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Comparative performance of stiff ODE solvers for simulating transport in heterogeneous porous media

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Introduction

Interested in large stiff systems of nonlinear ordinary differential equations in autonomous form

$$\frac{du}{dt} = g(u(t)), \qquad u(0) = u_0,$$

where $u \in \mathbb{R}^N$ and N is large.

- Arise from spatial discretisations of nonlinear time-dependent partial differential equations (transport in porous media)
- Explicit methods, e.g., forward Euler

$$u_{n+1} = u_n + \tau_n g(u_n)$$

- Implicit methods, e.g., backward Euler

$$u_{n+1} = u_n + \tau_n g(u_{n+1})$$

- For stiff systems: Implicit $\gg$ Explicit
- Exponential integrators v backward differentiation formulae (BDF)

Exponential integrators

An *exponential integrator* is any time integration method that involves the exponential of the Jacobian matrix.

Prototype method (exponential Euler method) Solve the linearised problem

$$\frac{du}{dt} = g_n + J_n(u - u_n)\,, \qquad J = \frac{\partial g}{\partial u}\,,$$

gives the time-stepping formula

$$u_{n+1} = u_n + \tau_n \varphi_1(\tau_n J_n) g_n\,, \qquad \varphi_1 = \frac{e^z - 1}{z}\,.$$

Exponential integrators are

- Explicit
- Stable in the entire complex plane (linear stability sense)

Krylov subspace methods for $\varphi(\tau J_n)b$

Extract an approximation from a small dimensional Krylov subspace

$$\mathcal{K}_m(J_n, b) = \operatorname{span}\left\{b, J_n b, \ldots, J_n^{m-1} b\right\} \subseteq \mathbb{R}^N .$$

To do this we construct an orthonormal basis for the subspace $V_m = [v_1, v_2, \ldots, v_m] \in \mathbb{R}^{N \times m}$ using Arnoldi's method:

$$J_n V_m = V_m H_m + \beta_m v_{m+1} e_m^T , \qquad H_m = V_m^T J_n V_m \in \mathbb{R}^{m \times m} .$$

Arnoldi's method requires only matrix-vector products with J_n. These products can be approximated efficiently and accurately using difference quotients

$$J_n v \approx \frac{g(u_n + \epsilon v) - g_n}{\epsilon}$$

involving function evaluations of $g(u)$. This avoids generating the need to form J_n.

Krylov subspace methods for $\varphi(\tau J_n)b$

Use FOM approximation in the Cauchy integral formula:

$$\begin{aligned}\varphi(\tau J_n)b &= \frac{1}{2\pi i}\int_\Gamma \varphi(\lambda)(\lambda I - \tau J_n)^{-1} b\, d\lambda \\ &\approx \frac{1}{2\pi i}\int_\Gamma \varphi(\lambda)\|b\|_2 V_m(\lambda I - \tau H_m)^{-1} e_1\, d\lambda \\ &= V_m \varphi(\tau H_m) e_1 \cdot \|b\|_2\,.\end{aligned}$$

Very accurate approximations can be obtained for $m \ll N$ so the matrix $\varphi(\tau H_m)$ can be computed cheaply (using diagonalisation or Padé approximation). Other Krylov approaches exist:

- Harmonic Ritz approximation
  (Hochbruck & Hochstenbach, 2009 and Carr, Turner & Ilic, 2011)
- First approximate $\varphi(z)$ using a rational function. Then use GMRES/FOM to approximate each of the terms in the partial fraction form
  (Schmelzer & Trefethen, 2007, Frommer & Simoncini, 2008 and Carr, Turner & Perré, 2012)

Higher order exponential integrators

Write the ODE system in the form

$$\frac{du}{dt} = g_n + J_n(u - u_n) + d(u)\,,$$

where $d(u) = g(u) - g_n - J_n(u - u_n)$.

Using the integrating factor e^{-tJ_n}:

$$\frac{d}{dt}\left(e^{-tJ_n}u(t)\right) = e^{-tJ_n}\left(g_n - J_n u_n\right) + e^{-tJ_n}d(u)\,.$$

Exact solution can be expressed as

$$u(t_{n+1}) = u_n + \tau_n \varphi_1(\tau_n J_n) g_n + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-t)J_n} d(u(t))\,dt\,.$$

This is the starting point for developing higher order methods.

Higher order exponential integrators

General class of methods. Consist of $(s-1)$ internal stages $\tilde{u}_{n,i}$ that approximate the solution at $t = t_n + c_i\tau_n$.

$$\tilde{u}_{n,i} = u_n + c_i\tau_n\varphi_1(c_i\tau_n J_n)g_n + \tau_n \sum_{j=1}^{i-1} a_{ij}(\tau_n J_n)d_{n,j}\,, \quad i = 2\ldots s$$

$$u_{n+1} = u_n + \tau_n\varphi_1(\tau_n J_n)g(u_n) + \tau_n \sum_{i=2}^{s} b_i(\tau_n J_n)d_{n,i}$$

The weights $b_i(z)$ and coefficients $a_{ij}(z)$ are linear combinations of the so called φ-functions

$$\varphi_1(z) = (e^z - 1)/z$$
$$\varphi_2(z) = (e^z - 1 - z)/z^2$$
$$\varphi_3(z) = (e^z - 1 - z - \tfrac{1}{2}z^2)/z^3\,, \quad \text{etc.}$$

Exponential Rosenbrock methods

`exprb32`: Third order method with second order embedded method: (Hochbruck & Ostermann, 2009)

$$
\begin{aligned}
\tilde{u}_{n,1} &= u_n + \tau_n \varphi_1(\tau_n J_n) g_n \\
u_{n+1} &= u_n + \tau_n \varphi_1(\tau_n J_n) g_n + 2\tau_n \varphi_3(\tau_n J_n) d_{n,1} \\
\hat{u}_{n+1} &= u_n + \tau_n \varphi_1(\tau_n J_n) g_n
\end{aligned}
$$

Two Krylov subspaces: J_n with g_n and $d_{n,1}$.

