Building and solving reduced models for the uncertain linear Boltzmann equation<br>(sometimes, intrusiveness is worth it)<br>Gaël Poëtte ${ }^{\dagger}$<br>$\dagger$ CEA, CESTA, DAM<br>F-33114 Le Barp, France

1 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)

44 Few simple test-cases

- Comparisons, performance considerations
- MC-gPC for $k_{\text {eff }}$ computations (work with E. Brun [28])
- Hybrid intrusive/non-intrusive computations

5 Conclusion

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## Motivations (and few notations) A very general class of problem

We are interested in the resolution of the linear Boltzmann equation

$$
\begin{aligned}
\partial_{t} u(\mathbf{x}, t, \mathbf{v})+\mathbf{v} \cdot \nabla u(\mathbf{x}, t, \mathbf{v})= & -v \sigma_{t}(\mathbf{x}, \mathbf{v}) u(\mathbf{x}, t, \mathbf{v}) \\
& +\int v \sigma_{s}\left(\mathbf{x}, \mathbf{v}, \mathbf{v}^{\prime}\right) u\left(\mathbf{x}, t, \mathbf{v}^{\prime}\right) \mathrm{d} \mathbf{v}^{\prime}
\end{aligned}
$$

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 $\left(t^{*}\right): U\left(\mathbf{x}, t^{*}\right)=\int u\left(\mathbf{x}, t^{*}, \mathbf{v}\right) \mathrm{d} \mathbf{v}$.

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 $\left(\sigma_{\alpha}\right)_{\alpha \in\{s, t\}}, u_{0}$, boundary conditions etc.
- We model them thanks to random variables of probability measure $X \sim \mathrm{~d} \mathcal{P}_{X}$
$\Longrightarrow$ We need to solve a stochastic PDE in order to propagate uncertainties

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

$$
\begin{aligned}
\partial_{t} u(\mathbf{x}, t, \mathbf{v}, X)+\mathbf{v} \cdot \nabla u(\mathbf{x}, & t, \mathbf{v}, X)+v \sigma_{t}(\mathbf{x}, \mathbf{v}, X) u(\mathbf{x}, t, \mathbf{v}, X) \\
& =\int v \sigma_{s}\left(\mathbf{x}, \mathbf{v}, \mathbf{v}^{\prime}, X\right) u\left(\mathbf{x}, t, \mathbf{v}^{\prime}, X\right) \mathrm{d} \mathbf{v}^{\prime}
\end{aligned}
$$

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

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

Now, in general, for our application, an MC scheme is used General properties of MC resolutions

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

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

(Central Limit theorem, see Lapeyre-Pardoux-Sentis [17]).
$\square$ We will abusively but concisely write the error is $e_{N_{M C}}=\mathcal{O}\left(\frac{1}{\sqrt{N_{M C}}}\right)$.

- The performance of the MC schemes can be studied by analyzing $\sigma_{\mathrm{Mc}}$.

■ Several schemes: analog, non-analog, with variance reduction technics...

