Thesis Review

Advanced Tools for Arbitrary Lagrangian-Eulerian Simulations
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Thesis Relevance

The thesis presents several methods to improve multi-material calculations in the indirect arbitrary Lagrangian-Eulerian (ALE) framework. The work is applied to both solids and fluids which is of particular relevance as ALE hydrocode applications are extended to genuinely multi-material, rather than simply multi-fluid. The work related to remapping of the stress tensor is of note as this topic is relatively new to the literature. The extension of the interface-aware sub-scale dynamics (IASSD) closure model to solids, and additionally to voids, presents several new developments to a method that is currently under wider development in the community and represents the most up-to-date capability of the framework. The work on analysing the local error of the swept and intersection remapping methods, together with the application of the error analysis to the development of a hybrid remapping method is also useful, particularly as calculations increase in fidelity – in terms of grid resolution and remapping additional quantities, such as the stress tensor, amongst other measures – and the associated computational expense also increases.

The partnerships with scientists at UK and US national laboratories further support the fact that the research is up-to-date and of interest to the active community.

Methods Utilised

The thesis builds upon a comprehensive literature survey, deriving numerical solutions to physical systems of equations. For the swept and intersection based remap analysis, rigorous algebraic error analysis is performed and exploited to compare methods, and used as a metric to determine which method is used in particular cells in the hybrid method. For the new Proportional Compressibility bulk step, and the additional constraints in the sub-scale step, optimisation of systems of linear constraints is employed. Numerical examples of varying complexity are used to evaluate the performance of the new methods. Simple one-dimensional tests are initially employed to clearly show key properties. Two-dimensional prescribed mesh motion tests are used to isolate remapping errors from hydrodynamics effects. Single variable and full ALE calculations are shown, with shaped charge simulations shown to replicate and compare performance against physical experiments. Comparison to analytic solutions has been used where possible, along with comparison between alternate implementations and options where applicable. Mesh resolution studies are included to show convergence rates and error analysis and attain the expected accuracy.

Thesis Goal

The thesis aims to address several aspects of the Lagrangian and remap phases of multi-material ALE calculations in terms of increased scope, and increased accuracy and efficiency. The goals of the thesis can be seen to have been achieved through several research articles published in a variety of peer-reviewed journals, included in Appendices A-E.

To improve the Lagrangian phase of the calculation, extensions of the IASSD framework to deal with solids and voids were proposed. Appendix A extends the IASSD method to voids (zero mass and energy materials) by reformulating the sub-scale flux limiters to allow massless materials in the limiter constraints, and to allow for void closure by allowing the void volume flux limiter to permit zero component volumes at the end of the sub-scale stage. Appendix B addresses the extension to solids by employing an additional optimisation constraint (normal stress) to the sub-scale flux calculation. Work in this regard also led to the development of a new Proportional Compressibility (PC) method for the bulk stage of the IASSD method, together with the directional switch to ensure the correct void opening behaviour at high and low speeds. Further development of the PC method would also offer the opportunity to provide a computationally cheaper (albeit potentially less accurate, compared to the developed IASSD method) closure model for multimaterial cells. Appendix B also extends the void treatment algorithm to allow for void opening within the sub-scale stage based upon a void seed method and by analysing the stress in the material components of the multimaterial cell.

To improve the remap phase of the calculation, a hybrid swept/intersection based remapping scheme is developed, and the conservative remap of the stress tensor has been examined. Appendix C performs a thorough numerical error analysis to compare the accuracy and performance of two popular remapping methods. The swept flux method is computationally cheap, but suffers from inherent approximations when dealing with symmetry preservation and at multimaterial interfaces. The intersection method ensures the correct quantities are always used in fluxes and does not suffer from symmetry preservation issues, but is computationally intensive. The analysis within the paper supports the literature in identifying cases where the swept flux method can have superior numerical accuracy compared to the intersection method. Following this result, Appendix D develops a hybrid swept/intersection method based on error estimators that allows the benefits of each method to be exploited in appropriate regions of the computational mesh, whilst minimising the computational expense by only using the expensive intersection method where symmetry preservation issues are present. Appendix E develops the methodology required to conservatively remap the stress tensor in simulations which deal with impact and fluid-solid interactions – a key requirement to exploit the developments made to the Lagrangian phase of ALE calculations via IASSD model extensions in Appendices A and B.

