

EGU21-1941: Global random walk solvers for fully coupled flow and transport in saturated/unsaturated porous media

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Coupled flow and transport model:

$$\frac{\partial}{\partial t} \theta(\psi, c) - \nabla \cdot [K(\theta(\psi, c)) \nabla (\psi + z)] = 0,$$

$$\frac{\partial}{\partial t} [\theta(\psi, c)c] - \nabla \cdot [D \nabla c - \mathbf{q}c] = R(c), \quad \mathbf{q} = -K(\theta(\psi, c)) \nabla (\psi + z).$$

- Richards and transport Eqs. fully coupled through $\theta(\psi, c)$ and $\theta(\psi, c)c$
- Richards Eq. parabolic-elliptic degenerate ($\theta = f(\psi, c) \leftrightarrow \theta(\psi > 0) = \text{const}$)
- Strongly nonlinear $K(\theta(\psi, c))$ (e.g., van Genuchten-Mualem model)
- Solution approach:
 - explicit FD + $L(\psi_{i,j,k}^{s+1} - \psi_{i,j,k}^s)$, iterations until $\|\psi^{s+1} - \psi^s\| \leq \varepsilon$
 - ψ & $c \approx n_{i,j,k}^s / \mathcal{N}$, $\mathcal{N} = 10^{24}$ random walkers $\equiv$ GRW
 - jump probabilities $r_\psi(K) \leq 1/(2d)$, $r_c(D, \mathbf{q}) \leq 1/(2d)$, $d = 1, 2$

$\Rightarrow$ GRW algorithms for both flow and transport are free of numerical diffusion

<https://arxiv.org/abs/2011.12889>

<https://github.com/PMFlow/RichardsEquation> (Matlab codes)

Global Random Walk

RW $\equiv$ Particle Tracking on lattices with diffusion coefficient $D = r(d\Delta x)^2/2\Delta t$:

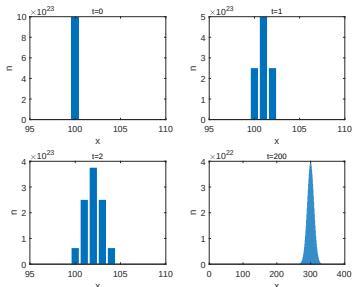
$$X_{t+1} = X_t + v\Delta x + \xi d, \quad v = \lfloor V\Delta t/\Delta x \rfloor, \quad P(\xi = \pm 1) = r/2, \quad P(\xi = 0) = (1 - r).$$

GRW $\equiv$ counting the number of particles at lattice sites

unbiased GRW ($d \geq 1$):

$$n_{i,t} = \delta n_{i+v,t} + \delta n_{i+v-d,t} + \delta n_{i+v+d,t}$$

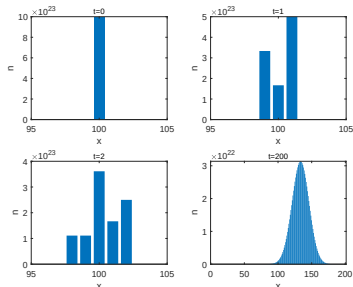
$$\overline{\delta n_{i+v,t}} = (1-r)\overline{n_{i,t}}, \quad \overline{\delta n_{i+v\pm d,t}} = \frac{r}{2}\overline{n_{i,t}}$$



biased GRW ($d = 1$):

$$n_{i,t} = \delta n_{i,t} + \delta n_{i-1,t} + \delta n_{i+1,t}$$

$$\overline{\delta n_{i,t}} = (1-r)\overline{n_{i,t}}, \quad \overline{\delta n_{i\pm 1,t}} = \frac{1}{2}(r \pm v)\overline{n_{i,t}}$$



Note: $v \leq r$ implies $\text{Pé} = V\Delta x/D \leq 2$ in BGRW codes.

Straightforward quantification of numerical diffusion: consider a 2-dim. diffusion with constant diffusion and drift coefficients $D = \text{const}$ and $V_x = 0$, $V_z = \text{const}$, compute D_x and D_z from the 2-nd centered moment of the numerical solution and estimate errors $\varepsilon_{D_x} = |D_x - D|/D$ and $\varepsilon_{D_z} = |D_z - D|/D$ at fixed $t = T$.

Estimation of numerical diffusion for BGRW, GRW and FV codes.

	$\Delta x = \Delta z$	$T/\Delta t$	Pé	ε_{D_x}	ε_{D_z}
BGRW	0.1	2	3.31	7.55e-02	2.60e-01
	0.05	9	1.65	1.90e-16	1.48e-15
	0.01	239	0.33	4.16e-16	1.02e-15
	0.005	960	0.17	2.93e-15	3.63e-15
GRW	0.1	4	3.31	1.94e-16	6.14e-16
	0.05	4	1.65	6.60e-17	8.05e-16
	0.01	19	0.33	1.94e-16	4.79e-16
	0.005	39	0.17	2.10e-15	8.92e-16
TPFA- Finite Volume	0.1	5	3.31	9.16e-03	1.99e-01
	0.05	10	1.65	4.69e-03	9.94e-02
	0.01	50	0.33	9.58e-04	1.99e-02
	0.005	100	0.17	5.38e-04	9.89e-03

Flow GRW with L -scheme linearization

FD scheme with backward discretization in time of 1dim Richards equation

$$\theta(\psi_{i,k}) - \theta(\psi_{i,k-1}) = \frac{\Delta t}{\Delta z^2} \left\{ [K(\psi_{i+1/2,k})(\psi_{i+1,k} - \psi_{i,k}) - K(\psi_{i-1/2,k})(\psi_{i,k} - \psi_{i-1,k})] + (K(\psi_{i+1/2,k}) - K(\psi_{i-1/2,k})) \Delta z \right\}$$