`exprb43`: Fourth order method with third order embedded method: (Hochbruck & Ostermann, 2009)

$$
\begin{aligned}
\tilde{u}_{n,1} &= u_n + \tfrac{\tau_n}{2} \varphi_1(\tfrac{\tau_n}{2} J_n) g_n \\
\tilde{u}_{n,2} &= u_n + \tau_n \varphi_1(\tau_n J_n) g_n + \tau_n \varphi_1(\tau_n J_n) d_{n,1} \\
u_{n+1} &= u_n + \tau_n \varphi_1(\tau_n J_n) g_n + \tau_n \left[16\varphi_3(\tau_n J_n) - 48\varphi_4(\tau_n J_n)\right] d_{n,1} \\
&\quad + \tau_n \left[-2\varphi_3(\tau_n J_n) + 12\varphi_4(\tau_n J_n)\right] d_{n,2} \\
\hat{u}_{n+1} &= u_n + \tau_n \varphi_1(\tau_n J_n) g_n + 16\tau_n \varphi_3(\tau_n J_n) d_{n,1} - 2\tau_n \varphi_3(\tau_n J_n) d_{n,2}
\end{aligned}
$$

Three Krylov subspaces: J_n with g_n, $d_{n,1}$ and $d_{n,2}$.

Backward differentiation formulae

Evaluate ODE system at $t = t_{n+1}$ to give

$$\frac{du}{dt}(t_{n+1}) = g(u_{n+1})$$

For a BDF of order q: Interpolate the solution at (t_{n+1-i}, u_{n+1-i}), $i = 0, \ldots, q$ using a polynomial of degree q:

$$u(t) \approx \sum_{i=0}^{q} \ell_i(t) u_{n+1-i} \qquad \ell_i(t) = \prod_{\substack{j=0 \\ j \neq i}}^{q} \frac{t - t_{n+1-j}}{t_{n+1-i} - t_{n+1-j}}$$

where $\ell_i(t)$ are the usual Lagrange interpolating polynomials.

Differentiate interpolant and evaluate at $t = t_{n+1}$ to obtain

$$\frac{du}{dt}(t_{n+1}) \approx \sum_{i=0}^{q} \ell_i'(t) u_{n+1-i}$$

Backward differentiation formulae

This leads to a system of nonlinear equations

$$f(u_{n+1}) = u_{n+1} - \gamma_n g(u_{n+1}) + a_n = 0\,,$$

where $a_n = \sum_{i=1}^{q} \alpha_{n,i}/\alpha_{n,0} u_{n+1-i}$, $\alpha_{n,i} = \tau_n \ell_i'(t_{n+1})$ and $\gamma_n = \tau_n/\alpha_{n,0}$.

All comparisons made using the CVODE module of the Suite of Nonlinear and Differential/Algebraic Equation Solvers (SUNDIALS)[1] (Hindmarsh et al. 2005)

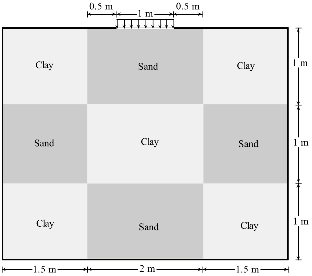
- Employs Newton iteration with a preconditioned GMRES method.
- Periodically adjusts the order, with the goal of maximizing the stepsize τ_n
- At every step, the local error is estimated and the time step adjusted to satisfy user prescribed error tolerances

[1] https://computation.llnl.gov/casc/sundials/main.html

Test Problem: Water infiltration

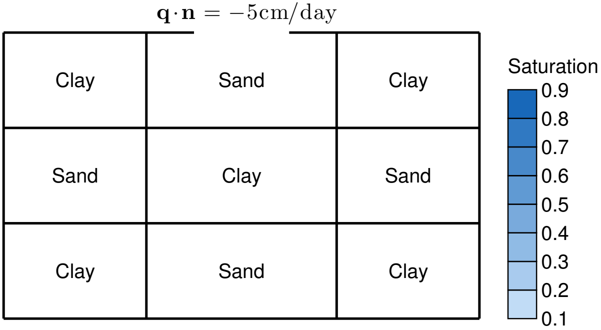
The test problem is derived from a spatial discretisation of Richards' equation for unsaturated flow of water in heterogeneous soils (Kirkland et al., 1992 and Carr, Moroney & Turner, 2011)

$$\begin{cases} \dfrac{\partial\theta}{\partial t} = \nabla \cdot q\,, \quad q = -K(h)(\nabla h + e_y) \\ \text{on } 0 < x < 5 \text{ and } 0 < y < 3 \\ \\ \text{Initial condition} \\ h = -500 \qquad \text{at } t = 0 \\ \\ \text{Boundary conditions} \\ q \cdot n = -5 \quad \text{on } 2 < x < 3 \text{ and } y = 3 \\ q \cdot n = 0 \qquad \text{elsewhere} \end{cases}$$



The problem is discretised on a uniform 132×132 grid by central differences, so that the dimension of the resulting ODE problem is $N = 16641$.

