Measure valued and statistical solutions of systems of balance laws.

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Systems of balance laws

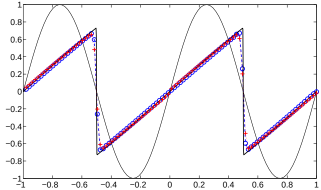
- Nonlinear systems of PDEs of form:

$$\mathbf{U}_t + \mathrm{div}(\mathbf{F}(\mathbf{U})) = \mathbf{B}(x, t, \mathbf{U}).$$

- Examples:
  - Shallow water equations with bottom topography (Geophysics, Oceanography)
  - Euler equations with gravitation (Climate Science).
  - Stratified MHD equations (Astrophysics).
- Special case: Conservation laws (Source $\mathbf{B} \equiv 0$).

Solution framework: Entropy solutions

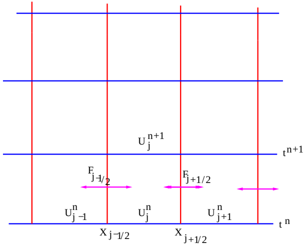
- Hyperbolicity: Finite speed of propagation.
- Nonlinearity$\Rightarrow$ Shock formation.



- Weak solutions (in the sense of distributions).
- Weak solutions are not necessarily unique.
- Additional admissibility criteria: Entropy conditions.

Standard numerical Methods

- Finite volume schemes: Discrete balance.



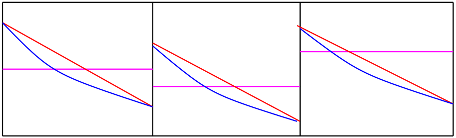
- Numerical flux:
  - Exact (approximate) Riemann solver: Godunov, Roe, HLL.
- Non-oscillatory piecewise polynomial reconstruction:
  - TVD, ENO, WENO, DG.
- SSP Runge-Kutta time stepping.

Discretization of Source terms

- Need to preserve steady states (Hydrostatic equilibrium):
- Ensure Discrete version of

$$\operatorname{div}(\mathbf{F}(\mathbf{U})) \approx \mathbf{B}(x, t, \mathbf{U}).$$

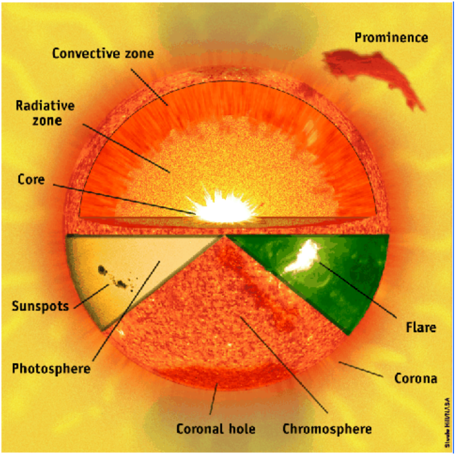
- Hydrostatic reconstruction $\Rightarrow$ Well-balanced schemes



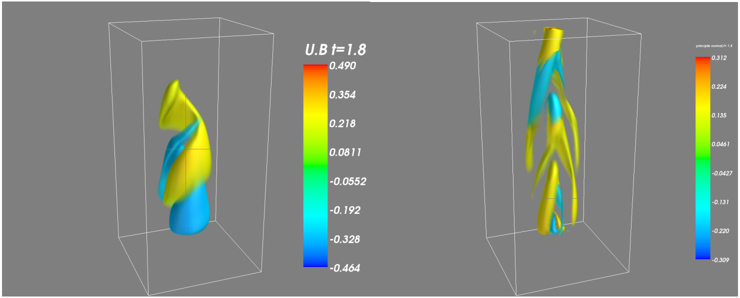
- Above framework is Highly successful in practice.

Ex 1: Simulating waves in the Solar atmosphere

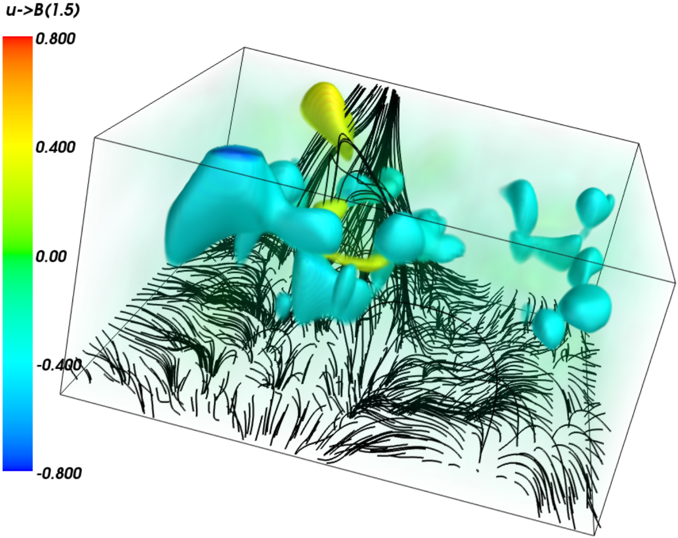
- Stratified MHD equations (Simulations of Fuchs,McMurry,SM,Waagan,2010,2011)



Alfven Waves in a synthetic solar atmosphere

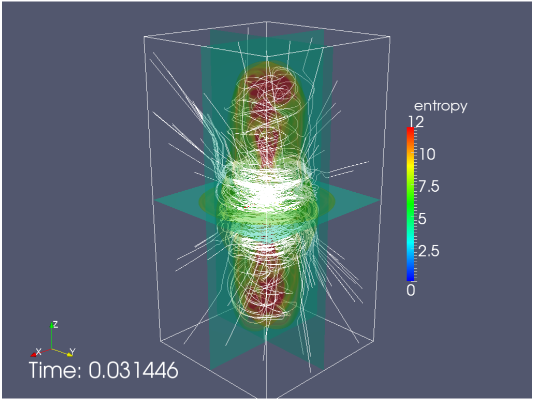


Chromospheric waves from SOHO data

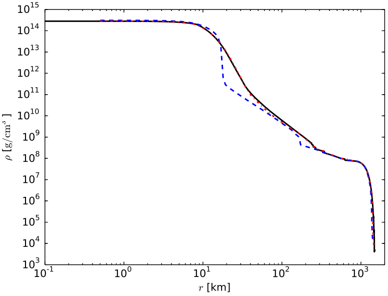


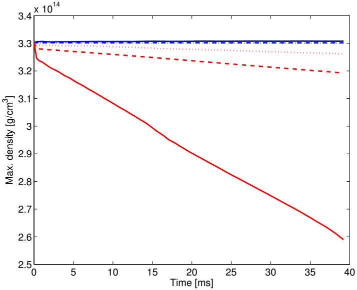
Ex 2: Simulating Supernova Core Collapse

- Stratified MHD with Neutrino transport and Self gravity (Käppeli, SM, 2014,2015)



