Efficient simulation of unsaturated flow in heterogeneous soils using an exponential integrator

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Exponential Integrators

Consider systems of initial value problems of the form

$$\frac{du}{dt} = g(u); \qquad u(0) = u_0.$$

where $u \in \mathbb{R}^N$ and $g : \mathbb{R}^N \supset D \to \mathbb{R}^N$. Exponential integrators solve these systems via the application of a function of the Jacobian matrix $J(u) = \partial g / \partial u$ on a vector v – either the matrix exponential or a closely related function:

$$\varphi(A) = A^{-1}(e^A - I) = I + \tfrac{1}{2}A + \tfrac{1}{6}A^2 + \dots$$

Recently, these methods have found application in the numerical integration of stiff problems.

The attractiveness of these methods is that they can **perform very well without the need for preconditioning** unlike implicit integrators, which require approximation to $A^{-1}v$.

Model: Richards' equation

Pressure-driven flow in porous media can be modelled using Darcy's law:

$$q = -K(h)\left(\nabla h + e_z\right),$$

where q is the Darcy flux vector, h is pressure head, K is the hydraulic conductivity and e_z is the unit vector in the vertical direction, oriented upwards.

Assuming incompressibility, conservation of mass requires that

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (K(h)\nabla h) + \frac{\partial K(h)}{\partial z}.$$

which gives the well-known mixed-form of Richards' Equation where θ is the volumetric moisture content.

Closure conditions: van Genuchten model

The effective saturation in unsaturated soil is defined as

$$S_e(h) = \left(1 + (-\alpha h)^n\right)^{-m} \ ,$$

where α and n are empirically-derived soil parameters and $m = 1 - 1/n$.

In terms of the effective saturation, the moisture content and hydraulic conductivity are given for unsaturated flow by

$$\theta(h) = \theta_{\text{res}} + \big(\theta_{\text{sat}} - \theta_{\text{res}}\big) S_e$$
$$K(h) = K_{\text{sat}} \sqrt{S_e} \left(1 - \left(1 - S_e^{1/m}\right)^m\right)^2$$

where θ_{res} and θ_{sat} are the residual and saturated moisture content respectively.

Spatial discretisation: Finite Volume Method (FVM)

Using the finite volume method on a 2D rectangular mesh and integrating over a control volume of volume $\Delta x_i \times \Delta y_j$ the following spatially discrete form of Richards' equation is obtained:

$$\frac{d\theta_p}{dt} = \frac{1}{\Delta z_j}\left(q_{i,j-1/2} - q_{i,j+1/2}\right) + \frac{1}{\Delta x_i}\left(q_{i-1/2,j} - q_{i+1/2,j}\right) ,$$

where indices on the flux vector q denote its normal derivative approximated at a representative point on the control volume face.

Enacting the chain rule on the left hand side to obtain

$$\frac{dh_p}{dt} = \frac{1}{C(h_p)}\left[\frac{1}{\Delta z_j}\left(q_{i,j-1/2} - q_{i,j+1/2}\right) + \frac{1}{\Delta x_i}\left(q_{i-1/2,j} - q_{i+1/2,j}\right)\right] ,$$

where $C(h) = d\theta/dh$ is known as the specific moisture capacity.

Exponential Euler Method (EEM)

The exponential Euler method is derived by linearising $g(u)$ about $t = t_n$. At each step this results in the linear initial value problem:

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

where $J_n = J(u_n)$ to advance the solution from $t = t_n$ to $t = t_{n+1}$.

The exact solution of this problem determines the EEM scheme:

$$\begin{aligned} u_{n+1} &= u_n + J_n^{-1}(e^{\tau_n J_n} - I)g_n \\ &= u_n + \tau_n \varphi(\tau_n J_n) g_n \end{aligned}$$

We note that the method is A-stable and second-order accurate:

$$\text{Global error} \sim \mathcal{O}(\tau_n^2) \qquad \text{Local error} \sim \mathcal{O}(\tau_n^3)$$

Numerical challenge: How do we compute $\varphi(\tau_n J_n) g_n$?

Project onto the Krylov subspace $\mathcal{K}_m(J_n, g_n) = \mathrm{span}\left\{g_n, \ldots, J_n^{m-1} g_n\right\}$:

$$\varphi(\tau_n J_n) g_n \approx \beta V_m \varphi(\tau_n H_m) e_1,$$

where $\beta = \|g_n\|_2$ and Arnoldi's method is used to generate the decomposition

$$J_n V_m = V_m H_m + \beta_m v_{m+1} e_m^T, \tag{1}$$

where V_m is a matrix whose column vectors form an orthonormal basis for $\mathcal{K}_m(J_n, g_n)$, $\beta_m = \|v_{m+1}\|_2$ and e_m is the mth canonical basis vector in $\mathbb{R}^m$. The difference quotient:

$$J(u) w \approx \frac{g(u + \varepsilon w) - g(u)}{\varepsilon}$$

is used to approximate the Jacobian-vector products required in Arnoldi's method, removing the need to explicitly form J_n.

