

# Scaling up of an underground waste disposal model with random source terms

F. Smaï<sup>1</sup>, O. Gipouloux<sup>1</sup>

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Setting the problem

A model of random  
sources

Simulation on a  
synthesized case

Deterministic limit  
equation

Global error estimate

Random corrector

# Plan

## Setting the problem

- Transport equation
- Geometry of sources
- Randomness of the sources

## A model of random sources

- Altered glass model
- Introduction of the randomness

## Simulation on a synthesized case

- Geometry and physical characteristics
- Observables

## Deterministic limit equation

- Theoretical result
- Distribution of  $u^\varepsilon$  vs  $u^0$

## Global error estimate

## Random corrector

- Pointwise result
- Vectorial result

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# Setting the problem

## Transport equation

- ▶ We consider a convection-diffusion problem describing the transport of radionuclide in porous media :

$$\begin{aligned}\partial_t u^\varepsilon - \nabla(a(x)\nabla u^\varepsilon - \mathbf{b}(x)u^\varepsilon) + \lambda u^\varepsilon &= Q^\varepsilon && \text{in } [0; T] \times \mathcal{D} \\ u^\varepsilon &= 0 && \text{in } \{0\} \times \mathcal{D} \\ (a(x)\nabla u^\varepsilon - \mathbf{b}(x)u^\varepsilon) \cdot \mathbf{n}(x) &= 0 && \text{in } [0; T] \times (\partial\mathcal{D} \setminus \Gamma_d) \\ u^\varepsilon &= 0 && \text{in } [0; T] \times \Gamma_d\end{aligned}$$

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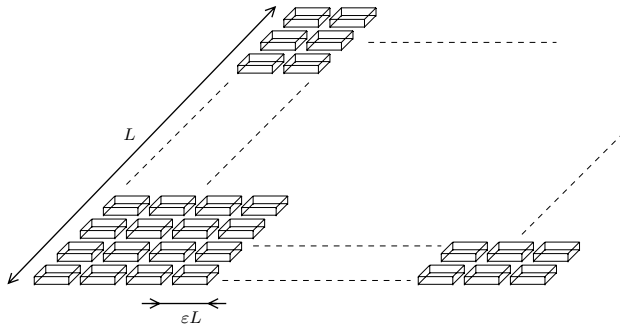
$$\begin{aligned}\partial_t u^\varepsilon - \nabla(a(x)\nabla u^\varepsilon - \mathbf{b}(x)u^\varepsilon) + \lambda u^\varepsilon &= Q^\varepsilon && \text{in } [0; T] \times \mathcal{D} \\ u^\varepsilon &= 0 && \text{in } \{0\} \times \mathcal{D} \\ (a(x)\nabla u^\varepsilon - \mathbf{b}(x)u^\varepsilon) \cdot \mathbf{n}(x) &= 0 && \text{in } [0; T] \times (\partial\mathcal{D} \setminus \Gamma_d) \\ u^\varepsilon &= 0 && \text{in } [0; T] \times \Gamma_d\end{aligned}$$

- ▶ The superscript  $\varepsilon$  on the concentration,  $u^\varepsilon$ , and on the source term,  $Q^\varepsilon$ , is related to spatial periodicity of sources

# Setting the problem

## Geometry of sources

- ▶ The small parameter  $\varepsilon$  characterizes the ratio between the size of the whole disposal site and the size of one source



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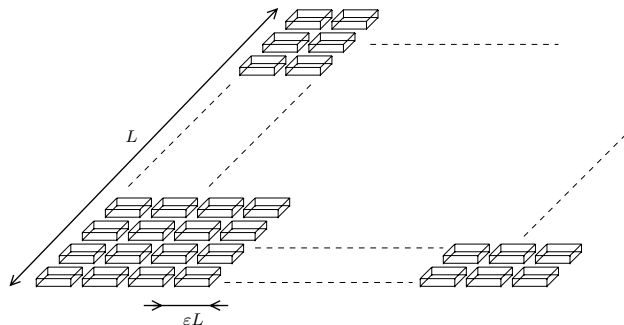
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# Setting the problem

## Geometry of sources

- ▶ The small parameter  $\varepsilon$  characterizes the ratio between the size of the whole disposal site and the size of one source



