotone: if $u_j^n \leq v_j^n$ then $u_j^{n+1} \leq v_j^{n+1}$.
  - Discrete L^1 contractive: $\sum |u_j^{n+1} - u_j^n| \leq \sum |u_j^n - u_j^{n-1}|$
  - *TVD*: $\sum |u_{j+1}^{n+1} - u_j^{n+1}| \leq \sum |u_{j+1}^n - u_j^n|$
- Schemes Converge to the entropy solution as $\Delta x \rightarrow 0$.
- Convergence rate:

$$\|u - u^{\Delta x}\|_{L^\infty(\mathbb{R}_+, L^1(D))} \leq C(\Delta x)^{\frac{1}{2}}.$$

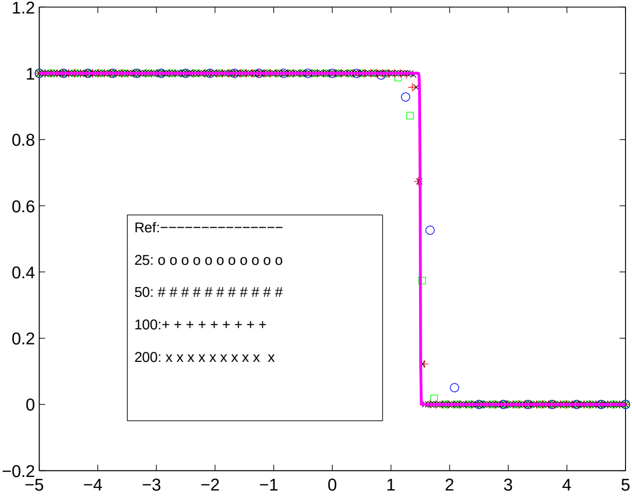
Num Ex:1, space time plot of u with Godunov scheme and $\Delta x = 0.01, CFL = 0.9$



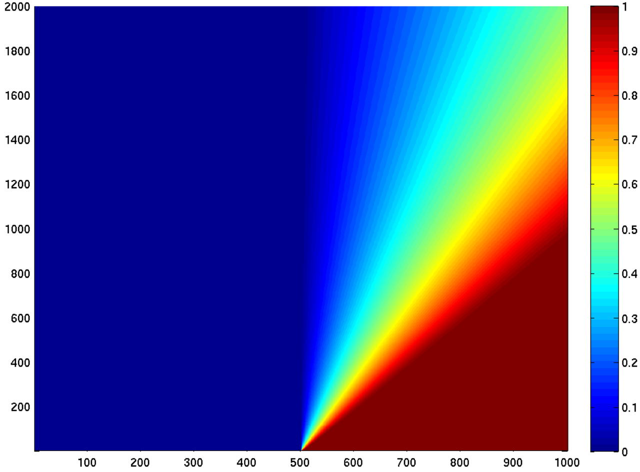
Num Ex:1, u at time $t = 3$ with Godunov scheme and $\Delta x = 0.01, CFL = 0.9$



Effect of Mesh refinement on the Godunov scheme



Num Ex:2, space time plot of u with Godunov scheme and $\Delta x = 0.1, CFL = 0.9$



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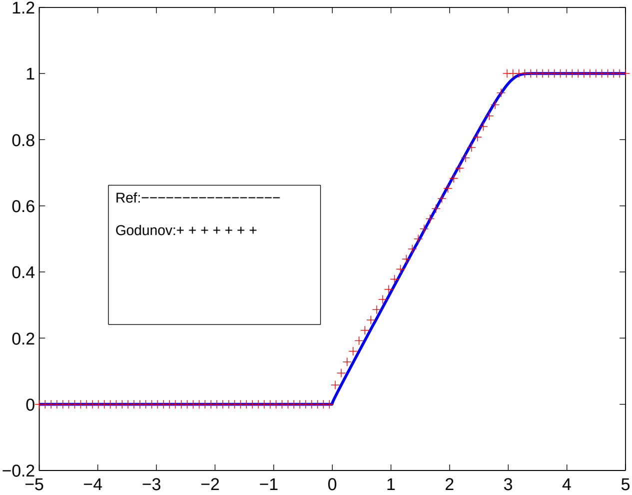


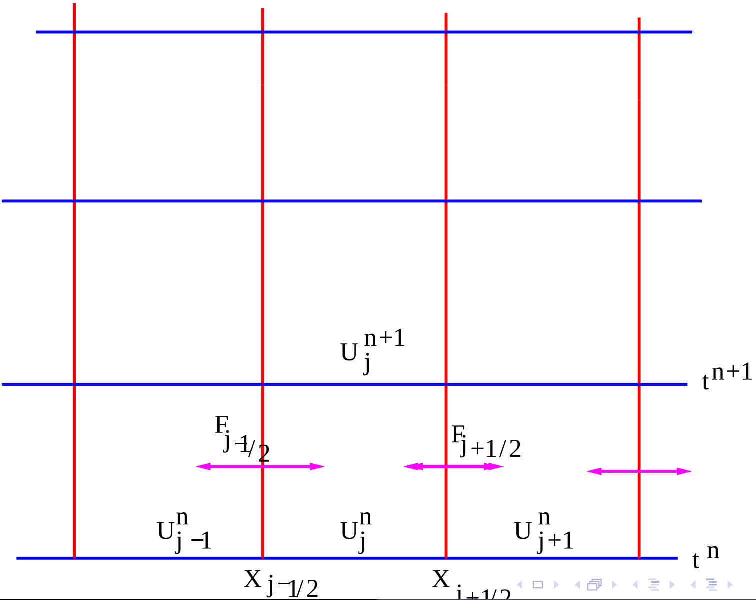
Systems of conservation laws

- Equations of the form,

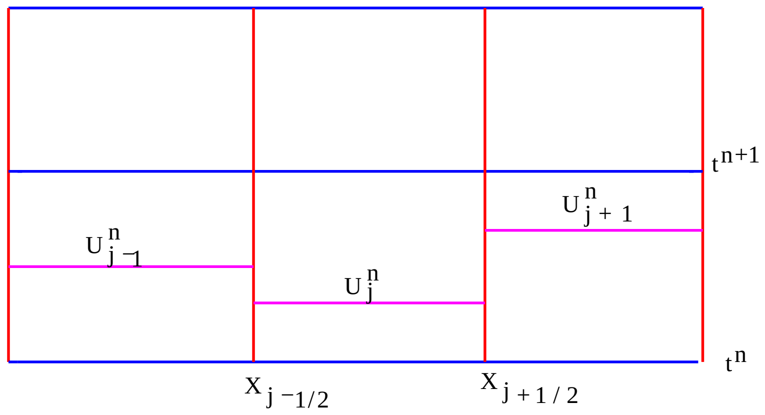
$$\mathbf{U}_t + (\mathbf{f}(\mathbf{U}))_x = 0,$$

- Where
  - $\mathbf{U}$: Vector of unknowns.
  - $\mathbf{f}$: Flux vector.
- Aim: Design numerical schemes to approximate systems.

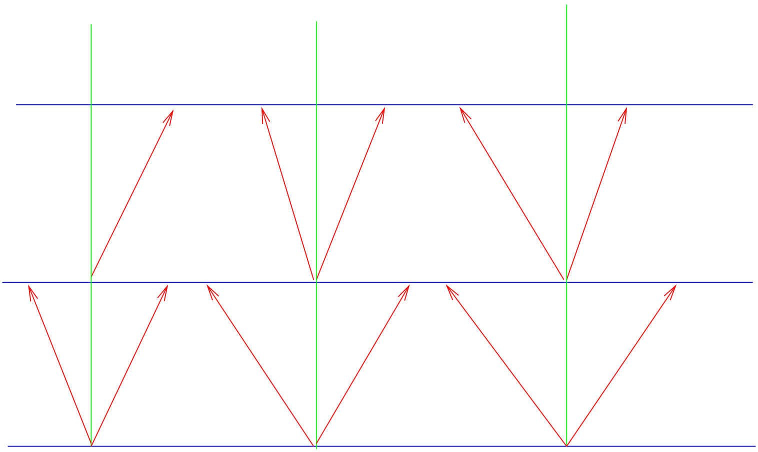
Finite volume grid



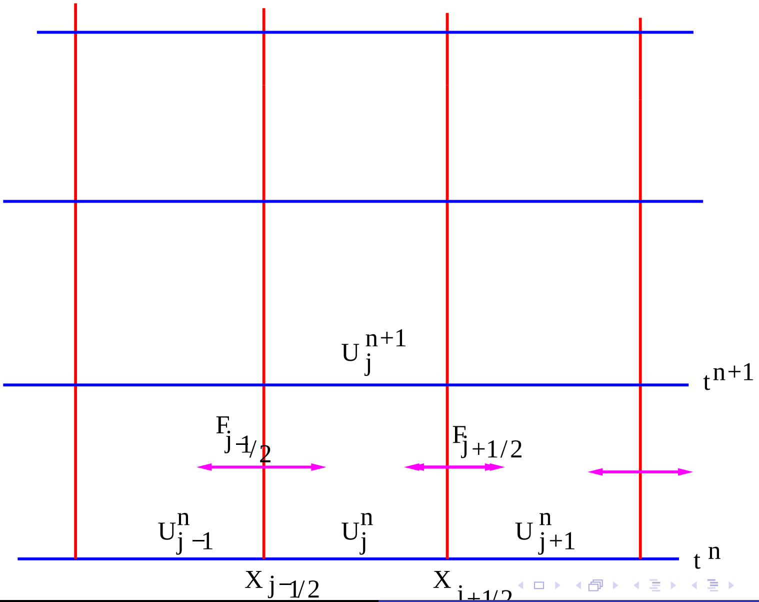
Riemann Problems



Riemann Problems



The grid



Finite volume scheme

- Scheme of form:

$$\mathbf{U}_j^{n+1} = \mathbf{U}_j^n - \frac{\Delta t}{\Delta x}(\mathbf{F}(\mathbf{U}_j^n, \mathbf{U}_{j+1}^n) - \mathbf{F}(\mathbf{U}_{j-1}^n, \mathbf{U}_j^n))$$

- Interface flux:

$$\mathbf{F}_{j+1/2} = \mathbf{F}(\mathbf{U}_j^n, \mathbf{U}_{j+1}^n) = \mathbf{f}(\mathbf{U}^h(x_{j+1/2}))$$

- Exact Riemann solver: Extremely Difficult to obtain explicit formulas !!!

Wave structure

- Linearizing $\mathbf{U}_t + (\mathbf{f}(\mathbf{U}))_x = 0$, about a state

$$\mathbf{U}_t + A\mathbf{U}_x = 0,$$

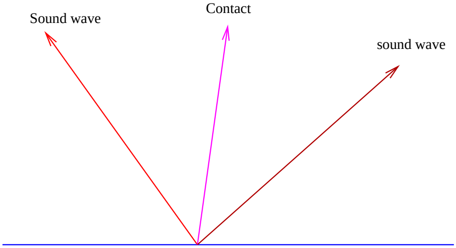
- Wave structure consists of
  - (Real) Eigenvalues of A: wave speeds (hyperbolicity).
  - Eigenvectors: Jumps and states.
- Let $\{\lambda_i, r_i, l_i\}$ be the eigen-system of A, then,

$$\begin{aligned}
\mathbf{U}_t + A\mathbf{U}_x &= 0, \\
\mathbf{U}_t + R\Lambda R^{-1}\mathbf{U}_x &= 0, \\
(R^{-1}\mathbf{U})_t + \Lambda(R^{-1}\mathbf{U})_x &= 0,
\end{aligned}$$

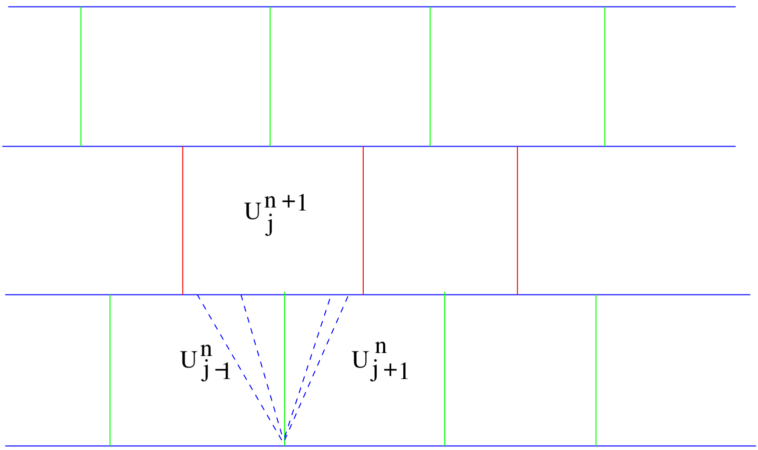
- System solved in terms of the characteristic variables $R^{-1}\mathbf{U}$

Riemann problem for Nonlinear system

- Consists of 3 possible families of Waves:
  - Shocks : Intersecting characteristics, Rankine-Hugoniot conditions.
  - Rarefaction waves: Lipschitz continuous, Self-Similar
  - Contact discontinuity: Parallel characteristics, linear waves.
- Example: Euler equations



Staggered Grid



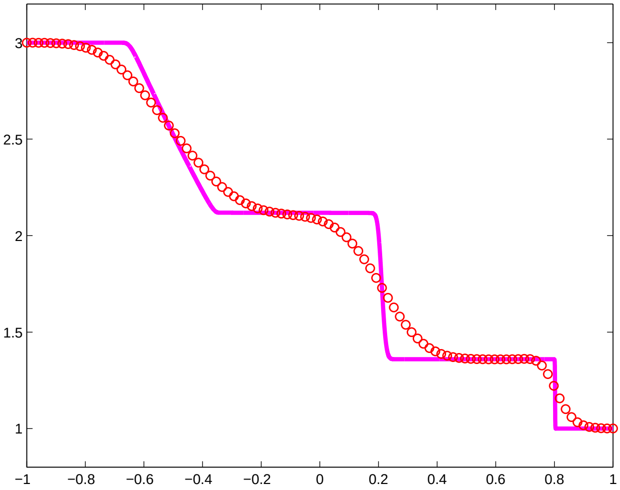
Central Schemes

- The grids at succeding time levels are staggered with respect to each other.
- Riemann problems are solved at each interface but the averaging is over the entire Riemann fan.
- Simplest first order scheme is of the form,

$$\mathbf{U}_j^{n+1} = \frac{1}{2}(\mathbf{U}_{j-1}^n + \mathbf{U}_{j+1}^n) - \frac{\lambda}{2}(\mathbf{F}(\mathbf{U}_{j+1}^n) - \mathbf{F}(\mathbf{U}_{j+1}^n))$$

- Well known Lax-Friedrichs Scheme.
- No explicit details about the Riemann solution are required.

Sod Shock tube: ρ with LxF scheme (100 mesh points)



Linearized Solvers: Roe flux

- Based on quasi-linear form of the equation:

$$\mathbf{U}_t + A(\mathbf{U})\mathbf{U}_x = 0,$$

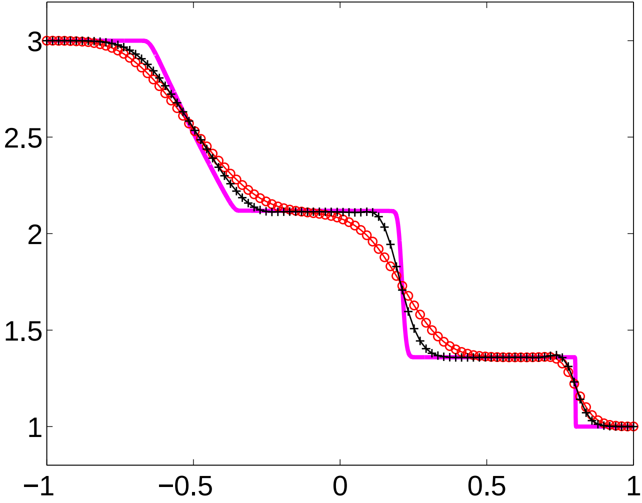
- Find a suitable state such that

$$\mathbf{F}(\mathbf{U}_r) - \mathbf{F}(\mathbf{U}_l) = A(\mathbf{U}_l, \mathbf{U}_r)(\mathbf{U}_r - \mathbf{U}_l),$$

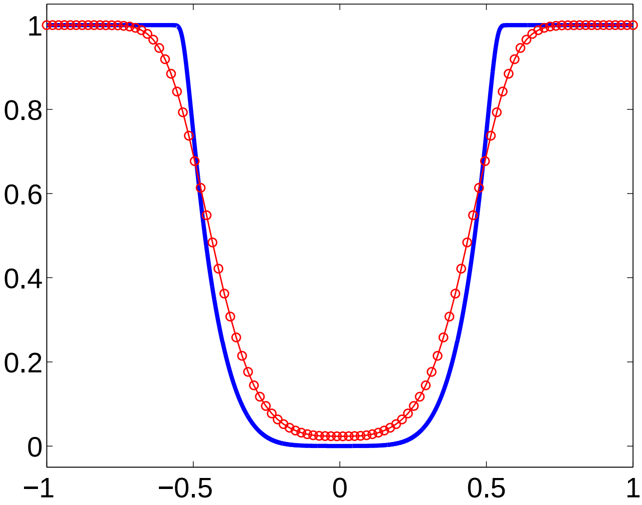
- $A(\mathbf{U}_l, \mathbf{U}_r)$ (Roe Matrix).
- Resulting scheme is

$$\mathbf{F}(\mathbf{U}_j, \mathbf{U}_{j+1}) = \frac{1}{2}(\mathbf{F}(\mathbf{U}_j) + \mathbf{F}(\mathbf{U}_{j+1}) - R_{j+1/2}|\Lambda|_{j+1/2}R^{-1}_{j+1/2}(\mathbf{U}_{j+1} - \mathbf{U}_j))$$

Sod shock tube: Roe vs LxF



Expansion problem: Roe vs. LxF



Non-linear solvers

- Roe solver: Not positivity preserving.
- Have to use non-linear Hartex-Lax-vanLeer (HLL) solvers.
- Approximate Riemann Problem with two-waves.
- Conservation:

$$\mathbf{F}(\mathbf{U}^*) - \mathbf{F}(\mathbf{U}_L) = s_L(\mathbf{U}^* - \mathbf{U}_L),$$
$$\mathbf{F}(\mathbf{U}_R) - \mathbf{F}(\mathbf{U}^*) = s_R(\mathbf{U}_R - \mathbf{U}^*),$$

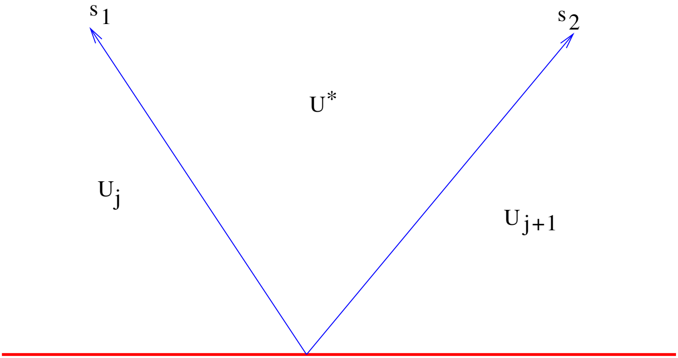
- Middle state:

$$\mathbf{u}^* = \frac{\mathbf{F}(\mathbf{U}_R) - \mathbf{F}(\mathbf{U}_L) - s^R_{j+1/2}\mathbf{U}_R + s^L_{j+1/2}\mathbf{U}_j}{s^L_{j+1/2} - s^R_{j+1/2}}$$

- Choice of wave speeds (Einfeldt)

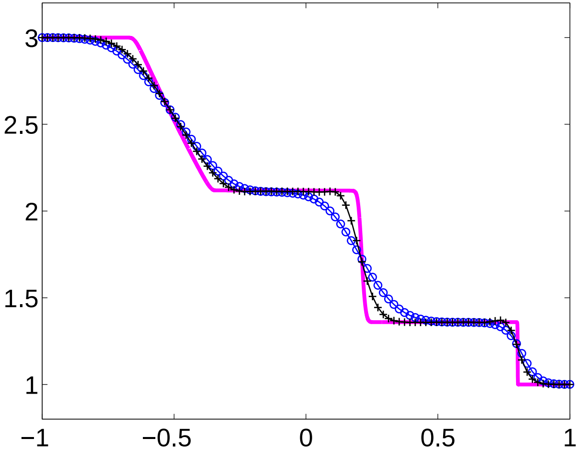
$$s^L_{j+1/2} = \min(\lambda^1_j, \lambda^1_{j+1/2}), \quad s^R_{j+1/2} = \max(\lambda^m_R, \lambda^m_{j+1/2})$$

HLL 2-Wave solver

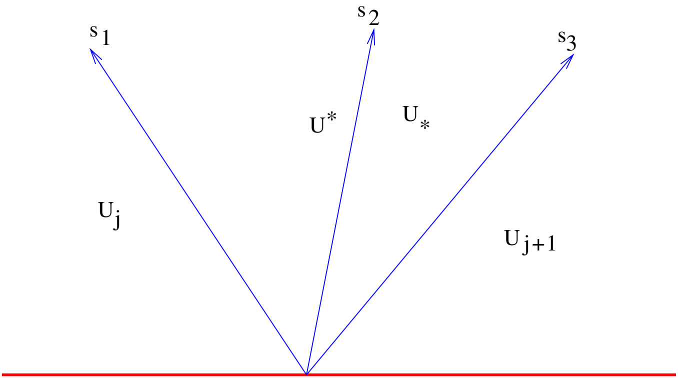


HLL 2 Wave Solver

Sod shock tube



HLL 3-Wave Solver



HLL 3–Wave Solver

HLL 3-wave solver

- Two middle states: $\mathbf{U}^*, \mathbf{U}_*$.
- Conservation equations

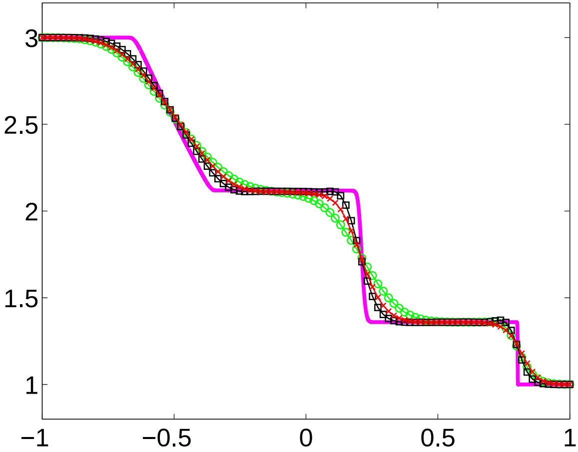
$$\mathbf{F}(\mathbf{U}^*) - \mathbf{F}(\mathbf{U}_L) = s_L(\mathbf{U}^* - \mathbf{U}_L),$$
$$\mathbf{F}(\mathbf{U}_*) - \mathbf{F}(\mathbf{U}^*) = s_M(\mathbf{U}_* - \mathbf{U}^*),$$
$$\mathbf{F}(\mathbf{U}_R) - \mathbf{F}(\mathbf{U}_L) = s_R(\mathbf{U}_R - \mathbf{U}_*),$$

- Middle speed $s_M = u_{L,R}^{\mathrm{Roe}}$.
- Special properties:

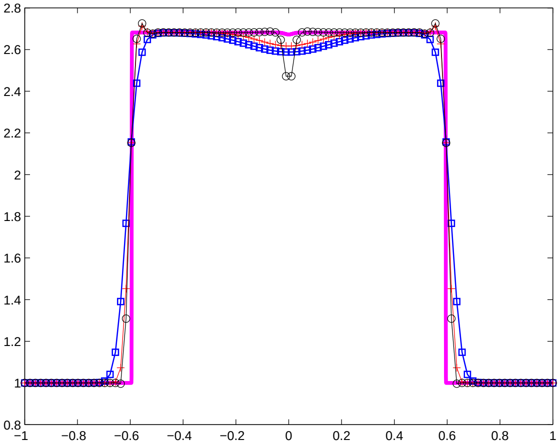
$$u_* = u^* = s_M, \quad p_* = p^*,$$

- Enables a unique solution.

