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Biased Global Random Walk, a Cellular Automaton for Diffusion

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GRW move particles on a lattice to simulate diffusion:

-a superposition of many particle tracking procedures;

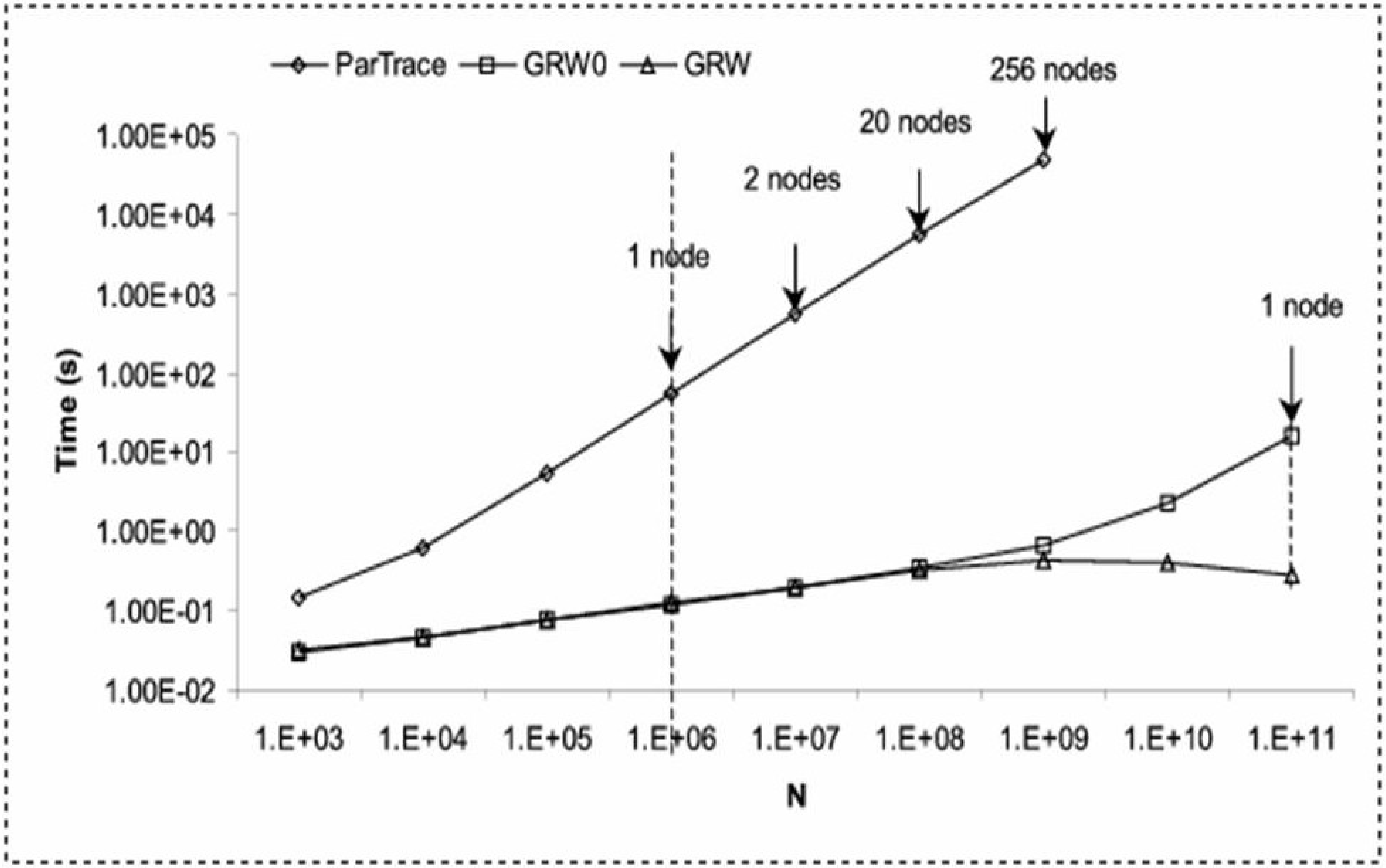
-a cellular automaton (CA) without exclusion principle;

