A kinetic approach to statistical inference for nonlinear waves

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based on joint work with

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Sensitivity of schemes I: Shocks and interfaces are related to *Nonlinear problems with non unique weak solutions*

Typical models include nonlinear evolution PDEs

$$u_t(t) + A(u(t)) = 0$$

Due to the singular structure of the solutions existence and uniqueness of (weak) solutions is very subtle

- (1) non-uniqueness of weak solutions - Conservation Laws, Hamilton Jacobi, Equations describing phase separation, ...
- (2) selection criteria for the physical relevant solution - CL: entropy solution, HJ: viscosity solution, geometric laws for propagating interfaces

A typical example: Scalar Conservation Laws

$$u_t(x,t) + \text{div} F(u(x,t)) = 0, \quad x \in R^d, t > 0.$$

Unique entropy solution:

$$\eta(u)_t + \text{div} S(u) \leq 0, \quad \text{in } \mathcal{D}'.$$

The entropy solution is characterized as the limit of viscosity approximations ("Viscosity solution") :

$$u^\epsilon \to u.$$

$$u^\epsilon_t(x,t) + \text{div} F(u^\epsilon(x,t)) = \epsilon \Delta u^\epsilon(x,t), \quad x \in R^d, t > 0.$$

- Relation to the design of schemes: artificial diffusion

Numerical schemes

"Reasonable" schemes do not perform always as we expect.

- oscillations (Ex. 1)
- convergence to the "wrong" solution (Ex. 2)

WHY?

Numerical schemes induce their own physics...

“Reasonable” schemes do not perform always as we expect.

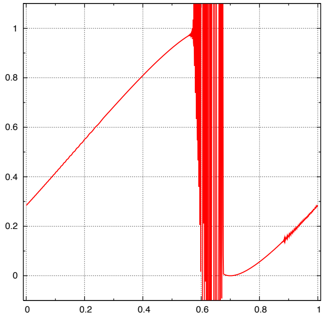
- each scheme corresponds to an approximation of the PDE

$$v_t^h(t) + A(v^h(t)) = B_h(h, v^h(t)),$$

  where $B_h(h, v^h(t))$ is a differential operator acting on v^h not always clear.

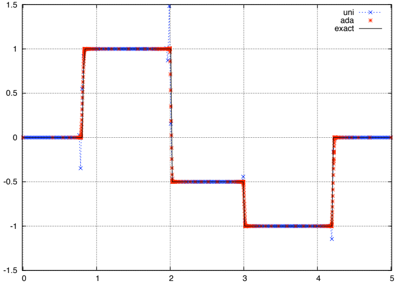
- this is a PDE that models the numerical scheme

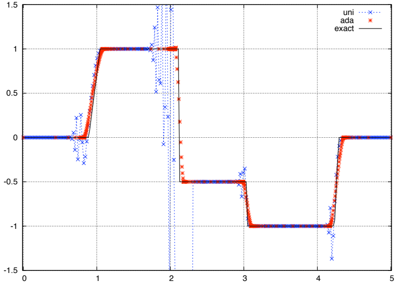
Oscillatory schemes



- Limit dynamics of such schemes refs: von Neumann 1943-44, Goodman and Lax 1988, Hou and Lax 1991, Brenier and Levy 2000 computational studies.
- PDEs: development of the theory of small dispersion limits (Lax, Levermore, Venakides,...)

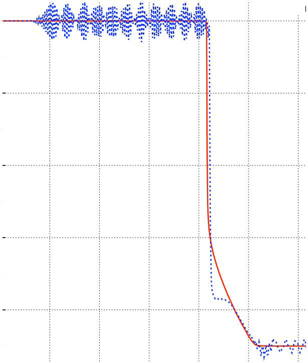
Introducing artificial diffusion in the scheme





Ex. 2: But still computations can be subtle...