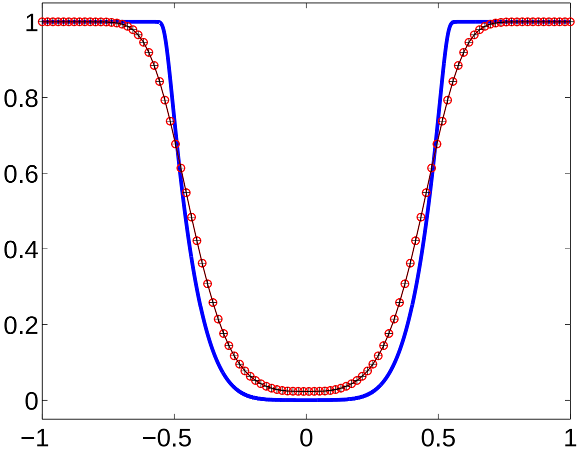
Sod shock tube



Double shocks



Expansion problem



Quality of Stable numerical approximation

- Key Indicator: Order of Accuracy.
- Consider the conservation law,

$$u_t + (f(u))_x = 0,$$

- Numerical scheme of the form,

$$v_j^{n+1} = H_{\Delta x}^{\Delta t}(\cdots, v_{j-1}^n, v_j^n, v_{j+1}^n, \cdots),$$

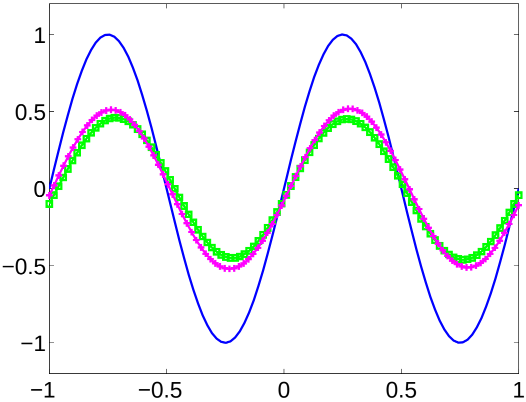
- Exact solution u, let $u(x_j, t^n) = u_j^n$, and

$$|u_j^{n+1} - H_{\Delta x}^{\Delta t}(\ldots, u_{j-1}^n, u_j^n, u_{j+1}^n, \ldots)| \leq C(\Delta x^p + \Delta t^q)$$

- The following orders of accuracy:
  - Spatial order: p,
  - Temporal order: q,

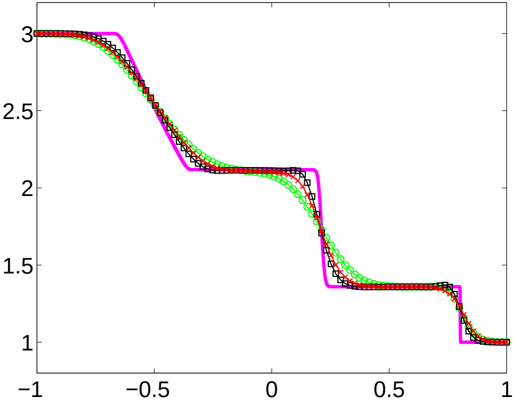
Order of accuracy: Example 1 (Linear advection)

- Upwind scheme is first-order accurate in both space and time !!!

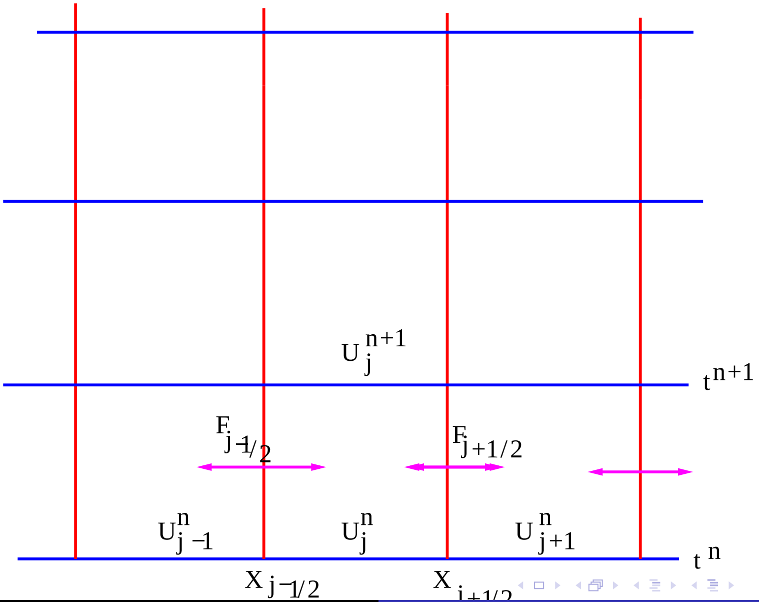


Order of accuracy: Example 2 (Euler Equations)

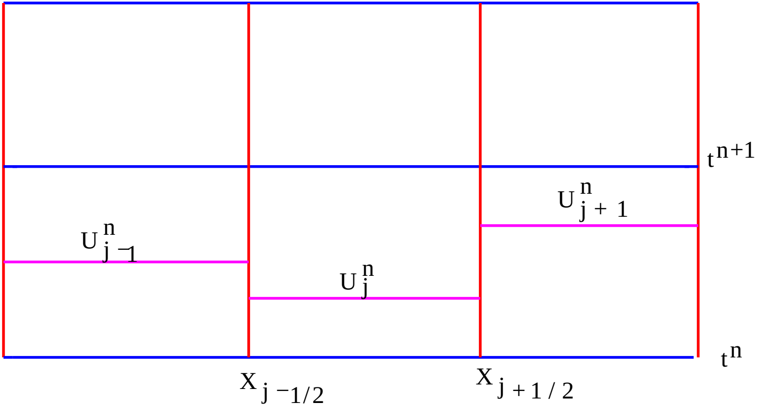
- Riemann solvers are first-order accurate in both space and time !!!



Finite volume grid



Riemann Problems



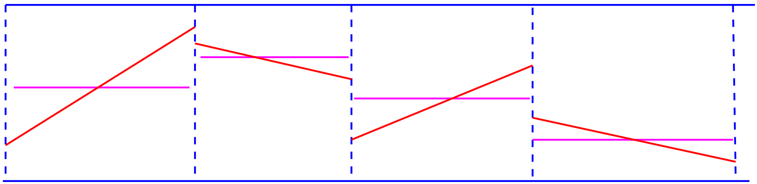
Godunov schemes

- Solution realized as: Cell-averages
- Piecewise constants in each cell.
- Replace Piecewise constants $\mapsto$ Piecewise linears in each cell.
- Given cell-averages u_j, reconstructed polynomial:

$$p_j(x) = u_j + u_j'(x - x_j),$$

- For smooth solutions, $|p_j(x) - u(x)| \leq C\Delta x^2$,
- Conservative reconstruction.

Piecewise-linear Reconstruction



Resulting scheme for $\mathbf{U}_t + (\mathbf{F}(\mathbf{U}))_x = 0$

- Semi-discrete Godunov scheme based on piecewise constants:

$$\frac{d}{dt}(\mathbf{U}_j(t)) + \frac{1}{\Delta x}(\mathbf{F}(\mathbf{U}_j, \mathbf{U}_{j+1}) - \mathbf{F}(\mathbf{U}_{j-1}, \mathbf{U}_j))$$

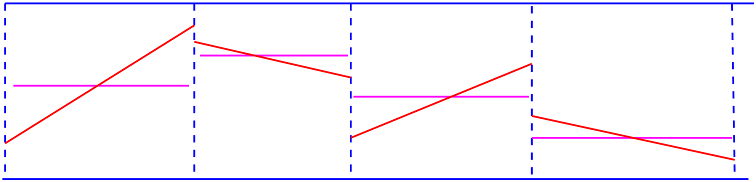
- Define edge values:

$$\mathbf{U}_j^+ = p_j(x_{j+1/2}), \mathbf{U}_j^- = p_j(x_{j-1/2}).$$

- Form of the Second-order scheme,

$$\frac{d}{dt}(\mathbf{U}_j(t)) + \frac{1}{\Delta x}(\mathbf{F}(\mathbf{U}_j^+, \mathbf{U}_{j+1}^-) - \mathbf{F}(\mathbf{U}_{j-1}^+, \mathbf{U}_j^-)) = 0.$$

Piecewise linear Reconstruction



Piecewise-linear Reconstruction

- Choice of Slopes:
  - Backward:
$$\mathbf{U}_j' = \frac{\mathbf{U}_j - \mathbf{U}_{j-1}}{\Delta x}$$
.
  - Forward:
$$\mathbf{U}_j' = \frac{\mathbf{U}_{j+1} - \mathbf{U}_j}{\Delta x}$$
.
  - Central
$$\mathbf{U}' = \frac{\mathbf{U}_{j+1} - \mathbf{U}_{j-1}}{\Delta x}$$
.
- Many, many other choices.

Choice of slope: Linear advection

- Choosing the Forward slope:

$$\frac{u_{j+1} - u_j}{\Delta x}$$

- Edge values,

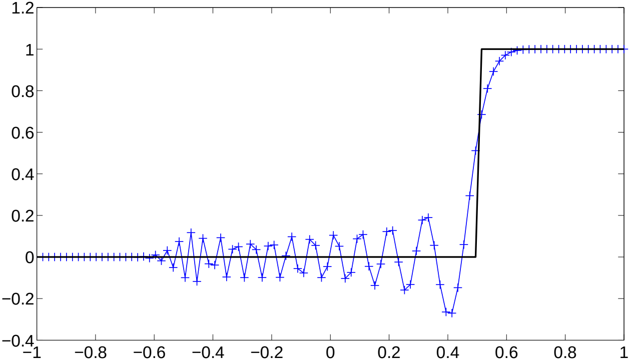
$$u_j^+ = \frac{u_j + u_{j+1}}{2}, u_j^- = \frac{u_{j+1}}{2} - \frac{3}{2}u_j,$$

- Second-order scheme is

$$\frac{d}{dt}u_j + \frac{u_{j+1} - u_{j-1}}{2\Delta x} = 0.$$

- Choice of slope is crucial.

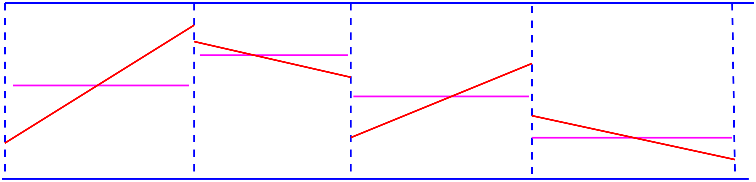
Linear Advection $a = 1$: Discontinuous solution



Clever choice of slopes

- We need non-oscillatory resolution of shocks.
- Reconstruction: Oscillatory for arbitrary choice of slopes.
- We need non-oscillatory reconstruction.
- Total variation: Indicator of oscillations.
- Require TVD piecewise linear reconstruction.

Piecewise linear reconstruction



TVD reconstruction

- Let $p_j(x) = \mathbf{U}_j + \mathbf{U}_j'(x - x_j)$
- Define,

$$(\mathbf{U}^{\Delta x}, p^{\Delta x}) = (\mathbf{U}_j, p_j(x)) \quad \text{if} \quad x_{j-1/2} \leq x < x_{j+1/2},$$

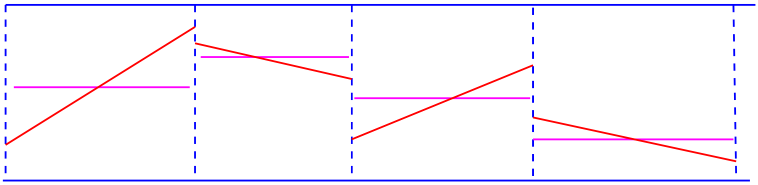
- Aim: Find slopes such that $TV(p^{\Delta x}) \leq TV(\mathbf{U}^{\Delta x})$.
- Solution: Use slope limiters: Minmod limiter:

$$u_j' = \mathrm{minmod}\{\frac{\mathbf{U}_{j+1} - \mathbf{U}_j}{\Delta x}, \frac{\mathbf{U}_j - \mathbf{U}_{j-1}}{\Delta x}\}$$

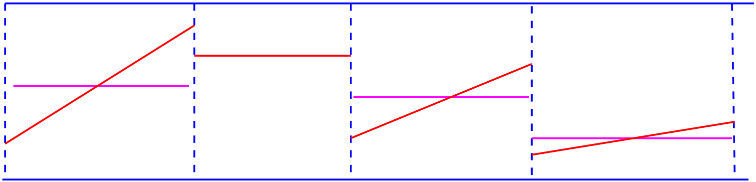
- Where

$$\mathrm{minmod}\{a, b\} = \begin{cases} 0, & \text{if} \quad sgn(a) \neq sgn(b), \\ sgn(a)\min\{|a|, |b|\}, & \text{otherwise}, \end{cases}$$

Piecewise linear Reconstructions



Minmod limiters



Other limiters

- MC limiter (Van Leer):

$$u'_j = M\{\frac{2(u_{j+1} - u_j)}{\Delta x}, \frac{u_{j+1} - u_{j-1}}{2\Delta x}, \frac{2(u_j - u_{j-1})}{\Delta x}\}$$

- Where

$$M\{a, b, c\} = \begin{cases} sgn(a)\min\{|a|, |b|, |c|\}, & \text{if} \quad sgn(a) = sgn(b) = sgn \\ 0, & \text{otherwise}, \end{cases}$$

- Superbee limiter:

Time integration

- Preceding schemes were semi-discrete.
- Can be time marched with Forward Euler.
- Second-order accuracy: Runge-Kutta methods
- Need to use second-order SSP RK methods.
- Developed by Gottlieb, Shu, Tadmor.

SSP:RK-2

- Consider the following semi-discrete scheme,

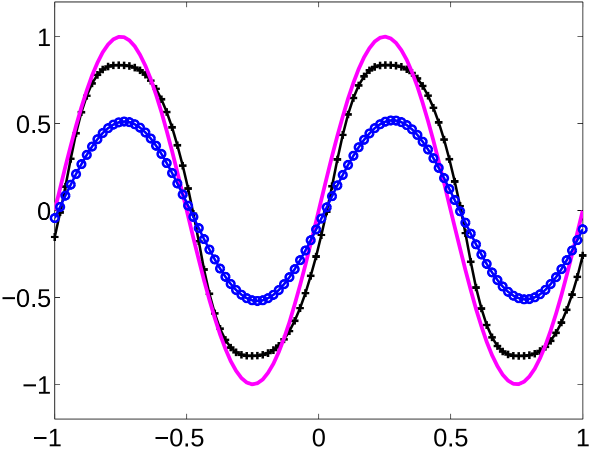
$$\frac{d}{dt}(u_j(t)) = H(u_{j-1}, u_j, u_{j+1}),$$

- SSP-RK2 is of the form,

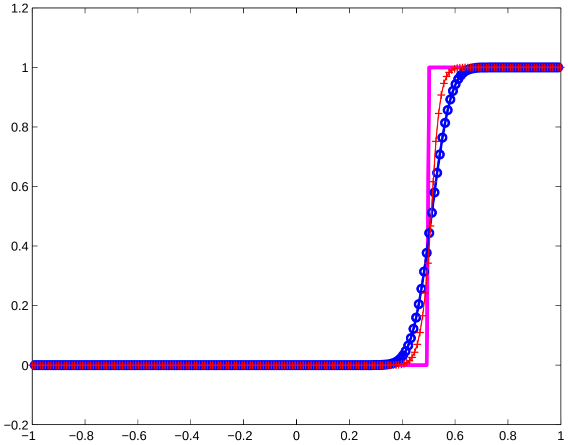
$$\begin{aligned} u_j^* &= u_j^n + \Delta t H(u_{j-1}^n, u_j^n, u_{j+1}^n), \\ u_j^{**} &= u_j^* + \Delta t H(u_{j-1}^*, u_j^*, u_{j+1}^*), \\ u_j^{n+1} &= \frac{1}{2}(u_j^n + u_j^{**}), \end{aligned}$$

- Time-integration is second-order accurate and *TVD*.

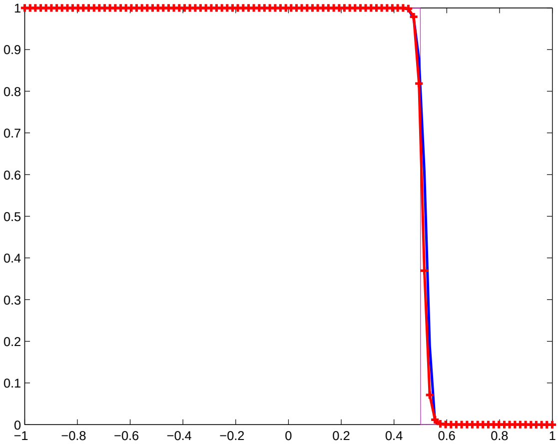
Linear advection: smooth solutions (comparison)



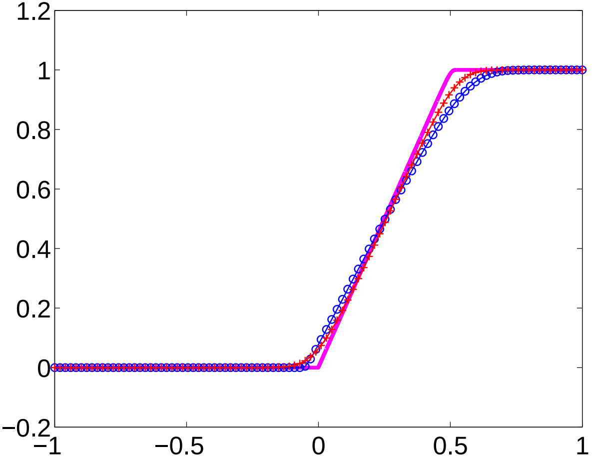
Linear advection: Discontinuities



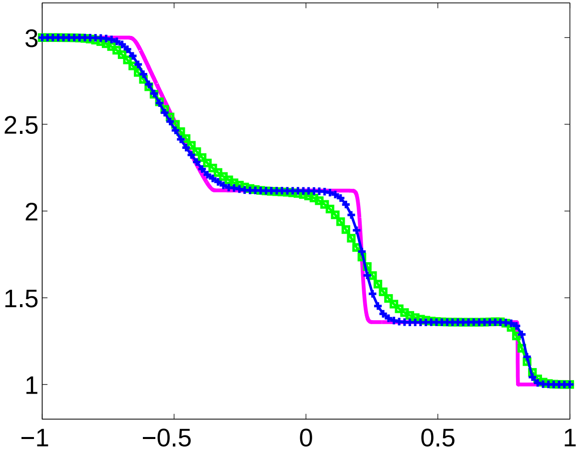
Burgers' equation: Shock



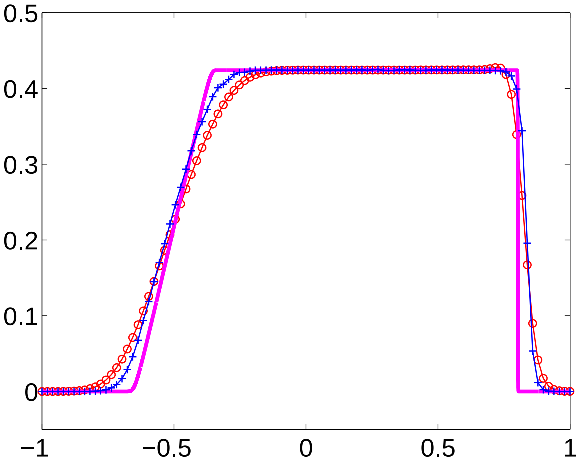
Burgers' equation: Rarefaction



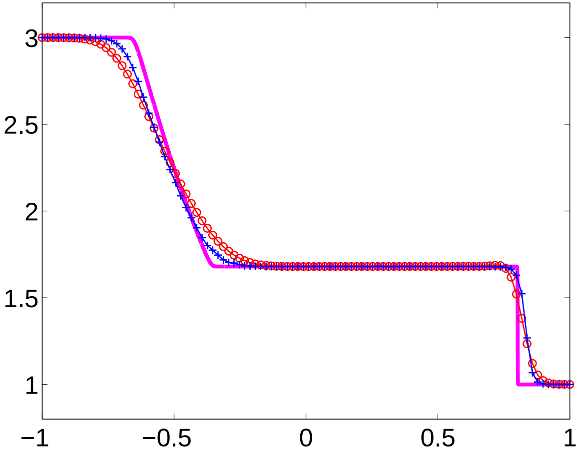
Sod shock tube ρ



Sod shock tube u



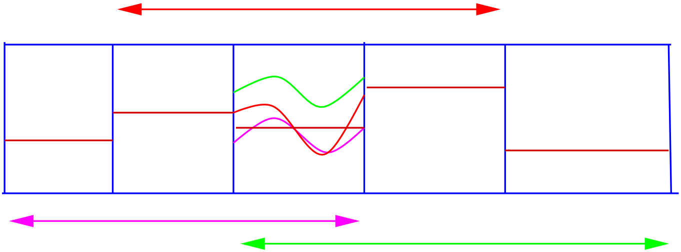
Sod shock tube p



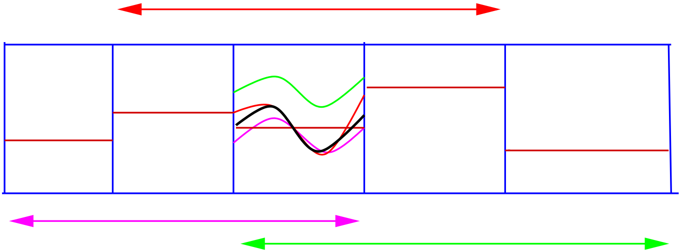
Even Higher-order schemes

- High-order ENO reconstructions Harten,Engquist,Osher, Chakravarty, 1985.
- High-order WENO reconstructions Shu,Osher 1989.
- High-order SSP-RK time-integration routines.

ENO reconstruction



WENO reconstruction



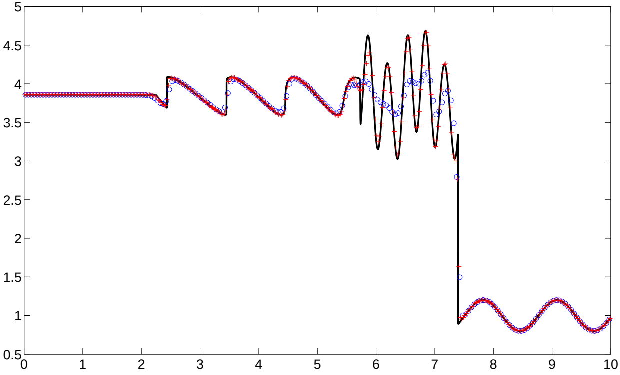
SSP-RK3

- Consider the following semi-discrete scheme,

$$\frac{d}{dt}(U_j(t)) = \mathcal{L}(U_j),$$

$$\begin{aligned}
U_j^{*} &= u_j^{n} + \Delta t \mathcal{L}(U_j^{n}) \\
U_j^{**} &= \frac{3}{4}U_j^{n} + \frac{1}{4}U_j^{*} + \frac{\Delta t}{4}\mathcal{L}(U_j^{*}) \\
U_j^{n+1} &= \frac{1}{3}U_j^{n} + \frac{2}{3}U_j^{**} + \frac{2\Delta t}{3}\mathcal{L}(U_j^{**}).
\end{aligned}$$

Shock-Turbulence interaction for Euler equations: Minmod vs. WENO5



Finite volumes in multi-dimensions

- Consider a 2-D conservation law,

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x + \mathbf{G}(\mathbf{U})_y = 0.$$

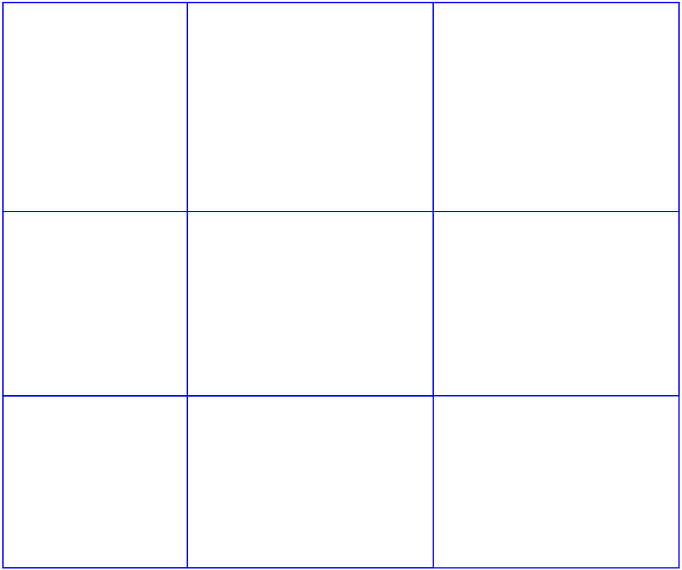
- The domain is divided into cells (control volumes).
- Consider a Cartesian mesh.
- Denote cell average as

$$\mathbf{U}_{i,j}(t) = \frac{1}{\Delta x \Delta y} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \mathbf{U}(x,y,t)dxdy,$$

- Integrating the conservation law over each cell,

$$\begin{aligned}\frac{d}{dt}\mathbf{U}_{i,j} = & \int_{y_{j-1/2}}^{y_{j+1/2}} (\mathbf{F}(\mathbf{U}(x_{i+1/2},y,t)) - \mathbf{F}(\mathbf{U}(x_{i-1/2},y,t)))dy \\ & + \int_{x_{i-1/2}}^{x_{i+1/2}} (\mathbf{G}(\mathbf{U}(x,y_{j+1/2},t)) - \mathbf{G}(\mathbf{U}(x,y_{j-1/2},t)))dx\end{aligned}$$

2-D Cartesian grid



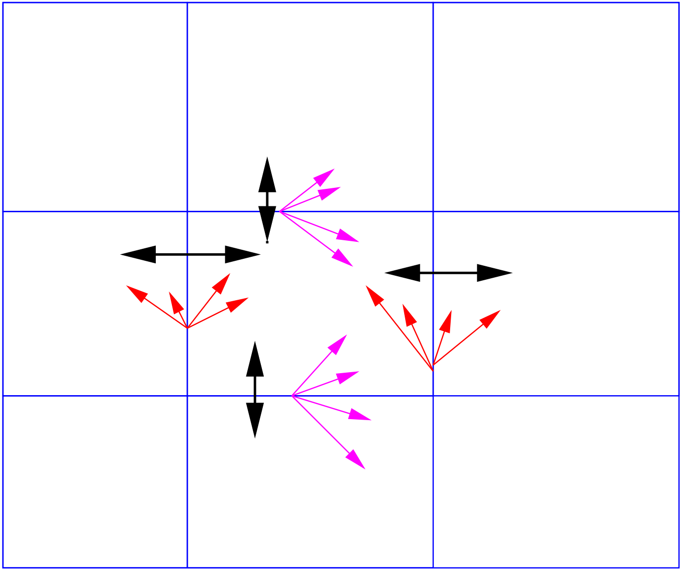
2D finite volumes

- Have to approximate interface fluxes.
- Solve Riemann problems in the normal direction
- Final form of the scheme,

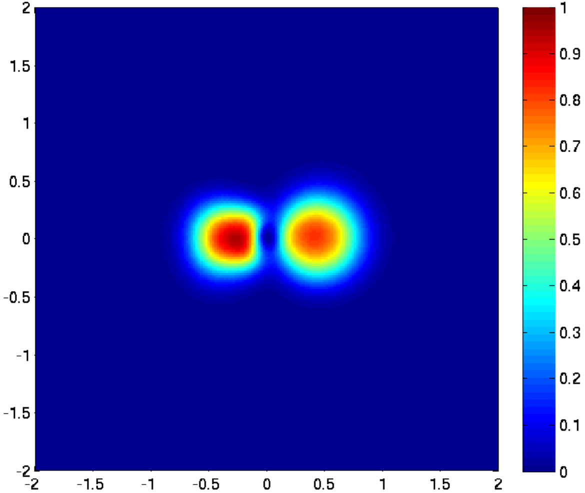
$$\frac{d}{dt}\mathbf{U_{i,j}} = -\frac{1}{\Delta x}(\mathbf{F}(\mathbf{U}_{i,j}, \mathbf{u}_{i+1,j}) - \mathbf{F}(\mathbf{u}_{i-1,j}, \mathbf{u}_{i,j})) - \frac{1}{\Delta y}(\mathbf{G}(\mathbf{u}_{i,j}, \mathbf{u}_{i,j+1}) - \mathbf{G}(\mathbf{u}_{i,j-1}, \mathbf{u}_{i,j})),$$

- $\mathbf{F}, \mathbf{G}$ are numerical fluxes in x- and y- directions.
- Defined by Exact or Approximate Riemann solvers in normal direction.

