Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Seminar for Applied Mathematics SAM

# Robust massively parallel MLMC-FVM solver for uncertainty quantification in nonlinear conservation laws

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# Hyperbolic nonlinear conservation laws

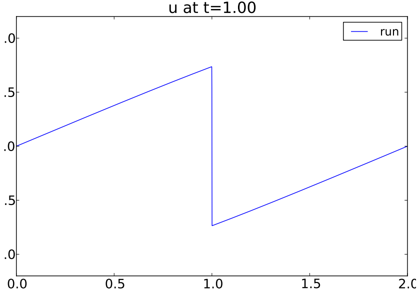
# (Non)linear hyperbolic conservation laws

Conservation of the physical quantities (mass, momentum, energy):

$$\begin{cases} \partial_t \mathbf{U}(\mathbf{x},t) + \operatorname{div} \mathbf{F}(\mathbf{U},\mathbf{x}) = 0, \\ \mathbf{U}(\mathbf{x},0) = \mathbf{U}_0(\mathbf{x}), \end{cases} \qquad \mathbf{x} \in \mathbb{R}^d,\ t > 0.$$

Burgers' equation:

$$\begin{cases} u_t + \left(\dfrac{u^2}{2}\right)_x = 0, \\ u(x,0) = \sin(\pi x). \end{cases}$$

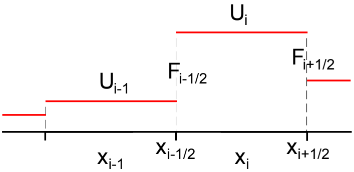



- Hyperbolicity: finite speed of propagation
- Nonlinearity: smooth initial data leads to solutions with shocks
- Weak solutions need to be considered (+ entropy conditions for uniqueness)
- No explicit solutions - numerical schemes (Finite Volume Method)

# Finite Volume Method (FVM)

- **1. Cell averages:**

$$\mathbf{U}_i \approx \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{U}(x,t)dx$$



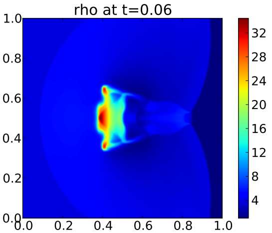

- **2. Semi-discrete formulation (ODE):**

$$\frac{\partial}{\partial t}\mathbf{U}_i + \frac{1}{\Delta x}\left(\mathbf{F}_{i+\frac{1}{2}} - \mathbf{F}_{i-\frac{1}{2}}\right) = 0$$

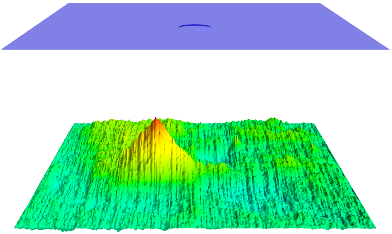
- **3. Approximate Riemann fluxes:** HLL, Godunov (Roe)
  - **High order reconstruction:** TVD (Van Leer), (W)ENO (Harten, Shu, Osher)

- **4. Time stepping:**
  - CFL: $\Delta t < \Delta x / (\text{max wave speed})$
  - Forward Euler (FE) $\mathbf{U}^{n+1} = \mathbf{U}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{F}_{i+\frac{1}{2}} - \mathbf{F}_{i-\frac{1}{2}}\right)$
  - SSP-RK2 (Gottlieb, Shu, Tadmor) $\mathbf{U}_i^{n+1} = \frac{1}{2}(\mathbf{U}_i^n + \mathrm{FE}(\mathrm{FE}(\mathbf{U}_i^n)))$

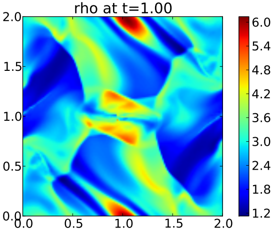
# Examples of (non)linear hyperbolic conservation laws



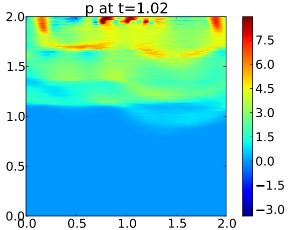

**Euler** cloud-shock interaction



**Shallow water** with varying topography




**MHD** Orszag-Tang vortex



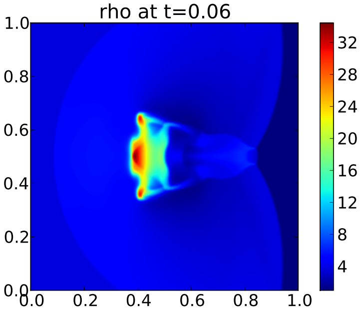

**Wave** propagation in porous medium

# Compressible Euler equations of gas dynamics

Question: What is the time evolution of density/pressure/velocity fields in compressible fluids?

$$\begin{cases} \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0, \\ (\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + p\mathbf{ID}) = 0, \\ E_t + \operatorname{div}((E + p)\mathbf{u}) = 0. \end{cases}$$

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




Density in cloud-shock interaction

- design of aircraft profiles
- gas turbines
- internal combustion engines
- ...

- uncertain cloud geometry/density
- uncertain shock size/location
- uncertain gas constant $\gamma$

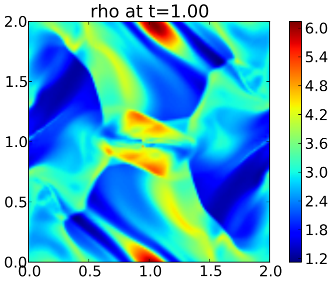
# Magnetohydrodynamics equations for plasma physics

Describes magnetic and density/pressure/velocity fields interaction in electrically conducting fluid.

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

- plasmas (e.g. in the sun)
- liquid metals
- various electrolytes

- HLL 3-wave and 5-wave solvers
  - not strictly hyperbolic
  - non-convex fluxes
  - div constraint
- Godunov-Powell source term
- positivity preserving (W)ENO




Density in Orszag-Tang vortex

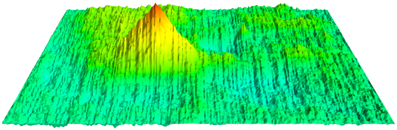
# Shallow water equation with varying bottom topography

Question: what is the time evolution of a tsunami wave caused by an earthquake?

$$\begin{cases} h_t + \mathrm{div}(h\mathbf{u}) = 0 \\ (h\mathbf{u})_t + \mathrm{div}(h\mathbf{u} \otimes \mathbf{u}) = -\nabla(ghb + \frac{1}{2}gh^2) \end{cases}$$

Important for:

- avalanche modeling
- debris slides
- atmospheric flows of weather prediction
- risk assessment of region flooding (due to tsunami or dam break)
- ...



Water level above bottom topography

- uncertain initial perturbation
- uncertain bottom topography
- ...