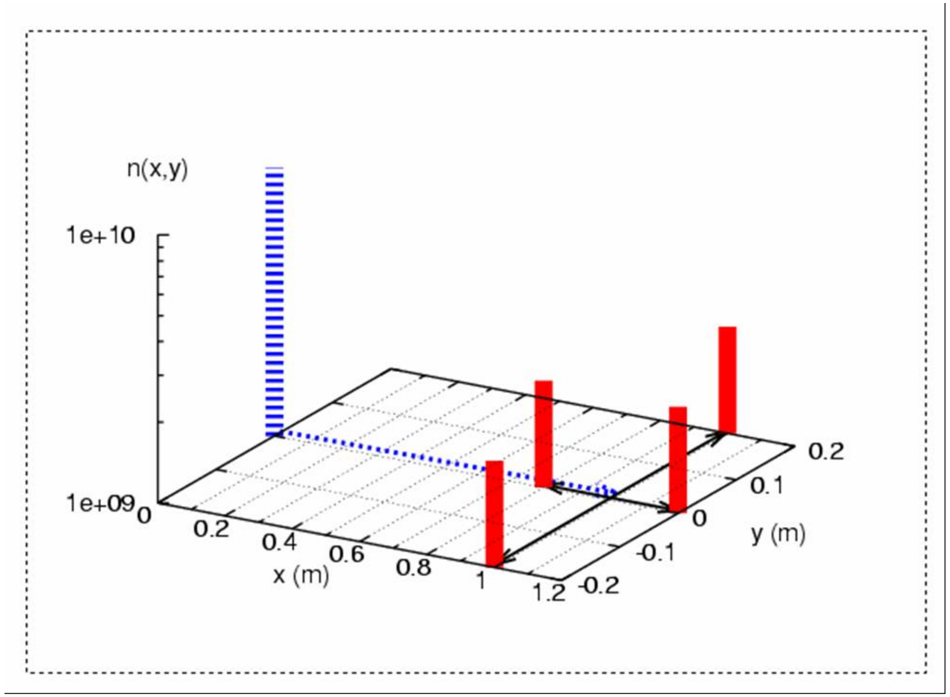
-inherently stable, free of round-of errors and numerical diffusion;

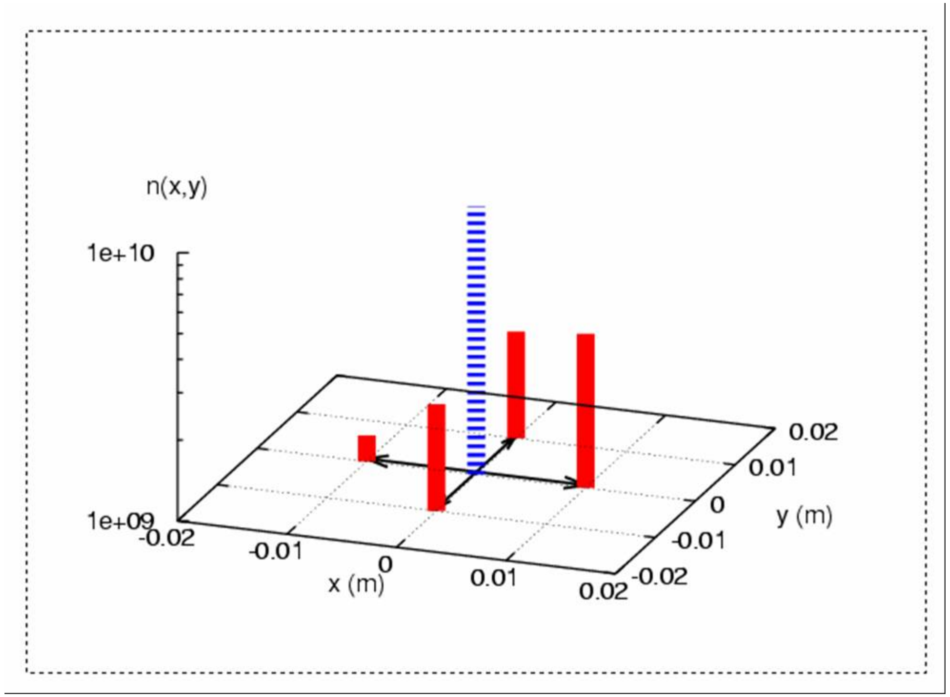
-self-averaging; the solution of the heat equation converges as
$\mathcal{O}(\delta x^2) + \mathcal{O}(1/\sqrt{N})$,
where δx is the lattice parameter and N is the total number of particles [*Vamoş et al.*, 2003].