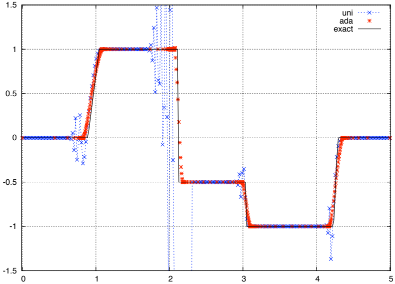
- $u_t + f(u)_x = au_{xx} + bu_{xxx}$,
- Transport, diffusion and dispersion



[LeFloch, Rohde 2000]

Part II : Statistics : Measure Valued Solutions

Why we would like to compute/study such solutions?



- The behaviour of approximations (and in some important cases of the “solution”) is not certain...
- The data might contain uncertainties : statistics for the corresponding solutions
- Uncertainty Quantifiaction

Statistics for an assembly of initial data

Consider the nonlinear conservation law:

$$u_t(x,t) + \mathrm{div} F(u(x,t)) = 0, \quad x \in R^d, t > 0.$$

To fix ideas, consider different solutions u_j, $j = 1, \ldots, J$, which correspond to different initial data u_j^0, $j = 1, \ldots, J$. Assume that all u_j satisfy the above PDE.

Is it possible to derive some kind of statistical inference without solving the PDE with all the different data (solving the PDE J times)?

It is natural to consider measures of the form

$$\frac{1}{J} \sum_{j=1}^{J} \delta_{u_j(x,t)} \,.$$

- Can we consider solutions of the PDE which are measure valued?
- What type of measures should we consider?
- Is it possible to have a theoretical framework which will support our computational approach?

Young measures

Let $\mathbf{M}(\mathbb{R}^m)$ be the set of all signed Radon measures on $\mathbb{R}^m$. We denote by $\mathbf{M}^+(\mathbb{R}^m)$ the set of all positive Radon measures and by $\mathbf{M}^{\mathbb{P}}(\mathbb{R}^m)$ the set of all probability measures over $\mathcal{B}(\mathbb{R}^m)$ that is,

$$\mathbf{M}^{\mathbb{P}}(\mathbb{R}^m) = \{\mu \in \mathbf{M}^+(\mathbb{R}^m), \mu(\mathbb{R}^m) = 1\}.$$

We call *young measure* a weakly* measurable mapping from Ω into $\mathbf{M}^{\mathbb{P}}(\mathbb{R}^m)$.The set of all young measures is denoted by $\mathbf{Y}(\Omega, \mathbb{R}^m)$.

Young Measures II

Let u_j a bounded sequence of approximations in $L^\infty(\Omega, \mathbb{R}^m)$. Then there exists a subsequence and a measure $\mu \in \mathbf{Y}(\Omega, \mathbb{R}^m)$, $\mu = \mu_{x,t}$, $(x,t) \in \Omega$, such that for $G \in C(\mathbb{R}^m)$,

$$G(u_j) \rightharpoonup \overline{G}, \quad \text{where} \quad \overline{G}(x,t) = \langle G, \mu_{x,t} \rangle = \int_{\mathbb{R}^m} G(\lambda) d\mu_{x,t}(\lambda).$$

- $$\langle G, \delta_{u(x,t)} \rangle = \int_{\mathbb{R}^m} G(\lambda) d\delta_{u(x,t)}(\lambda) = G(\, u(x,t))$$
- $$\langle id, \delta_{u(x,t)} \rangle = \int_{\mathbb{R}^m} \lambda \, d\delta_{u(x,t)}(\lambda) = u(x,t)$$

Measure-valued solutions (Di Perna)

A measure $\mu \in \mathbf{Y}(\Omega, \mathbb{R}^m)$ is said to be a measure-valued solution of the conservation law if it satisfies the expression

$$\int_{\Omega} \big(\langle id, \mu_{x,t}\rangle \cdot \phi_t + \langle f, \mu_{x,t}\rangle \cdot \phi_x\big) dxdt + \int_{\mathbb{R}} u_0 \cdot \phi(0,x) dx = 0, \quad (0.1)$$

for all $\phi \in C_0^\infty(\overline{\Omega})$.
This definition is an extension of weak solutions to allow measure valued solutions.