# Acoustic wave equation in heterogeneous medium

Question: What is the time evolution of the acoustic wave propagating through random medium?

$$p_{tt}(\mathbf{x},t) - \nabla\cdot(c(\mathbf{x})\nabla p(\mathbf{x},t)) = f(\mathbf{x})$$

$$\Downarrow$$

$$\begin{cases} p_t(\mathbf{x},t) - \nabla\cdot(c(\mathbf{x})\mathbf{u}(\mathbf{x},t)) = tf(\mathbf{x}), \\ \mathbf{u}_t(\mathbf{x},t) - \nabla p(\mathbf{x},t) = 0. \end{cases}$$

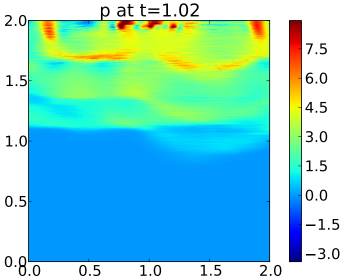
- sound/elastic wave propagation through geological layers
- structural mechanics

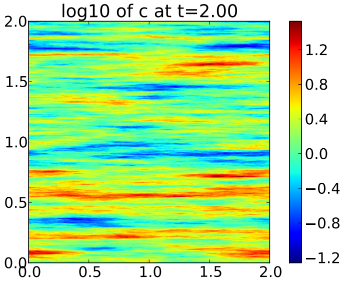
...

- $c(\mathbf{x})$ is often uncertain, e.g. **log-normal** with covariance:

  $$\mathrm{Cov}(\log c(\mathbf{x}), \log c(\mathbf{y})) = \sigma^2 e^{-\|\mathbf{x}-\mathbf{y}\|_\eta}$$

- parallel spectral FFT generator [1]




[1] Ravalec, Noetinger, Hu (Mathematical Geology, 2000)

# Stochastic (non)linear systems of balance laws

$\mathbf{U}(\mathbf{x}, 0)$, $\mathbf{F}(\cdot, \mathbf{x})$ and $\mathbf{S}(\cdot, \mathbf{x})$ are uncertain $\longrightarrow$ solution $\mathbf{U}(\mathbf{x}, t)$ is also uncertain:

$$\begin{cases} \dfrac{\partial}{\partial t}\mathbf{U}(\mathbf{x}, t, \omega) + \operatorname{div}\mathbf{F}(\mathbf{U}, \mathbf{x}, \omega) = \mathbf{S}(\mathbf{U}, \mathbf{x}, \omega), \\ \mathbf{U}(\mathbf{x}, 0, \omega) = \mathbf{U}_0(\mathbf{x}, \omega), \end{cases} \quad \forall \omega \in \Omega, \quad (\Omega, \mathcal{F}, \mathbb{P}). \tag{1.1}$$

## Well-posedness requirement

If uncertain input data (e.g. $\mathbf{U}_0$, $\mathbf{S}$) has finite mean and variance,

$\Downarrow$

**entropy solution** $\mathbf{U}(\mathbf{x}, t, \omega)$ **exists** and has **finite mean and variance**.

## Goals

- Theory for the existence of $\mathbf{U}(\mathbf{x}, t, \omega)$ and its statistical moments
- Numerical methods for the approximate statistical moments of $\mathbf{U}(\mathbf{x}, t, \omega)$

# Theory and numerical results on MLMC-FVM

for hyperbolic conservation laws

| | Scalar stochastic PDE | System of stochastic PDE |
|---|---|---|
| **Linear** | ▶ Linear advection<br>Theory + numerical results [2] | ▶ Acoustic wave<br>▶ Linear elasticity<br>Theory + numerical results [3] |
| **Nonlinear** | ▶ Burgers'<br>▶ Buckley-Leverett<br>Theory + numerical results [2] | ▶ Euler<br>▶ Magneto-hydrodynamics<br>▶ Shallow water [4]<br>Extensive numerical results [5] |

[2] Mishra, Schwab (Math. Comp., 2012)
[3] Šukys, Mishra, Schwab (MCQMC, 2013 (to appear))
[4] Mishra, Schwab, Šukys (SIAM J. Sci. Comput., 2012)
[5] Mishra, Schwab, Šukys (J. Comput. Phys., 2012)

# Short review of MC-FVM and MLMC-FVM

# Monte Carlo FVM algorithm (MC-FVM)

We are interested in $\mathbb{E}[\mathbf{U}(\mathbf{x}, t)]$ and $\mathbb{V}[\mathbf{U}(\mathbf{x}, t)]$ with $(\mathbf{x}, t)$ - fixed.

1. **Draw** $M$ i.i.d. samples of random quantities

$$\{\mathbf{U}_0^i(\cdot), \mathbf{F}^i(\cdot), \mathbf{S}^i(\cdot)\}, \quad i = 1, \dots, M.$$

2. For each draw, **solve** for approximate (FVM with $\Delta x$) entropy solutions

$$\{\mathbf{U}_0^i(\cdot), \mathbf{F}^i(\cdot), \mathbf{S}^i(\cdot)\} \quad \longrightarrow \quad \mathbf{U}^i(\cdot, t^n).$$

3. **Estimate statistics** of $\mathbb{E}[\mathbf{U}(\cdot, t^n)]$ with:

$$\boxed{E_M[\mathbf{U}_{\Delta x}^n(\cdot)] := \frac{1}{M} \sum_{i=1}^{M} \mathbf{U}^i(\cdot, t^n).}$$

# Error vs. Work for Monte Carlo FVM

Theorem [6]

- **scalar** CL with $\mathbf{U}_0 \in L^2(\Omega, \mathbf{V})$ and $\mathbf{F} \in L^\infty(\Omega, C^1(\mathbb{R}))$
- **linear systems** of CLs with $\mathbf{U}_0, \mathbf{S} \in L^2(\Omega, \mathbf{V})$ and $\sqrt{c} \in L^1(\Omega, L^\infty(\mathbf{D}))$

$$\|\mathbb{E}[\mathbf{U}(t^n)] - E_M[\mathbf{U}^n_{\Delta x}]\|_{L^2(\Omega;L^1)} \lesssim M^{-\frac{1}{2}} \|\mathbf{U}_0\|_{L^2(\Omega;L^1)} + t^n \Delta x^s \, \|\mathbf{U}_0\|_{L^\infty(\Omega;TV)}$$

FVM convergence rate is $s$. Constants depend on $\mathbf{U}_0, \mathbf{S}, \mathbf{F}$, **not** on $\Delta x$ or $M$.