Comparison with classical particle tracking

(3-dim heat equation, simulations for 10 time steps on a Cray3TE)







GRW state at $t = \delta t = 0.5$ days.

BGRW state at $t = \delta t = 0.0025$ days.

BGRW completely remove the overshooting errors!

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BGRW algorithm

The 2-dimensional BGRW is defined by the **local** *Cellular Automaton* (CA) rule

$$
\begin{aligned}
n(i,j,k) \quad = \quad & \delta n(i,j \mid i,j,k)+ \\
& \delta n(i+1,j \mid i,j,k) + \delta n(i-1,j \mid i,j,k)+ \\
& \delta n(i,j+1 \mid i,j,k) + \delta n(i,j-1 \mid i,j,k)
\end{aligned}
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$$

- $n(i,j,k)$ is the number of particles on the site $(x,y)=(i\delta x, j\delta y)$ at the time $t=k\delta t$
- n and δn are Bernoulli distributed random variables.

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- drift and diffusion coefficients of the transport problem:
  $V_x(x,y,t)$, $V_y(x,y,t)$, $D_x(x,y,t)$, $D_y(x,y,t)$

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- dimensionless parameters

$$v_x = V_x \frac{\delta t}{\delta x},\ v_y = V_y \frac{\delta t}{\delta y},\ r_x = D_x \frac{2\delta t}{\delta x^2},\ r_y = 2D_y \frac{2\delta t}{\delta y^2}$$

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- average over an ensemble of CA simulations:

$$\overline{\delta n}(i,j \mid i,j,k) = (1 - r_x - r_y)\, \overline{n}(i,j,k)$$
$$\overline{\delta n}(i \pm 1, j \mid i,j,k) = \tfrac{1}{2}(r_x \pm v_x)\overline{n}(i,j,k)$$
$$\overline{\delta n}(i, j \pm 1 \mid i,j,k) = \tfrac{1}{2}(r_y \pm v_y)\overline{n}(i,j,k)$$

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$$\frac{V_x\rho(x+\delta x,y,t)-V_x\rho(x-\delta x,y,t)}{2\delta x}+\frac{V_y\rho(x,y+\delta y,t)-V_y\rho(x,y-\delta y,t)}{2\delta y}=$$
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- i.e the forward-time centred-space finite difference scheme for the advection-diffusion (Fokker-Plank) equation

$$\partial_t\rho + \partial_x(V_x\rho) + \partial_y(V_y\rho) = \partial_x^2(D_x\rho) + \partial_y^2(D_y\rho)$$

Restriction for BGRW parameters

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- example: isotropic two-dimensional diffusion in groundwater
  - diffusion coefficient: $D_x = D_y = D = 0.01 \; m^2/day$
  - mean flow of $U = 1 \; m/day$ along the x axis
  - standard deviation $\sigma = 0.2 \; m/day$
- Assuming $r_x = r_y = r = 0.5$ and $V^{\max} = U + 5\sigma = 2 \; m/day \Rightarrow$ $\delta x \leq 2D/V_x^{\max} = 0.01 \; m$, $\delta t = 0.0025 \; day$

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- 3 cpu hours $\equiv$
  - simulations over 50 days (BGRW)
  - simulations over 1000 days (UGRW-unbiased algorithm)

BGRW supplies evaluations for UGRW

OBSERVABLES: 1st and 2-nd centered moments of the density

$$\mu_\alpha(t) = \int\int \alpha\rho(x,y,t)dxdy,\ \mu_{\alpha\alpha}(t) = \int\int (\alpha - \mu_\alpha)^2\rho(x,y,t)dxdy,$$

where α stands for x or y.