EEM with Krylov approximation

Proposition 1

Let the Arnoldi decomposition of J_n hold as defined in (1) and let $\tilde{J}_n = J_n - \beta_m v_{m+1} v_m^T$. The following statements are true:

(i) $\tilde{J}_n V_m = V_m H_m$;

(ii) $\varphi(\tau_n \tilde{J}_n) V_m = V_m \varphi(\tau_n H_m)$ and hence $\varphi(\tau_n \tilde{J}_n) g_n = \beta V_m \varphi(\tau_n H_m) e_1$;

(iii) $\tilde{J}_n g_n = J_n g_n$, provided $m \geq 2$;

(iv) The local error of the scheme

$$u_{n+1} = u_n + \tau_n \beta V_m \varphi(\tau_n H_m) e_1$$

is $\mathcal{O}(\tau_n^3)$, provided $m \geq 2$.

Proof.

(i) Follows from $v_m^T V_m = e_m^T$ and rearranging the Arnoldi decomposition

$$(J_n - \beta_m v_{m+1} v_m^T) V_m = V_m H_m \,.$$

(ii) Both results follow from the invariance of $\mathcal{K}_m(J_n, g_n)$ under $\tilde{J}_n$.

(iii) Consider

$$\tilde{J}_n g_n = J_n g_n - \beta_m v_{m+1} v_m^T g_n,$$

but the term $v_m^T g_n$ is zero, since v_m and $g_n = \beta v_1$ are two columns of V_m, and hence are orthogonal.

Proof. cont'd

(iv) We analyse the equivalent scheme

$$u_{n+1} = u_n + \tau_n \varphi(\tau_n \tilde{J}_n) g_n,$$

and expand to obtain

$$\begin{aligned} u_{n+1} &= u_n + \tau_n \varphi(\tau_n \tilde{J}_n) g_n \\ &= u_n + \tau_n \left(I + \frac{\tau_n}{2} \tilde{J}_n + \mathcal{O}(\tau_n^2) \right) g_n \\ &= u_n + \tau_n g_n + \frac{\tau_n^2}{2} \tilde{J}_n g_n + \mathcal{O}(\tau_n^3) \\ &= u_n + \tau_n g_n + \frac{\tau_n^2}{2} J_n g_n + \mathcal{O}(\tau_n^3), \end{aligned}$$

which agrees with the Taylor series expansion of u_{n+1} about $t = t_n$ to second order.

Local error control

Propose to use the difference between u_{n+1} and a second approximate solution $u_{n+1}^{(2)}$, computed using a two-step scheme with half-sized steps:

$$\begin{aligned} u_{n+1/2} &= u_n + \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}J_n)g_n \\ u_{n+1}^{(2)} &= u_{n+1/2} + \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}J_{n+1/2})g(u_{n+1/2}), \end{aligned}$$

where $J_{n+1/2} = J(u_{n+1/2})$.

Replacing $J_{n+1/2}$ with J_n, and $g(u_{n+1/2})$ with its orthogonal projection $V_m V_m^T g(u_{n+1/2})$ onto the space $\mathcal{K}_m(J_n, g_n)$ results in the following modified scheme

$$\begin{aligned} u_{n+1/2} &= u_n + \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}J_n)g_n \\ u_{n+1}^{(2)} &= u_{n+1/2} + \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}J_n)V_m V_m^T g(u_{n+1/2})\,. \end{aligned}$$

This allows all matrix function terms to be approximated using the existing Arnoldi decomposition:

$$\varphi(\tfrac{\tau_n}{2}J_n)g_n \approx \beta V_m \varphi(\tfrac{\tau_n}{2}J_n)e_1$$
$$\varphi(\tfrac{\tau_n}{2}J_n)V_m \approx V_m \varphi(\tfrac{\tau_n}{2}H_m),$$

and we obtain the final two-step scheme:

$$u_{n+1/2} = u_n + \tfrac{\tau_n}{2}\beta V_m \varphi(\tfrac{\tau_n}{2}H_m)e_1$$
$$u^{(2)}_{n+1} = u_{n+1/2} + \tfrac{\tau_n}{2}V_m \varphi(\tfrac{\tau_n}{2}H_m)V_m^T g(u_{n+1/2}).$$

Conclusion

The value of $u^{(2)}_{n+1}$ can be approximated using a single additional function evaluation!