## 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 \(p \in\left\{1, \ldots, N_{M C}\right\}\) do
    set \(s_{p}=t\) \#this will be the life time of particle \(p\)
    set \(\mathbf{x}_{p}=\mathbf{x}\)
    set \(\mathbf{v}_{p}=\mathbf{v}\)
    set \(w_{p}=\frac{1}{N_{M C}}\)
    while \(s_{p}>0\) and \(w_{p}>0\) do
        Sample \(\tau\) by inversing the cdf of an exponential law \(\tau=-\frac{\ln (\mathcal{U}([0,1]))}{v_{p} \sigma_{s}\left(\mathbf{x}_{p}, \mathbf{v}_{p}\right)}\)
        if \(\tau>s_{p}\) 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
            \(w_{p} \times=e^{-v \sigma_{a}\left(\mathbf{x}_{p}, \mathbf{v}_{p}\right) s_{p}}\)
        \#tally the contribution of particle \(p\)
        \(u(\mathbf{x}, t, \mathbf{v})+=w_{p} \times u_{0}\left(\mathbf{x}_{p}, \mathbf{v}_{p}\right)\)
            end
            else
            \#move the particle \(p\)
            \(\mathbf{x}_{p}-=\mathbf{v}_{p} \tau\),
            \#change the weight of the particle
            \(w_{p} \times=e^{-v \sigma_{a}\left(\mathbf{x}_{p}, \mathbf{v}_{p}\right) \tau}\)
                            Sample the velocity \(\mathbf{V}^{\prime}\) sampled from \(P_{S}\left(\mathbf{x}_{p}, \mathbf{v}^{\prime}, \mathbf{v}_{p}\right) \mathrm{d} \mathbf{v}^{\prime}\)
                            \(\mathbf{v}_{p}=\mathbf{V}^{\prime}\)
                            \#set the life time of particle \(p\) to:
                    \(s_{p}-=\tau\)
            end
    end
end
```

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11 is an arbitrary random variable of probability measure $\mathrm{d} \mathcal{P}_{X}$.
2 Discretization of $\left(X, \mathrm{~d} \mathcal{P}_{X}\right)$ by a quadrature with $N$ points $\left(X_{i}, w_{i}\right)_{i \in\{1, \ldots, N\}}$.
B $N$ independent solutions at points $\left(X_{i}, w_{i}\right)$ :

$$
\left(u\left(\mathbf{x}, t, \mathbf{v}, X_{i}\right), w_{i}\right)_{i \in\{1, \ldots, N\}}, \text { solutions of your favorite problem }
$$

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

$$
\begin{aligned}
\mathbb{E}[U](\mathbf{x}, t) & =\iint u(\mathbf{x}, t, \mathbf{v}, X) \mathrm{d} \mathbf{v d} \mathcal{P}_{X}, \\
\mathbb{E}\left[U^{2}\right](\mathbf{x}, t) & =\int\left(\int u(\mathbf{x}, t, \mathbf{v}, X) \mathrm{d} \mathbf{v}\right)^{2} \mathrm{~d} \mathcal{P}_{X}, \\
\mathbb{V}[U](\mathbf{x}, t) & =\mathbb{E}\left[U^{2}\right](\mathbf{x}, t)-(\mathbb{E}[U](\mathbf{x}, t))^{2}, \\
\ldots & =\ldots
\end{aligned}
$$

[5 Other examples of interesting statistical quantities will be given later

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$$
\begin{aligned}
\mathbb{E}[U](\mathbf{x}, t) & =\sum_{k=1}^{N} w_{i} U\left(\mathbf{x}, t, X_{i}\right)+\mathcal{O}\left(N^{\beta}\right) \\
\mathbb{E}\left[U^{2}\right](\mathbf{x}, t) & =\sum_{k=1}^{N} w_{i} U^{2}\left(\mathbf{x}, t, X_{i}\right)+\mathcal{O}\left(N^{\beta}\right) \\
\mathbb{V}[U](\mathbf{x}, t) & =\mathbb{E}\left[U_{N}^{2}\right](\mathbf{x}, t)-\left(\mathbb{E}\left[U_{N}\right](\mathbf{x}, t)\right)^{2}+\mathcal{O}\left(N^{\beta}\right) \\
\ldots & =\ldots
\end{aligned}
$$

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$11 X$ is an arbitrary random variable of probability measure $\mathrm{d} \mathcal{P}_{X}$.
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${ }^{3} N$ independent runs of a black box code at points $\left(X_{i}, w_{i}\right)$ :

$$
\left(u_{\Delta}\left(\mathbf{x}, t, \mathbf{v}, X_{i}\right), w_{i}\right)_{i \in\{1, \ldots, N\}}, \text { approximations } u_{\Delta}=u+\mathcal{O}(\Delta)
$$

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

$$
\begin{aligned}
\mathbb{E}[U](\mathbf{x}, t) & =\sum_{k=1}^{N} w_{i} U_{\Delta}\left(\mathbf{x}, t, X_{i}\right)+\mathcal{O}\left(N^{\beta}\right)+\mathcal{O}(\Delta) \\
\mathbb{E}\left[U^{2}\right](\mathbf{x}, t) & =\sum_{k=1}^{N} w_{i} U_{\Delta}^{2}\left(\mathbf{x}, t, X_{i}\right)+\mathcal{O}\left(N^{\beta}\right)+\mathcal{O}(\Delta) \\
\mathbb{V}[U](\mathbf{x}, t) & =\mathbb{E}\left[U_{N, \Delta}^{2}\right](\mathbf{x}, t)-\left(\mathbb{E}\left[U_{N, \Delta}\right](\mathbf{x}, t)\right)^{2}+\mathcal{O}\left(N^{\beta}\right)+\mathcal{O}(\Delta), \\
\ldots & =\ldots
\end{aligned}
$$

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

$$
e_{\Delta}^{N}=\underbrace{\mathcal{O}(\Delta)}_{\text {deterministic solver }}+\underbrace{\mathcal{O}\left(N^{\beta}\right)}_{\text {uncertainty integration }}
$$

- 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:
$\Delta=\Delta t, N^{\beta}=\frac{1}{\sqrt{2 \pi N_{G L}}}\left(\frac{e}{N_{G L}}\right)^{N_{G L}}$

$\Delta=\frac{1}{\sqrt{N_{M C}}}, N^{\beta}=\frac{1}{\sqrt{N_{M C}^{U Q}}}$


Interpretation of the previous non-intrusive results (using an MC scheme for the deterministic resolution)

- When running $N$ times the MC code: MC particles for ( $\mathbf{x}, t, \mathbf{v}$ ) and the experimental design for $X$ are tensorised.

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

- MC methods are integration methods supposed to avoid such tensorisation!
(Is it possible to have only $N_{M C}$ for the whole set of variables $(\mathbf{x}, t, \mathbf{v}, X)$ ?)
- Main difficulty: as always, finding the relevant linearisation $\Longrightarrow$ example of the equation satisfied by the second order moment


## Equation satisfied by the second moment

 The need for a relevant linearisation- The simplest statistical observable is the variance:

$$
\mathbb{V}[u](\mathbf{x}, t, \mathbf{v})=M_{2}(\mathbf{x}, t, \mathbf{v})-M_{1}^{2}(\mathbf{x}, t, \mathbf{v}) \text { with }
$$

$$
M_{2}(\mathbf{x}, t, \mathbf{v})=\int u^{2}(\mathbf{x}, t, \mathbf{v}, X) \mathrm{d} \mathcal{P}_{X}=\int m_{2}(\mathbf{x}, t, \mathbf{v}, X) \mathrm{d} \mathcal{P}_{X} .
$$

■ The equation satisfied by $u$ is

$$
\begin{aligned}
& \partial_{t} u(\mathbf{x}, t, \mathbf{v}, X)+\mathbf{v} \cdot \nabla u(\mathbf{x}, t, \mathbf{v}, X)=-v \sigma_{t}(\mathbf{x}, \mathbf{v}, X) u(\mathbf{x}, t, \mathbf{v}, X) \\
&+\int v \sigma_{s}\left(\mathbf{x}, \mathbf{v}, \mathbf{v}^{\prime}, X\right) u\left(\mathbf{x}, t, \mathbf{v}^{\prime}, X\right) \mathrm{d} \mathbf{v}^{\prime}
\end{aligned}
$$

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

- Let us multiply the transport equation by $u$ to obtain

$$
\begin{aligned}
& \partial_{t} \frac{u^{2}}{2}(\mathbf{x}, t, \mathbf{v}, X)+\mathbf{v} \cdot \nabla \frac{u^{2}}{2}(\mathbf{x}, t, \mathbf{v}, X)=-v \sigma_{t}(\mathbf{x}, \mathbf{v}, X) u^{2}(\mathbf{x}, t, \mathbf{v}, X) \\
&+u(\mathbf{x}, t, \mathbf{v}, X) \int v \sigma_{s}\left(\mathbf{x}, \mathbf{v}, \mathbf{v}^{\prime}, X\right) u\left(\mathbf{x}, t, \mathbf{v}^{\prime}, X\right) \mathrm{d}^{\prime}
\end{aligned}
$$

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

$$
\begin{aligned}
\partial_{t} m_{2}(\mathbf{x}, t, \mathbf{v}, X)+\mathbf{v} \cdot \nabla & m_{2}(\mathbf{x}, t, \mathbf{v}, X)=-2 v \sigma_{t}(\mathbf{x}, \mathbf{v}, X) m_{2}(\mathbf{x}, t, \mathbf{v}, X) \\
+ & 2 u(\mathbf{x}, t, \mathbf{v}, X) \int v \sigma_{s}\left(\mathbf{x}, \mathbf{v}, \mathbf{v}^{\prime}, X\right) u\left(\mathbf{x}, t, \mathbf{v}^{\prime}, X\right) \mathrm{d} \mathbf{v}^{\prime}
\end{aligned}
$$

which is nonlinear in general (i.e. if $\sigma_{s} \neq 0$ ).

■ Nonlinearity demands a splitting/linearisation hypothesis.

$$
\begin{aligned}
\partial_{t} m_{2}(\mathbf{x}, t, \mathbf{v}, X)+\mathbf{v} \cdot \nabla & m_{2}(\mathbf{x}, t, \mathbf{v}, X)=-2 v \sigma_{t}(\mathbf{x}, \mathbf{v}, X) m_{2}(\mathbf{x}, t, \mathbf{v}, X) \\
+ & 2 u(\mathbf{x}, t, \mathbf{v}, X) \int v \sigma_{s}\left(\mathbf{x}, \mathbf{v}, \mathbf{v}^{\prime}, X\right) u\left(\mathbf{x}, t, \mathbf{v}^{\prime}, X\right) \mathrm{d}^{\prime}
\end{aligned}
$$

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] ( $\mathcal{O}(\Delta t)$ 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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+ & 2 u(\mathbf{x}, t, \mathbf{v}, X) \int v \sigma_{s}\left(\mathbf{x}, \mathbf{v}, \mathbf{v}^{\prime}, X\right) u\left(\mathbf{x}, t, \mathbf{v}^{\prime}, X\right) \mathbf{d}^{\prime}
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- 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.
$\Longrightarrow$ 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 $\mathrm{d} \mathcal{P}_{X}(x)$, $\left(\phi_{k}\right)_{k \in \mathbb{N}}$ is the basis of orthonormal polynomials with respect to $\mathrm{d} \mathcal{P}_{X}(x)$ Let $u(X)$ be an unknown random variable with $\int u^{2}(X) \mathrm{d} \mathcal{P}_{X}<\infty$,
then $u_{P}(X)=\sum_{k=0}^{P} u_{k} \phi_{k}(X) \underset{P \rightarrow \infty}{\stackrel{L^{2}}{\longrightarrow}} u(X)$, where $u_{k}=\int u(X) \phi_{k}(X) \mathrm{d} \mathcal{P}_{X}$.

- Idea: compute the coefficients $\left(u_{k}\right)_{k \in\{0, \ldots, P\}}$ 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?

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

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

■ Let us plug $u^{P}$ in the transport equation and perform a Galerkin projection to get

$$
\begin{array}{ll}
\partial_{t} u_{0}+\mathbf{v} \cdot \nabla_{\mathbf{x}} u_{0} & =-v \int\left(\sigma_{t} \sum_{k \leq P} u_{k} \phi_{k}\right) \phi_{0} \mathrm{~d} \mathcal{P}_{X}+v \iint\left(\left(\sigma_{s} \sum_{k \leq P} u_{k} \phi_{k}\right) \phi_{0} \mathrm{~d} \mathcal{P}_{X}\right) \\
& \ldots \\
\partial_{t} u_{P}+\mathbf{v} \cdot \nabla_{\mathbf{x}} u_{P} & =-v \int\left(\sigma_{t} \sum_{k \leq P} u_{k} \phi_{k}\right) \phi_{P} \mathrm{~d} \mathcal{P}_{X}+v \iint\left(\left(\sigma_{s} \sum_{k \leq P} u_{k} \phi_{k}\right) \phi_{P} \mathrm{~d} \mathcal{P}_{X}\right)
\end{array}
$$

■ The reduced model is still linear $\Longrightarrow$ it can be solved by an MC scheme.
■ In fact, it can be solved by slightly modifying an already existing MC code [21]. Spectral convergence with respect to $P$

In [22], proof of spectral convergence as $P \rightarrow \infty$ for the gPC reduced model:
■ Let us defined the gPC developpement $u^{P}=\sum_{q=0}^{P} u_{q} \phi_{q}$ with $u_{q}=\int u \phi_{q} \mathrm{~d} \mathcal{P}_{X}$.
■ Define the space of functions

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

- Assume bounds on the cross-sections

$$
\begin{equation*}
\left\|v \sigma_{t}\right\|_{L^{\infty}(\mathcal{I} \times \Theta)}=\Sigma_{t}<\infty, \quad\left\|v \sigma_{s}\right\|_{L^{\infty}(\mathcal{I} \times \Theta)}=\Sigma_{s}<\infty \tag{1}
\end{equation*}
$$

## 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 $\forall t \in[0, T]$
$\left\|u(t)-u^{P}(t)\right\|_{L^{2}(\mathcal{I}, \Theta)}^{2} \leq e^{2\left(\Sigma_{t}+\Sigma_{s}\right) t}\left(\left\|u_{0}-u_{0}^{P}\right\|_{L^{2}(\mathcal{I}, \Theta)}^{2}+2\left(\Sigma_{s}+\Sigma_{t}\right) t\left\|u_{0}^{2}\right\|_{L^{2}(\mathcal{I}, \Theta)} \frac{D_{k}}{P_{\text {p. 15/35 }}^{k}}\right)$.

