RESEARCH STATEMENT:

COMPUTATIONAL PHYSICS and DISCRETE DIFFERENTIAL GEOMETRY

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0. Overview

In my research, I would like to apply discrete differential geometry to the study of computational physics, and apply computational physics to the study of discrete differential geometry — two areas that have a rich history of interaction [Arn66, Sma70, Sou70, FM74, MW74, MW01, GBRT13, GBY18]. As such, I hope to make contribution to both mathematics and physics.

Computational physics arose in the mid-twentieth century as a complement to theoretical and experimental physics, but has come in more recent years to provide an criterion to all areas of modern physics. In the graphics community, we mainly consider phenomena at the human scale, such as fluids and clothes. A deep question, which will require both discrete differential geometry and functional analytic methods, is to overcome the lack of analytic solvability of these problems — many aspects of computational physics have been mathematically well-established, but there are many aspects yet to make precise.

Discrete differential geometry is an emerging field studying discrete versions of smooth theories (usually from differential geometry). Instead of discretizing a problem based on approximations, one seeks for discrete definitions of mathematical objects, discusses their structural properties, and finds theorems analogous to their smooth counterparts. These discrete theories not only are bases for numerical methods, but also provide new insight in the smooth theory in return.

One of the most important arenas of interaction between computational physics and discrete differential geometry arises when one asks to classify the space of simulation process:

Question 1. *How do we represent physical quantities with different features in space*[1] *(such as grid, particles, etc)?*

Asking about the space is a way to more faithfully reflect features of the underlying mathematical equations. There are a wide variety of approaches to geometric numerical integration [HHIL06] that can be used to conserve energy, symplectic or Poisson Structures [MPS99], or remain on a Lie Group [CMO14]. It is fundamentally a discrete differential geometry question because the space is always need to be reduced into finite dimensional systems, and understanding these structures helps dramatically in the simulation.

My goal in this Research Statement is to review different aspect to answer Question 1 in fluid simulation, as well as the questions I am pursuing.

1. Grid Aspect

Marker-and-Cell discretization scheme [HW$^+$65, Bri15] is widely adopted in fluid simulation. With the equivalence to a Discrete Exterior Calculus scheme, offers a unified approach to the construction of discrete operators, backed by the rigor of differential topology.

Question 2. *How can we construct algorithms satisfying mass-conserving, shape-preserving, and the constancy condition?*

In multiphase flow simulations, two classes of methods of treating the interface exists: (1) interface capturing, wherein the interface front is represented by a set of connected marker points, and (2) interface tracking, in which a marker function is employed to identify each fluid phase.

Interface capturing methods employ an additional equation governing the evolution of marker function, and any change in the topology of the interface occurs automatically, i.e. without any specialized reconstruction. Due to this advantage, interface capturing methods, such as volume of fluid (VOF) [HN81, You82, HF00, SZ03, PJP04, JLCO14] and the level set (LS) [SSO94, OK05, OKZ07, Her08, Wac15] methods are more popular and widely applied in multiphase flow simulations.

Conjecture 1. *Phase Field could be written into commutative diagram to satisfy the above requirement.*

Unlike the artificially smoothed level set function, the phase field function places the phase ratio and the gradient of it together into the free energy function. In this way, the phase field function not only follows the convective phase state, but also minimizes the total free energy of the system. Interfaces are always consistent and do not have to be re-initialized [ZYF$^+$10]. It is easier to keep the volume constant without adding more system complexity [Jac99].

The evolution process of phase field is controlled by Ginzburg–Landau free energy as $\mathcal{F}(c, \boldsymbol{\gamma}) = \int_\Omega \psi(c) + \kappa\|\boldsymbol{\gamma}\|^2 \mathrm{d}\Omega$, where $\boldsymbol{\gamma} = \boldsymbol{\nabla} c$ is enhanced flow variable. Thus the evolution operator in this system is formally

[1] This space should have the capability to express topological changes, such as rupture and coalescence. In the corresponding representation, we would like to keep the interface between different material as sharp and clear as possible.

skew-symmetric, which constitutes a Dirac structure. Applying Green's Theorem, this system can be constituted as a port Hamiltonian system. According to Nishida et al. [NMI15], we can use a commutative diagram to represent the above port Hamilton system.

On the other hand, Wang et al. prove the boundedness of the conservative phase field equation for the first order Euler forward and predictor-corrector time integration schemes in the discrete exterior calculus framework [WJHS23].

Question 3. *How to design the Poisson bracket to integrate the kinetic and the Ginzburg–Landau free energy in discrete space?*

Nabizadeh et al. use B-spline to design divergence-consistent grid to represent divergence-free vector fields [NRCY$^+$24]. But unlike the continuous theory, the discrete space is in general not a Lie algebra. They use the adjoint of the embedding function (from continuous space to discrete space) to pullback the discrete Hamilton function.

Similarly, we can not equip the phase field with Lie algebra, due to the lack of additivity. So, *is it possible to provide an analogous basis for interpolation to expand the bounded phase field space?* Under this space, the port Hamiltonian system will degenerate into a finite-dimensional structure. For this structure, it is necessary to use the orthogonal collocation method to discretize and add the dynamic process through Symplectic integrators. Once this structure is obtained, we can perform corresponding energy error analysis and order proof in the discretized space.

