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Building and solving reduced models for the uncertain linear Boltzmann equation

(sometimes, intrusiveness is worth it)

Gaël Poëtte<sup>†</sup>

†CEA, CESTA, DAM F-33114 Le Barp, France

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- Motivations and objectives + the skeleton of an MC code
- 2 Non-intrusive applications and drawbacks in an MC context
- 3 Intrusive reduced modeling (sometimes, it is worth it)

#### 4 Few simple test-cases

- Comparisons, performance considerations
- MC-gPC for k<sub>eff</sub> computations (work with E. Brun [28])
- Hybrid intrusive/non-intrusive computations

# 5 Conclusion

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We are interested in the resolution of the linear Boltzmann equation

$$\partial_t u(\mathbf{x}, t, \mathbf{v}) + \mathbf{v} \cdot \nabla u(\mathbf{x}, t, \mathbf{v}) = -v\sigma_t(\mathbf{x}, \mathbf{v})u(\mathbf{x}, t, \mathbf{v}) \\ + \int v\sigma_s(\mathbf{x}, \mathbf{v}, \mathbf{v}')u(\mathbf{x}, t, \mathbf{v}') \,\mathrm{d}\mathbf{v}'.$$

Few constraints for the resolution:

- Dimension  $7 = 3(\mathbf{x}) + 1(t) + 3(\mathbf{v}) \Longrightarrow$  use of Monte-Carlo (MC).
- Need for accurate transient/late time  $(t^*)$ :  $U(\mathbf{x}, t^*) = \int u(\mathbf{x}, t^*, \mathbf{v}) d\mathbf{v}$ .

In this talk, we are interested in: Uncertainty Analysis

- Assume some parameters  $X \in \mathbb{R}^Q$  in the above PDE are uncertain
- General dependence w.r.t. X of  $(\sigma_{\alpha})_{\alpha \in \{s,t\}}$ ,  $u_0$ , boundary conditions etc.
- $\blacksquare$  We model them thanks to random variables of probability measure  $X \sim \mathsf{d}\mathcal{P}_X$
- $\implies$  We need to solve a stochastic PDE in order to propagate uncertainties

2 The uncertain linear Boltzmann equation A brief presentation of what is in [21]

We are interested in the resolution of the uncertain linear Boltzmann equation

$$\begin{aligned} \partial_t u(\mathbf{x}, t, \mathbf{v}, X) + \mathbf{v} \cdot \nabla u(\mathbf{x}, t, \mathbf{v}, X) + v \sigma_t(\mathbf{x}, \mathbf{v}, X) u(\mathbf{x}, t, \mathbf{v}, X) \\ &= \int v \sigma_s(\mathbf{x}, \mathbf{v}, \mathbf{v}', X) u(\mathbf{x}, t, \mathbf{v}', X) \, \mathrm{d}\mathbf{v}', \end{aligned}$$

where  $X \in \mathbb{R}^Q$  is a random variable of dimension Q sampled from  $d\mathcal{P}_X$ . <u>Few constraints for the resolution</u>:

- $7 + Q = 3(\mathbf{x}) + 1(t) + 3(\mathbf{v}) + Q(X)$  (independent) dimensions.
- $\blacksquare$  Statistics of  $U(\mathbf{x},t^*,X)=\int u(\mathbf{x},t^*,\mathbf{v},X)\mathrm{d}\mathbf{v}$

### About the resolution of the above stochastic PDE:

- Once a simulation device at hand to approximate the solution, the most straightforward uncertainty propagation method is the non-intrusive one.
- In our codes, the transport equation is often solved using **an MC scheme**.



- Inconditionally stable scheme: the time step can be the time of interest t\*. (MC schemes scale weakly in a replication domain context if ∆t is high enough)
- Positive scheme.
- Converging scheme (Law of large number, see Lapeyre-Pardoux-Sentis)
- Asymptotically, with  $u_p(\mathbf{x},t,\mathbf{v}) = w_p(t)\delta_{\mathbf{x}}(\mathbf{x}_p(t))\delta_{\mathbf{v}}(\mathbf{v}_p(t))$ , we have

$$\sqrt{N_{MC}} \left( \sum_{k=1}^{N_{MC}} u_p(\mathbf{x}, t, \mathbf{v}) - u(\mathbf{x}, t, \mathbf{v}) \right) \xrightarrow{\mathcal{L}} \mathcal{G}(0, \sigma_{\mathsf{MC}}),$$

(Central Limit theorem, see Lapeyre-Pardoux-Sentis [17]).

- We will abusively but concisely write the error is  $e_{N_{MC}} = \mathcal{O}\left(\frac{1}{\sqrt{N_{MC}}}\right)$ .
- $\blacksquare$  The performance of the MC schemes can be studied by analyzing  $\sigma_{\rm MC}$  .
- Several schemes: analog, **non-analog**, with variance reduction technics...

ок LA ИКСНЕЙСНЕ ѝ СПИЗИАТИ

Algorithmic sketch for the non-analog MC scheme (Backward formulation with constant per cell cross-sections)

set  $u(\mathbf{x}, t, \mathbf{v}) = 0$ for  $p \in \{1, ..., N_{MC}\}$  do set  $s_p = t \# this will be the life time of particle p$ set  $\mathbf{x}_n = \mathbf{x}$ set  $\mathbf{v}_n = \mathbf{v}$ set  $w_p = \frac{1}{N_{MC}}$ while  $s_{\mathcal{D}} > 0$  and  $w_{\mathcal{D}} > 0$  do  $\ln(\mathcal{U}([0,1]))$ Sample au by inversing the cdf of an exponential law au= $v_n \sigma_s(\mathbf{x}_n, \mathbf{v}_n)$ if  $\tau > s_{\mathcal{D}}$  then #move the particle p  $\mathbf{x}_p - = \mathbf{v}_p s_p$ #set the life time of particle p to zero:  $s_{p} = 0$ #change its weight  $w_p \times = e^{-v\sigma_a(\mathbf{x}_p, \mathbf{v}_p)s_p}$ #tally the contribution of particle p  $u(\mathbf{x}, t, \mathbf{v}) + = w_p \times u_0(\mathbf{x}_p, \mathbf{v}_p)$ e nd else #move the particle p  $\mathbf{x}_p - = \mathbf{v}_p \tau$ #change the weight of the particle  $w_p \times = e^{-v\sigma_a(\mathbf{x}_p, \mathbf{v}_p)\tau}$ Sample the velocity  $\mathbf{V}'$  sampled from  $P_s(\mathbf{x}_p, \mathbf{v}', \mathbf{v}_p) d\mathbf{v}'$  $\mathbf{v}_n = \mathbf{V}'$ #set the life time of particle p to:  $s_n - = \tau$ e nd end end