- ▶ In the case of identical and deterministic sources, the source term is written as

$$Q^\varepsilon(t, x) = \mathbf{1}_{B^\varepsilon}(x) \frac{1}{\varepsilon^\gamma} f(t)$$

# Setting the problem

## Randomness of the sources

- ▶ In the case of random sources, the source term becomes

$$Q^\varepsilon(\omega, t, x) = \mathbf{1}_{B^\varepsilon} \frac{1}{\varepsilon^\gamma} f_{\mathbf{z}}(\omega, t) \quad \text{with } \mathbf{z} = [x'/L\varepsilon] \in \mathbb{N}^{d-1}$$

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The concentration is now a random field :  $u^\varepsilon(\omega, t, x)$

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- ▶  $f_{\mathbf{z}}(\omega, t)$  describe the randomness of the source indexed by  $\mathbf{z}$
- ▶ We will assume that  $(f_{\mathbf{z}})_{\mathbf{z}}$  satisfies some conditions :
  - ▶ stationarity : all the  $f_{\mathbf{z}}$  follow the same law (we will note  $f(\omega, t)$ )
  - ▶ ergodicity : equivalence between the "spatial" and "probabilistic" means
  - ▶ conditions on "spatial" correlation at large distance

# A model of random sources

## Altered glass model

- ▶ In the altered glass model, the radionuclide release of a package is given by

$$f(t) = qe^{-\lambda t}Q_{VA}(t)$$

- ▶  $q$  : initial fraction of radionuclide in the package
- ▶  $qe^{-\lambda t}$  : fraction of radionuclide in the package at time  $t$
- ▶  $Q_{VA}(t)$  : velocity of the glass alteration

# A model of random sources

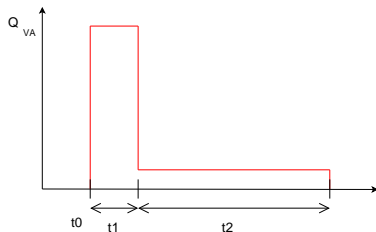
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$$Q_{VA}(t) = \begin{cases} M_1/t_1 & \text{if } 0 < t - t_0 \leq t_1 \\ M_2/t_2 & \text{if } 0 < t - t_0 - t_1 \\ & \leq t_0 + t_1 + t_2 \\ 0 & \text{otherwise} \end{cases}$$



# A model of random sources

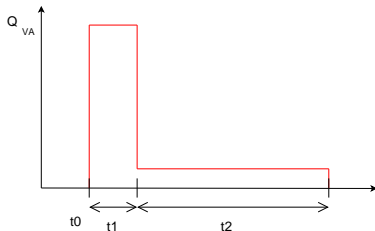
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- ▶ 4 parameters define the source behavior :  
 $q$  ("amplitude") and  $t_0$ ,  $t_1$  and  $t_2$  ("form")

# A model of random sources

## Introduction of the randomness

- ▶ In the following simulations, the 4 parameters ( $q, t_0, t_1$  and  $t_2$ ) are considered random, independent for a given source and independent from a source to another

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# A model of random sources

## Introduction of the randomness

- ▶ In the following simulations, the 4 parameters ( $q, t_0, t_1$  and  $t_2$ ) are considered random, independent for a given source and independent from a source to another
- ▶ Other models are possible, for instance models with spatial correlation, but the results are the same

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# Simulation on a synthesized case

## Geometry and physical characteristics

- ▶ Numerical tests are done on a simplified problem :

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# Simulation on a synthesized case

## Geometry and physical characteristics

- ▶ Numerical tests are done on a simplified problem :
  - ▶ Two dimensional geometry
  - ▶ Uniform diffusion tensor
  - ▶ No convection
  - ▶ Radioactive element :  $^{129}I$

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# Simulation on a synthesized case

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  - ▶ Radioactive element :  $^{129}I$
- ▶ Simulations are done with *Cast3m*, spatial discretization is EFMH
- ▶ Statistical values are estimated on samples of 2000 realizations

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# Simulation on a synthesized case

## Observables

- ▶ We observe the concentration

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# Simulation on a synthesized case