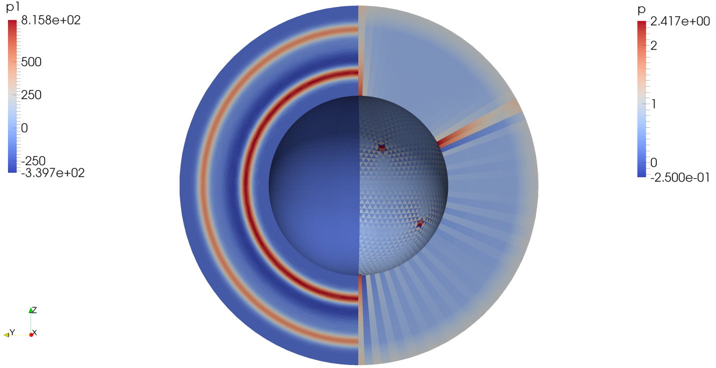
Well balanced vs. Naive Schemes





Ex 3: Simulation of Exoplanet atmospheres

- Stratified Euler on a sphere (By Grosheintz, Käppeli, SM, Heng,Forthcoming)

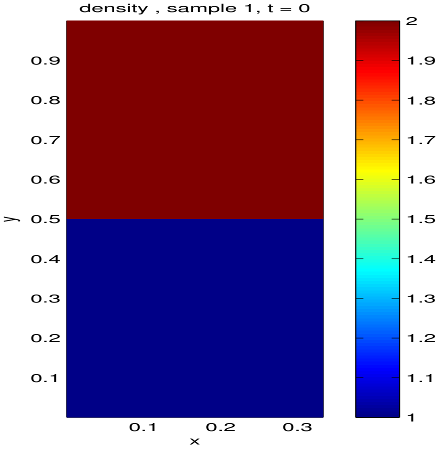


Problem I: What is the numerical error?

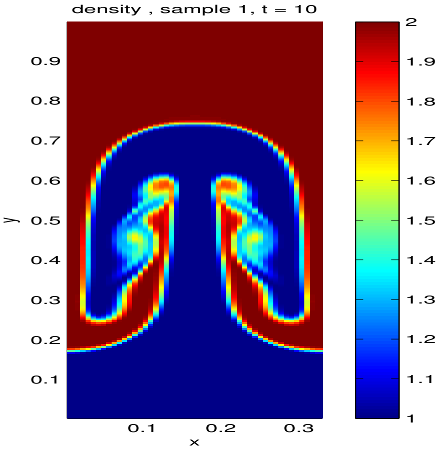
- Convergence: Fundamental question in Numerical analysis
- Does $\mathbf{U}^{\Delta x} \to \mathbf{U}$ as $\Delta x \to 0$?
- Rate of convergence ?
- Question of Convergence of numerical methods is open.
- Particularly for Multi-D systems.
- Empirical demonstration of convergence ?

Rayleigh-Taylor problem: Euler equations with gravity

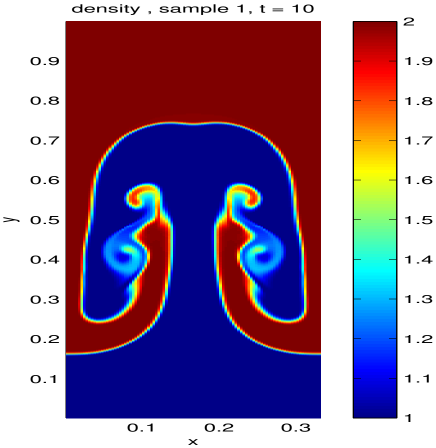
- Second-order well-balanced simulation of Käppeli, SM.



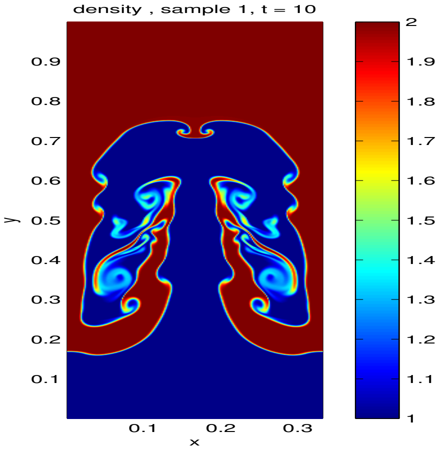
Numerical convergence: 2-D Rayleigh-Taylor problem 200×50 grid ($T = 10$)



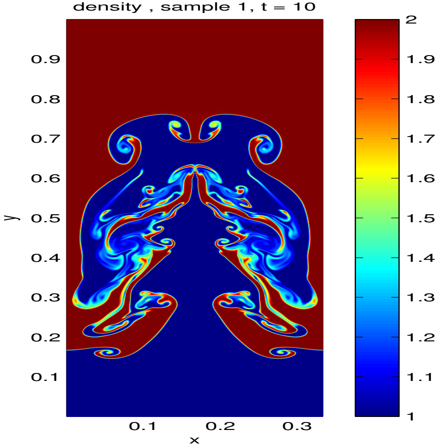
Numerical convergence: 2-D Rayleigh-Taylor problem 400×100 grid ($T = 10$)



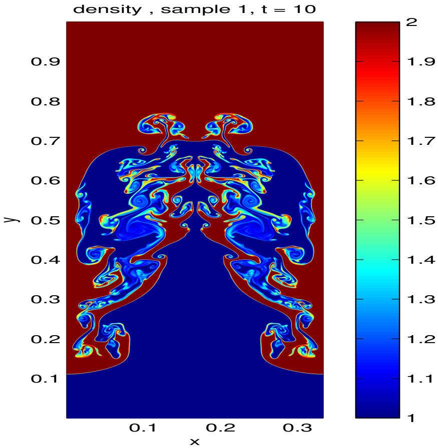
Numerical convergence: 2-D Rayleigh-Taylor problem 800×200 grid ($T = 10$)



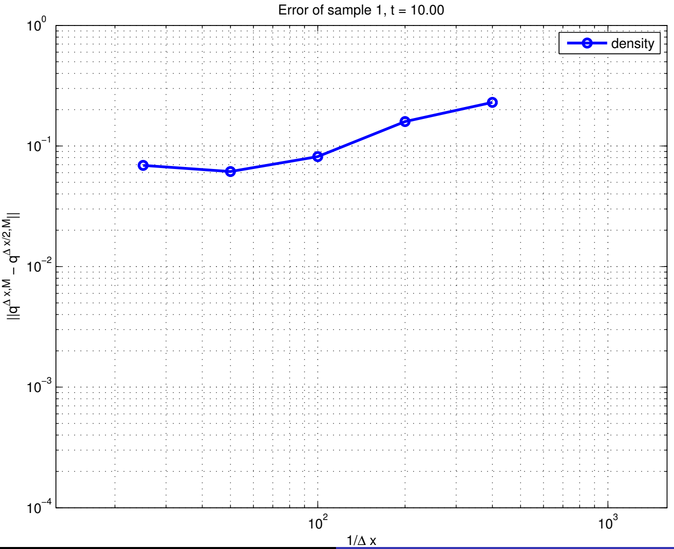
Numerical convergence: 2-D Rayleigh-Taylor problem 1600×400 grid ($T = 10$)