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- ${f I}$  X is an arbitrary random variable of probability measure d ${\cal P}_X.$
- 2 Discretization of  $(X, d\mathcal{P}_X)$  by a quadrature with N points  $(X_i, w_i)_{i \in \{1, \dots, N\}}$ .
- **3** N independent solutions at points  $(X_i, w_i)$ :

 $(u(\mathbf{x},t,\mathbf{v},X_i),w_i)_{i\in\{1,\dots,N\}},$  solutions of your favorite problem

4 Estimation of the statistical quantities of interest by numerical integration:

$$\mathbb{E}[U](\mathbf{x},t) = \iint u(\mathbf{x},t,\mathbf{v},X) d\mathbf{v} d\mathcal{P}_X,$$
  

$$\mathbb{E}[U^2](\mathbf{x},t) = \int \left(\int u(\mathbf{x},t,\mathbf{v},X) d\mathbf{v}\right)^2 d\mathcal{P}_X,$$
  

$$\mathbb{V}[U](\mathbf{x},t) = \mathbb{E}[U^2](\mathbf{x},t) - (\mathbb{E}[U](\mathbf{x},t))^2,$$
  
... = ...

Other examples of interesting statistical quantities will be given later



- $\blacksquare X$  is an arbitrary random variable of probability measure d $\mathcal{P}_X$ .
- 2 Discretization of  $(X, d\mathcal{P}_X)$  by a quadrature with N points  $(X_i, w_i)_{i \in \{1, ..., N\}}$ .
- 3 N independent runs of a black box code at points  $(X_i, w_i)$ :

 $(u(\mathbf{x},t,\mathbf{v},X_i),w_i)_{i\in\{1,\dots,N\}},$  solutions of your favorite problem

4 Estimation of the statistical quantities of interest by numerical integration:

$$\mathbb{E}[U](\mathbf{x},t) = \sum_{\substack{k=1\\N}}^{N} w_i U(\mathbf{x},t,X_i) + \mathcal{O}(N^{\beta}),$$
  
$$\mathbb{E}[U^2](\mathbf{x},t) = \sum_{\substack{k=1\\N}}^{N} w_i U^2(\mathbf{x},t,X_i) + \mathcal{O}(N^{\beta}),$$
  
$$\mathbb{V}[U](\mathbf{x},t) = \mathbb{E}[U_N^2](\mathbf{x},t) - (\mathbb{E}[U_N](\mathbf{x},t))^2 + \mathcal{O}(N^{\beta}),$$
  
$$\dots = \dots$$

5 Other examples of interesting statistical quantities will be given later



- **1** X is an arbitrary random variable of probability measure  $d\mathcal{P}_X$ .
- 2 Discretization of  $(X, d\mathcal{P}_X)$  by a quadrature with N points  $(X_i, w_i)_{i \in \{1, ..., N\}}$ .
- 3 N independent runs of a black box code at points  $(X_i, w_i)$ :

$$(u_{\Delta}(\mathbf{x}, t, \mathbf{v}, X_i), w_i)_{i \in \{1, \dots, N\}}, \text{ approximations } u_{\Delta} = u + \mathcal{O}(\Delta)$$

4 Estimation of the statistical quantities of interest by numerical integration:

$$\mathbb{E}[U](\mathbf{x},t) = \sum_{k=1}^{N} w_i U_{\Delta}(\mathbf{x},t,X_i) + \mathcal{O}(N^{\beta}) + \mathcal{O}(\Delta),$$
  

$$\mathbb{E}[U^2](\mathbf{x},t) = \sum_{k=1}^{N} w_i U_{\Delta}^2(\mathbf{x},t,X_i) + \mathcal{O}(N^{\beta}) + \mathcal{O}(\Delta),$$
  

$$\mathbb{V}[U](\mathbf{x},t) = \mathbb{E}[U_{N,\Delta}^2](\mathbf{x},t) - (\mathbb{E}[U_{N,\Delta}](\mathbf{x},t))^2 + \mathcal{O}(N^{\beta}) + \mathcal{O}(\Delta),$$
  
... = ...

5 Other examples of interesting statistical quantities will be given later



The error e for the UQ problem, on any statistical observable, is



 Illustration on a homogeneous uncertain problem for which an analytical solution for the variance can be built (see [21])

Convergence studies w.r.t. to  $\Delta$  and N for two different strategies:





When running N times the MC code: MC particles for (x, t, v) and the experimental design for X are tensorised.

(We need to deal with  $N(X) \times N_{MC}(\mathbf{x}, t, \mathbf{v})$  MC particles)

MC methods are integration methods supposed to avoid such tensorisation!

(Is it possible to have only  $N_{MC}$  for the whole set of variables  $(\mathbf{x}, t, \mathbf{v}, X)$ ?)

