Modeling uncertainties with kinetic equations

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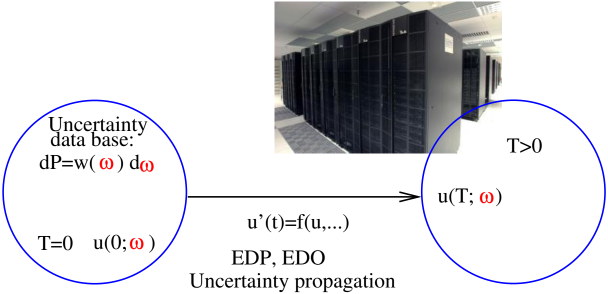
Section 1

Motivations

Need in applied sciences



- Assume the probability law is **given**

$$d\mathcal{P} = d\mu(\omega), \qquad d\mathcal{P} = e^{-\frac{(\omega-\omega_0)^2}{2\sigma}}d\omega, \quad \omega \in \mathbb{R}^P \text{ high stochastic dimension.}$$

- A popular idea to use chaos polynomials (Wiener 36') expansion

$$u(x,t,\omega) \approx u_N(x,t,\omega) = \sum_0^N u_n(x,t)p_n(\omega), \quad p_n \in P_n.$$

Conservation laws

Goal : model/propagate uncertainties in conservation laws

- Euler equations (Wiener 38', Lin-Su-Karniadakis 06', Glimm and al 06', ...)

$$\begin{cases} \partial_t \rho + \partial_x(\rho v) = 0, & \\ \partial_t(\rho v) + \partial_x(\rho v^2 + p_\omega) = 0, & p_\omega = (\gamma(\omega) - 1)\rho\varepsilon \\ \partial_t(\rho e) + \partial_x(\rho v e + p_\omega v) = 0, & e = \varepsilon + \frac{1}{2}v^2. \end{cases}$$

- Transport of the uncertain variable ω

$$\begin{cases} \partial_t U + \partial_x F(U, \omega) = 0, \\ \partial_t(\rho\omega) + \partial_x(\rho v \omega) = 0. \end{cases}$$

- In this presentation : model conservation law with uncertainties in the initial condition

$$\begin{cases} \partial_t u + \partial_x F(u) = 0, & F : \mathbb{R} \to \mathbb{R}, \\ u(x, \omega, 0) = u_0(x, \omega) & \end{cases}$$

Section 2

Kinetic formulations

Kinetic formulation of conservation laws

- The kinetic formulation of conservation laws (Perthame-Tadmor 91') writes

$$\begin{cases} \partial_t f_\varepsilon + a(\xi)\partial_x f_\varepsilon + \frac{1}{\varepsilon} f_\varepsilon = \frac{1}{\varepsilon} M(u_\varepsilon;\xi), \quad a(\xi) = F'(\xi), \ (\text{Burgers} : a(\xi) = \xi), \\ u_\varepsilon(x,t) = \int f_\varepsilon(x,\xi,t)d\xi, \\ f_\varepsilon(t=0) = M(u^{\text{init}};\xi), \end{cases}$$

For simplicity $u^{\text{init}} \geq 0$. The kinetic variable is $\xi \geq 0$.
The pseudo-Maxwellian is $M(u;\xi) = \mathbf{1}_{\{0<\xi<u\}}$.

- Under general conditions (Lions-Perthame-Tadmor 94'), the limit $\varepsilon \to 0^+$ is :
$u_\varepsilon(t) \to u(t)$ in L^1_x and $f_\varepsilon(t) \to M(u(t))$ in $L^1_{x\xi}$

$$\partial_t u + \partial_x F(u) = 0, \quad F : \mathbb{R} \to \mathbb{R}.$$

Moreover the limit is entropic (we will come back to that).

• Variables :
usual variables are the time t and space x,
additionally one has the kinetic variable ξ and the uncertain variable ω.