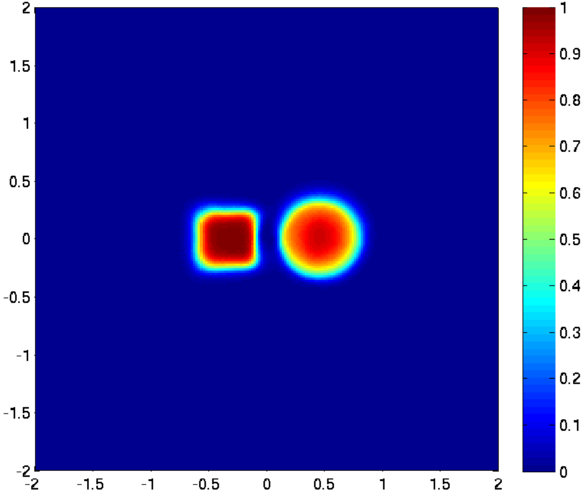
Normal Riemann problems



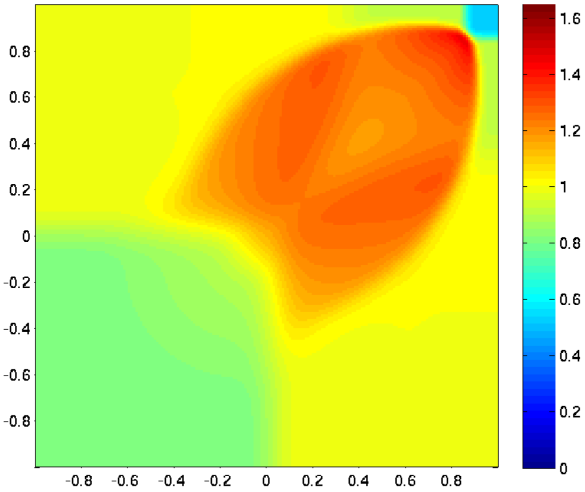
$2-D$ inhomogenous advection with rotation: First order



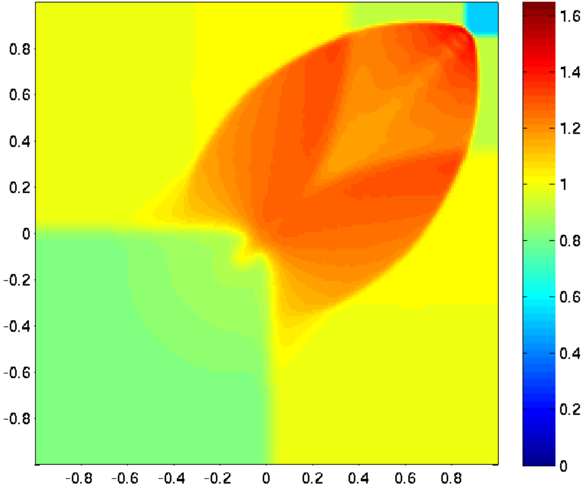
$2 - D$ inhomogenous advection with rotation: Second order



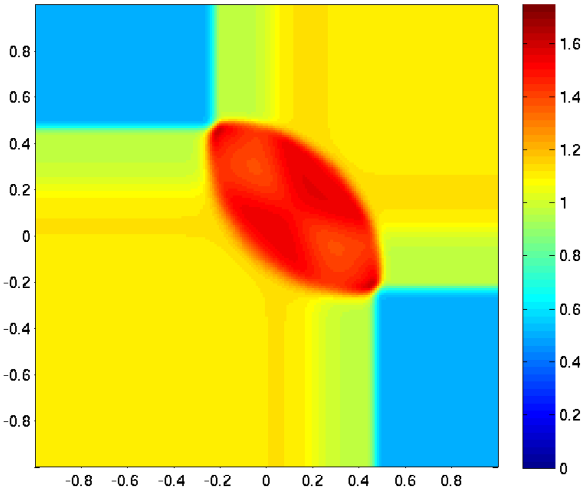
$2-D$ Euler: Mach vs. Regular reflection (First order)



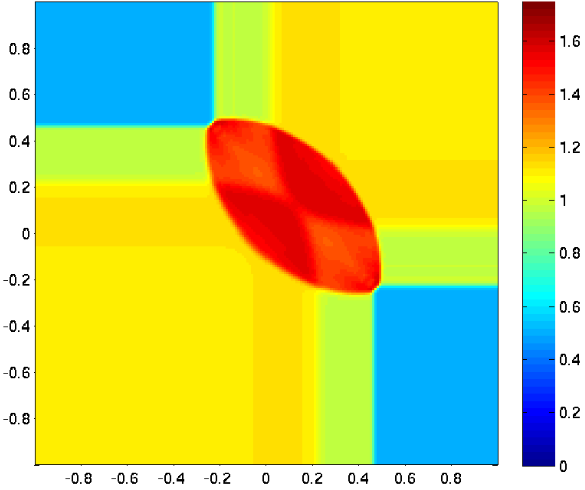
$2-D$ Euler: Mach vs. Regular reflection (Second order)



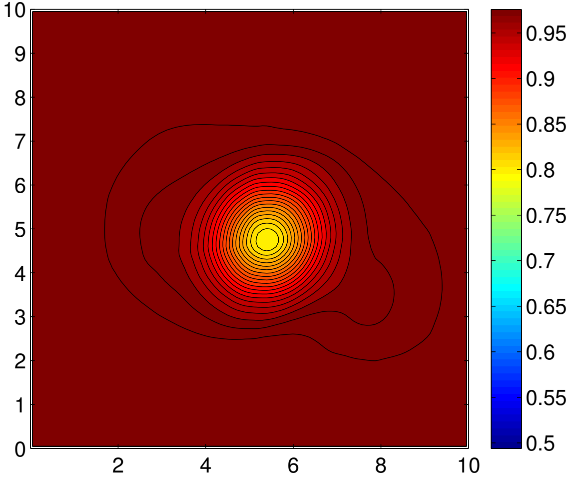
$2-D$ Euler: 2-Contact, 2-Rarefaction (First order)



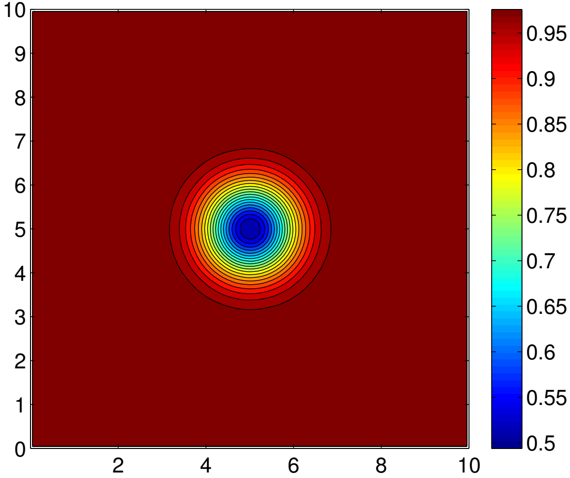
$2-D$ Euler: 2-Contact, 2-Rarefaction (Second order)



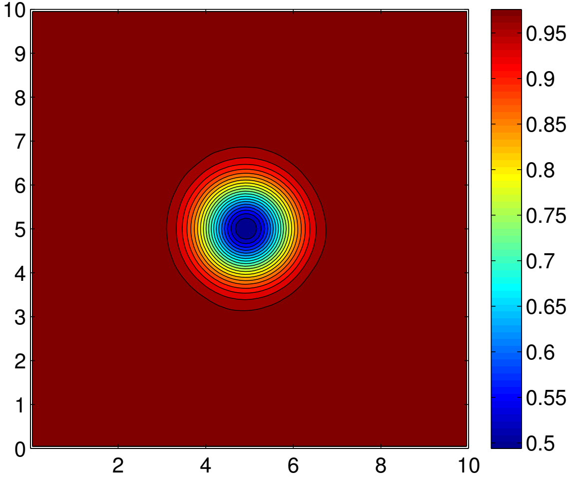
Advection of Euler vortex: TeCNO2



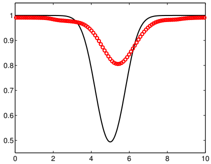
Advection of Euler vortex:TeCNO3



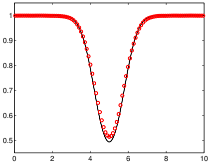
Advection of Euler vortex: TeCNO4



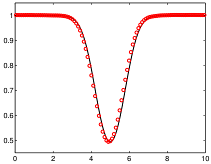
Advection of Euler vortex



(a) TeCNO2

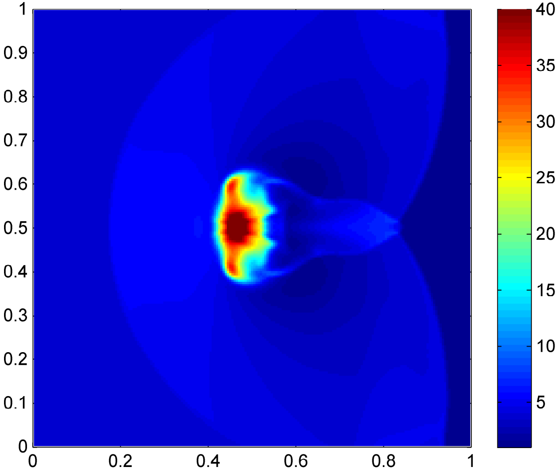


(b) TeCNO3

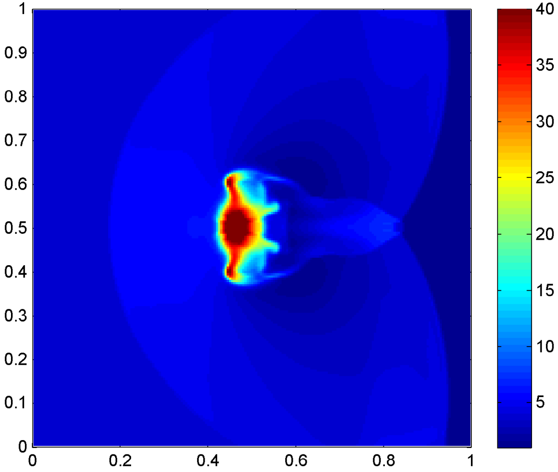


(c) TeCNO4

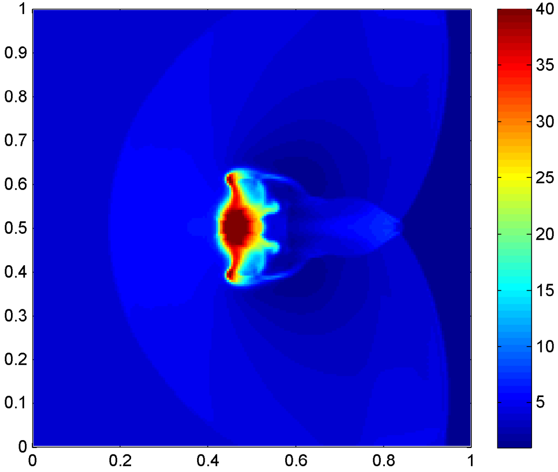
Euler: Cloud-Shock interaction: TeCNO2



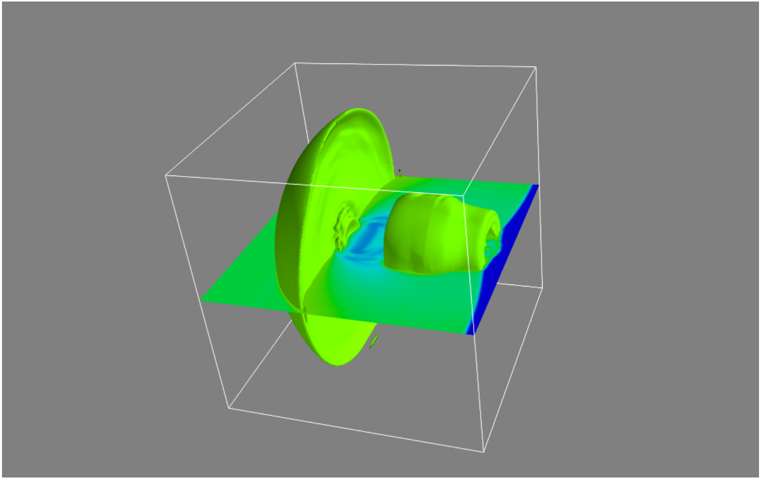
Euler: Cloud-Shock interaction: TeCNO3



Euler: Cloud-Shock interaction: TeCNO4



Euler: 3-D Cloud-Shock Interaction



Ideal MagnetoHydroDynamics (MHD) equations

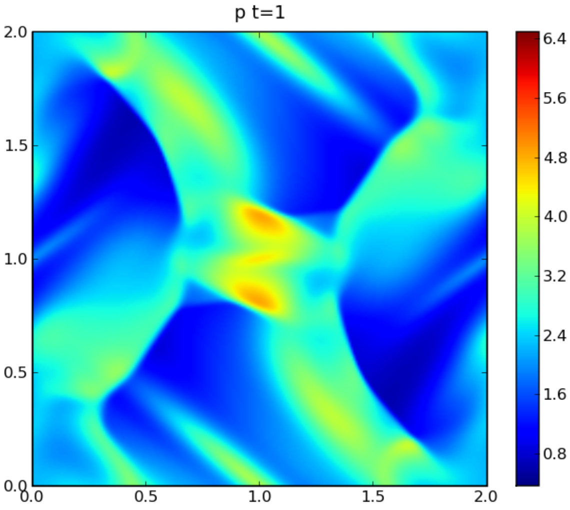
- $$\begin{aligned} \rho_t + \mathrm{div}(\rho \mathbf{u}) &= 0, \\ (\rho \mathbf{u})_t + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u} + (p + \frac{1}{2}|\mathbf{B}|^2)I - \mathbf{B} \otimes \mathbf{B}) &= 0, \\ E_t + \mathrm{div}((E + p + \frac{1}{2}|\mathbf{B}|^2)\mathbf{u} - (\mathbf{u} \cdot \mathbf{B})\mathbf{B}) &= 0, \\ \mathbf{B}_t + \mathrm{div}(\mathbf{u} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{u}) &= 0, \\ \mathrm{div}(\mathbf{B}) &= 0. \end{aligned}$$

- Together with equation of state

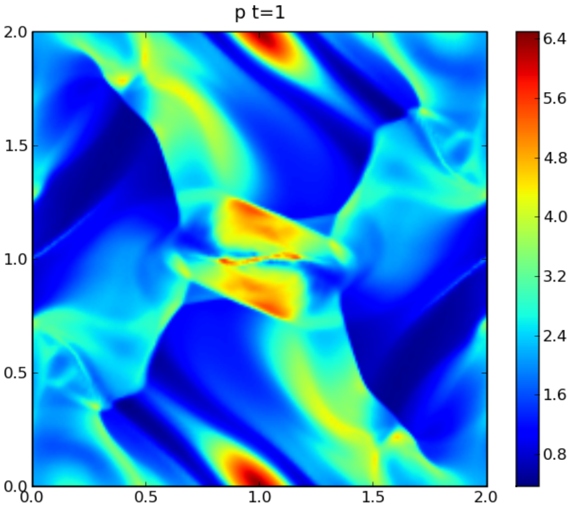
$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{1}{2}|\mathbf{B}|^2,$$

- Usual form of MHD in practice.

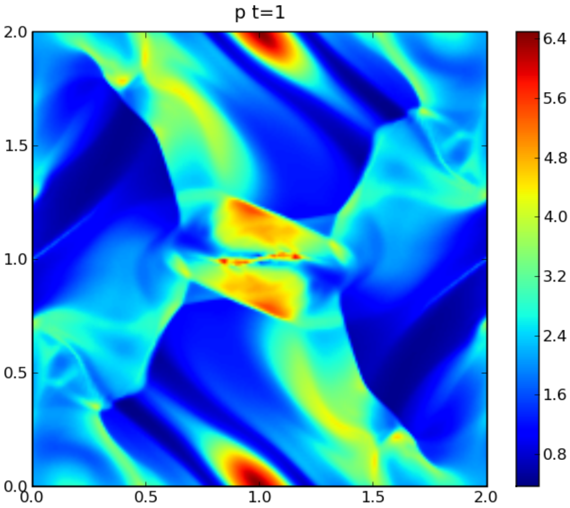
Orszag-Tang Vortex: Pressure (200 $\times$ 200 mesh) Ist Order



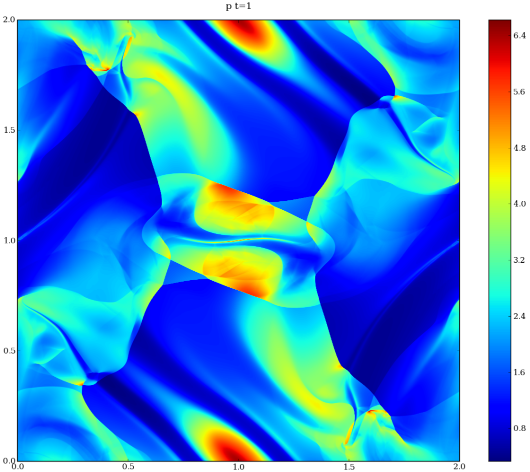
Orszag-Tang Vortex: Pressure (200 $\times$ 200 mesh) ENO



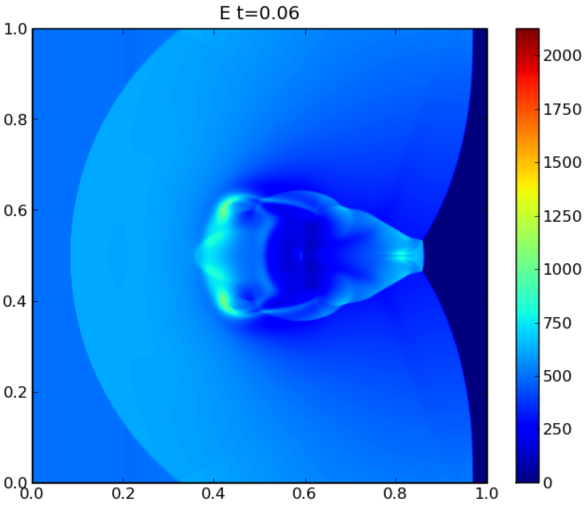
Orszag-Tang Vortex: Pressure (200 $\times$ 200 mesh) WENO



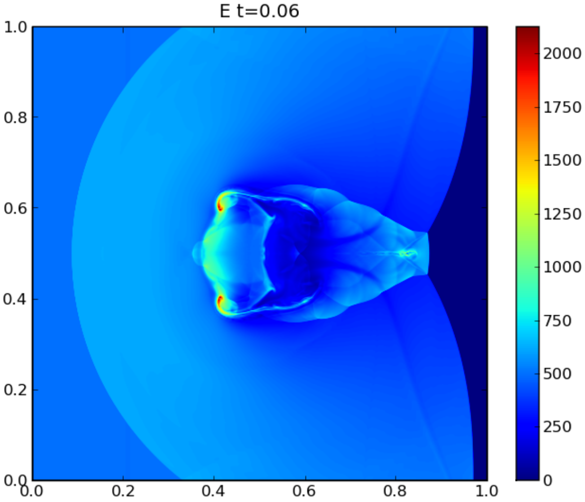
Highly resolved solution: WENO on 4000 × 4000 mesh



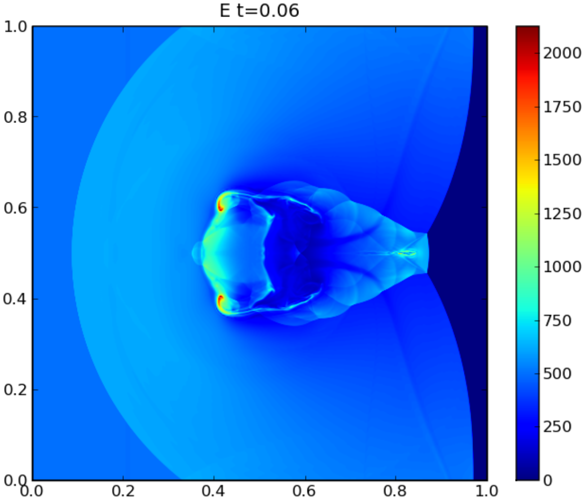
Cloud shock interaction: Energy (1600 × 1600 mesh) Ist Order



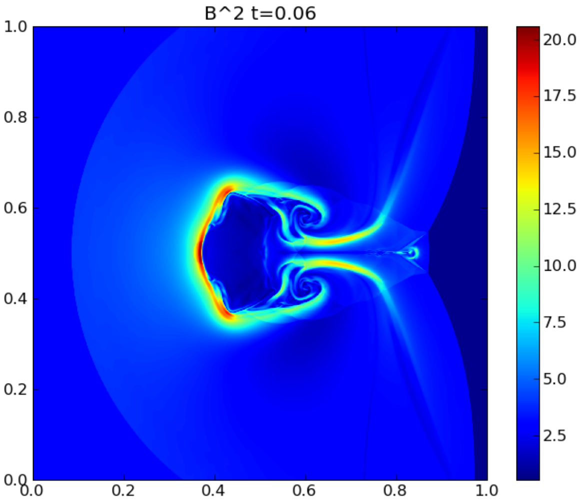
Cloud shock interaction: Energy (1600×1600 mesh) ENO



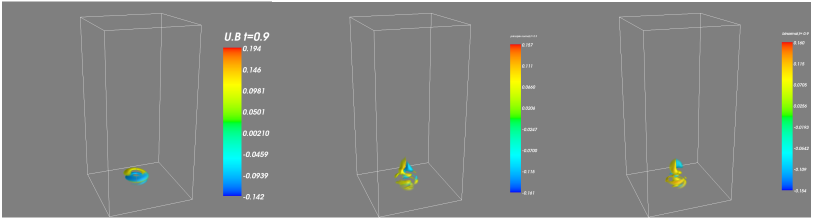
Cloud shock interaction : Energy (1600 × 1600 mesh) WENO



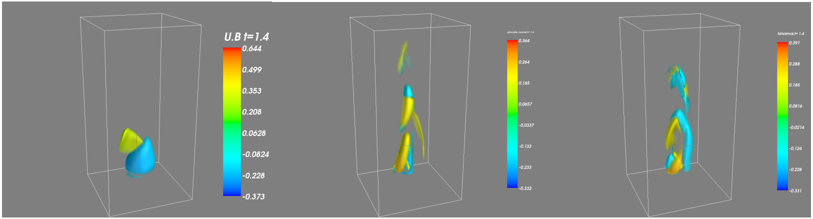
Cloud shock interaction : Magnetic pressure (4000×4000 mesh)



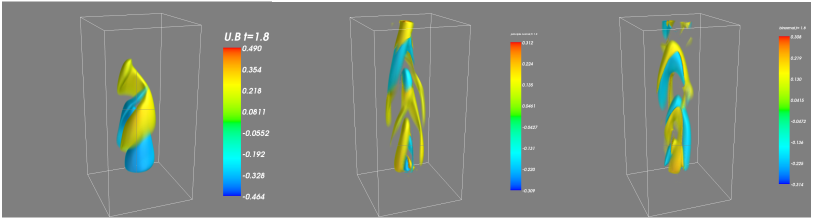
Alfven wave simulation: $T = 0.9$



Alfven wave simulation: $T = 1.4$



Alfven wave simulation: $T = 1.8$



$$\begin{aligned}\mathbf{U}_t + \mathrm{div}(\mathbf{F}(k(x,t),\mathbf{U})) &= S(x,t,\mathbf{U}),\\ \mathbf{U}(x,0) &= \mathbf{U}_0(x),\\ \mathbf{U}|_{\partial D} &= \mathbf{U}_b(x,t).\end{aligned}$$

- Uncertainty in determining:
  - Flux Coefficients (Equations of state, Material properties of porous media)
  - Initial data (Initial wave displacement in tsunamis)
  - Source terms (Bottom topography in shallow water waves)
  - Boundary data (Plasma circuit breakers)
- UQ: Given uncertainty in inputs $\Rightarrow$ Compute uncertainty in the solution.