```
for }k\in{0,\ldots,P} d
| set }\mp@subsup{u}{k}{}(\mathbf{x},t,\mathbf{v})=
end
for p\in{1,\ldots,N}\mp@subsup{N}{MC}{}}\mathrm{ do
    set }\mp@subsup{s}{p}{}=t\mathrm{ #this will be the remaining life time of particle p, it must go down to zero (backward)
    set }\mp@subsup{\mathbf{x}}{p}{}=\mathbf{x
    set }\mp@subsup{\mathbf{v}}{p}{}=\mathbf{v
    set w
    set }\mp@subsup{X}{p}{}=X\mathrm{ with }X\mathrm{ sampled from the probability measure d}\mp@subsup{\mathcal{P}}{X}{}\mathrm{ .
    while }\mp@subsup{s}{p}{}>0\mathrm{ and }\mp@subsup{w}{p}{}>0\mathrm{ do
        Sample \tau by inversing the cdf of an exponential law }\tau=-\frac{\operatorname{ln}(\mathcal{U}([0,1]))}{v\mp@subsup{\sigma}{S}{}(\mp@subsup{\mathbf{x}}{p}{},\mp@subsup{\mathbf{v}}{p}{},\mp@subsup{X}{p}{})
        if }\tau>\mp@subsup{s}{p}{}\mathrm{ then
            \mp@subsup{x}{p}{}
            sp}=
        wp}\times=\mp@subsup{e}{}{-v\mp@subsup{\sigma}{a}{}(\mp@subsup{\mathbf{x}}{p}{},\mp@subsup{\mathbf{v}}{p}{},\mp@subsup{X}{p}{})\mp@subsup{s}{p}{}
        #tally the contribution of particle p
        for }k\in{0,\ldots,P}\mathrm{ do
            uk
    end
        end
        else
            \mp@subsup{x}{p}{}-=}=\mp@subsup{\mathbf{v}}{p}{}\tau
            wp}\times=\mp@subsup{e}{}{-v\mp@subsup{\sigma}{a}{}(\mp@subsup{\mathbf{x}}{p}{},\mp@subsup{\mathbf{v}}{p}{},\mp@subsup{X}{p}{})\tau
            \mp@subsup{v}{p}{}}=\mp@subsup{\mathbf{V}}{}{\prime}\mathrm{ with }\mp@subsup{\mathbf{V}}{}{\prime}\mathrm{ sampled from }\mp@subsup{P}{S}{}(\mp@subsup{\mathbf{x}}{p}{},\mp@subsup{\mathbf{v}}{}{\prime},\mp@subsup{\mathbf{v}}{p}{},\mp@subsup{X}{p}{})\textrm{d}\mp@subsup{\mathbf{v}}{}{\prime
            #set the life time of particle p to:
            sp
        end
    end
end
```

$\Longrightarrow$ A converging MC scheme with simple modifications of an existing MC implementation [21]

- Back to the previous convergence study with the new reduced model

- With the new MC-gPC scheme: $N_{M C}^{U Q}=N_{M C}^{N_{N G}^{U Q}}$.
- The truncation order for this test-case is $P=1$.
- The error $e$ is now $e=\mathcal{O}\left(\frac{1}{\sqrt{N_{M C}}}\right)$ (for this test-pb at least!)
$\Longrightarrow$ but surely depends also more thoroughly on $P$ for other problems...

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$$
\left\{\begin{array}{l}
\partial_{t} u+v \omega \nabla_{x} u=-v \sigma_{s}(X) u+\int v \sigma_{s}(X) u \mathrm{~d} \omega^{\prime} \\
u(x, 0, \mathbf{v})=u_{0}(x)=\delta_{1}(x) .
\end{array}\right.
$$

We assume $X \sim \mathcal{U}([-1,1])$ with $\sigma_{s}(X)=\bar{\sigma}_{s}+\hat{\sigma}_{s} X$ with $\bar{\sigma}_{s}=1$ and $\hat{\sigma}_{s}=0.99$.
Mean and variance of $U(x, t=0 ., X)$


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





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









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


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






 Monokinetic monodimensional $(Q=1)$ uncertain problem

For the results obtained with the MC-gPC solver:
■ Non-intrusive gPC reference obtained for $N_{M C}=3.2 \times 10^{8}, N_{G L}=4, P=2$.

- taking $N_{M C}=3.2 \times 10^{8}, P=2 \Longrightarrow$ perfect agreement with the reference.

■ Performance considerations:
$=$ ni-gPC cost: $\quad N_{G L} \times$ averaged CPU time of $1 \quad$ run $\approx 4 \times 85.0 \mathrm{~s}$.
$=$ MC-gPC cost: $\quad 1 \times$ effective CPU time of the run $=1 \times 86.6 s$.
$\Longrightarrow \mathrm{MC}-\mathrm{gPC}$ is $\approx 4$ times faster than the non-intrusive application.


$$
\mathbb{V}[U](x, t=0.5)
$$



- 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 $\sigma_{s}, \sigma_{t}, \eta$

The configuration is the following:

- Set-up:

- The statistical outputs are the mean $\mathbb{E}[U]$, variance $\mathbb{V}[U]$ and Sobol indices $\mathbb{S}[U]$ profiles of $U(x, t, X)=\int u(x, t, \omega, X) \mathrm{d} \omega$ at time $t=1.0$.
For this test-case, a non-intrusive gPC reference can still be obtained

Sensitivity analysis in $3 D$ stochastic dimension Mean, variance and total Sobol indices

$$
\begin{aligned}
& \mathbb{E}[U](x, t=1) \\
& \\
& =10
\end{aligned}
$$



$\Longrightarrow$ Perfect agreement with the MC-gPC scheme and the references.

Perfect agreement non-intrusive gPC vs. MC-gPC on every statistical observables Few characteristics:
ni-gPC : $N_{G L}^{Q}=4^{3}=64$ points with $(P+1)^{Q}=(2+1)^{3}=27$ coefficients.

- MC-gPC: $\quad(P+1)^{Q}=(2+1)^{3}=27$ coefficients.
$\Longrightarrow$ same truncation order $P$ ensures the same accuracy.
Performance considerations:
- ni-gPC cost: $\quad N_{G L}^{Q}=4^{3} \times$ averaged CPU time of 1 run $\approx 64 \times 3 \min 52 s$.
- MC-gPC cost: $1 \times$ effective CPU time of the run $=1 \times 4 \min 50 s$.
$\Longrightarrow$ 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.
$\Longrightarrow$ Something to dig here? Additional cost comes from the tallying phase [21]
The tallying phase is the only one sensitive to the dimension $Q$.

On the new MC-gPC scheme (allowing to characterise $\delta_{X}$ ):

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

On the new MC-gPC scheme (allowing to characterise $\delta_{X}$ ):

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Let us focus on performance considerations

On the new MC-gPC scheme (allowing to characterise $\delta_{X}$ ):

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

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

On the new MC-gPC scheme (allowing to characterise $\delta_{X}$ ):

- Spectral convergence as $P$ grows of the gPC based reduced model in [22]
- Convergence with respect to $N_{M C}$ 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])

On the new MC-gPC scheme (allowing to characterise $\delta_{X}$ ):

- Spectral convergence as $P$ grows of the gPC based reduced model in [22]
- Convergence with respect to $N_{M C}$ 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]?)