Test Problem: Water infiltration



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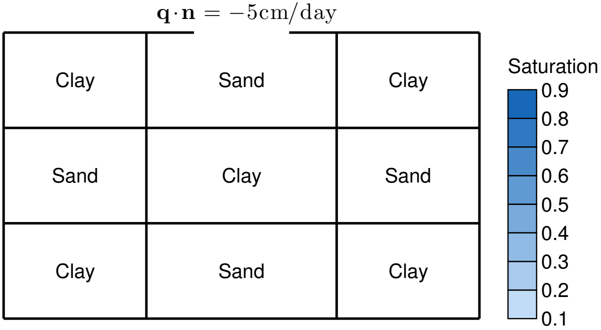

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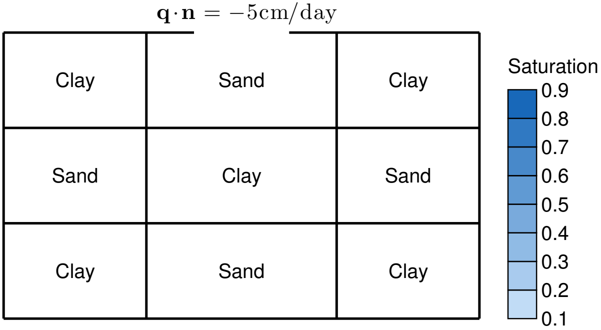

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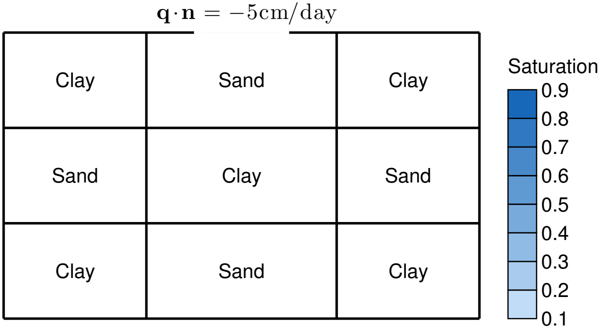

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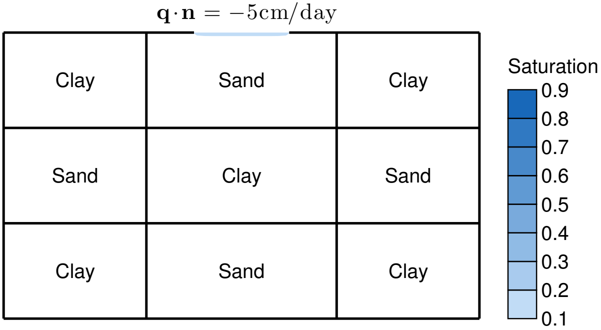

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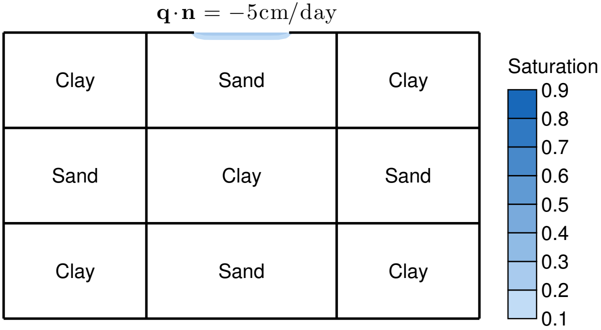

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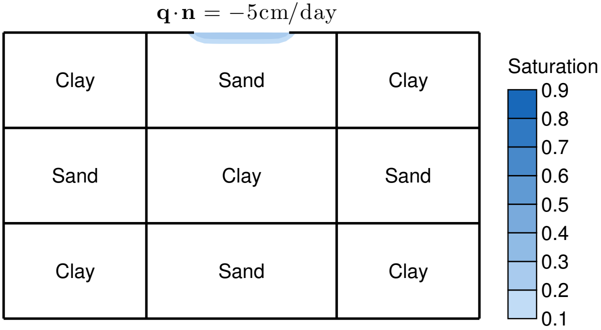

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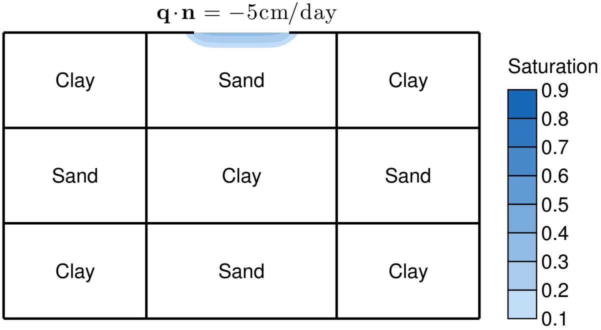

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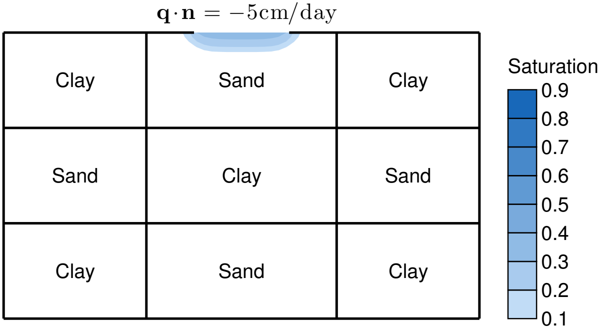

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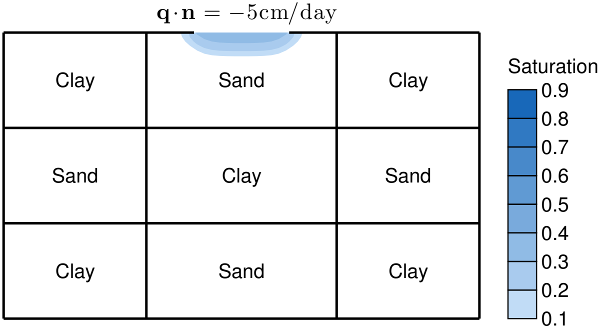

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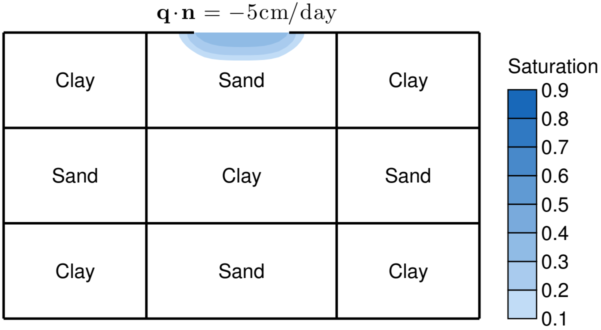