Numerical convergence: 2-D Rayleigh-Taylor problem
3200×800 grid ($T = 10$)



L^1 Error vs mesh resolution: 2-D Rayleigh-Taylor problem $T = 10$



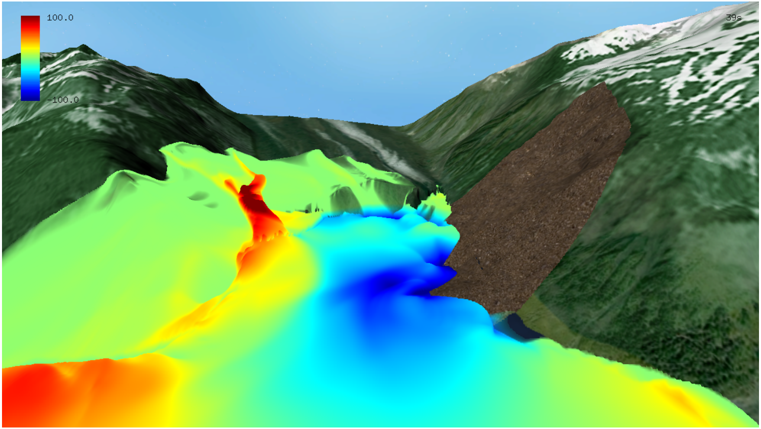
Problem 1: Lack of convergence for Conservation (Balance) laws

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

Lituya Bay Mega Tsunami, Alaska, 1958

- Earthquake induced rockslide tsunami.
- Highest recorded wave run-up: 524 m !!!
- Simulation of Asuncion, Castro, SM, Sukys, Sanchez, 2014:
  - Two-layer shallow water model.
  - Robust finite volume scheme for Non-conservative hyperbolic system
  - Optimized GPU implementation.

Run-up at $T = 39s$



Criticism of the simulation

- Three Crucial Model parameters
  - Ratio of inter-layer densities.
  - Coloumb friction.
  - Inter-layer friction.
- Measurement of parameters is highly uncertain.
- No reliability of the simulation.

Problem 2: Uncertainty

- Model inputs: are obtained by Measurements:
  - Initial conditions.
  - Boundary data.
  - Coefficients.
  - Parameters.
- Measurements are Uncertain.
- Uncertain Inputs $\Rightarrow$ Uncertain Solutions (Outputs).
- Modeling and computation of this uncertainty is Uncertainty Quantification (UQ)

Challenges

- Lack of Convergent methods.
- Linked to the lack of global well-posedness results for entropy (admissible) solutions.
- UQ
- A promising solution that kills two birds with one stone
- Measure valued solutions
- Statistical solutions
- Follow up to the lecture of Tadmor
- Trailer for the lecture of Fjordholm

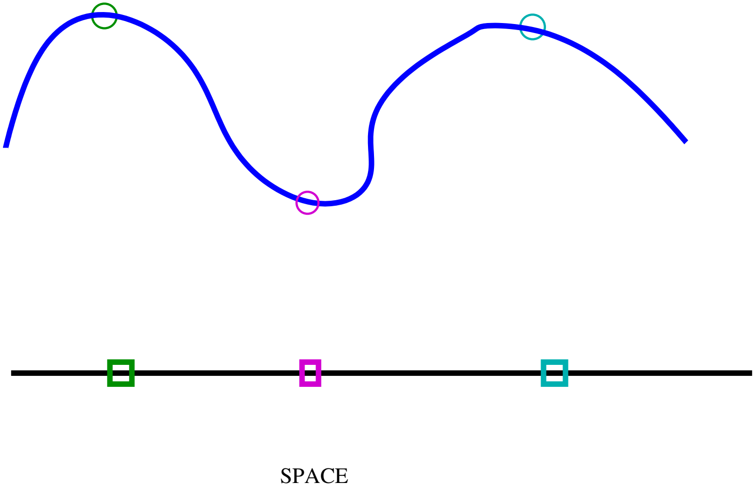
Entropy measure valued solutions

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

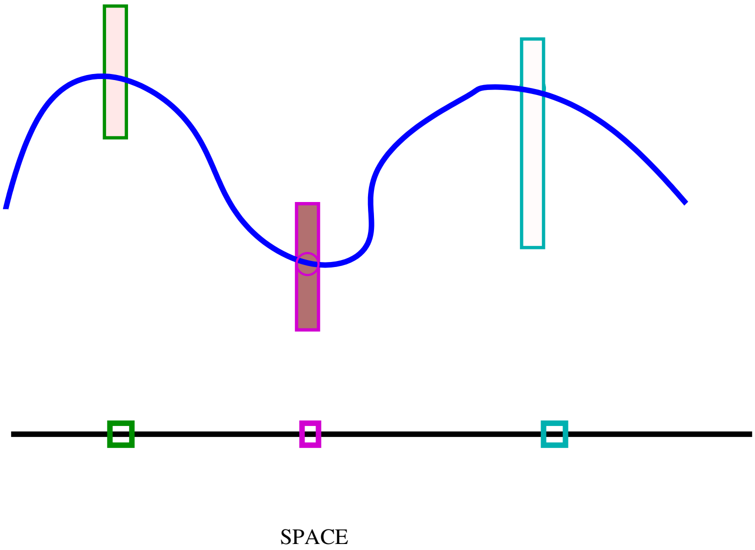
$$\langle g, \nu_{x,t} \rangle := \int_P g(\lambda) d\nu_{x,t}(\lambda)$$

- 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)

Weak solutions (time snapshot)



Measure valued solutions (time snapshot)



Generalized Cauchy problem for $\mathbf{U}_t + \mathrm{div}(\mathbf{F}(\mathbf{U})) = \mathbf{B}(x, t, \mathbf{U})$

$$\langle \nu_{x,t}, ID\rangle_t + \mathrm{div}(\langle \nu_{x,t}, \mathbf{F}\rangle) = \langle \nu_{x,t}, \mathbf{B}(x,t,\cdot)\rangle \quad \text{in} \quad \mathcal{D}'(D)$$
$$\nu_{x,0} = \sigma_x, \quad \text{a.e } x \in \mathbb{R}.$$

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

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

  - Initial data attained in the sense of mean.
- Efficient Construction 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 $\overline{D} \subset \mathbb{R}^m$:

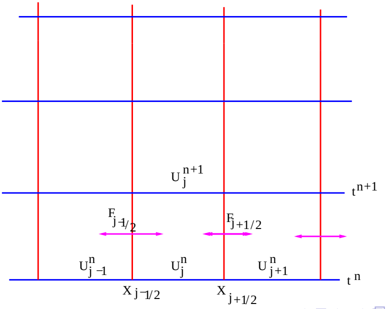
$$\sigma_x(\overline{D}) := \mathcal{P}\left(\{\omega \in \Omega : \mathbf{U}_0(\omega, x) \in \overline{D}\right),$$

Step 2: Numerical approximations

- Standard semi-discrete finite volume scheme:

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

- 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,Tadmor Forthcoming) with Generalized young measures.
- Numerical schemes satisfy L^2 bounds (Entropy estimate).