## Observables

- ▶ We observe the concentration
  - ▶ in two points :  $x_A$  and  $x_B$
  - ▶ and at two time :  $t_1 = 10^5$  *ans* and  $t_2 = 10^6$  *ans*

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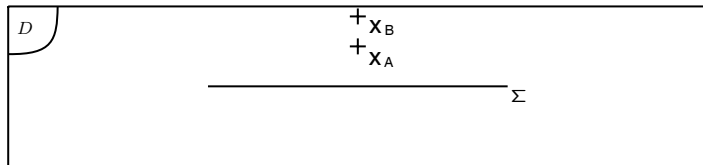
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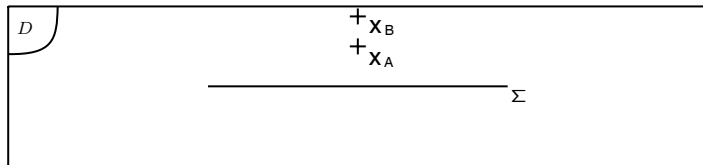
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- ▶  $x_A$  is taken far from the domain boundaries
- ▶  $x_B$  is taken near from the top boundary



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  - ▶ in two points :  $x_A$  and  $x_B$
  - ▶ and at two time :  $t_1 = 10^5$  ans and  $t_2 = 10^6$  ans
- ▶  $x_A$  is taken far from the domain boundaries
- ▶  $x_B$  is taken near from the top boundary
- ▶  $t_1$  corresponds to the time when concentration in  $x_A$  becomes significant
- ▶  $t_2$  corresponds to the time when concentration in  $x_B$  becomes significant



# Deterministic limit equation

## Theoretical result

When  $\varepsilon \rightarrow 0$ ,  $u^\varepsilon$  converges (in  $L^2$  a.s.) to  $u^0$  solution of :

$$\partial_t u^0 + Au^0 = F \quad \text{in } [0; T] \times \mathcal{D}$$

$$u^0 = 0 \quad \text{in } \{0\} \times \mathcal{D}$$

$$(a(x)\nabla u^0 - \mathbf{b}(x)u^0) \cdot \mathbf{n}(x) = 0 \quad \text{in } [0; T] \times (\partial\mathcal{D} \setminus \Gamma_d)$$

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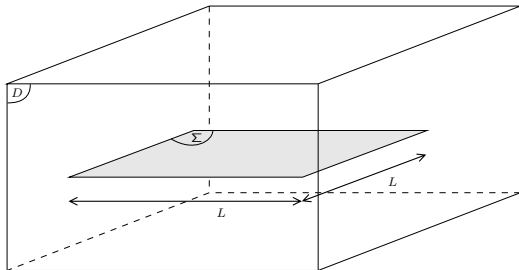
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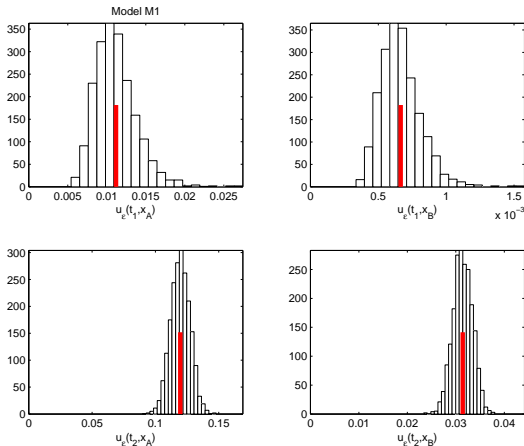
$$u^0 = 0 \quad \text{in } [0; T] \times \Gamma_d$$

with  $F(t, x) = K_{source} \mathbf{E}[f(\cdot, t)] \delta_\Sigma(x)$



# Deterministic limit equation

Distribution of  $u^\varepsilon$  vs  $u^0$



Comparison, for  $\varepsilon = 1/30$ , between the distribution of the r.v.  $u^\varepsilon(t, x)$  (in black) and  $u^0(t, x)$  (in red)

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# Global error estimate

This convergence result can be completed by an estimate of the mean global error

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# Global error estimate

This convergence result can be completed by an estimate of the mean global error

- ▶ Under some assumptions on the spatial correlation, we have the following estimate

