DE LA RECHERCHE À L'INDUSTRIE

An intrusive MC scheme for the uncertain (non)linear Boltzmann equation

(Sometimes, intrusiveness is worth it)

Gaël Poëtte

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

ETICS, 4-9 oct. 2020, Oléron

1. A particular context (MC resolution of the deterministic transport equation)
2. Non-intrusive computation of the Sobol indices for the transport equation
3. The gPC intrusive MC scheme for the uncertain linear Boltzmann equation
4. Test-cases, comparisons, performance considerations
5. Preliminary results on nonlinear problems (k_{eff} computations and photonics)

1. A particular context (MC resolution of the deterministic transport equation)
2. Non-intrusive computation of the Sobol indices for the transport equation
3. The gPC intrusive MC scheme for the uncertain linear Boltzmann equation
4. Test-cases, comparisons, performance considerations
5. Preliminary results on nonlinear problems (k_{eff} computations and photonics)

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

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

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

- $7+Q = 3(\mathbf{x}) + 1(t) + 3(\mathbf{v}) + Q(X)$ (independent) dimensions.
- Statistics (but above all Sobol indices) 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:

- General dependence w.r.t. X of $(\sigma_\alpha)_{\alpha\in\{s,t\}}$, u_0, boundary conditions etc.
- In our case, *deterministic* transport equation is solved with **an MC scheme**.

$\Longrightarrow$ But before let us give details on the MC resolution of the transport equation...

- 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

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

  (Central Limit theorem, see Lapeyre-Pardoux-Sentis [6]).
- We will abusively but concisely write the error is $e_{N_{MC}} = \mathcal{O}\left(\frac{1}{\sqrt{N_{MC}}}\right)$.
- Inconditionally stable scheme: the time step can be the time of interest t^*.
  (MC schemes scale weakly in a replication domain context if Δt is high enough)

Algorithmic sketch for the non-analog MC scheme *(Backward formulation)*

set $u(\mathbf{x}, t, \mathbf{v}) = 0$

for $p \in \{1, \dots, N_{MC}\}$ 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 $w_p = \frac{1}{N_{MC}}$

  while $s_p > 0$ *and* $w_p > 0$ do

    Sample τ by inversing the cdf of an exponential law $\tau = -\frac{\ln(\mathcal{U}([0,1]))}{v_p \sigma_s(\mathbf{x}_p, s_p, \mathbf{v}_p)}$

    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

      $w_p \times = e^{-v\sigma_a(\mathbf{x}_p, s_p, \mathbf{v}_p) s_p}$

      #tally the contribution of particle p

      $u(\mathbf{x}, t, \mathbf{v}) + = w_p \times u_0(\mathbf{x}_p, \mathbf{v}_p)$

    end

    else

      #move the particle p

      $\mathbf{x}_p - = \mathbf{v}_p \tau,$

      #change the weight of the particle

      $w_p \times = e^{-v\sigma_a(\mathbf{x}_p, s_p, \mathbf{v}_p)\tau}$

      Sample the velocity $\mathbf{V}'$ sampled from $P_s(\mathbf{x}_p, s_p, \mathbf{v}', \mathbf{v}_p)d\mathbf{v}'$

      $\mathbf{v}_p = \mathbf{V}'$

      #set the life time of particle p to:

      $s_p - = \tau$

    end

  end

end

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

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

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

$$\begin{aligned}
\mathbb{E}[U](\mathbf{x},t) &= \iint u(\mathbf{x},t,\mathbf{v},X)\mathrm{d}\mathbf{v}\mathrm{d}\mathcal{P}_X \approx \sum_{k=1}^{N} w_i U(\mathbf{x},t,X_i) + \mathcal{O}(N^\beta),\\
\mathbb{E}[U^2](\mathbf{x},t) &= \int \left(\int u(\mathbf{x},t,\mathbf{v},X)\mathrm{d}\mathbf{v}\right)^2 \mathrm{d}\mathcal{P}_X \approx \sum_{k=1}^{N} w_i U^2(\mathbf{x},t,X_i) + \mathcal{O}(N^\beta),\\
\mathbb{V}[U](\mathbf{x},t) &= \mathbb{E}[U^2](\mathbf{x},t) - (\mathbb{E}[U](\mathbf{x},t))^2,\\
\dots &= \dots
\end{aligned}$$

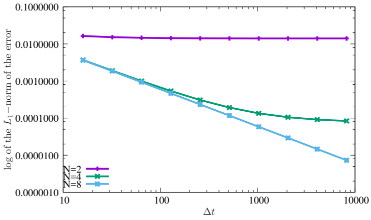
5. Same idea for the computation of Sobol indices [12, 5], of interest for us.

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

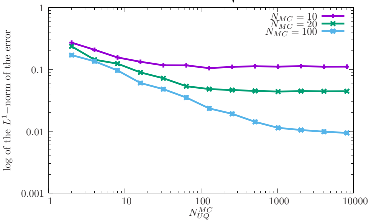
$$e_\Delta^N = \underbrace{\mathcal{O}(\Delta)}_{\text{deterministic solver}} + \underbrace{\mathcal{O}(N^\beta)}_{\text{uncertainty integration}} .$$

- Illustration on a homogeneous uncertain problem for which an analytical solution for the variance can be built (see [8])
- Convergence studies w.r.t. to Δ and N for two different strategies:

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



$$\Delta = \frac{1}{\sqrt{N_{MC}}},\ N^\beta = \frac{1}{\sqrt{N_{MC}^{UQ}}}$$



Interpretation of the previous non-intrusive results

Why having resort for to an intrusive reduced model?

- When running N times the MC code:
  MC particles for $(\mathbf{x}, t, \mathbf{v})$ 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 $(\mathbf{x}, t, \mathbf{v}, X)$?

A gPC-based reduced model for uncertain transport
(order P is the new linearisation parameter)

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

- Let us defined the gPC developpement

$$u^P(\mathbf{x},t,\mathbf{v},X)=\sum_{q=0}^{P}u_k(\mathbf{x},t,\mathbf{v})\phi_k(X) \text{ with } u_k(\mathbf{x},t,\mathbf{v})=\int u(\mathbf{x},t,\mathbf{v},X)\phi_k(X)\mathrm{d}\mathcal{P}_X.$$

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

$$\begin{cases}\partial_t u_0+\mathbf{v}\cdot\nabla_{\mathbf{x}}u_0 & =-v\int\left(\sigma_t\sum_{k\leq P}u_k\phi_k\right)\phi_0\mathrm{d}\mathcal{P}_X+v\iint\left(\left(\sigma_s\sum_{k\leq P}u_k\phi_k\right)\phi_0\mathrm{d}\mathcal{P}_X\right)\\ \dots & \dots\\ \partial_t u_P+\mathbf{v}\cdot\nabla_{\mathbf{x}}u_P & =-v\int\left(\sigma_t\sum_{k\leq P}u_k\phi_k\right)\phi_P\mathrm{d}\mathcal{P}_X+v\iint\left(\left(\sigma_s\sum_{k\leq P}u_k\phi_k\right)\phi_P\mathrm{d}\mathcal{P}_X\right)\end{cases}$$

- 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* [8].

The gPC intrusive non-analog MC scheme as in [8]
(Backward formulation)

```
for k ∈ {0, ..., P} do
    set u_k^X(x, t, v) = 0
end
for p ∈ {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 x_p = x
    set v_p = v
    set w_p = 1/N_MC
    set X_p = X with X sampled from the probability measure dP_X .
    while s_p > 0 and w_p > 0 do
        Sample τ by inversing the cdf of an exponential law τ = − ln(U([0,1])) / (v σ_s(x_p, s_p, v_p, X_p))
        if τ > s_p then
            x_p −= v_p s_p,
            s_p = 0
            w_p ×= e^{−v σ_a(x_p, s_p, v_p, X_p) s_p}
            #tally the contribution of particle p
            for k ∈ {0, ..., P} do
                u_k^X(x, t, v) += w_p × u_0(x_p, v_p, X_p) φ_k^X(X_p)
            end
        end
        else
            x_p −= v_p τ,
            w_p ×= e^{−v σ_a(x_p, s_p, v_p, X_p) τ}
            v_p = V' with V' sampled from P_s(x_p, s_p, v', v_p, X_p) dv'
            #set the life time of particle p to:
            s_p −= τ
        end
    end
end
```

In [9], proof of spectral convergence as $P \to \infty$ 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

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

- Assume bounds on the cross-sections

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

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

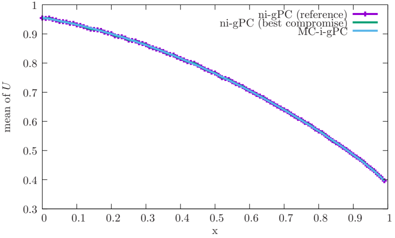
Spectral accuracy holds in the following sense: for all $k \in \mathbb{N}$ such that $u \in H^k(\Theta)$, there exists a constant D_k such that $\forall t \in [0, T]$

$$\left\| u(t) - u^P(t) \right\|^2_{L^2(\mathcal{I},\Theta)} \leq e^{2(\Sigma_t + \Sigma_s)t} \left(\left\| u_0 - u_0^P \right\|^2_{L^2(\mathcal{I},\Theta)} + 2(\Sigma_s + \Sigma_t)t \|u_0^2\|_{L^2(\mathcal{I},\Theta)} \frac{D_k}{P^k} \right).$$

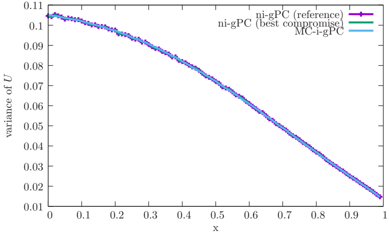
Sensitivity analysis in $3D$ stochastic dimension

Mean, variance and total Sobol indices: uncertain σ_s, σ_t, η

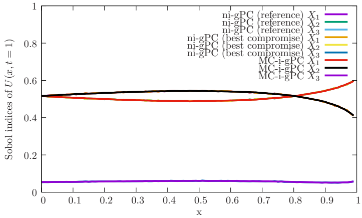
$\mathbb{E}[U](x, t = 1)$



$\mathbb{V}[U](x, t = 1)$



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



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

Sensitivity analysis in $3D$ stochastic dimension

Performance considerations

Perfect agreement non-intrusive gPC vs. MC-i-gPC on every statistical observables

Few characteristics:

- n-i gPC : $N_{GL}^Q = 4^3 = 64$ points with $(P+1)^Q = (2+1)^3 = 27$ coefficients.
- MC-i-gPC: $(P+1)^Q = (2+1)^3 = 27$ coefficients.