- linearized by adding a stabilization term $L(\psi_{i,k}^{s+1} - \psi_{i,k}^s)$ and performing

$s = 1, 2, \dots$ iterations until $\|\psi_k^s - \psi_k^{s-1}\| \leq \varepsilon_a + \varepsilon_r \|\psi_k^s\|$;

- with $r_{i\pm 1/2,k}^s = K(\psi_{i\pm 1/2,k}^s) \Delta t / (L \Delta z^2)$ and $\psi_{i,k}^s \approx n_{i,k}^s a / \mathcal{N}$, a equal to a unit length $\Rightarrow$

$$n_{i,k}^{s+1} = \left[1 - (r_{i+1/2,k}^s + r_{i-1/2,k}^s) \right] n_{i,k}^s + r_{i+1/2,k}^s n_{i+1,k}^s + r_{i-1/2,k}^s n_{i-1,k}^s + \lfloor \mathcal{N} f^s \rfloor,$$

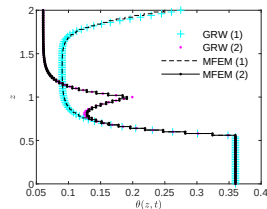
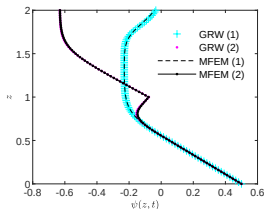
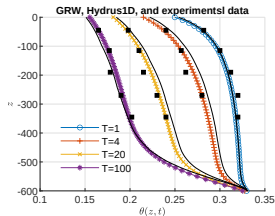
where $f^s = (r_{i+1/2,k}^s - r_{i-1/2,k}^s) \Delta z - [\theta(n_{i,k}^s) - \theta(n_{i,k-1}^s)] / L$.

The solution is obtained with the **BGRW algorithm**

$$n_{j,k}^s = \delta n_{j,j,k}^s + \delta n_{j-1,j,k}^s + \delta n_{j+1,j,k}^s,$$

$$\overline{\delta n_{j,j,k}^s} = [1 - (r_{j-1/2,k}^s + r_{j+1/2,k}^s)] \overline{n_{j,k}^s}, \quad \overline{\delta n_{j\mp 1/2,j,k}^s} = r_{j\mp 1/2,k}^s \overline{n_{j,k}^s}.$$

Validation tests of the flow GRW algorithms were done by comparisons with experimental data, exact analytical solutions, and reference MFEM solutions.



Left: comparison between measured water content in a free drainage experiment, Hydrus 1D solutions, and GRW solutions for 1dim unsaturated flow.

Middle: pressure profiles computed with GRW solver and Richy MFEM for soil column with constant pressure at the bottom and variable flux at the top, for constant (scenario 1) and $K_{saturated}$ with jump at half height (scenario 2).

Right: water content for the same scenarios as in the middle panel.

GRW solutions for fully coupled flow and reactive transport

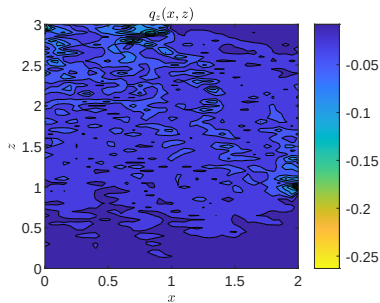
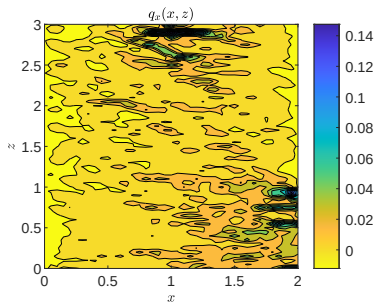
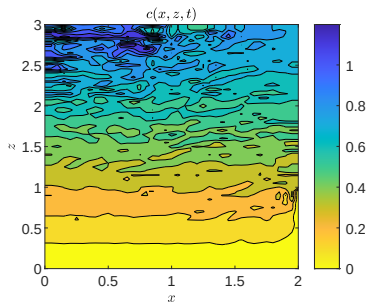
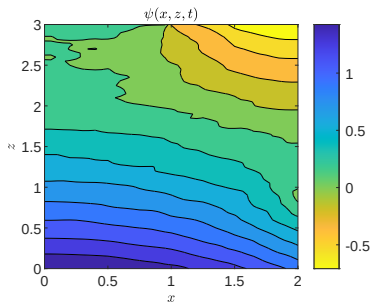
- $\theta(\psi)$ and $K(\theta(\psi))$ are given by the van Genuchten-Mualem model

$$\Theta(\psi) = \begin{cases} (1 + (-\alpha\psi)^n)^{-m}, & \psi < 0 \\ 1, & \psi \geq 0, \end{cases}$$
$$K(\Theta(\psi)) = \begin{cases} K_{sat} \Theta(\psi)^{\frac{1}{2}} \left[1 - \left(1 - \Theta(\psi)^{\frac{1}{m}} \right)^m \right]^2, & \psi < 0 \\ K_{sat}, & \psi \geq 0, \end{cases}$$

where θ_{res} , θ_{sat} , represent the residual and saturated water content, respectively and K_{sat} is the saturated hydraulic conductivity.

- K_{sat} is modeled as space random function with Gaussian correlation
- the flow and transport are coupled in both directions through $\theta(\psi, c) = \theta(\gamma(c)\psi)$, where $\gamma(c) = 1/[1 - b \ln(c/a + 1)]$
- the nonlinear reaction term is specified as $R(c) = 10^{-3}c/(1 + c)$ [<https://arxiv.org/abs/2011.12889>, Sect. 5]

Solutions for loam soil parameters



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Thank you for your visit!