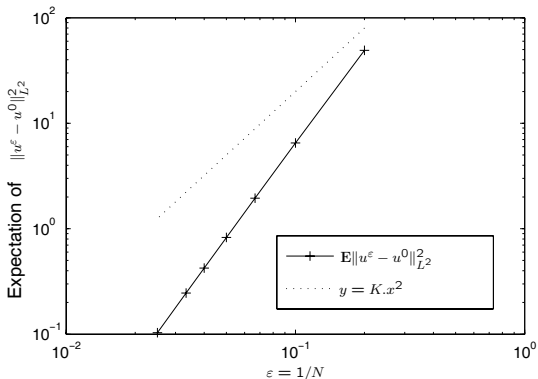
$$\mathbf{E} \left[ \|u^\varepsilon - u^0\|_{L^2(0,T;L^2(\mathcal{D}))}^2 \right] \leq C_1(\varepsilon^2 + \varepsilon^{2\gamma})$$

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$$\mathbf{E} \left[ \|u^\varepsilon - u^0\|_{L^2(0,T;L^2(\mathcal{D}))}^2 \right] \leq C_1(\varepsilon^2 + \varepsilon^{2\gamma})$$



# Random corrector

- ▶  $u^0$  is a good "candidate" to approximate  $u^\varepsilon$

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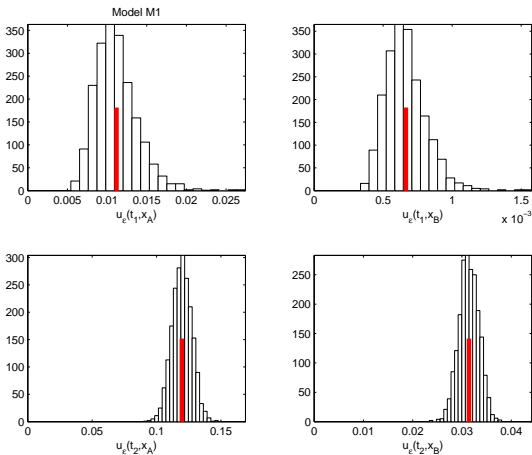
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- ▶  $u^0$  is a good "candidate" to approximate  $u^\varepsilon$
- ▶ But  $u^0$  is deterministic and give only the mean behavior of  $u^\varepsilon$



red :  $u^0$

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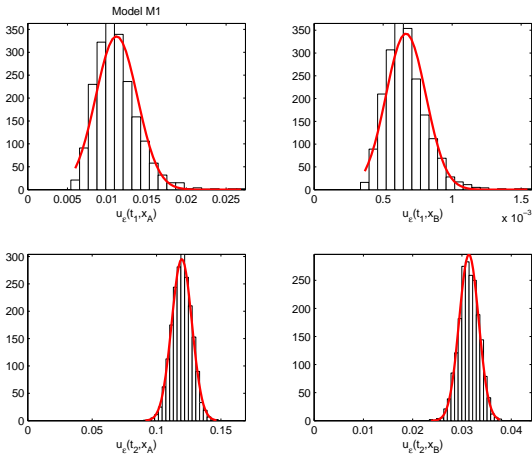
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# Random corrector

- ▶  $u^0$  is a good "candidate" to approximate  $u^\varepsilon$
- ▶ But  $u^0$  is deterministic and give only the mean behavior of  $u^\varepsilon$
- ▶ Therefore we introduce a "random" corrector



red :  $u^0 +$  random corrector

# Random corrector

## Pointwise result (1/3)

- ▶ With additional mixing conditions, the random variable

$$\frac{1}{\varepsilon^{(d-1)/2}}(u^\varepsilon(t, x) - u^0(t, x))$$

converges in law toward a Gaussian random variable

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- ▶ This limit Gaussian r.v. is zero mean and the covariance  $\sigma^2(t, x)$  is given by :

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- ▶ This limit Gaussian r.v. is zero mean and the covariance  $\sigma^2(t, x)$  is given by :

$$\sigma^2(t, x) = \int_0^t \int_0^t \int_{\Sigma} G(t, s, x, y') G(t, r, x, y') \bar{c}(s, r) dy' ds dr$$