Number of samples to equilibrate MC and FVM errors:

$$M = \mathcal{O}((\Delta x)^{-2s})$$

$$\Downarrow$$

$$\text{error} \;\sim (\text{Work})^{-s/(d+1+2s)} \xrightarrow[s \gg d]{} -1/2$$

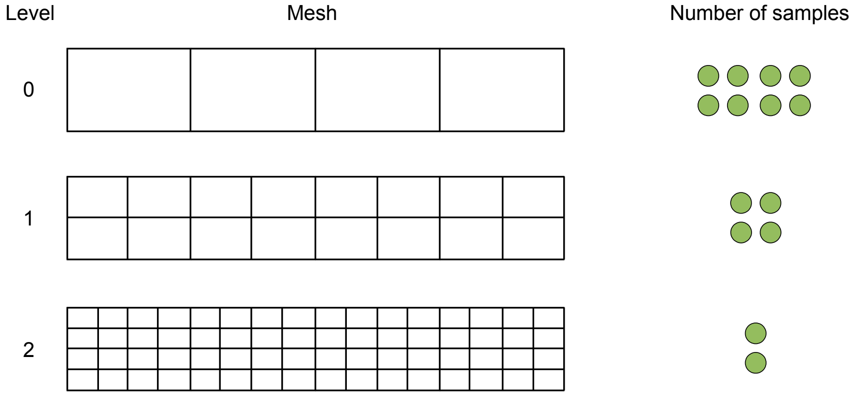
Expensive!

[6]Mishra, Schwab (Math. Comp., 2012); Šukys, Mishra, Schwab (MCQMC, 2012)

# Multi-Level Monte Carlo[7] FVM method (MLMC-FVM)

- **Nested levels** of resolution

$$\Delta x_\ell = \mathcal{O}(2^{-\ell}\Delta x_0), \quad \ell \in \mathbb{N}_0.$$




[7] Introduced by Heinrich (1999); Giles (2008); Barth, Schwab, Zollinger (2011).

# Multi-Level Monte Carlo FVM method (MLMC-FVM)

1. **Draw** $M_\ell$ i.i.d. samples of random quantities for each level $\ell$

$$\{\mathbf{U}^i_{0,\ell}(\cdot), \mathbf{F}^i_\ell(\cdot), \mathbf{S}^i_\ell(\cdot)\}, \qquad i = 1, \dots, M.$$

2. For each draw $i$ and level $\ell$, **solve** (with FVM)

$$\{\mathbf{U}^i_{0,\ell}(\cdot), \mathbf{F}^i_\ell(\cdot), \mathbf{S}^i_\ell(\cdot)\} \quad \longrightarrow \quad \mathbf{U}^i_\ell(\cdot, t^n).$$

3. **Estimate statistics:**

$$\mathbb{E}[\mathbf{U}(\cdot, t^n)] = \mathbb{E}\left[\mathbf{U}_0(\cdot, t^n)\right] + \sum_{\ell=1}^{\infty} \mathbb{E}\left[\mathbf{U}_\ell(\cdot, t^n) - \mathbf{U}_{\ell-1}(\cdot, t^n)\right].$$

Fix $L > 0$ and estimate each term in the telescoping sum using MC-FVM

$$E^L[\mathbf{U}^n_{\Delta x_L}(\cdot)] = E_{M_0}[\mathbf{U}_0(\cdot, t^n)] + \sum_{\ell=1}^{L} E_{M_\ell}[\underbrace{\mathbf{U}_\ell(\cdot, t^n) - \mathbf{U}_{\ell-1}(\cdot, t^n)}_{\text{variance} \to 0 \text{ as } \ell \to \infty}].$$

# Error vs. Work for Multi-Level Monte Carlo FVM

Theorem [8]

- **scalar** CL with $\mathbf{U}_0 \in L^2(\Omega, \mathbf{V})$ and $\mathbf{F} \in L^\infty(\Omega, C^1(\mathbb{R}))$
- **linear systems** of CLs with $\mathbf{U}_0, \mathbf{S} \in L^2(\Omega, \mathbf{V})$ and $\sqrt{c} \in L^1(\Omega, L^\infty(\mathbf{D}))$

$$\left\|\mathbb{E}[\mathbf{U}(t^n)] - E^L[\mathbf{U}^n_{\Delta x_L}]\right\|_{L^2(\Omega;\mathbf{V})} \leq C_1 \Delta x_L^s + C_2 \sum_{\ell=0}^{L} M_\ell^{-\frac{1}{2}} \Delta x_\ell^s + C_{\mathrm{MC}} M_0^{-\frac{1}{2}}.$$

FVM convergence rate is $s$. $C_{1,2,\mathrm{MC}}$ depend on $\mathbf{U}_0, \mathbf{S}, t^n, \mathbf{F}$, **not** on $L, \Delta x_\ell, M_\ell$.

Equilibrate MC and FVM errors:

$$M_\ell = \left(\frac{C_2}{C_1}\right)^2 \times 2^{2(L-\ell)s}$$

Error $\lesssim$ Work$^{-s/(d+1)}$ log(Work)

Optimize[9] MC and FVM errors for $M_\ell$:

$$M_\ell = \left(\frac{C_2}{C_1}\right)^2 \times 2^{\frac{2}{3}(L-\ell)(s+d+1)}$$

Error $\lesssim$ Work$^{-s/(d+1)}$

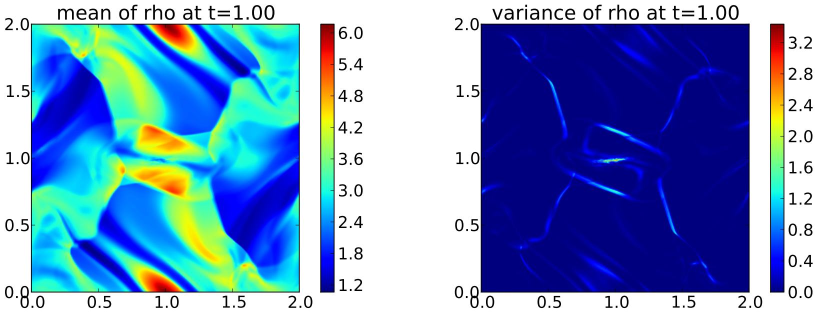
**!** Same complexity as a single FVM solve. Constants differ by $\sqrt{M_L}$.