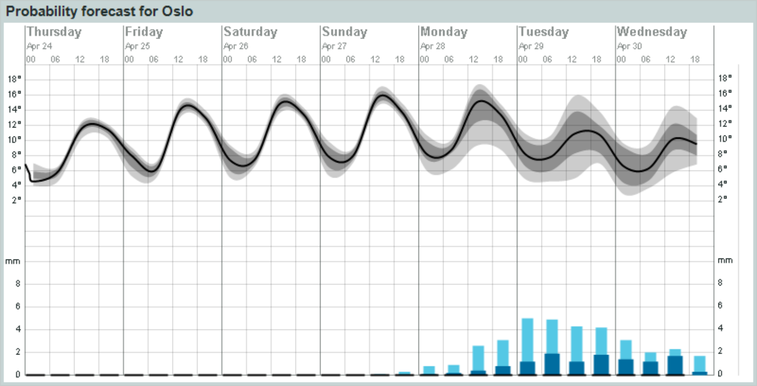
Computing the EMVS

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

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

- 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).
- Almost any quantity of interest can be written as an admissible observable

Typical measurements: Weather



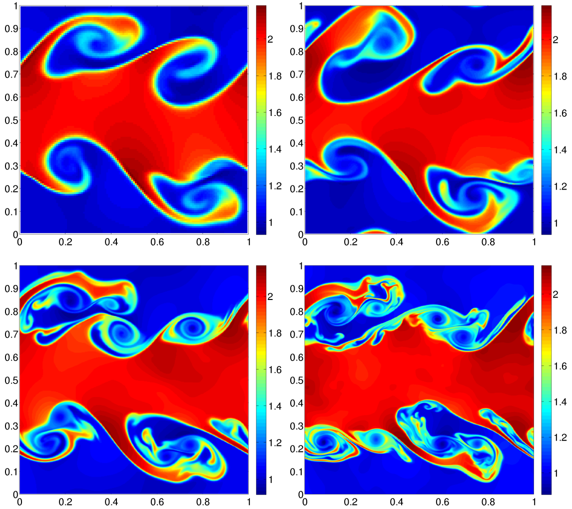
Monte Carlo approximation

- We need to compute:

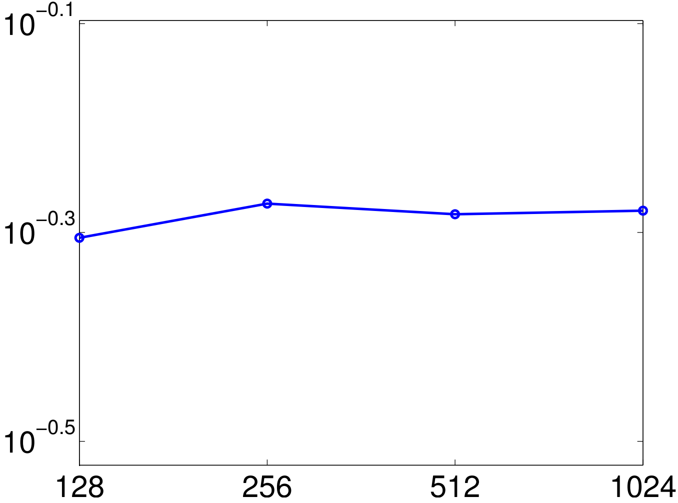
$$\begin{aligned}\langle g, \nu_{x,t}^{\Delta x}\rangle &= \int_P g(\lambda) d\nu_{x,t}^{\Delta x}(\lambda) \\ &= \int_\Omega g(\mathbf{U}^{\Delta x}(x,t,\omega)) d\mathcal{P}(\omega) \quad \text{(Definition of law)} \\ &\approx \frac{1}{M} \sum_{1 \le i \le M} g(\mathbf{U}_i^{\Delta x}(x,t)) \quad \text{(MC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

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

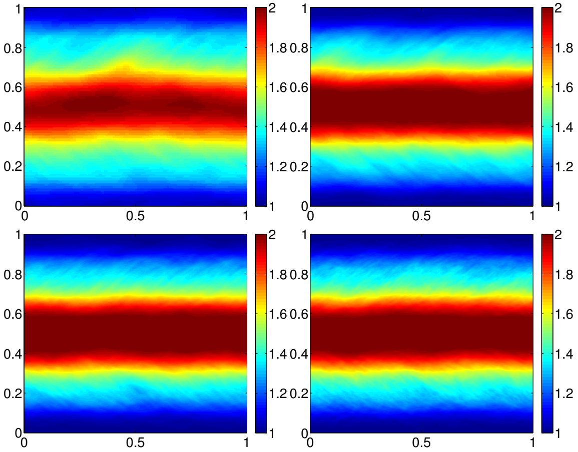
KH (Sample): Density at different resolutions



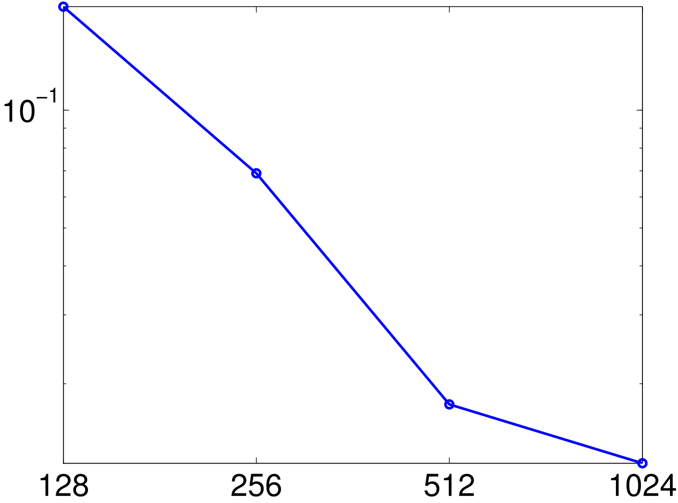
Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