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where α stands for x or y.

- velocity of the center of mass

$$\mathcal{V}_\alpha = d\mu_\alpha/dt$$

- effective diffusion coefficients

$$\mathcal{D}_{\alpha\alpha} = \mu_{\alpha\alpha}/(2t)$$

- The deviations from BGRW $\Delta\mathcal{V}_\alpha$ and $\Delta\mathcal{D}_{\alpha\alpha}$ are used to estimate overshooting errors:

$$\varepsilon(\mathcal{V}_\alpha) = \sqrt{\frac{1}{T}\sum_{k=0}^{k=T}(\Delta\mathcal{V}_\alpha)^2(k)},\ \varepsilon(\mathcal{D}_{\alpha\alpha}) = \sqrt{\frac{1}{T}\sum_{k=0}^{k=T}(\Delta\mathcal{D}_{\alpha\alpha})^2(k)}$$

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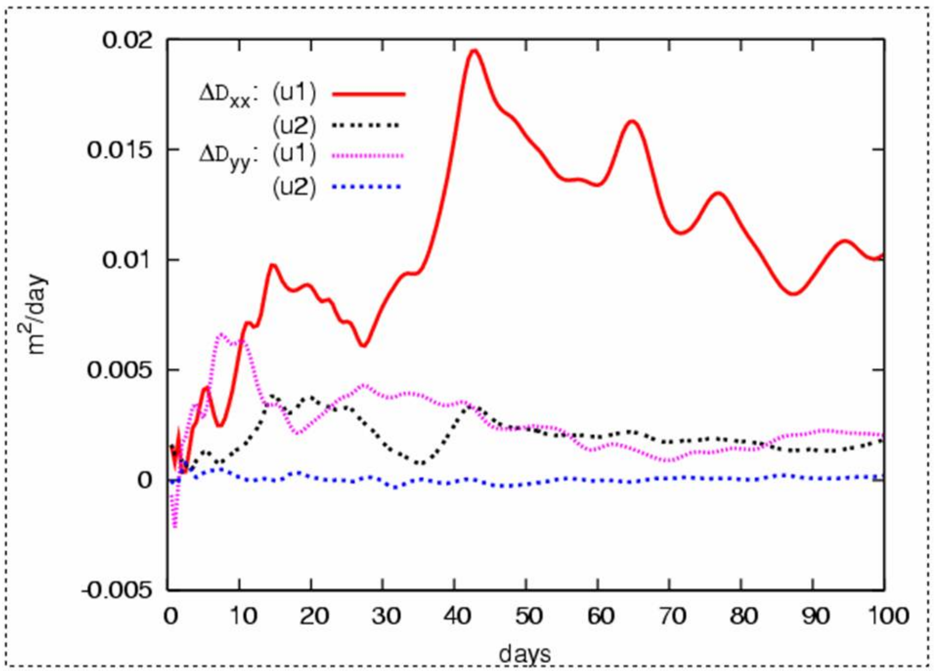
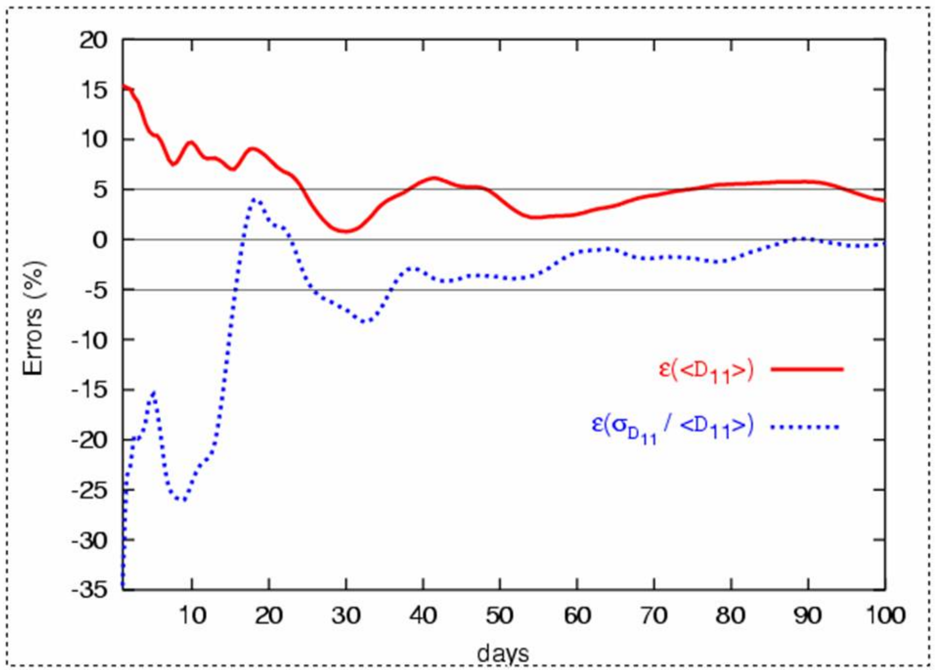
Evaluations of UGRW errors for the sets of parameters