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

$$
\left\{\begin{array}{l}
\mathbf{v} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \mathbf{v})+v \sigma_{t}(\mathbf{x}, \mathbf{v}) u(\mathbf{x}, \mathbf{v})=v \sigma_{s}(\mathbf{x}, \mathbf{v}) \int P_{s}\left(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}^{\prime}\right) u\left(\mathbf{x}, \mathbf{v}^{\prime}\right) \mathrm{d} \mathbf{v}^{\prime}  \tag{2}\\
\quad+\frac{v \nu_{f}(\mathbf{x}, \mathbf{v}) \sigma_{f}(\mathbf{x}, \mathbf{v})}{k_{\text {eff }}} \int P_{f}\left(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}^{\prime}\right) u\left(\mathbf{x}, \mathbf{v}^{\prime}\right) \mathrm{d} \mathbf{v}^{\prime} \\
u(\mathbf{x}, \mathbf{v})=u_{b}(\mathbf{v}), \quad \mathbf{x} \in \partial \mathcal{D}, \quad \frac{\mathbf{v}}{v} \cdot n_{s}<0, \text { with }|\mathbf{v}|=v
\end{array}\right.
$$

- The above equation can be more concisely rewritten as

$$
\left\{\begin{array}{l}
L u=\frac{1}{k_{\text {eff }}} F u  \tag{3}\\
B u .
\end{array}\right.
$$

$\Longrightarrow$ we are looking for $u$ the fixed point of the above equation
■ The power iteration method [5] consists in choosing the $n^{t h}$ iteration of the algorithm as

$$
\left\{\begin{array}{l}
L u^{n}=\frac{1}{k_{\text {eff }}^{n-1}} F u^{n-1},  \tag{4}\\
B u^{n},
\end{array} \text { where } k_{\text {eff }}^{n}=k_{\text {eff }}^{n-1} \times \frac{\int_{\mathcal{D}} \int_{\mathcal{V}} u^{n}(\mathbf{x}, \mathbf{v}) \mathrm{d} \mathbf{x d} \mathbf{v}}{\int_{\mathcal{D}} \int_{\mathcal{V}} u^{n-1}(\mathbf{x}, \mathbf{v}) \mathrm{d} \mathbf{x d} \mathbf{v}} .\right.
$$

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

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

$$
\left\{\begin{array}{l}
\mathbf{v} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \mathbf{v})+v \sigma_{t}(\mathbf{x}, \mathbf{v}) u(\mathbf{x}, \mathbf{v})=v \sigma_{s}(\mathbf{x}, \mathbf{v}) \int P_{s}\left(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}^{\prime}\right) u\left(\mathbf{x}, \mathbf{v}^{\prime}\right) \mathrm{d} \mathbf{v}^{\prime}  \tag{2}\\
\quad+\frac{v \nu_{f}(\mathbf{x}, \mathbf{v}) \sigma_{f}(\mathbf{x}, \mathbf{v})}{k_{\text {eff }}} \int P_{f}\left(\mathbf{x}, \mathbf{v} \cdot \mathbf{v}^{\prime}\right) u\left(\mathbf{x}, \mathbf{v}^{\prime}\right) \mathrm{d} \mathbf{v}^{\prime} \\
u(\mathbf{x}, \mathbf{v})=u_{b}(\mathbf{v}), \quad \mathbf{x} \in \tilde{\mathcal{D}}, \quad \frac{\mathbf{v}}{v} \cdot n_{s}<0, \text { with }|\mathbf{v}|=v
\end{array}\right.
$$

- The above equation can be more concisely rewritten as

$$
\left\{\begin{array}{l}
L u=\frac{1}{k_{\text {eff }}} F u  \tag{3}\\
B u .
\end{array}\right.
$$

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

- Modified power iteration method [28]:

$$
\left\{\begin{array}{l}
\partial_{t} u^{n}+L u^{n}=\frac{1}{k_{\text {eff }}^{n-1}} F u^{n},  \tag{4}\\
u_{0}=u^{n-1}, \\
B u^{n},
\end{array} \quad \text { where } k_{\text {eff }}^{n}=k_{\text {eff }}^{n-1} \times \frac{\int_{\mathcal{D}} \int_{\mathcal{V}} u\left(\mathbf{x}, t^{n}, \mathbf{v}\right) \mathbf{d} \mathbf{x d} \mathbf{v}}{\int_{\mathcal{D}} \int_{\mathcal{V}} u\left(\mathbf{x}, t^{n-1}, \mathbf{v}\right) \mathrm{d} \mathbf{x d} \mathbf{v}}\right.
$$

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

- Modified power iteration method [28] with uncertainties:
$\begin{cases}\partial_{t} u^{n}+L^{X} u^{n}=\frac{1}{k_{\text {eff }}^{n-1}} F^{X} u^{n}, & \\ u_{0}=u^{n-1}, & , k_{\text {eff }}^{n}(X)=k_{\text {eff }}^{n-1}(X) \times \frac{\iint u\left(\mathbf{x}, t^{n}, \mathbf{v}, X\right) \mathrm{d} \mathbf{x d} \mathbf{v}}{\iint u\left(\mathbf{x}, t^{n-1}, \mathbf{v}, X\right) \mathrm{d} \mathbf{x d} \mathbf{v}} .\end{cases}$
Asymptotically as $n \times \Delta t \rightarrow \infty$, 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:

$$
\left\{\begin{array}{l}
\partial_{t} u^{n}+L^{X} u^{n}=\frac{1}{k_{\text {eff }}^{n-1}} F^{X} u^{n}, \\
u_{0}=u^{n-1}, \\
B^{X} u^{n},
\end{array}, k_{\text {eff }}^{\text {new }, k}=\int k_{\text {eff }}^{\text {old }, P}(X) \frac{\iint u^{P}\left(\mathbf{x}, t^{n}, \mathbf{v}, X\right) \mathrm{d} \mathbf{x d} \mathbf{v}}{\iint u^{P}\left(\mathbf{x}, t^{n-1}, \mathbf{v}, X\right) \mathrm{d} \mathbf{x d} \mathbf{v}} \phi_{k}(X) \mathrm{d} \mathcal{P}_{X} .\right.
$$

Asymptotically as $n \times \Delta t \rightarrow \infty$, 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=sampleUncertain Particles \(\left(N_{M C}\right)\)
    set \(U_{\text {old }}^{0}=1\)
    set \(U_{\text {new }}^{0}=1\)
    set \(k_{\text {eff }}^{0}=1\)
    for \(k \in\{1, \ldots, P\}\) do
        \(U_{\text {old }}^{k}=0\)
        \(U_{\text {new }}^{k}=0\)
        \(k_{\text {eff }}^{k}=1\)
    end
    while iter < iter max do
        \#Apply \(\overline{M C}-g P C\) during time step \(\left[t^{n}, t^{n}+\Delta t\right]\)
        \(\left(U_{\text {new }}^{k}\right)_{k \in\{0, \ldots, P\}}=\) trackUncertainParticlesWithMC-gPC(list_of_particles, \(\Delta t, k_{\text {eff }}^{0}, \ldots, k_{\text {eff }}^{P}\) )
        \#build punctual uncertain values
            \(\left(U_{\text {new }}^{P}\left(X_{g}\right)\right)_{g \in\left\{1, \ldots, N_{G}\right\}}=\) buildPunctualValues \(\left(\left(X_{g}\right)_{g \in\left\{1, \ldots, N_{G}\right\}},\left(U_{\text {new }}^{k}\right)_{k \in\{0, \ldots P\}}\right)\)
            \(\left(U_{\text {old }}^{P}\left(X_{g}\right)\right)_{g \in\left\{1, \ldots, N_{G}\right\}}=\) buildPunctualValues \(\left(\left(X_{g}\right)_{g \in\left\{1, \ldots, N_{G}\right\}},\left(U_{\text {old }}^{k}\right)_{k \in\{0, \ldots P\}}\right)\)
            \(\left(k_{\text {eff }}^{P}\left(X_{g}\right)\right)_{g \in\left\{1, \ldots, N_{G}\right\}}=\) buildPunctualValues \(\left(\left(X_{g}\right)_{g \in\left\{1, \ldots, N_{G}\right\}},\left(k_{\text {eff }}^{k}\right)_{k \in\{0, \ldots P\}}\right)\)
```

