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Organisers: Matthias Möller, Robert Jan Labeur and Deborah Sulsky

TIME INTEGRATION ERRORS AND ENERGY CONSERVATION PROPERTIES OF THE STORMER VERLET METHOD APPLIED TO MPM

Martin Berzins

Scientific Computing and Imaging Institute University of Utah Salt Lake City, UT 84112 USA
mb@sci.utah.edu

The great practical success of the Material Point Method (MPM) in solving many challenging problems nevertheless raises some open questions regarding the fundamental properties of the method. as grid crossing and null-space errors and for example nonlinear stability. The question of the energy conservation of the method has been addressed by Bardenhagen and Love and Sulsky but has not been considered further. In this work both the time integration errors and the energy conservation of MPM is extended by including the impact of particle movement and grid-crossing and a different time integration approach. It is shown that the properties of the spatial methods used play an important role in time accuracy and in conservation. In particular it is shown that a lack of smoothness in the spatial basis functions results in a loss of time accuracy. Furthermore it is shown that it is helpful for the basis functions to possess a commutative property. The error in energy conservation is evaluated and as a result, a more accurate method based upon the Stormer-Verlet method is applied. This method is symplectic and very widely used in many applications such as molecular dynamics and planetary orbits and even dates back to Newton. An analysis of this method as applied to MPM is undertaken and the method is shown to have globally second order accuracy in energy conservation and locally third order accuracy of energy conservation in time. This is in contrast to the globally first order accuracy both in the solution and in energy conservation of the the Symplectic Euler Methods that are used in many MPM calculations This theoretical accuracy is demonstrated numerically on standard MPM test examples

ON THE INCOMPATIBILITY OF TRADITIONAL LAGRANGIAN MECHANICS AND THE MATERIAL POINT METHOD

W.M. Coombs[a], C.E. Augarde, T.J. Charlton, Y.G. Motalgh and L. Wang

Department of Engineering, Durham University, UK
[a]w.m.coombs@durham.ac.uk

The material point method [D. Sulsky, Z. Chen, H. Schreyer, A particle method for history-dependent materials, *Computer Methods in Applied Mechanics and Engineering* 118 (1994) 179-196] is marketed as the technique to solve problems involving large deformations, particularly in areas where conventional mesh-based methods struggle. However, there are issues with combining the method with traditional total and updated Lagrangian statements of equilibrium. These issues are associated with the basis functions, and particularity their derivatives, of material point methods normally being defined based on an unformed, and sometimes regular, background mesh. It is possible to map the basis function spatial derivatives using the deformation at a material point but this introduces additional algorithm complexity and computational expense. This paper will first present the issues associated with conventional Lagrangian statements of equilibrium and then proposes a new statement which is ideal for material point methods as it satisfies equilibrium on the undeformed background mesh at the start of a load step. The resulting weak form statement of equilibrium for the proposed *previously converged* formulation is

$$\int_{\varphi_{t_n}(\Omega)} (\tilde{P}_{ij}(\nabla_{\tilde{X}}\eta)_{ij} - b_i\eta_i)\mathrm{d}v - \int_{\varphi_{t_n}(\partial\Omega)} (t_i\eta_i)\mathrm{d}s = 0, \tag{1}$$

where φ_{t_n} is the motion of the material body, with domain Ω, evaluated at the previously converged (or for the first load step, the initial) state, $\tilde{X}_i$. The body is subject to tractions, t_i, on the boundary of the domain (with surface, s), $\partial\Omega$, and body forces, b_i, acting over its volume, v. The weak form is derived assuming a field of admissible virtual displacements, η_i. $\tilde{P}_{ij}$ is the Cauchy stress pulled back to the previously converged state $\tilde{P}_{ij} = \Delta J\, \sigma_{im}(\Delta F^{-1})_{jm}$, where ΔF_{ij} is the increment in the deformation gradient over the current loadstep, $\Delta J = \det(\Delta F_{ij})$ is the incremental volume ratio and σ_{ij} is the Cauchy stress. The above weak statement is combined with a linear relationship between elastic logarithmic strains and Kirchhoff stresses and the multiplicative decomposition of the deformation gradient into elastic and plastic components. The resulting equations are discretised by a set of material points that represent the solid body.