Issues

- How to model uncertainty in inputs ??
- Mathematical framework for uncertain solutions.
- Efficient numerical methods for UQ.

Modeling Input Uncertainty

- Use the Probabilistic framework a la Kolmogorov.
- Complete Probability space:
  - Ω (Set of Outcomes)
  - Σ (σ-algebra (field) of Events)
  - $\mathbb{P} : \Omega \mapsto [0, 1]$ with $\mathbb{P}(\Omega) = 1$ (Probabilty measure).

Random fields

- Use Random fields to model Uncertain:
  - Initial data.
  - Boundary conditions.
  - Fluxes.
  - Sources.
- $(\Omega, \Sigma, \mathbb{P})$ is a complete probability space.
- Random field $\mathbf{U} : (\Omega, \Sigma) \mapsto (\mathcal{F}, \mathcal{B}(\mathcal{F}))$ measurable
- $\mathcal{F}$ is a function space (separable Banach space) with Borel σ-algebra $\mathcal{B}(\mathcal{F})$
- For $\omega \in \Omega$, $\mathbf{U}(\omega) \in \mathcal{F}$.
- Example: Random initial data (scalar conservation laws):

$$u_0 : (\Omega, \Sigma) \mapsto (L^1(\mathbb{R}^d), \mathcal{B}(L^1(\mathbb{R}^d)))$$
$$u_0(., \omega) \in L^\infty(\mathbb{R}^d) \cap BV(\mathbb{R}^d), \mathbb{P} - a.s.$$

Representation of Random fields I: Parametric representation

- Random field represented by a finite number of parameters (Random Variables).
- Example I: Euler equations – Sod Shock tube – Uncertain initial location + amplitude:

$$
\mathbf{U}_0(x,\omega) = \begin{cases} \mathbf{U}_l + \alpha(\omega) & \text{if} \quad x \leq \beta(\omega), \\ \mathbf{U}_r & \text{if} \quad x > \beta(\omega), \end{cases}
$$

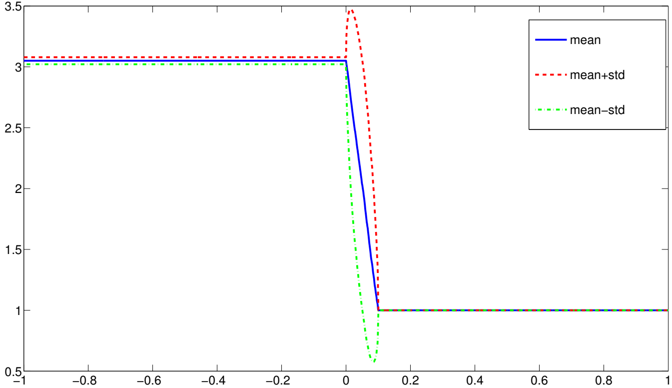
$$
\alpha \sim 0.05\mathcal{U}[-1,1]
$$

$$
\beta \sim 0.2\mathcal{U}[-1,1]
$$

- 2 Uniformly distributed random parameters.

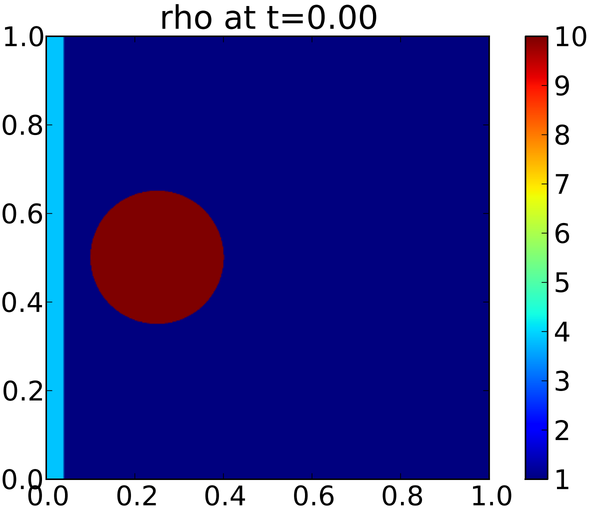
Euler equations – Sod Shock tube – Uncertain initial location + amplitude

- Mean ± Standard deviation.



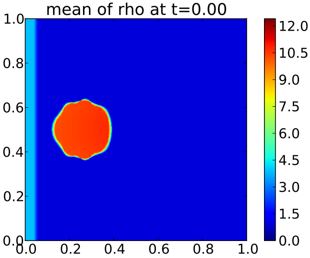
Ex II: Euler equations - Cloud shock interaction

- Deterministic Initial data:



Ex II: Euler equations - Cloud shock interaction

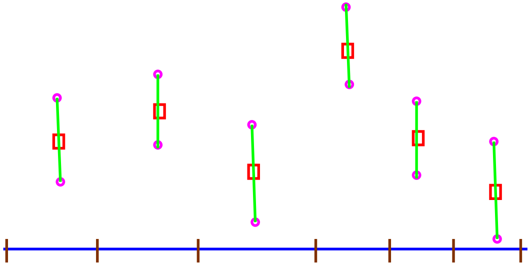
- Uncertain initial data in terms of 11 uniformly distributed parameters:



- Uncertainty in Shock location, amplitude, Bubble location, amplitude and geometry.

Ex III: Shallow water equations– bottom topography

- Real data bottom topography given by Digital Terrain Models.
- Typical representation:

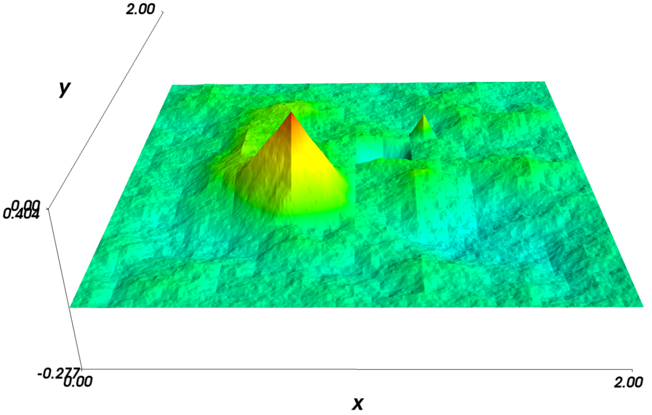


- Interpolation using hierarchical hat basis (SM, Schwab, Sukys, 2013)

Bottom topography: one sample (realization)

Hierarchical hat basis representation

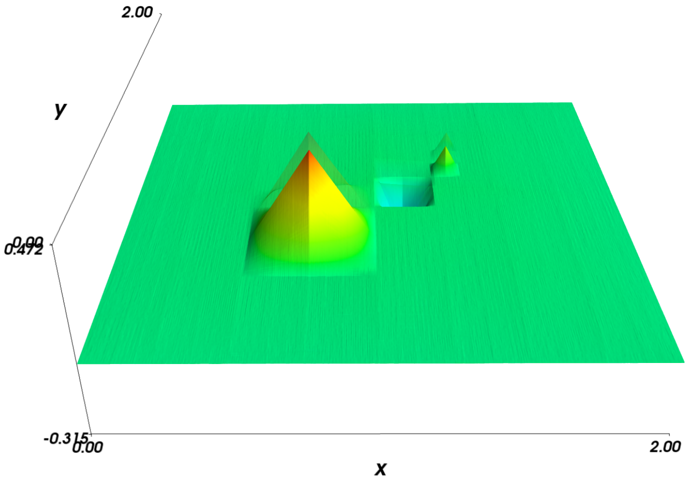
- 962 Random parameters !!!



Bottom topography: mean and standard deviation

Hierarchical hat basis representation

- 962 Random parameters !!!



Representation of random fields II: Karhunen-Loeve expansions

- Bi-orthogonal decomposition (a la Fourier Series).
- A prototypical example:
  - Centered random field $f : \Omega \mapsto L^2(D)$ with $\mathbb{E}(f) = 0$
  - Covariance function: $C \in L^2(D \times D)$ with

$$C_f(x, y) := \mathbb{E}(f(x, \omega)f(y, \omega)).$$

  - Covariance operator: $K_C : L^2(D) \mapsto L^2(D)$:

$$K_{C_f}[g](x) = \int_D K_{C_f}(x, y)g(y)dy.$$

  - K_C is a Compact $++$ operator !!!
  - $\Rightarrow$ possess orthonormal eigensystem (λ_k, f_k) over L^2

$$K_C[f_k] = \lambda_k f_k$$

Karhunen-Loeve expansions (Contd...)

- Hence, Random field f is

$$f(x,\omega) = \sum_{k=1}^{\infty} Z_k(\omega) f_k(x)$$

$$Z_k := \int_D f(x,\omega) f_k(x) dx$$

- Z_k's are Uncorrelated random variables as

$$\mathbb{E}(Z_i Z_j) := \lambda_j \delta_{ij}.$$

- General form of KL expansion:

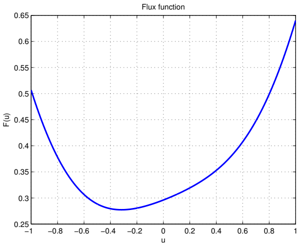
$$f = \overline{f} + \sum \sqrt{\lambda_k} Z_k g_k.$$

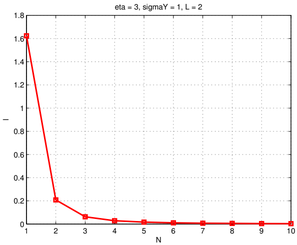
- Best L^2 truncated N-term approximation !!!
- PCA, POD are similar.

Ex I: Perturbed Burgers' flux

- Has the KL expansion:

$$f(\omega; u) = f(\mathbf{y}; \mathbf{u})\Big|_{\mathbf{y}=\mathbf{Y}(\omega)} = \frac{\mathbf{u}^2}{2} + \delta\Big(\sum_{\mathbf{j}\geq 1} \mathbf{y_j}\sqrt{\lambda_{\mathbf{j}}}\mathbf{\Phi_j}(\mathbf{u})\Big),$$





- Represented as a Gaussian process with exponential covariance: $C_Y(u_1, u_2) = \sigma_Y^2 e^{-|u_1-u_2|/\eta}$, and

Ex II: Rock permeability for seismic imaging

- Seismic Acoustic pulses modeled by Wave equation:

$$p_{tt} + div(\mathbf{c}\nabla p) = 0.$$

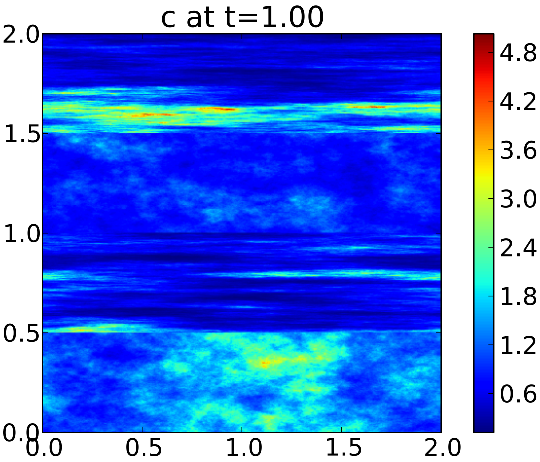
- Rewritten as a linear system of conservation laws.
- $\mathbf{c}$ is the rock permeability coefficient
- Highly uncertain – modeled by a log normal Gaussian random field:

$$\log(\mathbf{c}(x,\omega)) := \log(\overline{c}(x)) + \sum_{k=1}^{\infty} \sqrt{\lambda_k} Z_k(\omega) g_k(x).$$

- Many different Covariance functions.
- Need Spectral FFT + Upscaling for efficient generation.

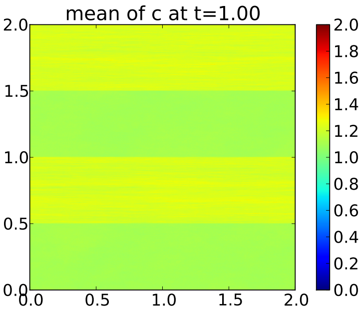
Ex II: 2-D log normal layered permeability field (sample)

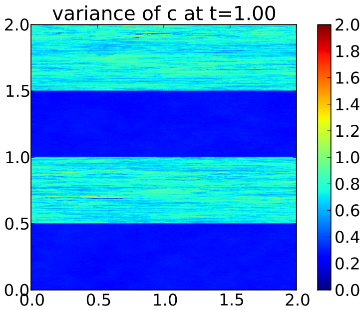
- $\approx$ 1000 uncertain parameters !!!



Ex II: 2-D log normal layered permeability field (statistics)

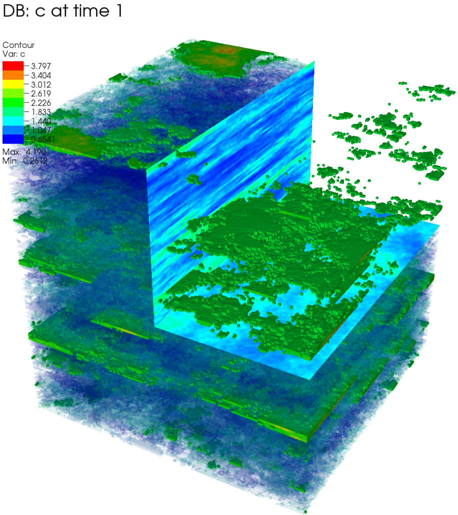
- ≈ 1000 uncertain parameters !!!





Ex II: 3-D log normal layered permeability field (sample)

- $\approx 10^6$ uncertain parameters !!!



Mathematical framework (scalar case)

- Random scalar conservation laws:

$$u_t(x,t,\omega) + \mathrm{div}(f(\omega; u(x,t,\omega))) = 0.$$
$$u(x,0,\omega) = u_0(x,\omega).$$

- with initial data and flux:

$$u_0 : (\Omega, \Sigma) \mapsto (L^1(\mathbb{R}^d), \mathcal{B}(L^1(\mathbb{R}^d)))$$
$$f : (\Omega, \Sigma) \mapsto (C^1(\mathbb{R}^1; \mathbb{R}^d); \mathcal{B}(C^1(\mathbb{R}; \mathbb{R}^d)))$$

Random entropy solution

- Solution is a random field that satisfies,
  - Measurability: $u : \Omega \in \omega \mapsto u(x, t; \omega)$ is measurable from (Ω, Σ) to $C((0, T); L^1(\mathbb{R}^d))$.
  - Weak solution: u satisfies the integral identity:

$$\int_{\mathbb{R}^d \times \mathbb{R}_+} (u(x,t,\omega)\varphi_t(x,t) + \langle f(\omega; u(x,t,\omega), \nabla\varphi(x,t)\rangle)dxdt + \int_{\mathbb{R}^d} u(x,0,\omega)\varphi(x,0)dx = 0.$$

    for $\mathbb{P}$-a.e $\omega \in \Omega$.
  - Entropy conditions: satisfied for all entropy-entropy flux pairs and for $\mathbb{P}$-a.e $\omega \in \Omega$.

Well-posedness theorem: SM, Schwab, 2010, SM et al 2012.

- For sufficiently regular u_0,:
  - Existence: There exists a unique random entropy solution

$$u : \Omega \ni \omega \mapsto C_b(0, T; L^1(\mathbb{R}^d))$$

  - Construction:

$$u(\cdot, t; \omega) = S(t)u_0(\cdot, \omega) \;, \quad t > 0, \; \omega \in \Omega$$

  - Stability: $\mathbb{P}$-a.s $\omega \in \Omega$,

$$\begin{aligned} \|u\|_{L^k(\Omega; C(0,T; L^1(\mathbb{R}^d)))} &\leq \|u_0\|_{L^k(\Omega; L^1(\mathbb{R}^d))} \;, \\ \|S(t)\,u_0(\cdot,\omega)\|_{(L^1\cap L^\infty)(\mathbb{R}^d)} &\leq \|u_0(\cdot,\omega)\|_{(L^1\cap L^\infty)(\mathbb{R}^d)} \\ TV(S(t)u_0(\cdot,\omega)) &\leq TV(u_0(\cdot,\omega)) \end{aligned}$$

Higher moments for random initial data

- Initial data satisfies,

$$u_0 \in L^r(\Omega; L^1(\mathbb{R}^d)).$$

- k-point correlation function

$$u(x_1, t_1; \omega) \otimes \cdots \otimes u(x_k, t_k; \omega) \in L^{r/k}(\Omega; L^1(\mathbb{R}^{kd})).$$

- k-th Moment:

$$\mathcal{M}^k u(t_1, \dots, t_k) := \mathbb{E}[u(\cdot, t_1; \omega) \otimes \cdots \otimes u(\cdot, t_k; \omega)] \in L^1(\mathbb{R}^{kd}).$$

- Stability:

$$\left\| \left(\mathcal{M}^k u\right)(t_1, ..., t_k) \right\|_{L^1(\mathbb{R}^d)^{(k)}} \leq \|u_0\|^r_{L^r(\Omega; L^1(\mathbb{R}^d))}.$$

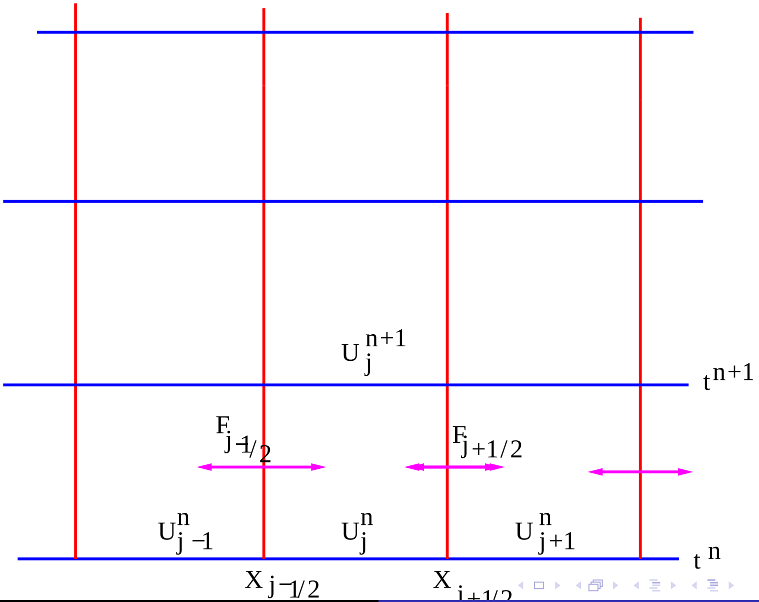
Schemes for random conservation laws

- Conservation law with uncertain initial data:

$$
\begin{aligned}
u_t(x,t,\omega) + \mathrm{div}(f(u(x,t,\omega))) &= 0. \\
u(x,0,\omega) &= u_0(x,\omega).
\end{aligned}
$$

- Discretization of Physical space-time.
- Standard Finite volume method

Finite volume Grid



Standard FVM

- Of the form:

$$u_j^{n+1} - u_j^n + \frac{\Delta t}{\Delta x}(F_{j+1/2} - F_{j-1/2}) = 0$$

- Have the following convergence rate:

$$\|u(.,t) - u_\tau(.,t)\|_{L^1(\mathbb{R}^d)} \leq C\Delta x^s.$$

- Work estimate:

$$\mathrm{Work}_\tau = \mathcal{O}(\Delta x^{-(d+1)}).$$

- Accuracy vs. Work:

$$\|u(.,t) - u_\tau(.,t)\|_{L^1(\mathbb{R}^d)} \leq C(\mathrm{Work}_\tau)^{-\frac{s}{d+1}}.$$

Schemes for random conservation laws

- Random conservation law:

$$u_t(x,t,\omega) + \mathrm{div}(f(\omega; u(x,t,\omega))) = 0.$$
$$u(x,0,\omega) = u_0(x,\omega).$$

- Need to discretize the probability space.
- Statistical sampling methods: Monte Carlo (**MC**) method.

MCFVM

- The MC algorithm:
  - Draw M i.i.d samples for the initial data and flux: $\{u_0^i, f^i\}_{1 \leq i \leq M}$.
  - For each sample: Solve conservation law by FVM to obtain u_τ^i.
  - Sample statistics:

$$\mathcal{M}^1 u(\cdot, t) \approx E_M[u_\tau(\cdot, t)] := \frac{1}{M}\sum_{i=1}^{M} u_\tau^i(\cdot, t).$$

$$\mathcal{M}^k u(t_1, \dots, t_k) := \frac{1}{M}\sum_{i=1}^{M} \underbrace{\left(u_\tau^i(\cdot, t_1) \otimes \cdots \otimes u_\tau^i(\cdot, t_k)\right)}_{k-\text{times}}.$$

MCFVM: Properties, SM, Schwab, 2010.

- Convergence:

$$\|\mathbb{E}[u(\cdot,t)] - E_M[u_\tau(\cdot,t;\omega)]\|_{L^2(\Omega;L^1(\mathbb{R}^d))} \leq C_{\mathrm{stat}} M^{-\frac{1}{2}} + C_{\mathrm{st}} \Delta x^s.$$

- Number of samples: $M = \mathcal{O}(\Delta x)^{-2s}$.
- Accuracy vs. Work:

$$\|\mathbb{E}[u(\cdot,t)] - E_M[u_\tau(\cdot,t;\omega)]\|_{L^2(\Omega;L^1(\mathbb{R}^d))} \leq C(\mathrm{Work}_\tau)^{-\frac{s}{d+1+2s}}.$$

- Slow convergence $\Rightarrow$ very high computational cost.

Multi-level Monte Carlo (MLMC) FVM:

- Heinrich 1995: Quadrature.
- Giles 2002: Stochastic ODEs.
- Barth, Schwab, Zollinger 2010: Elliptic PDEs.