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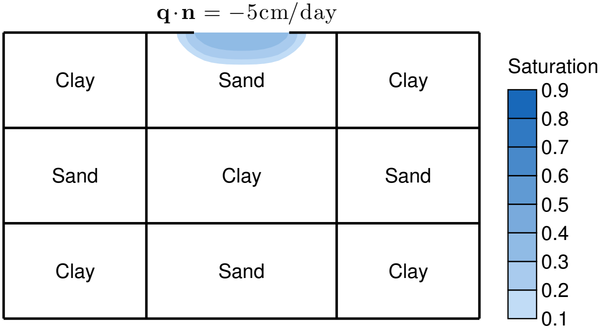

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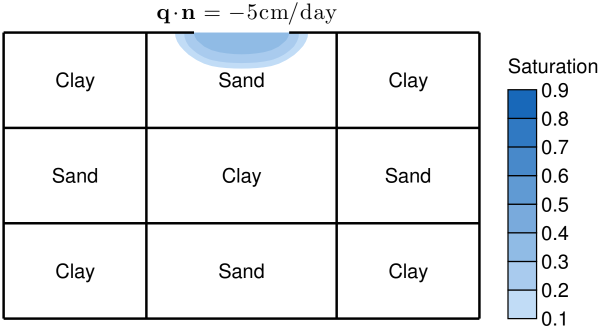

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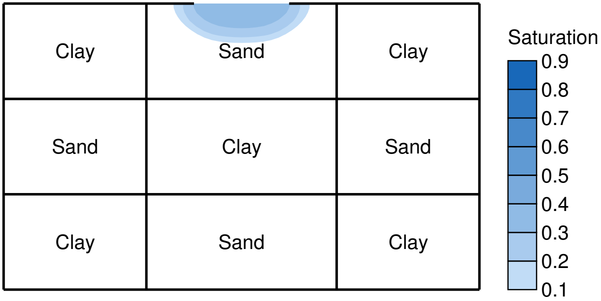
$\mathbf{q} \cdot \mathbf{n} = -5\text{cm/day}$



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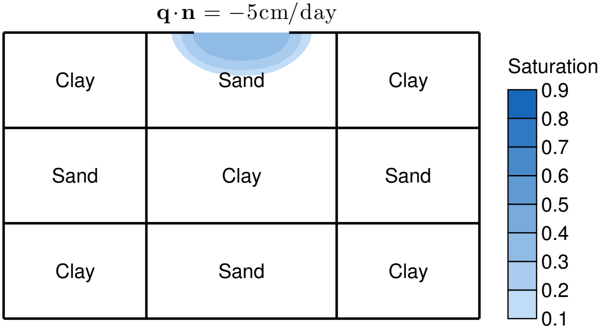

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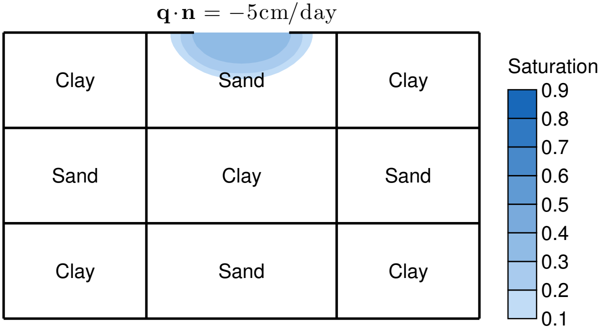

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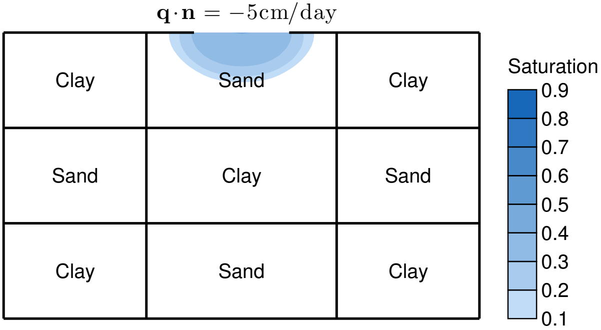

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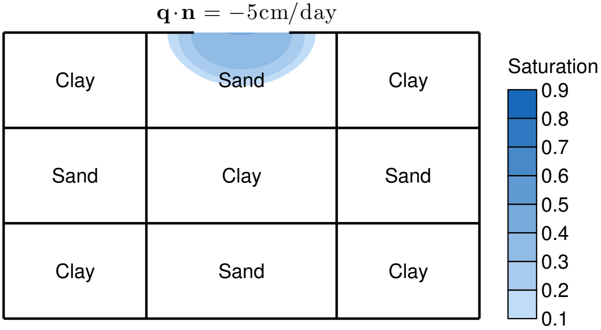

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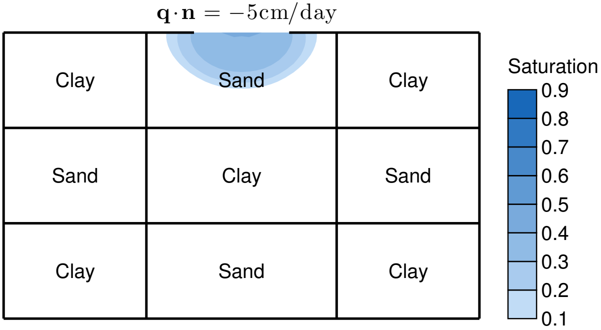

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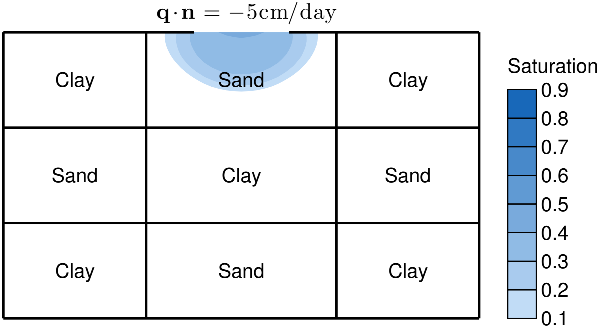

