Optimal-Transportation Meshfree (OTM) Approximation Schemes

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ABSTRACT

Approximation schemes based on Optimal Transportation theory (e.g., [2]), when combined with with meshfree interpolation (cf., e.g., [1]) and *material point* sampling [3] supply a powerful alternative to the strictly Lagrangian or Eulerian paradigms that combines some of the best attributes of both. A simple case in point is furnished by Euler flows over time dependent domains, e.g., resulting from fluid-structure interaction. For these systems, inertia competes with free energy in determining the flow of mass. Conveniently, the free energy of a fluid can be expressed directly in terms of its mass density and the resulting action can also be expressed directly in terms of the mass density. A class of semi-discrete actions that is well-suited to computation is [3]

$$A_d(\rho_1,\ldots,\rho_{N-1}) = \sum_{k=0}^{N-1}\left\{\frac{1}{2}\frac{\mathcal{T}_2(\rho_k,\rho_{k+1})}{(t_{k+1}-t_k)^2} - \frac{1}{2}[U(\rho_k)+U(\rho_{k+1})]\right\}(t_{k+1}-t_k)\,, \qquad (1)$$

which is expressed directly in terms of densities ρ_0, ρ_1, ..., ρ_k, ... ρ_N at the discrete times t_0, t_1, ..., t_k, ... t_N. In this expression, the functional $U(\rho)$ gives the total internal energy of the fluid and ρ_0 and ρ_N are presumed given. We note that, in (1), the inertial part of the action is given by the Wasserstein distance $\mathcal{T}_2(\rho_k,\rho_{k+1})$ between consecutive mass densities. Further extensions to solid flows, which requires consideration of more general actions, and to viscous and inelastic behavior are presented in [3]. The discrete equations of motion follow by rendering the semi-discrete (1) action stationary and supply a central-difference-like time discretization of the equations of motion of the fluid.

In order to obtain a fully discrete action for computations, the semi-discrete action (1) needs to be discretized in space. The scope of this discretization is three-fold and it concerns: i) the discretization of the volume measure $\mathcal{L}$; ii) the discretization of the mass densities ρ_k; and iii) the discretization of the incremental transportation maps $\varphi_{k\to k+1}$. We achieve the first of these spatial discretizations simply by approximating the usual Lebesgue measure $\mathcal{L}$ by discrete measures of the form: $\mathcal{L}_{h,k} = \sum_{p=1}^{M} \upsilon_{p,k}\delta_{x_{p,k}}$, concentrated at *material points* $x_{p,k}$, each of which is assigned a discrete volume $\upsilon_{p,k}$. We achieve the second spatial discretization simply by identifying the discrete mass distributions as measures that are absolutely continuous with respect to the discrete volume measure $\mathcal{L}_{h,k}$, i.e., $\rho_{h,k}(x) = \sum_{p=1}^{M}\rho_{p,k}\upsilon_{p,k}\delta\big(x-x_{p,k}\big)$. The quantity $m_p = \rho_{p,k}\upsilon_{p,k}$ may be regarded as the mass *carried* by material point p. A weak reformulation of the continuity equation then shows that discrete mass is conserved if and only if m_p is constant and independent of time. Finally, the incremental transportation maps $\varphi_{k\to k+1}$ may be interpolated by *max-ent meshfree interpolation* [1]. By continuously updating these shape functions,

(a) (b)

Figure 1: Snapshots of an OTM simulation of the ballistic penetration of a 152.4mm x 152.4mm x 0.5mm Al6061-T6 plate by a nylon 6/6 cylindrical projectile with length 1.8mm and diameter 1.8mm at velocity 5.2km/s. The plate and projectile are modeled by 2,042,320 material points and 1,660,470 degrees of freedom. The simulation was performed on LLNL's Hera using 2048 mpi tasks in 24 hours.

unconfined flows can be computed free of mesh-entanglement obstructions. This combination of optimal transportation and meshfree interpolation has been termed *Optimal-Transportation Meshfree* (OTM) approximation in [3].

As in other material-point methods, seizing contact is obtained for free simply by cancelation of linear momenta, which greatly facilitates the simulation of complex contact configurations such as arise as a result of fragmentation. Finally, fracture and fragmentation can be account for by means of the eigenfracture method [4], a provably convergent material-point erosion method. Figure 1 shows a typical application of OTM to the simulation of a hypervelocity impact experiment consisting of nylon projectile striking an aluminum plate at 5.4 km/s. The ability of OTM to simulate extreme conditions of material response, including high pressures, strain rates and temperatures, large inelastic deformations, phase transitions such as melting, transport properties such as viscosity, and failure mechanisms such as fracture and fragmentation, is noteworthy.

References

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