Particle Simulation of Unsaturated Flows … in Porous Media

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1. Particle method

2. Porous media

3. Unsaturated flows

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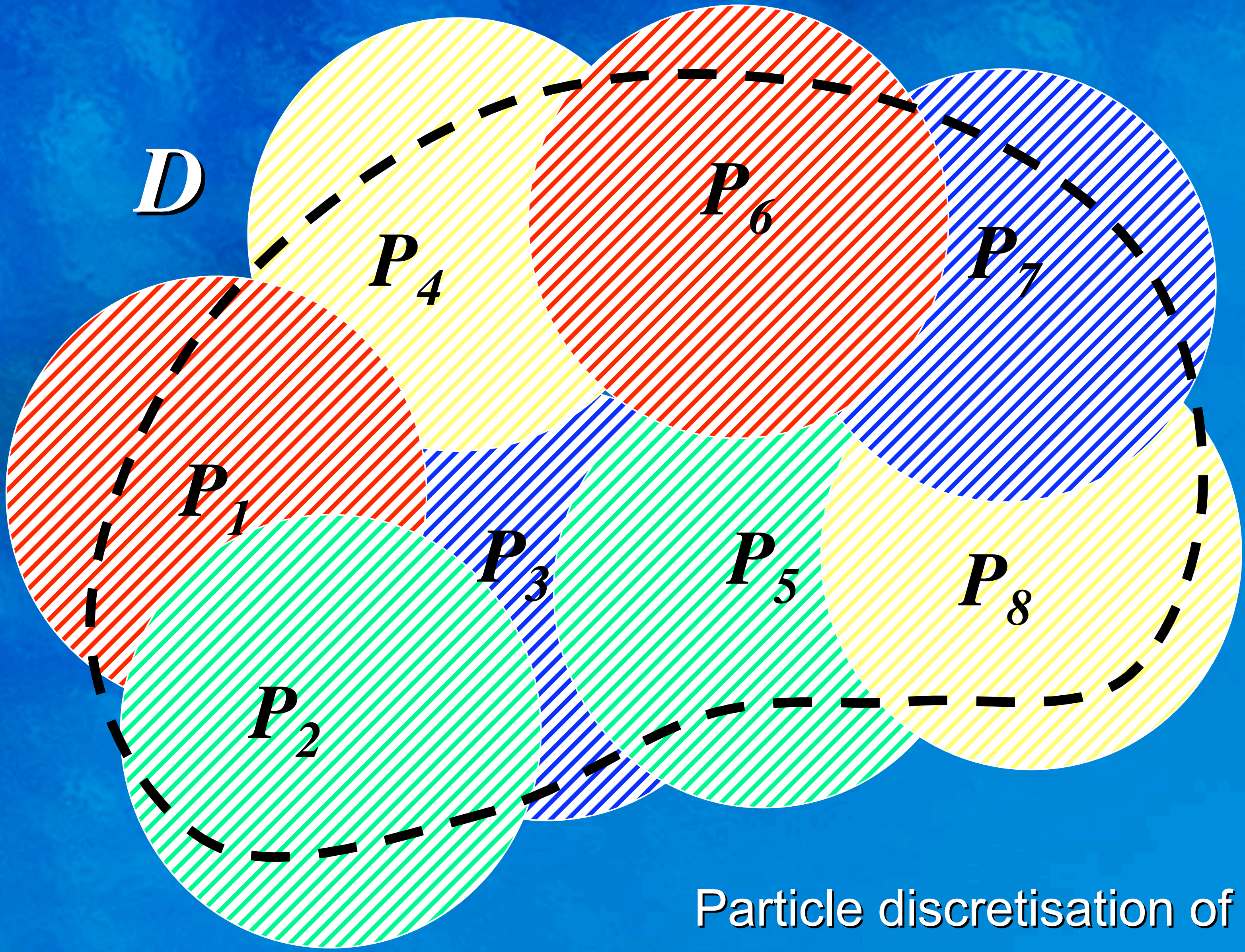
1. Particle method

Particle discretisation :

- position : $$\underline{X}_i = \frac{\iiint_{p_i} \underline{x}\, dv(\underline{x})}{\iiint_{p_i} dv(\underline{x})}$$
- transported quantity : $$\Theta_i = \iiint_{P_i} \theta(\underline{x},t)\, dv(\underline{x})$$
- "shape" : $$\varsigma_\varepsilon(\underline{X}_i - \underline{x}) = \frac{1}{\varepsilon^3} \exp\left(- \frac{(\underline{X}_i - \underline{x})^2}{\varepsilon^2} \right)$$

Function approximation :

$$\Rightarrow \quad \boxed{\theta_h(\underline{x},t) = \sum_i \Theta_i \varsigma_\varepsilon(\underline{X}_i - \underline{x})}$$