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

Performance considerations:

- n-i gPC cost: $N_{GL}^Q = 4^3 \times$averaged CPU time of 1 run$\approx 64 \times 3min52s$.
- MC-i-gPC cost: $1\times$effective CPU time of the run$= 1 \times 4min50s$.

$\Longrightarrow$ It is ≈ 50 times faster than the non-intrusive application.

- But the cost of a MC-i-gPC run is $\approx 1.26\times$ the cost of a non-intrusive one.

$\Longrightarrow$ Additional cost comes from the *tallying phase* (see [8] for details)

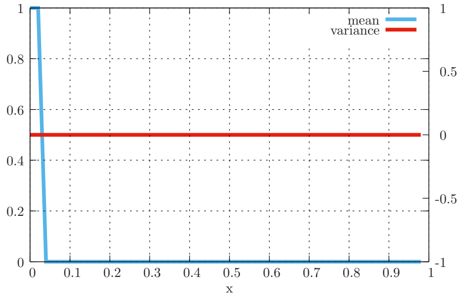
The tallying phase is the only one sensitive to the dimension Q.

A simplified configuration (also presented in [9])
(with uncertain anisotropic scattering)

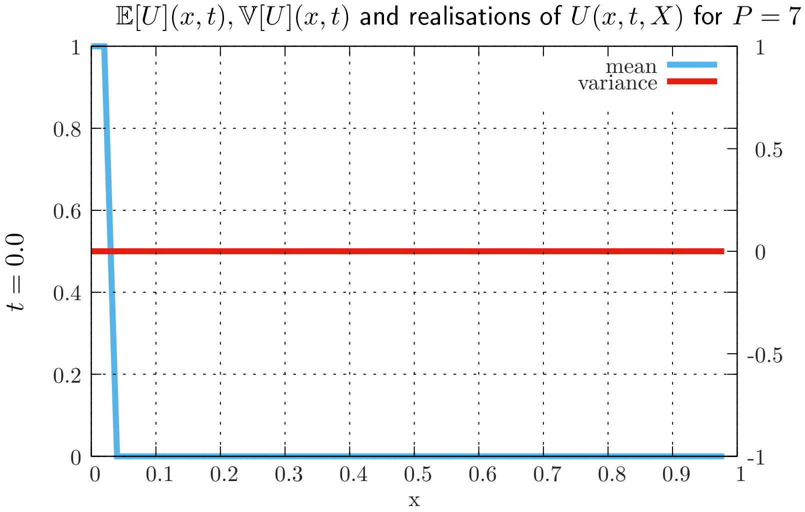
$$\begin{cases} \partial_t u + v\omega\nabla_x u = -v\sigma_s u + \displaystyle\int v\sigma_s P_s(X) u \, \mathrm{d}\omega', \\ u(x,0,\mathbf{v}) = u_0(x) = \mathbf{1}_{[0,\frac{1}{50}]}(x). \end{cases}$$

We assume $X \sim \mathcal{U}([-1,1])$ with $P_s(\omega', X)\mathrm{d}\omega' = \mathbf{1}_{[0,U(X)]}(\omega')$,
where $X \longrightarrow U(X) = 0.8^{\frac{(X+1)}{2}}$ maps $X \sim \mathcal{U}([-1,1])$ into $U(X) \sim \mathcal{U}([0, 0.8])$.

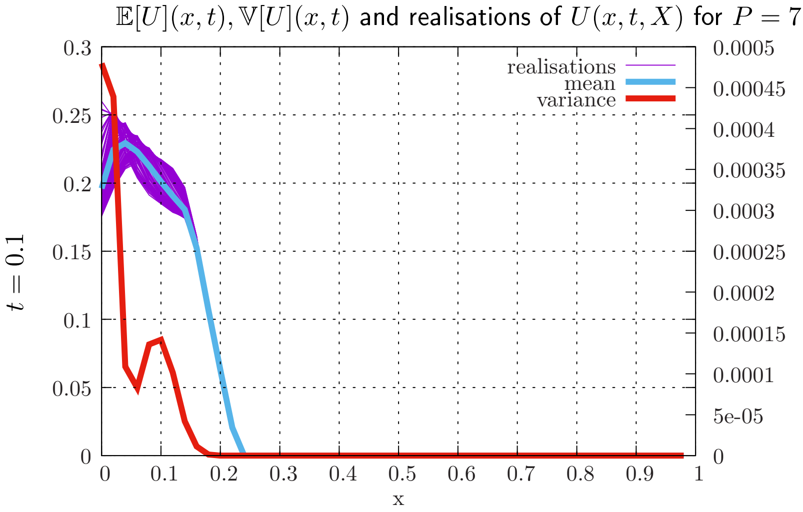
Mean and variance of $U(x, t = 0., X)$



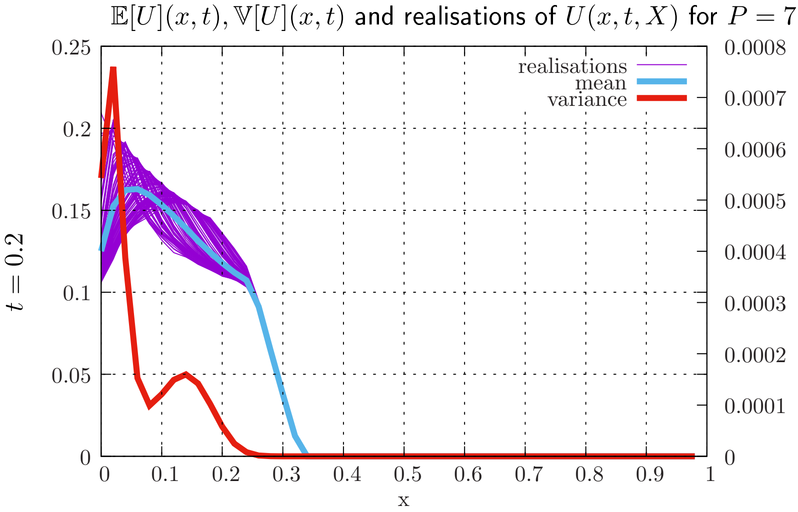
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

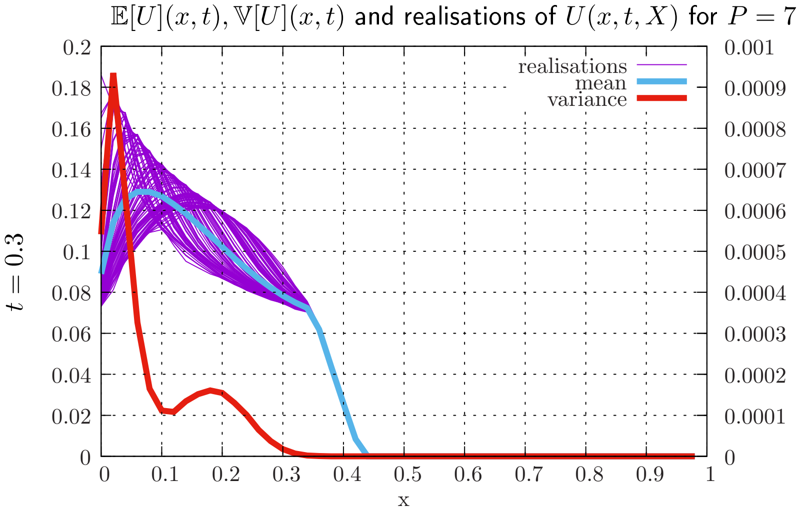


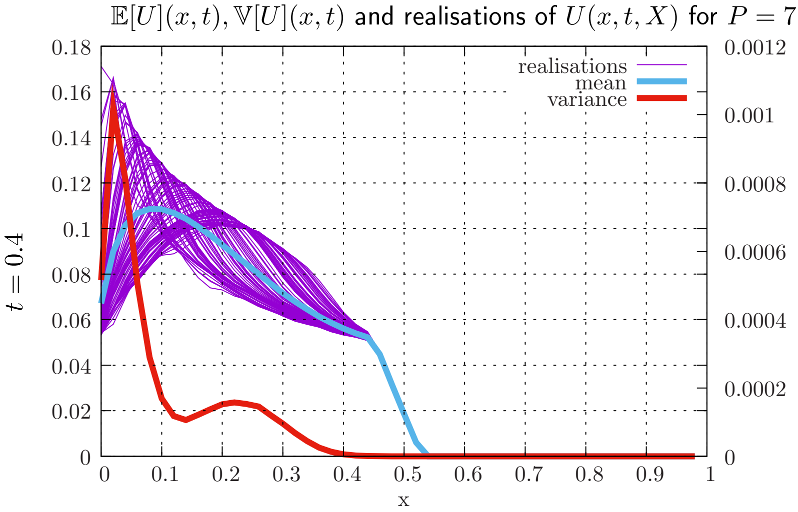
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

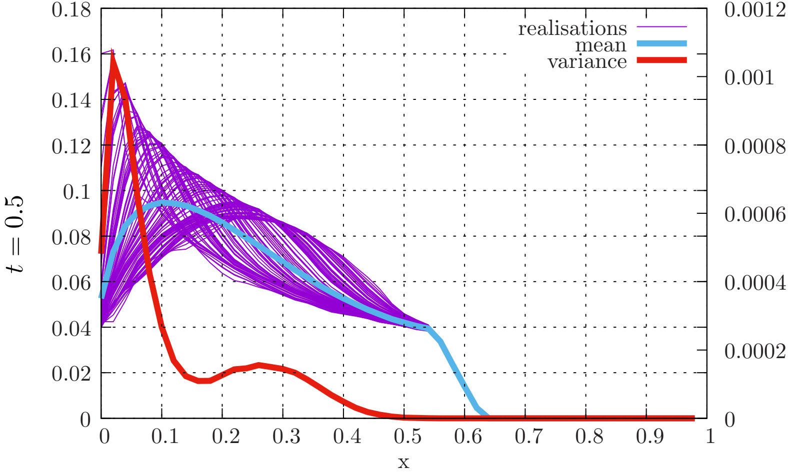



$\mathbb{E}[U](x,t), \mathbb{V}[U](x,t)$ and realisations of $U(x,t,X)$ for $P=7$
realisations
mean
variance
$t = 0.3$
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.001
0.0009
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x