Similarly, a young measure $\mu \in \mathbf{Y}(\Omega, \mathbb{R}^m)$ which fulfils the additional relation

$$\int_{\Omega} \big(\langle \eta, \mu_{x,t}\rangle \cdot \phi_t + \langle Q, \mu_{x,t}\rangle \cdot \phi_x\big) dxdt + \int_{\mathbb{R}} u_0 \cdot \phi(0,x) dx \geq 0, \quad (0.2)$$

for all $\phi \in C_0^\infty(\Omega)$ with $\phi \geq 0$ is called an *entropy measure-valued solution* of the conservation law.

Questions / Problems

- Measure valued solutions allow for a statistical analysis of the problem
- Computational methods tailor made for computing measure valued solutions...
- What do we compute?? We need a solid stability framework to justify the computations.
- Available results concentrated to initial data of the form

  $$\delta_{u^0(x)}.$$

  Uniqueness is lost for general measure valued initial data
- The definition of Entropy Measure Valued solutions has to be enhanced in order to allow a more consistent theory with non-atomic initial value, see, e.g., the recent results of Fjordholm, Mishra on corrolation measures

Relationship with kinetic models : Computational methods

Approximation theory of Young measures

(Roubicek // Pedregal 1996-7)
Suppose that for every $h > 0$ there exist a continuous linear projector $P_h : L^1(\Omega; C_0(S)) \to L^1(\Omega; S_h) = P_h(L^1(\Omega; C(S)))$ where S_h is a finite subspace of $C(S)$ and $S \subset \mathbb{R}^d$. Let further $\mathbf{Y}_h(\Omega, S)$ be the set of all Young measures which map Ω into $(S_h)^*$.

Lemma

The spaces $P_h^*(L_w^\infty(\Omega; \mathbf{M}^{\mathbb{P}}(S))$ and $L_w^\infty(\Omega; (S_h)^*)$ are isomorphic. In particular if

$$P_h^*(\mathbf{Y}(\Omega, S)) \subset \mathbf{Y}(\Omega, S)$$

then

$$P_h^*(\mathbf{Y}(\Omega, S)) \cong \mathbf{Y}_h(\Omega, S).$$

If $\mathbf{Y}_h(\Omega, S)$ is a space of approximate Young measures, then given an $\mu \in \mathbf{Y}(\Omega, S)$ there exist only one $\bar{\mu} \in \mathbf{Y}_h(\Omega, S)$ such that

$$\int_\Omega \langle \phi, \bar{\mu}_{x,t} \rangle dxdt = \int_\Omega \langle P_h \phi, \mu_{x,t} \rangle dxdt \qquad (0.3)$$

for all $\phi \in L^1(\Omega; C(S))$.

A specific choice

Let S_h be a finite element subspace of $C(S)$, then the interpolation operator of the form

$$P_h(\phi(x,t,\xi)) = \sum_{i=1}^{n} \phi(x,t,\xi_i)\upsilon_i(\xi) \qquad (0.4)$$

can be used.

Here $\{\upsilon_i\}_{i=1}^n$ is a standard nodal basis of S_h and $\{\xi_i \in S\}_{i=1}^n$ are the mesh points.

Explicit representation of the approximate Young measure

It is essential now to see the form of the approximate measure:

$$\int_\Omega \langle \phi, \bar{\mu}_{x,t} \rangle dxdt = \int_\Omega \langle \sum_{i=1}^{n} \phi(x,t,\xi_i) v_i(\xi), \mu_{x,t} \rangle dxdt$$

$$= \sum_{i=1}^{n} \int_\Omega \phi(x,t,\xi_i) \langle v_i(\xi), \mu_{x,t} \rangle dxdt = \sum_{i=1}^{n} \int_\Omega \alpha_i(x,t) \int_S \phi(x,t,\lambda) d\delta_{\xi_i}(\lambda) dxdt$$