(u1): $\delta x = 0.1\ m$, $\delta t = 0.5\ day$, $r = 0.25$

(u2): $\delta x = 0.01\ m$, $\delta t = 0.1\ day$, $r = 0.408$

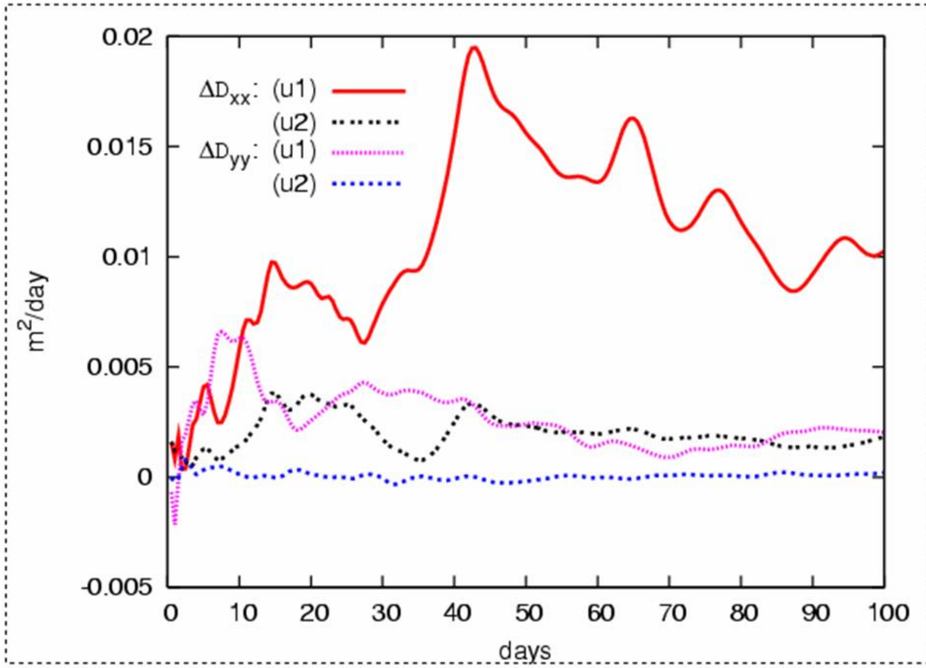
	$\varepsilon(\mathcal{V}_x)$	$\varepsilon(\mathcal{V}_y)$	$\varepsilon(\mathcal{D}_{xx})$	$\varepsilon(\mathcal{D}_{yy})$
(u1)	0.02359 m/day	0.01716 m/day	0.01317 m^2/day	0.00257 m^2/day
(u2)	0.00612 m/day	0.00524 m/day	0.00312 m^2/day	0.00039 m^2/day