            \#update the \(g P C\) coefficients of the eigenvalue
            for \(k \in\{0, \ldots, P\}\) do
                \(k_{\text {eff }}^{k} \leftarrow \sum_{g=1}^{N_{G}} k_{\text {eff }}^{P}\left(X_{g}\right) \times \frac{U_{\text {new }}^{P}\left(X_{g}\right)}{U_{\text {old }}^{P}\left(X_{g}\right)} \phi_{k}\left(X_{g}\right) w_{g}\)
            end
            \#update the old number of physical particles
            for \(k \in\{0, \ldots, P\}\) do
                    \(U_{\text {old }}^{k} \leftarrow U_{\text {new }}^{k}\)
    end
    iter++
    end
    
## Uncertain $\mathrm{k}_{\text {eff }}$ computations

 Work in collaboration with E. Brun (DES), see [28]$\square$ Uncertain $k_{\text {eff }}$ computations with uncertain $\sigma_{a}, \sigma_{s}, \sigma_{f}, \nu$ on UD2O-1-0-SL [30]
$95 \%$ confidence intervals on $u$

$95 \%$ confidence intervals on $k_{\text {eff }}$


- UD2O-H2O(1)-1-0-SL problem [30], uncertain interface UD2O/H2O



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
E These hybrid computations are competitive w.r.t. a full non-intrusive simulation.