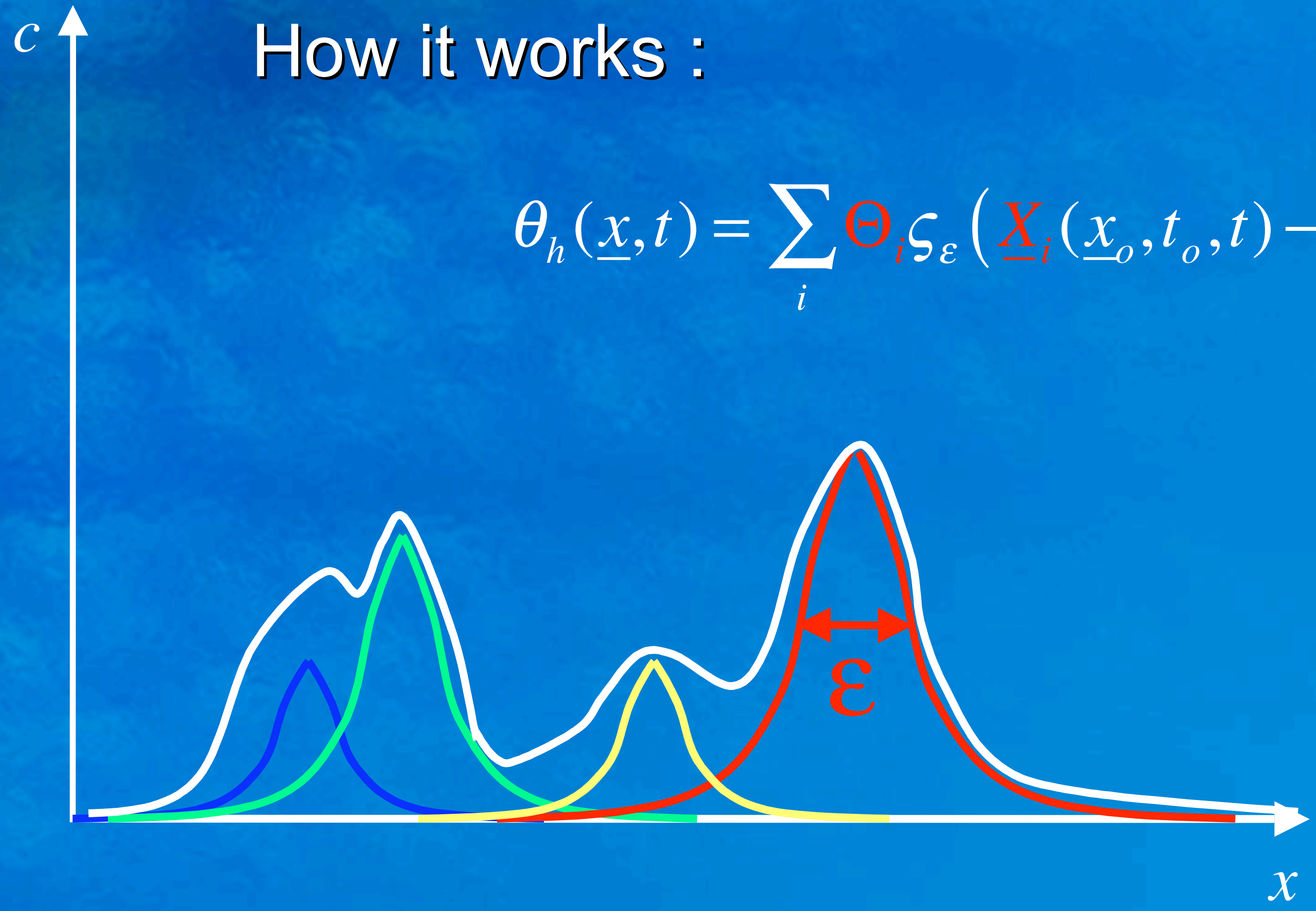


Particle discretisation of ***D***

1. Particle method

How it works :

$$\theta_h(\underline{x},t) = \sum_i \Theta_i \varsigma_\varepsilon\left(\underline{X}_i(\underline{x}_o,t_o,t) - \underline{x}\right)$$



1. Particle method

- Differential equation in convective form :

$$\frac{\partial \theta}{\partial t} + \mathrm{div}\left(\underline{U}\theta\right) = S(\theta) \qquad \theta = \theta(\underline{x}, t), \underline{x} \in D, \quad t_o \leq t \leq T$$