Main difficulty: as always, finding the relevant linearisation
 ⇒ example of the equation satisfied by the second order moment



The simplest statistical observable is the variance:  $\mathbb{V}[u](\mathbf{x}, t, \mathbf{v}) = M_2(\mathbf{x}, t, \mathbf{v}) - M_1^2(\mathbf{x}, t, \mathbf{v})$  with

$$M_2(\mathbf{x}, t, \mathbf{v}) = \int u^2(\mathbf{x}, t, \mathbf{v}, X) \mathrm{d}\mathcal{P}_X = \int m_2(\mathbf{x}, t, \mathbf{v}, X) \mathrm{d}\mathcal{P}_X.$$



 $\blacksquare$  The equation satisfied by u is

$$\partial_t u(\mathbf{x}, t, \mathbf{v}, X) + \mathbf{v} \cdot \nabla u(\mathbf{x}, t, \mathbf{v}, X) = -v\sigma_t(\mathbf{x}, \mathbf{v}, X)u(\mathbf{x}, t, \mathbf{v}, X) + \int v\sigma_s(\mathbf{x}, \mathbf{v}, \mathbf{v}', X)u(\mathbf{x}, t, \mathbf{v}', X)d\mathbf{v}',$$

and is linear so why do we need a relevant linearisation?



**\blacksquare** Let us multiply the transport equation by u to obtain

$$\begin{split} \partial_t \frac{u^2}{2}(\mathbf{x}, t, \mathbf{v}, X) + \mathbf{v} \cdot \nabla \frac{u^2}{2}(\mathbf{x}, t, \mathbf{v}, X) &= -v\sigma_t(\mathbf{x}, \mathbf{v}, X)u^2(\mathbf{x}, t, \mathbf{v}, X) \\ &+ u(\mathbf{x}, t, \mathbf{v}, X)\int v\sigma_s(\mathbf{x}, \mathbf{v}, \mathbf{v}', X)u(\mathbf{x}, t, \mathbf{v}', X)\mathrm{d}\mathbf{v}', \end{split}$$

in which it remains to make  $u^2 = m_2$  appear.



If u is solution of the uncertain transport equation, quantity  $m_2$  is solution of  $\partial_t m_2(\mathbf{x}, t, \mathbf{v}, X) + \mathbf{v} \cdot \nabla m_2(\mathbf{x}, t, \mathbf{v}, X) = -2v\sigma_t(\mathbf{x}, \mathbf{v}, X)m_2(\mathbf{x}, t, \mathbf{v}, X)$  $+2u(\mathbf{x}, t, \mathbf{v}, X) \int v\sigma_s(\mathbf{x}, \mathbf{v}, \mathbf{v}', X)u(\mathbf{x}, t, \mathbf{v}', X)d\mathbf{v}',$ 

which is nonlinear in general (i.e. if  $\sigma_s \neq 0$ ).

Nonlinearity demands a splitting/linearisation hypothesis.

$$\begin{split} \partial_t m_2(\mathbf{x},t,\mathbf{v},X) + \mathbf{v}\cdot\nabla m_2(\mathbf{x},t,\mathbf{v},X) &= -2v\sigma_t(\mathbf{x},\mathbf{v},X)m_2(\mathbf{x},t,\mathbf{v},X) \\ &+ 2u(\mathbf{x},t,\mathbf{v},X)\int v\sigma_s(\mathbf{x},\mathbf{v},\mathbf{v}',X)u(\mathbf{x},t,\mathbf{v}',X)\mathrm{d}\mathbf{v}', \end{split}$$

which is nonlinear in general (i.e. if  $\sigma_s \neq 0$ ).

- The most common linearisation strategies for this type of quadratic operator:
  - Nanbu-like method [6]  $(\mathcal{O}(\Delta t) \text{ splitting})$ (would need small time steps in very collisional media)
  - Bird-like method [4] ( $\mathcal{O}(\Delta t)$  splitting). (would also need small time steps in some regimes)
  - Posttreatment of a count rate file from an analog resolution [7]  $\mathcal{O}(\Delta t)$ . (explosion of the I/O and file size close to criticity)

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  - Bird-like method [4] (O(\Delta t) splitting).
     (would also need small time steps in some regimes)
  - Posttreatment of a count rate file from an analog resolution [7]  $\mathcal{O}(\Delta t)$ . (explosion of the I/O and file size close to criticity)
  - AND we need a linearisation working for other statistical quantities too.
  - $\implies$  We here only suggest a new linearisation (with respect to P introduced later). (see [21, 22, 23, 24, 28, 9, 20] for other physical applications)

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 Convergence theorem for generalised Polynomial Chaos [33, 8, 35, 32, 12] (also called stochastic finite elements in the literature [31, 13, 11, 34, 14])

Let X be an arbitrary r.v. of probability measure  $d\mathcal{P}_X(x)$ ,  $(\phi_k)_{k\in\mathbb{N}}$  is the basis of orthonormal polynomials with respect to  $d\mathcal{P}_X(x)$ Let u(X) be an unknown random variable with  $\int u^2(X) d\mathcal{P}_X < \infty$ ,

then 
$$u_P(X) = \sum_{k=0}^P u_k \phi_k(X) \xrightarrow[P \to \infty]{L^2} u(X)$$
, where  $u_k = \int u(X) \phi_k(X) \mathrm{d}\mathcal{P}_X$ .

Idea: compute the coefficients (u<sub>k</sub>)<sub>k∈{0,...,P}</sub> during the MC resolution
Of course, one can obtain the coefficients non-intrusively [15, 10, 19, 29, 18]
How do we use that convergence theorem?

A gPC-based reduced model for uncertain transport (order P is the new linearisation parameter... Looks like  $P_n$  models...)

