Méthode particulaire & transport en milieux poreux

MABordeaux : Héloise Beaugendre, Iraj Mortazavi,

EGID Bordeaux : Olivier Atteia,

LOMC Le Havre : Elie Rivoalen, Anthony Beaudoin,

IEC Nancy : Antoine Lejay,

LIMSI Orsay :Olivier Le Maître, Lionel Mathelin,

LEA Poitiers : Serge huberson,

Objectives :

Particle method

- streamlines methods+ diffusion.
- uncertain transport.
- real-life application.

Particle method

convection-dispersion equation

$$\frac{\partial c}{\partial t} + \mathrm{div}(\vec{u}\ c) = \mathrm{div}\left(\overline{\overline{D}} \cdot \overrightarrow{\mathrm{grad}}(c)\right) - \lambda c + S$$

c : concentration field

u : velocity field

D : dispersion tensor $D_{11} = \frac{u_1^2}{|\vec{u}|}\nu_l + \frac{u_2^2}{|\vec{u}|}\nu_t, \quad D_{12} = \frac{u_1 u_2}{|\vec{u}|}(\nu_l - \nu_t) = D_{21}$

$$D_{22} = \frac{u_2^2}{|\vec{u}|}\nu_l + \frac{u_1^2}{|\vec{u}|}\nu_t$$

The actual field data are only partially known

$\rightarrow$ uncertainties

Particle method

- Lagrangian particles discretisation $\left(\vec{X}_i, C_i\right)$
  - X_i : particles positions
  - C_i : particle weight (concentration integrated on a particle..)
- Approximated cocentration

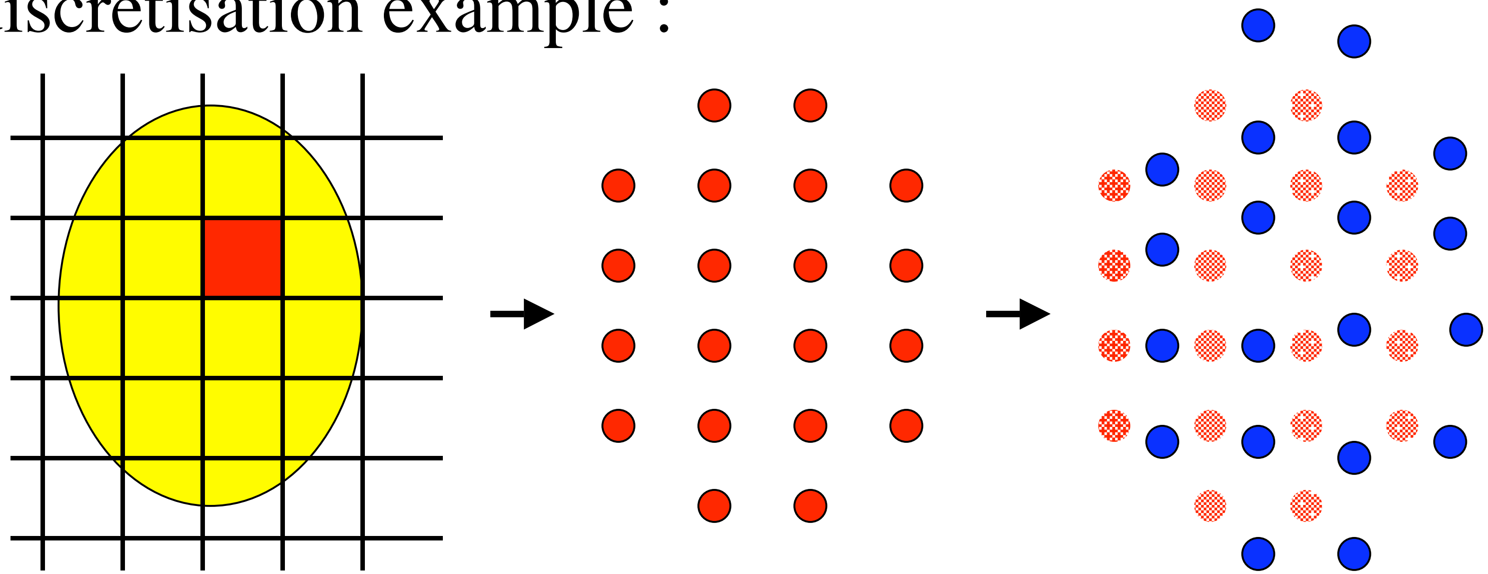
$$c_\varepsilon(\vec{x},t) = \sum_I C_i \varsigma_\varepsilon\left(\vec{X}_i - \vec{x}\right)$$

- ς_ε : regular "approximation" of the Dirac measure

$$\varsigma_\varepsilon(\vec{x}) = \frac{1}{\varepsilon^d}\varsigma\left(\frac{|\vec{x}|}{\varepsilon}\right), \quad \int_{R^d} \varsigma(\vec{x})dx = 1, \quad \int_{R^d} \vec{x}^m \varsigma(\vec{x})dx = 0 \quad 0 < m < M$$

Particle method

discretisation example :



→ Three discretisation parameters :

- h : particle volume
- ε : regularisation parameter
- Δt : time step

Particle method

"fluid" particles = lagrangian coordonnates

$$\underbrace{\frac{\partial c_\varepsilon}{\partial t} + \mathrm{div}\left(\vec{u}\; c_\varepsilon\right)} = \mathrm{div}\left(\overline{\overline{\mathrm{D}}} \cdot \overrightarrow{\mathrm{grad}}(c_\varepsilon)\right) \underbrace{- \lambda c_\varepsilon + S}$$

$$\frac{d\vec{X}_i}{dt} = \vec{U}\left(\vec{X}_i, t\right)$$

$$\frac{dC_i}{dt} = \lambda C_i + \int_{P_i} S\; dv$$

- Particles are convected with the Darcy velocity
- Particles weight are modified according to the remaining terms

Particle method

dispersion :

$$\frac{\partial c_\varepsilon}{\partial t} + \mathrm{div}\left(\vec{u}\ c_\varepsilon\right) = \underbrace{\mathrm{div}\left(\overline{\overline{\mathrm{D}}} \cdot \overrightarrow{\mathrm{grad}}(c_\varepsilon)\right)} - \lambda c_\varepsilon + S$$

alternatives :

1. random walk $\vec{X}_i(t+\Delta t) = \vec{X}_i(t) + \sqrt{\Delta t}\,\eta_i, \quad C_i(t+\Delta t) = C_i(t)$

2. dispersion velocity $\dfrac{d\vec{X}_i}{dt} = \dfrac{\overline{\overline{D}} \cdot \overrightarrow{\mathrm{grad}}(c_\varepsilon)}{c_\varepsilon}, \quad C_i(t+\Delta t) = C_i(t)$

3. approximated integrale solution (PSE)

$$\vec{X}_i(t+\Delta t) = \vec{X}_i(t), \qquad \frac{dC_i}{dt} = \int_{R^d} H(\vec{X}_i - \vec{X}_j)\left(C_i - C_j\right)$$