- Lagrangian coordinates

$$\frac{d\tilde{\theta}}{dt} = S(\tilde{\theta}) \qquad \tilde{\theta} = \tilde{\theta}(\underline{\chi}), \qquad \underline{\chi} = \underline{\chi}(\underline{x}_o, t_o, t)$$

$$\frac{d\underline{\chi}}{dt} = \underline{U}$$

1. Particle method

- spatial operator :
  1. derive from an integral form (green fuction or the previous ς_ε)

$$S(\theta)\big|_x \rightarrow \iiint_{\mathrm{supp}(\theta)} \left(\theta(\underline{x},t)-\theta(\underline{x}',t)\right) N(\underline{x},\underline{x}',t)\,dv(\underline{x}')$$

  2. Monte Carlo (random walk)
  3. convective form

$$S(\theta) = \mathrm{div}\left(S'(\theta)\right) \rightarrow S(\theta) = \text{-}\mathrm{div}\left(\underline{U}_s\theta\right) \text{ , } \underline{U}_s = \text{-}S'(\theta)/\theta$$

$$\frac{\partial\theta}{\partial t} + \mathrm{div}\left(\underline{U}\theta\right) = S(\theta) \rightarrow \boxed{\frac{\partial\theta}{\partial t} + \mathrm{div}\left(\left(\underline{U}+\underline{U}_s\right)\theta\right) = 0}$$

1. Particle method

Boundary conditions

- $\underline{U}_\gamma = \underline{0}$ integral formulation

  $\rightarrow$ boundary integral equation (ex:)

$$\theta(\underline{x},t) = \iiint_{\mathrm{supp}(\theta)} \theta(\underline{x}',t) G(\underline{x},\underline{x}',t) dv(\underline{x}') = \theta_\gamma(\underline{x},t) \quad x \in \partial D$$

- $\underline{U}_\gamma \neq \underline{0}$ prescribed flux $\rightarrow$ particles generation

$$\underline{x} \in \partial D \; : \left. \begin{matrix} \phi_\theta \\ \underline{U}_\gamma \end{matrix} \right| \quad \Rightarrow \quad \left| \begin{matrix} \underline{X}_i = \underline{X}_\gamma + \underline{U}_\gamma \left(\delta t/2\right) \\ \Theta_i = \phi_\theta \delta t \end{matrix} \right.$$

2. Porous media

Flow + Transport

flow : saturated $\rightarrow$ Darcy

unsaturated $\rightarrow$ Richard

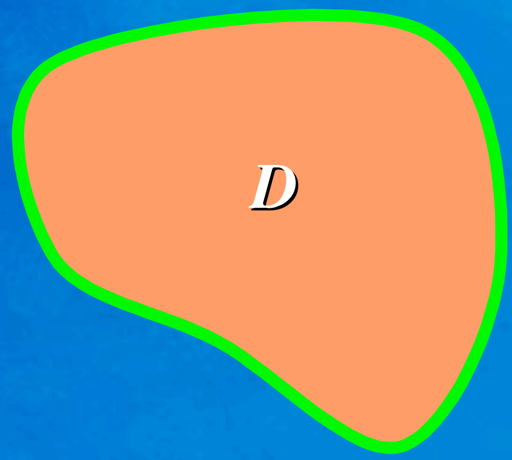
Output : velocity field $\vec{U}$

transport = advection + dispersion + …

$$\frac{\partial c}{\partial t} + \mathrm{div}\left(\underline{U}c\right) = \mathrm{div}\left(\overline{\overline{K}} \cdot \underline{\mathrm{grad}c}\right) + S(c)$$

2. Porous media

Darcy :



$$-\Delta p = S_p$$

$$\underline{U} = -\overline{\overline{K}} \cdot \underline{\mathrm{grad}}\, p$$

$$+ \text{boundary conditions}$$

Integral solution :