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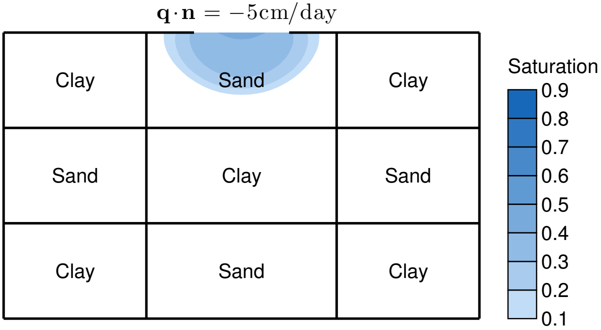

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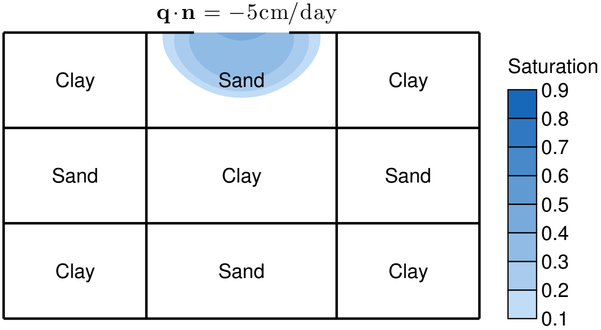

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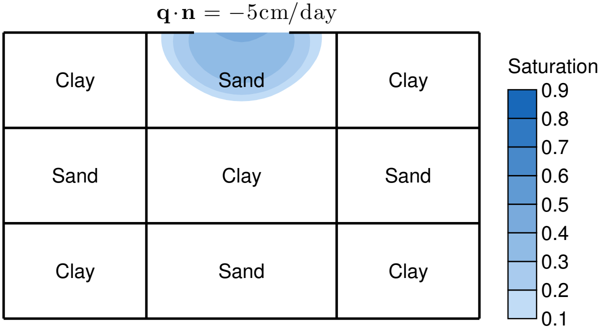

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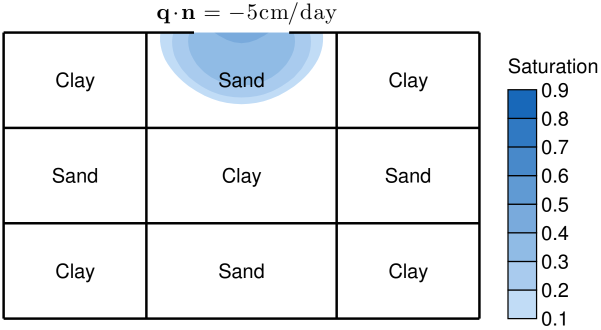

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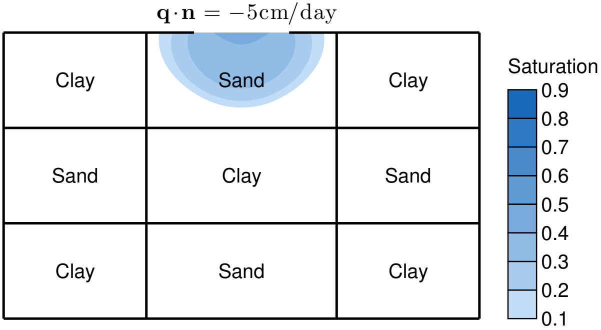

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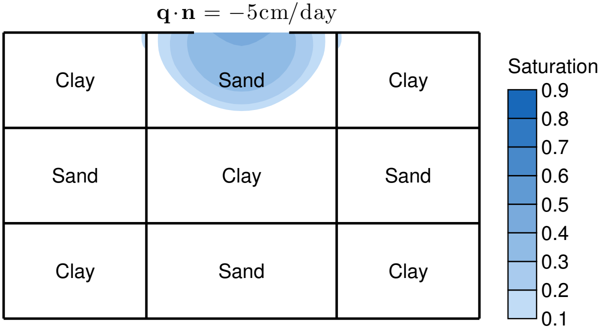

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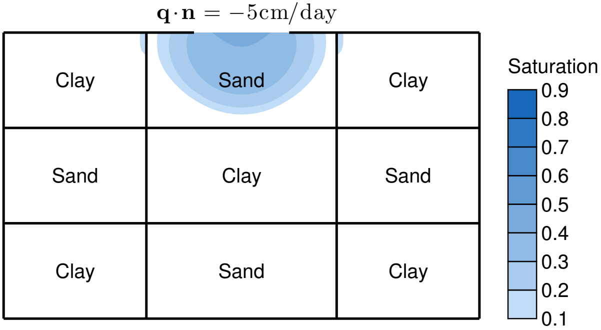

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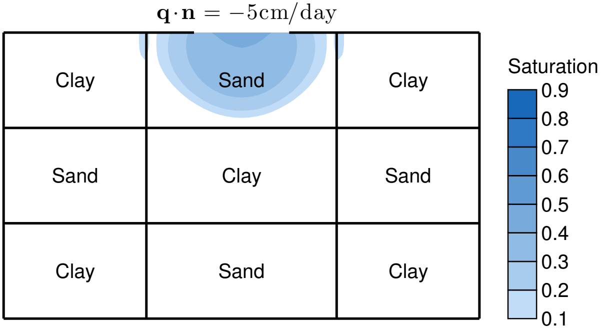

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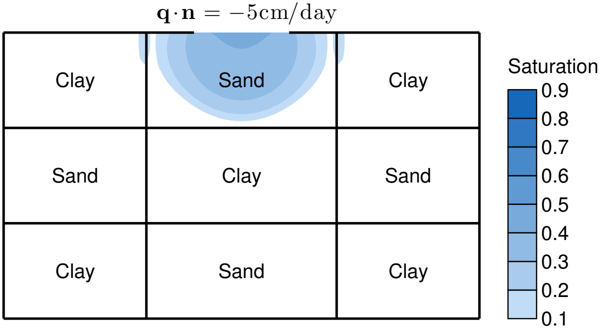