## Efficient hybrid intrusive/non-intrusive computations Once again, the previous 3D example...

- 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 $\sigma_{t}\left(X_{1}\right), \sigma_{s}\left(X_{2}\right)$,
= but not yet the uncertainties on $\eta\left(X_{3}\right)$.
- Then we can quite easily
= run the MC-gPC solver to propagate the uncertainties with respect to $X_{1}, X_{2}$
- several times, for several values of $\left(X_{3}^{i}, w_{i}\right)_{i \in\{1, \ldots, N\}} \sim\left(X_{3}, \mathrm{~d} \mathcal{P}_{X_{3}}\right)$.
- To know how in details see [26] (intensive use of the orthonormality property of the $\left.\left(\phi_{k}\right)_{k \in\{0, \ldots, P\}}\right)$
- Comparisons of the mean and variance MC-gPC vs. hybrid ni-gPC /MC-gPC $\Longrightarrow$ excellent agreement!


- Now, the costs of each numerical strategies are given by
$-\quad$ new MC-gPC: cost $=1 \times$ CPU time of 1 run $\quad=1 \times 1 \mathrm{~min} 25 \mathrm{~s}$.
- ni-gPC: cost $=64 \times$ CPU time of 1 run $=64 \times 0 \mathrm{~min} 54 \mathrm{~s}=58 \mathrm{~min} 06 \mathrm{~s}$.
$-\quad$ hybrid $: \quad \operatorname{cost}=4 \times \operatorname{CPU}$ time of 1 run $\quad=4 \times 0 \min 58 s=3 \mathrm{~min} 52 \mathrm{~s}$.
- Gains:

| - | new MC-gPC | $:$ | vs. | ni-gPC | $\times$ | 41.0 |  |
| :--- | :---: | :--- | :--- | :---: | :---: | :---: | :--- |
| - | new MC-gPC | $:$ | vs. | hybrid ni-gPC / MC-gPC | $\times$ | 0.36 | (loss) |
| - | hybrid ni-gPC / MC-gPC | $:$ | vs. | ni-gPC | $\times$ | 15.0 | p. $33 / 35$ |

1 Motivations and objectives + the skeleton of an MC code
(2) Non-intrusive applications and drawbacks in an MC context

33 Intrusive reduced modeling (sometimes, it is worth it)

4 Few simple test-cases
. - Comparisons, performance considerations

- MC-gPC for $k_{\text {eff }}$ computations (work with E. Brun [28])
- Hybrid intrusive/non-intrusive computations

5 Conclusion

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 $u^{P} \xrightarrow[P \rightarrow \infty]{\longrightarrow} u$ )
- Convergence of the MC-gPC scheme in [21]
(design of converging numerical schemes such that $u_{N_{M C}}^{P} \xrightarrow[N_{M C} \rightarrow \infty]{\longrightarrow} u^{P}$ )
(only simple modifications of an existing MC code are necessary)
(Test-cases up to 6D stochastic dimensions)
- Applications to $k_{\text {eff }}$ 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... $\times 4$ faster than MC-gPC)
(+ some efficient hybrid intrusive/non-intrusive applications)


## Question?

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

77 Uncertain analytical solution and convergence study

주 A 6-D uncertain problem with sensitivity analysis
@ Verification of the theorem and (non-)optimality

IIC A beautiful animation

Uncertain photonic computations An uncertain nonlinear stiff system [24]

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

$$
\left\{\begin{array}{l}
\frac{1}{c} \partial_{t} I(x, t, \omega, X)+\omega \cdot \nabla I(x, t, \omega, X)+\sigma_{t}(E(x, t, X), X) I(x, t, \omega, X) \\
\quad=\sigma_{a}(E(x, t, X), X) B(E(x, t, X))+\sigma_{s}(E(x, t, X), X) \int I\left(x, t, \omega^{\prime}, X\right) \mathrm{d} \omega^{\prime},  \tag{5}\\
\partial_{t} E(x, t, X)=c \sigma_{a}(E(x, t, X), X) \int\left(I\left(x, t, \omega^{\prime}, X\right)-B(E(x, t, X))\right) \mathrm{d} \omega^{\prime}, \\
X \sim \mathrm{~d} \mathcal{P}_{X} .
\end{array}\right.
$$

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

- Uncertain photonics with uncertain $\sigma_{a}, C_{v}$



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

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

If A beautiful animation

The solutions are given by

$$
\begin{align*}
M_{1}^{U}(t)=\mathbb{E}[U(t, X)] & =\frac{1}{2} U_{0} e^{-v \bar{\sigma}_{a} t} \frac{e^{v \hat{\sigma}_{s} t}-e^{-v \hat{\sigma}_{s} t}}{\hat{\sigma}_{s} t v} \\
M_{2}^{U}(t)=\mathbb{E}\left[U^{2}(t, X)\right] & =\frac{1}{4} U_{0}^{2} e^{-2 v \bar{\sigma}_{a} t} \frac{e^{2 v \hat{\sigma}_{s} t}-e^{-2 v \hat{\sigma}_{s} t}}{\hat{\sigma}_{s} t v},  \tag{6}\\
\mathbb{V}[U](t) & =M_{2}^{U}(t)-\left(M_{1}^{U}(t)\right)^{2} .
\end{align*}
$$