Streamlines + dispersion

1. Streamlines+ dispersion

Streamlines method :

- Mixed discretisation : particles + grid
  - flow (Darcy) computed on the grid
  - Transport with particles method
- Exact streamlines for the approximated velocity field
- Unstructured mesh possible (finite element type)

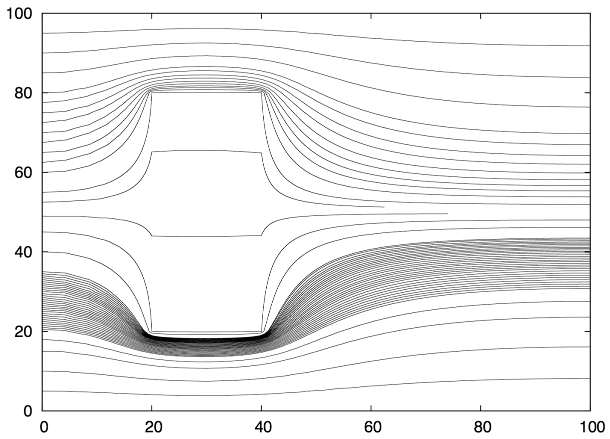
1. Streamlines + dispersion

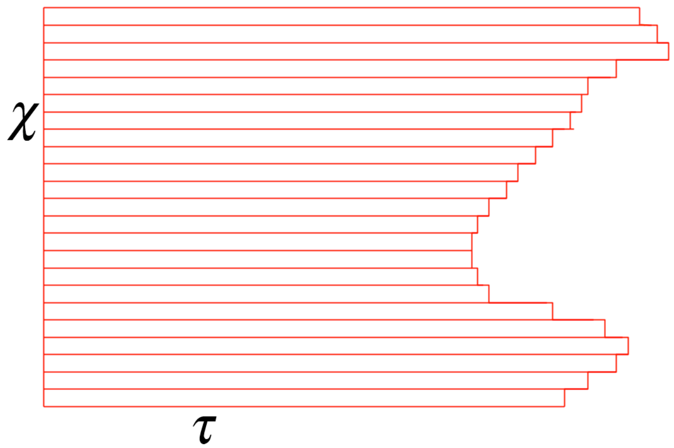
New point of view :

- Streamlines ⇒ mapping of the computational domain

$$(x, y) \rightarrow (\chi, \tau)$$

  - χ is the origin f the streamline containing (x, y)
  - τ is the time to go from the streamline origin to (x, y)





1. Streamlines + dispersion

Dispersion modeling :

particles method → 3 alternatives

- Particle strength exchange (PSE)
  - Necessitates a full coverage of the computational domain → boundary conditions
- Dispersion velocity
- Random walk
  - Respect the streamlines point of view, but the streamlines have to be re-computed for each new data set → CPU time consuming

1. Streamlines+ dispersion

Conclusions

$\Rightarrow$ at this stage, PSE is still the best possible choice!

Solution : 2 directions to be explored

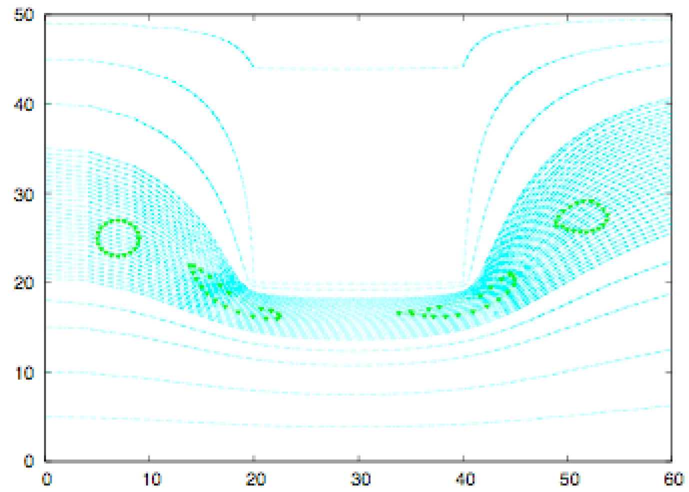
1. keep the streamlines constant
2. accelerate the "dispersed" streamlines computation

1. Streamlines + dispersion

1 : keep the streamline constant :

$\rightarrow$ contour transport method

- use the dispersion velocity
- Move the iso-value markers along a line of the (χ, τ) grid



1. Streamlines + dispersion

non conservative dispersion velocity = one single equation for the two (three in 3D!) velocity components

$$\frac{\partial c}{\partial t}+\left(\vec{U}\cdot\overrightarrow{\text{grad}}(c)\right)=\text{div}\left(\overline{\overline{D}}\cdot\overrightarrow{\text{grad}}(c)\right)$$

$$\Rightarrow\ \frac{\partial c}{\partial t}+\left(\left(\vec{U}+\vec{U}_D\right)\cdot\overrightarrow{\text{grad}}(c)\right)=0\ ,\qquad \boxed{\vec{U}_D\cdot\overrightarrow{\text{grad}}(c)=-\text{div}\left(\overline{\overline{D}}\cdot\overrightarrow{\text{grad}}(c)\right)}$$

The particle move along a streamline :

$\vec{\tau}$: streamline tangent

$\rightarrow$ one (two in 3D) equation(s) $\boxed{\vec{U}_D=U_D\vec{\tau}}$

1. Streamlines + dispersion

2. Accelerate the dispersed streamlines computation

   → streamtubes method :