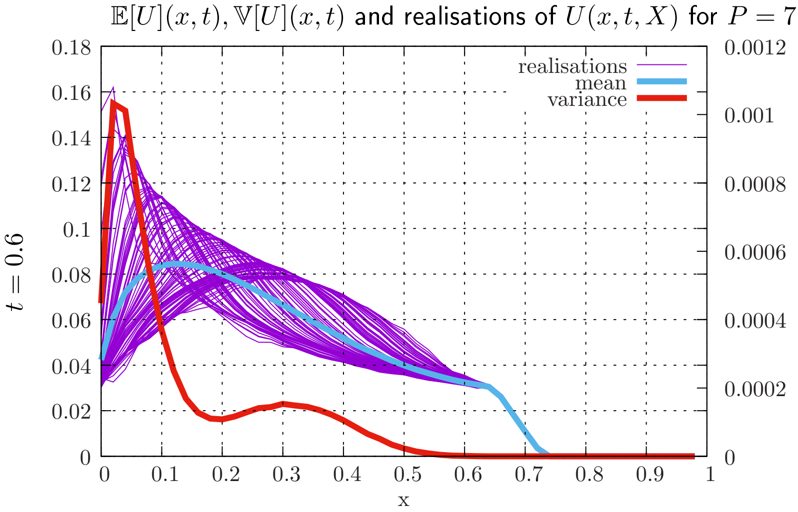

$\mathbb{E}[U](x,t), \mathbb{V}[U](x,t)$ and realisations of $U(x,t,X)$ for $P = 7$
$t = 0.4$
realisations
mean
variance
x
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

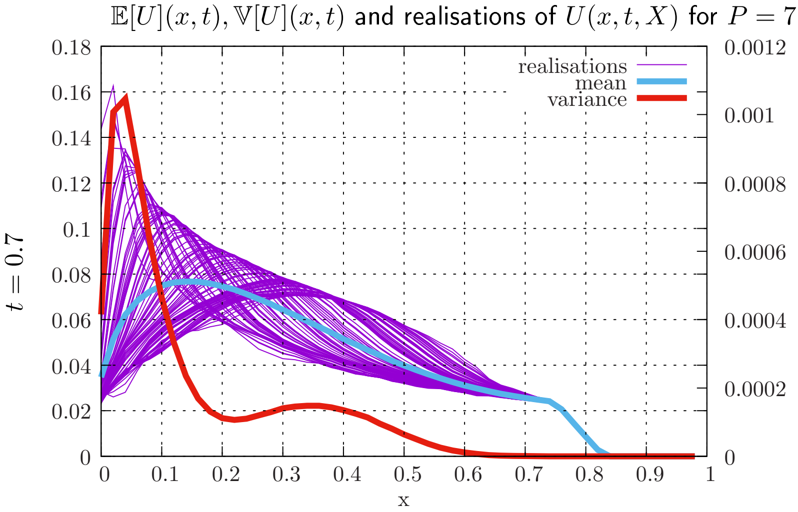
$\mathbb{E}[U](x,t), \mathbb{V}[U](x,t)$ and realisations of $U(x,t,X)$ for $P=7$

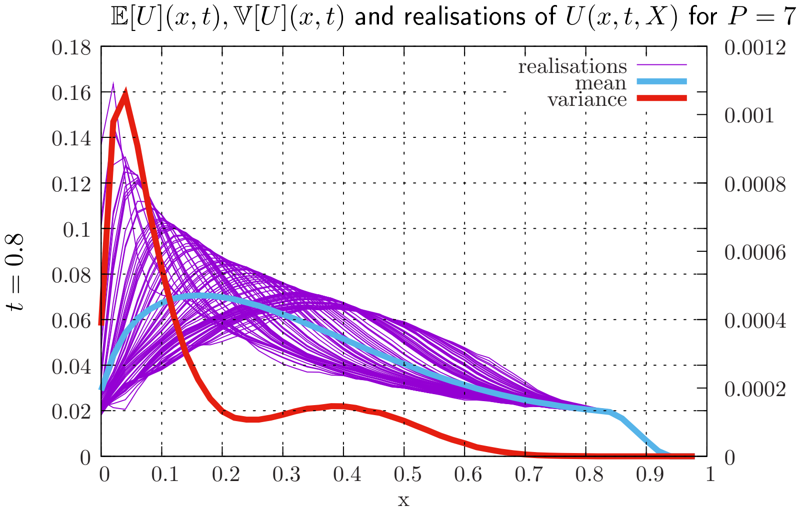


Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

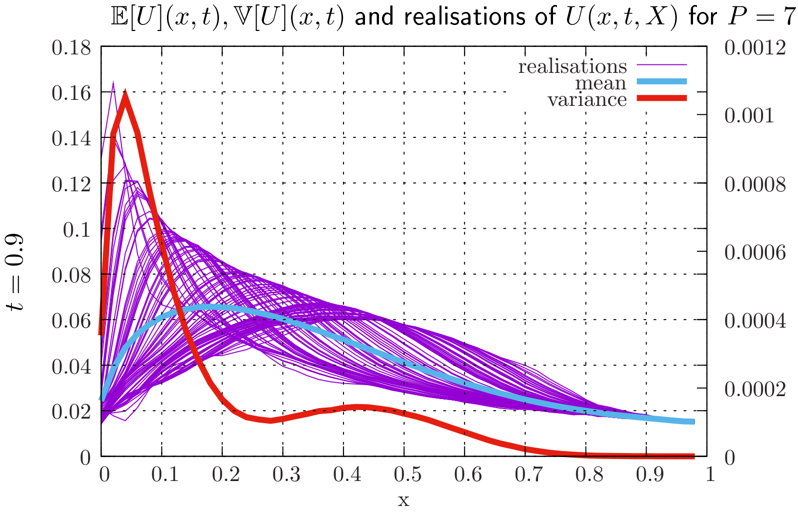


Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



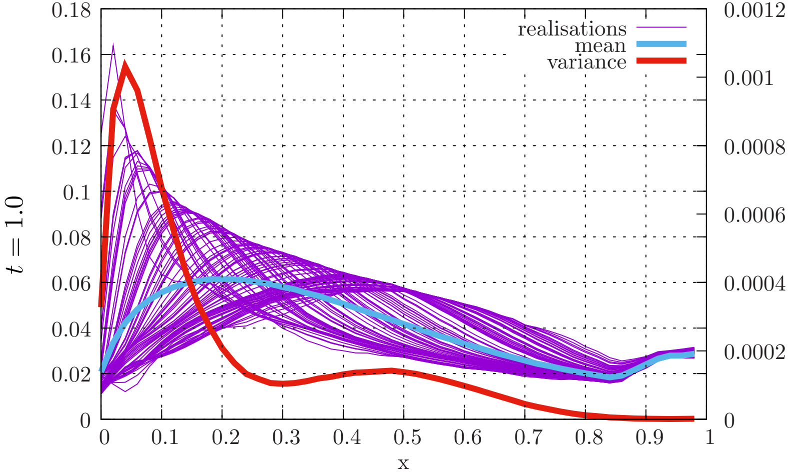

$\mathbb{E}[U](x,t), \mathbb{V}[U](x,t)$ and realisations of $U(x,t,X)$ for $P=7$
realisations
mean
variance
$t = 0.8$
x
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.0002
0.0004
0.0006
0.0008
0.001
0.0012

Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

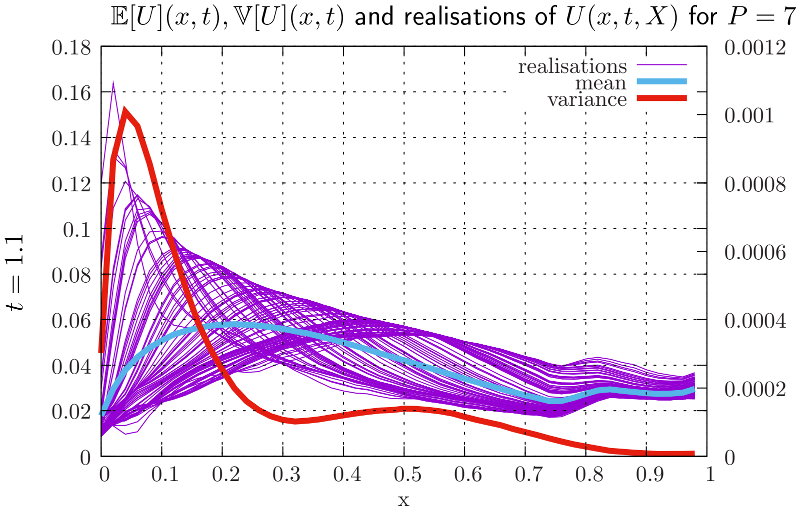


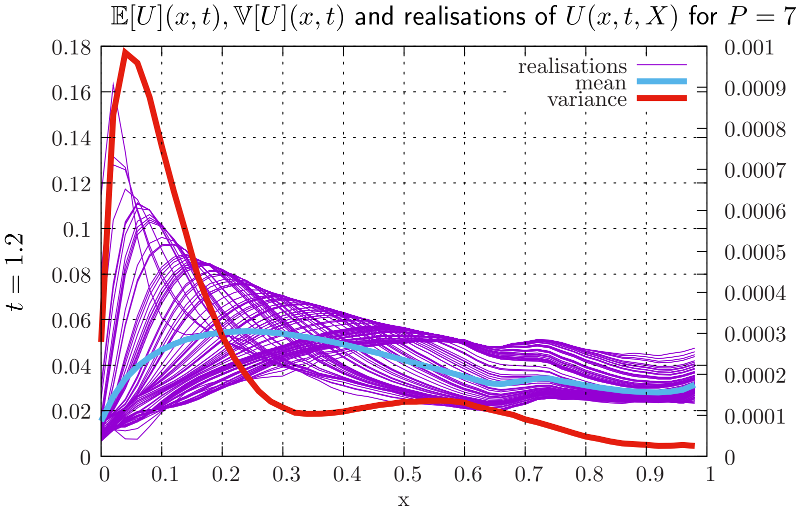
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