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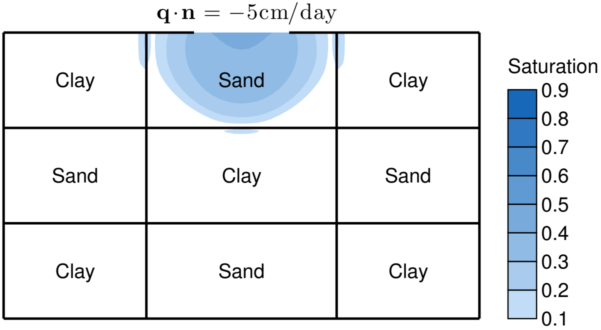

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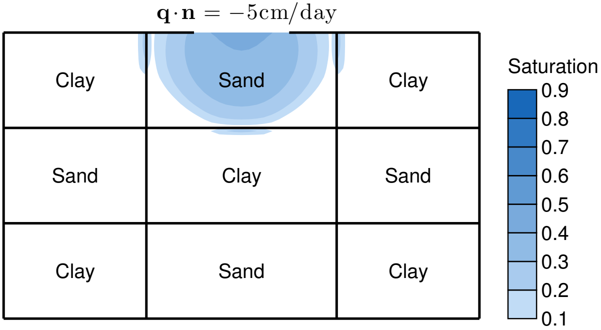

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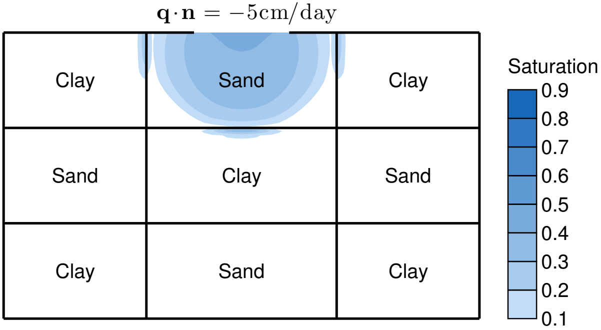

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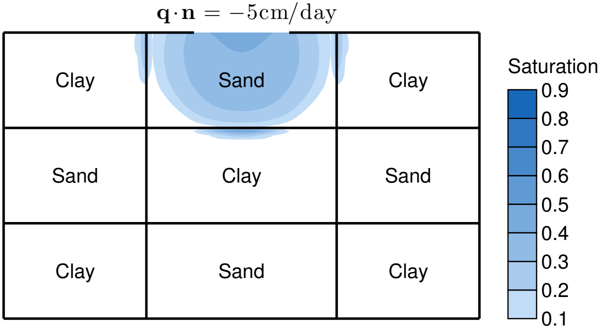

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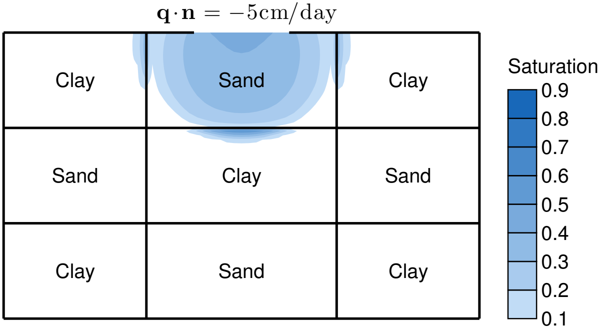

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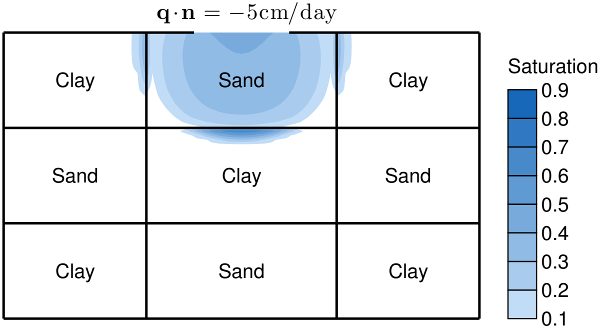

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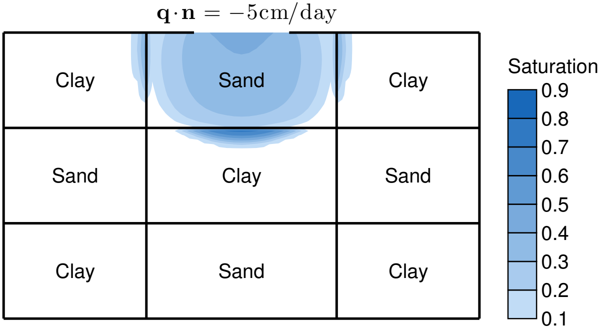

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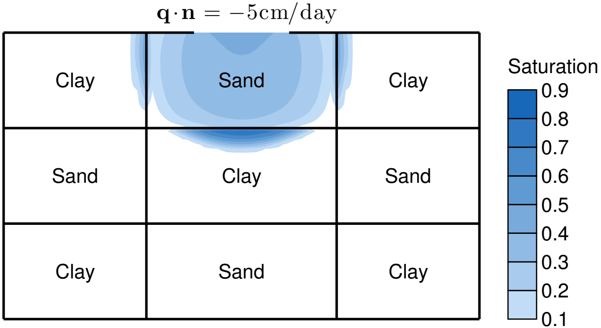