- local gradient → dispersion
- dispersion

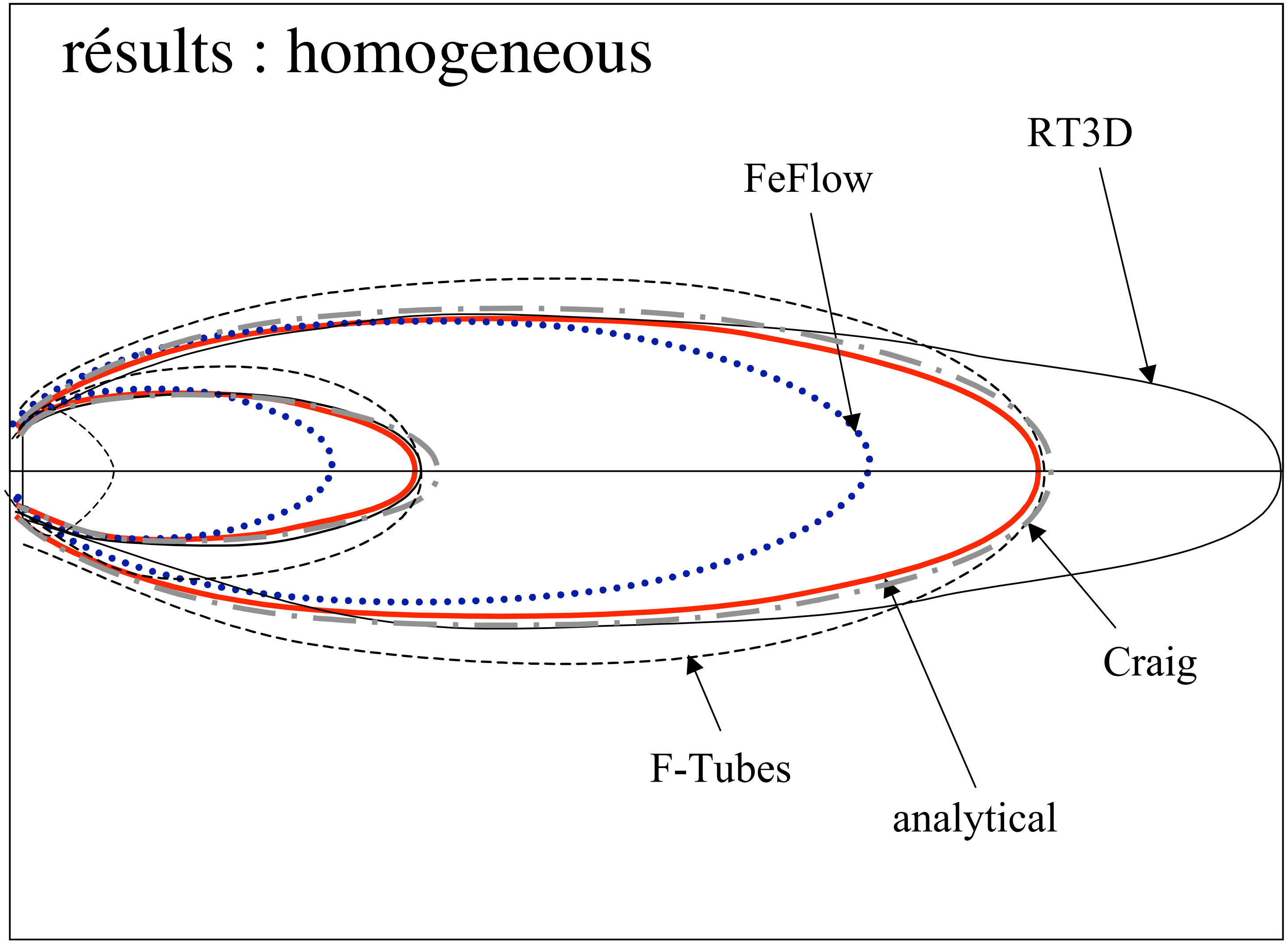
  → streamtube expansion

  → opening angle θ

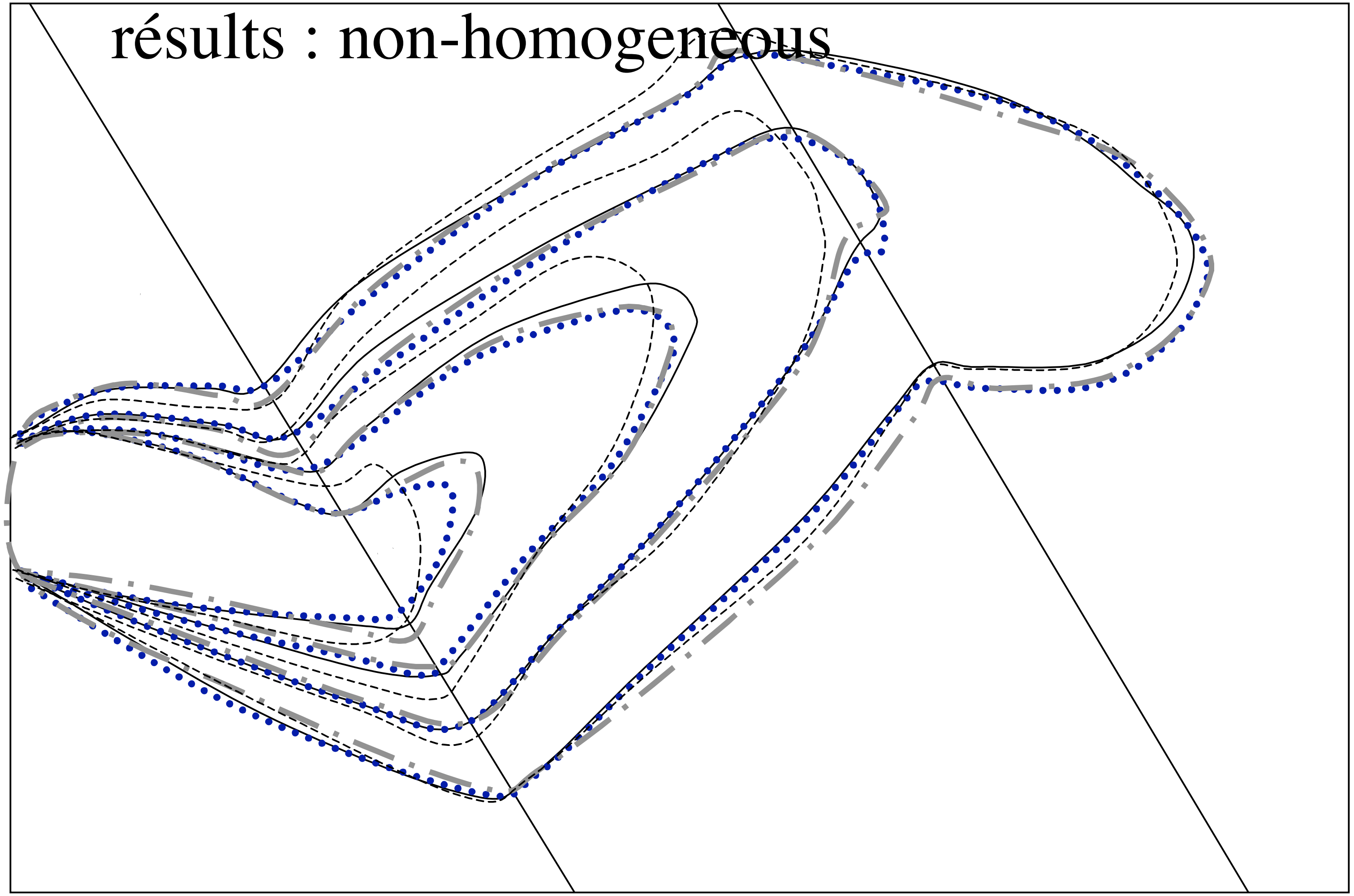
  → tabulated according to a local explicit solution

  Example : cleary solution for plume dispersion

1. Streamlines + dispersion



1. Streamlines + dispersion



2. uncertain transport

2. uncertain transport

Transport in porous media with partially known characteristics

asumption :

the velocity field and the dispersion tensor are parametrised using a set of random variables with well-defined probability

2 alternatives :