The numerical analysis framework is demonstrated using a number of large deformation elasto-plastic problems with both the standard and the generalised interpolation [S.G. Bardenhagen, E.M. Kober, The generalized interpolation material point method, *Computer Modeling in Engineering and Sciences* 5 (2004) 477-495] material point methods, with a specific focus on the convergence towards analytical solutions. Although the formulation is implemented within a implicit material point method, the proposed framework can be applied to all existing material point methods and adopted for both implicit and explicit analysis.

A LOCALLY CONSERVATIVE PARTICLE-MESH STRATEGY FOR HYPERBOLIC CONSERVATION LAWS

Jakob Maljaars[a] and Robert Jan Labeur[b]

Faculty of Civil Engineering and Geosciences, Delft University of Technology,
Stevinweg 1, 2600, GA Delft, The Netherlands
[a]j.m.maljaars@tudelft.nl, [b]r.j.labeur@tudelft.nl

In an attempt to reconcile the advantages of a Lagrangian method with those of an Eulerian method, hybrid particle-mesh methods make combined use of Lagrangian particles and an Eulerian mesh. Particularly, using Lagrangian particles to account for the advective transport entails the promise of ruling out numerical diffusion and avoiding stabilization of the advection term. Simultaneously, the Eulerian mesh admits an efficient discretization of constitutive relations.

Despite many successful applications, it is not surprising that such an approach tends to have difficulties in unifying accuracy and exact conservation. Most notably so, since information is repeatedly projected back-and-forth between a discrete set of Lagrangian particles and an Eulerian mesh field.

In this contribution, a particle-mesh interaction strategy on arbitrary meshes is presented in which the aforementioned issue is fundamentally overcome. Central to the presented approach is to cast the particle-mesh interaction as a PDE-constrained minimization problem in such a way that, from a mesh-perspective, the transported Lagrangian particle field satisfies a hyperbolic conservation law. Loosely stated, the constrained particle-mesh projection for a scalar-valued field ψ_p defined on the Lagrangian particles reads

$$\min_{\psi_h} J = \sum_p \frac{1}{2}\left(\psi_h(\mathbf{x}_p(t), t) - \psi_p(t)\right)^2 \tag{1}$$

such that a scalar hyperbolic conservation law is satisfied in a weak sense.

with ψ_h the state variable to be approximated in an appropriate function space. Furthermore, the summation over p runs over all particles in the domain of interest.

Starting from Eq. (1), the optimality system for the scalar-valued constrained particle-mesh projection is derived, and - by introducing a facet-based control variable - it is shown that a hybridized Discontinuous Galerkin (HDG) framework naturally provides the ingredients required for the optimality control. Several properties of the resulting particle-mesh projection are derived, including consistency and local conservation. Furthermore, an efficient solution strategy using *static condensation* is proposed. Key features of the constrained particle-mesh projection are highlighted for a number of scalar advection benchmarks, demonstrating high-order accuracy and the absence of numerical diffusion.

The presented approach is believed be useful for a range of applications. In particular, it is shown how the particle-mesh projections can serve as a building block for mass conservative density tracking in multi-phase flows. To give attendees a headstart to apply the presented work to their own challenges, core functionality is made available under an open-source license in LEoPart[1].

A HIGH-ORDER B-SPLINE MATERIAL POINT METHOD

R. Tielen[a], E.D. Wobbes, M. Möller and C. Vuik

Delft Institute of Applied Mathematics, Delft University of Technology, the Netherlands.
[a]r.p.w.m.tielen@tudelft.nl

The Material Point Method (MPM) [1] has shown to be succesful in simulating problems that involve large deformations and history-dependent material behaviour. MPM can be considered as a hybrid Eulerian-Langranian method that combines the use of a set of particles, called material points, with a fixed background grid. The equations of motion are solved on this background grid within a variational framework, typically adopting piece-wise linear (Lagrangian) basis functions. Integrals resulting from the variational formulation are then approximated by using the material points as quadrature points.

