Material Point Methods and Multiphysics for Fracture and Multiphase Problems

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Material point methods (MPM) provide an intriguing new path for the design of algorithms that are poised to scale to billions of cores [4]. These methods are particularly important for simulating various phases in the presence of extreme deformation and topological change. This brings about the possibility of new simulations enabled at the exascale for a variety of phenomena in high energy multiphysics problems as well as general problems in multiphase flow. Examples of the MPM method are emerging in ice-sheet models for climate simulation as well as more traditional explosive-related simulations. The crux of these algorithms lies in their ability to use a hybrid Langrangian/Eulerian approach to leverage accuracy inherent in particle based advection with the use of a background grid to discretize stress derivatives without the necessity of a high quality mesh on the particles. Material is primarily represented on each particle, with the background grid being used as a "scratch pad". This makes treatment of multiple phases very natural as each particle can be assigned with an individual constitutive model. This also allows for general parallelism models based on independent particle interactions to be applied to these methods, in fact MPM simulations are currently some of the most scalable [2] and include versions for various architectures such as GPUs[1]. These aspects have proven the methods to be very effective for numerous applications over the years due to their relative ease of implementation and efficiency. In particular, this is true in the context of methods that treat extreme deformation and high-energy events. Despite recent advances in parallel implementations of MPM, it remains relatively undiscovered in the petascale community and is therefore ripe for discovery and advancement, and filled with mathematical challenges. For emerging exascale architectures, appropriate algorithmic development will involve techniques that leverage parallelism on each node to treat the different regions of the material during the Eulerian phase as these are typically the most computationally burdensome components of the calculations. This includes treatment of implicit time stepping calculations that involve non-linear solution of equations over a complicated subset of the background Eulerian grid. Retaining stability and accuracy with diverse treatments requires careful consideration. It is likely that exascale architectures will have different levels of parallelism and latency in order to achieve the unprecedentedly levels of concurrency. Treating different phases of the calculations with different techniques is fundamental to achieving the highest levels of parallelsm. However, significant care must be take to assure that hybrid methods maintain the levels of convergence and stability afforded by single method approaches. Important topics for discussion in this are are the ability to map these problems to heterogenous architectures and the trade-offs between various MPM algorithmic design choices.

Exascale computations will allow for spatial and temporal resolutions many orders of magnitude beyond what is currently possible. This increased resolution will provide the enabling technology for many new scientific studies. For example, the MPM simulations done in Figures 1 and 2 were done with approximately one million spatial degrees of freedom and provided simulations on the scale of one meter with the resolution of about one centimeter [3]. At the exascale, we could likely scale such simulations up to the size of a kilometer without sacrificing the one centimeter spatial samples. This would allow for incredibly accurate and detailed simulations of much larger-scale phenomena. While MPM has been around for years, much additional mathematical research is required to ensure stability, consistency, and accuracy for multiphase, high energy problems at this scale. An important area for discussion is the benefits of explicit methods versus implicit and semi-implicit formulations. For instance, a semi-implicit treatment can naturally be handled over the Eulerian grid alone. This leads to relative simplicity as well as conditioning of linear systems that

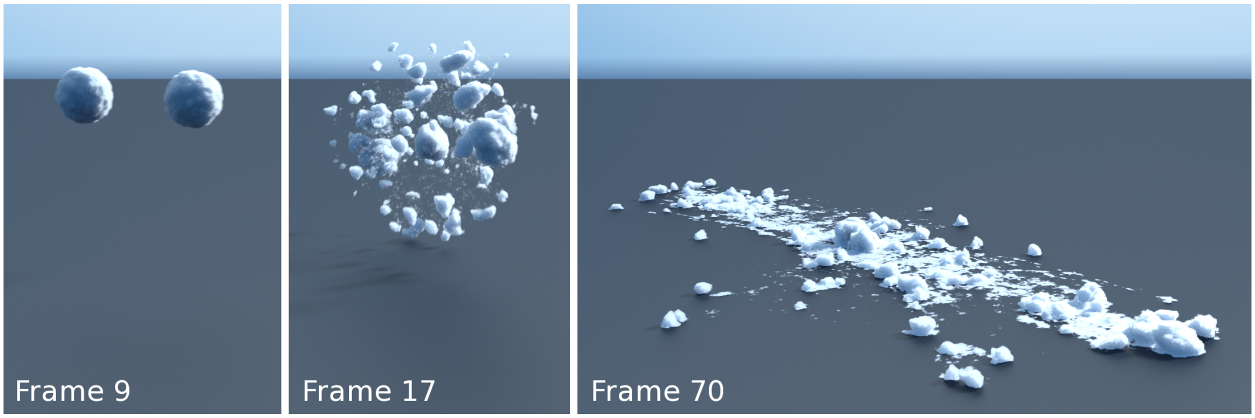

Figure 1: Simulation of granular materials colliding and undergoing complex topological change.

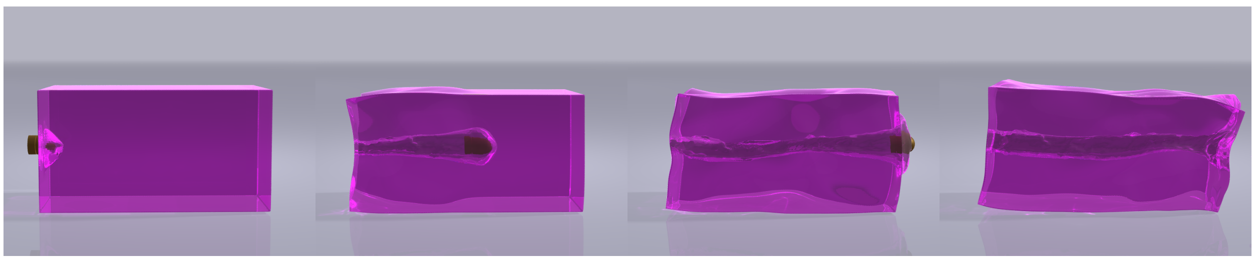

Figure 2: Simulation of a high speed projective colliding with a hyperelastic solid.

is more predictable and manageable than treatments that also address the particles. While the use of an implicit scheme allows for a time step that is at least an order of magnitude larger than what an explicit scheme would allow, and taking fewer time steps improves the dynamics by reducing the damping effects caused by transferring data between the particles and the grid, it does still require the solution of a sparse linear system arising for a discrete elliptic PDE and these will be increasingly difficult to solve at extremely high grid resolution. The efficient solution of these types of systems at the exascale will be a difficult research problem to solve. This type of problem is of course ubiquitous for many other competing techniques for the relevant problems. This is not by any means a new discussion, but it should be considered in the context of the MPM where the constraints of the underlying physical system involve different issues with regard to accuracy and stability.

References

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