- particle location = probability density function
- "spectral" particle method

2. uncertain transport

- uncertainty define an abstract probability space *(Θ,Σ,dμ)*

$$\vec{u} = \begin{bmatrix} u_1(\theta) \\ u_2(\theta) \end{bmatrix}, \quad \overline{\overline{D}} = \begin{bmatrix} D_{11}(\theta) & D_{12}(\theta) \\ D_{12}(\theta) & D_{22}(\theta) \end{bmatrix}$$

- Stochastic problem :

$$\frac{\partial c(\theta)}{\partial t} + \mathrm{div}\left(\vec{u}(\theta)\ c(\theta)\right) = \mathrm{div}\left(\overline{\overline{D}}(\theta) \cdot \overrightarrow{\mathrm{grad}}(c(\theta))\right)$$

2. uncertain transport

$\xi = (\xi_1(\theta), \xi_2(\theta), \ldots, \xi_N(\theta))$: set of N independent random variables with domain Ξ and known probability density function p_ξ

Uncertain data parametrized using ξ :

- $u(\theta) \Rightarrow u(\xi(\theta))$
- $D(\theta) \Rightarrow D(\xi(\theta))$

Solution in (Ξ, B_Ξ, p_ξ)

- $c(x,t;\theta) \Rightarrow c(x,t;\xi(\theta))$

Uncertain transport

first method

- Contour marker : uncertain particle location
- Dispersion velocity :
  - → convection-dispersion equation
  - → convection equation
  - → probability density function for each X_i

second method

- Spectral stochastic method
- Galerkin projection on Polynomial chaos basis
- Particle discretisation of the set of PDE for each stochastic mode
- Stochastic expansion for each C_i

2. uncertain transport

"spectral" stochastic method

$\left\{\psi_0,\psi_1,...\psi_p(\xi)\right\}$ set of random functionals in ξ

- $\left\langle\psi_\alpha,\psi_\beta\right\rangle = E\left[\psi_\alpha\psi_\beta\right] = \delta_{\alpha\beta}$
- $S = \mathrm{span}\left\{\psi_0,\psi_1,...\psi_p\right\}$
- dim(S)=$p+1$

Concentration field expansion on S

$$C(\vec{x},t;\xi) = \sum_{\alpha=0}^{p} C^\alpha(\vec{x},t)\psi_\alpha(\xi)$$

Solve the sochastic equation → equations for the stochastic modes $C^\alpha(\vec{x},t)$

2. uncertain transport

Galerkin projection :

$$\frac{\partial C^{\alpha}}{\partial t} + \sum_{\beta=0}^{p} \operatorname{div}\left(u_{\alpha\beta} c^{\beta}\right) = \sum_{\beta=0}^{p} \operatorname{div}\left(\overline{\overline{D}}_{\alpha\beta} \cdot \overrightarrow{\operatorname{grad}}\left(c^{\beta}\right)\right)$$

$$u_{\alpha\beta} = \left\langle u \psi_{\beta} \psi_{\alpha} \right\rangle, \qquad \overline{\overline{D}}_{\alpha\beta} = \left\langle \overline{\overline{D}} \psi_{\beta} \psi_{\alpha} \right\rangle$$

Stochastic particle solution :

$$C(\vec{x},t;\xi) = \sum_{m=1}^{M} \sum_{\alpha=0}^{p} C^{\alpha}(\vec{x},t) \psi_{\alpha}(\xi) \varsigma_{\varepsilon}\left(\vec{x} - \vec{X}_{m}(t)\right)$$

2. uncertain transport

Galerkin projection :

$$\frac{\partial C^{\alpha}}{\partial t} + \sum_{\beta=0}^{p} \mathrm{div}\left(u_{\alpha\beta} c^{\beta}\right) = \sum_{\beta=0}^{p} \mathrm{div}\left(\overline{\overline{D}}_{\alpha\beta} \cdot \overrightarrow{\mathrm{grad}}\left(c^{\beta}\right)\right)$$

$$u_{\alpha\beta} = \left\langle u \psi_{\beta} \psi_{\alpha} \right\rangle, \qquad \overline{\overline{D}}_{\alpha\beta} = \left\langle \overline{\overline{D}} \psi_{\beta} \psi_{\alpha} \right\rangle$$

Stochastic particle solution :

$$C(\vec{x},t;\xi) = \sum_{m=1}^{M} \sum_{\alpha=0}^{p} C^{\alpha}(\vec{x},t) \psi_{\alpha}(\xi) \varsigma_{\varepsilon}\left(\vec{x} - \vec{X}_{m}(t)\right)$$

- stochastic weight
- deterministic position

2. uncertain transport

Decomposition : $\vec{u}(\xi) = \vec{U} + \vec{u}\,'(\xi) \qquad \vec{U} = \langle \vec{u} \rangle, \quad \langle \vec{u}\,' \rangle = 0$

$$\frac{\partial C^{\alpha}}{\partial t} + \mathrm{div}\left(Uc^{\alpha}\right) = -\sum_{\beta=0}^{p} \mathrm{div}\left(u'_{\alpha\beta}\, c^{\beta}\right) + \sum_{\beta=0}^{p} \mathrm{div}\left(\overline{\overline{D}}_{\alpha\beta} \cdot \overrightarrow{\mathrm{grad}}\left(c^{\beta}\right)\right)$$

$$u'_{\alpha\beta} = \left\langle u \psi_{\beta} \psi_{\alpha} \right\rangle, \qquad \overline{\overline{D}}_{\alpha\beta} = \left\langle \overline{\overline{D}} \psi_{\beta} \psi_{\alpha} \right\rangle$$

- Particles convected with the mean flow <U>
- Convection by u' with PSE
- Dispersion term with PSE

2. uncertain transport

Uncertain velocity

$$u(\theta) = \upsilon(\theta)\begin{bmatrix}\cos(\gamma)\\ \sin(\gamma)\end{bmatrix}$$

- $\gamma = 45^{o}$
- $\upsilon(\theta)$ random variable uniformely distributed on