The use of piecewise-linear basis functions leads however to unphysical oscillations (so called 'grid crossing errors') in the numerical solution, due to the discontinuity of the gradient of these basis functions. Furthermore, the use of material points as integration points leads to a quadrature rule of which the quality is uncertain.

Recently, different strategies have been proposed to overcome these shortcomings. The use of quadratic B-spline basis functions within MPM (i.e. B-spline MPM [2]) completely removes grid-crossing errors, due to the C^1-continuity of the basis functions. The application of a Taylor Least-Squares (TLS) reconstruction [3] has shown to lead to more accurate integration, while conserving the total mass and momentum within MPM.

In this talk, we present prelimenary results obtained with a novel implementation of B-spline MPM within the C++ library G+Smo [4]. In this implementation, a TLS reconstruction to approximate the integrals in the variational formulation is included. Furthermore, it enables the use of MPM within a high performance computing (HPC) framework. Numerical results, obtained for different two-dimensional benchmarks, show that this version of the MPM potentially shows $\mathcal{O}(h^{p+1})$ spatial convergence.

References

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APPLICATION OF BOUNDARY CONDITIONS IN MPM

P.J. Vardon[a], G. Remmerswaal, M. Bolognin and M.A. Hicks

Geo-Engineering Section, Faculty of Civil Engineering and Geosciences,
Delft University of Technology, the Netherlands
[a]P.J.Vardon@tudelft.nl

The material point method (MPM) typically has two discretisations; one for the simulated bodies (into material points or material point clusters) and the second for a (background) mesh where the analysis is undertaken. Moreover, both fluid and solid mechanics (and coupled problems) are able to be simulated via MPM. Boundary conditions have, in general, been applied to background mesh locations, where the calculation takes place, although sometimes they are applied to individual material points. However, this is only for ease of the computation. In this work, the general conditions required for a complete description of the boundary conditions have been outlined. In addition, special treatment required when boundary conditions are applied to the material discretisation is outlined.

TOWARDS AN OSCILLATION FREE (IMPLICIT) MATERIAL POINT METHOD

P.J. Vardon[a], M.A. Hicks and G. Remmerswaal

Geo-Engineering Section, Faculty of Civil Engineering and Geosciences,
Delft University of Technology, the Netherlands
[a]P.J.Vardon@tudelft.nl

The material point method (MPM) suffers from a series of numerical inaccuracies which are often termed oscillations. These oscillations were addressed in the finite element method via the use of Gauss locations for the integration points; however these are typically abandoned for MPM. A number of proposed changes have been made and presented in literature, and mainly tested using 1D problems, e.g. compacting columns. Moreover, generally explicit formulations have been used, which eliminate the stiffness matrix, but utilise very small timesteps, resulting in long computation times. A detailed investigation of the causes of numerical inaccuracies and proposed improvement methods (both novel and proposed in literature) has been carried out. As a result, a proposed method to virtually eliminate the observed inaccuracies is presented.

COMPARISON AND UNIFICATION OF MATERIAL POINT AND OPTIMAL TRANSPORTATION MESHFREE METHODS

Elizaveta Wobbes[a], Roel Tielen, Matthias Möller and Cornelis Vuik

Delft Institute of Applied Mathematics, Delft University of Technology, Netherlands
[a]e.d.wobbes@tudelft.nl

Both the Material Point Method (MPM) [1] and Optimal Transportation Meshfree (OTM) method [2] have been developed for efficient and robust integration of the weak form equations that originate from applications in computational mechanics. However, the methods are derived in a different fashion and have been studied independently of one another. In this study, we provide a direct step-by-step comparison of the MPM and OTM algorithms. Based on this comparison, we derive the conditions, under which the two approaches can be related to each other, thereby bridging the gap between the MPM and OTM communities. In addition, we introduce a novel unified approach that combines the design principles from B-spline MPM (BSMPM) and OTM methods. The proposed approach is significantly cheaper than the standard OTM method and allows for the use of a consistent mass matrix without stability issues that are typically encountered in MPM computations.

References

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