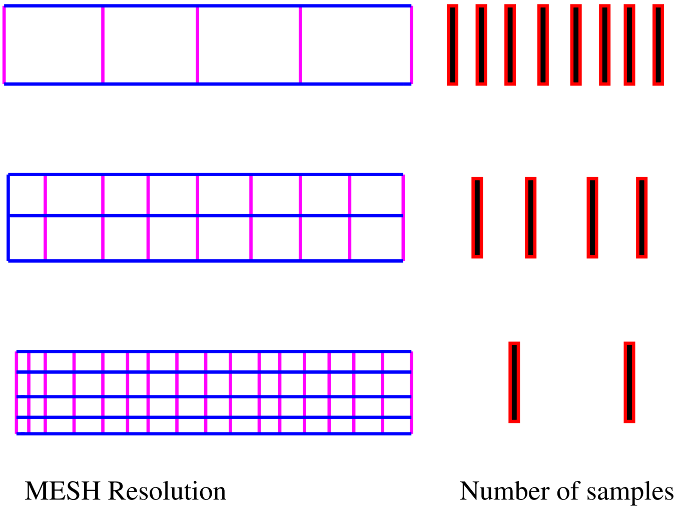
Multi-level Monte Carlo (MLMC) FVM: SM, Schwab, 2010

- MLMCFVM algorithm:
  - Different nested levels of resolution: l.
  - Draw M_l i.i.d samples for the initial data: $\{u^i_{l,0}\}_{1 \le i \le M_l}$.
  - For each draw: Solve conservation law by FVM to obtain $u^i_{l,\tau}$.
  - Sample statistics: with $u_{\tau,-1} = 0$,

$$\mathcal{M}^1 u(\cdot,t) \approx E^L[u(\cdot,t)] = \sum_{\ell=0}^{L} E_{M_\ell}[u_{\tau,\ell}(\cdot,t) - u_{\tau,\ell-1}(\cdot,t)]$$

$$\mathcal{M}^k u(t_1,\dots,t_k) := \sum_{\ell=0}^{L} E_{M_\ell}[u^{(k)}_{\tau,\ell}(\cdot,t) - u^{(k)}_{\tau,\ell-1}(\cdot,t)]$$

MLMCFVM



MLMCFVM: Properties

- Convergence:

$$\|\mathbb{E}[u(\cdot,t)] - E^L[u_\tau(\cdot,t,\omega)]\|_{L^2(\Omega;L^1(\mathbb{R}^d))} \leq C_1 \Delta x_L^s + C_3 M_0^{-\frac{1}{2}} + C_2 \left\{ \sum_{\ell=0}^{L} M_\ell^{-\frac{1}{2}} \Delta x_\ell^s \right\}$$

- Level dependent number of samples: $M_l = \mathcal{O}\left(\frac{\Delta x_l^{2s}}{\Delta x_L^{2s}}\right)$
- Accuracy vs. Work: If $0 \leq s < (d+1)/2$,

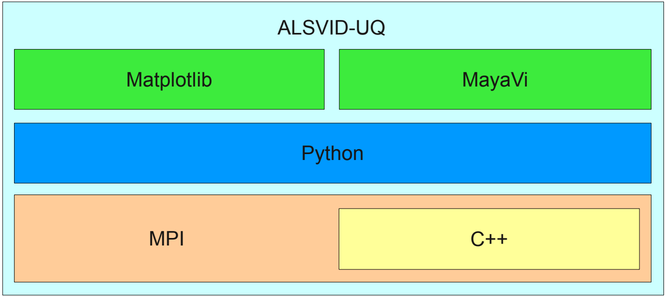
$$\|\mathbb{E}[u(\cdot,t)] - E^L[u_\tau(\cdot,t;\omega)]\|_{L^2(\Omega;L^1(\mathbb{R}^d))} \leq C(\mathrm{Work})^{-\frac{s}{d+1}} \log(\mathrm{Work})$$

- Same as the deterministic FVM !!!!!
- Sparse tensor higher moments computation with same efficiency.

Implementation of MC methods

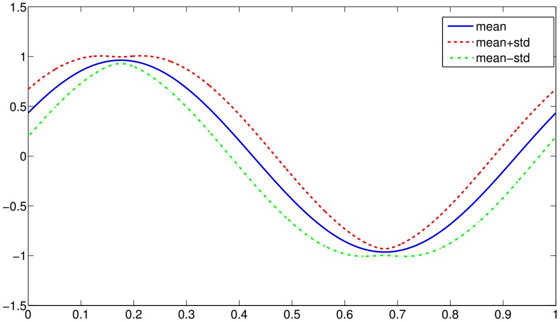
- Both MC and MLMC FVM are non-intrusive.
- Works with *any* spatio-temporal discretization.
- Interesting issues for parallelization.

ALSVID-UQ

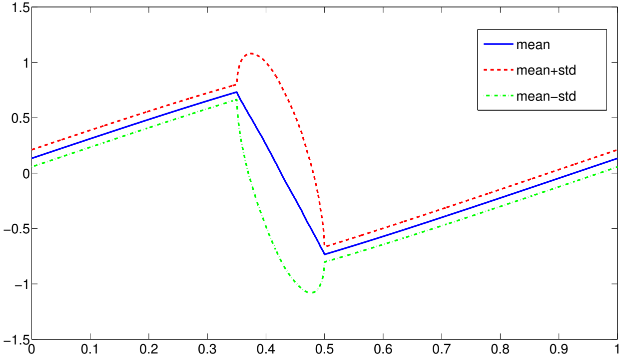


1-D Burgers' with uncertain initial phase

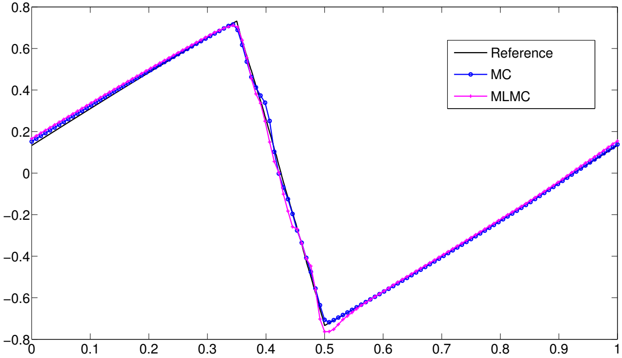
- 1 random parameter.



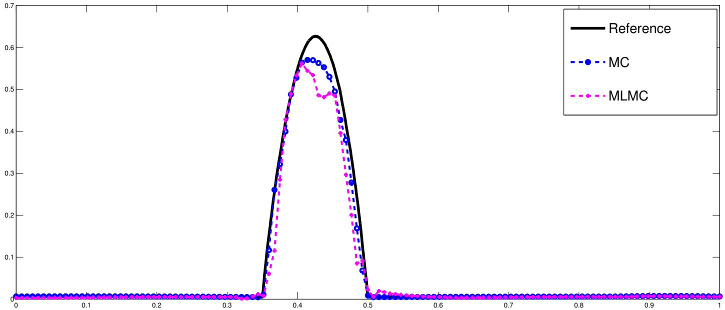
Mean ± Standard deviation



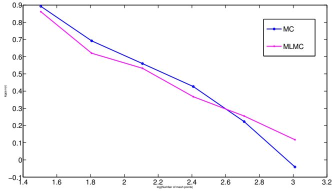
Mean: MC vs MLMC



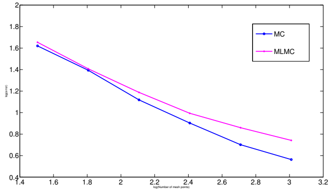
Variance: MC vs MLMC



log(resolution) vs. log(relative error)

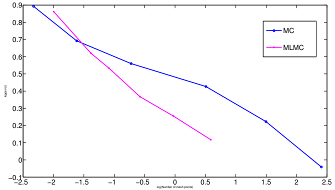


(d) mean

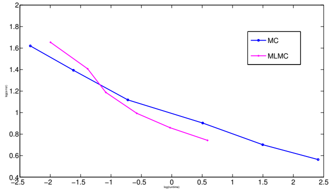


(e) variance

log(runtime) vs. log(relative error)



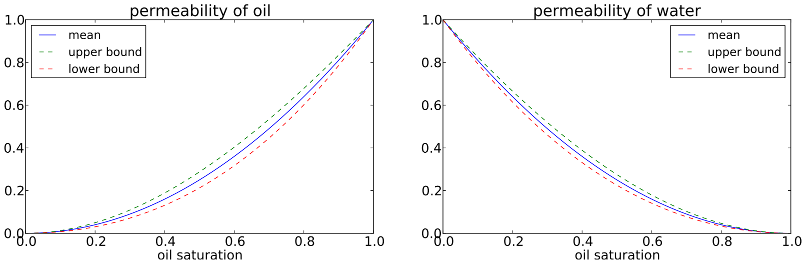
(f) mean



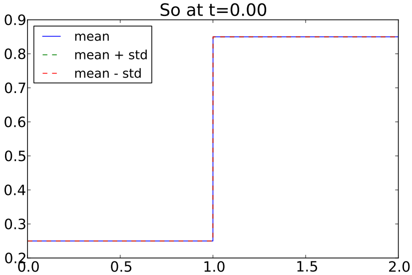
(g) variance

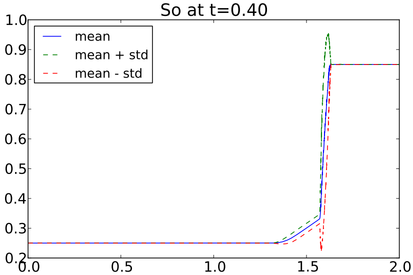
Buckley Leverette with uncertain relative permeabilities

- 2 random parameters.

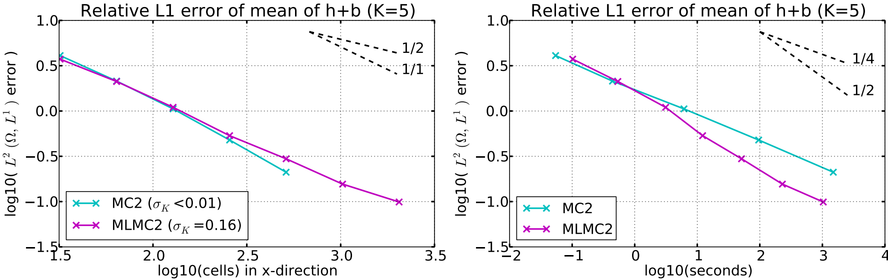


Buckley Leverette: mean $\pm$ std of Water saturation

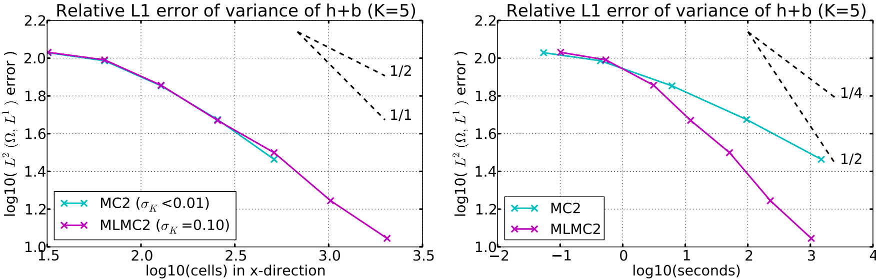




Buckley Leverette: convergence of mean



Buckley Leverette: convergence of variance



Linear systems of conservation laws

- Random linear systems of conservation laws:

$$\mathbf{U}_t(x,t,\omega) + \sum_{r=1}^{d} \frac{\partial}{\partial \mathbf{x}_r}\Big(\mathbf{A}_r(\mathbf{x},\omega)\mathbf{U}\Big) = 0.$$

$$\mathbf{U}(x,0,\omega) = \mathbf{U}_0(x,\omega).$$

- with uncertain initial data an flux:

$$\mathbf{U}_0 : (\Omega,\Sigma) \mapsto (L^2(\mathbf{D}), \mathcal{B}(L^2(\mathbf{D}))$$

$$\mathbf{A}_r : (\Omega,\Sigma) \mapsto (C^1(\mathbf{D})^{m\times m}; \mathcal{B}(C^1(\mathbf{D})^{m\times m})$$

Random Weak solution

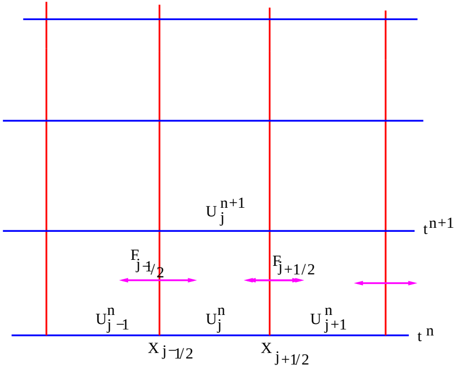
- Solution is a random field that satisfies,
  - Measurability: $\mathbf{U} : \Omega \in \omega \mapsto \mathbf{U}(x, t; \omega)$ is measurable from (Ω, Σ) to $C((0, T); L^2(\mathbf{D}))$.
  - Weak solution: $\mathbf{U}$ satisfies the integral identity:

$$\int\limits_{\mathbb{R}^d \times \mathbb{R}_+} \left(\mathbf{U} \cdot \varphi_t + \sum_{r=1}^{d} \mathbf{A}_r \mathbf{U} \cdot \frac{\partial}{\partial \mathbf{x}_r} \varphi \right) d\mathbf{x} dt + \int\limits_{\mathbb{R}^d} \mathbf{U}_0 \cdot \varphi(t = 0) \, d\mathbf{x} = 0.$$

  for $\mathbb{P}$-a.e $\omega \in \Omega$.
- THM (SM, Schwab, Sukys 2014): Random weak solutions exist and are unique.

Schemes for Linear systems I: FVM

- Standard Finite volume method to discretize Space-time.



- Under suitable assumptions on initial data + coefficients $\mathbf{A}_r$, FVM Convergence rate:

$$\|\mathbf{U} - \mathbf{U}^{\Delta x}\|_{L^2} \leq C \Delta x^s$$

Schemes for Linear systems II: MCFVM

- The MC algorithm:
  - Draw M i.i.d samples for the initial data and flux: $\{\mathbf{U}_0^i, \mathbf{A}_r^i\}_{1 \le i \le M}$.
  - For each sample: Solve linear system by FVM to obtain $\mathbf{U}_\tau^i$.
  - Sample statistics:

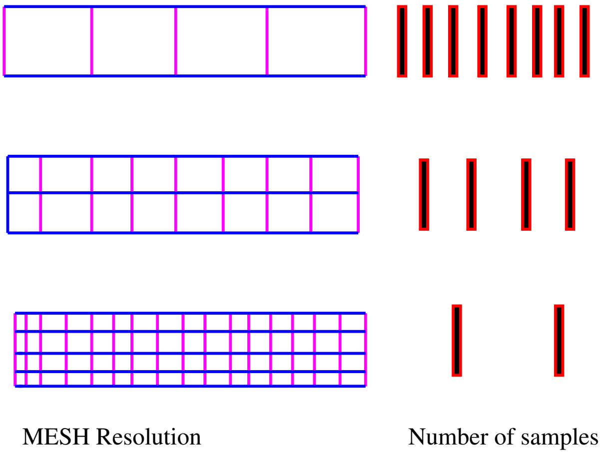
$$\mathbb{E}(\mathbf{U}(\cdot, t)) \approx E_M[\mathbf{U}_\tau(\cdot, t)] := \frac{1}{M} \sum_{i=1}^{M} \mathbf{U}_\tau^i(\cdot, t).$$

- Convergence (SM,Schwab,Sukys,2014):

$$\|\mathbb{E}[\mathbf{U}(\cdot, t)] - E_M[\mathbf{U}_\tau(\cdot, t; \omega)]\|_{L^2(\Omega; L^2(\mathbf{D}))} \le C_{\mathrm{stat}} M^{-\frac{1}{2}} + C_{\mathrm{st}} \Delta x^s.$$

- Slow convergence $\Rightarrow$ very high computational cost.

Schemes for Linear systems III: MLMCFVM-SM,Schwab,Sukys 2014



MLMCFVM for linear systems

- Convergence:

$$\|\mathbb{E}[\mathbf{U}(\cdot,t)] - E^L[\mathbf{U}_\tau(\cdot,t,\omega)]\|_{L^2(\Omega;L^2(\mathbb{R}^d))} \leq C_1 \Delta x_L^s + C_3 M_0^{-\frac{1}{2}} + C_2 \left\{ \sum_{\ell=0}^{L} M_\ell^{-\frac{1}{2}} \Delta x_\ell^s \right\}$$

- Proper choice of $M_\ell \Rightarrow$ Same complexity as deterministic FVM !!!

Ex : Seismic imaging

- Seismic Acoustic pulses modeled by Wave equation:

$$p_{tt} + div(\mathbf{c}\nabla p) = 0.$$

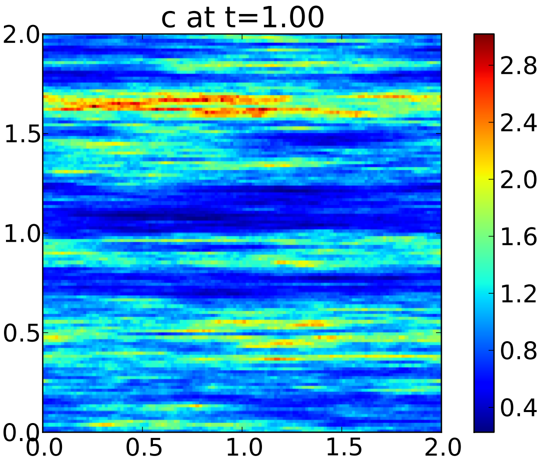
- Rewritten as a linear system of conservation laws.
- **c** is the rock permeability coefficient
- Highly uncertain – modeled by a log normal Gaussian random field:

$$\log(\mathbf{c}(x,\omega)) := \log(\overline{c}(x)) + \sum_{k=1}^{\infty} \sqrt{\lambda_k} Z_k(\omega) g_k(x).$$

- Many different Covariance functions.
- Need Spectral FFT + Upscaling for efficient generation.

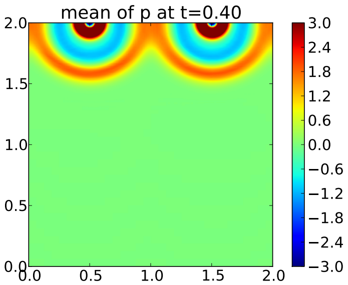
Ex : 2-D log normal layered permeability field (sample)

- $\approx$ 1000 uncertain parameters !!!



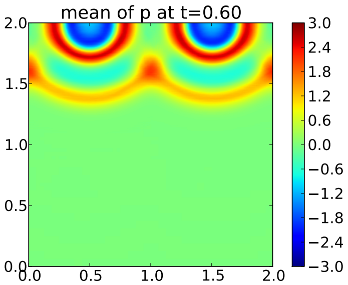
Ex : 2-D log normal layered permeability field $T = 0.4$

- $\approx$ 1000 uncertain parameters !!!



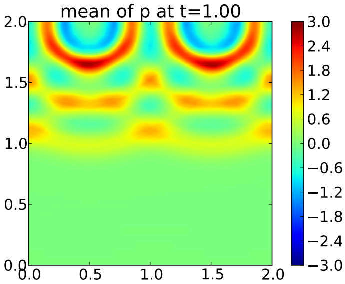
Ex : 2-D log normal layered permeability field $T = 0.6$

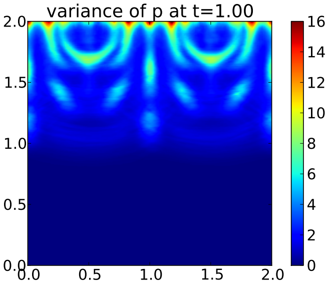
- $\approx$ 1000 uncertain parameters !!!



Ex : 2-D log normal layered permeability field $T = 1.0$

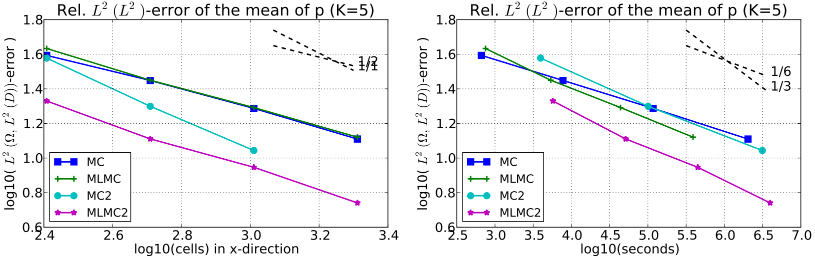
- $\approx$ 1000 uncertain parameters !!!





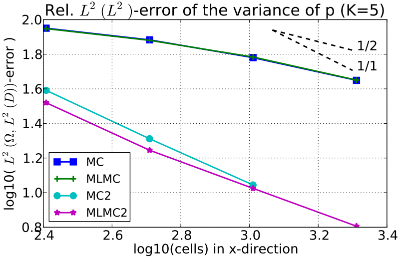
Convergence of mean

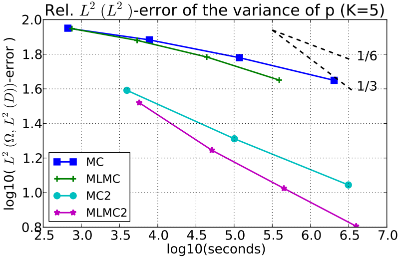
- $\approx$ 1000 uncertain parameters !!!



Convergence of variance

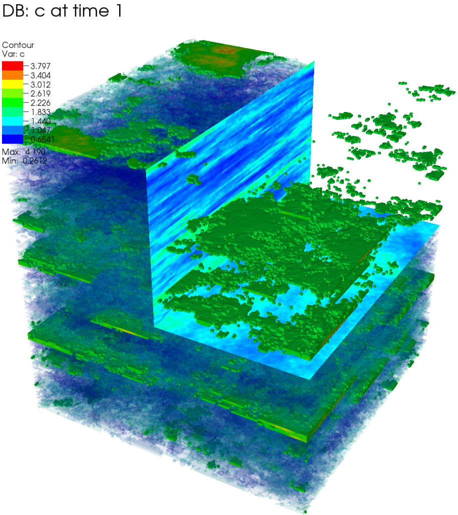
- $\approx$ 1000 uncertain parameters !!!





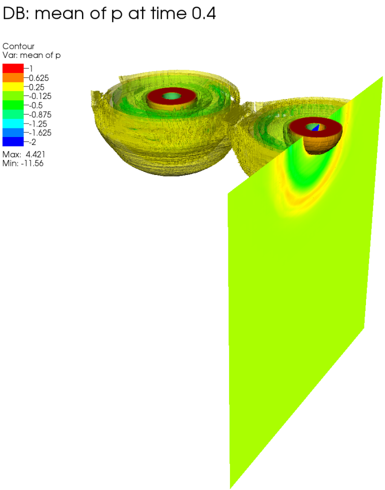
Ex II: 3-D log normal layered permeability field (sample)

- $\approx 10^6$ uncertain parameters !!!



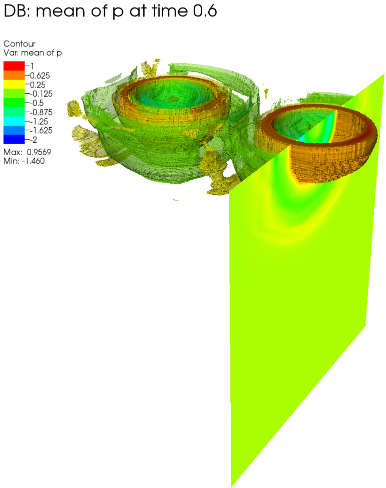
Ex II: Mean at $T = 0.4$

- $\approx 10^6$ uncertain parameters !!!



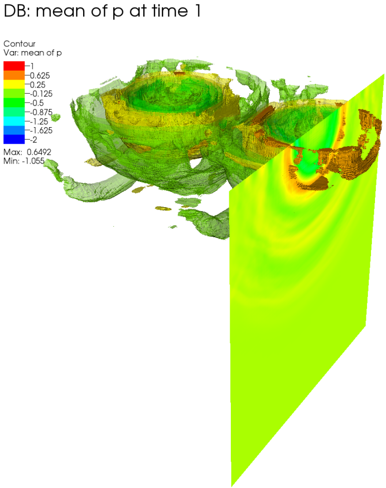
Ex II: Mean at $T = 0.6$

- $\approx 10^6$ uncertain parameters !!!



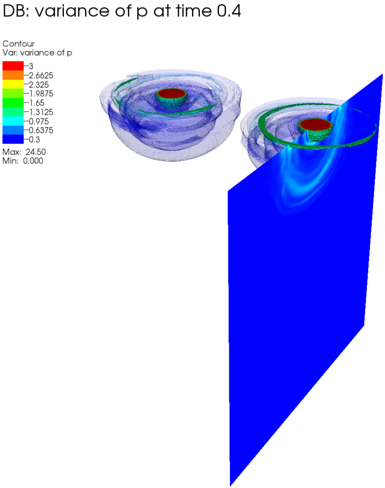
Ex II: Mean at $T = 1.0$

- $\approx 10^6$ uncertain parameters !!!



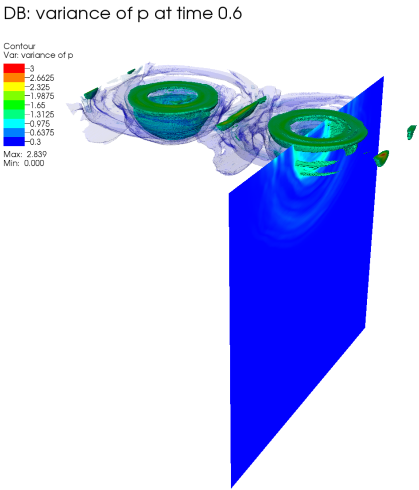
Ex II: Variance at $T = 0.4$

- $\approx 10^6$ uncertain parameters !!!



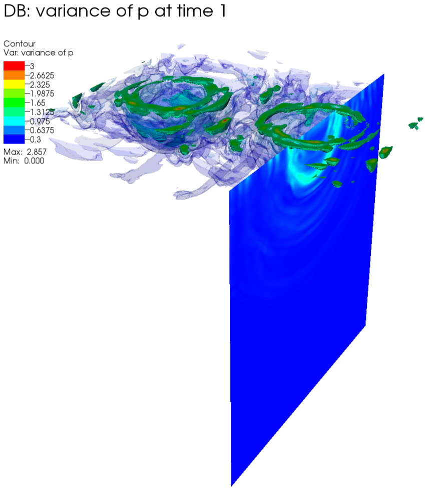
Ex II: Variance at $T = 0.6$

- $\approx 10^6$ uncertain parameters !!!