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

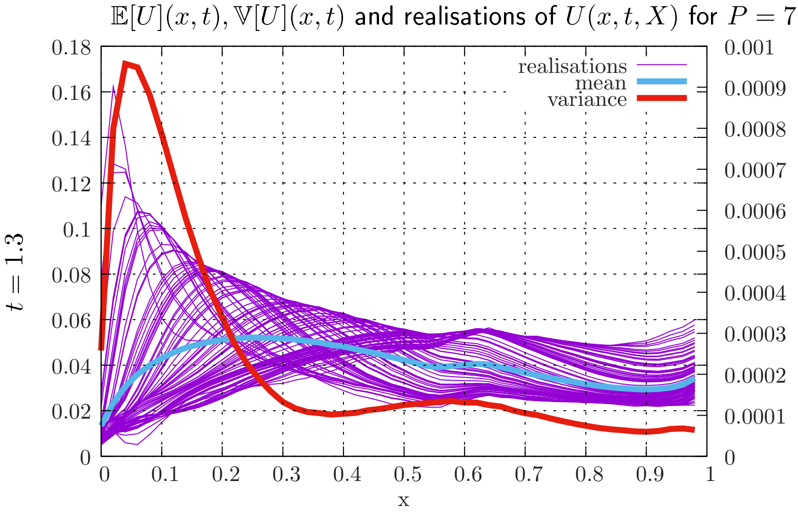


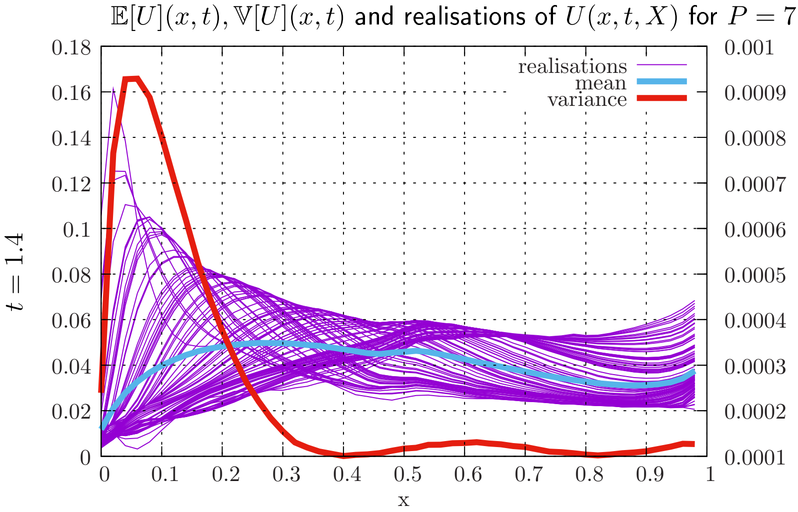
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



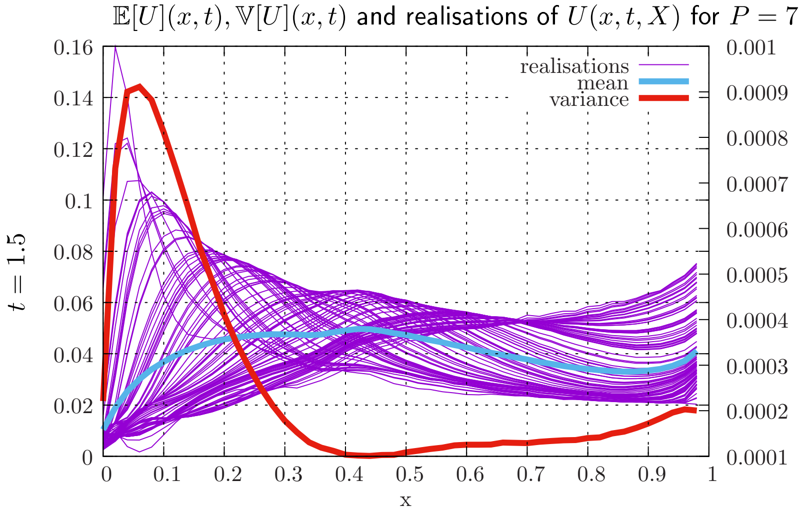

$\mathbb{E}[U](x,t), \mathbb{V}[U](x,t)$ and realisations of $U(x,t,X)$ for $P=7$
$t = 1.2$
realisations
mean
variance
x
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.0001
0.0002
0.0003
0.0004
0.0005
0.0006
0.0007
0.0008
0.0009
0.001

Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

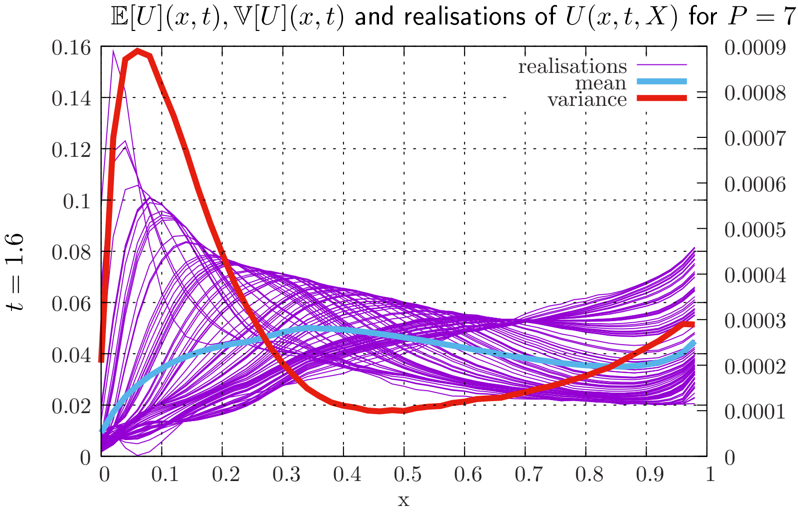



$\mathbb{E}[U](x,t), \mathbb{V}[U](x,t)$ and realisations of $U(x,t,X)$ for $P=7$
$t = 1.4$
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.001
0.0009
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
x
realisations
mean
variance

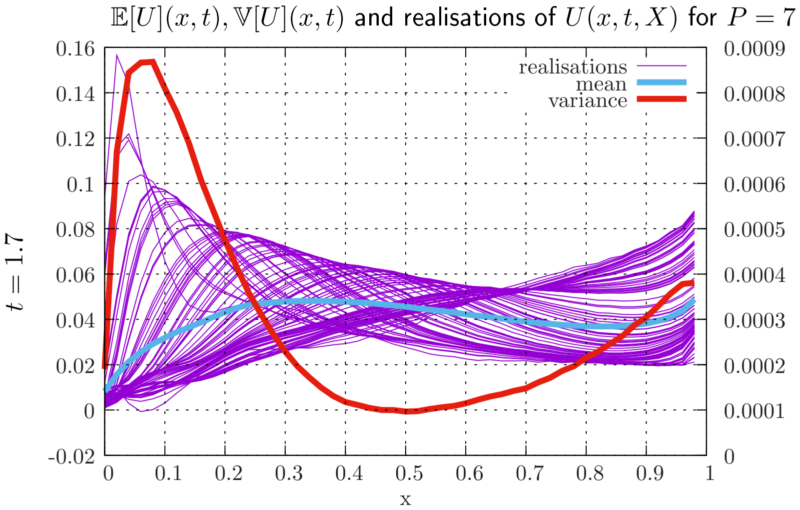
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



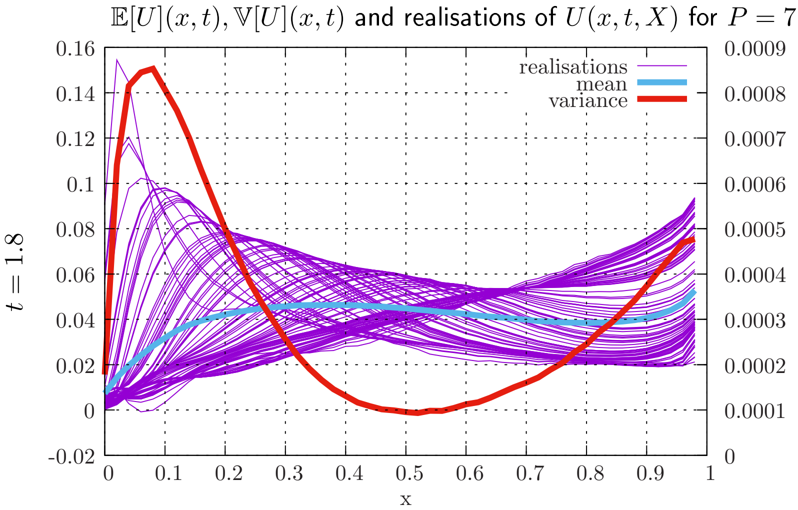
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



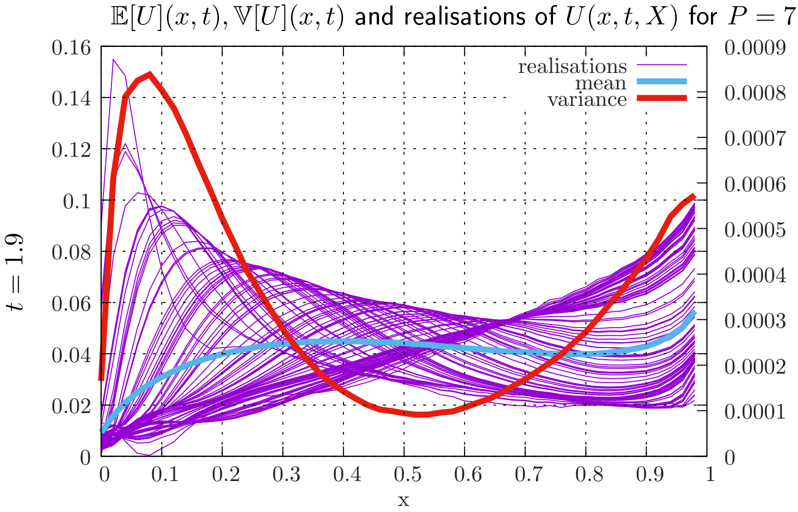
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