[8] Mishra, Schwab (Math. Comp., 2012); Šukys, Mishra, Schwab (MCQMC, 2012)
[9] Giles (Oper. Res., 2008)

Numerical experiments
and
error convergence

# MHD: MLMC-FVM for Orszag-Tang vortex

with uncertain initial magnetic field (2 sources of uncertainty)



# MHD: MLMC-FVM for Orszag-Tang vortex

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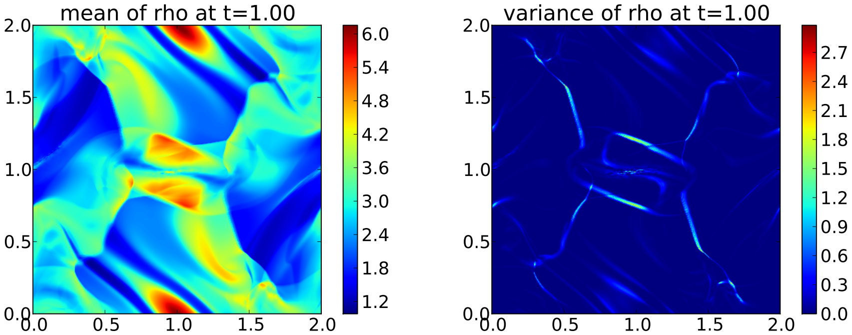
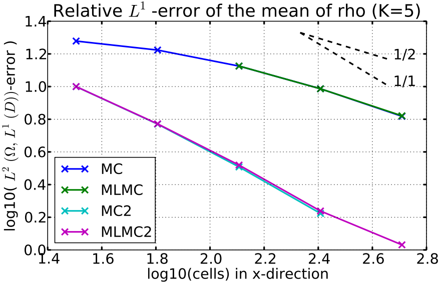
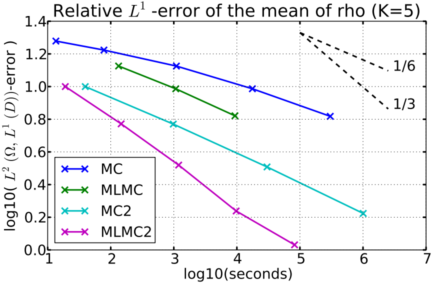



| $L$ | $M_L$ | grid size | CFL | cores | runtime | efficiency |
|---|---|---|---|---|---|---|
| 7 | 4 | 2048x2048 | 0.475 | 128 | 5:02:14 | 98.4% |

# MHD: Orszag-Tang vortex - convergence for mean

with 2 sources of uncertainty

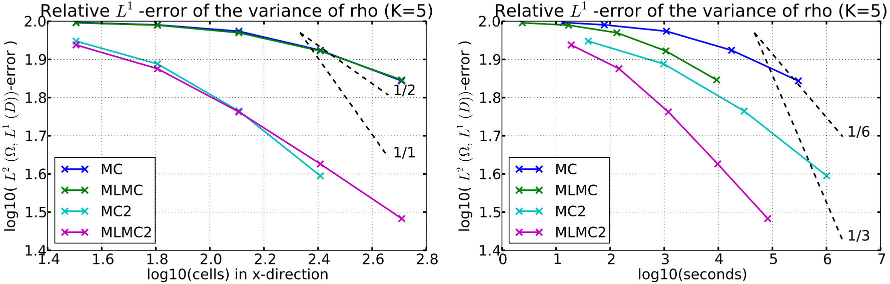



Convergence rates coincide with the rigorous theory for SCL!

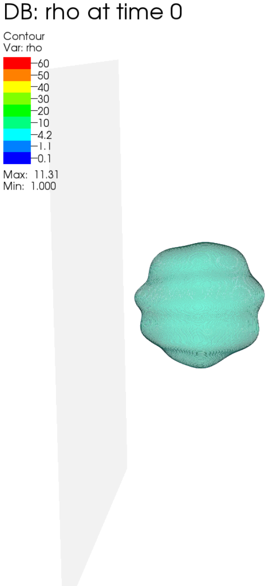
# MHD: Orszag-Tang vortex - convergence for variance

## with 2 sources of uncertainty



# Euler: FVM for cloud shock - one sample

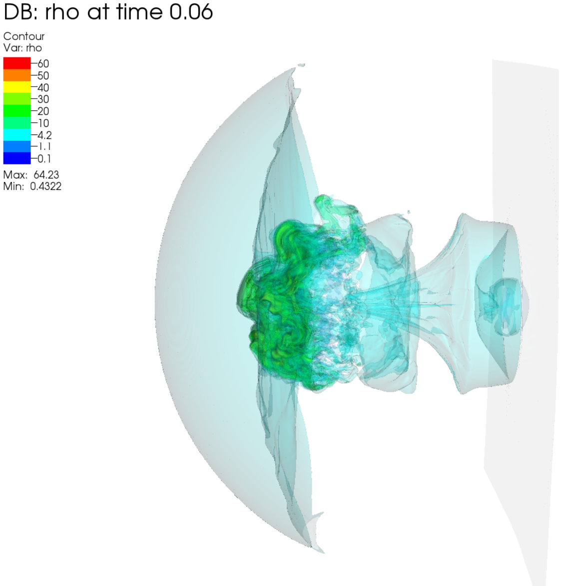
with uncertain shock location/magnitude and geometry of the cloud




| | |
|---|---|
| $L$ | 0 |
| $M_L$ | 1 |
| cells | 1 Billion |
| CFL | 0.475 |
| cores | 4096 |
| runtime | 4:29:44 |
| eff. | 95.7% |

# Euler: FVM for cloud shock - one sample

## with uncertain shock location/magnitude and geometry of the cloud

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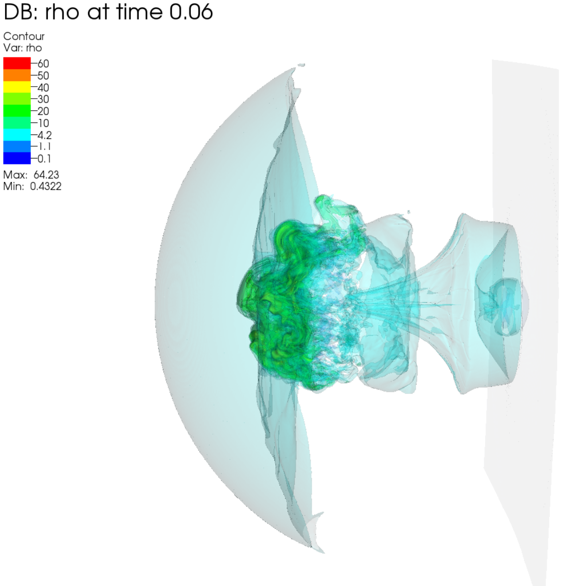
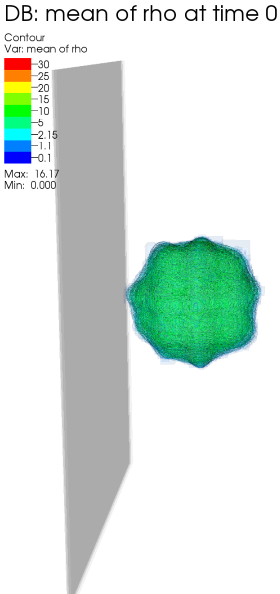
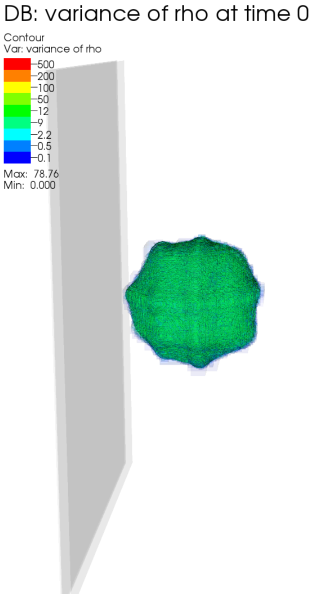



| | |
|---|---|
| $L$ | 0 |
| $M_L$ | 1 |
| cells | 1 Billion |
| CFL | 0.475 |
| cores | 4096 |
| runtime | 4:29:44 |
| eff. | 95.7% |

