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# A variable-stepsize Jacobian-free exponential integrator for simulating transport in heterogeneous porous media: Application to wood drying

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ABSTRACT

A Jacobian-free variable-stepsize method is developed for the numerical integration of the large, stiff systems of differential equations encountered when simulating transport in heterogeneous porous media. Our method utilises the exponential Rosenbrock–Euler method, which is explicit in nature and requires a matrix–vector product involving the exponential of the Jacobian matrix at each step of the integration process. These products can be approximated using Krylov subspace methods, which permit a large integration stepsize to be utilised without having to precondition the iterations. This means that our method is truly "Jacobian-free" – the Jacobian need never be formed or factored during the simulation. We assess the performance of the new algorithm for simulating the drying of softwood. Numerical experiments conducted for both low and high temperature drying demonstrates that the new approach outperforms (in terms of accuracy and efficiency) existing simulation codes that utilise the backward Euler method via a preconditioned Newton–Krylov strategy.



## 1. Introduction

We study time integration methods for ODE systems resulting from semi-discretised (i.e., discretised in space) coupled nonlinear transport equations encountered in wood drying applications. For such stiff problems, Newton–Krylov methods based on an implicit method (e.g. the backward Euler method or a higher-order backward differentiation formula (BDF) [9]) are often preferred [30]. Implicit methods are often favoured because they have favourable stability properties (in the linear stability sense) when compared with standard explicit methods (e.g. Adams–Bashforth methods, explicit Runge–Kutta methods etc.), which means that the time step is usually less restricted by stability constraints. The computational requirements of Newton–Krylov methods are dominated by the solution of a large linear system involving a sparse Jacobian matrix at each Newton iteration. When the Jacobian matrix is nonsymmetric, the preferred method is usually the generalised minimal residual method (GMRES) [25], since it minimises the 2–norm of the residual vector (over the given Krylov subspace) at each iteration. A common characteristic of Krylov subspace methods such as GMRES is that they require only matrix–vector products with the Jacobian matrix. This is attractive from a computational perspective as such products can be approximated by a finite difference approximation that requires a single function evaluation (see, e.g. [13, Ch. 3]). However, preconditioning is essential for a successful application of a Newton–Krylov method [14], which usually means that all or part of the Jacobian matrix must be generated in order to form the preconditioner matrix.

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The focus of this paper is the convective drying of softwood, which is a process that involves coupled heat and mass transfer within an extremely heterogeneous and anisotropic porous material. Softwood exhibits rapid variation in density from the light-coloured earlywood to the dark-coloured latewood across a growth ring (see Fig. 1). The mesoscopic model presented in [20,21], which features three coupled nonlinear transport equations, captures this heterogeneity through the density of the porous medium, $\rho_0$, and via the density variation of material properties such as the capillary pressure, permeability, diffusivity and conductivity that feature in the equations (see Section 2.1 and 2.2). Unfortunately, the mesoscopic approach requires considerable refinement of the mesh to sufficiently capture the heterogeneous structure, which means that the study of time integration methods is imperative to the efficiency of the drying simulation. Current state-of-the-art wood drying simulation codes [32,33] employ a Newton–Krylov method based on the first-order BDF method, the well-known backward Euler method. Within these codes, heuristics based on the convergence speed of the GMRES and Newton iterations are used for time step adaptation purposes.

Over the last decade, there has been an increase in interest in applying exponential integrators to ODE systems resulting from spatially-discretised PDEs (see, e.g. [11,30]). One of the simplest examples of an exponential integrator (see, e.g. [12,16] for a comprehensive review of the class of methods) is the exponential Rosenbrock–Euler method, which can be applied to initial value problems taking the form

$$\frac{d\mathbf{u}}{dt} = \mathbf{g}(\mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0, \tag{1}$$

where $\mathbf{u} \in \mathbb{R}^N, \ \mathbf{g} : \mathbb{R}^N \supset D \to \mathbb{R}^N$ is a nonlinear function of $\mathbf{u}$ and $\mathbf{u}_0$ is the initial solution at $t = 0$. We note that in the context of semi-discretised PDEs, the vector $\mathbf{u}$ contains the unknowns at the nodes in the mesh. At each step of the integration process, a linearised version of (1) taking the form

$$\frac{d\mathbf{u}}{dt} = \mathbf{g}(\mathbf{u}_n) + \mathbf{J_g}(\mathbf{u}_n)(\mathbf{u} - \mathbf{u}_n), \quad \mathbf{u}(t_n) = \mathbf{u}_n,$$

is solved exactly to obtain

$$\mathbf{u}(t) = \mathbf{u}_n + (t - t_n)\varphi((t - t_n)\mathbf{J_g}(\mathbf{u}_n))\mathbf{g}(\mathbf{u}_n), \quad t > t_n,$$

where $\mathbf{J_g} \in \mathbb{R}^{N\times N}$ is the Jacobian matrix of $\mathbf{g}$ and the so-called $\varphi$-function is defined as $\varphi(z) = (e^z - 1)/z$. This in turn defines the explicit second-order exponential Rosenbrock–Euler method [3,11,16], given by

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \tau_n\varphi(\tau_n\mathbf{J_g}(\mathbf{u}_n))\mathbf{g}(\mathbf{u}_n), \tag{2}$$

which relates the approximate solution at time level $n + 1$ $(t = t_{n+1})$ to the approximate solution at time level $n$ $(t = t_n)$ with stepsize $\tau_n = t_{n+1} - t_n$. This strategy has appeared in the literature in several papers (see, e.g. [3,11,12,16,22,27]). We note that in previous work by two of the current authors [3,4] the scheme (2) was called the exponential Euler method. In this paper, however, we will follow the recent review work by Hochbruck and Ostermann [12] and use the name exponential

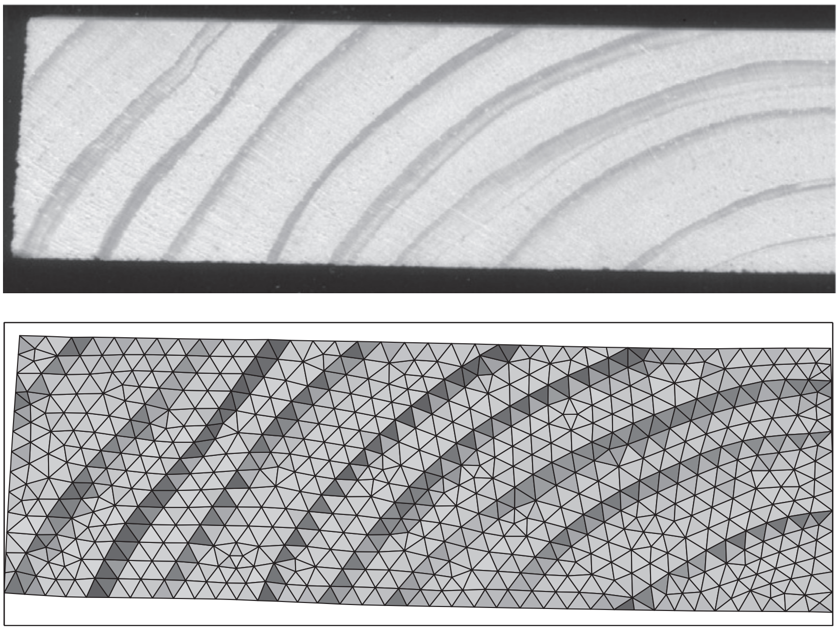

**Fig. 1.** Meshing of a board cross-section of softwood consisting of 633 nodes and 1163 elements.