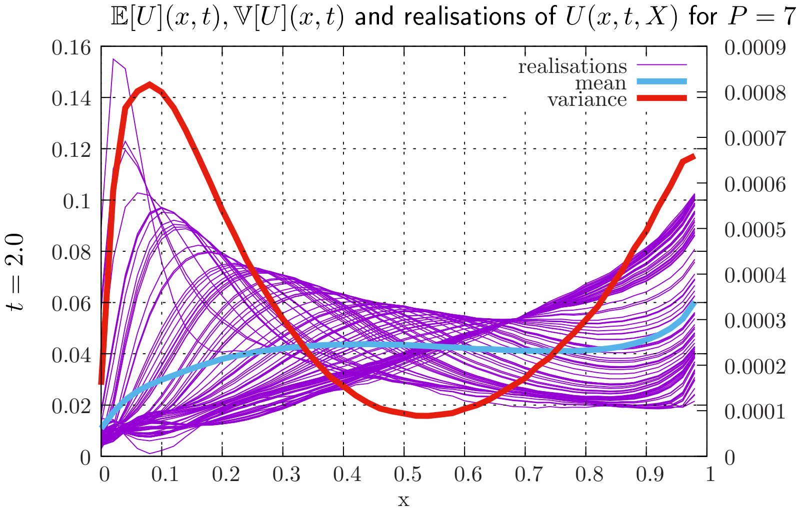
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



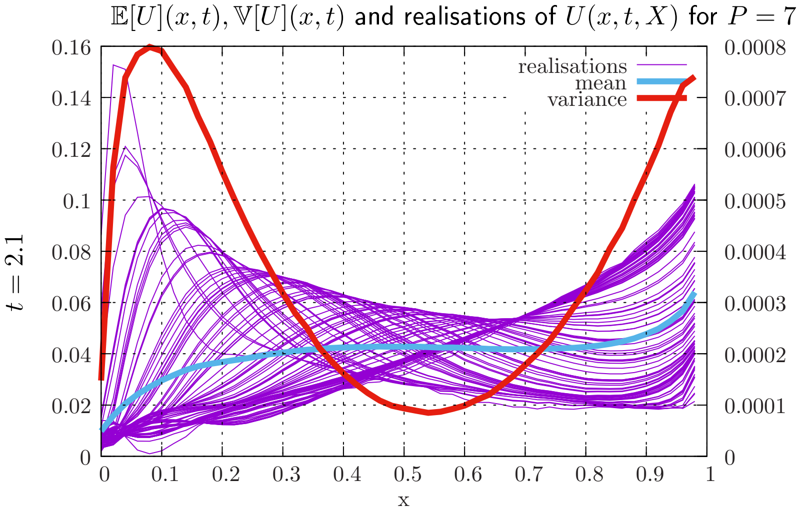
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



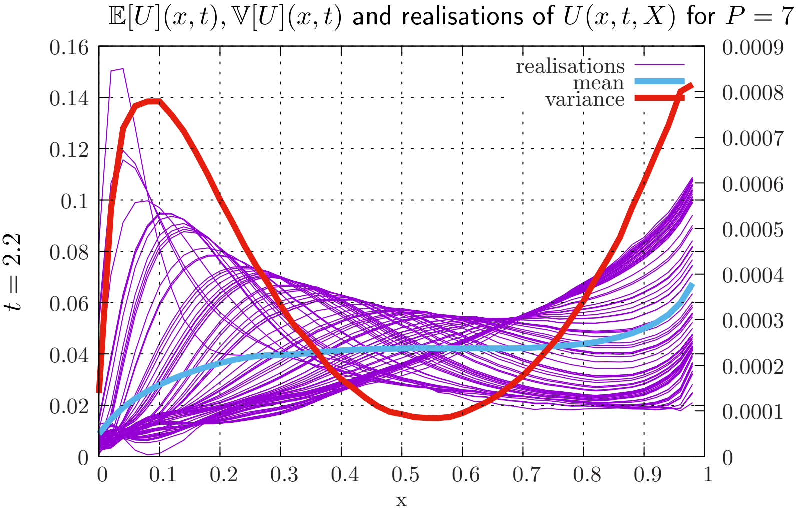
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



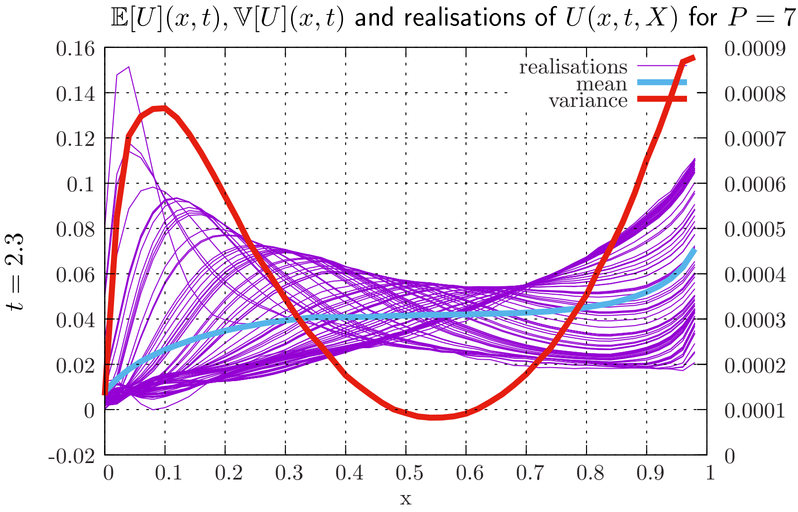
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



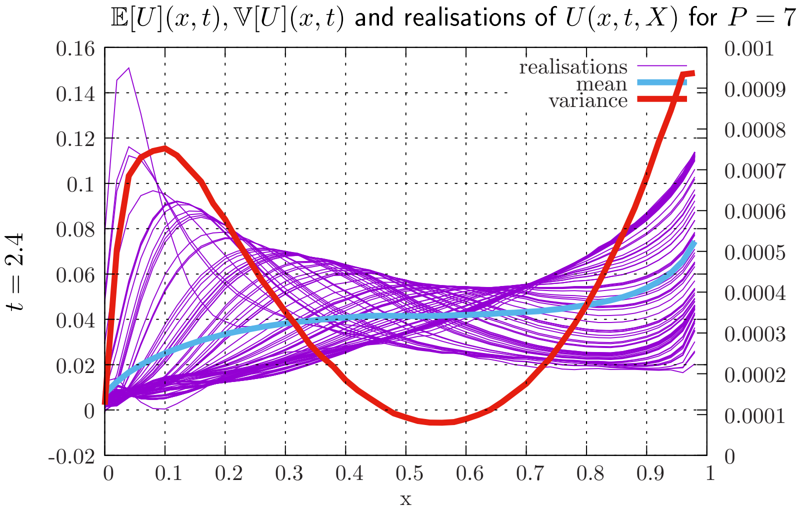
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



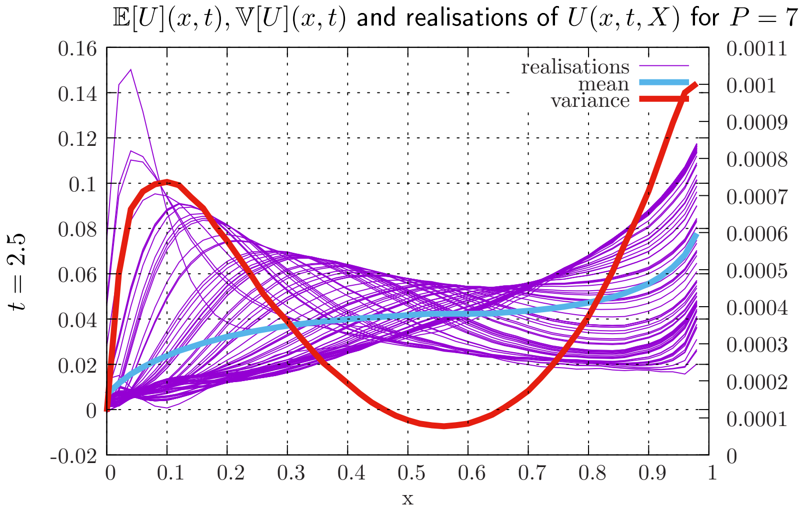
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



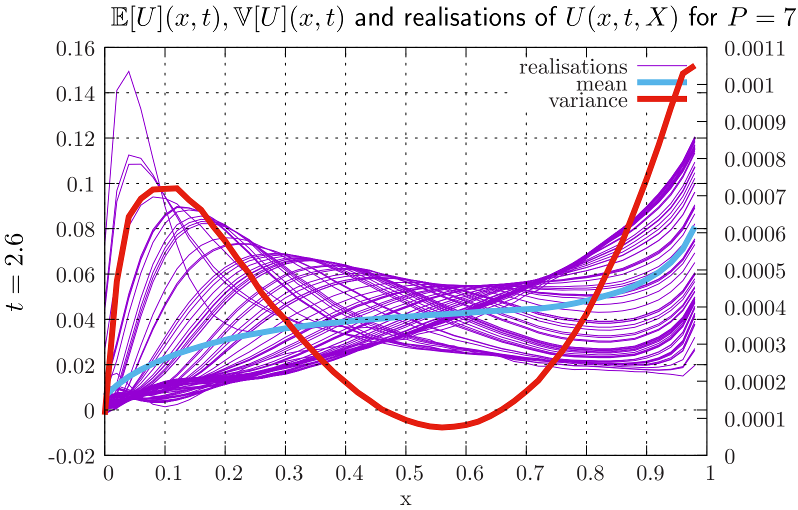
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