# Euler: MLMC-FVM for cloud shock - mean and variance

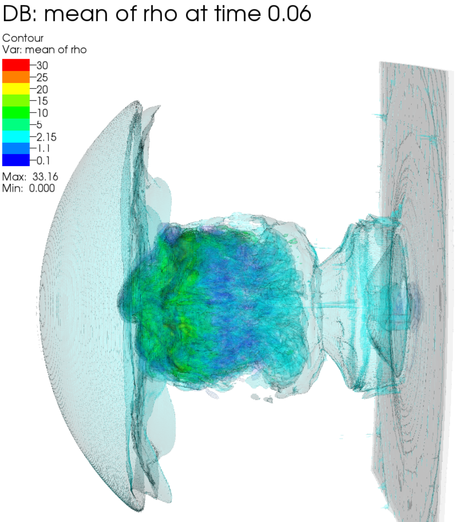
with uncertain shock location/magnitude and geometry of the cloud

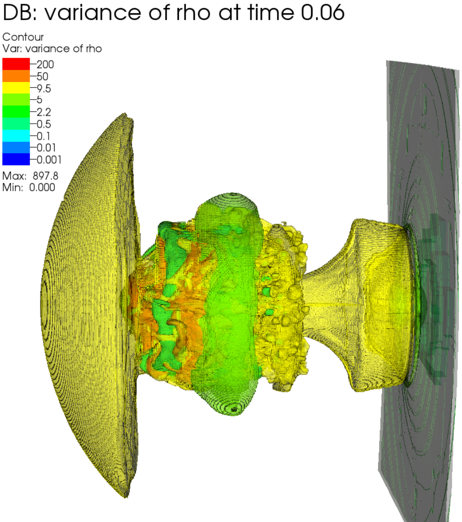


# Euler: MLMC-FVM for cloud shock - mean and variance

## with uncertain shock location/magnitude and geometry of the cloud



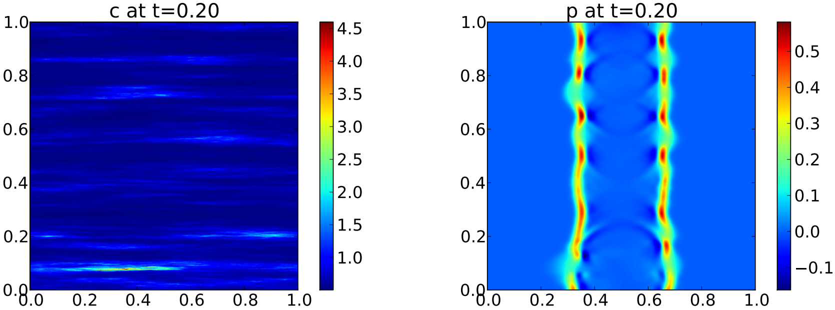




| $L$ | $M_L$ | grid size | CFL | cores | runtime | efficiency |
|---|---|---|---|---|---|---|
| 6 | 4 | 1024x1024x1024 | 0.475 | 21844 | 4:49:42 | 93.9% |

A numerical experiment
with stochastic flux

# Wave equation: log-normal material coefficient

$$p_{tt}(\mathbf{x},t,\omega) - \nabla\cdot\left(c(\mathbf{x},\omega)\nabla p(\mathbf{x},t,\omega)\right) = 0$$




Coefficient $c(\mathbf{x},\omega)$ is assumed to be **log-normal**, determined by its covariance

$$\mathrm{Cov}(\log c(\mathbf{x},\cdot), \log c(\mathbf{y},\cdot)) = k(\|\mathbf{x}-\mathbf{y}\|_\eta) = \sigma^2 \exp\left(-\sqrt{\sum_{r=1}^{d}\frac{|\mathbf{x}_r-\mathbf{y}_r|^2}{\eta_r^2}}\right)$$

where

- covariance kernel $k : \mathbb{R} \to \mathbb{R}_+$
- correlation lengths in each direction $\eta = \{\eta_1, \ldots, \eta_d\} \in \mathbb{R}_+^d$ (anisotropy)

# Naive generation of log-normal coefficient in 1d

Given: kernel $k$ with the specified variance $\sigma^2$, correlation lengths $\eta = \{\eta_1, \dots, \eta_d\}$.

Goal: generate random coefficients $\mathbf{c}_i = c(\mathbf{x}^i, \omega)$ at cell mid-points $\{\mathbf{x}^i\} \in \mathbb{R}^N$ with

$$\mathrm{Cov}(\mathbf{c}_i, \mathbf{c}_j) := k(\|\mathbf{x}^i - \mathbf{x}^j\|_\eta), \quad i, j \in \{1, \dots, N\}.$$

Naive generation:

1. Find a factorization $\mathbf{C} = \mathbf{L}\mathbf{L}^\top$ of the s.p.d. covariance matrix $\mathbf{C} \in \mathbb{R}^{N \times N}$

$$\mathbf{C}_{ij} = \mathrm{Cov}(\mathbf{c}_i, \mathbf{c}_j).$$

2. Draw a Gaussian i.i.d. vector

$$\mathbf{g} \in \mathbb{R}^N, \quad \mathbf{g}_i \sim \mathcal{N}(0, 1).$$

3. Compute the values of $\mathbf{c}_i$ by

$$\mathbf{c} = \mathbf{L}\mathbf{g}.$$

Drawback: $\mathbf{C} = \mathbf{L}\mathbf{L}^\top$ is very expensive, only storage is $\mathcal{O}(N^2) \gg \mathcal{O}(N)$.

# Spectral generation of log-normal coefficient in 1d [10]

Stationary kernel $\Longrightarrow$ circulant covariance matrix $\mathbf{C}$.

Spectral generation: $\mathcal{O}(N\log(N))$

1. FFT transforms of kernel $\mathbf{k} = k(\|\mathbf{x}^1 - \mathbf{x}^i\|_\eta)$ and Gaussian vector $\mathbf{g}$

$$\hat{\mathbf{k}} = \mathsf{FFT}(\mathbf{k}) \in \mathbb{R}^N_+, \qquad \hat{\mathbf{g}} = \mathsf{FFT}(\mathbf{g}) \in \mathbb{C}^N.$$

   $\mathbf{k}$ is even $\Longrightarrow$ $\hat{\mathbf{k}}$ is real. $\hat{\mathbf{k}}$ are eigenvalues of s.p.d. $\mathbf{C}$ $\Longrightarrow$ $\hat{\mathbf{k}}$ are positive.