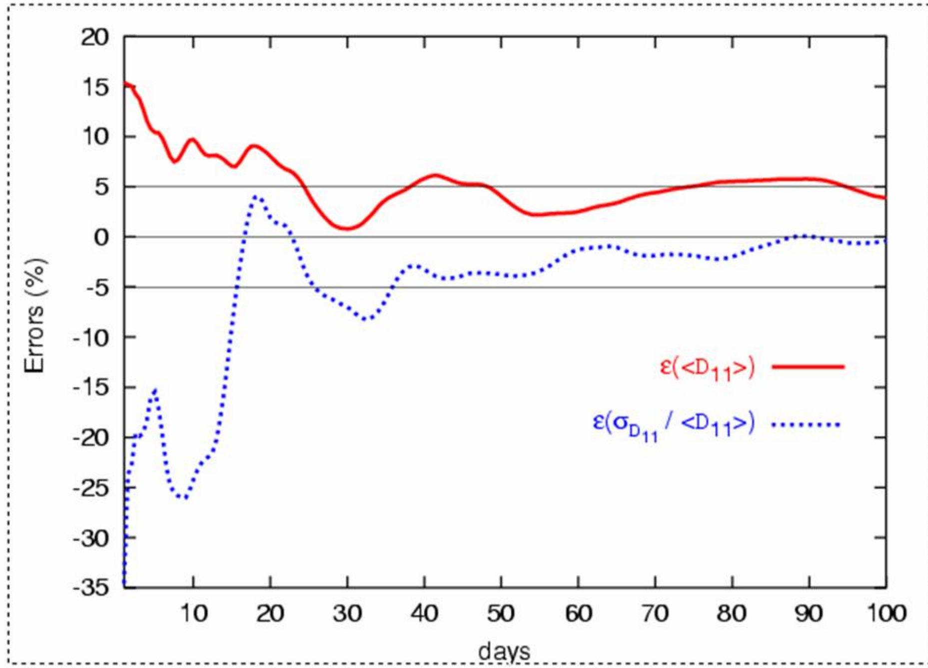




Single realization

Averages over ensemble of velocity





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