Ex II: Variance at $T = 1.0$

- $\approx 10^6$ uncertain parameters !!!



Non-Linear systems of conservation laws

- Random non-linear systems of conservation laws:

$$\mathbf{U}_t(x,t,\omega) + \mathrm{div}\,(\mathbf{F}(\omega,\mathbf{u}(x,t,\omega))) = 0.$$
$$\mathbf{U}(x,0,\omega) = \mathbf{U}_0(x,\omega).$$

- with uncertain initial data and flux:

$$\mathbf{U}_0 : (\Omega,\Sigma) \mapsto (L^1(\mathbf{D})^m, \mathcal{B}((L^1(\mathbf{D}))^m)$$
$$\mathbf{F} : (\Omega,\Sigma) \mapsto (C^1(\mathbf{D})^m; \mathcal{B}(C^1(\mathbf{D})^m)$$

Random Entropy solution

- Solution is a random field that satisfies,
  - Measurability: $\mathbf{U} : \Omega \in \omega \mapsto \mathbf{U}(x, t; \omega)$ is measurable from (Ω, Σ) to $(C((0, T); L^1(\mathbf{D})))^m$.
  - Weak solution: $\mathbf{U}$ satisfies the integral identity:

$$\int\limits_{\mathbb{R}^d \times \mathbb{R}_+} \left(\mathbf{U} \cdot \varphi_t + \sum_{r=1}^{d} \mathbf{F}_r(\mathbf{U}) \cdot \frac{\partial}{\partial \mathbf{x}_r} \varphi \right) d\mathbf{x} dt + \int\limits_{\mathbb{R}^d} \mathbf{U}_0 \cdot \varphi(t = 0) \; d\mathbf{x} = 0.$$

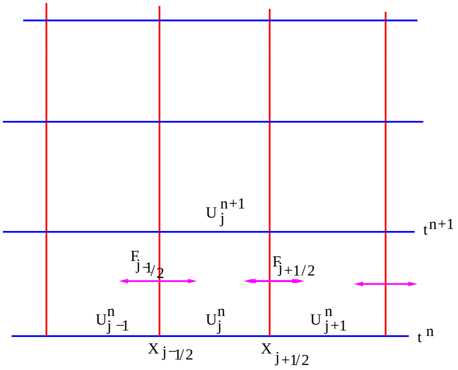
    for $\mathbb{P}$-a.e $\omega \in \Omega$.
- Entropy condition to be satisfied $\mathbb{P}$ a.s.

Wellposedness

- Deterministic problem:
  - Wellposedness of 1-d + small data (Glimm, Bianchini-Bressan).
  - NO global existence results in multi-D.
  - NON-UNIQUENESS of entropy solutions in multi-D (DeLellis-Szekelyhidi).
- Random entropy solutions
  - NO Wellposedness results !!!

Schemes for Nonlinear systems I: FVM

- Standard Finite volume method to discretize Space-time.



- NO rigorous convergence results for any scheme !!!
- Can Postulate Convergence rate ??:

$$\|\mathbf{U} - \mathbf{U}^{\Delta x}\|_{L^1} \leq C \Delta x^s$$

Schemes for NonLinear systems II: MCFVM

- The MC algorithm:
  - Draw M i.i.d samples for the initial data and flux: $\{\mathbf{U}_0^i, \mathbf{A}_r^i\}_{1 \le i \le M}$.
  - For each sample: Solve linear system by FVM to obtain $\mathbf{U}_\tau^i$.
  - Sample statistics:

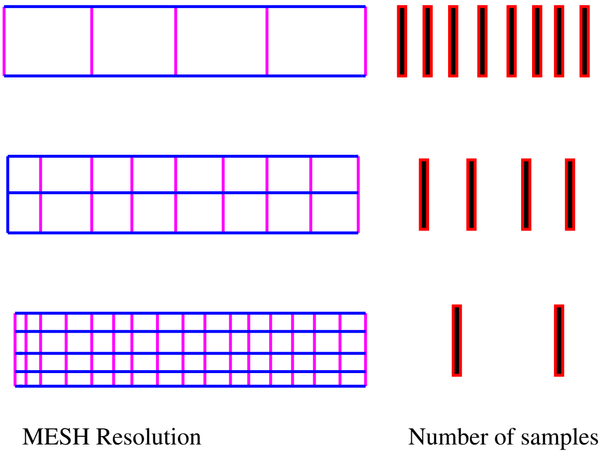
$$\mathbb{E}(\mathbf{U}(\cdot, t)) \approx E_M[\mathbf{U}_\tau(\cdot, t)] := \frac{1}{M}\sum_{i=1}^{M} \mathbf{U}_\tau^i(\cdot, t).$$

- Postulated Convergence:

$$\|\mathbb{E}[\mathbf{U}(\cdot, t)] - E_M[\mathbf{U}_\tau(\cdot, t; \omega)]\|_{L^2(\Omega; L^1(\mathbf{D}))} \le C_{\text{stat}} M^{-\frac{1}{2}} + C_{\text{st}} \Delta x^s.$$

- Slow convergence $\Rightarrow$ very high computational cost.

Schemes for NonLinear systems III: MLMCFVM-SM,Schwab,Sukys 2012



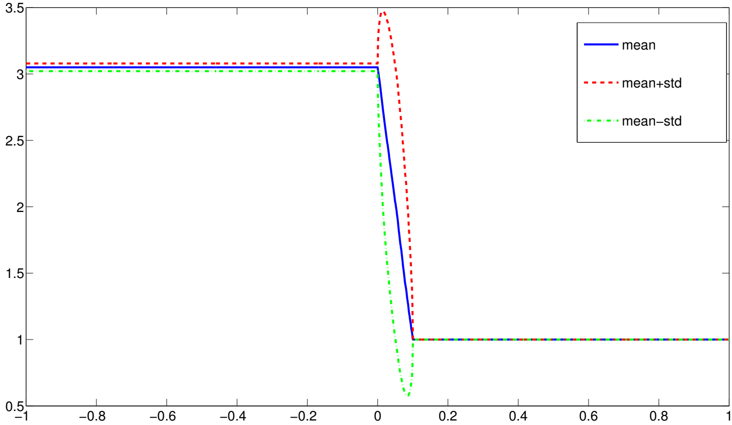
MLMCFVM for nonlinear systems

- Postulated Convergence:

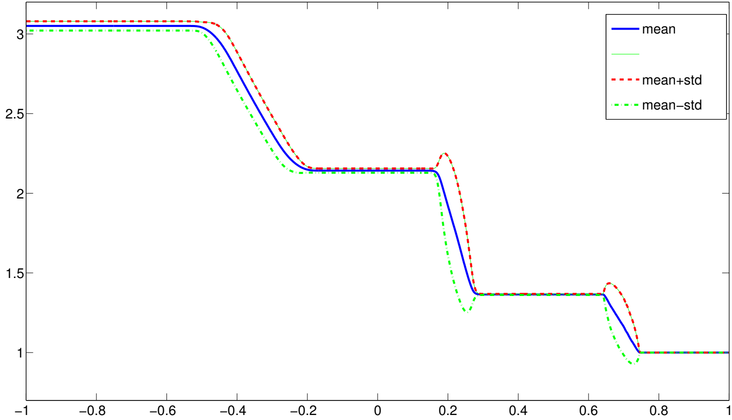
$$\|\mathbb{E}[\mathbf{U}(\cdot,t)] - E^L[\mathbf{U}_\tau(\cdot,t,\omega)]\|_{L^2(\Omega;L^1(\mathbb{R}^d))} \leq C_1 \Delta x_L^s + C_3 M_0^{-\frac{1}{2}} + C_2 \left\{ \sum_{\ell=0}^{L} M_\ell^{-\frac{1}{2}} \Delta x_\ell^s \right\}$$

- Proper choice of $M_\ell \Rightarrow$ Same complexity as deterministic FVM !!!

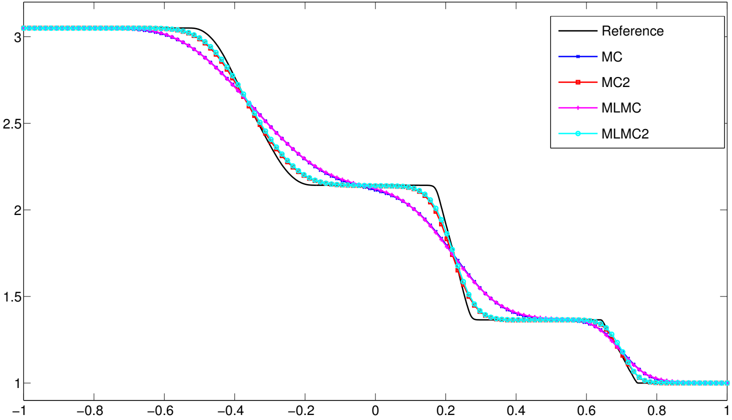
Euler equations with uncertain shock location and amplitude



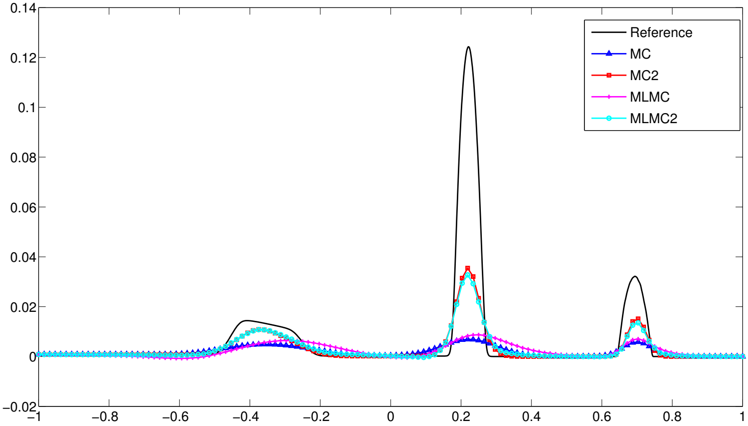
Mean ± Standard deviation



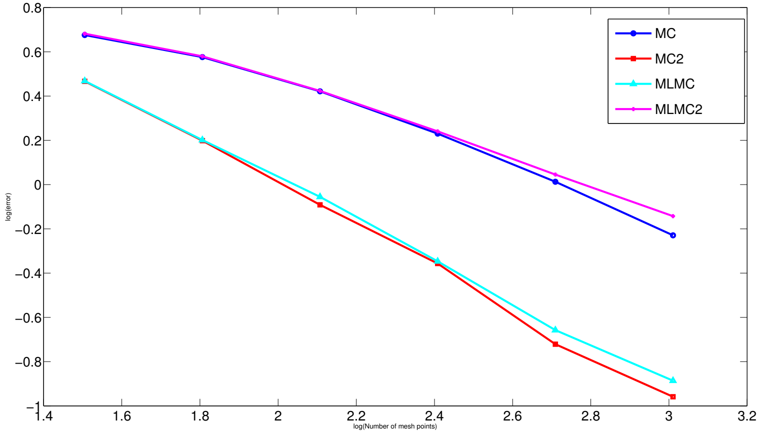
Mean: MC vs MLMC



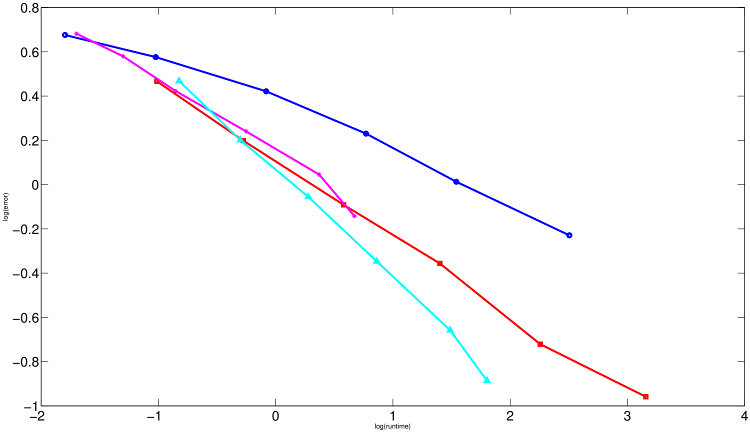
Variance: MC vs MLMC



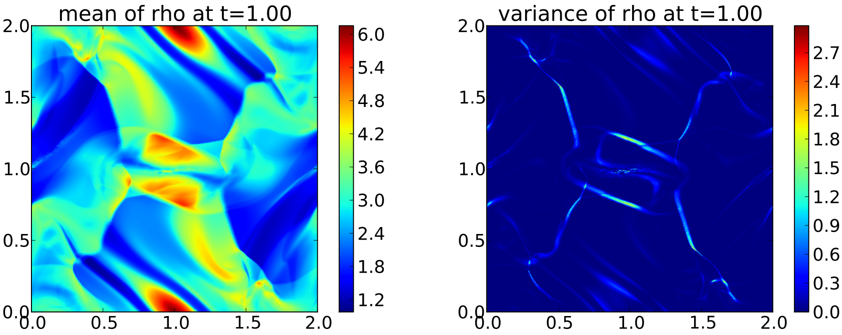
log(resolution) vs. log(relative error in mean)



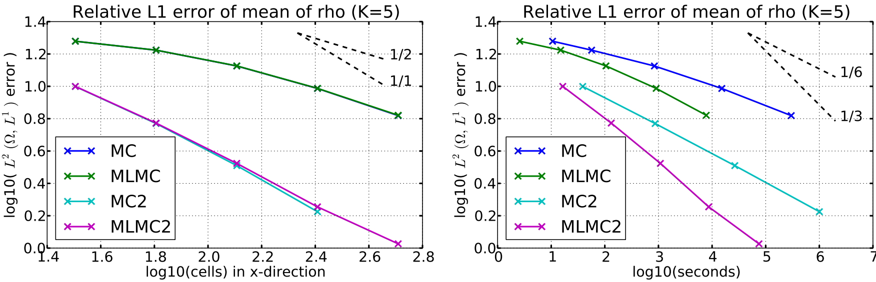
log(runtime) vs. log(relative error in mean)



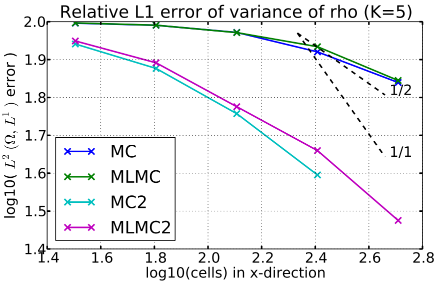
Uncertain Orszag-Tang vortex for MHD (2 Sources of uncertainty)

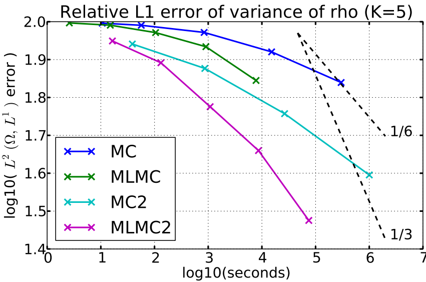


Uncertain Orszag-Tang vortex for MHD (Convergence of mean)

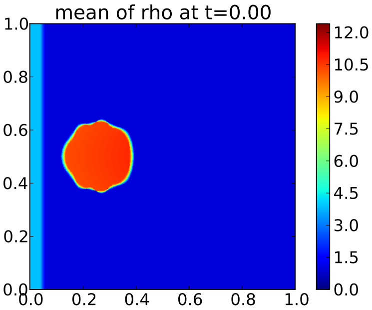


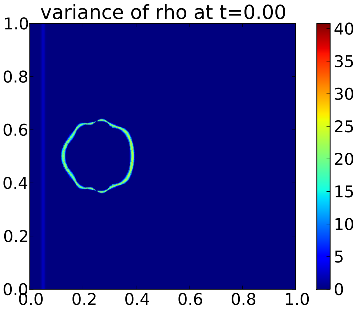
Uncertain Orszag-Tang vortex for MHD (Convergence of variance)



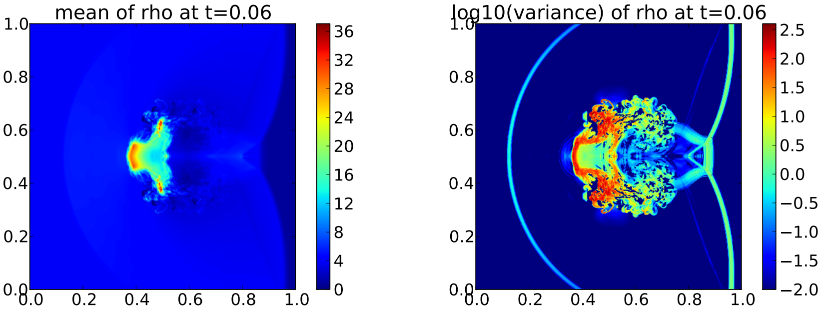


Euler: Cloud shock interaction with uncertain initial data (11 sources of uncertainty)

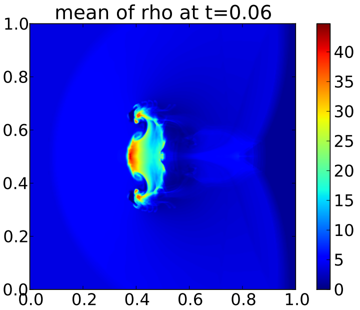


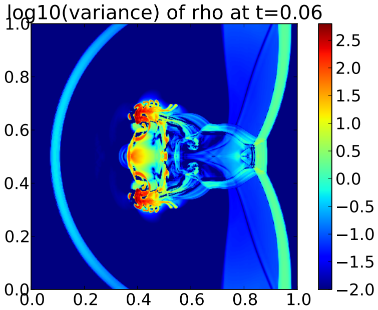


Euler: Cloud shock interaction with uncertain initial data (11 sources of uncertainty)



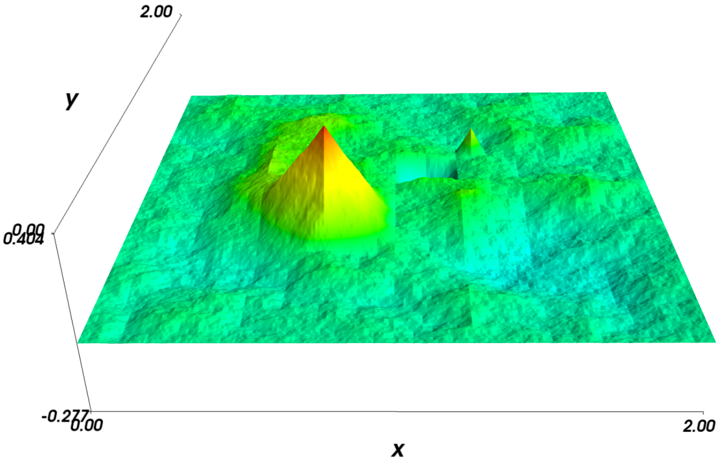
Euler: Cloud shock interaction with uncertain equations of state





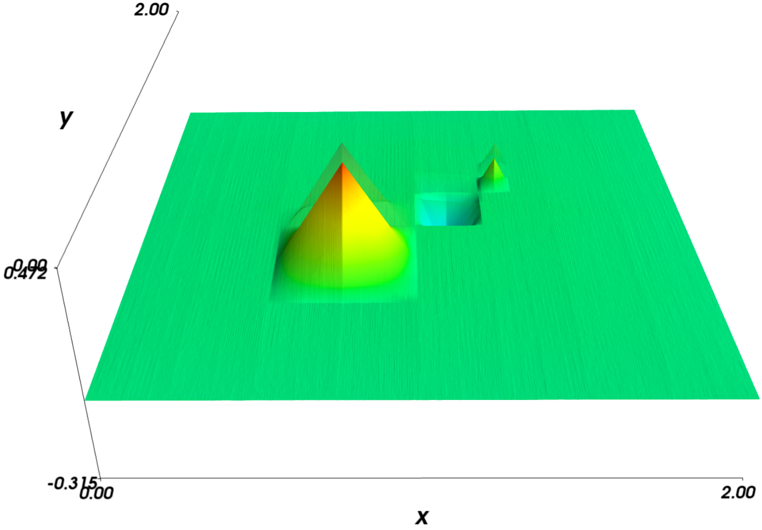
Bottom topography: one sample (realization)

Hierarchical hat basis representation



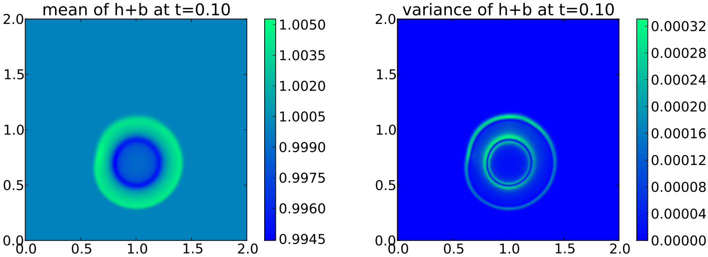
Bottom topography: mean and standard deviation

Hierarchical hat basis representation



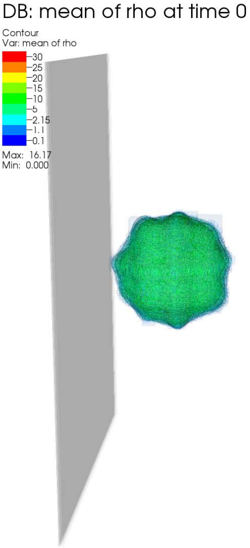
MLMC solution for perturbation of a lake-at-rest

uncertain magnitude of the perturbation, hierarchical hat basis topography

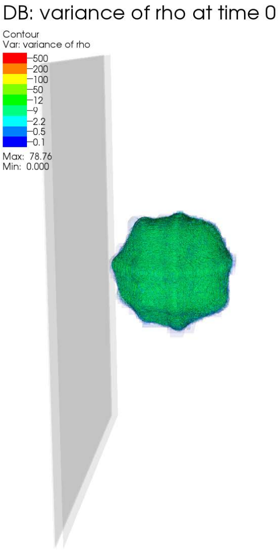


$\approx 10^3$-dimensional problem!

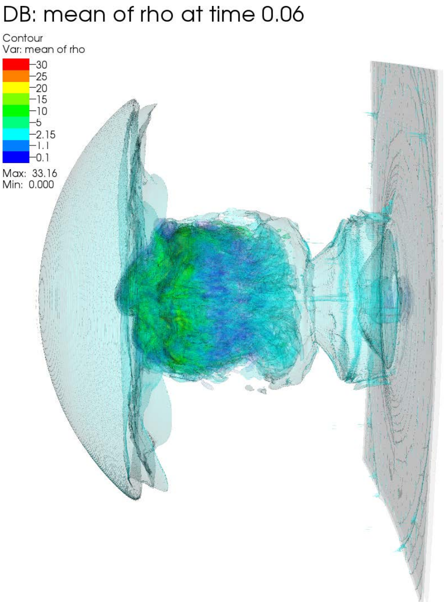
3D Euler– Initial Mean



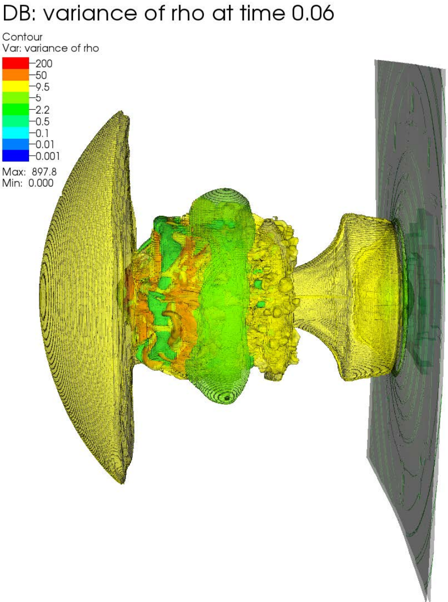
3D Euler– Initial Variance



3D Euler– Mean



3D Euler– Variance



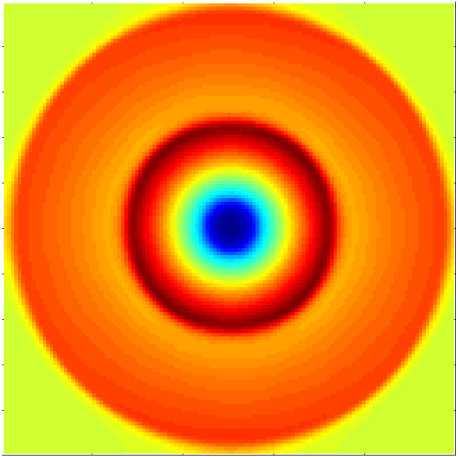
UQ for nonlinear systems ISSUE I: Convergence

- Convergence of both MC + MLMCFVM relies on:
- Postulated convergence of FVM:

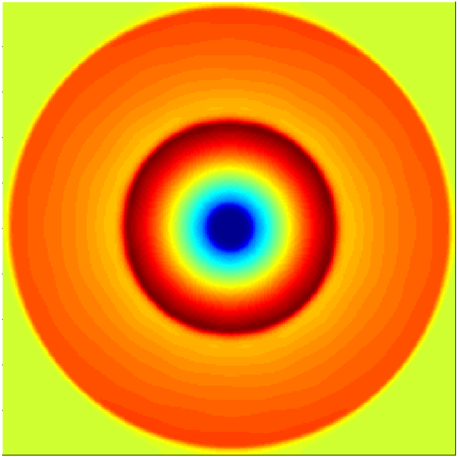
$$\|\mathbf{U} - \mathbf{U}^{\Delta x}\|_{L^p} \leq C \Delta x^s$$

- for some s, p.
- Widely expected to hold !!!
- Is this TRUE ?