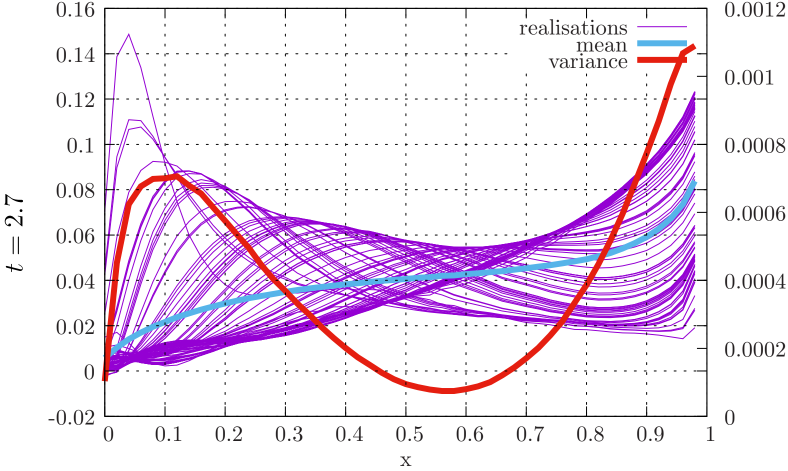
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



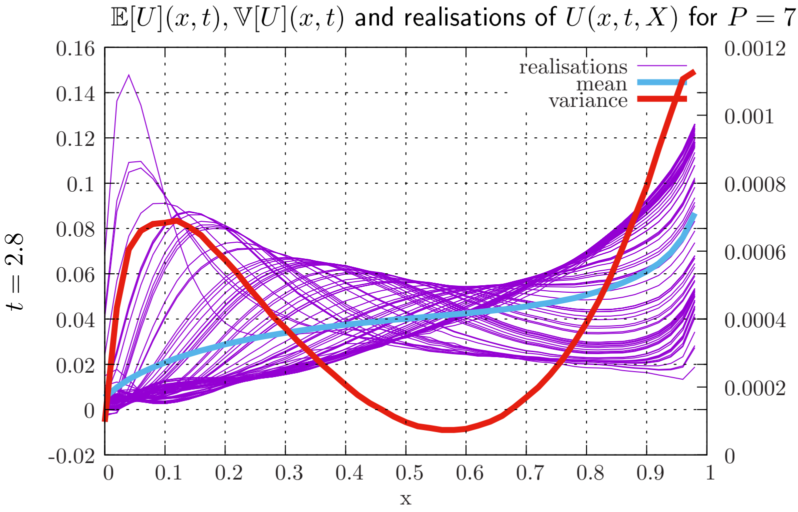
Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



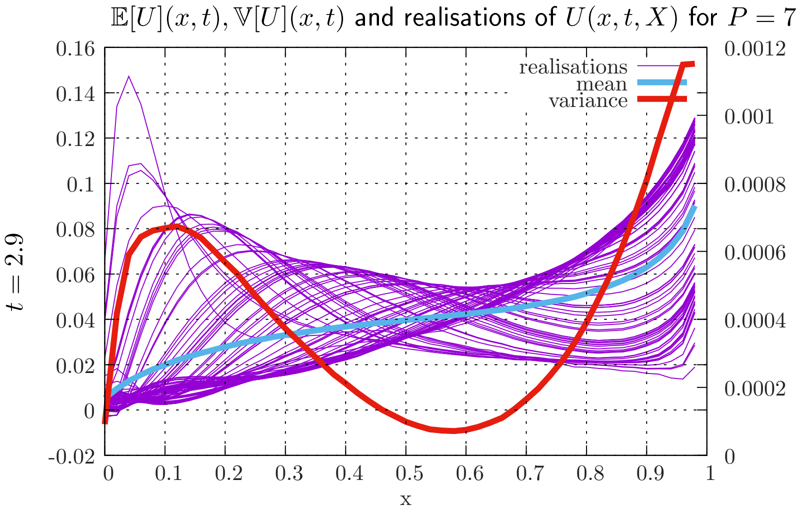
$\mathbb{E}[U](x,t), \mathbb{V}[U](x,t)$ and realisations of $U(x,t,X)$ for $P = 7$



Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)

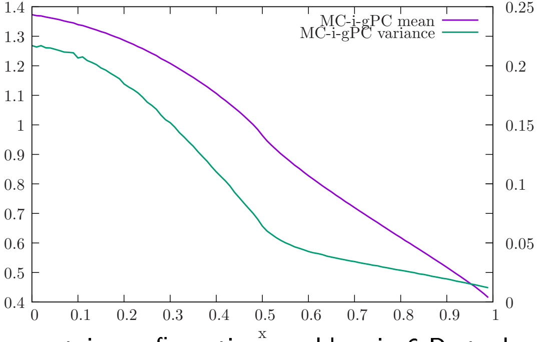


Uncertain linear Boltzmann equation
(with uncertain anisotropic scattering)



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

Mean and Variance of $U(x, t = 1, X)$



A two layered uncertain configuration: problem in 6-D stochastic dimension.

- each layer of media has uncertain σ_t, σ_s, η
- We need the sensitivity indices (Sobol indices) of $U(x, t, X)$.

To obtain the above solution:

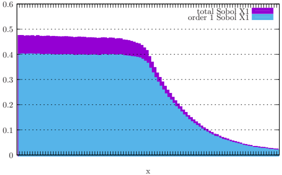
- Run 1.024×10^9 particles, $(P + 1)^6 = 729$ on 1024 proc. in $750s$.
- n-i gPC would need, same accuracies and restitution times, 131072 proc.

A two layered uncertain material: sensitivity analysis in 6D

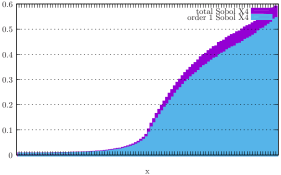
Total and first order Sobol indices

σ_s

$\mathbb{S}_1^{\text{tot}}[U](x, t = 1)$ vs. $\mathbb{S}_1^1[U](x, t = 1)$

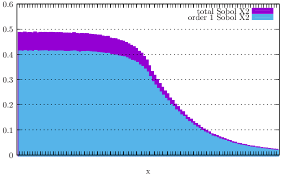


$\mathbb{S}_4^{\text{tot}}[U](x, t = 1)$ vs. $\mathbb{S}_4^1[U](x, t = 1)$

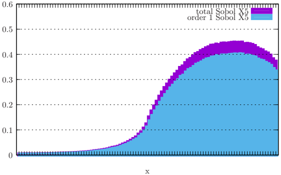


σ_t

$\mathbb{S}_2^{\text{tot}}[U](x, t = 1)$ vs. $\mathbb{S}_2^1[U](x, t = 1)$

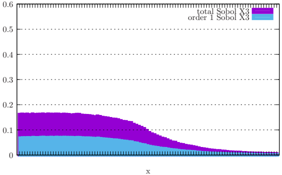


$\mathbb{S}_5^{\text{tot}}[U](x, t = 1)$ vs. $\mathbb{S}_5^1[U](x, t = 1)$

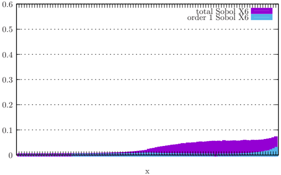


η

$\mathbb{S}_3^{\text{tot}}[U](x, t = 1)$ vs. $\mathbb{S}_3^1[U](x, t = 1)$



$\mathbb{S}_6^{\text{tot}}[U](x, t = 1)$ vs. $\mathbb{S}_6^1[U](x, t = 1)$



1 A particular context (MC resolution of the deterministic transport equation)

2 Non-intrusive computation of the Sobol indices for the transport equation

3 The gPC intrusive MC scheme for the uncertain linear Boltzmann equation

4 Test-cases, comparisons, performance considerations

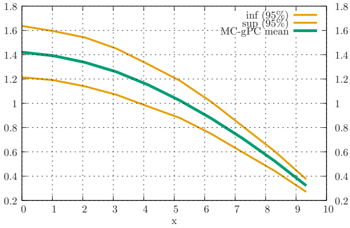
5 Preliminary results on nonlinear problems (k_{eff} computations and photonics)

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

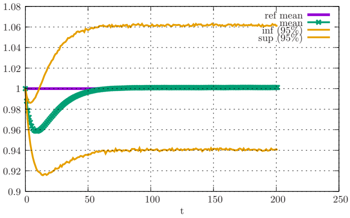
$$\begin{cases} \mathbf{v} \cdot \nabla_{\mathbf{x}} u(\mathbf{x},\mathbf{v}) + v\sigma_t(\mathbf{x},\mathbf{v})u(\mathbf{x},\mathbf{v}) = v\sigma_s(\mathbf{x},\mathbf{v}) \int P_s(\mathbf{x},\mathbf{v}\cdot\mathbf{v}')u(\mathbf{x},\mathbf{v}')d\mathbf{v}', \\ \qquad + \dfrac{v\nu_f(\mathbf{x},\mathbf{v})\sigma_f(\mathbf{x},\mathbf{v})}{k_{\text{eff}}} \int P_f(\mathbf{x},\mathbf{v}\cdot\mathbf{v}')u(\mathbf{x},\mathbf{v}')d\mathbf{v}', \\ u(\mathbf{x},\mathbf{v}) = u_b(\mathbf{v}), \quad \mathbf{x} \in \partial\mathcal{D}, \quad \frac{\mathbf{v}}{v}\cdot n_s < 0, \text{ with } |\mathbf{v}| = v. \end{cases} \tag{2}$$

- Need for additional numerical tools (stochastic power iteration), see [11].
- Uncertain k_{eff} computations with uncertain $\sigma_a, \sigma_s, \sigma_f, \nu$

Statistics of $x \to \int u(x,\omega,X)d\omega$



Statistics of k_{eff}

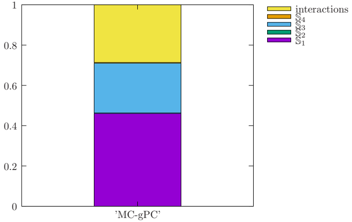


- We are interested in taking into account uncertainties on k_{eff} , u such that