• Consider

$$\begin{cases} \partial_t f_\varepsilon^N + a(\xi)\partial_x f_\varepsilon^N + \frac{1}{\varepsilon} f_\varepsilon^N = \frac{1}{\varepsilon} M^N(u_\varepsilon^N; \xi, \omega), \\ u_\varepsilon^N(x, \omega, t) = \int f_\varepsilon^N(x, \xi, \omega, t) d\xi, \\ f_\varepsilon^N(t = 0) = M^N(u^{\text{init}}; \xi, \omega), \end{cases}$$

where $0 \leq M^N(u_\varepsilon^N; \xi, \omega) \leq 1$ is a suitable **polynomial approximation** of M.

• Strategy : **construct M^N, study properties and pass to the limit $\varepsilon \to 0$ and $N \to \infty$.**

Convolutions with polynomial kernels

Convolution

$$M^N(u_\varepsilon^N;\xi) = G^N *_\omega M(u_\varepsilon^N;\xi) = \int G^N(\omega,\omega')M(u_\varepsilon^N(\omega');\xi)d\mu(\omega') \in P_\omega^N$$

with kernel $G^N(\omega,\omega') = \sum_{n=0}^N c_n p_n(\omega)p_n(\omega')$, with p_n the orthonormal basis of polynomials for the measure $d\mu(\omega)$ and where c_n are appropriate coefficients,
and where G^N is a **Kernel Polynomial Method** (Weisse and al, 2006)

$$G^N \geq 0, \quad \int G^N(\omega,\omega')d\mu(\omega') = 1. \tag{1}$$

Basic example : Take $d\mu(\omega) = \frac{d\omega}{\pi\sqrt{1-\omega^2}}$, on $\omega \in I = (-1,1)$, and Tchebycheff orthonormal polynomials $p_n(\omega) = T_n(\omega) = \cos(n \operatorname{arcos} \omega)$, $-1 \leq \omega \leq 1$. The Fejer kernel G_F^N is defined by the coefficients

$$c_0 = 1 \text{ and } c_n = 2\frac{N+1-n}{N+1}, \quad 1 \leq n \leq N$$

$$f_F^N(\omega) = c_0\mu_0 + 2\sum_{n=1}^N c_n\mu_n T_n(\omega), \qquad \mu_n = \int_I f(\omega')T_n(\omega')d\mu(\omega')$$

$$f_F^N(\cos t) = \int_0^{2\pi} f(\cos u)K_F^N(t-u)du, \quad K_F^N(u) = \frac{1}{2\pi(N+1)}\left(\frac{\sin(N+1)\frac{u}{2}}{\sin\frac{u}{2}}\right)^2 \geq 0.$$

A priori estimates

$$\begin{cases} \partial_t f_\varepsilon^N + a(\xi).\nabla f_\varepsilon^N + \frac{1}{\varepsilon} f_\varepsilon^N = \frac{1}{\varepsilon} G^N *_\omega M(u_\varepsilon^N; \xi, \omega), \\ u_\varepsilon^N(x,\omega,t) = \int f_\varepsilon^N(x,\xi,\omega,t) d\xi. \end{cases}$$

• L^∞ bounds : $0 \leq f_\varepsilon^N \leq 1$, $0 \leq u_\varepsilon^N \leq U_M := \sup_{x,\omega} u^{\text{init}}(x,\omega)$,
$f_\varepsilon^N(x,\xi,\omega,t) \equiv 0$ for $\xi \geq U_M$.

• Entropy bounds $S''(\xi) \geq 0$:
$\partial_t \int S'(\xi) f_\varepsilon^N(x,\xi,\omega,t) d\xi d\mu(\omega) + \text{div} \int a(\xi) S'(\xi) f_\varepsilon^N(x,\xi,\omega,t) d\xi d\mu(\omega) \leq 0$

• Propagation of classical BV bounds :
$\int |\nabla_x f_\varepsilon^N| dx d\xi d\mu(\omega) \leq C^{\text{init}}$, $\int |\nabla_x u_\varepsilon^N| dx d\mu(\omega) \leq C^{\text{init}}$,
$\int \left|\partial_t f_\varepsilon^N(t)\right| dx d\xi d\mu(\omega) \leq \int \left|\partial_t f_\varepsilon^N(0)\right| dx d\xi d\mu(\omega) \leq C^{\text{init}}$,
$\int \left|\partial_\xi f_\varepsilon^N(t)\right| dx d\xi d\mu(\omega) \leq e^{-\frac{t}{\varepsilon}} \int \left|\partial_\xi f_\varepsilon^N(0)\right| dx d\xi d\mu(\omega) + C$

• Plus new BV estimates with respect to ω, using the convolution structure.