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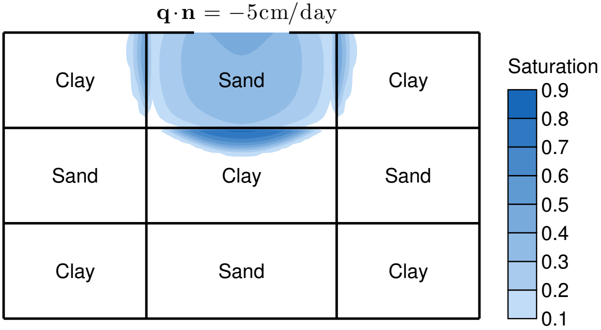

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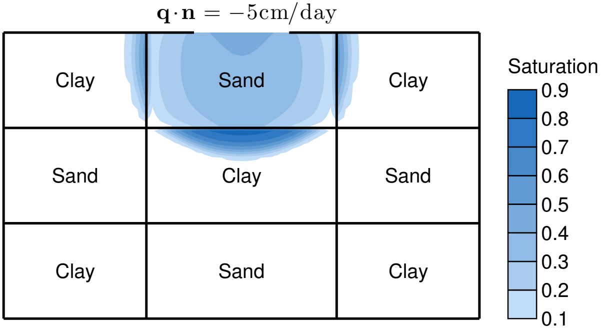

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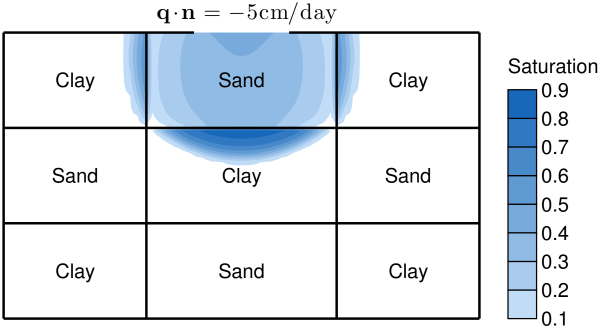

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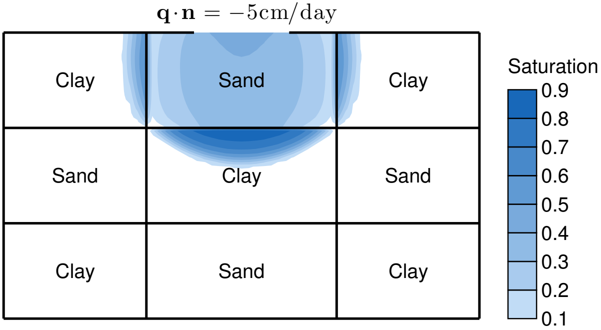

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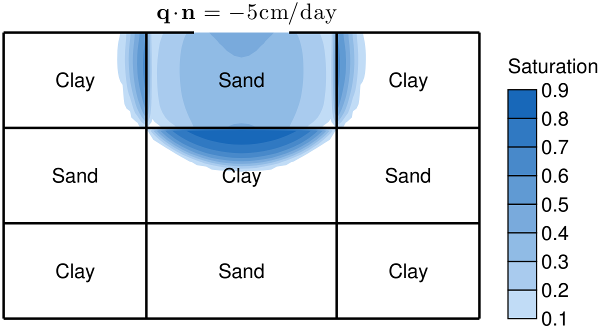

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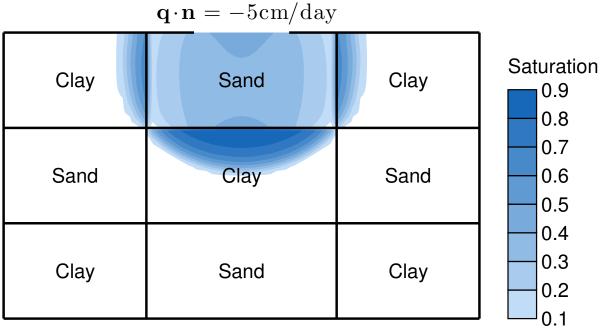

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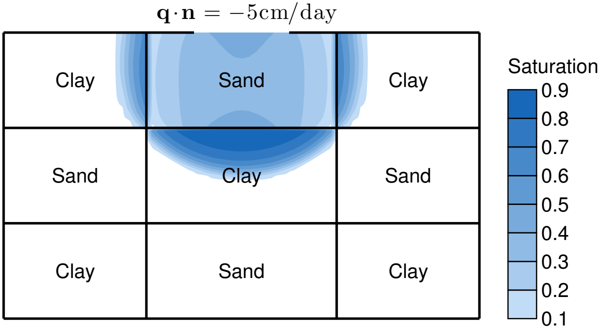

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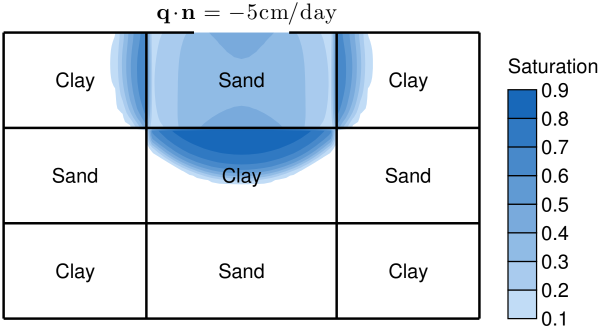