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


The error $e$ for the UQ problem is now $e=\mathcal{O}\left(\frac{N_{M C}^{U Q}}{\sqrt{N_{M C}}}\right)$ (for this test-pb at least ! )

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

17 Uncertain analytical solution and convergence study

8 A 6-D uncertain problem with sensitivity analysis
[9 Verification of the theorem and (non-)optimality

II A beautiful animation

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

The configuration is the following:

- Similar three first points $(v=1, \ldots)$
- The material is composed of two layers of different media, $A$ and $B$ with $\mathcal{D}_{A}=\left[0, \frac{1}{2}\right]$ and $\mathcal{D}_{B}=\left[\frac{1}{2}, 1\right]$ 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 $\left(X^{i}\right)_{i \in\{A, B\}}=\left(X_{1}^{i}, X_{2}^{i}, X_{3}^{i}\right)_{i \in\{A, B\}}$ with

$$
\begin{array}{lll}
\sigma_{t}(x, t, X) & =\sum_{i \in\{A, B\}}\left[\bar{\sigma}_{t}^{i}+\widehat{\sigma}_{t_{X}^{i}}^{i} X_{1}^{i} \mathbf{1}_{\mathcal{D}_{i}}(x),\right. & \forall x \in \mathcal{D}, t \in \mathbb{R}^{+}, \\
\sigma_{s}\left(x, t, \omega, \omega^{\prime}, X\right) & =\sum_{i \in\{A, B\}}\left[\bar{\sigma}_{s}^{i}+\widehat{\sigma}_{s}^{i} X_{2}^{i}\right] \mathbf{1}_{\mathcal{D}_{i}}(x), & \forall x \in \mathcal{D}, t \in \mathbb{R}^{+},  \tag{7}\\
\eta(x, t, X) & =\sum_{i \in\{A, B\}}\left[\bar{\eta}^{i}+\widehat{\eta}^{i} X_{3}^{i}\right] \mathbf{1}_{\mathcal{D}_{i}}(x), & \forall x \in \mathcal{D}, t \in \mathbb{R}^{+},
\end{array}
$$

- $\left(X_{1}^{i}, X_{2}^{i}, X_{3}^{i}\right)_{i \in\{A, B\}}$ are independent uniformly distributed RV s on $[-1,1]$.
- For the next computations, the mean quantities are set to

$$
\begin{array}{ll}
\bar{\sigma}_{t}^{A}=1.0, \bar{\sigma}_{s}^{A}=1.3, \bar{\eta}^{A}=1.0, & \widehat{\sigma}_{t}^{A}=0.4, \widehat{\sigma}_{s}^{A}=0.4, \widehat{\eta}^{A}=0.4 \\
\bar{\sigma}_{t}^{B}=1.0, \bar{\sigma}_{s}^{B}=0.9, \bar{\eta}^{B}=1.0, & \widehat{\sigma}_{t}^{B}=0.4, \widehat{\sigma}_{s}^{B}=0.4, \widehat{\eta}^{B}=0.4
\end{array}
$$

- Statistical observables: mean, variance, Sobol indices as before

For this test-case, a non-intrusive gPC reference is too costly


- Run $1.024 \times 10^{9}$ particles, $\left(P+{ }^{x}\right)^{6}=729$ on 1024 proc. in 750 s .

■ ni-gPC would need, same accuracies and restitution times, 131072 proc.
New problem: suppose now we want the variance to be lesser that $0.05 \forall x \in \mathcal{D}$
$\Longrightarrow$ How should we work on the uncertain parameters?
$\Longrightarrow$ On which ones?
$\Longrightarrow$ Of how much should we reduce their respective uncertainties?

## A two layered uncertain material: sensitivity analysis in 6D

 Total and first order Sobol indices

$$
\mathbb{S}_{2}^{\text {tot }}[U](x, t=1) \text { vs. } \mathbb{S}_{2}^{1}[U](x, t=1)
$$



$$
\mathbb{S}_{3}^{\operatorname{tot}}[U](x, t=1) \text { vs. } \mathbb{S}_{3}^{1}[U](x, t=1)
$$



$$
\mathbb{S}_{4}^{\text {tot }}[U](x, t=1) \text { vs. } \mathbb{S}_{4}^{1}[U](x, t=1)
$$




$$
\mathbb{S}_{6}^{\text {tot }}[U](x, t=1) \text { vs. } \mathbb{S}_{6}^{1}[U](x, t=1)
$$



By running several calculations with decreasing variances on $\sigma_{t}^{A}$ and $\sigma_{s}^{A}$ we get:



Answer to the problem:
Enough reducing the uncertainties on $X_{1}, X_{2}$ of only a factor 3 .
$\Longrightarrow$ 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
(8) A 6-D uncertain problem with sensitivity analysis

9 Verification of the theorem and (non-)optimality

II A beautiful animation

- Back to the previous convergence study with the new reduced model w.r.t. $P$ :
 same with a numerical resolution

- 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.
- Spectral convergence w.r.t. $P$ and MC resolution:

- Spectral convergence is recovered also in practice $\forall$ 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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11 A beautiful animation








Uncertain linear Boltzmann equation (with uncertain anisotropic scattering)

 (with uncertain anisotropic scattering)
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$\mathbb{E}[U](x, t), \mathbb{V}[U](x, t)$ and realisations of $U(x, t, X)$ for $P=7$


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