Let us build a gPC based reduced model for the uncertain transport equation

Let us defined the gPC developpement

$$u^{P}(\mathbf{x},t,\mathbf{v},X) = \sum_{q=0}^{P} u_{k}(\mathbf{x},t,\mathbf{v})\phi_{k}(X) \text{ with } u_{k}(\mathbf{x},t,\mathbf{v}) = \int u(\mathbf{x},t,\mathbf{v},X)\phi_{k}(X) \mathrm{d}\mathcal{P}_{X}.$$

 $\blacksquare$  Let us plug  $u^P$  in the transport equation and perform a Galerkin projection to get

$$\partial_{t}u_{0} + \mathbf{v} \cdot \nabla_{\mathbf{x}}u_{0} = -v \int \left(\sigma_{t} \sum_{k \leq P} u_{k}\phi_{k}\right) \phi_{0} d\mathcal{P}_{X} + v \iint \left(\left(\sigma_{s} \sum_{k \leq P} u_{k}\phi_{k}\right) \phi_{0} d\mathcal{P}_{X}\right) \\ \cdots \\ \partial_{t}u_{P} + \mathbf{v} \cdot \nabla_{\mathbf{x}}u_{P} = -v \int \left(\sigma_{t} \sum_{k \leq P} u_{k}\phi_{k}\right) \phi_{P} d\mathcal{P}_{X} + v \iint \left(\left(\sigma_{s} \sum_{k \leq P} u_{k}\phi_{k}\right) \phi_{P} d\mathcal{P}_{X}\right) \right)$$

The reduced model is still linear  $\implies$  it can be solved by an MC scheme.

In fact, it can be solved by slightly modifying an already existing MC code [21].

## A gPC-based reduced model for uncertain transport Spectral convergence with respect to P

In [22], proof of spectral convergence as  $P 
ightarrow \infty$  for the gPC reduced model:

- Let us defined the gPC developpement  $u^P = \sum_{q=0}^{P} u_q \phi_q$  with  $u_q = \int u \phi_q d\mathcal{P}_X$ .
- Define the space of functions

$$H^{k}(\Theta) = \left\{ u \in L^{2}_{\Theta} \Big| \int \sum_{l=0}^{k} (u^{(l)})^{2} \mathrm{d}\mathcal{P}_{X} < \infty \right\}.$$

Assume bounds on the cross-sections

$$\|v\sigma_t\|_{L^{\infty}(\mathcal{I}\times\Theta)} = \Sigma_t < \infty, \quad \|v\sigma_s\|_{L^{\infty}(\mathcal{I}\times\Theta)} = \Sigma_s < \infty.$$
(1)

Theorem (Convergence of the *P*-truncated gPC reduced model approximation)

Spectral accuracy holds in the following sense: for all  $k \in \mathbb{N}$  such that  $u \in H^k(\Theta)$ , there exists a constant  $D_k$  such that  $\forall t \in [0,T]$ 

$$\left\| u(t) - u^{P}(t) \right\|_{L^{2}(\mathcal{I},\Theta)}^{2} \leq e^{2(\Sigma_{t} + \Sigma_{s})t} \left( \left\| u_{0} - u_{0}^{P} \right\|_{L^{2}(\mathcal{I},\Theta)}^{2} + 2(\Sigma_{s} + \Sigma_{t})t \|u_{0}^{2}\|_{L^{2}(\mathcal{I},\Theta)} \frac{D_{k}}{P^{k}} \right).$$

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# The gPC intrusive non-analog MC scheme as in [21] (Backward formulation with constant per cell cross-sections)

for  $k \in \{0, ..., P\}$  do set  $u_{\mathbf{k}}(\mathbf{x}, t, \mathbf{v}) = 0$ end for  $p \in \{1, ..., N_{MC}\}$  do set  $s_p = t \# this$  will be the remaining life time of particle p, it must go down to zero (backward) set  $\mathbf{x}_n = \mathbf{x}$ set  $\mathbf{v}_n = \mathbf{v}$ set  $w_p = \frac{1}{NMC}$ set  $X_{\mathcal{D}} = X$  with X sampled from the probability measure d  $\mathcal{P}_{\mathbf{X}}$ . while  $s_p > 0$  and  $w_p > 0$  do Sample  $\tau$  by inversing the cdf of an exponential law  $\tau = -\frac{\ln(\mathcal{U}([0,1]))}{v\sigma_s(\mathbf{x}n,\mathbf{y}n,\mathbf{x}n)}$ if  $\tau > s_n$  then  $\mathbf{x}_n - = \mathbf{v}_n s_n$ sn = 0 $w_p \times = e^{-v\sigma_a(\mathbf{x}_p, \mathbf{v}_p, \mathbf{X}_p)s_p}$ #tally the contribution of particle p for  $k \in \{0, ..., P\}$  do  $u_k(\mathbf{x}, t, \mathbf{v}) + = w_p \times u_0(\mathbf{x}_p, \mathbf{v}_p, X_p) \phi_k(X_p)$ e nd e nd else  $\mathbf{x}_p - = \mathbf{v}_n \tau$  $w_p \times = e^{-v\sigma_a(\mathbf{x}_p, \mathbf{v}_p, \mathbf{X}_p)\tau}$  $\mathbf{v}_p = \mathbf{V}'$  with  $\mathbf{V}'$  sampled from  $P_s(\mathbf{x}_p, \mathbf{v}', \mathbf{v}_p, \mathbf{X}_p) d\mathbf{v}'$  $\#_{set}^{P}$  the life time of particle p to:  $s_n - = \tau$ e nd end end

 $\Rightarrow$  A converging MC scheme with simple modifications of an existing MC implementation [21]  $_{p.~16/35}$ 



Back to the previous convergence study with the new reduced model



 $\blacksquare$  With the new MC-gPC scheme:  $N_{MC}^{UQ}=N_{MC}^{N_{MC}^{UQ}}$  .

- The truncation order for this test-case is P = 1.
- The error e is now  $e = O\left(\frac{1}{\sqrt{N_{MC}}}\right)$  (for this test-pb at least!)

but surely depends also more thoroughly on P for other problems...