# Random corrector

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where

$$\bar{c}(t, s) = \lim_{N \rightarrow \infty} \frac{s_d^2 L^{d+1}}{N^{d-1}} \int_{[0, N]^{d-1}} \int_{[0, N]^{d-1}} R(t, s, y, z) \mathbf{1}_{\tilde{B}}(y) \mathbf{1}_{\tilde{B}}(z) dy dz$$

# Random corrector

## Pointwise result (1/3)

- ▶ With additional mixing conditions, the random variable

$$\frac{1}{\varepsilon^{(d-1)/2}} (u^\varepsilon(t, x) - u^0(t, x))$$

converges in law toward a Gaussian random variable

- ▶ This limit Gaussian r.v. is zero mean and the covariance  $\sigma^2(t, x)$  is given by :

$$\sigma^2(t, x) = \int_0^t \int_0^t \int_{\Sigma} G(t, s, x, y') G(t, r, x, y') \bar{c}(s, r) dy' ds dr$$

where

$$\bar{c}(t, s) = \lim_{N \rightarrow \infty} \frac{s_d^2 L^{d+1}}{N^{d-1}} \int_{[0, N]^{d-1}} \int_{[0, N]^{d-1}} R(t, s, y, z) \mathbf{1}_{\tilde{B}}(y) \mathbf{1}_{\tilde{B}}(z) dy dz$$

$$R(t, s, y, z) = \text{Cov} [f_{[y]}(\cdot, t), f_{[z]}(\cdot, s)]$$

# Random corrector

## Pointwise result (2/3)

- ▶ We rescale  $\frac{1}{\varepsilon^{(d-1)/2}}(u^\varepsilon(t, x) - u^0(t, x))$  according to  $\sigma$  in order to compare it with the standard normal law (mean=0, covariance=1)

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- ▶ We quantify the distance between an empirical distribution and a probability law

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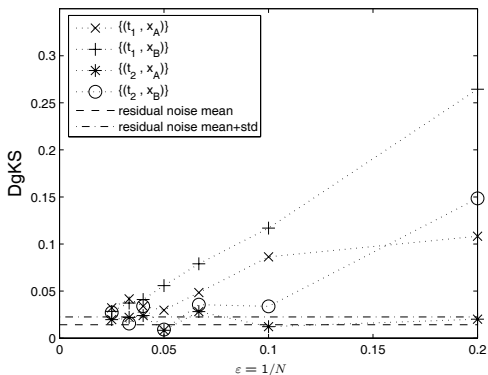
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- ▶ We quantify the distance between an empirical distribution and a probability law



# Random corrector

## Pointwise result (3/3)

- ▶ For  $G(\omega, t, x)$  a Gaussian r.v. with parameters  $(0, \sigma(t, x))$ ,

$$\bar{u}^\varepsilon(\omega, t, x) \equiv u^0(t, x) + \varepsilon^{(d-1)/2} G(\omega, t, x)$$

is an approximation (in law) of  $u^\varepsilon(\omega, t, x)$

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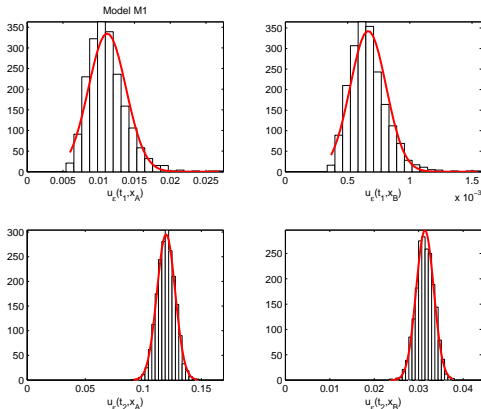
# Random corrector

## Pointwise result (3/3)

- For  $G(\omega, t, x)$  a Gaussian r.v. with parameters  $(0, \sigma(t, x))$ ,

$$\bar{u}^\varepsilon(\omega, t, x) \equiv u^0(t, x) + \varepsilon^{(d-1)/2} G(\omega, t, x)$$

is an approximation (in law) of  $u^\varepsilon(\omega, t, x)$



Distribution of  $u^\varepsilon(t, x)$  (in black) and distribution of  $\bar{u}^\varepsilon(t, x)$  (in red) 16 / 21