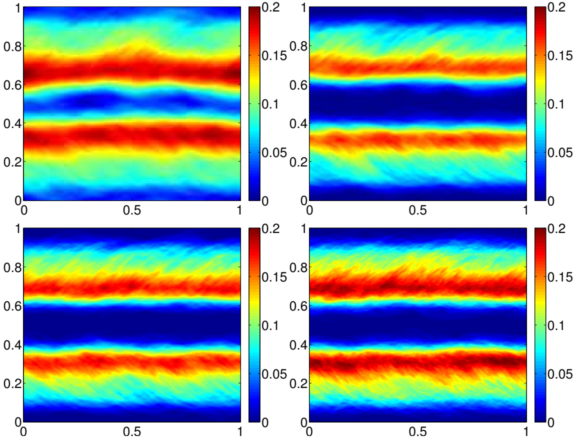
KH mean on different meshes (200 samples)



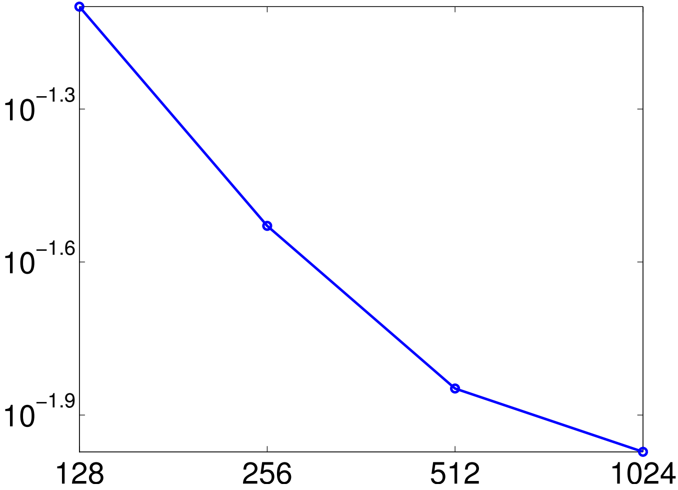
Mean: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



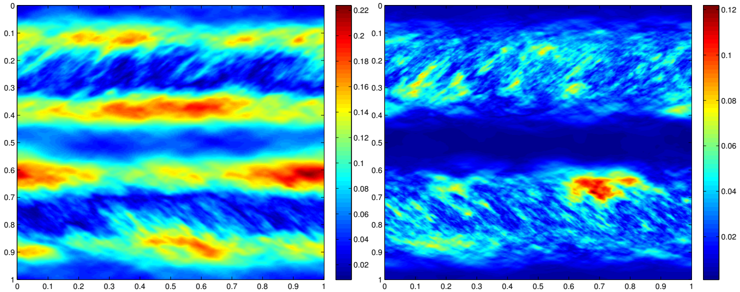
KH variance on different meshes (200 samples)



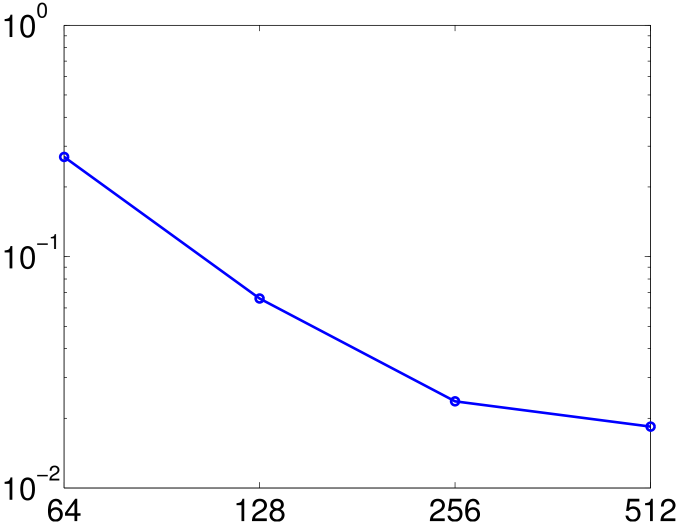
Variance: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



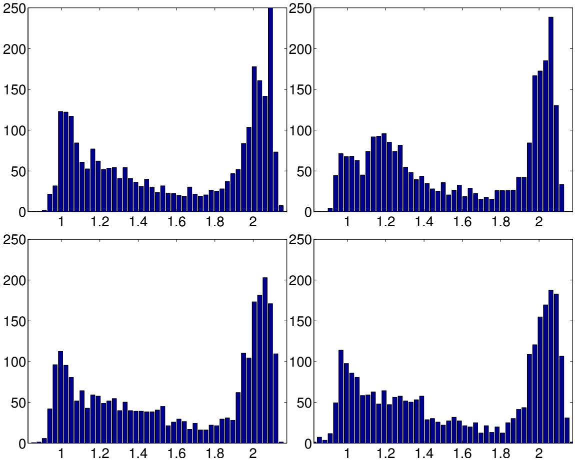
Wasserstein distances $\mathcal{W}_1(\nu^{\Delta x}, \nu^{\Delta x/2})$ for different resolutions



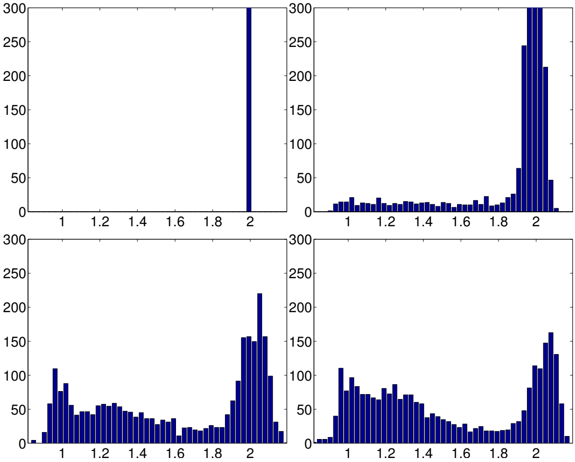
Cauchy rates in $L^1(\mathcal{W}_1)$



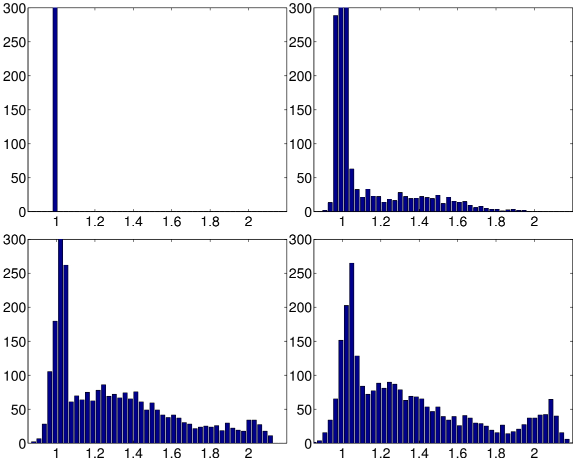
Convergence of PDFs



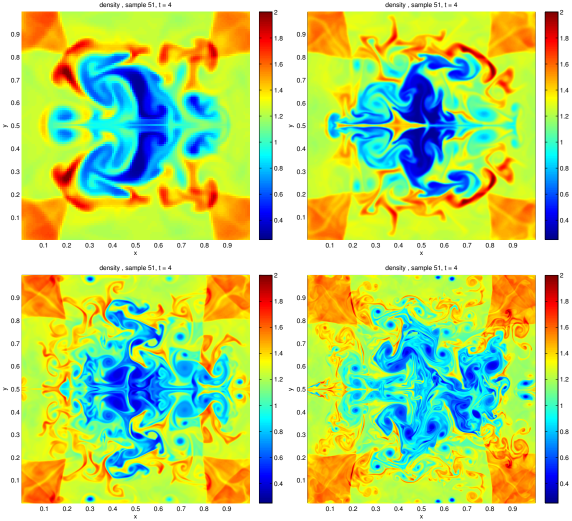
Atomic initial measure ⇒ Non-atomic young measure