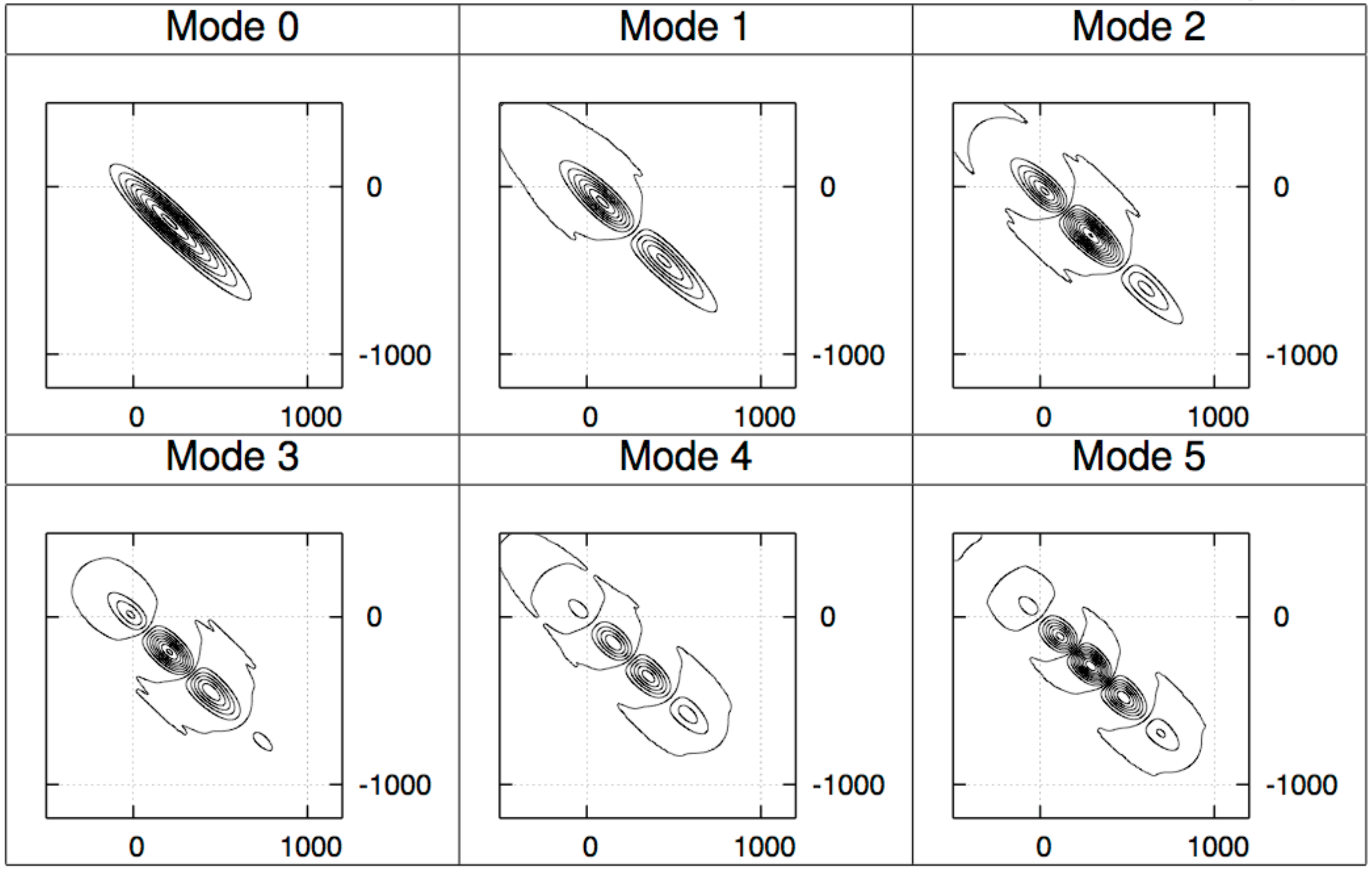
[-0.5, 0.5]

$$\upsilon(\theta) = 1 + 0.5\xi(\theta)$$

- $\psi_{\alpha}(\xi)$: α^{th} order Legendre polynomial
- $\nu_l = 100\ \nu_t$
- Initial conditions : gaussian injection

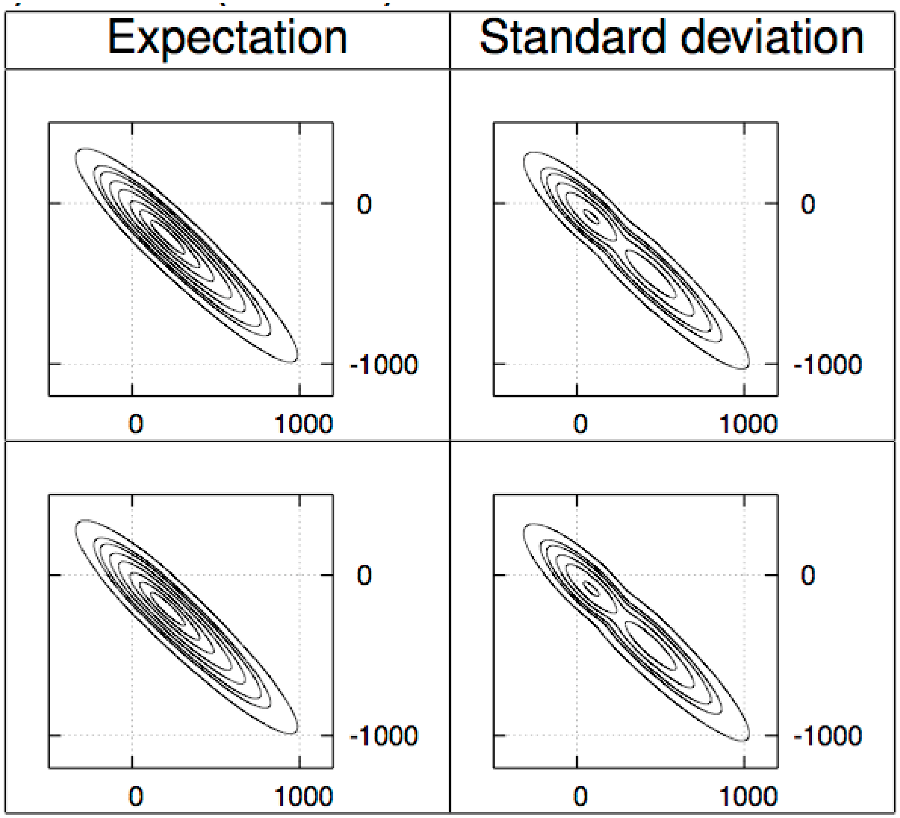
2. uncertain transport

- First stochatic modes (500 days)



2. uncertain transport

Particles position :



discrétisation parameter :