$$= \int_\Omega \int_S \phi(x,t,\lambda) d[\sum_{i=1}^{n} \alpha_i(x,t) \delta_{\xi_i}(\lambda)] dxdt = \int_\Omega \langle \phi, \sum_{i=1}^{n} \alpha_i(x,t) \delta_{\xi_i} \rangle dxdt$$

for all $\phi \in L^1(\Omega; C(S))$ where $\alpha_i(x,t) = \langle v_i, \mu_{x,t} \rangle$ and δ is the Dirac measure. Therefore,

$$\bar{\mu}_{x,t} = \sum_{i=1}^{n} \alpha_i(x,t) \delta_{\xi_i}. \tag{0.5}$$

- The functions α_i here are unknowns and need to be determined in order to compute the measure $\bar{\mu}$
- The approximation of a young measure μ is equivalent to the determination of the action of μ on every basis function v_i of the space S_h.

Approximation of Measure-valued solutions of conservation laws

Substituting μ with $\bar{\mu}$ in the definition of measure valued solutions of the CL ($u_0 = 0$)

$$\int_{\Omega} \big(\langle id, \bar{\mu}_{x,t}\rangle \cdot \phi_t + \langle A, \bar{\mu}_{x,t}\rangle \cdot \phi_x\big) dxdt \approxeq 0.$$

Hence,

$$\int_{\Omega} \big(\langle id, \sum_{i=1}^{n} \alpha_i(x,t)\delta_{\xi_i}\rangle \cdot \phi_t + \langle A, \sum_{i=1}^{n} \alpha_i(x,t)\delta_{\xi_i}\rangle \cdot \phi_x\big) dxdt \approxeq 0 \Rightarrow$$

$$\int_{\Omega} \big(\sum_{i=1}^{n} \xi_i \alpha_i(x,t) \cdot \phi_t + \sum_{i=1}^{n} A(\xi_i)\alpha_i(x,t) \cdot \phi_x\big) dxdt \approxeq 0.$$

Thus, one may conclude

$$\sum_{i=1}^{n} \xi_i \alpha_i(x,t)_t + \sum_{i=1}^{n} A(\xi_i)\alpha_i(x,t)_x \approxeq 0. \tag{0.6}$$

A family of approximate models

Considering the system

$$\xi_i \alpha_i(x,t)_t + A(\xi_i)\alpha_i(x,t)_x = M_i(x,t), \qquad \text{for } i = 1, \dots, n \tag{0.7}$$

- n equations with n unknowns α_i
- we need $\sum_{i=1}^{n} M_i(x,t) = 0$
- conditions on M_i which will lead to approximations of the entropy measure valued solution
- are these systems meaningful ?
- discrete kinetic model
- uniqueness within a class (??)

Relationship with kinetic models : Stability / Uniqueness

Motivation on the choice of M_i

To answer the above questions we need to go back to the kinetic formulation of the CL.
A function $f(x,t,\xi) \in L^\infty(0,+\infty; L^1(\mathbb{R}^2))$ is called a kinetic solution of the scalar conservation law if

$$\frac{\partial f(x,t,\xi)}{\partial t} + A'(\xi)\frac{\partial f(x,t,\xi)}{\partial x} = \frac{\partial m(t,x,\xi)}{\partial \xi} \qquad \text{in } \mathcal{D}' \tag{0.8}$$

where m is a bounded nonnegative measure on $(\mathbb{R} \times \mathbb{R} \times (0,+\infty))$ and

$$f = \chi_{u(x,t)}. \tag{0.9}$$

Here, $u(x,t)$ is the entropy solution of the CL and χ_λ is given by

$$\chi_\lambda(\xi) = \begin{cases} 1 \text{ if } 0 < \xi \le \lambda \\ -1 \text{ if } \lambda \le \xi < 0 \\ 0 \text{ otherwise} \end{cases}$$