Convergence for all $t \geq 0$ (Jackson kernels)

• **The limit is a weak solution** $N^2\varepsilon \to \infty$: Consider the Jackson kernels. There exists $f \in L^1_{loc}(\mathcal{D}_0)$ such that $\lim_{\varepsilon \to 0} \left\| f^N_\varepsilon - f \right\|_{L^1_{loc}(\mathcal{D}_0)} = 0$ and

$$\partial_t f + a(\xi)\partial_x f = \partial_\xi m \qquad \text{weak solution}$$

where $m \geq 0$ is a measure, and $f = M(u;\xi)$ with $u = \int f d\xi$.
"So" (Lions-Perthame-Tadmor 94') : u is the solution (a.e.).

• **Strong error bounds** $N\varepsilon \to \infty$: Moreover

$$\left\| f^N_\varepsilon(t) - G^N *_\omega f_\varepsilon(t) \right\|_{L^1_{x\xi\mu}} \leq C \frac{t}{\varepsilon} \int_0^{2\pi} |f(\cos(t+\alpha) - f(\cos t)| \, dt \approx \frac{Ct}{N\varepsilon}.$$

• **Projected equations** $\varepsilon = \frac{1}{N+1}$ fixed : One gets for
$u^N_{\varepsilon,i}(x,t) = \int f^N_{\varepsilon,i}(x,\xi,\omega,t) d\xi d\mu(\omega)$, $f^N_{\varepsilon,i}(x,\omega,t) = \int f^N_\varepsilon(x,\xi,\omega,t) T_i(\omega) d\xi$

$$\partial_t u^N_{\varepsilon,i} + \partial_x \int a(\xi) f^N_{\varepsilon,i} d\xi = -h_N(i) u^N_{\varepsilon,i}, \quad h_N(i) > 0 \text{ for } i > 0.$$

Kinetic polynomials and optimal control

• Reminder Brenier 83' : the indicatrix function is the minimum of a certain minimization problem

$$\mathbf{1}_{\{0<\xi<u\}} = M(u;\cdot) = \underset{\{0\le g\le 1 | |\int g d\xi = u \ge 0\}}{\operatorname{argmin}} \int_0^\infty g(\xi) S'(\xi) d\xi, \qquad \forall S,\ S'' > 0.$$

• Generalize : Minimization of weighted L^1 norms, under convex constraints

$$M^N(u^N) = \underset{g^N \in K^N(u^N)}{\operatorname{argmin}} \int_0^\infty \int_I g^N(\xi,\omega) S'(\xi) d\xi d\mu(\omega), \quad \text{for admissible } S,$$

where

$$K^N(u^N) = \left\{ g^N(\cdot,\cdot) \in P^N_\omega,\ u^N(\omega) = \int_0^\infty g^N(\xi,\omega) d\xi,\ 0 \le g^N \le 1 \text{ for } \omega \in I \right\}$$

A remark

Make the assumption : for all $u^N \geq 0$ there exists a unique M^N (we call it a kinetic polynomial) such that

$$M^N(u^N) = \underset{g^N \in K^N(u^N)}{\operatorname{argmin}} \int_0^\infty \int_I g^N(\xi, \omega) S'(\xi) d\xi d\mu(\omega), \quad \text{for a given } S.$$

Then the solution of

$$\begin{cases} \partial_t f_\varepsilon^N + a(\xi)\partial_x f_\varepsilon^N + \frac{1}{\varepsilon} f_\varepsilon^N = \frac{1}{\varepsilon} M^N(u_\varepsilon^N; \xi, \omega), \\ u_\varepsilon^N(x, \omega, t) = \int f_\varepsilon^N(x, \xi, \omega, t) d\xi, \\ f_\varepsilon^N(t = 0) = M^N(u^{\text{init}}; \xi, \omega), \end{cases}$$

is in bounds, $0 \leq f^N \leq 1$, and is conservative

$$\partial_t u_\varepsilon^N(x, \omega, t) + \partial_x G_\varepsilon^N(x, \omega, t) d\xi = 0,$$

$$u_\varepsilon^N = \int_\xi f_\varepsilon^N d\xi, \quad G_\varepsilon^N(x, \omega, t) = \int_\xi a(\xi) f_\varepsilon^N d\xi.$$

This last property does not hold with the convolution method.