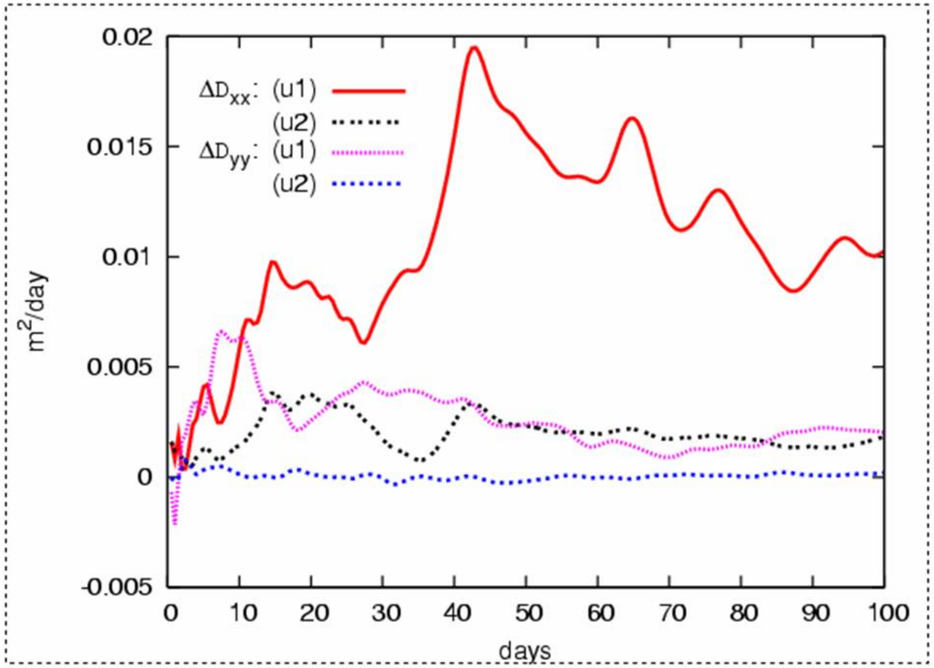
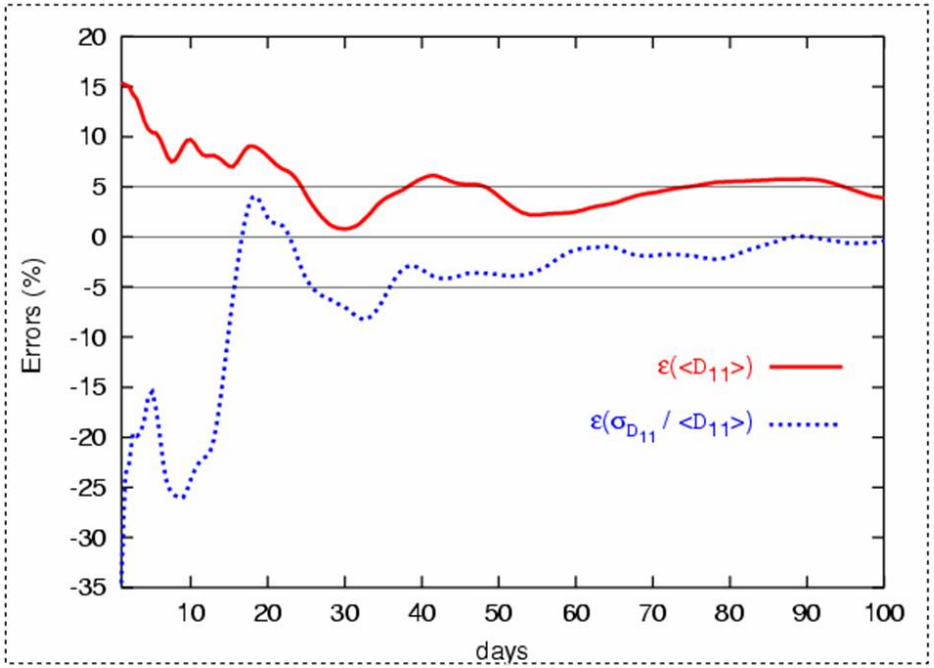
(u2: $\delta x = 0.01\ m\ \&\ \delta t = 0.1\ day$) necessary for given velocity