2. Decomposition $\mathbf{C} = \mathbf{L}\mathbf{L}^\top = \mathbf{L}\mathbf{L}$: take the square root of $\hat{\mathbf{k}}$:

$$\hat{\mathbf{l}} \in \mathbb{R}^N_+, \quad \hat{\mathbf{l}}_i = \sqrt{\hat{\mathbf{k}}_i}.$$

3. "Matrix-vector" multiplication $\mathbf{c} = \mathbf{L}\mathbf{g} = \mathbf{k} * \mathbf{g}$ corresponds to

$$\mathbf{c} = \mathsf{IFFT}(\hat{\mathbf{l}} \cdot \hat{\mathbf{g}}).$$

4. Steps 1 - 3 are parallelized using `FFTW` library.

[10] Ravalec, Noetinger, Hu (Mathematical Geology, 2000)

# Coupling generated samples on two mesh levels

The MLMC-FVM requires MC estimates of the coupled differences

$$E_{M_\ell}[\mathbf{U}_\ell - \mathbf{U}_{\ell-1}] = \sum_{i=m}^{M_\ell}[\mathbf{U}_\ell(\omega_m) - \mathbf{U}_{\ell-1}(\omega_m)].$$

Requirements for coupling $\mathbf{c}^{\ell-1} \in \mathbb{R}^{N/2}$ to $\mathbf{c}^{\ell} \in \mathbb{R}^{N}$:

- the same realization of $\mathbf{c}(\omega_m)$,
- diffferent mesh resolutions, $\ell$ and $\ell - 1$, i.e. $\mathbf{c}^{\ell}(\omega_m)$ and $\mathbf{c}^{\ell-1}(\omega_m)$.

**Naive method:** average the coefficient $\mathbf{c}_i^{\ell-1} = \frac{1}{2}\left(\mathbf{c}_{2i}^{\ell} + \mathbf{c}_{2i+1}^{\ell}\right)$.

- separable kernel $k(\cdot)$: method is appropriate
- non-separable $k(\cdot)$: $\mathbf{k}^{\ell}$ needs to be computed from $\mathbf{k}^{L}$, for all $0 \leq \ell < L$.

**Better method:** filter the Gaussian vector $\mathbf{g}^{\ell}$ from level $\ell$ to $\ell - 1$ by averaging,

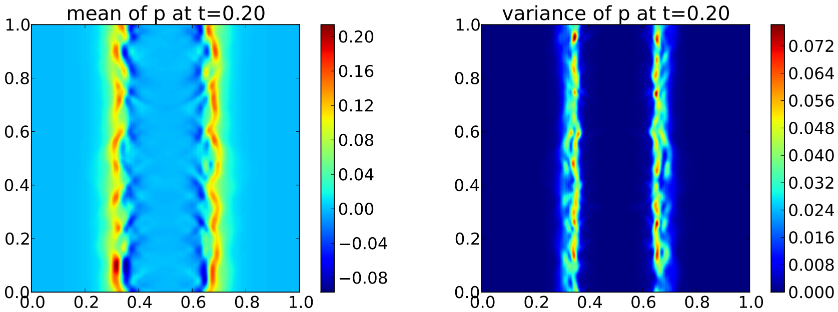
$$\mathbf{g}_i^{\ell-1} = \frac{\mathbf{g}_{2i}^{\ell} + \mathbf{g}_{2i+1}^{\ell}}{2} \sim \mathcal{N}(0,1), \quad i = 1, \ldots, N/2.$$

Afterwards, proceed as before,

$$\hat{\mathbf{k}}^{\ell-1} = \mathrm{FFT}(\mathbf{k}^{\ell-1}) \in \mathbb{R}_+^{N/2}, \qquad \hat{\mathbf{g}}^{\ell-1} = \mathrm{FFT}(\mathbf{g}^{\ell-1}) \in \mathbb{C}^{N/2}, \qquad \ldots$$

# Wave equation: mean and variance of acoustic pressure

For random log-normally distributed material coefficient




| $L$ | $M_L$ | grid size | CFL | cores | runtime | efficiency |
|---|---|---|---|---|---|---|
| 8 | 4 | 2048x2048 | 0.9 | 86 | 0:06:45 | 82.1% |

Notice the low efficiency due to very heterogeneous samples.

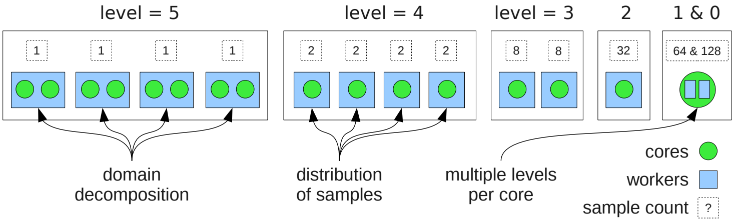
MLMC algorithm is non-intrusive

$\downarrow$

Parallelization

# Static and adaptive load balancing for parallel MLMC-FVM

## Parallelization over levels, samples and subdomains




- computational work at level $\ell$: $M_\ell$ samples at resolution $\Delta x_\ell$:

$$\mathrm{Work}_{M_\ell}(\Delta x_\ell) = M_\ell \cdot \mathrm{Work}^{\mathrm{sample}}(\Delta x_\ell) = M_\ell \cdot \mathcal{O}(N_{\mathrm{cells}} N_t) \approx M_\ell \cdot K \Delta x^{-(d+1)}.$$

Deterministic flux,
small variance in input data

⇓

Static (compile-time) balancing

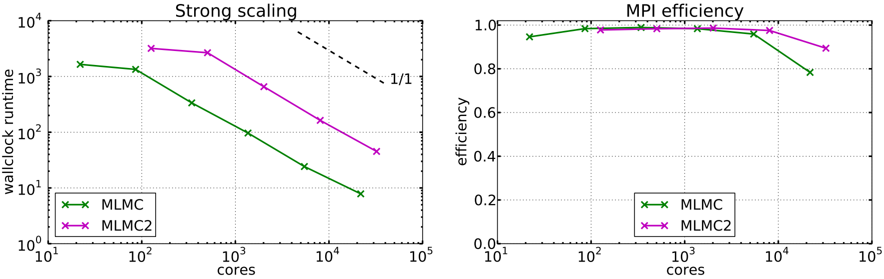
Stochastic flux,
large variance in input data

⇓

Adaptive (run-time) balancing

# Linear (strong) scaling of static load balancing

(with domain decomposition)




**Strong and weak scaling** up to 40 000 cores with high efficiency.
(Cray XE6, CSCS)

# Adaptive load balancing algorithm

Generalization of "greedy" algorithm for "workers" with non-uniform speed of execution

**Setup:** "Workers" $\mathcal{G}_j$ with "computing capacities" $C_j$.
**Loads:** (computed in parallel)

$$\text{Load}_\ell^i = \lambda_\ell^i \Delta x^{-(d+1)}, \qquad \ell = 0, \dots, L, \quad i = 1, \dots, M_\ell.$$

**Recursive rule: (2-approximation of optimal balancing)**[11]
Assign the **largest** $\text{Load}_\ell^i$ to the worker $\mathcal{G}_j$ for which the total load is **minimized**.