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$$\begin{cases} \partial_t u + v\omega \nabla_x u = -v\sigma_s(X)u + \int v\sigma_s(X)u \,\mathrm{d}\omega', \\ u(x,0,\mathbf{v}) = u_0(x) = \delta_1(x). \end{cases}$$

We assume  $X \sim \mathcal{U}([-1,1])$  with  $\sigma_s(X) = \overline{\sigma}_s + \hat{\sigma}_s X$  with  $\overline{\sigma}_s = 1$  and  $\hat{\sigma}_s = 0.99$ .



















Uncertain linear Boltzmann equation (with uncertain cross-section, no absorption)






























































### Comparisons MC-gPC vs. classical non-intrusive gPC [21] Monokinetic monodimensional (Q = 1) uncertain problem

For the results obtained with the MC-gPC solver:

- Non-intrusive gPC reference obtained for  $N_{MC} = 3.2 \times 10^8, N_{GL} = 4, P = 2.$
- taking  $N_{MC} = 3.2 \times 10^8, P = 2 \Longrightarrow$  perfect agreement with the reference.
- Performance considerations:
  - ni-gPC cost:  $N_{GL} \times$  averaged CPU time of 1 run  $\approx 4 \times 85.0s$ .
  - **\_** MC-gPC cost:  $1 \times \text{effective CPU time of the run} = 1 \times 86.6s.$
  - $\implies$  MC-gPC is  $\approx 4$  times faster than the non-intrusive application.



## Application to a sensitivity analysis problem Mean, variance and total Sobol indices

### Sobol's indices: powerful, reliable but costly tool for sensitivity analysis [16]



Sensitivity analysis test-problem in the following slide:

- A 3-D problem with uncertainties affecting  $\sigma_s,\sigma_t,\eta$ 

Sensitivity analysis in 3D stochastic dimension Case presentation

The configuration is the following:

Set-up:

 $\begin{array}{c} u_0(x, \omega, X) = 1 \\ \\ \\ Domain \ \mathcal{D} = [0, 1] \\ \\ X = (X_1, X_2, X_3) \ independent \ uniform \ on \ [-1, 1] \\ \\ \sigma_t(X) = \sigma_t(X_1) = \overline{\sigma}_t + \hat{\sigma}_t X_1 \\ \\ \sigma_s(X) = \sigma_t(X_2) = \overline{\sigma}_s + \hat{\sigma}_s X_2 \\ \\ \eta(X) = \eta(X_3) = \overline{\eta} + \hat{\eta} X_3 \\ \\ \eta(X) = \eta(X_3) = \overline{\eta} + \hat{\eta} X_3 \\ \\ \end{array}$  wall  $\begin{array}{c} \\ \\ \\ \\ \end{array}$ 

• The statistical outputs are the mean  $\mathbb{E}[U]$ , variance  $\mathbb{V}[U]$  and Sobol indices  $\mathbb{S}[U]$  profiles of  $U(x,t,X) = \int u(x,t,\omega,X) d\omega$  at time t = 1.0.

For this test-case, a non-intrusive gPC reference can still be obtained





Perfect agreement non-intrusive gPC vs. MC-gPC on every statistical observables <u>Few characteristics</u>:

ni-gPC : N<sup>Q</sup><sub>GL</sub> = 4<sup>3</sup> = 64 points with (P + 1)<sup>Q</sup> = (2 + 1)<sup>3</sup> = 27 coefficients.
 MC-gPC: (P + 1)<sup>Q</sup> = (2 + 1)<sup>3</sup> = 27 coefficients.

 $\implies$  same truncation order P ensures the same accuracy.

### Performance considerations:

- ni-gPC cost: N<sup>Q</sup><sub>GL</sub> = 4<sup>3</sup>×averaged CPU time of 1 run≈ 64 × 3min52s.
   MC-gPC cost: 1×effective CPU time of the run= 1 × 4min50s.
- $\implies$  It is  $\approx 50$  times faster than the non-intrusive application.
  - But the cost of a MC-gPC run is  $\approx 1.26 \times$  the cost of a non-intrusive one.
- $\implies$  Something to dig here? Additional cost comes from the *tallying phase* [21]

The tallying phase is the only one sensitive to the dimension Q.



- Spectral convergence as P grows of the gPC based reduced model in [22]
- Convergence with respect to N<sub>MC</sub> of the MC-gPC solver in [21] for fixed P (many other properties are studied in [21, 22])



- Spectral convergence as P grows of the gPC based reduced model in [22]
- Convergence with respect to N<sub>MC</sub> of the MC-gPC solver in [21] for fixed P (many other properties are studied in [21, 22])

Let us focus on performance considerations



- Spectral convergence as P grows of the gPC based reduced model in [22]
- Convergence with respect to N<sub>MC</sub> of the MC-gPC solver in [21] for fixed P (many other properties are studied in [21, 22])

MC-gPC (1 run/ $N_{MC}$  particles) vs. non-intrusive gPC (N runs/ $N_{MC}$  particles)



- Spectral convergence as P grows of the gPC based reduced model in [22]
- Convergence with respect to N<sub>MC</sub> of the MC-gPC solver in [21] for fixed P (many other properties are studied in [21, 22])

MC-gPC allows important gains in comparison to non-intrusive gPC (accelerations between  $\times 4$  to more that  $\times 50$ , see [21])



- Spectral convergence as P grows of the gPC based reduced model in [22]
- Convergence with respect to  $N_{MC}$  of the MC-gPC solver in [21] for fixed P (many other properties are studied in [21, 22])

But the linear Boltzmann equation is scarcely used as such (is MC-gPC still efficient on  $k_{\text{eff}}$  computations [28]? Coupled with nonlinear physics [24]?)