Order of two-step scheme

Proposition 2

Let the Arnoldi decomposition of J_n hold as defined in (1) and let $\tilde{J}_n = J_n - \beta_m v_{m+1} v_m^T$ as in Proposition 1. The local error of the scheme:

$$u_{n+1/2} = u_n + \tfrac{\tau_n}{2}\beta V_m \varphi(\tfrac{\tau_n}{2} H_m) e_1$$
$$u_{n+1}^{(2)} = u_{n+1/2} + \tfrac{\tau_n}{2} V_m \varphi(\tfrac{\tau_n}{2} H_m) V_m^T g(u_{n+1/2}),$$

is $\mathcal{O}(\tau_n^3)$ provided $m \geq 2$.

Proof.

We analyse the equivalent scheme:

$$\begin{aligned} u_{n+1/2} &= u_n + \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}\tilde{J}_n)g_n \\ u_{n+1}^{(2)} &= u_{n+1/2} + \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}\tilde{J}_n)V_m V_m^T g(u_{n+1/2}). \end{aligned}$$

Expanding:

$$\begin{aligned} \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}\tilde{J}_n)g_n &= \frac{\tau_n}{2}g_n + \frac{\tau_n^2}{8}J_n g_n + \mathcal{O}(\tau_n^3) \\ g(u_{n+1/2}) &= g_n + \frac{\tau_n}{2}J_n g_n + \mathcal{O}(\tau_n^2) \\ V_m V_m^T g(u_{n+1/2}) &= g_n + \frac{\tau_n}{2}J_n g_n + \mathcal{O}(\tau_n^2) \\ \tfrac{\tau_n}{2}\varphi(\tfrac{\tau_n}{2}\tilde{J}_n)V_m V_m^T g(u_{n+1/2}) &= \frac{\tau_n}{2}\left(I + \frac{\tau_n}{4}\tilde{J}_n + \mathcal{O}(\tau_n^2)\right)g(u_{n+1/2}) \\ &= \frac{\tau_n}{2}g_n + \frac{3\tau_n^2}{8}J_n g_n + \mathcal{O}(\tau_n^3) \end{aligned}$$

Substituting:

$$u_{n+1}^{(2)} = u_n + \tau_n g_n + \frac{\tau_n^2}{2}J_n g_n + \mathcal{O}(\tau_n^3)$$

Stepsize adjustment

Conclusion

$\Delta_n = u_{n+1} - u_{n+1}^{(2)}$ is an order equivalent approximation to the local error incurred by EEM during one integration step.

Time step (τ_n) adjusted according to the value of $\|\Delta_n\|_{\text{WRMS}}$ with $\|\cdot\|_{\text{WRMS}}$ defined by:

$$\|y\|_{\text{WRMS}} = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\frac{y_i}{w_i} \right)^2 \right)^{1/2},$$

where the weights $w_i = \text{RTOL} \cdot |y_i| + \text{ATOL}$ and ATOL_i and RTOL are the given absolute and relative error tolerances.

Backward differentiation formulae (BDF)

Current state-of-play sees the time integration of spatially-discrete forms of Richards' equation performed using variable-stepsize variable-order implementations of the BDF.

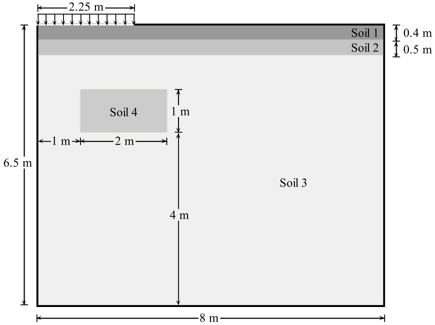
Require the solution of a nonlinear system of equations at each time step:

$$f(u_{n+1}) \equiv \alpha_{n,0} u_{n+1} - \tau_n g(u_{n+1}) + a_n = 0.$$

In this work, we compared our variable-stepsize implementation of EEM to these methods, as implemented in the CVODE module of the Suite of Nonlinear and Differential/Algebraic Equation Solvers (SUNDIALS)[1].

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

Test Problems



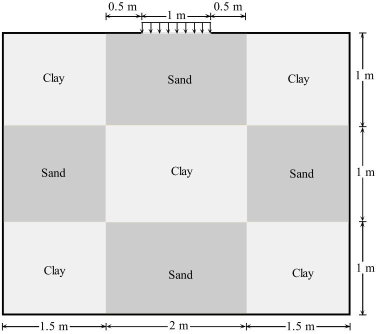
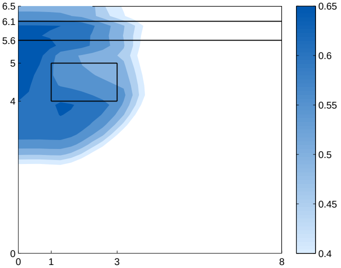


Figure: Schematic representations of the test problems: Forsyth *et al.*'s problem (left) and Kirkland *et al.*'s problem (right).