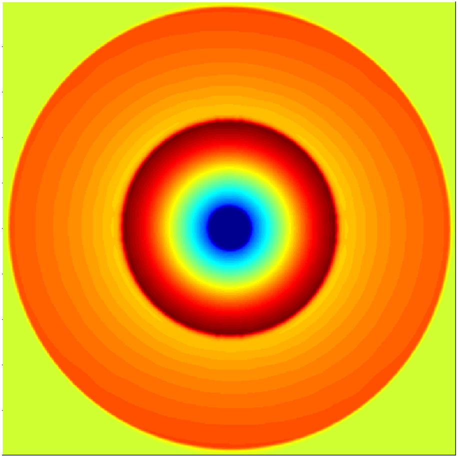
Numerical convergence Example 1: 2-D Radial shock tube 128^2 grid



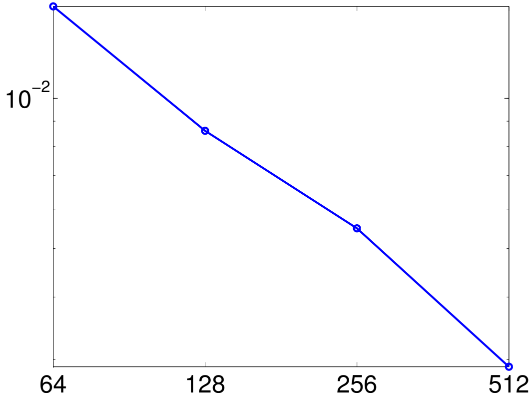
Numerical convergence Example 1: 2-D Radial shock tube 256^2 grid



Numerical convergence Example 1: 2-D Radial shock tube 512^2 grid



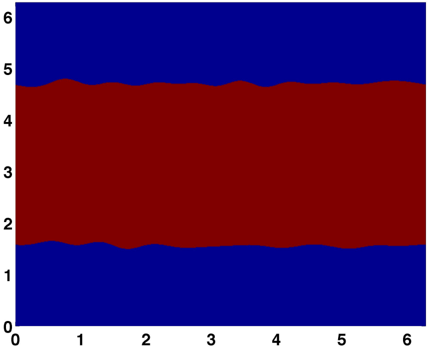
L^1 Error vs mesh resolution Example 1: 2-D Radial shock tube



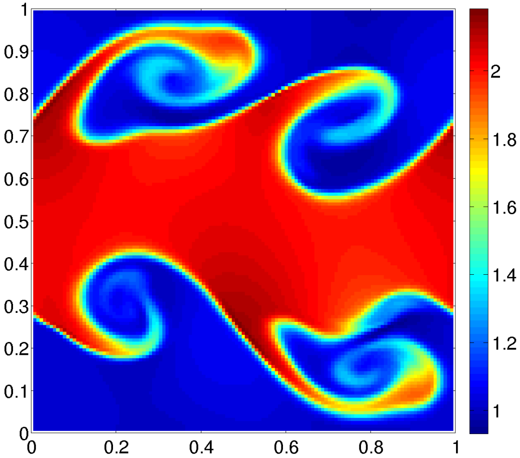
• Suggests L^1 convergence of approximate solutions to Entropy solutions

Ex II: Kelvin-Helmholtz problem: Compressible Euler equations

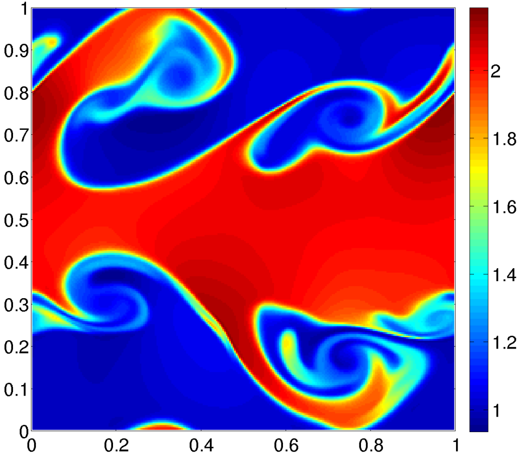
- Finite volume TeCNO3 simulation of Fjordholm, Käpelli, SM, Tadmor, 2014.



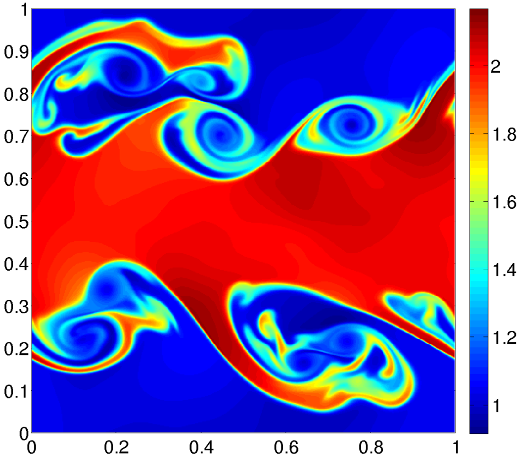
Numerical convergence: 2-D Kelvin-Helmholtz problem 128^2 grid ($T = 2$)



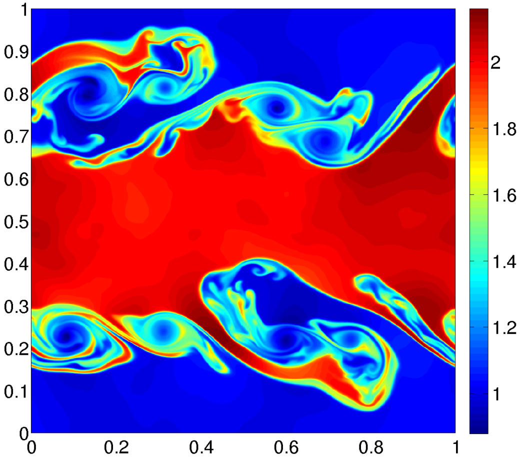
Numerical convergence: 2-D Kelvin-Helmholtz problem 256^2 grid $T = 2$



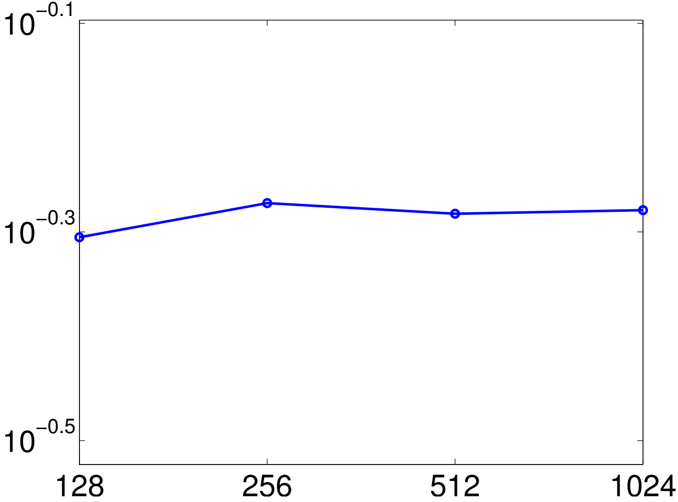
Numerical convergence: 2-D Kelvin-Helmholtz instability 512^2 grid $T = 2$



Numerical convergence: 2-D Kelvin-Helmholtz instability 1024^2 grid $T = 2$



L^1 Error vs mesh resolution: 2-D Kelvin-Helmholtz instability $T = 2$



Problem : Lack of convergence

- Suggests Lack of convergence to any function.
- Refining resolution reveals more small scale phenomena.
- Many Other examples like Richtmeyer-Meshkov problem.
- Generic to Unstable and Turbulent flows.
- Similar behavior for all numerical schemes.

Status Update

- MC-MLMC UQ methods assume Convergence of FVM !!!
- NO observed convergence of any numerical scheme in multi-D (in general).
- Linked to
  - Lack of Global existence results for Entropy solutions of deterministic problem.
  - NON-uniqueness of entropy solutions !!!
- $\Rightarrow$ Lack of Well-posedness of Random entropy solutions
- Search for a different Solution framework

Entropy measure valued solutions

- Pioneered by DiPerna (early to mid 80's).
- Contributions from Majda, Murat, Tartar.
- Solutions are Young measures i.e, space-time parametrized probability measures $\nu_{x,t}$.
- With action:

$$\langle g, \nu_{x,t} \rangle := \int_P g(\lambda) d\nu_{x,t}(\lambda)$$

- Characterizes weak limits of sequences of bounded functions.
- MVS assigns a probability distribution (likely value) for a.e point in space-time (one-point statistics)

Generalized Cauchy problem for $\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = 0$

$$\langle ID, \nu \rangle_t + \langle \mathbf{F}, \nu \rangle_x = 0, \quad \text{in} \quad \mathcal{D}'(D)$$
$$\nu_{x,0} = \sigma_x, \quad \text{a.e } x \in \mathbb{R}.$$

- EMVS satisfies:
  - Weak solution.
  - Entropy condition: $\langle S, \nu \rangle_t + \langle \mathbf{Q}, \nu \rangle_x \leq 0$
  - Initial data (DiPerna)

$$\lim_{t \to 0+} \int_{\mathbb{R}} \varphi(x) \langle ID, \nu_{x,t} \rangle dx = \int_{\mathbb{R}} \varphi(x) \langle ID, \sigma_x \rangle dx$$

  - σ_x models Uncertainty in initial data (EMVS is an UQ framework).
- Efficient Computation of EMVS: Algorithm designed by Fjordholm, Käppeli, SM, Tadmor (FKMT), 2014.

Step 1: Preparation of initial data

- Let $\{\Omega, \Sigma, \mathcal{P}\}$ be a complete probability space.
- Find random field $\mathbf{U}_0 : \Omega \mapsto L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$, such that:
- σ_x be the LAW of the random field $\mathbf{U}_0$ i.e, for all Borel subsets $\overline{D} \subset \mathbb{R}^m$:

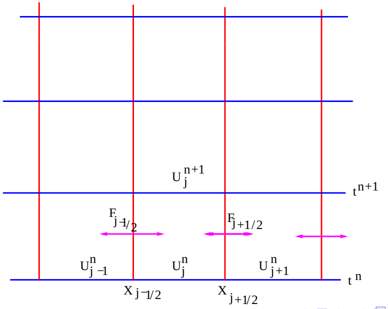
$$\sigma_x(\overline{D}) := \mathcal{P}\left(\{\omega \in \Omega : \mathbf{U}_0(\omega, x) \in \overline{D}\right),$$

Step 2: Numerical approximations

- Standard semi-discrete finite volume scheme:

$$\frac{d}{dt}\mathbf{U}_j^{\Delta x}(t) + \frac{1}{\Delta x}(\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}) = 0$$
$$\mathbf{U}_j^{\Delta x}(0,\omega) = \mathbf{U}_0(x_j,\omega)$$
$$\mathbf{U}^{\Delta x}|_{[x_{j-1/2},x_{j+1/2})} = \mathbf{U}_j^{\Delta x}.$$

- On the grid:



Step 3: Abstract Convergence criteria, Fjordholm, Käppeli, SM, Tadmor 2014

- Let $\nu_{x,t}^{\Delta x}$ be the law of the random field $\mathbf{U}^{\Delta x}$
- Thrm: $\nu_{x,t}^{\Delta x}$ is a young measure on phase space.

Step 3: Abstract Convergence criteria, (Contd..)

- L^∞ bounds:

$$\|\mathbf{U}^{\Delta x}\|_{L^\infty} \leq C, \quad \text{a.e } \omega$$

.

- Discrete entropy inequality:

$$\frac{d}{dt} S(\mathbf{U}_j(t)) + \frac{1}{\Delta x}(Q_{j+1/2} - Q_{j-1/2}) \leq 0$$

- Weak BV bounds (for a.e. ω):

$$\int_0^T \sum_j |\mathbf{U}_{j+1} - \mathbf{U}_j|^{p+1} dt \leq C.$$

• Thrm: Then, $\nu^{\Delta x} \rightharpoonup \nu$ (EMVS of the system).

Convergent schemes

- Schemes satisfy Discrete entropy inequality + Weak BV bound:
  - TeCNO schemes (Fjordholm, SM, Tadmor 2012).
  - Space-time DG schemes (Hiltebrand, SM, 2013).
- Assumption of L^∞ bound.
- Relaxed in (Fjordholm,SM 2014) with Generalized young measures.
- Numerical schemes satisfy L^2 bounds (Entropy estimate).

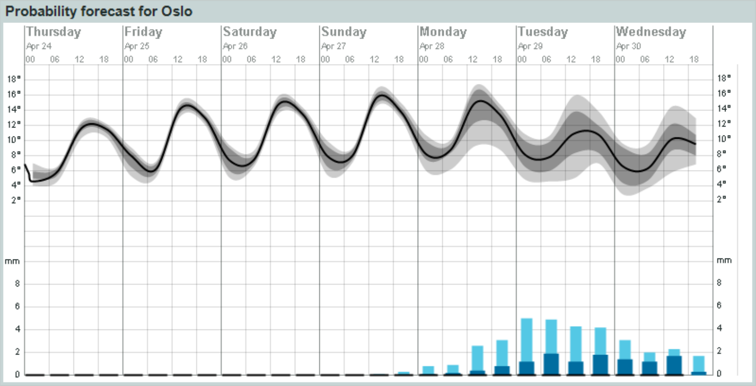
Computing the EMVS

- Narrow convergence $\Rightarrow$ as $\Delta x \to 0$, convergence of

$$\int_{D_t} \psi(x,t)\langle g, \nu_{x,t}^{\Delta x}\rangle dxdt \to \int_{D_t} \psi(x,t)\langle g, \nu_{x,t}\rangle dxdt$$

- Sense of convergence: Statistics of functionals of interest
- Precisely the outputs of measurement
- Typical observables:
  - $g(\lambda) = \lambda$ (Mean).
  - $g(\lambda) = \lambda \otimes \lambda$ (Variance).

Typical measurements: Weather



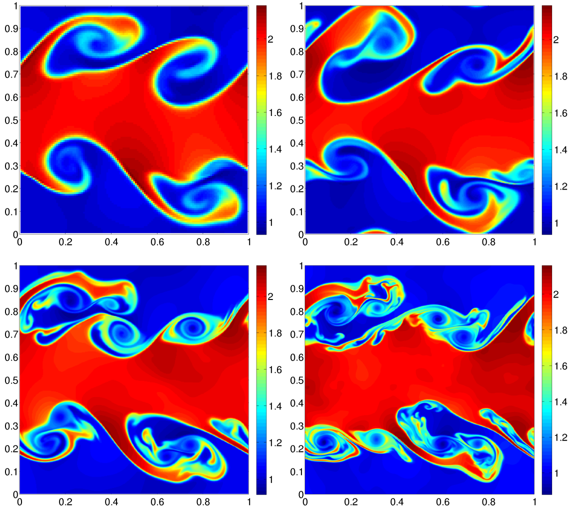
Monte Carlo approximation

- We need to compute:

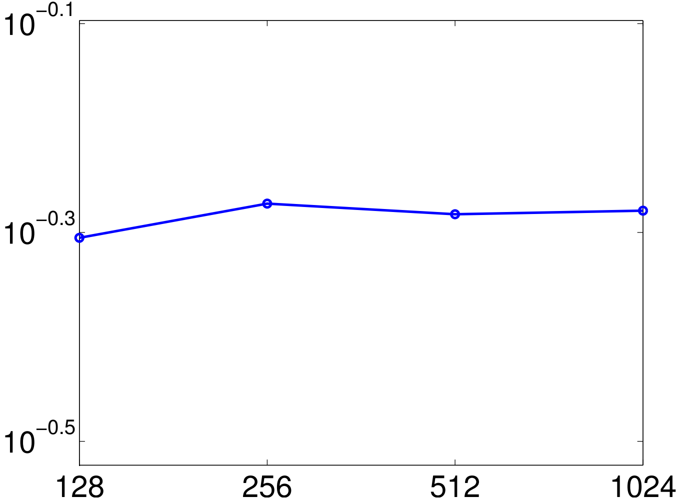
$$\begin{aligned}\langle g, \nu_{x,t}^{\Delta x} \rangle &= \int_P g(\lambda) d\nu_{x,t}^{\Delta x}(\lambda) \\ &= \int_{\Omega} g(\mathbf{U}^{\Delta x}(x,t,\omega)) d\mathcal{P}(\omega) \quad \text{(Definition of law)} \\ &\approx \frac{1}{M} \sum_{1 \le i \le M} g(\mathbf{U}_i^{\Delta x}(x,t)) \quad \text{(MC approximation).}\end{aligned}$$

- $\mathbf{U}_i^{\Delta x}$ are M i.i.d samples
- Convergence proof as $M \to \infty$ (Fjordholm, Käppeli, SM, Tadmor,,2014).

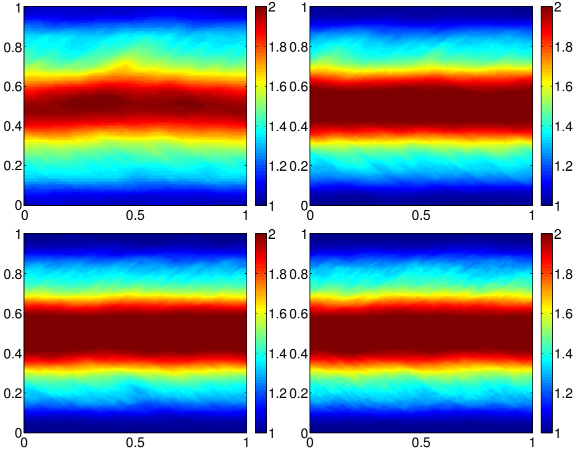
KH (Sample): Density at different resolutions



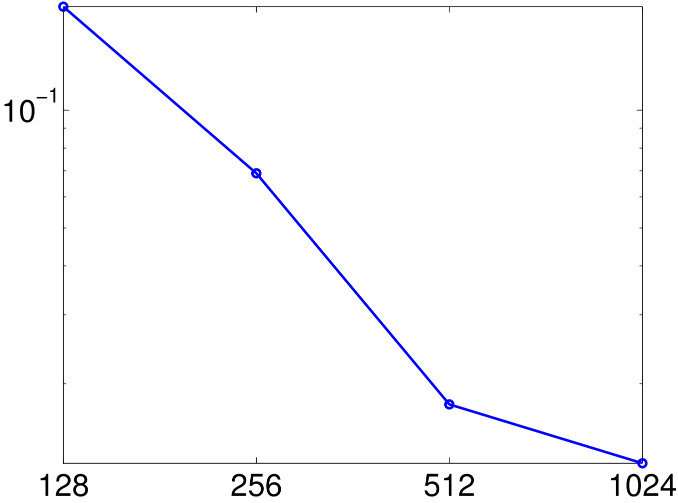
Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



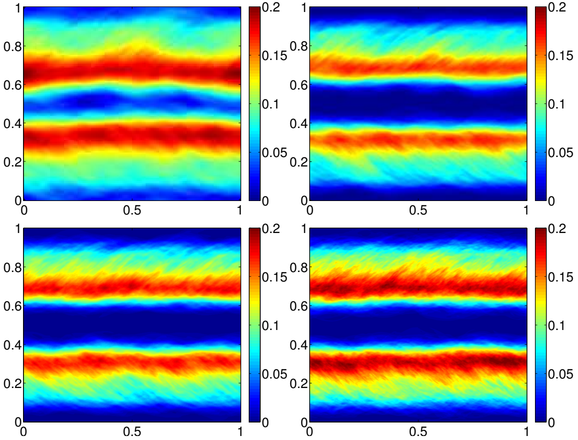
KH mean on different meshes (200 samples)



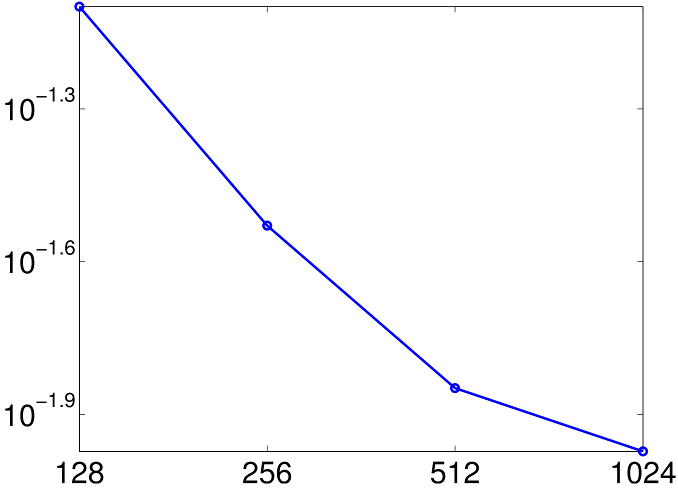
Mean: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



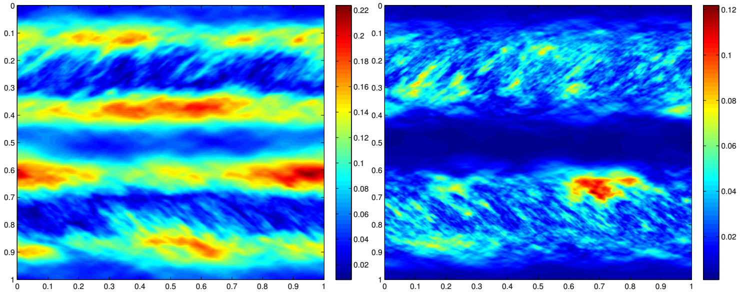
KH variance on different meshes (200 samples)



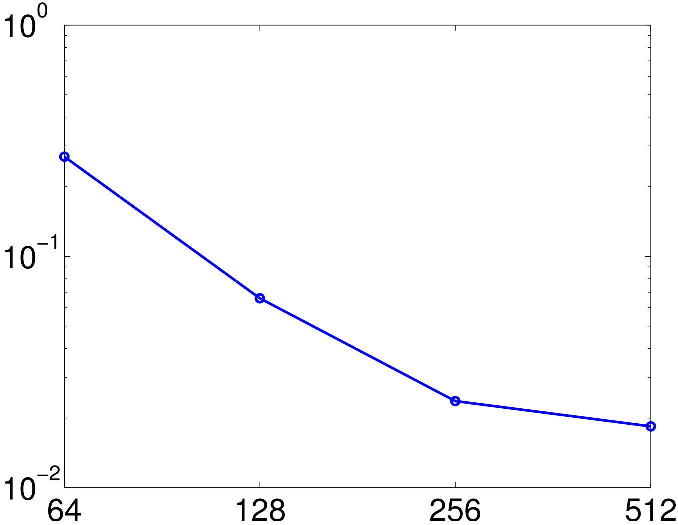
Variance: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



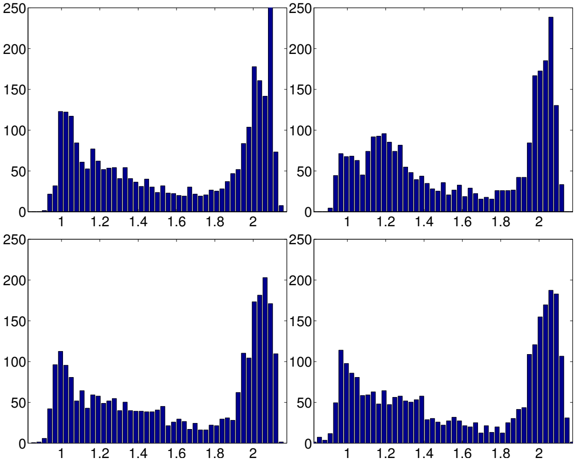
Wasserstein distances $\mathcal{W}_1(\nu^{\Delta x}, \nu^{\Delta x/2})$ for different resolutions



