Gradient Operator Optimization for 3D Unstructured Meshes (LA-UR-15-21404)

S. Coffing[1], **M. T. Bement, J. Fung, M. A. Kenamond, and B. M. Smith**

Computational Physics Division, Los Alamos National Laboratory, NM, USA.

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ABSTRACT

FLAG is a code that solves the arbitrary Lagrangian-Eulerian (ALE) form of the conservation equations to model multi-material and multi-physics problems [1]. The particular ALE algorithm implemented in FLAG can be split into three main steps: performing a Lagrangian solution update, generating a new computational mesh with improved characteristics, and remapping the Lagrangian solution onto the new mesh. A particularly costly and repeated operation in a remapping step is the calculation of discrete gradients of various solution quantities, such as density or pressure. The gradient operator reconstructs field quantities at the nodes of a mesh by using the averaged fields and geometries of the surrounding zones.

FLAG's gradient operator is only implemented serially, is not optimized, and cannot be parallelized due to data race conditions. Furthermore, FLAG employs MPI primarily to achieve parallelization by using single-core computation spread to a number of number of processors – utilizing the many-core and multi-core processing power of the next generation architecture is a current challenge of similar 3D unstructured mesh simulation codes [2]. The gradient algorithm used in FLAG is similar to the algorithms used in many unstructured fluid dynamics codes and comparable to commonly used spatial operators. As such, FLAG's gradient operator serves as an excellent case for testing parallelization of spatial operators on a 3D unstructured mesh.

Starting with a mini-application designed to simulate the basic features of FLAG, a variety of gradient operator alternatives and optimizations were tested. The most successful of those algorithms were then implemented directly into FLAG to demonstrate their computational performance compared to the currently used methods. They include different renumbering schemes, data restructuring, and connectivity inversion. This research also investigates the feasibility of a hybrid OpenMP and MPI parallelization solution for FLAG and similar hydrocodes. Preliminary research suggests over 20 times the performance increase of the current methods and the initial tests suggest that the new alternative gradients will translate well to multi-core, multi-processor environments.

References

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[1]Corresponding Author; sxc@lanl.gov