h= 10

Δt= 1

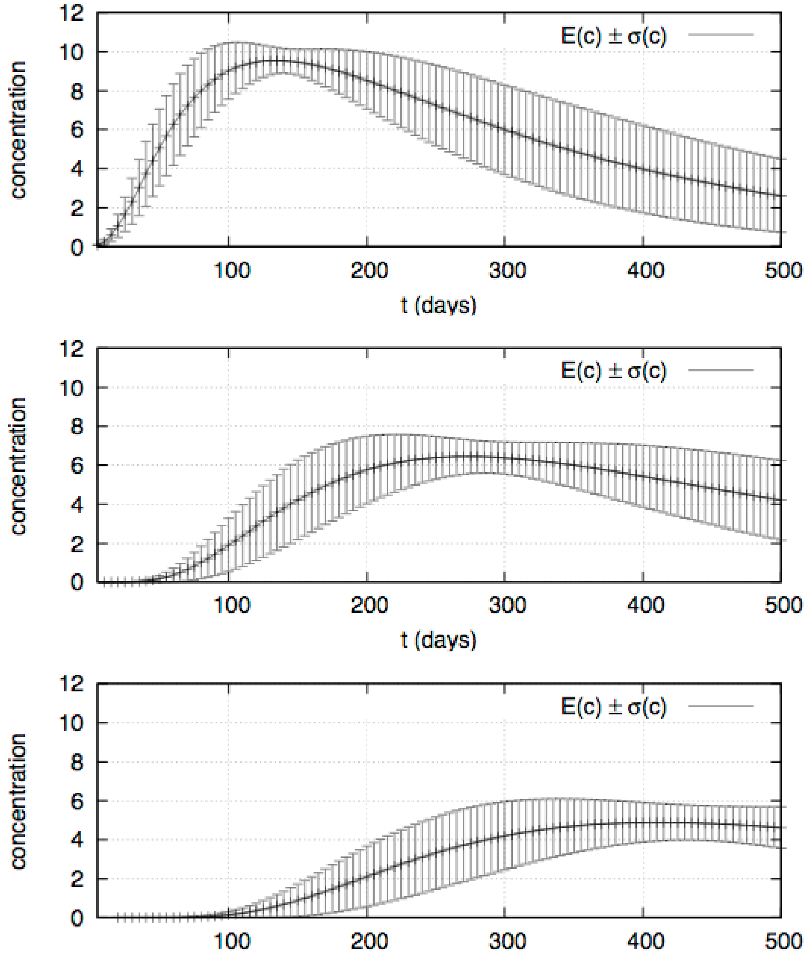
regularisation : 4th ordre

$N_o = 6$

2. uncertain transport

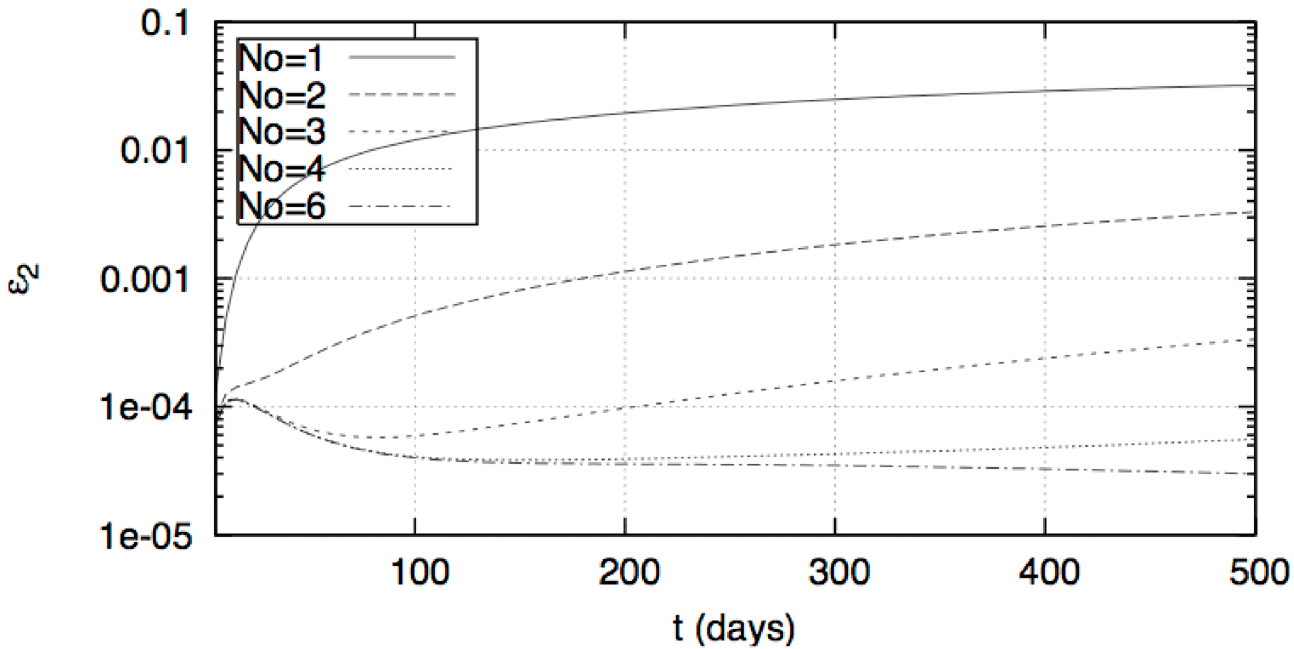
Concentrations statistic

Expectation and standard deviation at points
(25, -25),
(125,-125),
(225,-225)



2. uncertain transport convergence

Stochastic expansion order



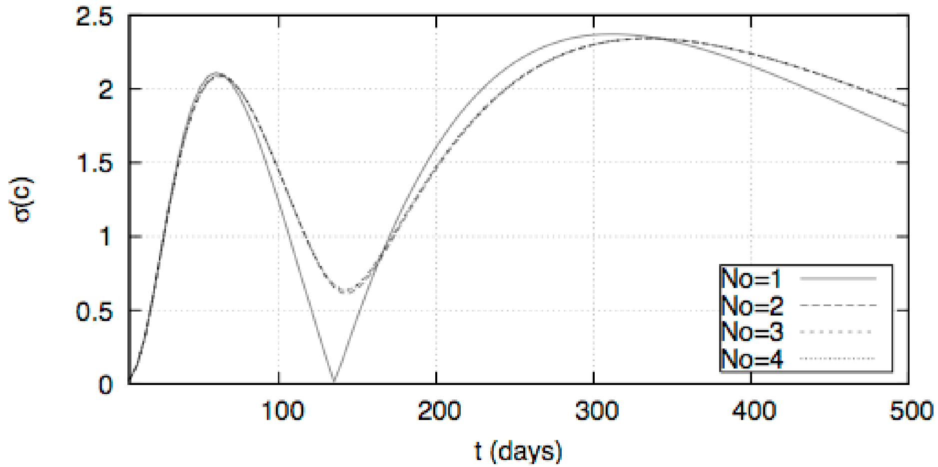
$$\varepsilon_2 = \sum_{i=1}^{M} \frac{E\left[\left(\tilde{c}(x_i,t,.) - c^{ex}(x_i,t,.)\right)^2\right]}{M}$$

2. uncertain transport convergence

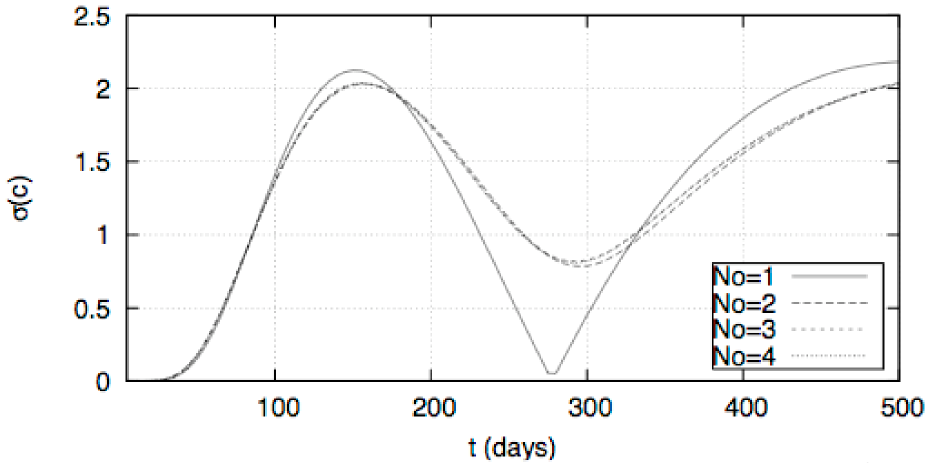
Stochastic expansion-2

Standard deviation

(25,-25)