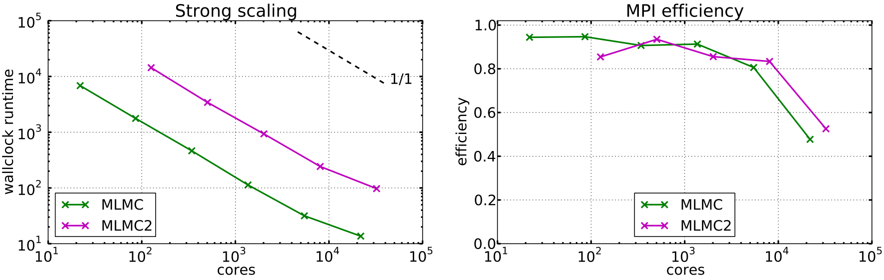
## Pseudocode

$\mathcal{L} = \{\text{Load}_\ell^i : \ell = 0, \dots, L, i = 1, \dots, M_\ell\}$
**while** $\mathcal{L} \neq \emptyset$ **do**
  $\text{Load}_\ell^i = \max \mathcal{L}$
  $\mathcal{G}_j = \arg\min_{\mathcal{G}_j} \sum \left\{ \text{Load}/C_j : \text{Load} \in \mathcal{G}_j \cup \text{Load}_\ell^i \right\}$
  $\mathcal{G}_j = \mathcal{G}_j \cup \text{Load}_\ell^i$
  $\mathcal{L} = \mathcal{L} \backslash \text{Load}_\ell^i$
**end while**

[11] Šukys (PPAM 2013)

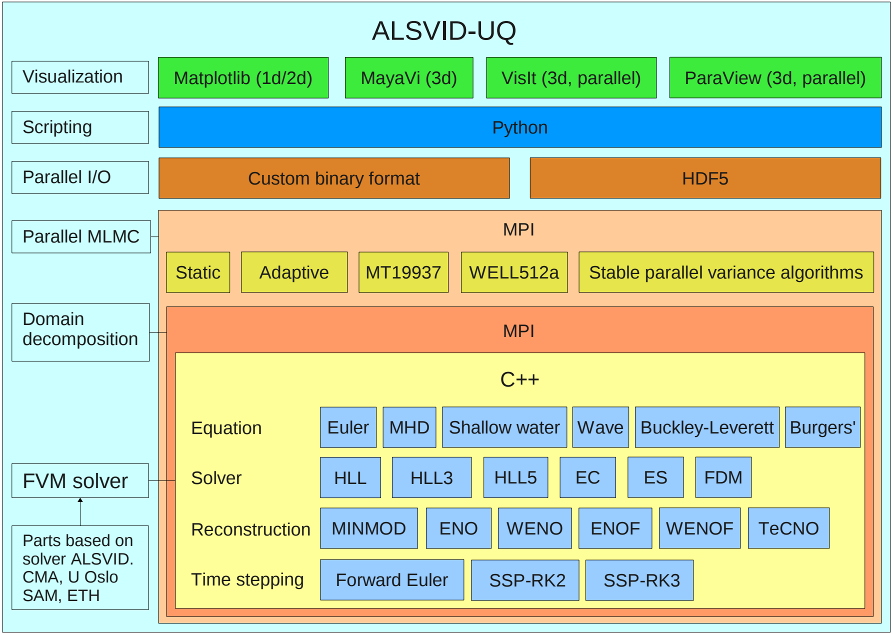
# Linear (strong) scaling of adaptive load balancing

(with domain decomposition)



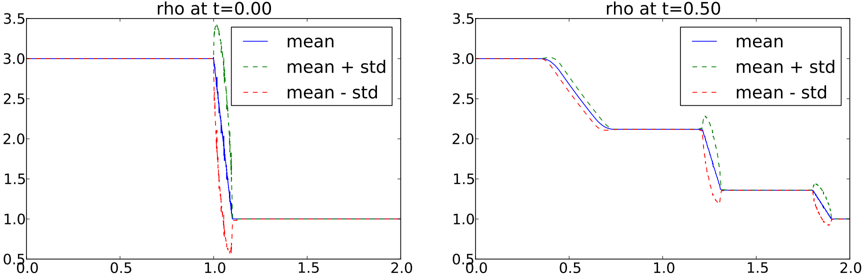

**Strong and weak scaling** up to 10 000 cores with high efficiency.
(Cray XE6, CSCS)

# Parallel MLMC-FVM implementation: ALSVID-UQ



# MLMC-FVM solution of the Sod shock tube

## with uncertain initial shock location




| $L$ | $M_L$ | grid size | CFL | cores | runtime | efficiency |
|---|---|---|---|---|---|---|
| 12 | 16 | 32768 | 0.475 | 104 | 1:49:49 | 99.1% |

Here, only mean and variance are provided.
How about a complete empirical probability density function?

# Empirical probability density

## Random initial data for Sod shock tube

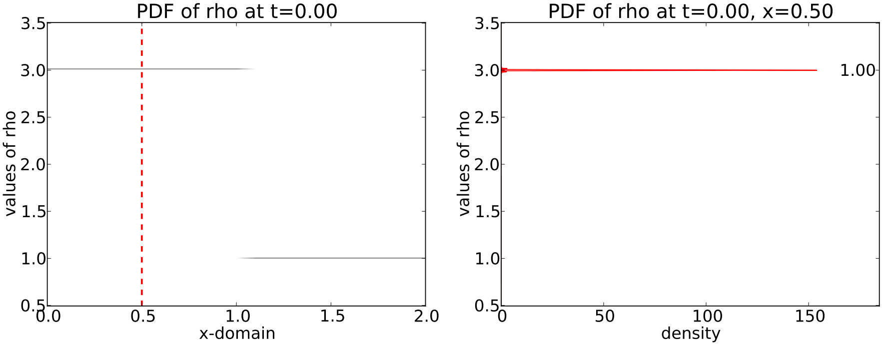



Figure: Initial empirical probability density of $\rho$ at $T = 0$.