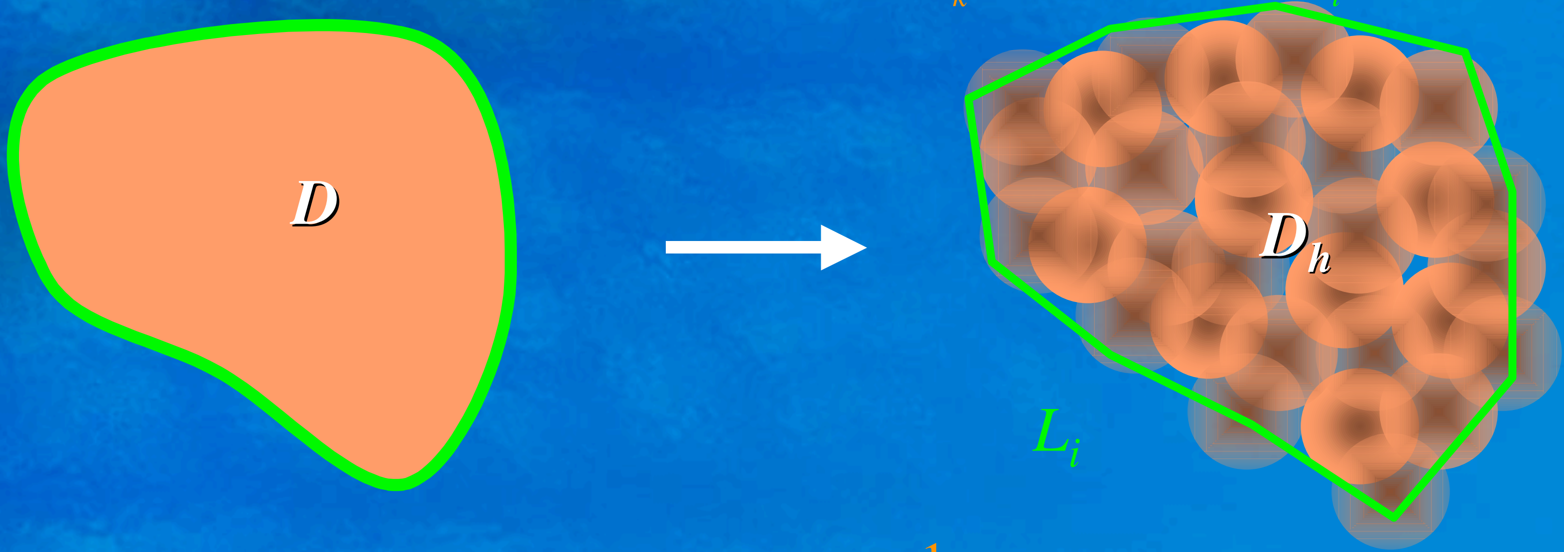
$$p(\underline{x}) = \frac{1}{2\pi} \underbrace{\int_{\partial D} \sigma(\vec{x}')\log(\underline{x}-\underline{x}')^2\, dl(\underline{x}')}_{\text{boundary conditions}} + \frac{1}{2\pi} \underbrace{\iint_{D} S(\underline{x}')\log(\underline{x}-\underline{x}')^2\, ds(\underline{x}')}_{\text{sources}}$$

2. Porous media

Darcy discretisation :

$$D \approx D_h, \qquad \partial D \approx \partial D_h$$

$$D_h = \bigcup_k P_k, \qquad \partial D_h = \bigcup_i L_i$$



Particle (sources only) : $S_h(\underline{x}) = \frac{1}{2\pi}\sum_k S_k \varsigma_\varepsilon(\underline{x} - \underline{X}_k)$

$$p_h(\underline{x}) = \frac{1}{2\pi}\sum_i \sigma_i \int_{L_i} \log(\underline{x} - \underline{x}')^2 \, dl(\underline{x}') + \frac{1}{2\pi}\sum_k S_k \log(\underline{x} - \underline{X}_k)^2$$

2. Porous media

Particle method for Darcy problem :

+ easy account for complex geometry

+ direct construction procedure

- boundary integral formulation fo Poisson Eq

- computational cost

  (even with fast summation algorithm)

- non uniform $K \rightarrow$ no explicit green function known

  $\rightarrow$ other integral formulation (PSE)

2. Porous media

Transport

$$\frac{\partial c}{\partial t} + \mathrm{div}\left(\underline{U}c\right) = \mathrm{div}\left(\overline{\overline{D}} \cdot \underline{\mathrm{grad} c}\right) + S(c)$$

Dispersion velocity

$$\frac{\partial c}{\partial t} + \mathrm{div}\left(\underline{U}c\right) = \mathrm{div}\left(\underbrace{\left(\frac{\overline{\overline{D}} \cdot \underline{\mathrm{grad} c}}{c}\right)}_{-\underline{U}_D} c\right) + S(c)$$

Advection equation

$$\frac{\partial c}{\partial t} + \mathrm{div}\left(\underline{U}c\right) + \mathrm{div}\left(\underline{U}_D c\right) = S(c)$$

$$\Leftrightarrow \begin{cases} \dfrac{dc(\underline{X})}{dt} = 0 \\ \dfrac{d\underline{X}}{dt} = \underline{U} + \underline{U}_D \end{cases}$$

