MULTIRESOLUTION SIMULATIONS USING REMESHED PARTICLES

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Summary We present an overview and recent advances for remeshed particle framework for simulations of continuum systems. The framework relies on a Lagrangian formulations of the momentum equation and on the remeshing of distorted computational elements on a regularized grid. We demonstrate the relationship of this method with other numerical schemes such as finite difference methods and particle-in-cell techniques for fluid and solid simulations. We present wavelet adapted grids for this framework and its implementation in multicore/GPU architectures. Results include simulations of vortex reconnection at high Re, flows of multiple swimmers and solids undergoing large deformations.

PARTICLE METHODS

Particle methods for the simulation of fluids and solids are often distinguished by their grid based counterparts by the flexibility in the location and interactions of the computational elements. Indeed the simulation of the motion of interacting particles is a deceivingly simple, yet powerful and natural computational technique to simulate systems across scales. Techniques such as Molecular Dynamics (MD) for simulations of protein folding, Dissipative Particle Dynamics (DPD) for simulation of blood flow and Smoothed Particle Hydrodynamics for astrophysics are all realizations of particle methods that are based on tracking a set of interacting particles. Particles can be viewed as objects carrying a physical property of a system, that is being simulated through the solution of ordinary differential equations that determine the trajectories and the evolution of the properties carried by the particles. Particle methods such as MD,DPD, SPH have a computational structure with a large number of common abstractions that helps in their computational implementation in particular in many/multi core architectures. Furthermore particle methods are distinguished by the fact that the computational elements are discrete representatives of the simulated physical systems.

At the same time it is important to consider a key distinction in simulations using particles: On one hand the *approximation of conservation laws* by suitably formulated particle interactions and on the other *models of physical systems* represented by interacting particles. In the first category we consider techniques such as Vortex Methods(VM), SPH and Material Point Method while in the second we may consider techniques such as MD and DPD.
In continuum (fluid or solid) simulations particles are implemented along with a Lagrangian formulation of the continuum equations, as in the velocity-vorticity formulation of the Navier-Stokes equations. The *key common characteristic* of continuum particle methods is the approximation of the conservation laws by replacing the differential operators through equivalent integral operators that are in turn discretized on the particle locations. The adaptivity of the method ensures that particles adapt to the transport velocity and further adaptivity can be incorporated so that particle location and size conforms with the strain field.

Common Themes

Particle methods for flow simulations, such as VM and SPH(see [1,2]and references therein) approximate the Lagrangian form of the conservation laws by replacing the derivative operators through equivalent integral operators that are in turn discretized on the particle locations. The related *Meshless particle methods* (see [3] and references therein) for simulations in mechanics are Galerkin type methods distinguished by the irregularity of their computational elements. In these methods derivative operators are approximated by solving systems of equations to construct conservative, discrete mollifier kernels leading to Partition of Unity Methods.We note a number of alternative particle techniques has been developed for simulations in mechanics. The Material Point Method (MPM) [4] relies on a dual representation of the systems on grids and particles and as such it is closely related to the remeshed particle methods for flow simulations. Another particle based method, peridynamics [5], relies on transforming differential operators into integrals that are then discretized by particles as quadrature points. We note again the striking similarity on the integral formulation these methods with the particle methods for flow simulations.

REMESHING AND WAVELET ADAPTED GRIDS

As particle methods operate on the Lagrangian formulation of the respective conservation laws they avoid the explicit discretization of the non-linear convective term and the associated stability constraints. This formulation enables an automatic adaptivity of the computational elements albeit only due to the convection field of the flow. This adaptation, however, comes at the expense of the regularity of the particle distribution, deteriorating the accuracy of the method. Particle regularity and in turn convergence of particle methods can be guaranteed by remeshing the particle locations on a regular grid (see [2] and references therein). During remeshing quantities carried by the particles are transported (for example through moment conserving interpolation techniques) onto the grid nodes and only grid nodes with significant

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weights are maintained and transformed anew into particles that will be transported in a Lagrangian fashion.
This "momentary" regularity of the particle locations enables a number of advances:

- Fast and efficient computation of derivatives
- Implementation of fast grid based field solvers
- Introduction of efficient multi resolution capabilities
- Numerical analysis of remeshed particle method and linking with other seemingly disparate numerical methods.
- Efficient implementation on multicore/GPU architectures

I consider in fact the latter issue as a key advantage pod particle methods as it demonstrates that even grid based schemes such as finite differences can be expressed as remeshed particle methods [6]. We have extended the formulation of remeshed particle methods to simulations of bodies with non-linear elastic stress strain relationships undergoing large deformations. There are also direct connections with the particle-in-cell formalism of the material point method and we introduce remeshing in order to enhance its accuracy in cases of large deformations. Furthermore the present framework can be linked to techniques such as peridynamics. We note that remeshing does not limit the capability of the method to handle problems of flow-structure interaction involving complex boundaries when the resumed particle method is combined with immersed boundary and penalization techniques.

Wavelet Adapted Grids and Particles

We note that in Lagrangian simulations of continuum systems involving large deformations *beyond adaptivity as dictated by the flow map it is necessary to employ particle methods with different resolution requirements as dictated by the physics of the flow*. In order to simulate physical systems involving sharp gradients and discontinuities we have introduced methods with Lagrangian adaptivity enhanced by the multiresolution capabilities of wavelets [7].
In these techniques during the remeshing of the particles we analyze quantities of interest using wavelets and associate grid nodes for the remeshed particles with non-negligible wavelet coefficients. This enables a nested representation of the quantity of interest and enables fast computations through the user of fast and These methods are developed in parallel with a software framework which maps effectively the resulting data structures to multicore computer architectures.
We will demonstrate the generalized capabilities of this framework and present a unified multiresolution particle simulation technique for problems of flow-structure interaction.

Multiresolution Simulations on Multicores and GPUs

Particle methods can be viewed as N-body solvers and as such they can easily exploit the capabilities of massively parallel computer architectures albeit at a nominal cost that scales with the square of the computational elements. It is possible however to combine the multi resolution capabilities of the remeshed particle methods with the capabilities of emerging heterogeneous multicore/multi-GPU architectures, with a cost that scales also linearly with the number of computational elements. A highly efficient parallel implementation is achieved by introducing the concept of wavelet blocks, exploiting the task-based parallelism for CPU cores, and by managing asynchronously an array of GPUs by means of OpenCL and CUDA [8]. We report the performance improvements on flow simulations using two million wallet adapted particles by employing up to 12 cores and 6 GPUs compared to the single-core execution and observe up to a 100-fold speedup for the heterogeneous part and an overall speedup of 30.

CONCLUSIONS

We have presented an overview of remeshed particle methods demonstrating the convergence of the method and its relationship to techniques such as finite differences and particle in cell techniques. Furthermore we have presented wavelet adapted particle methods and their implementation on multi/GPU based architectures that indicate the capability of this simulation technique of simulations across physical systems and scales.

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