# Empirical probability density at a rarefaction

## Sod shock tube, MLMC-FVM approximation

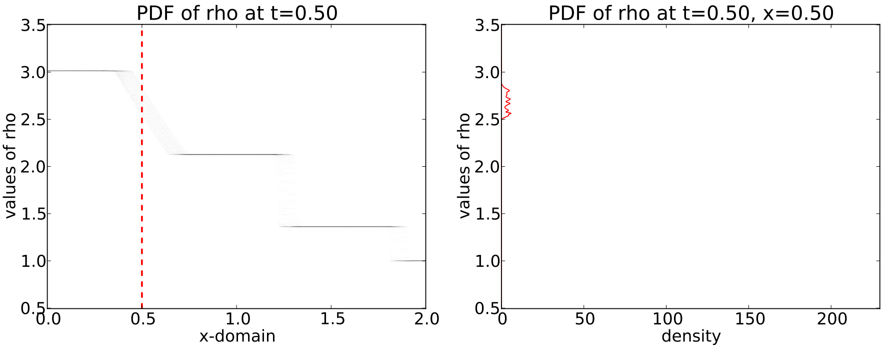



Figure: Empirical probability density of $\rho$ at $T = 0.5$.

| $L$ | $M_L$ | grid size | CFL | cores | runtime |
|---|---|---|---|---|---|
| 8 | 8 | 4096 | 0.475 | 1 | 0:44:53 |

# Empirical probability density at a contact discontinuity

## Sod shock tube, MLMC-FVM approximation

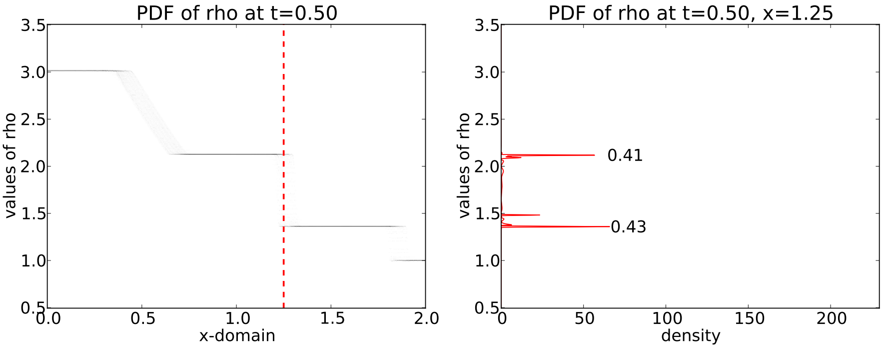



Figure: Empirical probability density of $\rho$ at $T = 0.5$.

| $L$ | $M_L$ | grid size | CFL | cores | runtime |
|---|---|---|---|---|---|
| 8 | 8 | 4096 | 0.475 | 1 | 0:44:53 |

# Empirical probability density at a shock

## Sod shock tube, MLMC-FVM approximation

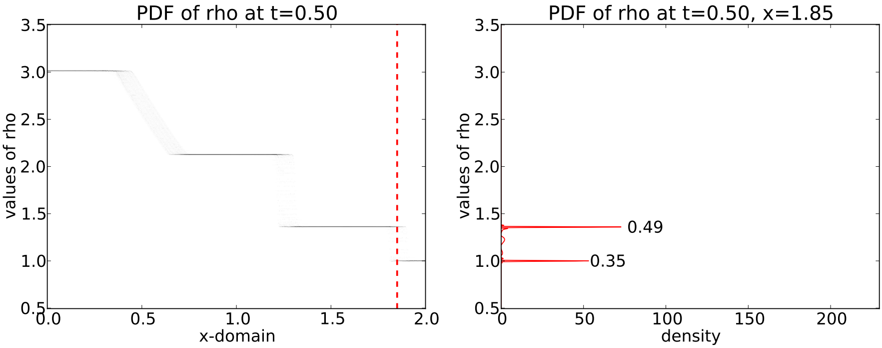



Figure: Empirical probability density of $\rho$ at $T = 0.5$.

| $L$ | $M_L$ | grid size | CFL | cores | runtime |
|---|---|---|---|---|---|
| 8 | 8 | 4096 | 0.475 | 1 | 0:44:53 |

# Summary for MLMC-FVM method

- applications: **Euler**, **MHD**, **shallow water**, **Buckley-Leverett**, **wave, etc.**
- flexible w.r.t. the origin of the uncertainty: $\mathbf{U}_0, \mathbf{S}, c, \mathbf{F}$

- optimal computational complexity (same as for deterministic systems)
- 2-3 orders of magnitude speed-up of MLMC-FVM vs. MC-FVM
- linear complexity w.r.t. stochastic dimension (unlike in gPC)

- low regularity requirements
- non-intrusive - deterministic FVM solvers can be reused
- easily parallelizable and scalable (tested up to 40 000 cores)

- algorithmic fault tolerant parallelization:
  - lost samples (due to node failures) are dropped
  - MLMC-FVM error bound is still valid, in the sense of expected accuracy
  - NO checkpoint/restore needed from the system
  - the algorithm is guaranteed to finish during a given time span
  - collaboration with S. Pauli and P. Arbenz [12]

[12] Pauli, Arbenz and Schwab (SAM Report No. 2012-24, PARCO 2013)

# Joint work in progress with

- Siddhartha Mishra
  - SAM, ETH Zürich, Switzerland
- Christoph Schwab
  - SAM, ETH Zürich, Switzerland

- Other collaborators:
  - Stefan Pauli
  - Florian Müller
  - Svetlana Tokareva
  - Franziska Weber
  - Luc Grosheintz
  - Manuel Kohler


- Part of ETH interdisciplinary research grant
  - CH1-03 10-1

- Grant from the Swiss National Supercomputing Centre (CSCS)
  - Project ID S366

# Publications (JŠ, S. Mishra, Ch. Schwab)

List available at: http://www.sam.math.ethz.ch/~sukysj

- *MLMC-FVM: uncertainty quantification in nonlinear systems of balance laws.* **UQLNCSE**, 2013 (to appear).
- *MLMC-FVM for stochastic linear hyperbolic systems.* **MCQMC 2012** (to appear).
- *Adaptive load balancing for massively parallel multi-level Monte Carlo solvers.* **PPAM 2013** (to appear).
- *MLMC-FVM for shallow water equations with uncertain topography.* **SIAM J. Sci. Comput., 34(6)**, B761–B784, 2012.
- *MLMC-FVM for nonlinear systems of conservation laws in multi-dimensions.* **J. Comp. Phys., 231(8)**, 3365–3388, 2012.
- *Sparse tensor MLMC-FVM for conservation laws with random initial data.* **Math. Comp., 280**, 1979–2018, 2012.
- *Static load balancing for multi-level Monte Carlo finite volume solvers.* **PPAM 2011, Part I, LNCS 7203**, 245–254. Springer, Heidelberg 2012.
- **ALSVID-UQ:** http://www.sam.math.ethz.ch/alsvid-uq.