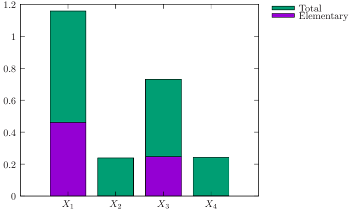
$$\begin{cases} \mathbf{v}\cdot\nabla_{\mathbf{x}}u(\mathbf{x},\mathbf{v})+v\sigma_t(\mathbf{x},\mathbf{v})u(\mathbf{x},\mathbf{v}) = v\sigma_s(\mathbf{x},\mathbf{v})\displaystyle\int P_s(\mathbf{x},\mathbf{v}\cdot\mathbf{v}')u(\mathbf{x},\mathbf{v}')d\mathbf{v}', \\ \qquad +\dfrac{v\nu_f(\mathbf{x},\mathbf{v})\sigma_f(\mathbf{x},\mathbf{v})}{k_{\text{eff}}}\displaystyle\int P_f(\mathbf{x},\mathbf{v}\cdot\mathbf{v}')u(\mathbf{x},\mathbf{v}')d\mathbf{v}', \\ u(\mathbf{x},\mathbf{v}) = u_b(\mathbf{v}), \quad \mathbf{x}\in\partial\mathcal{D}, \quad \frac{\mathbf{v}}{v}\cdot n_s<0, \text{ with } |\mathbf{v}|=v. \end{cases} \quad (2)$$

- Need for additional numerical tools (stochastic power iteration), see [11].
- Uncertain k_{eff} computations with uncertain $\sigma_a, \sigma_s, \sigma_f, \nu$

Elementary & interactions on k_{eff}



Total and elementary on k_{eff}



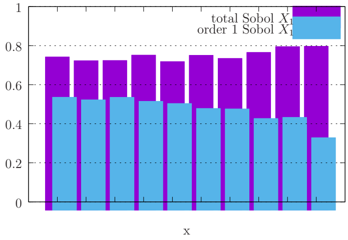
Uncertain k_{eff} computations
Work in collaboration with E. Brun (DES), see [11]

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

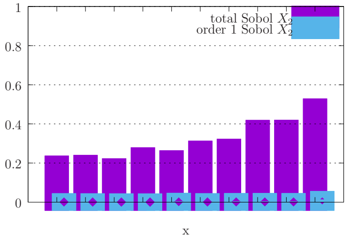
$$\left\{\begin{array}{l} \mathbf{v}\cdot\nabla_{\mathbf{x}}u(\mathbf{x},\mathbf{v})+v\sigma_t(\mathbf{x},\mathbf{v})u(\mathbf{x},\mathbf{v})=v\sigma_s(\mathbf{x},\mathbf{v})\int P_s(\mathbf{x},\mathbf{v}\cdot\mathbf{v}')u(\mathbf{x},\mathbf{v}')d\mathbf{v}', \\ \qquad +\dfrac{v\nu_f(\mathbf{x},\mathbf{v})\sigma_f(\mathbf{x},\mathbf{v})}{k_{\text{eff}}}\int P_f(\mathbf{x},\mathbf{v}\cdot\mathbf{v}')u(\mathbf{x},\mathbf{v}')d\mathbf{v}', \\ u(\mathbf{x},\mathbf{v})=u_b(\mathbf{v}),\quad \mathbf{x}\in\partial\mathcal{D},\quad \frac{\mathbf{v}}{v}\cdot n_s<0,\ \text{with } |\mathbf{v}|=v. \end{array}\right. \qquad (2)$$

- Need for additional numerical tools (stochastic power iteration), see [11].
- Uncertain k_{eff} computations with uncertain $\sigma_a, \sigma_s, \sigma_f, \nu$

Sobol indice for $\sigma_a(X_1)$



Sobol indice for $\sigma_s(X_2)$

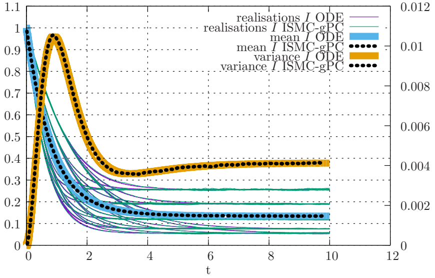


- We are interested in taking into account uncertainties on I, E solutions of

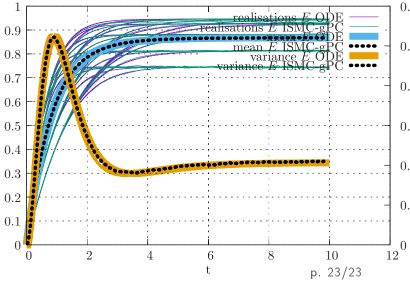
$$\begin{cases} \frac{1}{c}\partial_t I(x,t,\omega,X) + \omega\cdot\nabla I(x,t,\omega,X) + \sigma_t(E(x,t,X),X) I(x,t,\omega,X) \\ \qquad = \sigma_a(E(x,t,X),X)B(E(x,t,X)) + \sigma_s(E(x,t,X),X)\int I(x,t,\omega',X)\mathrm{d}\omega', \\ \partial_t E(x,t,X) = c\sigma_a(E(x,t,X),X)\int \left(I(x,t,\omega',X) - B(E(x,t,X))\right)\mathrm{d}\omega', \\ X \sim \mathrm{d}\mathcal{P}_X. \end{cases} \tag{3}$$

- Need for additional theoretical material (for wellposedness), see [10].
- Uncertain photonics with uncertain σ_a, C_v

$t, X \to I^{p_{1D}=4}(t,X)$



$t, X \to E^{p_{1D}=4}(t,X)$

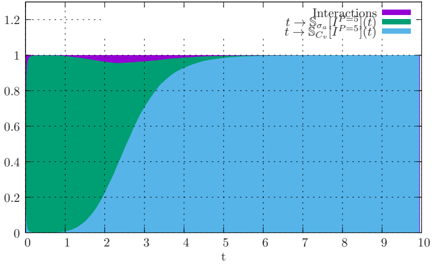


- We are interested in taking into account uncertainties on I, E solutions of

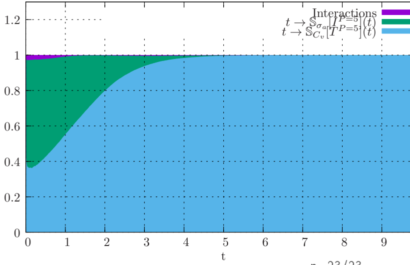
$$\begin{cases} \frac{1}{c}\partial_t I(x,t,\omega,X) + \omega\cdot\nabla I(x,t,\omega,X) + \sigma_t(E(x,t,X),X)I(x,t,\omega,X) \\ \qquad = \sigma_a(E(x,t,X),X)B(E(x,t,X)) + \sigma_s(E(x,t,X),X)\int I(x,t,\omega',X)\mathrm{d}\omega', \\ \partial_t E(x,t,X) = c\sigma_a(E(x,t,X),X)\int \left(I(x,t,\omega',X) - B(E(x,t,X))\right)\mathrm{d}\omega', \\ X \sim \mathrm{d}\mathcal{P}_X. \end{cases} \tag{3}$$

- Need for additional theoretical material (for wellposedness), see [10].
- Uncertain photonics with uncertain σ_a, C_v

$t \to \mathbb{S}_i[I^{P=5}](t),\ i \in \{\sigma_a, C_v, \{\sigma_a, C_v\}\}$



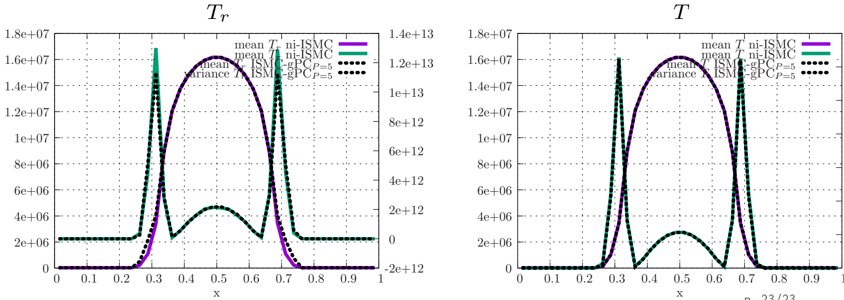
$t \to \mathbb{S}_i[T^{P=5}](t),\ i \in \{\sigma_a, C_v, \{\sigma_a, C_v\}\}$



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

$$\left\{\begin{aligned} &\frac{1}{c}\partial_t I(x,t,\omega,X) + \omega\cdot\nabla I(x,t,\omega,X) + \sigma_t(E(x,t,X),X) I(x,t,\omega,X) \\ &\qquad\quad = \sigma_a(E(x,t,X),X) B(E(x,t,X)) + \sigma_s(E(x,t,X),X)\int I(x,t,\omega',X)\mathrm{d}\omega', \\ &\partial_t E(x,t,X) = c\sigma_a(E(x,t,X),X)\int \left(I(x,t,\omega',X) - B(E(x,t,X))\right)\mathrm{d}\omega', \\ &X \sim \mathrm{d}\mathcal{P}_X. \end{aligned}\right. \tag{3}$$

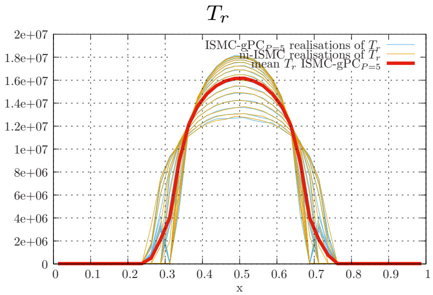
- Need for additional theoretical material (for wellposedness), see [10].
- Uncertain photonics with uncertain σ_a, C_v

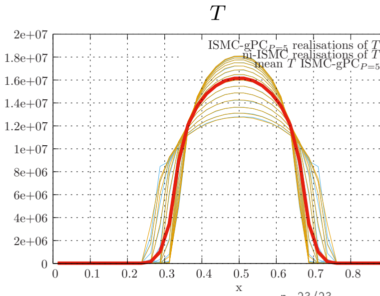


- We are interested in taking into account uncertainties on I, E solutions of

$$\begin{cases} \frac{1}{c}\partial_t I(x,t,\omega,X) + \omega\cdot\nabla I(x,t,\omega,X) + \sigma_t(E(x,t,X),X)I(x,t,\omega,X) \\ \qquad = \sigma_a(E(x,t,X),X)B(E(x,t,X)) + \sigma_s(E(x,t,X),X)\int I(x,t,\omega',X)\mathrm{d}\omega', \\ \partial_t E(x,t,X) = c\sigma_a(E(x,t,X),X)\int \left(I(x,t,\omega',X) - B(E(x,t,X))\right)\mathrm{d}\omega', \\ X \sim \mathrm{d}\mathcal{P}_X. \end{cases} \quad (3)$$

- Need for additional theoretical material (for wellposedness), see [10].
- Uncertain photonics with uncertain σ_a, C_v





Conclusion:

- Spectral convergence w.r.t. P of the MC-i-gPC reduced models in [9].
- Convergence w.r.t N_{MC} of the MC-i-gPC scheme for fixed P in [8].
- The MC-i-gPC scheme is still sensitive to the curse of dimensionality *via*:
  - The storing in memory of $(P+1)^Q$ gPC coefficients,

  $\Longrightarrow$ but we can focus on parts of the spatial or velocity domain to store less
  - The tallying of the MC particles contributions,

  $\Longrightarrow$ but this phase can certainly benefit some shared memory accelerations (vectorisation of the polynomial construction, modified Chebyshev algorithm).
- The MC-i-gPC scheme allows important gains for low stochastic dimensions (interesting results at least for Q ranging from 1 to 10)

ϕsics Nonlinear physics (neutronics, photonics...) but need for additional material

Perspectives:

UQ MC-i-gPC scheme is compatible with other indices (HSIC [4] for example)

HPC Test the vectorisation acceleration and tackle higher dimensions

Questions?