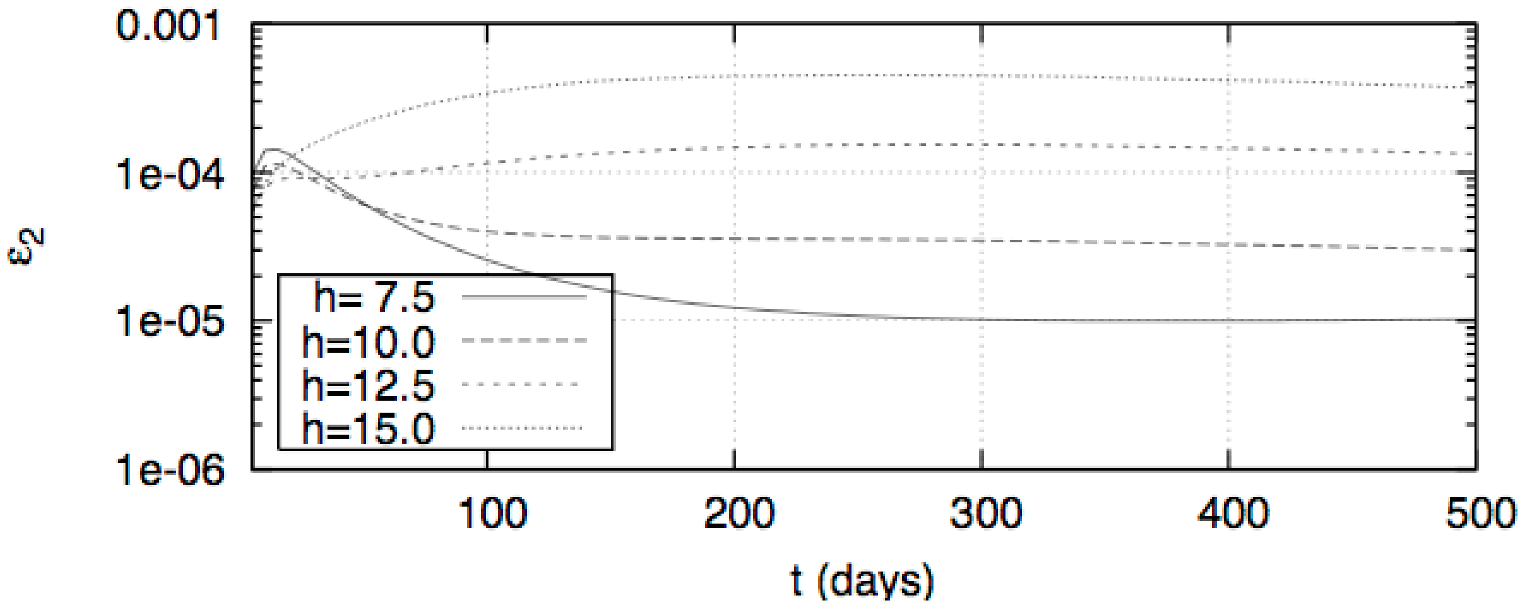


(125,-125)