Benchmark solutions: Forsyth *et al.*'s problem

Material	θ_{res}	θ_{sat}	K_{sat} (ms^{-1})	α (m^{-1})	n
Soil 1	0.1020	0.3680	9.153×10^{-5}	3.34	1.982
Soil 2	0.0985	0.3510	5.445×10^{-5}	3.63	1.632
Soil 3	0.0859	0.3250	4.805×10^{-5}	3.45	1.573
Soil 4	0.0859	0.3250	4.805×10^{-4}	3.45	1.573



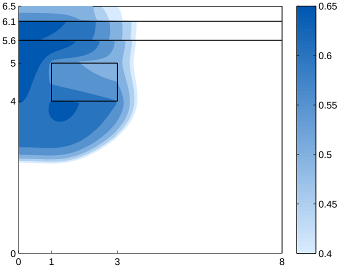


Figure: Saturation profiles for the benchmark solutions of Forsyth *et al.*'s problem at 30 days.

Benchmark solutions: Kirkland *et al.*'s problem

Material	θ_{res}	θ_{sat}	$K_{\text{sat}}\ (\text{ms}^{-1})$	$\alpha\ (\text{m}^{-1})$	n
Clay	0.1060	0.4686	1.516×10^{-6}	1.04	1.3954
Sand	0.0286	0.3658	6.262×10^{-5}	2.80	2.2390

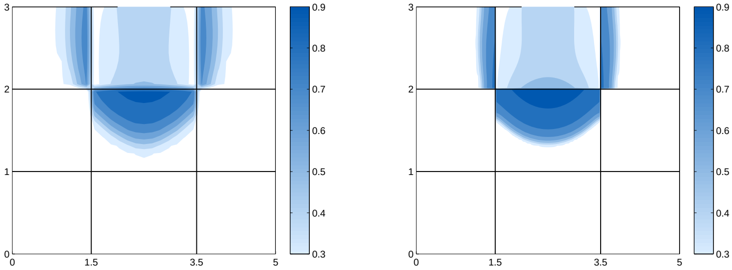


Figure: Saturation profiles for the benchmark solutions of Kirkland *et al.*'s problem at 12.5 days.

Solver statistics

		COARSE MESH				FINER MESH			
ATOL/RTOL	METHOD	ERROR	EVALS	STEPS	FAILS	ERROR	EVALS	STEPS	FAILS
Forsyth *et al.*'s problem									
10^{-3}	EEM	$5.77E-3$	704	101	0	$5.70E-2$	6416	267	0
	BDF(2)	$9.50E-3$	1313	335	0	$1.85E-2$	7601	843	1
	BDF(5)	$1.22E-3$	991	225	1	$5.19E-3$	6754	685	1
10^{-5}	EEM	$1.41E-4$	2284	441	0	$1.73E-4$	15023	1316	1
	BDF(2)	$3.83E-4$	4689	1515	2	$5.54E-4$	29046	4431	2
	BDF(5)	$1.18E-5$	1748	494	5	$8.86E-6$	11834	1675	4
10^{-7}	EEM	$9.40E-6$	9864	2037	2	$4.53E-6$	40054	6181	4
	BDF(2)	$1.94E-5$	20655	7018	3	$3.03E-5$	128423	20416	5
	BDF(5)	$5.81E-8$	3055	937	10	$8.34E-8$	21547	3213	18
Kirkland *et al.*'s problem									
10^{-3}	EEM	$1.70E-3$	1066	158	4	$1.43E-2$	9936	1112	5
	BDF(2)	$5.29E-3$	2287	505	1	$7.85E-3$	11078	1309	1
	BDF(5)	$1.87E-3$	1990	352	1	$1.53E-3$	9357	1044	4
10^{-5}	EEM	$8.59E-5$	3760	720	8	$2.73E-4$	17223	2185	7
	BDF(2)	$2.04E-4$	7874	2269	3	$3.12E-4$	41780	6112	2
	BDF(5)	$2.65E-6$	2973	748	14	$2.43E-6$	16903	2272	10
10^{-7}	EEM	$5.39E-6$	15905	3287	8	$7.25E-6$	66931	14015	10
	BDF(2)	$9.47E-6$	33659	10566	3	$1.28E-5$	183209	28663	3
	BDF(5)	$2.89E-7$	5226	1474	17	$1.56E-7$	31047	4502	16

Summary

- Provided a practical variable-stepsize implementation of the exponential Euler method (EEM).
- Introduced a new second-order variant of the scheme that enables the local error to be estimated at the cost of a single additional function evaluation.
- New EEM implementation outperformed sophisticated implementations of the backward differentiation formulae (BDF) of order 2 and was competitive with BDF of order 5 for moderate to high tolerances.