2. Porous media

Transport Discretisation :

$$c_h(\underline{x},t)=\sum_k C_k \varsigma_\varepsilon(\underline{x}-\underline{X}_k)$$

$$\left.\begin{array}{l}\dfrac{dc(\underline{X})}{dt}=0\\[2ex] \dfrac{d\underline{X}}{dt}=\underline{U}+\underline{U}_D\end{array}\right\}\Rightarrow\left\{\boxed{\begin{array}{l}\dfrac{dC_k}{dt}=0\\[2ex] \dfrac{d\underline{X}_k}{dt}=\underline{U}_h+\underline{U}_{Dh}\end{array}}\right.$$

$$\underline{\mathrm{grad}}\left(c_h(\underline{x},t)\right)=\sum_k C_k\,\underline{\mathrm{grad}}\left(\varsigma_\varepsilon(\underline{x}-\underline{X}_k)\right)$$

$$\rightarrow \qquad \underline{U}_{Dh}=-\frac{\sum_k C_k\,\underline{\mathrm{grad}}\left(\varsigma_\varepsilon(\underline{x}-\underline{X}_k)\right)}{\sum_k C_k \varsigma_\varepsilon(\underline{x}-\underline{X}_k)}$$

2. Porous media

Particle method for transport equation

- \+ currently used with random walk
- \+ advection : no stability condition
- \+ easy treatment of non-uniform dispersion
- \+ no dissipation (local conservation)
- \- computational cost …?
- \- instabilities for discontinuous dispersion

2. Porous media

Unsaturated (Richard)

- Two – phase flow
- Localised gaz inclusions
  - θ : unknown water content $\theta = \dfrac{V_{tot} - V_{gaz}}{V_{tot}},$
  - gravitation → density contrast : $\rho_{\mathrm{gaz}} \ll \rho_{\mathrm{water}}$
- Richard's equation :

$$\boxed{\frac{\partial\theta}{\partial t} + \mathrm{div}\left(\bar{\bar{K}}(\theta)\cdot\left(\underline{\mathrm{grad}}\,\theta + \underline{e}_z\right)\right) = 0}$$

2. Porous media

Why particle method ?

+ discontinuous initial data
+ localised information

- requires a specific discretisation of the spatial operators
  - $\rightarrow$ two solutions :
    - convective formulation
    - particle Strength exchange

- CPU time consuming due to particle/particle interactions
  - $\rightarrow$ fast summation algorithm
    - $\approx$ Multigrid integral evaluation

3. Unsaturated flow

Richard's equation + dispersion velocity :

$$\frac{\partial\theta}{\partial t}+\mathrm{div}\left(\bar{\bar{K}}(\theta)\cdot\left(\underline{\mathrm{grad}}\theta+\underline{e}_z\right)\right)=0 \quad \Rightarrow \quad \frac{\partial\theta}{\partial t}+\mathrm{div}\left(\vec{U}_k\theta\right)=0$$

$$\vec{U}_k=-\bar{\bar{K}}(\theta)\cdot\left(\underline{\mathrm{grad}}\theta+\underline{e}_z\right)/\theta$$

Discretisation :

$$\theta_h(\underline{x},t)=\sum_i\Theta_i\varsigma_\varepsilon(\underline{X}_i-\underline{x}), \qquad \underline{\mathrm{grad}}\theta_h(\underline{x},t)=\sum_i\Theta_i\mathrm{grad}\varsigma_\varepsilon(\underline{X}_i-\underline{x})$$

$$\frac{d\Theta_k}{dt}=0$$

$$\frac{d\underline{X}_k}{dt}=\underline{U}+\bar{\bar{K}}(\theta_h(\underline{X}_k))\left(\underline{\mathrm{grad}}(\theta_h(\underline{X}_k))+\underline{e}_z\right)\Big/\left(\sum_j\Theta_j\varsigma_\varepsilon\left(X_k-X_j\right)\right)$$

3. Unsaturated flow

Richard's equation + PSE

Hydraulic diffusion :

$$\frac{\partial \theta}{\partial t} + \mathrm{div}\left(\bar{\bar{K}}(\theta) \cdot \left(\underline{\mathrm{grad}}\theta + \underline{e}_z \right) \right) = 0 \quad \Rightarrow$$

$$\bar{\bar{E}} = \bar{\bar{K}}(\theta)\underline{\mathrm{grad}}\theta, \quad S_e = \frac{\theta_r - \theta}{\theta_r - \theta_s}$$

$$\frac{\partial S_e}{\partial t} + \mathrm{div}\left(\bar{\bar{K}} \cdot \underline{e}_z \right) = \mathrm{div}\left(\bar{\bar{E}} \cdot \underline{\mathrm{grad}} S_e \right)$$

S_e : effective saturation

θ_r : residual moisture

K : permeability

E : hydraulic diffusivity

3. Unsaturated flow

Richard's equation + PSE

diffusion operator → integral operator :

$$\operatorname{div}\left(\overline{\overline{E}}\cdot\underline{\operatorname{grad}}S_e\right)=\int_{R^d}\left(\overline{\overline{E}}(\underline{x})+\overline{\overline{E}}(\underline{x}')\right)\cdot\left(S_e(\underline{x}')-S_e(\underline{x})\right)\eta_\varepsilon\left(\left|\underline{x}'-\underline{x}\right|\right)dv(\underline{x}')$$