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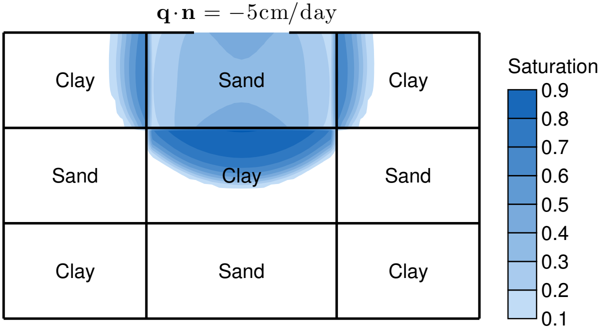
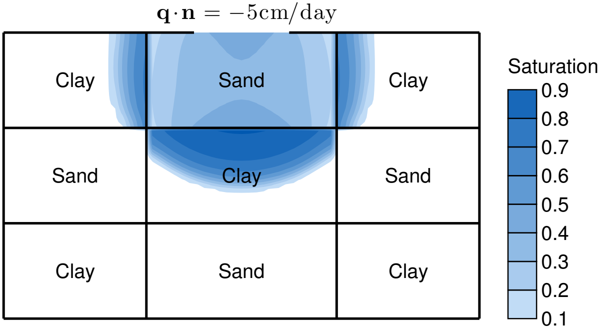
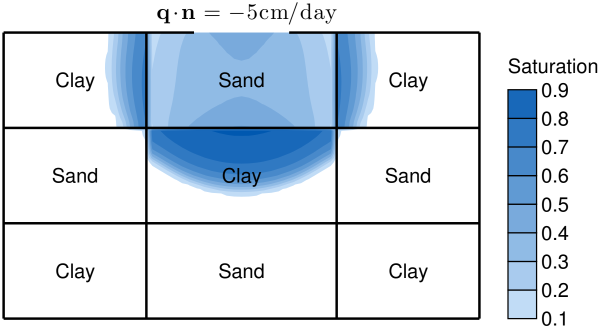


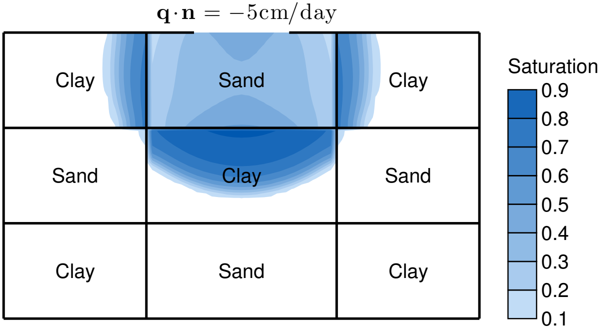
Test Problem: Water infiltration



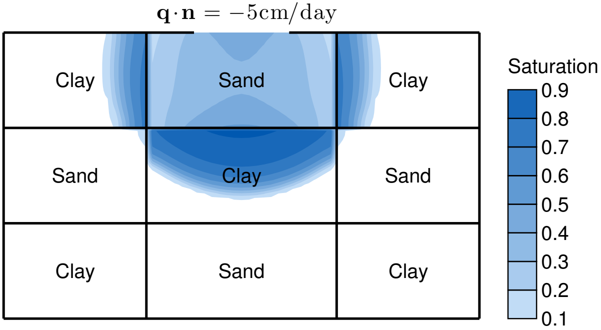
Test Problem: Water infiltration



Test Problem: Water infiltration

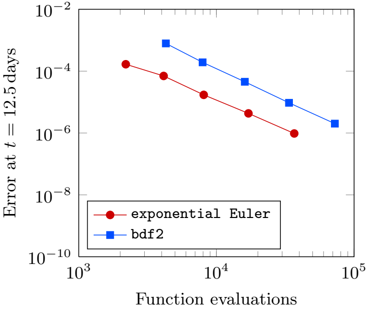


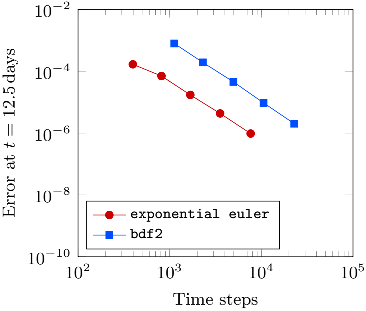
Test Problem: Water infiltration



Test Problem: Water infiltration

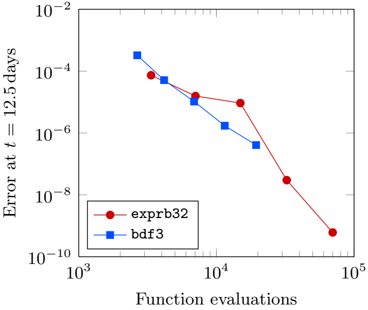
Methods of order 2

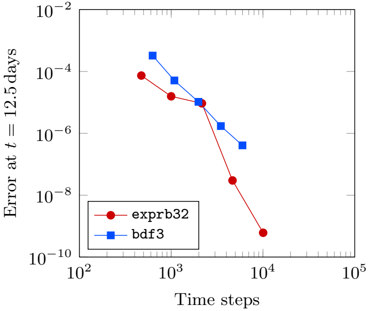




Test Problem: Water infiltration

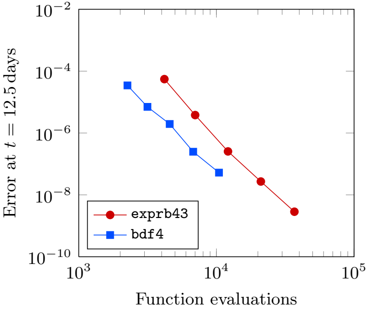
Methods of order 3

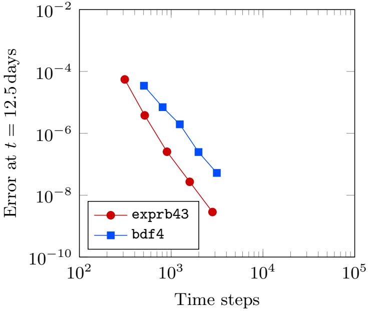




Test Problem: Water infiltration

Methods of order 4





Conclusions

Summary

- exponential integrators can be competitive with state-of-the-art methods for transport phenomena problems
- performance declines slightly in terms of function evaluations for higher order methods

Current work / Future plan

Higher order methods involve multiple products of matrix functions and vectors

$$\varphi(\tau_n J_n) g_n\,, \qquad \varphi(\tau_n J_n) d_{n,1}\,, \qquad \varphi(\tau_n J_n) d_{n,2}\,.$$

However, all Krylov subspaces are with the same Jacobian matrix. How can we reuse some of the information from one Krylov subspace to the next?