# A Block-Preconditioned Jacobian-Free Multiscale Method

by

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# ABSTRACT

In this dissertation, we develop a Jacobian-free multiscale modeling technique that circumvents explicit computation of Jacobian at the macro-scale by using a Newton-Krylov process. Effective preconditioning is necessary for the Krylov subspace iterations (e.g., GMRES) to enhance computational efficiency. This is challenging since no explicit information regarding the Jacobian matrix is available. The block preconditioning technique developed in this work overcomes this problem by effectively deflating the spectrum of the Jacobian matrix at the current Newton step using information of only the Krylov subspaces corresponding to the Jacobian matrices in the previous Newton steps and their representations on those subspaces. This approach is optimal and results in exponential convergence of the GMRES iterations within each Newton step. Hence, expensive microscale computations are minimized. The technique has been shown to scale well on massively parallel machines. The effectiveness of the approach is demonstrated through numerical examples. The action of a single block of the preconditioner per GMRES step scales linearly as the number of degrees of freedom of the macroscale problem as well as the dimension of the invariant subspace of the preconditioned Jacobian matrix. A particularly interesting application of this method is being pursued in computing the mechanical response of polycrystalline aggregates of FCC metal subject to neutron irradiation with dislocation and defect density-based hardening rules that is shown to capture the experimentally observed grain-level phenomena.