Discretisation :

$$\int_{P_i}\left(\operatorname{div}\left(\overline{\overline{E}}\cdot\underline{\operatorname{grad}}S_e\right)\right)dv$$

$$\approx\sum_j\left(\overline{\overline{E}}(\underline{X}_i)+\overline{\overline{E}}(\underline{X}_j)\right)\left(S_e(\underline{X}_j)\int_{P_i}dv-S_e(\underline{X}_i)\int_{Pj}dv\right)\eta_\varepsilon\left(\left|\underline{X}_j-\underline{X}_i\right|\right)$$

$$\Rightarrow\quad S_i^{n+1}=S_i^n+\delta t\sum_j\left(\overline{\overline{E}}_i^n+\overline{\overline{E}}_j^n\right)\left(S_i^n\left|P_j\right|-S_j^n\left|P_i\right|\right)\eta_\varepsilon\left(\left|\underline{X}_j^n-\underline{X}_{i_i}^n\right|\right)$$

3. Unsaturated flow

Numerical results :

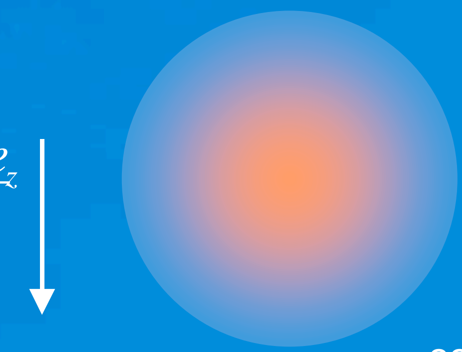
Evolution of a water drop in an unsaturated medium

- Unbounded 2D domain
- Van Genuchten's model for the soil water retention curve
- adimensionalised Richard's equation

  only function of Van Genuchten's parameter (**n = 6**)
- guassian initial condition :

$$S_e(\underline{X},0) = S_{\max} \exp\left(- \frac{\left|\underline{x}^2\right|}{\lambda^2} \right)$$