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

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

References I

G.A. Bird.
Molecular Gas Dynamics and the Direct Simulation of Gas Flows.
Number vol. 1 in Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Clarendon Press, 1994.

A. V. Bobylev and K. Nanbu.
Theory of collision algorithms for gases and plasmas based on the boltzmann equation and the landau-fokker-planck equation.
Phys. Rev. E, 61:4576–4586, Apr 2000.

Cacucci and Dan G.
Handbook of Nuclear Engineering, volume 1.
Springer Science & Business Media, 2010.

Sebastien Da Veiga.
Global sensitivity analysis with dependence measures.
Journal of Statistical Computation and Simulation, 85(7):1283–1305, Aug 2014.

Bertrand Iooss and Paul Lemaître.
A review on global sensitivity analysis methods.
In C. Meloni and G. Dellino, editors, *Uncertainty management in Simulation-Optimization of Complex Systems: Algorithms and Applications*. Springer, 2015.

B. Lapeyre, E. Pardoux, and R. Sentis.
Méthodes de Monte Carlo pour les équations de transport et de diffusion.
Number 29 in Mathématiques & Applications. Springer-Verlag, 1998.

G. Poëtte.
Contribution à l'analyse mathématique et numérique des systèmes de lois de conservation incertains et de l'équation de boltzmann linéaire et non-linéaire.
Habilitation à Diriger des Recherches, Université ??, 201?

References II

G. Poëtte.
A gPC-intrusive Monte-Carlo scheme for the resolution of the uncertain linear Boltzmann equation.
accepted to J. Comp. Phys., 2018.

G. Poëtte.
Spectral convergence of the generalized Polynomial Chaos reduced model obtained from the uncertain linear Boltzmann equation.
Preprint submitted to Mathematics and Computers in Simulation, 2019.

G. Poëtte.
Combining Implicit Semi-analog Monte Carlo (ISMC)
and Monte Carlo generalised Polynomial Chaos (MC-gPC)
for efficient uncertainty propagation for photonics.
Preprint, 2020.

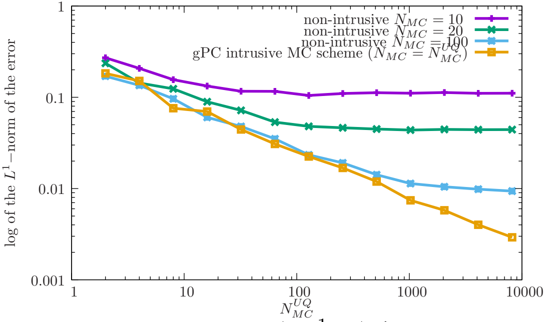
G. Poëtte and E. Brun.
Efficient uncertain k_{eff} computations with the Monte-Carlo resolution of generalised Polynomial Chaos Based reduced models.
Preprint, 2020.

I. Sobol.
Sensitivity estimates for nonlinear mathematical models.
Matematicheskoe Modelirovanie, 2:112–118, 1990.
in Russian, translated in English in Sobol, I. (1993). Sensitivity analysis for non-linear mathematical models. Mathematical Modeling & Computational Experiment (Engl. Transl.), 1993, 1, 407–414.

The solutions are given by

$$\begin{aligned} M_1^U(t) = \mathbb{E}[U(t,X)] &= \tfrac{1}{2}U_0 e^{-v\overline{\sigma}_a t}\frac{e^{v\hat{\sigma}_s t} - e^{-v\hat{\sigma}_s t}}{\hat{\sigma}_s t v}, \\ M_2^U(t) = \mathbb{E}[U^2(t,X)] &= \tfrac{1}{4}U_0^2 e^{-2v\overline{\sigma}_a t}\frac{e^{2v\hat{\sigma}_s t} - e^{-2v\hat{\sigma}_s t}}{\hat{\sigma}_s t v}, \\ \mathbb{V}[U](t) &= M_2^U(t) - (M_1^U(t))^2. \end{aligned} \quad (4)$$

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



The error e for the UQ problem is now $e = \mathcal{O}(\frac{1}{\sqrt{N_{MC}}})$ **(for this test-pb at least!)**

The configuration is the following:

- $v = 1$, $x \in \mathcal{D} = [0,1]$, subdivided into $N_x = 100$ cells $\cup_{i=1}^{N_x} \mathcal{D}_i = \mathcal{D}$.
- Specular left boundary condition (at $x = 0$) and vacuum right one (at $x = 1$).
- Initially, the density of particles is homogeneous and deterministic, equal to 1.
- The medium is pure $\sum_{m=1}^{M} \sigma_\alpha^m \eta_m = \sigma_\alpha \eta, \forall \alpha \in \{s,t\}$ and homogeneous.
- It is uncertain and depends on three parameters $X = (X_1, X_2, X_3)$ such that

$$\begin{array}{llll}
\sigma_t(x,t,X) & = \sigma_t(X_1) & = \overline{\sigma}_t + \widehat{\sigma}_t X_1, & \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \\
\sigma_s(x,t,\omega,\omega',X) & = \sigma_s(X_2) & = \overline{\sigma}_s + \widehat{\sigma}_s X_2, & \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \forall(\omega,\omega') \in \mathcal{S}^2, \\
\eta(x,t,X) & = \eta(X_3) & = \overline{\eta} + \widehat{\eta} X_3, & \forall x \in \mathcal{D}, t \in \mathbb{R}^+,
\end{array}$$

- (X_1, X_2, X_3) are independent uniformly distributed RVs on $[-1,1]$.
- For the next computations, the mean quantities are set to
  $\overline{\sigma}_t = 1.0$, $\overline{\sigma}_s = 0.9$, $\overline{\eta} = 1.0$ and the ones controling the variability to
  $\widehat{\sigma}_t = 0.4$, $\widehat{\sigma}_s = 0.4$, $\widehat{\eta} = 0.4$.
- 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**

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 $\mathcal{D}_A = [0, \frac{1}{2}]$ 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

$$\begin{aligned} \sigma_t(x,t,X) &= \sum_{i \in \{A,B\}} \left[\overline{\sigma}_t^i + \widehat{\sigma}_t^i X_1^i\right] \mathbf{1}_{\mathcal{D}_i}(x), \quad \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \\ \sigma_s(x,t,\omega,\omega',X) &= \sum_{i \in \{A,B\}} \left[\overline{\sigma}_s^i + \widehat{\sigma}_s^i X_2^i\right] \mathbf{1}_{\mathcal{D}_i}(x), \quad \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \\ \eta(x,t,X) &= \sum_{i \in \{A,B\}} \left[\overline{\eta}^i + \widehat{\eta}^i X_3^i\right] \mathbf{1}_{\mathcal{D}_i}(x), \quad \forall x \in \mathcal{D}, t \in \mathbb{R}^+, \end{aligned} \tag{6}$$

- $(X_1^i, X_2^i, X_3^i)_{i \in \{A,B\}}$ are independent uniformly distributed RVs on $[-1, 1]$.
- For the next computations, the mean quantities are set to

$$\begin{aligned} &\overline{\sigma}_t^A = 1.0,\ \overline{\sigma}_s^A = 1.3,\ \overline{\eta}^A = 1.0, \qquad \widehat{\sigma}_t^A = 0.4,\ \widehat{\sigma}_s^A = 0.4,\ \widehat{\eta}^A = 0.4, \\ &\overline{\sigma}_t^B = 1.0,\ \overline{\sigma}_s^B = 0.9,\ \overline{\eta}^B = 1.0, \qquad \widehat{\sigma}_t^B = 0.4,\ \widehat{\sigma}_s^B = 0.4,\ \widehat{\eta}^B = 0.4, \end{aligned}$$

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

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

6 Why do we need a relevant linearisation?

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

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

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

- Let us multiply the transport equation by u to obtain

$$\partial_t \frac{u^2}{2}(\mathbf{x},t,\mathbf{v},X) + \mathbf{v}\cdot\nabla\frac{u^2}{2}(\mathbf{x},t,\mathbf{v},X) = -v\sigma_t(\mathbf{x},t,\mathbf{v},X)u^2(\mathbf{x},t,\mathbf{v},X) + u(\mathbf{x},t,\mathbf{v},X)\int v\sigma_s(\mathbf{x},t,\mathbf{v},\mathbf{v}',X)u(\mathbf{x},t,\mathbf{v}',X)\mathbf{dv}',$$

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

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

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

- Nonlinearity demands a splitting/linearisation hypothesis.
- The most common linearisation strategies for this type of quadratic operator:
  - Nanbu-like method [2] ($\mathcal{O}(\Delta t)$ splitting)
    (would need small time steps in very collisional media)
  - Bird-like method [1] ($\mathcal{O}(\Delta t)$ splitting).
    (would also need small time steps in very collisional media)
  - Posttreatment of a count rate file from an analog resolution [3] $\mathcal{O}(\Delta t)$.
    (explosion of the I/O and file size close to criticity)
  - We here only suggest a new linearisation (with respect to P introduced later).
    (see [8, 9, 7])