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New preconditioning strategy for Jacobian-Free solvers coupled with advanced discretization methods

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Numerical algorithms for nonlinear PDEs employ often implicit or explicit-implicit time integration schemes that result in a system of nonlinear discrete equations. Another key component of these algorithms is the spatial discretization of PDEs. The current practice of using unstructured meshes that conform to the physical domain or solution features reduces accuracy of the conventional discretization methods. New advanced discretization methods that remain accurate on unstructured meshes become more complex. However, the potential impact of modern discretization methods on multi-physics simulations has not been yet realized because the additional complexity cannot be managed by existing nonlinear solvers.

Variably saturated flow in porous media is a critical process in a wide variety of environmental applications, including contaminant transport in the subsurface and carbon cycling in degrading permafrost. This flow process is often modeled by the nonlinear PDE which is referred to as the Richards' equation. In Richard's formulation the flow model is considered under the assumption that the gas phase is immobile. This simplification also makes Richards' equation a strongly nonlinear parabolic PDE, creating significant challenges for the performance of nonlinear solvers.

The implicit discretization in time of its mixed-form is the standard approach for this type of applications since it enables large time steps and locally conserve mass. This scheme leads to a nonlinear discrete system of equations that must be solved at each time step. Typically, this solution is obtained by discretizing PDEs and then solving the resulting system of nonlinear discrete equations with a Newton-Raphson-type method. This approach is widely used in the case of cartesian grids with isotropic or grid-aligned anisotropic permeabilities, for which the two-point flux approximation of the flux is accurate. The Jacobian matrix is computed by differentiating the discrete nonlinear system of equations analytically with respect to the discrete pressure unknowns. This discrete Jacobian matrix is non-symmetric but positive definite, and for certain upwinding formulations, naturally picks up the appropriate upwinding needed for stability of the first-order derivatives. However, complexity and cost do increase if complex models of porosity or density are incorporated, particularly if these models require interpolation of tabular data. The geometric complexity of the subsurface environment requires to handle non-orthogonal and unstructured meshes. To discretize the flow model in these settings advanced discretization methods are essential. These methods offer accurate schemes on general meshes, but close-from formulas for the analytic Jacobian may not exist, e.g slope-limiting methods, nonlinear discretization schemes. For these discrete systems an implementation of the standard Newton-Raphson-type nonlinear solvers becomes very problematic. Although, this complexity in the discretization is manageable, it is problematic for the direct analytic differentiating of the nonlinear discrete system, as it is costly or overly complex to evaluate and the resulting Jacobian matrix may be singular. Therefore, development of Jacobian-Free solvers has attracted a lot of interest in the past decade.

Several Jacobian-Free methods have become quite popular in the recent years. Methods, such as the Jacobian-Free Newton-Krylov method, only require the action of the Jacobian matrix on a vector, which is approximated via the numerical computation of the Gateaux derivative. Accelerated fixed-point methods such as Anderson Mixing and Nonlinear Krylov Acceleration (NKA) methods are design to extend the power of linear iterative schemes to the nonlinear case. In all of these methods the preconditioner plays a crucial role for the efficacy of a nonlinear solver. The standard preconditioning approach is based on a linearized counterpart of the original discrete system. The strong nonlinearity in the coefficients limits the efficacy of that approach and results in the growth of nonlinear iterations.

We propose and analyze a new preconditioning strategy that is based on a stable discretization of the continuum Jacobian. The underlying idea in this work is to reverse the order of the discretization and linearization steps in the development of the nonlinear solver. Specifically, by performing the linearization step first, the analytic Jacobian of the continuum model is derived and then analyzed to establish requirements for accurate and stable discretizations. This strategy allows us to take full advantage of advanced discretization methods and control properties of intermediate solutions. For example, we may use monotone schemes for the diffusive term in the Jacobian and upwinded schemes for the advective term. This not only leads to an efficient preconditioner but also allows us to control its numerical properties.

The proposed strategy was tested in simulations of water infiltration into a partially saturated layered medium in steady-state and transient regimes on non-orthogonal subsurface topology with heterogeneous permeabilities and water retention models. These experiments demonstrate that the new preconditioner improves convergence of the existing Jacobian-Free solvers 3-20 times.