Entropy inequality

Moreover it satisfies the entropy inequality

$$\frac{d}{dt}\int_\xi\int_\omega\int_x f^N(x,\xi,\omega,t)dxS'(\xi)d\xi d\mu(\omega)$$

$$=\frac{1}{\varepsilon}\int_x\left(\int_\xi\int_\omega M^N S'(\xi)d\xi d\omega-\int_\xi\int_\omega f^N S'(\xi)d\xi d\omega\right)\leq 0.$$

Note that it passes (at least formally) to the limit $\varepsilon\to 0$: one gets the equation

$$\partial_t u^N(x,\omega,t)+\partial_x G^N(x,\omega,t)d\xi=0,\quad G^N(x,\omega,t)=\int_\xi a(\xi)M^N(u^N)d\xi$$

which satisfies the entropy inequality

$$\partial_t\int_\xi a(\xi)M^N(u^N)d\xi+\partial_x\int_\xi a(\xi)M^N(u^N)S'(\xi)d\xi\leq 0.$$

Designing M^N is the issue

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Conclusion

For simplicity rewrite the time and space variables as $t \leftarrow \xi$ and $x \leftarrow \omega$. Set $S'(\xi) = S'(t) = t$ for simplicity. Consider the interval $x \in I = [0, 1]$. write $n = N$. The problem rewrites as :

Given a given non negative polynomial $\mathbf{u_n} \in P_n^+(I)$, find

$$v_n(t) \in U_n \equiv \{w_n \in P_n \mid 0 \le w_n(x) \le 1 \text{ for all } x \in I\}$$

with the constraint

$$\int_0^T v_n(t,x)dt = \mathbf{u_n}(x) \quad x \in I,$$

such that

$$v_n = \text{argmin} \int_0^T \int_I w_n(t,x)\ tdtdx.$$

:(the structure of U_n is complex with an infinite number of constraints and the functional is linearly degenerate.
:) it can interpreted in the setting of Optimal Control.

Reformulation

Set

$$y_n(t,x) = \int_0^T v_n(t,x)dt.$$

The problem writes : Find a control $v_n(t) \in U_n$ such that the state y_n

$$\frac{d}{dt} y_n = v_n, \quad y_n(0) = 0,$$

reaches the objective $y_n(T) = \mathbf{u_n}$ and minimizes the cost function

$$C(v_n) = \int_0^T \int_I v_n(t,x) t dt dx.$$

First obvious result : if $T \geq \|\mathbf{u_n}\|_{L^\infty}$ then

$$v_n^{\text{non opt.}}(t,x) = \frac{\mathbf{u_n(x)}}{\|\mathbf{u_n}\|_{L^\infty}}$$

is a (a priori) non optimal solution.

Properties

• Wish/claim : there exists a unique solution $v_n(t)$ to the Optimal control problem. Hint of the proof : mix the Bojanic-Devore theorem (one-sided L^1 polynomial approximation) with optimal control.

• **Theorem** (Pontryagin maximum principle) : for all optimal trajectories, there exists a multiplier $\lambda_n \in P_n$ such that

- either the trajectory is normal

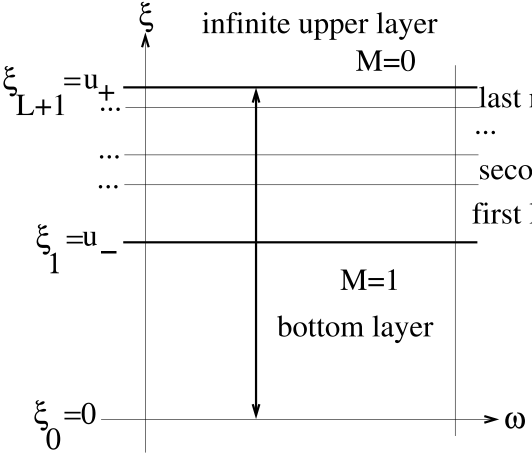
$$v_n(t) = \text{argmax}_{w_n \in U_n} \int_0^1 (\lambda_n(x) - t) w_n(x) dx$$

- or the trajectory is abnormal

$$v_n(t) = \text{argmax}_{w_n \in U_n} \int_0^1 \lambda_n(x) w_n(x) dx.$$

• Next simulations are with the AMPL code, very popular in the Optimal Control community.