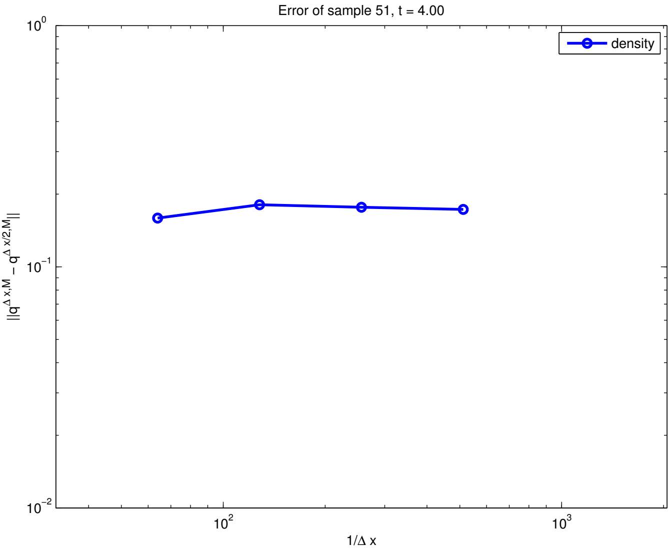
Atomic initial measure ⇒ Non-atomic young measure



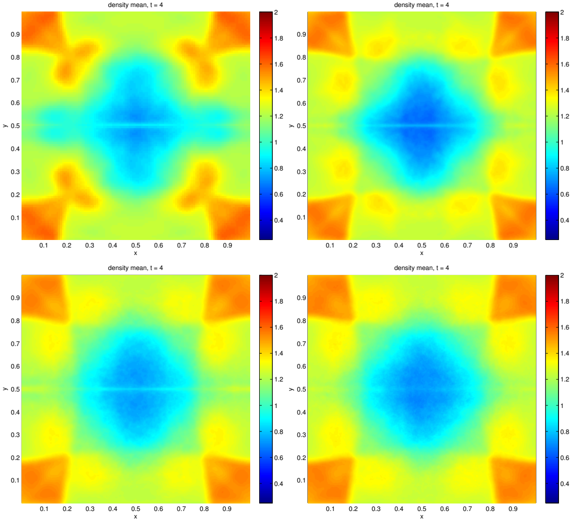
Richtmeyer Meshkov (Sample): Density



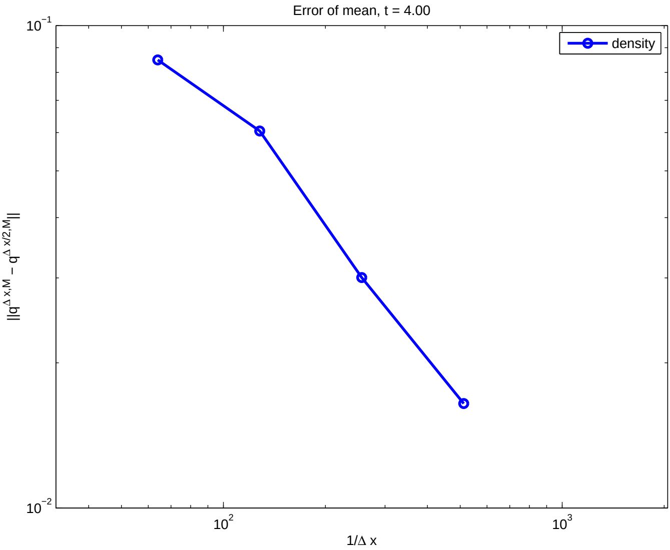
Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



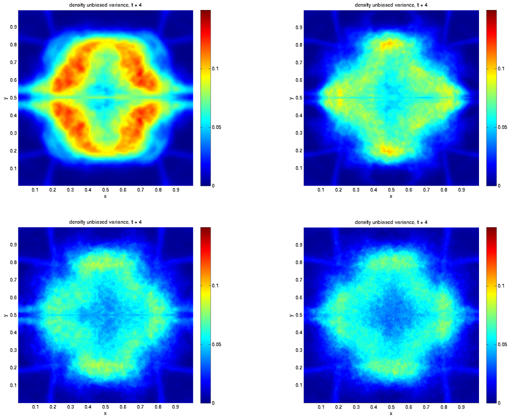
RM mean on different meshes (200 samples)



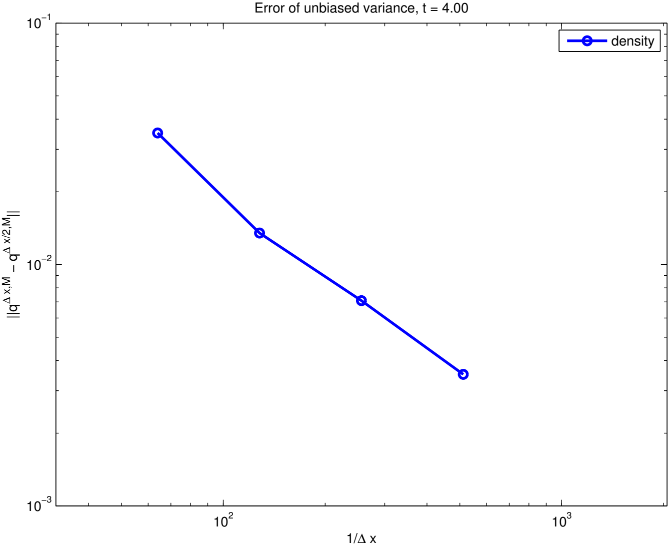
Mean: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



RM variance on different meshes (200 samples)



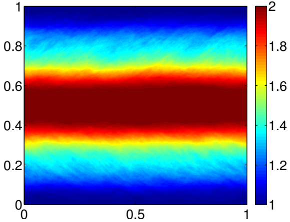
Variance: Cauchy rates $\|\mathbf{U}^{\Delta x} - \mathbf{U}^{\Delta x/2}\|_{L^1}$



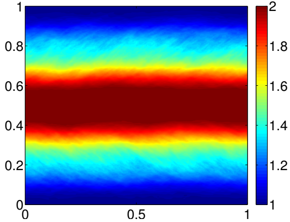
MVS Issues I: Uniqueness (stability) ?