 $\blacksquare$  We are interested in taking into account uncertainties on  $k_{
m eff}$  , u such that

$$\begin{pmatrix} \mathbf{v} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \mathbf{v}) + v\sigma_t(\mathbf{x}, \mathbf{v}) u(\mathbf{x}, \mathbf{v}) = v\sigma_s(\mathbf{x}, \mathbf{v}) \int P_s(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}') u(\mathbf{x}, \mathbf{v}') d\mathbf{v}', \\ + \frac{v\nu_f(\mathbf{x}, \mathbf{v})\sigma_f(\mathbf{x}, \mathbf{v})}{k_{\text{eff}}} \int P_f(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}') u(\mathbf{x}, \mathbf{v}') d\mathbf{v}', \\ u(\mathbf{x}, \mathbf{v}) = u_b(\mathbf{v}), \quad \mathbf{x} \in \partial \mathcal{D}, \quad \frac{\mathbf{v}}{v} \cdot n_s < 0, \text{ with } |\mathbf{v}| = v. \end{cases}$$

$$(2)$$

The above equation can be more concisely rewritten as

$$\left(\begin{array}{c}
Lu = \frac{1}{k_{\text{eff}}}Fu, \\
Bu.
\end{array}\right)$$
(3)

 $\implies$  we are looking for u the fixed point of the above equation

lacksquare The power iteration method [5] consists in choosing the  $n^{th}$  iteration of the algorithm as

$$\begin{cases} Lu^{n} = \frac{1}{k_{\text{eff}}^{n-1}} Fu^{n-1}, \\ Bu^{n}, \end{cases} \text{ where } k_{\text{eff}}^{n} = k_{\text{eff}}^{n-1} \times \frac{\int_{\mathcal{D}} \int_{\mathcal{V}} u^{n}(\mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}}{\int_{\mathcal{D}} \int_{\mathcal{V}} u^{n-1}(\mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}}. \end{cases}$$
(4)

Asymptotically as  $n o \infty$ , the solution  $u^n pprox u^{n-1} pprox u^\infty$  solves (3).



lacksim We are interested in taking into account uncertainties on  $k_{ extsf{eff}}$  , u such that

$$\begin{aligned} \mathbf{v} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \mathbf{v}) + v\sigma_t(\mathbf{x}, \mathbf{v}) u(\mathbf{x}, \mathbf{v}) &= v\sigma_s(\mathbf{x}, \mathbf{v}) \int P_s(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}') u(\mathbf{x}, \mathbf{v}') d\mathbf{v}', \\ &+ \frac{v\nu_f(\mathbf{x}, \mathbf{v})\sigma_f(\mathbf{x}, \mathbf{v})}{k_{\text{eff}}} \int P_f(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}') u(\mathbf{x}, \mathbf{v}') d\mathbf{v}', \\ \mathbf{v}(\mathbf{x}, \mathbf{v}) &= u_b(\mathbf{v}), \quad \mathbf{x} \in \partial \mathcal{D}, \quad \frac{\mathbf{v}}{v} \cdot n_s < 0, \text{ with } |\mathbf{v}| = v. \end{aligned}$$

$$(2)$$

The above equation can be more concisely rewritten as

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Lu = \frac{1}{k_{\text{eff}}}Fu, \\
Bu.
\end{array}\right)$$
(3)

 $\implies$  we are looking for u the fixed point of the above equation

Modified power iteration method [28]:

$$\begin{aligned} \partial_t u^n + L u^n &= \frac{1}{k_{\text{eff}}^{n-1}} F u^n, \\ u_0 &= u^{n-1}, \\ B u^n, \end{aligned} \qquad \text{where } k_{\text{eff}}^n = k_{\text{eff}}^{n-1} \times \frac{\int_{\mathcal{D}} \int_{\mathcal{V}} u(\mathbf{x}, t^n, \mathbf{v}) d\mathbf{x} d\mathbf{v}}{\int_{\mathcal{D}} \int_{\mathcal{V}} u(\mathbf{x}, t^{n-1}, \mathbf{v}) d\mathbf{x} d\mathbf{v}}. \end{aligned}$$
(4)

Asymptotically as  $n \times \Delta t \to \infty$ , the solution  $u^n \approx u^{n-1} \approx u^\infty$  solves (3).



Modified power iteration method [28] with uncertainties:

 $\left\{ \begin{array}{l} \partial_t u^n + L^X u^n = \frac{1}{k_{\mathrm{eff}}^{n-1}} F^X u^n, \\ u_0 = u^{n-1}, \\ B^X u^n, \end{array} \right. \text{, } k_{\mathrm{eff}}^n(X) = k_{\mathrm{eff}}^{n-1}(X) \times \frac{\int \int u(\mathbf{x}, t^n, \mathbf{v}, X) \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v}}{\int \int u(\mathbf{x}, t^{n-1}, \mathbf{v}, X) \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v}}. \end{array}$ 

Asymptotically as  $n \times \Delta t \to \infty$ , the solution  $u^n \approx u^{n-1} \approx u^\infty$  solves (3).

Need for additional numerical tools (stochastic power iteration):

- The blue part is solved by application of MC-gPC at every iterations
- The red part remains to be discretized



Modified power iteration method [28] with uncertainties:

$$\begin{array}{l} \partial_t u^n + L^X u^n = \frac{1}{k_{\text{eff}}^{n-1}} F^X u^n, \\ u_0 = u^{n-1}, \\ B^X u^n, \end{array} , \ k_{\text{eff}}^{\text{new},k} = \int k_{\text{eff}}^{\text{old},P}(X) \frac{\iint u^P(\mathbf{x},t^n,\mathbf{v},X) \mathrm{d} \mathbf{x} \mathrm{d} \mathbf{v}}{\iint u^P(\mathbf{x},t^{n-1},\mathbf{v},X) \mathrm{d} \mathbf{x} \mathrm{d} \mathbf{v}} \phi_k(X) \mathrm{d} \mathcal{P}_X \\ \end{array}$$

Asymptotically as  $n \times \Delta t \to \infty$ , the solution  $u^n \approx u^{n-1} \approx u^\infty$  solves (3).