- Lions, Perthame, Tadmor 95
- equivalence to the entropy formulation of the CL

Kinetic formulation and Young measures

A function $f(x,t,\xi) \in L^\infty(0,+\infty; L^1(\mathbb{R}^2))$ is called a generalized kinetic solution of the scalar conservation law with initial data f_0, if for all $\phi \in D([0,+\infty) \times \mathbb{R} \times \mathbb{R})$ we have

$$\int_0^\infty \int_{\mathbb{R}^2} f(t,x,\xi) \left[\frac{\partial \phi(x,t,\xi)}{\partial t} + A'(\xi) \frac{\partial \phi(x,t,\xi)}{\partial x} \right] dx d\xi dt \\ = \int_0^\infty \int_{\mathbb{R}^2} m(t,x,\xi) \frac{\partial \phi(x,t,\xi)}{\partial \xi} dx d\xi dt - \int_{\mathbb{R}^2} f_0(x,\xi) \phi(0,x,\xi) dx d\xi \tag{0.10}$$

where m is a bounded nonnegative measure on $(\mathbb{R} \times \mathbb{R} \times (0,+\infty))$ and

$$|f(x,t,\xi)| = sgn(\xi) f(x,t,\xi) \leq 1 \tag{0.11a}$$

$$f = \int_{\mathbb{R}} \chi_\lambda(\xi) d\nu_{x,t}(\lambda). \tag{0.11b}$$

- $\nu_{x,t}$ is a Young measure associated to f
- LPT 95, Perthame and Tzavaras 2000, Perthame- Book 2002, Panov 1998, Debussche and Vovelle 2013

Choice of M_i : Diffusion approximations

Consider now, for each $\epsilon > 0$ the parabolic equation

$$\partial_t u + \partial_x A(u) = \epsilon u_{xx}, \quad x \in \mathbb{R}, \quad t > 0. \tag{0.12}$$

The corresponding kinetic formulation of this equation is given by

$$\frac{\partial \chi_u(\xi)}{\partial t} + A'(\xi)\frac{\partial \chi_u(\xi)}{\partial x} - \epsilon \frac{\partial^2 \chi_u(\xi)}{\partial x^2} = \epsilon \left(\frac{\partial \delta(\xi - u)}{\partial \xi} \left(\frac{\partial u}{\partial x}\right)^2 \right) = \frac{\partial m^\epsilon}{\partial \xi}$$

- G.-Q. Chen and B. Perthame 2003.
- Recall

$$\int_{\mathbb{R}} \chi_u(\xi)\, d\xi = u$$

- Our aim is first to consider schemes introducing artificial diffusion

Approximation by viscosity: Generalised viscous kinetic solutions : Uniqueness

A function $f(x,t,\xi) \in L^\infty(0,+\infty; L^1(\mathbb{R}^2))$ is called a generalized viscus kinetic solution of the scalar conservation law with initial data f_0, if for all $\phi \in D([0,+\infty) \times \mathbb{R} \times \mathbb{R})$ we have

$$\int_0^\infty \int_{\mathbb{R}^2} f(t,x,\xi) \left[\frac{\partial \phi(x,t,\xi)}{\partial t} + A'(\xi) \frac{\partial \phi(x,t,\xi)}{\partial x} \right] dx d\xi dt$$

$$= - \int_0^\infty \int_{\mathbb{R}^2} B_\varepsilon(x) \frac{\partial f(x,t,\xi)}{\partial x} \, \frac{\partial \phi(x,t,\xi)}{\partial x} dx d\xi dt$$

$$+ \int_0^\infty \int_{\mathbb{R}^2} m(t,x,\xi) \frac{\partial \phi(x,t,\xi)}{\partial \xi} dx d\xi dt - \int_{\mathbb{R}^2} f_0(x,\xi) \phi(0,x,\xi) dx d\xi$$

where m is a bounded nonnegative measure on $(\mathbb{R} \times \mathbb{R} \times (0,+\infty))$ and $|f(x,t,\xi)| = sgn(\xi) f(x,t,\xi) \le 1$