Feasible solution : constant one layer the other



Numerical scheme (with the feasible solution)

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Conclusion

Let a 1D mesh $j\Delta x$. Consider

$$\frac{\overline{u}_j^N - u_j^N}{\Delta t} + \frac{F^N[u_j^N] - F^N[u_{j-1}^N]}{\Delta x} = 0,$$

unknown $u_j^N \in P^N(\omega)$ is a polynomial in ω of degree N (fixed) in cell j, flux $F^N[u_j^N] \in P^N(\omega)$ in cell j is constructed with the kinetic polynomial formula for the Burgers equation

$$F^N[u^N]_n = \sum_{l \geq 0} (F(\xi_{l+1}) - F(\xi_l)) \int h_l^N(\omega) p_n(\omega) d\mu(\omega), \quad F(\xi) = \frac{\xi^2}{2}.$$

Assume init. is bounded : $0 \leq U_m \leq u_j^N(\omega) \leq U_M < \infty$, $\forall j$ and $\forall \omega \in I$.

Theorem : Assume the CFL condition $U_M \Delta t \leq \Delta x$. Then

$$U_m \leq \overline{u}_j^N(\omega) \leq U_M, \quad \forall j \text{ and } \forall \omega \in I.$$

Proof. Either use the kinetic formulation, or prove directly.

Numerical illustration : Burgers equation

Set up : $d\mu(\omega) = \frac{d}{\pi\sqrt{1-\omega^2}}$, $N = 2$.

The moments model is explicit

$$\partial_t \begin{pmatrix} a \\ b \\ c \end{pmatrix} + \partial_x \begin{pmatrix} \frac{a^2+b^2+c^2}{2} \\ ab + \frac{bc}{\sqrt{2}} \\ ac + \frac{b^2}{2\sqrt{2}} \end{pmatrix} = 0.$$

Compare solutions of

- the moment model,
- the kinetic polynomial method with feasible solution,
- and the standard non intrusive approach (quadrature points, close to MC).

N-convergence for Burgers eq.

Consider the system of $N+1$ conservation laws with $d\mu(\omega) = d\omega$

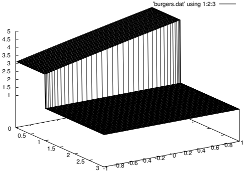
$$\begin{cases} \partial_t u_0 + \partial_x \int_{-1}^{1} \frac{\left(\sum_{n\le N} u_n \varphi_n(\omega)\right)^2}{2} \varphi_0(\omega) d\omega = 0, \\ \dots \\ \partial_t u_n + \partial_x \int_{-1}^{1} \frac{\left(\sum_{n\le N} u_n \varphi_n(\omega)\right)^2}{2} \varphi_N(\omega) d\omega = 0. \end{cases}$$

•There is an entropy-entropy flux pair $\Longrightarrow$ hyperbolicity

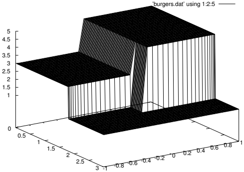
$$\partial_t \frac{\sum_{n\le N} |u_n|^2}{2} + \partial_x \int_\Theta \frac{\left(\sum_{n\le N} u_n \varphi_n(\omega)\right)^3}{3} d\omega \le 0.$$

Shock

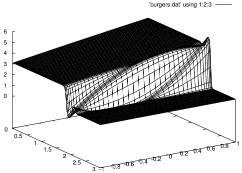
$$u^{\text{ini}}(x,\omega) = \begin{cases} 3 & \text{for } x < 1/2 \text{ and } -1 < \omega < 0, \\ 5 & \text{for } x < 1/2 \text{ and } 0 < \omega < 1, \\ 1 & \text{for } 1/2 < x \text{ and } -1 < \omega < 1. \end{cases}$$