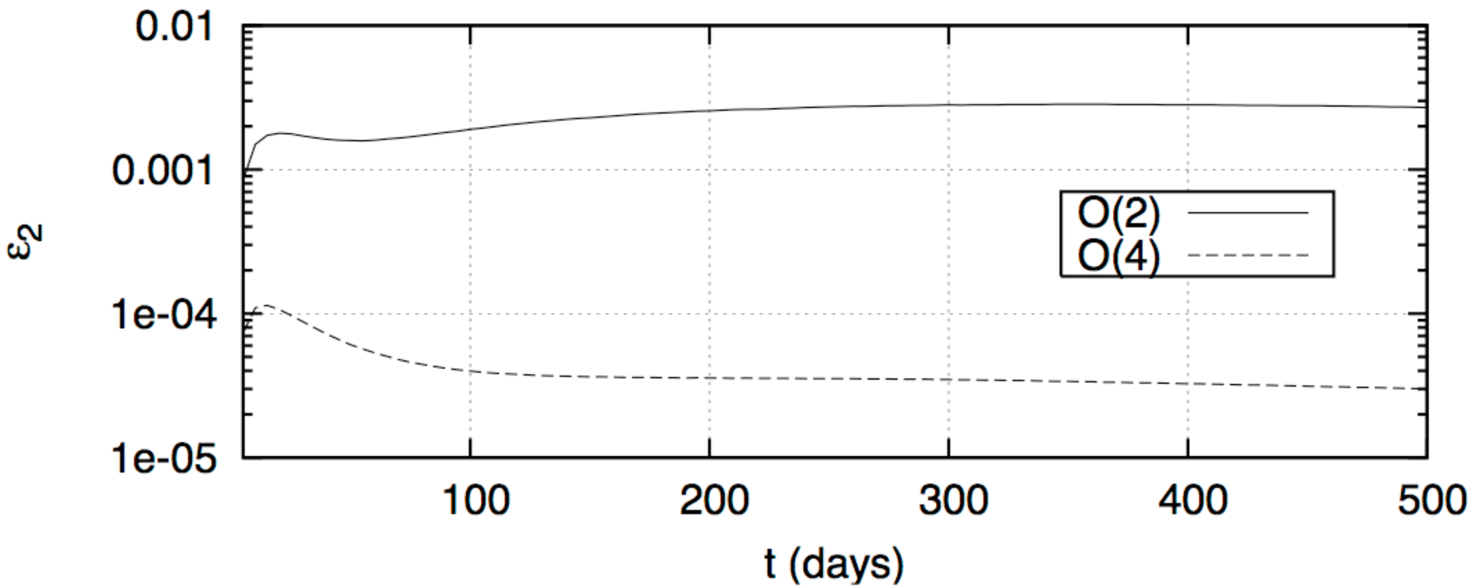
2. uncertain transport
convergence

Initial discretisation parameter *h*



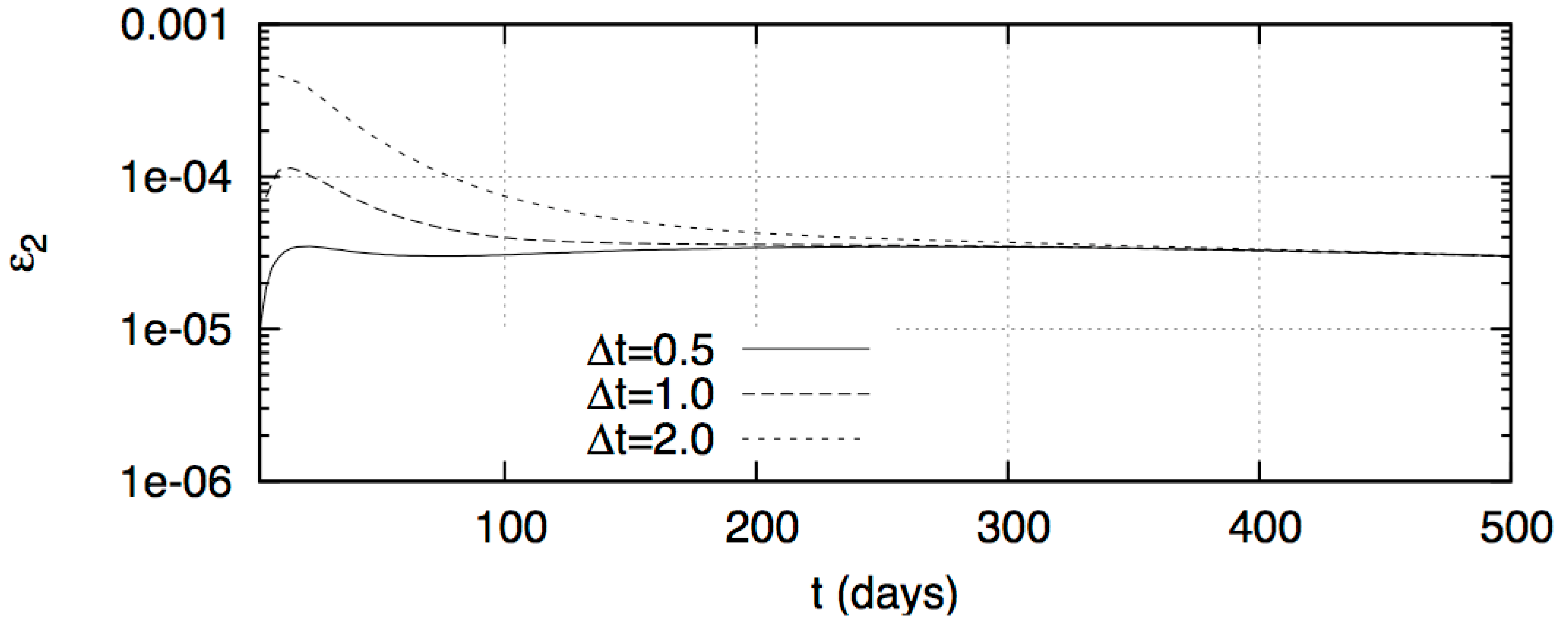
2. uncertain transport convergence

Regularisation order



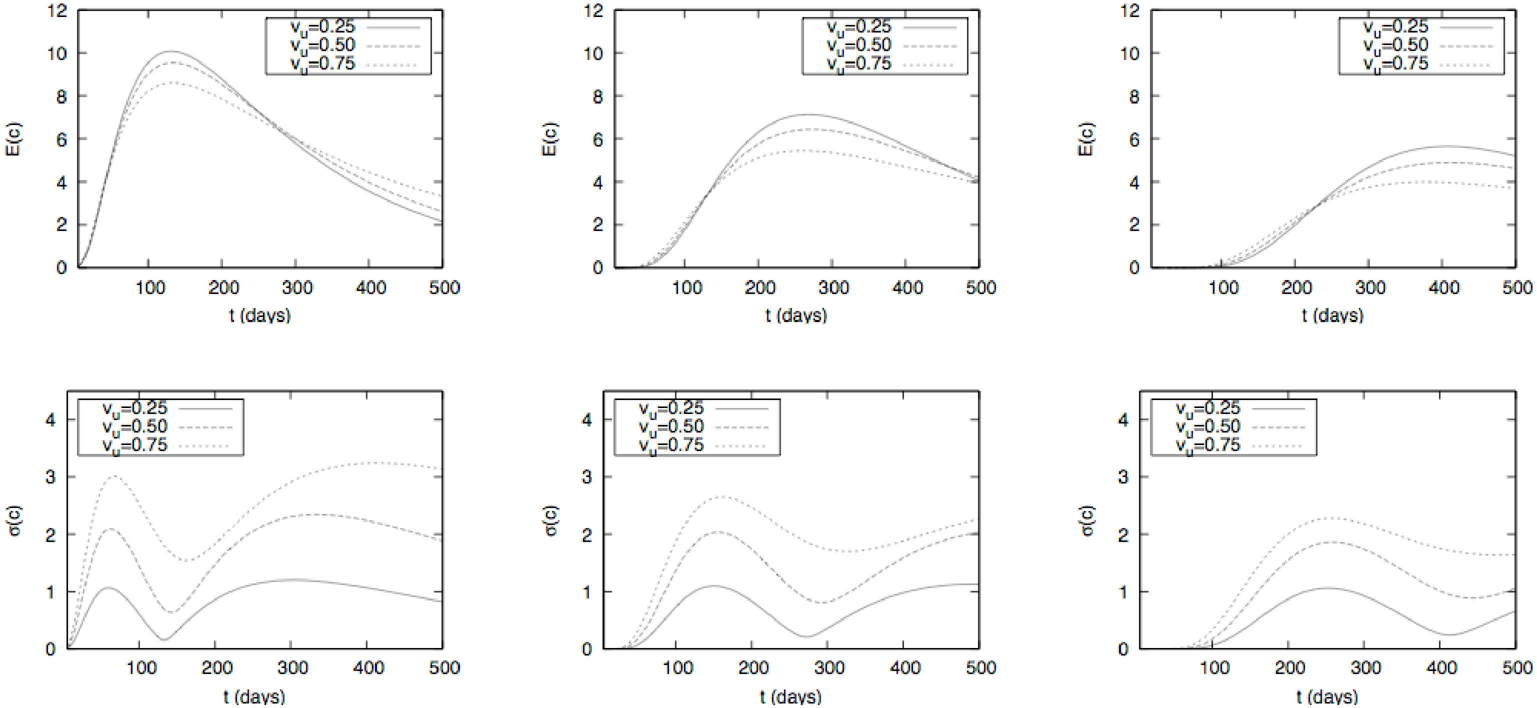
2. uncertain transport convergence

Time step



2. uncertain transport

Velocity vairability



Moyenne

déviation standard

(25,-25) (125,-125) (225,-225)

Conclusions

1. streamlines + dispersion
   – Streamlines methods ≠ particles methods
2. uncertain transport
   – Pdf limited to lower order
   – simulations for non uniform velocity
   – uncertainty on dispersion parameters ν_t, ν_l

to be done

– heterogeneous and discontinuous media with large contrast

(….)