$$f = \int_{\mathbb{R}} \chi_\lambda(\xi) d\nu_{x,t}(\lambda).$$

- $\nu_{x,t}$ is a Young measure associated to f

Approximation by viscosity: Monte-Carlo sampling

To fix ideas, consider different approximations $u_j,\ j = 1, \ldots, J$, which correspond to different initial data $u_j^0,\ j = 1, \ldots, J$. Assume that all u_j satisfy

$$\partial_t u + \partial_x A(u) = \epsilon u_{xx}, \quad x \in \mathbb{R}, \quad t > 0. \tag{0.13}$$

then we would like to study the behaviour of the measure

$$\frac{1}{J} \sum_{j=1}^{J} \delta_{u_j} \, .$$

- each δ_{u_j} corresponds the kinetic function χ_{u_j} and all these functions satisfy

$$\frac{\partial \chi_u(\xi)}{\partial t} + A'(\xi) \frac{\partial \chi_u(\xi)}{\partial x} - \epsilon \frac{\partial^2 \chi_u(\xi)}{\partial x^2} = \epsilon \left(\frac{\partial \delta(\xi - u)}{\partial \xi} \left(\frac{\partial u}{\partial x} \right)^2 \right) = \frac{\partial m^\epsilon}{\partial \xi}$$

- Then, to the sample above, we associate the kinetic function,

$$f^J(t, x, \xi) = \frac{1}{J} \sum_{j=1}^{J} \chi_{u_j(t,x)}(\xi) \, . \tag{0.14}$$

- Due to the linearity of the principal part of the viscous kinetic formulation, each such f^J satisfies the generalised , (here $B_\epsilon = I$), for an appropriate measure m' and for $f_0(x, \xi) = \frac{1}{J} \sum_{j=1}^{J} \chi_{u_j^0(x)}(\xi)$.

Analysis/design of schemes

- $\nu_{x,t}$ is a Young measure associated to f
- discretisation through approximate Young measures will lead to schemes introducing artificial diffusion
- $\|B_\varepsilon\|_{L^\infty} \to 0$ as $\varepsilon \to 0$
- straightforward extension in multi-D

Analysis : several questions

- what do we compute?
- Uniqueness of the generalised kinetic solutions with general initial data within a class
- Convergence of the approximate kinetic models
- Convergence of viscosity Monte-Carlo samplings
- Convergence of the fully discretised approximate kinetic models
- Systems ??
- Other approximations??

Generalised kinetic solutions of viscosity approximations: Uniqueness III

Theorem

In addition to the previous hypothesis, assume that the defect measures are functions of f and $\bar{f}$ satisfying (up to regularisation and as $\|B\|_{L^\infty}, \|\bar{B}\|_{L^\infty} \to 0$)

- $\langle m(\nu) - \bar{m}(\bar{\nu}), \nu - \bar{\nu} \rangle \leq 0,$
- $m = 0$, *if* $f = 0$.
- *Assume further that the initial data satisfy* $\bar{f}(0, x, \xi) = f(0, x, \xi)$.
- *Then as both* $\|B\|_{L^\infty}, \|\bar{B}\|_{L^\infty} \to 0$

$$\|f - \bar{f}\|_{L^2} \to 0\,.$$

Remarks

- preliminary result –possible improvements
- interesting analytical questions are posed
- Uniqueness of measure valued solutions within a class : Fjordholm, Mishra ARMA 2018 : Correlation measures
- Relationship to UQ : Despres and Perthame // S. Jin
- Systems : quite difficult // however this approach hinges on approximating kinetic models and not on equivalent kinetic formulations for the limiting problem.

Are parametrised Young measures appropriate for statistical studies?

- The main spaces used in statistical studies of PDEs are Probability spaces defined on function spaces: The computation of such measures is very expensive and not always robust.
- Young measures : much simpler objects which are easier to handle computationally. However the information they provide is restricted compared to measures on function spaces.
- Analogy to PDEs : very weak solutions + wPDE imply smoothness : Young measure solutions + appropriate equations provide more structure (e.g., weak-strong uniqueness)

Χρόνια Πολλά Μάκη!!!