- 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.

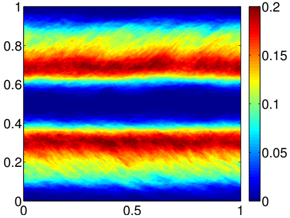
Stability vis a vis different numerical schemes



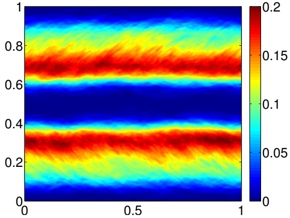
(a) Mean, TeCNO3



(b) Mean, FISH

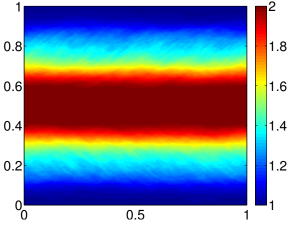


(c) Variance, TeCNO3

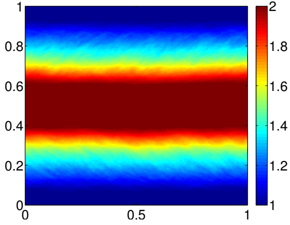


(d) Variance, FISH

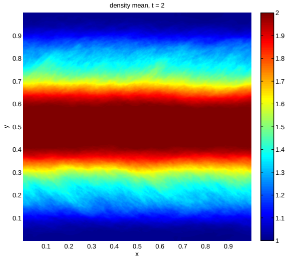
Stability vis a vis different types of perturbations: Mean



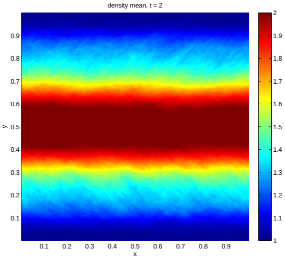
(e) Phase



(f) Amplitude

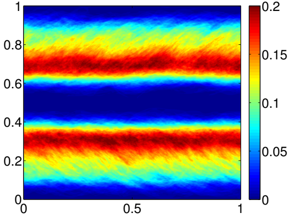


(g) Uniform

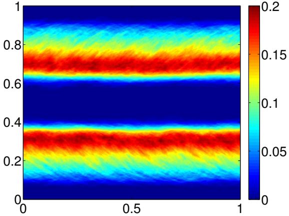


(h) Normal

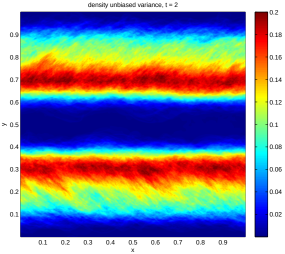
Stability vis a vis different types of perturbations: Variance



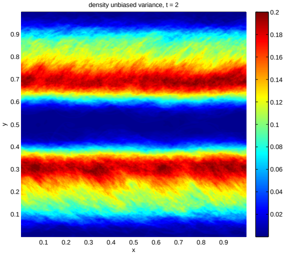
(i) Phase



(j) Amplitude



(k) Uniform



(l) Normal

Stability of MVS ?

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

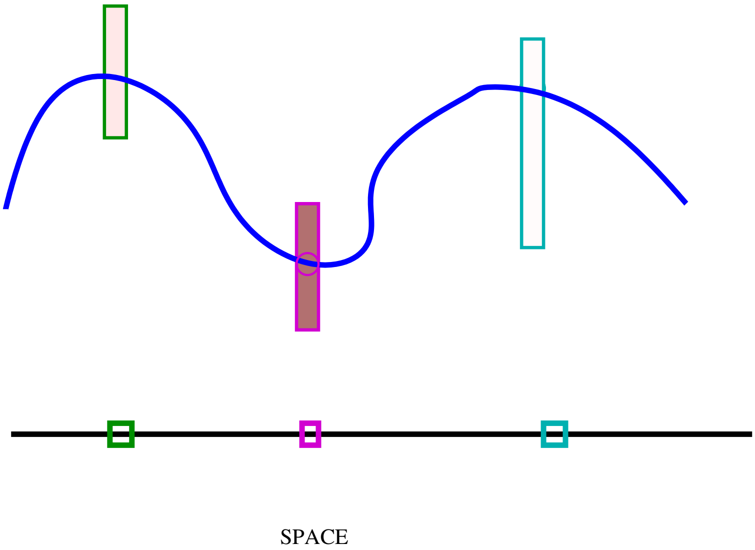
MVS as a UQ framework

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

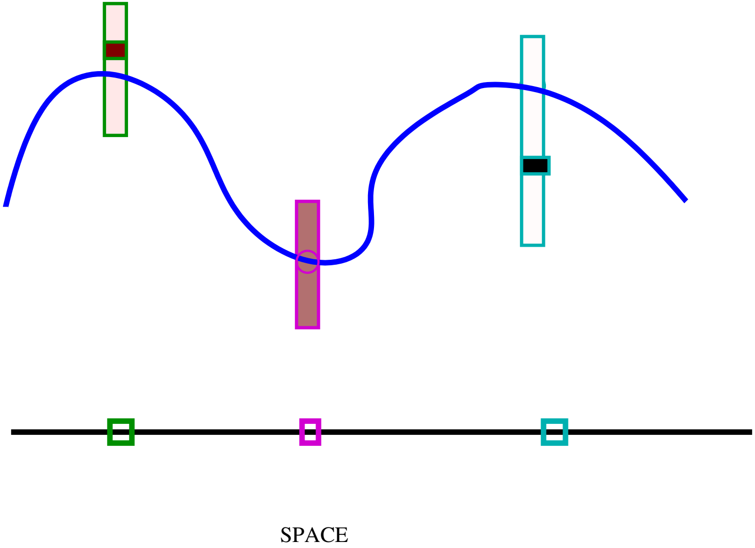
$$\begin{aligned} \langle \nu, ID \rangle_t + \mathrm{div} \langle \nu, \mathbf{F} \rangle &= \langle \nu, \mathbf{B} \rangle, \quad \text{in} \quad \mathcal{D}'(D) \\ \nu_{x,0} &= \sigma_x, \quad \text{a.e } x \in \mathbb{R}. \end{aligned}$$

  - 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 !!!