# Random corrector

## Vectorial result (1/3)

- ▶ This result can be extended by taking in account the correlation of the random field between time/space point

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## Vectorial result (1/3)

- ▶ This result can be extended by taking in account the correlation of the random field between time/space point
- ▶ Instead of a unique point  $(t, x)$ , now we consider a set of points

$$\{(t^1, x^1), \dots, (t^k, x^k)\}$$

# Random corrector

## Vectorial result (1/3)

- ▶ This result can be extended by taking in account the correlation of the random field between time/space point
- ▶ Instead of a unique point  $(t, x)$ , now we consider a set of points

$$\{(t^1, x^1), \dots, (t^k, x^k)\}$$

- ▶ and the random variable  $u^\varepsilon(t, x)$  is replaced by the random vector

$$(u^\varepsilon(t^j, x^j))_{j=1, \dots, k}$$

# Random corrector

## Vectorial result (2/3)

- ▶ Under additional assumptions on the time randomness, the random vector

$$\left( \varepsilon^{-(d-1)/2} (u^\varepsilon(t^j, x^j) - u^0(t^j, x^j)) \right)_{j=1, \dots, k}$$

converges in law toward a Gaussian random vector

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- ▶ This Gaussian limit vector is zero mean and its covariance matrix is given by :

$$\sigma^{i,j} = \int_0^{t^i} \int_0^{t^j} \int_{\Sigma} G(t^i, s, x^i, y') G(t^j, r, x^j, y') \bar{c}(s, r) dy' ds dr$$

# Random corrector

## Vectorial result (3/3)

- ▶ We rescale  $(\varepsilon^{-(d-1)/2}(u^\varepsilon(t^j, x^j) - u^0(t^j, x^j)))_{j=1, \dots, k}$  according to  $\sigma$  in order to compare it with standard normal law (mean=0, covariance= $Id$ )

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- ▶ We generalize the Kolmogorov-Smirnov distance to random vectors

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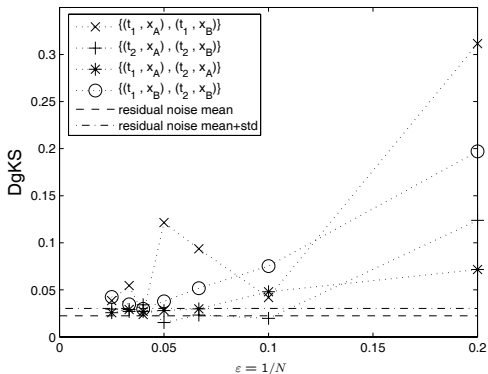
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# Conclusion

- ▶ Taking in account uncertainties in the source term behavior in a scaling up approach

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# Conclusion

- ▶ Taking in account uncertainties in the source term behavior in a scaling up approach
  - ▶ Deterministic approximation associated to a "global" source term

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# Conclusion

- ▶ Taking in account uncertainties in the source term behavior in a scaling up approach
  - ▶ Deterministic approximation associated to a "global" source term
  - ▶ Random corrector including spatial and time correlations

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# Conclusion

- ▶ Taking in account uncertainties in the source term behavior in a scaling up approach
  - ▶ Deterministic approximation associated to a "global" source term
  - ▶ Random corrector including spatial and time correlations
- ▶ Numerical validation on a synthesized model

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# Conclusion

- ▶ Taking in account uncertainties in the source term behavior in a scaling up approach
  - ▶ Deterministic approximation associated to a "global" source term
  - ▶ Random corrector including spatial and time correlations
- ▶ Numerical validation on a synthesized model
  - ▶ Effective computation of the deterministic approximation and the random corrector

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# Conclusion

- ▶ Taking in account uncertainties in the source term behavior in a scaling up approach
  - ▶ Deterministic approximation associated to a "global" source term
  - ▶ Random corrector including spatial and time correlations
- ▶ Numerical validation on a synthesized model
  - ▶ Effective computation of the deterministic approximation and the random corrector
  - ▶ Theoretical convergences are numerically verified

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# References



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