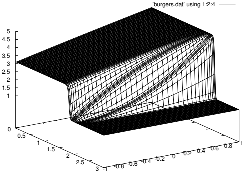
projection of the initial data



exact solution $t = 0.4$



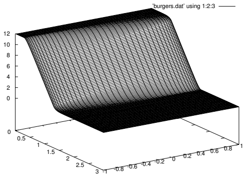
moment solution $t = 0.4$



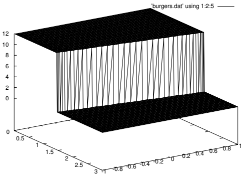
new method $t = 0.4$

Compressive solution

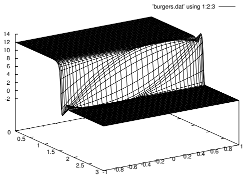
$$u^{\mathrm{ini}}(x,\omega) = \begin{cases} 12 & \text{for } x - \omega/5 < 1/2, \\ 1 & \text{for } x - \omega/5 < 3/2, \\ 12 - 11\,(x - \omega/5 - 1/2) & \text{in between.} \end{cases}$$



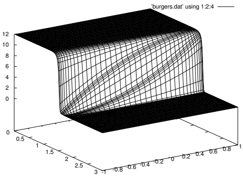
projection of the initial data



exact solution $t = 0.1$



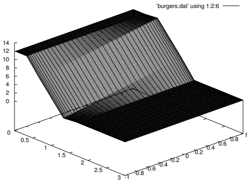
moment solution $t = 0.1$



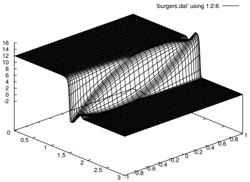
new method $t = 0.1$

Non intrusive moments with quadrature points

Use $\omega_1 = -\sqrt{\frac{3}{4}}$, $\omega_2 = 0$ and $\omega_3 = \sqrt{\frac{3}{4}}$. Then reconstruct.



reconstructed initial data



reconstructed solution at $t = 0.1$

The test is performed with the compressive initial data.

Initialization of the shock problem is ambiguous at $t = 0$.

Larger N (with a moment method, Poette PHD)

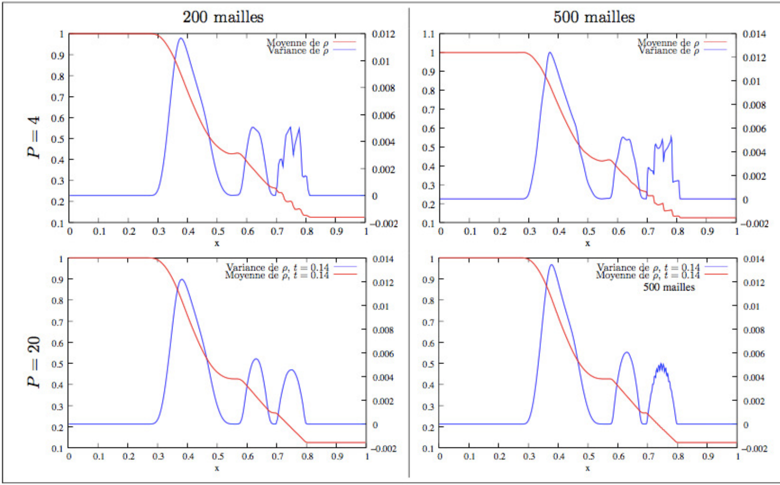


FIG. 5.18 – Problème de Riemann stochastique de conditions initiales (5.63). Les calculs sont effectués

Conclusion

- The kinetic formulation of conservation laws is a convenient tool for the analysis of conservation laws with intrusive uncertainties.
- The theory of convolution-based method is OK, but the practice not clear due the spurious damping.
- The alternative is kinetic polynomials (Maxwellian plus polynomials) which are at their infancy.

  The theory is full of open problems : existence, uniqueness, error estimates, ...and connection with optimal control.

Two issues were not addressed in this talk :

interpretation of the results in terms of **probability** ; the curse of dimension $\omega \in \mathbb{R}^{\textbf{large}}$.