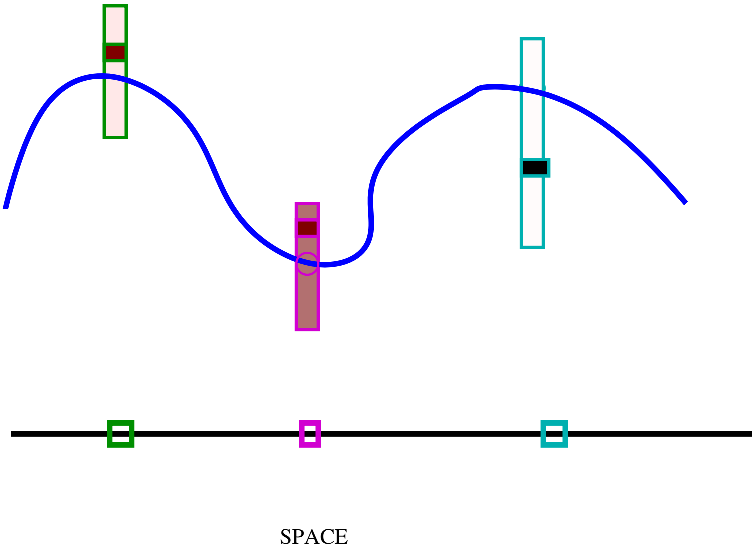
Measure valued solutions (time snapshot)



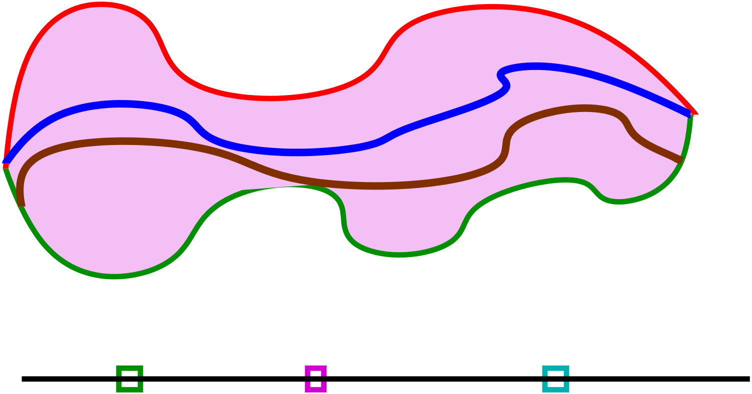
Two-point correlations (time snapshot)



Multi-point correlations (time snapshot)



Statistical Solutions



SPACE

Statistical solutions

- Developed by Fjordholm, Lanthaler, SM, forthcoming.
- 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 Liouville 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, SM, 2015 shows:
  - 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.
- Details in talk by Ulrik S. Fjordholm.

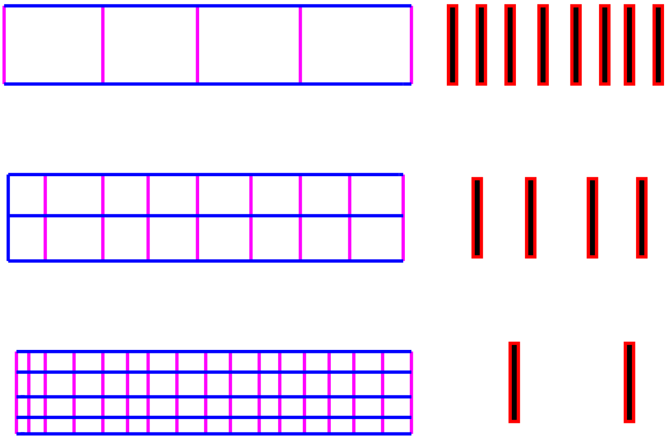
MVS Issue II: Computational cost

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

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

- 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.

MLMC



MESH Resolution

Number of samples

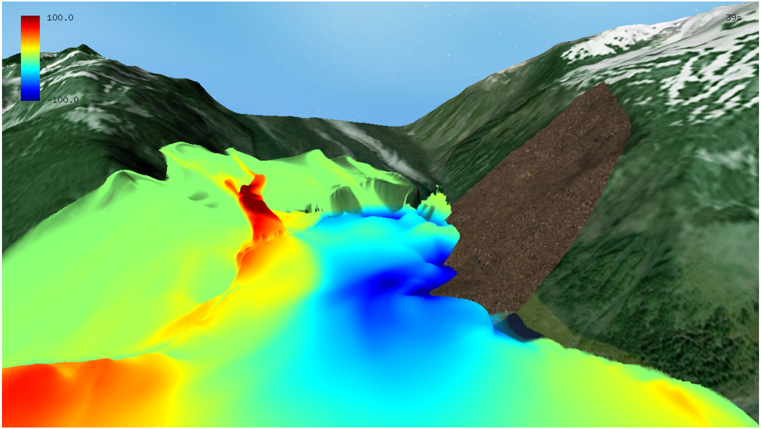
MLMC-FKMT algorithm: Lye, SM, forthcoming

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

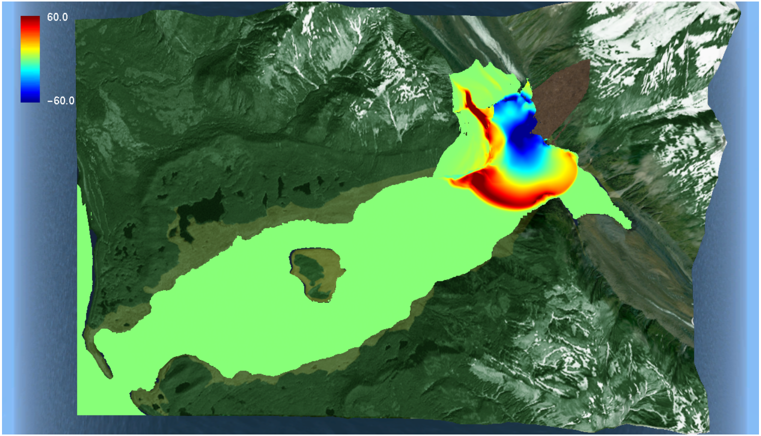
$$\langle g, \nu_{x,t}^{\tau} \rangle = \sum_{l=0}^{L} \sum_{i=1}^{M_l} \frac{1}{M_l} \left(g(\mathbf{U}_i^{\tau,l}(x,t)) - g(\mathbf{U}_i^{\tau,l-1}(x,t)) \right)$$

- Convergence of ν^{τ} to EMVS.
- Considerably Reduced Computational Cost.
- Numerical experiments in progress.

Run-up at $T = 39s$



Run-up Mean at $T = 39s$



Run-up Variance at $T = 39s$

Summary

- Problems with State of the art schemes:
  - Lack of Convergence on mesh refinement.
    - Generic to unstable and Turbulent flows.
    - Linked with lack of Wellposedness.
  - Uncertainty quantification
- A Statistical solution framework:
  - Measure Valued solutions.
  - Statisical solutions.
  - Approximation by convergent algorithms.
  - Promising description of multi-dimensional complex flows.
- Open questions:
  - Uniqueness of admissible statistical solutions.
  - Rigorous description of Turbulent flows.
  - Optimally complex numerical algorithms.
  - Non-conservative problems.
  - HPC implementation.

Atomic initial measure ⇒ Non-atomic young measure