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Parallel Algorithms and Software for Nuclear, Energy, and Environmental Applications. Part I: Multiphysics Algorithms

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Abstract. There is a growing trend within energy and environmental simulation to consider tightly coupled solutions to multiphysics problems. This can be seen in nuclear reactor analysis where analysts are interested in coupled flow, heat transfer and neutronics, and in nuclear fuel performance simulation where analysts are interested in thermomechanics with contact coupled to species transport and chemistry. In energy and environmental applications, energy extraction involves geomechanics, flow through porous media and fractured formations, adding heat transport for enhanced oil recovery and geothermal applications, and adding reactive transport in the case of applications modeling the underground flow of contaminants. These more ambitious simulations usually motivate some level of parallel computing. Many of the physics coupling efforts to date utilize simple code coupling or first-order operator splitting, often referred to as loose coupling. While these approaches can produce answers, they usually leave questions of accuracy and stability unanswered. Additionally, the different physics often reside on distinct meshes and data are coupled via simple interpolation, again leaving open questions of stability and accuracy.

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This paper is the first part of a two part sequence on multiphysics algorithms and software. Part I examines the importance of accurate time and space integration and that the degree of coupling used for the solution should match the requirements of the simulation. It then discusses the preconditioned Jacobian-free Newton Krylov solution algorithm that is used for both multiphysics and multiscale solutions. Part II [1] presents the software framework; the Multiphysics Object Oriented Simulation Environment (MOOSE) and discusses applications based on it.

AMS subject classifications: 65M12, 65M60, 65Y05, 65Z05, 65H10

Key words: Multiphysics simulation, Jacobian-free Newton Krylov, finite element applications, physics-based preconditioning.

1 Introduction

The use of multiphysics simulation is growing rapidly with the interest in more realistic and higher fidelity analysis of energy and environmental systems. This increase in activity is typically attributed to increasing computer power, but in truth, advanced numerical methods are playing an equal role. The phrase "multiphysics simulation" is used to describe analyses which include disparate physical phenomena. Examples of multiphysics problems in the nuclear energy field include coupling fluid flow, heat transfer and neutron kinetics for reactor dynamics, coupling fluid flow and structural dynamics to consider fluid-structure interactions for nuclear fuel rod fretting, and coupling nonlinear thermomechanics with contact, fission product behavior, and species transport to study fuel performance. In energy and environmental applications, one encounters problems involving most of the above physics; energy extraction involves geomechanics, flow through porous media and fractured formations, adding heat transport for enhanced oil recovery and geothermal applications, and adding reactive transport in the case of applications modeling the underground flow of contaminants. In addition to multiphysics coupling, most of these problems also have multiscale issues to resolve.

Important in higher fidelity multiphysics simulation are considerations of time integration and spatial discretization of the coupled system. It is popular to employ first-order operator splitting, or even explicit coupling of different codes, to perform the time integration. While this approach can produce results, it can also produce significant time integration error [2] and stability issues [3].

This paper (Part I of a two part sequence) discusses a modern multiphysics algorithm, the Jacobian-Free Newton-Krylov method (JFNK) combined with physics based preconditioning [4]. This approach can typically compete well with operator splitting, while significantly reducing time integration error and stability concerns. The first part of this presentation describes the JFNK methodology and its use in both a multiphysics and multiscale setting. Part II [1] describes an evolving software framework MOOSE [5] which utilizes this algorithmic basis and enables rapid development of multiphysics engineering analysis tools.