Need for additional numerical tools (stochastic power iteration):

- The blue part is solved by application of MC-gPC at every iterations
- The red part is remapped onto the gPC basis

# The stochastic power iteration with MC-gPC, [28] (main sketch)

#### begin

```
#initialisation of a population of particles
list of particles=sampleUncertainParticles(NMC)
set U_{old}^0 = 1
set U_{\text{new}}^0 = 1
set k_{\text{eff}}^0 = 1
for k \in \{1, \ldots, P\} do
          U_{\text{old}}^{\hat{k}} = 0
         U_{new}^k = 0
k_{eff}^k = 1
end
while iter < iter max do
          #Apply \overline{MC}-gPC during time step [t^n, t^n + \Delta t]
          (U_{\mathsf{new}}^k)_{k \in \{0, \dots, P\}} = \mathsf{trackUncertainParticlesWithMC-gPC(list_of_particles, \Delta t, k_{\mathsf{eff}}^0, \dots, k_{\mathsf{eff}}^P)
          #build punctual uncertain values
         (U_{\mathsf{new}}^P(X_g))_{g \in \{1,...,N_G\}} = \mathsf{buildPunctualValues}((X_g)_{g \in \{1,...,N_G\}}, (U_{\mathsf{new}}^k)_{k \in \{0,...P\}})
         (U_{\mathsf{old}}^P(X_g))_{q \in \{1,..,N_G\}} = \mathsf{buildPunctualValues}((X_g)_{g \in \{1,..,N_G\}}, (U_{\mathsf{old}}^k)_{k \in \{0,..,P\}})
         (k_{\text{eff}}^P(X_g))_{g \in \{1,...,N_G\}} = \text{buildPunctualValues}((X_g)_{g \in \{1,...,N_G\}}, (k_{\text{eff}}^k)_{k \in \{0,...,P\}})
         #update the gPC coefficients of the eigenvalue
         for k \in \{0, ..., P\} do
                   k_{\text{eff}}^{k} \leftarrow \sum_{k}^{N_{G}} k_{\text{eff}}^{P}(X_{g}) \times \frac{U_{\text{new}}^{P}(X_{g})}{U_{\text{rul}}^{P}(X_{g})} \phi_{k}(X_{g}) w_{g} 
         e nd
          #update the old number of physical particles
         for k \in \{0, ..., P\} do
                   U_{\text{old}}^{\hat{k}} \leftarrow U_{\text{new}}^{k}
          e nd
          iter++
```

end



 $\Rightarrow$  Gains of more than a factor imes 10 with respect to ni-gPC on these benchmarks [28]

In this section, we would like to take few lines to discuss about what intrusive uncertainty propagation codes (independently of the physics of interest) can bring:

- previous test-cases: we saw situations in which intrusiveness is worth it (from  $\times 2$  to  $\times 40$  computational gains)
- Still, intrusiveness can be more or less costly in terms of development (even if the modifications are simple, the verification always takes time)

Having these points in mind, we would like to show that:

- hybrid non-intrusive/intrusive simulations are at hand as soon as an intrusive code is available
- These hybrid computations are competitive w.r.t. a full non-intrusive simulation.



- Back to the previous 3D problem with the new reduced model
- Assume that the developments are ready in order to take into account
  - **\_** the uncertainties on  $\sigma_t(X_1), \sigma_s(X_2),$
  - but not yet the uncertainties on  $\eta(X_3)$ .
- Then we can quite easily
  - $\blacksquare$  run the MC-gPC solver to propagate the uncertainties with respect to  $X_1, X_2$
  - several times, for several values of  $(X_3^i, w_i)_{i \in \{1,...,N\}} \sim (X_3, d\mathcal{P}_{X_3})$ .
- To know how in details see [26]

(intensive use of the orthonormality property of the  $(\phi_k)_{k \in \{0,...,P\}}$ )

## The previous homogeneous uncertain configuration Back to the 3D problem

Comparisons of the mean and variance MC-gPC vs. hybrid ni-gPC /MC-gPC => excellent agreement!



- Motivations and objectives + the skeleton of an MC code
- Non-intrusive applications and drawbacks in an MC context
- Intrusive reduced modeling (sometimes, it is worth it)

### 4 Few simple test-cases

- Comparisons, performance considerations
- MC-gPC for k<sub>eff</sub> computations (work with E. Brun [28])
- Hybrid intrusive/non-intrusive computations

### 5 Conclusion

### The MC-gPC solver for the uncertain transport equation Summary

See also (things I do not have time to detail):

- Spectral convergence w.r.t. P of the gPC reduced models in [22] (fast convergence of the solution of the reduced model  $u^P \xrightarrow[P \to \infty]{} u$ )
- Convergence of the MC-gPC scheme in [21] (design of converging numerical schemes such that  $u^P_{N_{MC} \ N_{MC} \rightarrow \infty} u^P$ ) (only simple modifications of an existing MC code are necessary) (Test-cases up to 6D stochastic dimensions)
- Applications to k<sub>eff</sub> computations in neutronics [28] (design of a stochastic eigenvalue/eigenvector solver based on the material of this talk)
- Applications to stiff nonlinear photonic problems [24] (proof of the wellposedness of the gPC based reduced model)
- Study of the numerical MC noise on the gPC coefficients [25] (MC noise comparisons MC-gPC vs. non-intrusive gPC on the coefficients)
- Improvements of MC-gPC [27]

(design of a new multigroup MC scheme for the gPC reduced model) (less noisy, less sensitive to the curse of dimensionality but also less simple... ×4 faster than MC-gPC) (+ some efficient hybrid intrusive/non-intrusive applications)

### Question?

Commissariat à l'Énergie Atomique et aux Énergies Alternatives CEA/DAM/DIF, F-91297, Arpajon

T. +33 (0)1 69 28 40 00







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# **6** Some uncertain photonic applications: MC-gPC combined to ISMC