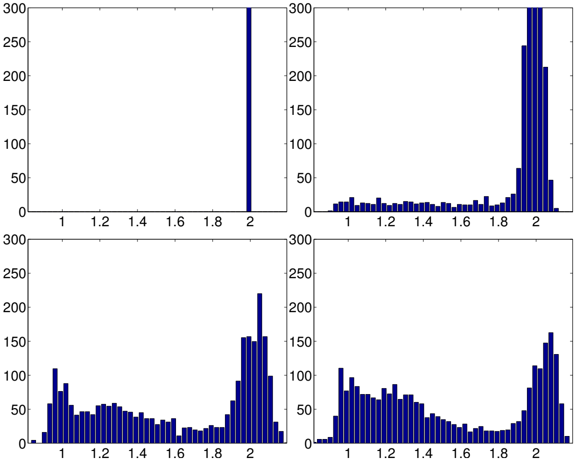
Cauchy rates in $L^1(\mathcal{W}_1)$



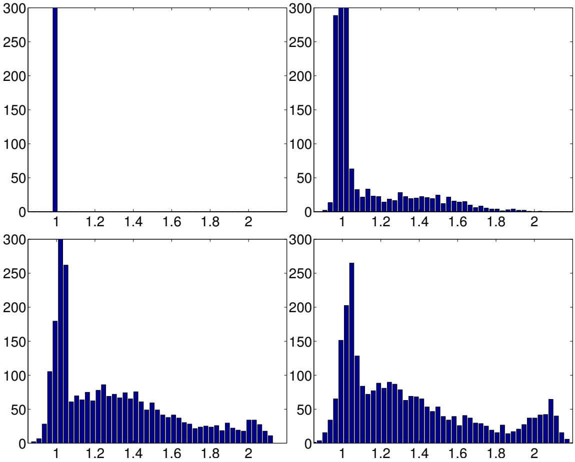
Convergence of PDFs



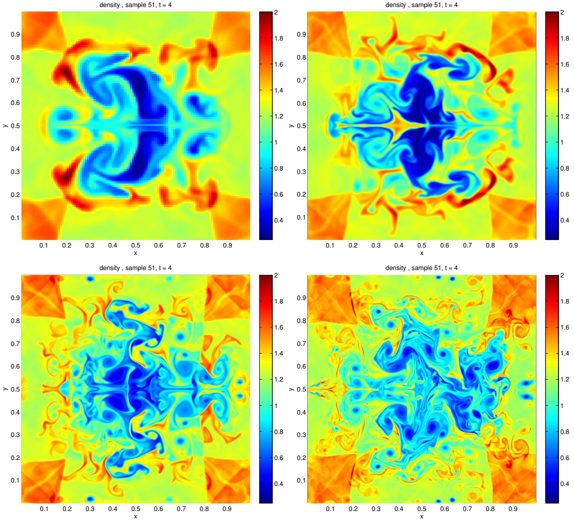
Atomic initial measure ⇒ Non-atomic young measure



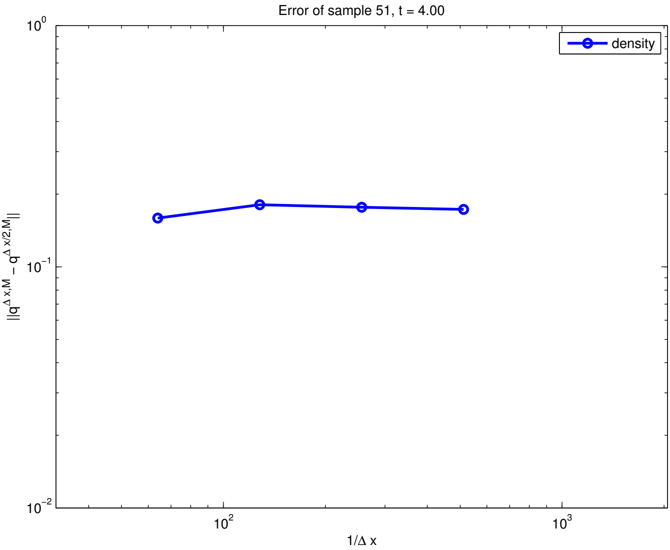
Atomic initial measure ⇒ Non-atomic young measure



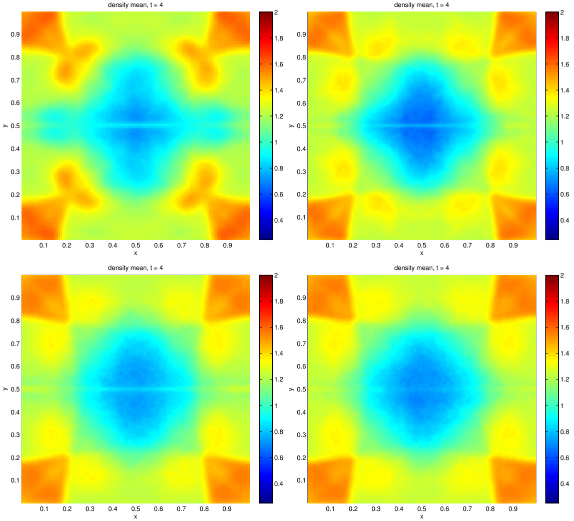
Richtmeyer Meshkov (Sample): Density



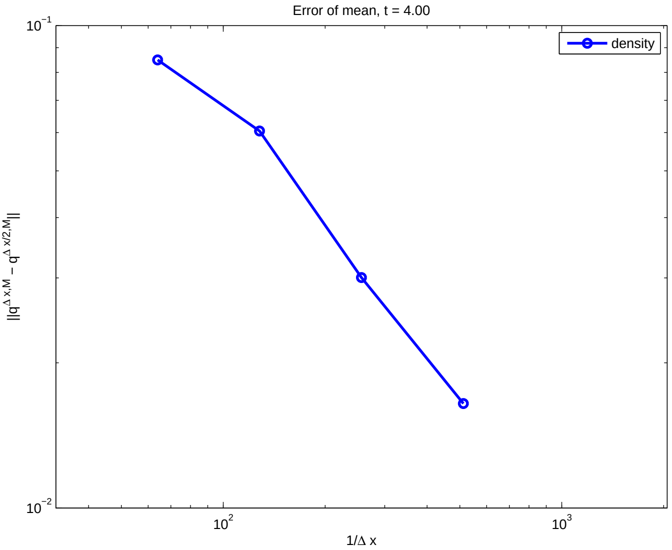
Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



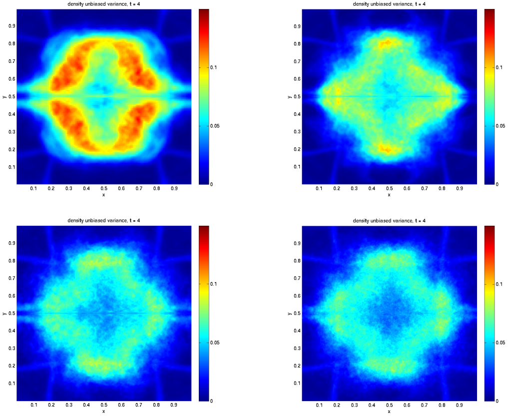
RM mean on different meshes (200 samples)



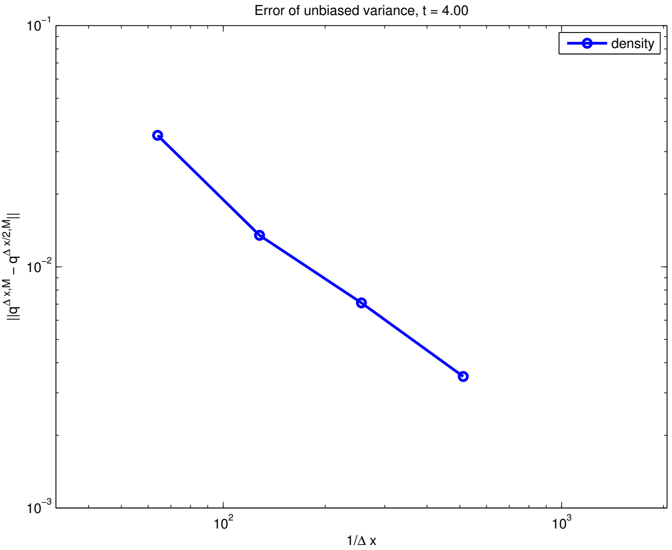
Mean: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



RM variance on different meshes (200 samples)



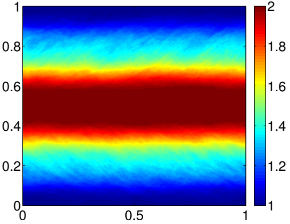
Variance: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



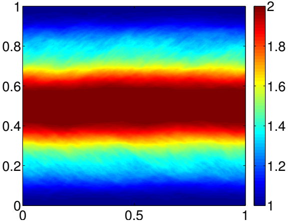
MVS Issues I: Uniqueness (stability) ?

- A generic admissible (entropy) MVS is Not unique.
- Similar construction a la DeLellis, Szekelyhidi.
- However, computed MVS seems to very stable wrt
  - Different numerical schemes.
  - Different types of initial perturbations.

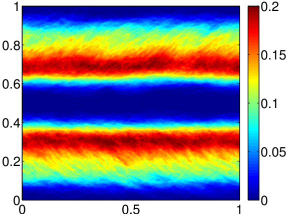
Stability vis a vis different numerical schemes



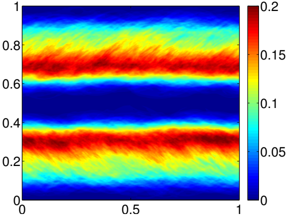
(h) Mean, TeCNO3



(i) Mean, FISH

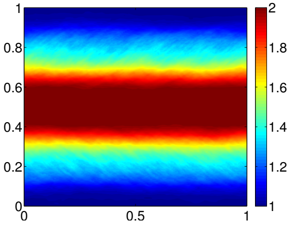


(j) Variance, TeCNO3

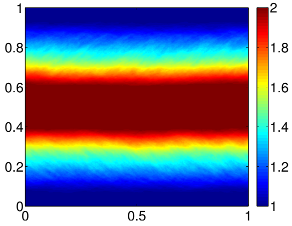


(k) Variance, FISH

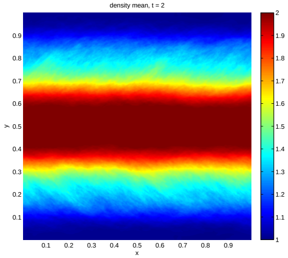
Stability vis a vis different types of perturbations: Mean



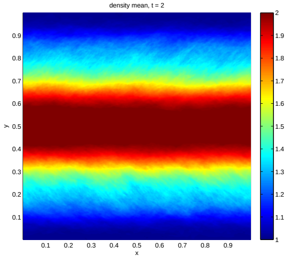
(l) Phase



(m) Amplitude

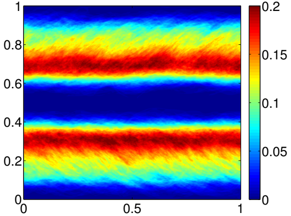


(n) Uniform

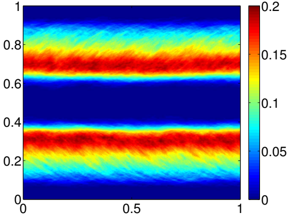


(o) Normal

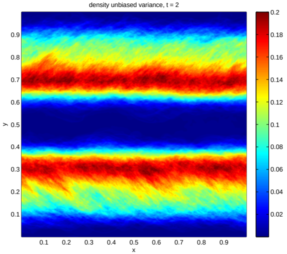
Stability vis a vis different types of perturbations: Variance



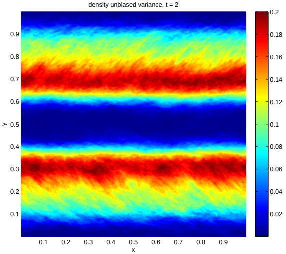
(p) Phase



(q) Amplitude



(r) Uniform



(s) Normal

Stability of MVS ?

- Numerical experiments suggest that computed solution is stable !!
- Additional selection criteria for the computed solution ?

MVS as a UQ framework

- MVS is an UQ framework for Uncertain initial data + coefficients.
- MV Cauchy problem:

$$\langle ID, \nu \rangle_t + \operatorname{div} \langle \mathbf{F}, \nu \rangle = 0, \quad \text{in} \quad \mathcal{D}'(D)$$
$$\nu_{x,0} = \sigma_x, \quad \text{a.e } x \in \mathbb{R}.$$

  - Initial Young measure σ_x represents 1-pt statistics.
  - 1-pt statistics evolved by MVS $\nu_{x,t}$.
  - DOESNOT account for Spatial correlations in initial data or solutions !!!
- Spatially independent initial data $\Rightarrow$ Spatially correlated solutions !!!

Statistical solutions

- Developed by Fjordholm, Lanthaler, SM, 2015.
- Statistical solution $\mu \in \mathrm{Prob}(L^p(D))$ i.e, probability measure on a function space.
- THM: Completely characterized by all k-point correlation measures.

$$\mu_t \Longleftrightarrow \begin{cases} \nu^1_{x,t} \\ \nu^2_{x_1,x_2,t} \\ \dots \\ \nu^k_{x_1,x_2,\dots,x_k,t} \\ \dots \end{cases}$$

- Identification through Cylindrical test functions.

Statistical solutions (Contd)

- Infinite dimensional Lioville equation characterized by,

$$\partial_t \langle \nu^k_{x_1,x_2,\dots,x_k,t}, \xi_1\xi_2\dots\xi_k\rangle + \sum_{i=1}^{k} \partial_{x_i} \langle \nu^k_{x_1,x_2,\dots,x_k,t}, \xi_1\xi_2\dots \mathbf{F}(\xi_i)\dots\xi_k\rangle = 0, \quad \forall k \in \mathbb{N}$$

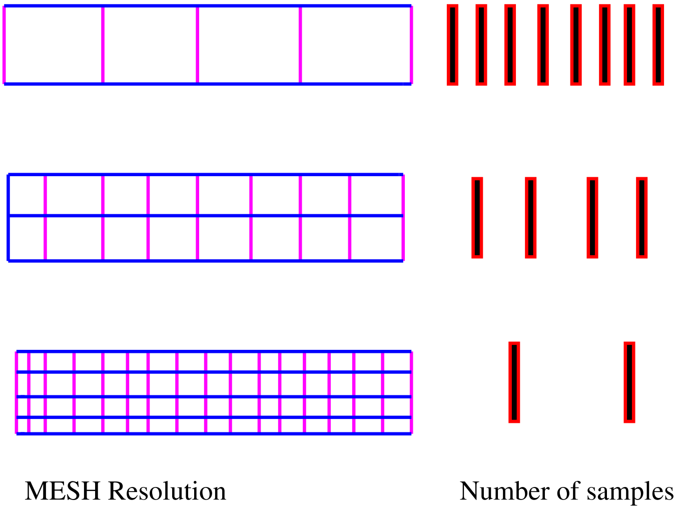
- $+$ Suitable Entropy conditions.
- Fjordholm, Lanthaler, SM, 2015 show:
  - Existence of statistical solutions.
  - Approximation of statistical solutions using the FKMT algorithm !!!
- Promising description of Turbulent flows.
- UQ framework that accounts for correlations.
- Uniqueness of statistical solutions is very much open.

MVS Issue II: Computational cost

- Phase space integrals by Monte Carlo (MC) sampling:

$$\langle g, \nu_{x,t}^{\Delta x} \rangle \approx \frac{1}{M} \sum_{1 \leq i \leq M} g(\mathbf{U}_i^{\Delta x}(x,t)).$$

- MC converges at rate $\mathcal{O}\left(\frac{1}{\sqrt{M}}\right)$
- Slow convergence $\Rightarrow$ Extreme computational cost.
- Possible solution: Multi-level Monte Carlo (MLMC) methods.


MESH Resolution
Number of samples

MLMC-FKMT algorithm: Lye, SM, in preparation

- Different nested levels of resolution: l.
- Draw M_l i.i.d samples for the initial random field: $\{\mathbf{U}^i_{l,0}\}_{1 \le i \le M_l}$.
- For each draw: Solve conservation law by numerical scheme to obtain $\mathbf{U}^i_{\tau,l}$.
- Sample statistics: with $u_{\tau,-1} = 0$,

$$\langle g, \nu^\tau_{x,t} \rangle = \sum_{l=0}^{L} \sum_{i=1}^{M_l} \frac{1}{M_l} \left(g(\mathbf{U}_i^{\tau,l}(x,t)) - g(\mathbf{U}_i^{\tau,l-1}(x,t)) \right)$$

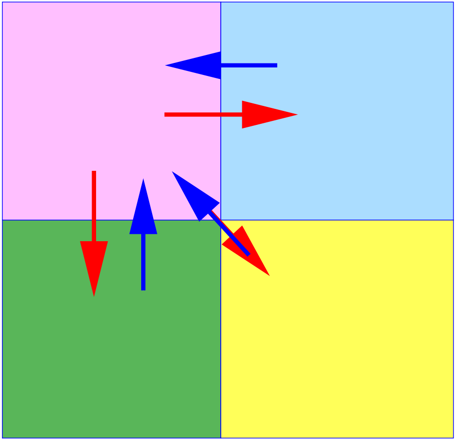
- Convergence of ν^τ to EMVS.
- Complexity estimate + Numerical experiments – Work in progress !!!

Implementation : Special care

- Online computation of variance !!
- A Good Pseudo-random number generator !!
  - **WELL**-series of pseudo random number generators:
  - We used WELL512a:
    - buffer size: 16
    - period length: $2^{512} - 1$
    - very good equidistribution
    - fast: takes 33 sec for 10^9 draws

Parallel implementation I

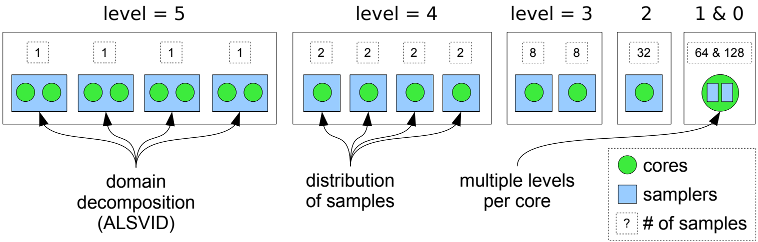
- Domain decomposition for the FMV solver.



- Use MPI for message passing between processors.

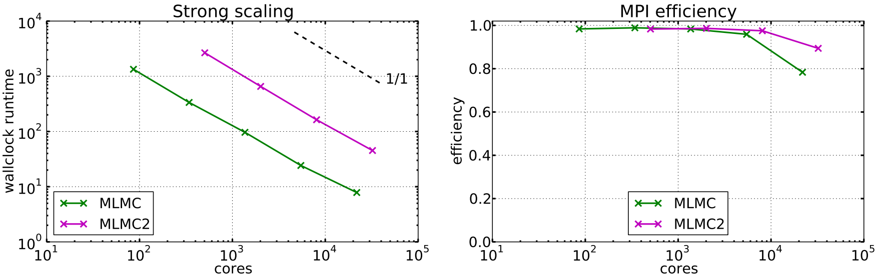
Parallel implementation II

- Static load balancing procedure for MLMC – SM, Schwab, Sukys 2012.

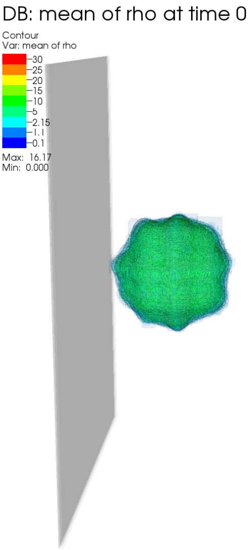


- A Dynamic load balancing version – Sukys, 2013.

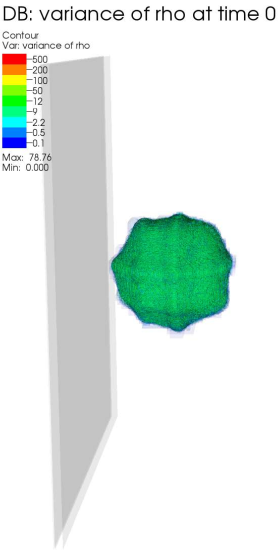
Strong scaling atleast upto 50000 processors



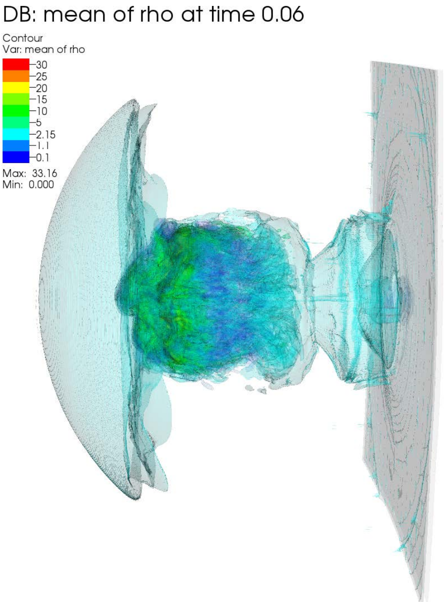
3D Euler– Initial Mean



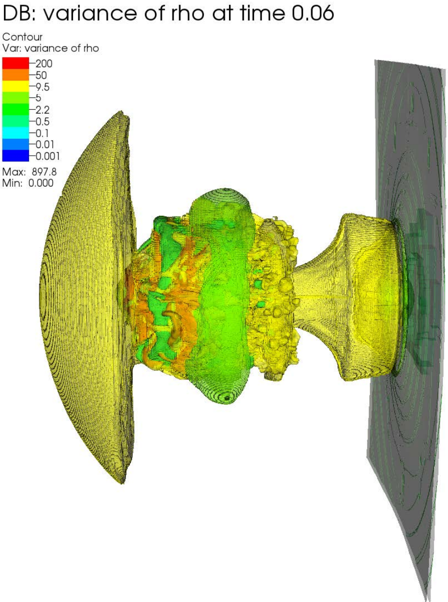
3D Euler– Initial Variance



3D Euler– Mean (Cost: 5 hours on 50000 processors)



3D Euler– Variance (Cost: 5 hours on 50000 processors)

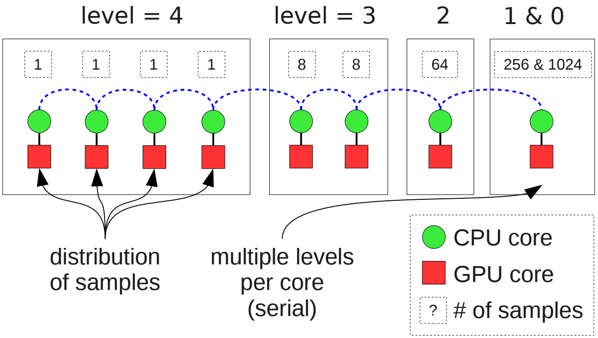


Emerging massively parallel HPC architectures: Piz Daint (CSCS, Switzerland)

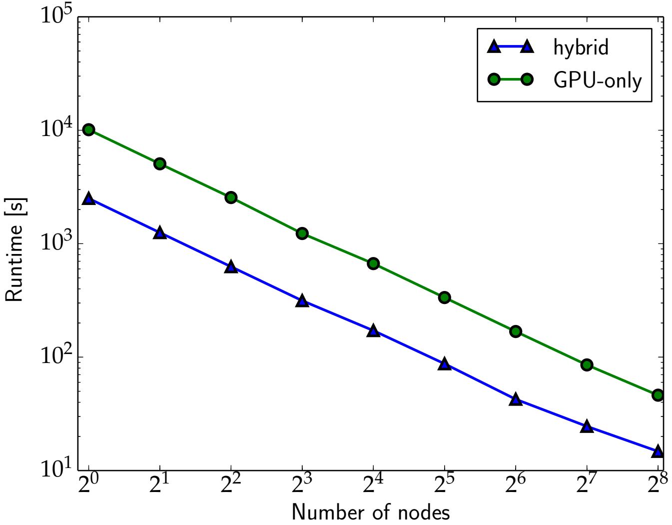
- Hybrid CRAYXC30 machine. (6-th in Top500)
- 5272 compute nodes (115000 cores)
- Each nodes consists of Intel Xeon E5-2670 (CPU) and NVIDIA TESLA 20 X (GPU) !!!
- Peak performance: 7.78 petaflops.

Hybrid MLMC

- Based on Dynamic load allocation algorithm (Grosheintz, SM, Sukys, forthcoming).
  - Master-Slave type load distributor.
  - CPU fast for coarse resolution but GPU fast for fine resolution.



Hybrid MLMC is efficient



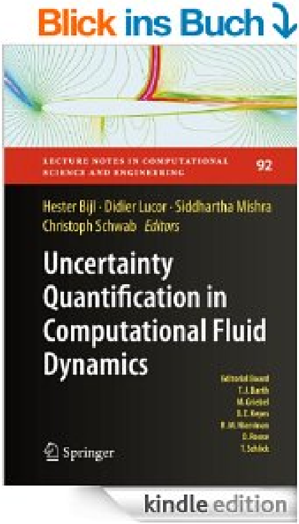
Summary

- Modeling of uncertain inputs + solutions:
  - Random fields (Scalar conservation laws, linear systems)
  - Young measures (Nonlinear systems)
- Computation of Uncertainty:
  - MC (slow but robust)
  - MLMC (fast)
- Massively parallel implementation on hybrid architectures.

MLMCFVM: Advantages over Stochastic Galerkin and Collocation methods (if they work)

- Ability to handle very large dimensions.
- low regularity requirements:
  - SGL and SCL methods need high regularity wrt stochastic variables.
  - For non-linear hyperbolic systems: Discontinuities in stochastic variables.
- Totally Non-intrusive and readily parallelizable.

More from



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