Scientific Value

Correctly updating component material properties in the Lagrangian phase of ALE calculations is important to avoid unphysical behaviours adversely affecting the evolution of a calculation featuring material interfaces within computational cells. Existing closure model methods have typically taken a simplified approach based on limited information about the multimaterial cell. This in turn then results in material values produced which can be outside of the local material maxima and minima. In the case of solid-fluid and solid/fluid-void interactions, utilisation of the sub-cell topology, and material properties is especially important to capture the correct physical behaviour in simulations. The IASSD method shown in the thesis addresses these issues.

Efficient remapping tools, such as the hybrid swept/intersection method in the thesis, allow calculations to increase the fidelity of the computational mesh and reduce the cost of remapping additional variables. This allows the multimaterial ALE method to be utilised in a wider range of applications and communities. Correctly remapping key quantities such as the stress tensor ensures that calculation behaviour in key regions (for example void opening/closure, spall, solid interactions) is physically correct, and not as a result of numerical artefacts.

Overall Evaluation

The thesis provides a thorough description of the background motivation and the compatible ALE scheme used in the calculations. The closure model extensions for void treatment and solid materials are useful additions to the IASSD framework, showing the importance of correctly treating material interfaces in multimaterial Lagrangian cells. The error analysis and proposal of a hybrid swept/intersection remap scheme offer both computational efficiency and numerical accuracy improvements. The development of the new approach to remap the stress tensor is a useful addition, highlighting the need to correctly treat this quantity in order to preserve symmetry and conservation.

A number of areas could be clarified via discussion, or represent opportunities for future work, for example:

Comparison to other closure models would be useful where possible. For example, Fig. 3.2, the performance of the Tipton pressure relaxation scheme, or the EC/PC methods could also be shown to give wider context.

Comparison to slide calculations where void closure test cases are performed (e.g. in Sections 6.5, 6.6, Appendix A Section 6.2.1, Appendix B Section 5.1) would show whether the behaviour of the closure model matches methods where the material interfaces are conformal, and where no analytic solution may be available.

Additional explanation of features seen in the projectile impact example shown in Appendix A, Fig. 25 would be useful. At t=4.5 and t=6, plate material appears to be entrained in the projectile. This is not present in the equivalent gas-background calculation shown in Figure 26. This could therefore point to this behaviour being a feature of the void closure model rather then the material interface reconstruction scheme used in both calculations.

For the swept and intersection hybrid remap method, further explanation of remapping between neighbouring cells identified for differing methods would be useful. A cell calculating the flux using intersections will utilise scalar quantities from corner elements as well as edge elements. The neighbouring cell calculating the flux using the swept method will only utilise scalar quantities from edge elements. Does this introduce any inconsistencies? Perhaps not for the common edge, but for other edge fluxes in the cell? Would such an issue be exaggerated for meshes using arbitrary polygon cells with enhanced connectivity?

For remap calculations, the assumption is made that node movement remains confined to within the neighbouring cells. Has this been confirmed for ALE calculations? When using the ALE10 approach, the mesh relaxer may need to significantly alter the mesh quality. Is there any evidence to support over-advection is not happening, and that is not adversely affecting the error analysis or choice of swept/intersection calculation?

In several cases, the use of the L1 norm (e.g, Appendix C and D) may have allowed compensating errors to mislead performance evaluations. For example, Appendix D Fig. 4, using equation (14) the symmetric properties of the test case shows over- and under- errors can cancel out. Analysis is backed up with additional methods, however there may be the potential for incorrect conclusions to be drawn upon the performance of each method.

The intersection remap method uses the correct intersection volumes with the correct corresponding scalar values. The swept method uses an approximation of the scalar field by only taking from the edge neighbour with a mis-matched flux volume. An explicit example of how the intersection remap can perform worse than the swept approach would be useful.

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In ALE calculations using the hybrid remap method, is the identification of swept and intersection cells only done once? If it is only done once, which scalar field controls this choice? If it is done multiple times, are there any issues where cells are identified for alternate methods for different scalar fields?

Overall, the thesis presents a significant quantity of high quality of work and I recommend it for presentation and defence.

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