7 Uncertain analytical solution and convergence study

8 A 6-D uncertain problem with sensitivity analysis

9 Verification of the theorem and (non-)optimality

🔟 A beautiful animation



 $\blacksquare$  We are interested in taking into account uncertainties on I, E solutions of

$$\begin{aligned} \frac{1}{c} \partial_t I(x,t,\omega,X) + \omega \cdot \nabla I(x,t,\omega,X) + \sigma_t(E(x,t,X),X)I(x,t,\omega,X) \\ &= \sigma_a(E(x,t,X),X)B(E(x,t,X)) + \sigma_s(E(x,t,X),X) \int I(x,t,\omega',X) \mathrm{d}\omega', \\ \partial_t E(x,t,X) &= c\sigma_a(E(x,t,X),X) \int \left(I(x,t,\omega',X) - B(E(x,t,X))\right) \mathrm{d}\omega', \\ X \sim \mathrm{d}\mathcal{P}_X. \end{aligned}$$
(5)

Need for additional theoretical material (for wellposedness), see [24].

lacksquare Uncertain photonics with uncertain  $\sigma_a, C_v$ 



Gain  $\times 20$  for this problem, see [24]

### Some uncertain photonic applications: MC-gPC combined to ISMC

# 7 Uncertain analytical solution and convergence study

### 8 A 6-D uncertain problem with sensitivity analysis

## 9 Verification of the theorem and (non-)optimality

### 🔟 A beautiful animation

A homogeneous uncertain configuration Analytical solution for statistical observables



Convergence studies w.r.t. the # of points of the experimental design N:



(6)

- 6 Some uncertain photonic applications: MC-gPC combined to ISMC
- 7 Uncertain analytical solution and convergence study

## 8 A 6-D uncertain problem with sensitivity analysis

- g Verification of the theorem and (non-)optimality
- 🔟 A beautiful animation

A two layered uncertain material: sensitivity analysis in 6D Case presentation

The configuration is the following:

- Similar three first points (v = 1,...)
- The material is composed of two layers of different media, A and B with  $\mathcal{D}_A = [0, \frac{1}{2}]$  and  $\mathcal{D}_B = [\frac{1}{2}, 1]$  such that  $\mathcal{D}_A \cup \mathcal{D}_B = \mathcal{D} = [0, 1]$ .
- Both media are pure, homogeneous and considered uncertain.
- Each depends on three parameters  $(X^i)_{i \in \{A,B\}} = (X_1^i, X_2^i, X_3^i)_{i \in \{A,B\}}$  with

$$\begin{aligned} \sigma_t(x,t,X) &= \sum_{i \in \{A,B\}} \left[ \overline{\sigma}_t^i + \widehat{\sigma}_t^i X_1^i \right] \mathbf{1}_{\mathcal{D}_i}(x), \quad \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \\ \sigma_s(x,t,\omega,\omega',X) &= \sum_{i \in \{A,B\}} \left[ \overline{\sigma}_s^i + \widehat{\sigma}_s^i X_2^i \right] \mathbf{1}_{\mathcal{D}_i}(x), \quad \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \\ \eta(x,t,X) &= \sum_{i \in \{A,B\}} \left[ \overline{\eta}^i + \widehat{\eta}^i X_3^i \right] \mathbf{1}_{\mathcal{D}_i}(x), \quad \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \end{aligned}$$
(7)

- $\label{eq:constraint} \blacksquare \ (X_1^i, X_2^i, X_3^i)_{i \in \{A,B\}} \text{ are independent uniformly distributed RVs on } [-1,1].$
- For the next computations, the mean quantities are set to  $\overline{\sigma}_t^A = 1.0, \ \overline{\sigma}_s^A = 1.3, \ \overline{\eta}^A = 1.0, \qquad \widehat{\sigma}_t^A = 0.4, \ \widehat{\sigma}_s^A = 0.4, \ \widehat{\eta}^A = 0.4, \ \overline{\sigma}_t^B = 1.0, \ \overline{\sigma}_t^B = 0.4, \ \widehat{\sigma}_s^B = 0.4, \ \widehat{\eta}^B = 0.4, \$

■ Statistical observables: mean, variance, Sobol indices as before For this test-case, a non-intrusive gPC reference **is too costly** 

p. 27/35

A two layered uncertain material: sensitivity analysis in 6D Mean, variance and setting of the problem



■ Run  $1.024 \times 10^9$  particles,  $(P + 1)^6 = 729$  on 1024 proc. in 750s.

■ ni-gPC would need, same accuracies and restitution times, 131072 proc. New problem: suppose now we want the variance to be lesser that  $0.05 \forall x \in D$ 

- → How should we work on the uncertain parameters?
- → On which ones?
- → Of how much should we reduce their respective uncertainties?

A two layered uncertain material: sensitivity analysis in 6D Total and first order Sobol indices



p. 29/35



Answer to the problem:

Enough reducing the uncertainties on  $X_1, X_2$  of only a factor 3.

 $\implies$  the study has been made possible by the new scheme.

- 6 Some uncertain photonic applications: MC-gPC combined to ISMC
- 7 Uncertain analytical solution and convergence study
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Back to the previous convergence study with the new reduced model w.r.t. P:



Spectral convergence is recovered also in practice (youpi!)

- The previous mathematical analysis is probably not optimal (we here obtain even faster convergence rates!)
- This is encouraging once an MC discretization will be introduced.



Back to the previous convergence study with the new reduced model w.r.t. P:



Spectral convergence is recovered also in practice (youpi!)

- The previous mathematical analysis is probably not optimal (we here obtain even faster convergence rates!)
- This is encouraging once an MC discretization will be introduced.

22 The previous homogeneous uncertain configuration Back to the analytical solution for statistical observables (variance)

### Spectral convergence w.r.t. P and MC resolution:



■ Spectral convergence is recovered also in practice ∀ times of interest T
 ■ The gPC accuracy is below the MC error for relatively small P

- 6 Some uncertain photonic applications: MC-gPC combined to ISMC
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