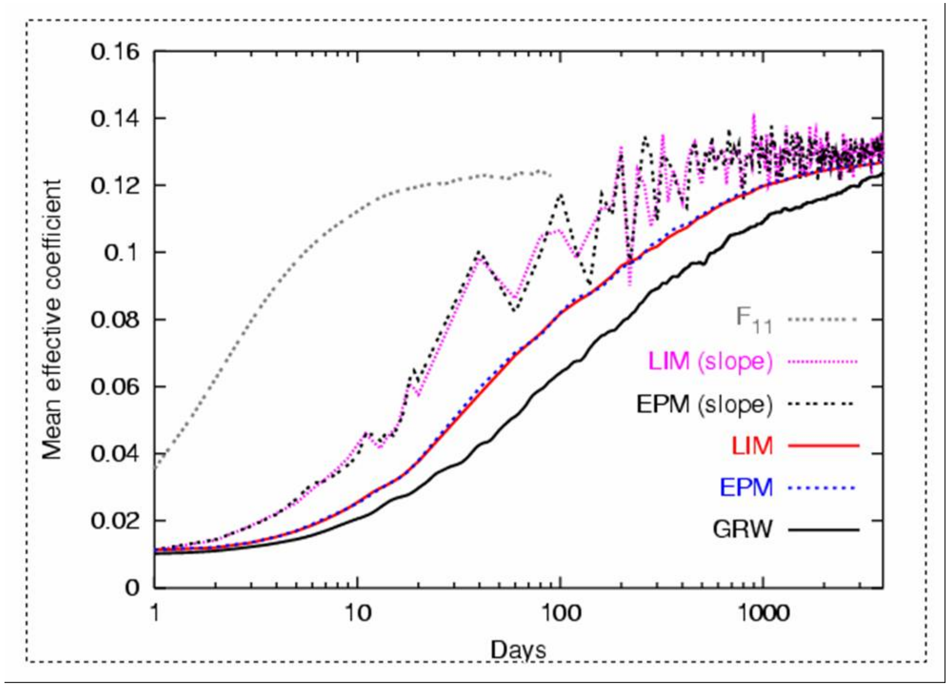
Single realization

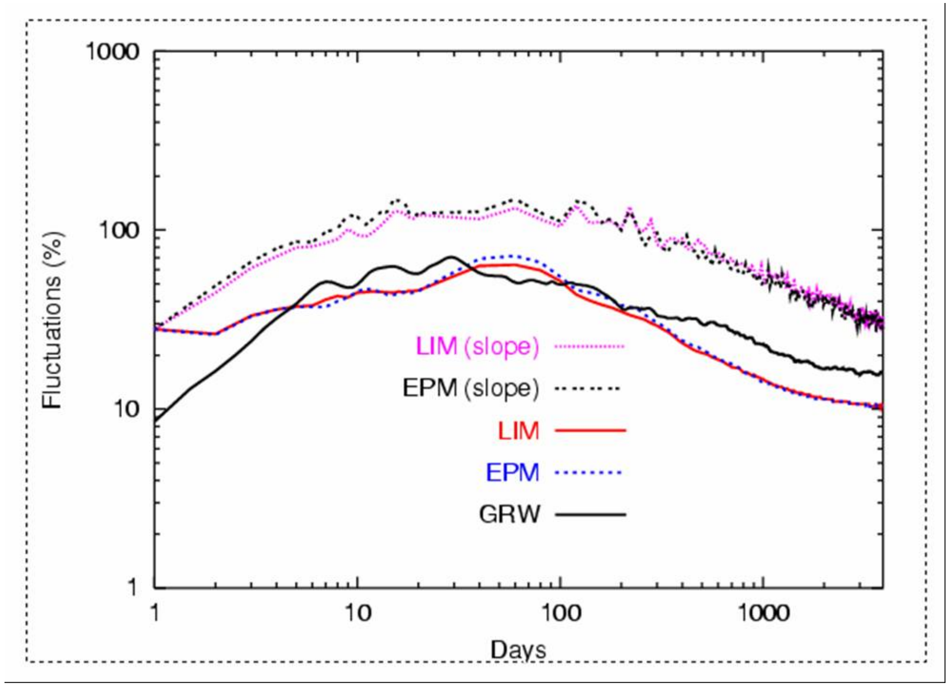
Averages over ensemble of velocity

(u2: $\delta x = 0.01\ m\ \&\ \delta t = 0.1\ day$) necessary for given velocity

(u1: $\delta x = 0.10\ m\ \&\ \delta t = 0.5\ day$) enough for reliable statistics

GRW supplies evaluations for 1-st order approximations in hydro-geology





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Conclusions

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- The local CA property makes BGRW algorithm naturally parallel.

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- The local CA property makes BGRW algorithm naturally parallel.
- Efficient large scale simulations are possible when BGRW is used conjointly with UGRW.
- GRW procedures are appropriate for reaction-diffusion problems: the number of particles can be as large as the real number of molecules of various species involved in chemical reactions.

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Thank you for your attention!