$-g\,\underline{e}_z$



3. Unsaturated flow

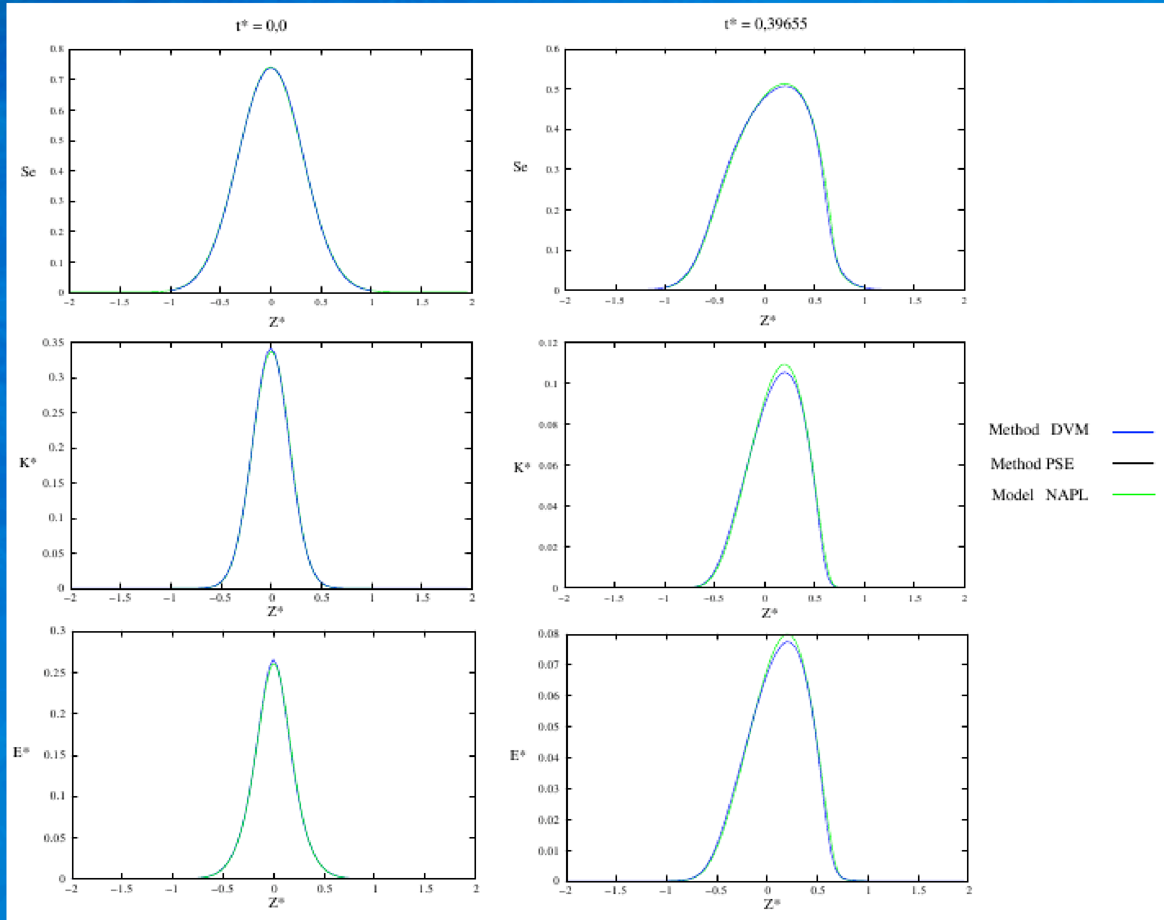
Physical parameters

initial final

S_e : effective saturation

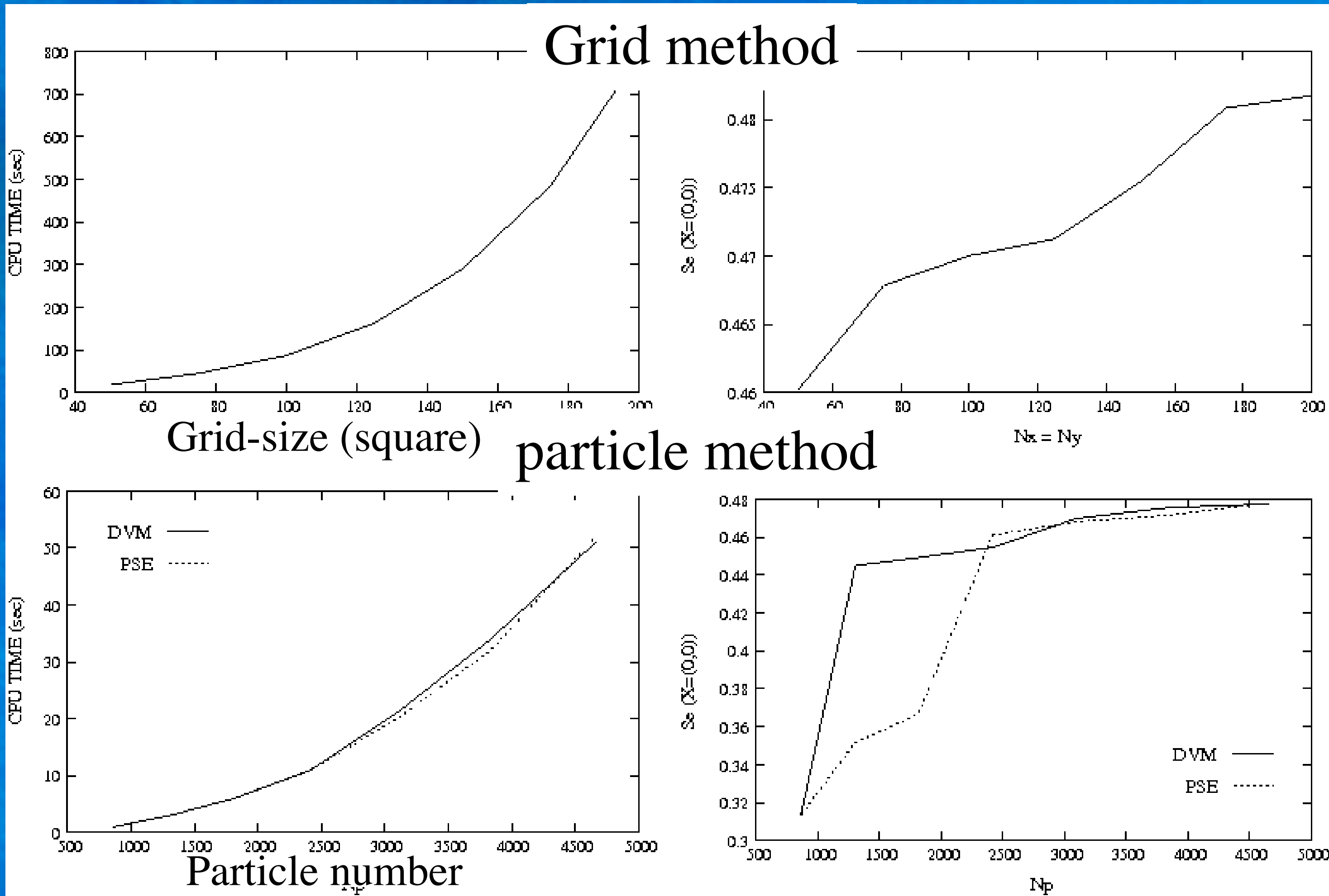
$\bar{\bar{K}}$: permeability

$\bar{\bar{E}}$: hydraulic diffusivity



3. Unsaturated flow

Discretisation error



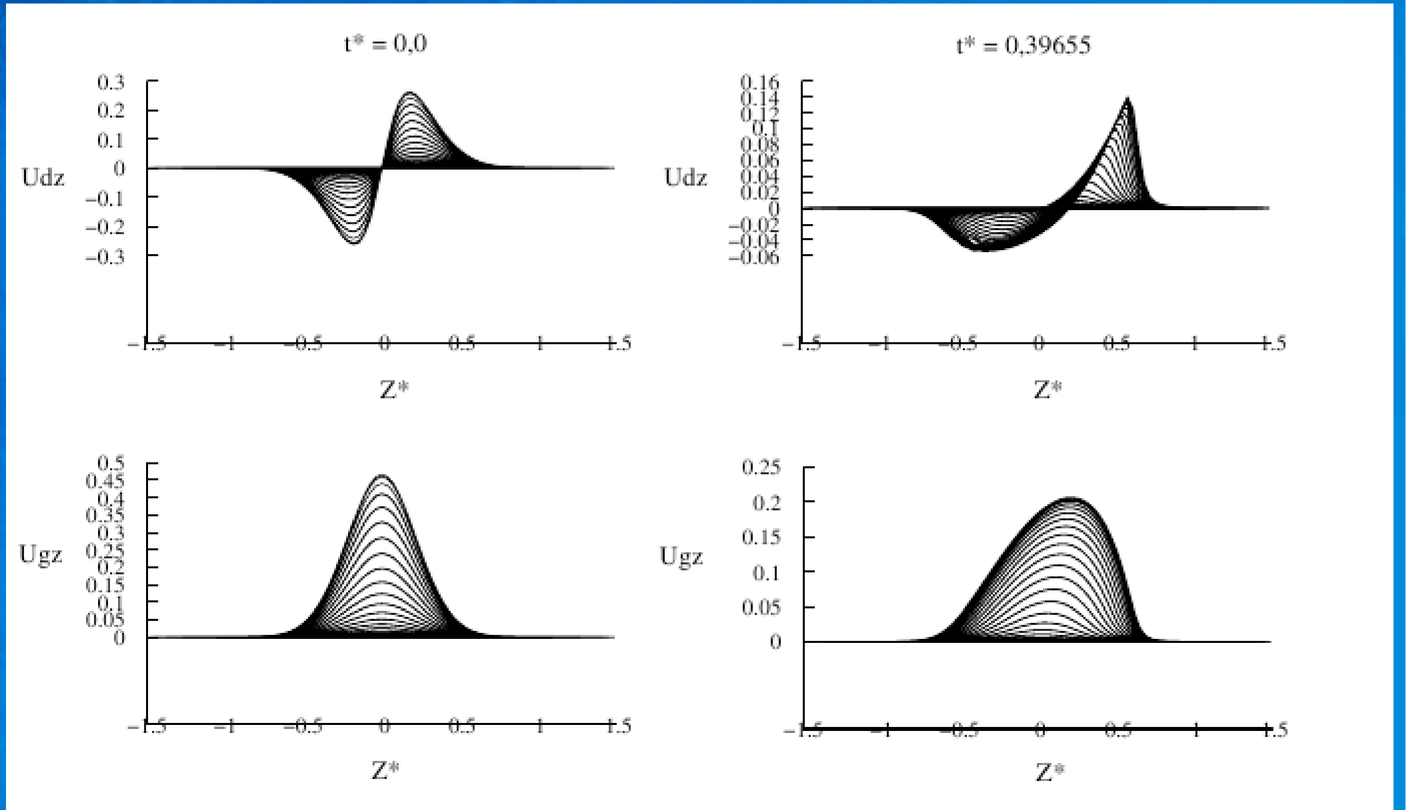
3. Unsaturated flow

infiltration and diffusion velocities vertical component

$$\underline{U}_k = \underline{U}_g + \underline{U}_d$$

$$\underline{U}_g = \frac{\overline{\overline{K}}(\theta)}{\theta}\,\underline{e}_z$$

$$\underline{U}_d = -\overline{\overline{E}}(\theta)\cdot\underline{\mathrm{grad}}(\theta)$$



Conclusion

Particle method = unusual approach

- Darcy :
  - boundary integral equations
  - Grid-particle method recommanded
- transport :
  - currently used in the Monte-Carlo version
  - low numerical dispersion
- unsaturated :
  - only one previous attempt (L. Rossi)
  - Usefull for unbouded flow perturbation