Question 4. *Represent better boundary details and changing domain for discrete exterior calculus.*

Question 5. As the Neural Network could compress the large amount of velocity data needed to evaluate these long-tern characteristics [DYZ$^+$23], and could model the symmetry transformations and the corresponding generators [KS20, CCCH22, LT22, FMM$^+$23]. *How can we keep the simulation process on the orbit of group action even if using Neural Network?*

2. Meshfree Aspect

Due to the lack of additivity, using particles to carry the fraction of volume is a promising way to attain the multiphase feature [Mon05, GK18, LRS20]. But it is known that the standard particle method (which is equivalent to the element-free Galerkin method with an Eulerian kernel and nodal quadrature) has two sources of instability: (1) rank deficiency of the discrete equations, and (2) distortion of the material instability. The former is known as the particle inconsistency and the latter leads to the so-called tensile instability.

Question 6. *How to describe the particle system independent of specific distribution without sufficiently dense?*

Naturally, we can use $\mathcal{P}$ tp denote the index set for the particles. The time-dependent state $(\boldsymbol{x}_p(t), \boldsymbol{u}_p(t))_{p\in\mathcal{P}}$ of the system would travel under a Lie group action by a generator $\boldsymbol{v} \in \mathfrak{X}_{\mathrm{div}}(W)$. And Nabizadeh et al. show the evolution under Lie group integrator becomes an energy preserving integrator in the limit where the particle density approaches a continuum[NRCY$^+$24].

Conjecture 2. *Pointwise divergence-free velocity field could help keep particle consistency.*

Chang et al. reconstruct streamfunctions from the velocity data on a grid to obtain the exact divergence-free flow interpolation [CPAB22]. But for free-surface and multi-phase fluid, the domain would get nonzero genus and with a few obstacles removed, there are velocities that cannot be expressed by streamfunctions.

To overcome this, we need different gauge for the inside and outside part of domain respectively. For the space to be extrapolated, there are no physical requirement. What one expects is a pointwise divergence-free velocity field distribution consistent with the dominant fluid's internal velocity. We could add some bridges to connect the dominate phase to form simple connected domain.

On the other hand, Liu et al. place uniform-distributed virtual particles to exert pressure, and to give an objective perspective on avoiding tensile instability [LHG$^+$24]. But although particle method has C^1 kernel consistency for the interior regions, for the boudary regions, it does not even have C^0 kernel consistency. The particles would not keep divergence-free out of interior. And as the distribution of the particle could not keep continuum all the time, the divergence is almost everywhere not 0.

Question 7. *Is it possible to get pointwise divergence-free velocity field only by particles?*

Question 8. As a Monte Carlo simulation could become a pointwise estimator for each substep with flexible integration with existing velocity-based techniques [SBH24], *how can we evaluate only a small number of positions and produce unbiased results?*

3. Hybrid Eulerian-Lagrangian Aspect

Question 9. *How to couple continuum-discrete solvers to ensure the conservation of relevant quantities.*

This difficulty arises because the conservation equations at the two scales are formulated for fundamentally different properties. Therefore, bridging the gap between micro- and macro- quantities is crucial but extremely difficult to achieve. In the review on continuum-discrete solvers, Rui Sun and Heng Xiao, based on physical reasoning and their experience with CFD-DEM simulations, pointed out that an ideal scheme should meet the following five requirements [SX15]:

(a) conserve relevant physical quantities;

(b) be able to handle particles both in the interior cells and the cells near boundaries without producing artifacts, including physical boundaries and processor boundaries in parallel computing;

(c) be able to achieve relatively mesh-independent results;

(d) be convenient for implementation in parallel, three-dimensional CFD solvers based on unstructured meshes with arbitrary cell shapes;

(e) be able to produce smooth fields even with the presence of a few large particles in relatively small cells.

If the above requirements could be met, proposing a flexible and easy-to-implement framework can make the conservation structure more concrete, providing physical benchmarks for steady-state conditions.

Conjecture 3. *Use Hodge star $\star$ to complete the dual between particles and girds.*

The physical quantities on both sides of the Hodge star operator in the commutative diagram could be stored on particles and meshes, respectively. Phase proportions and gradients are stored on particles, while corresponding statistics are calculated on the mesh. The chemical potential gradient is then derived from these statistics to update the particle states. This relationship ensures the conservation of total flux in the Hamiltonian sense.

Adding particles outside the mesh allows for more comprehensive spatial sampling. The particle splitting algorithm based on mass flow ensures that the phase proportions recorded on Lagrangian convective particles do not exceed boundaries, thus preserving shape. The port-Hamiltonian system provides a physical basis for the transfer of information between particles and meshes under the phase field.

Question 10. *How to integrate finite particles to the Poisson bracket?*

However, this operator only utilizes the commutative diagram derived from the port Hamiltonian to construct a numerical algorithm for phase field information, and has only been tested for phase separation scenarios. For a rigorous analysis and quantitative calculation of the Hamiltonian, it is necessary to design a metric in a divergence-free velocity field space. Only with this metric can we obtain more precise physical entities of exterior differential operators and differential forms, thereby achieving natural pairing of the variables we select. On the other hand, to provide a computational process for our particle grid separation strategy, we should design the corresponding Poisson brackets for derivation, rather than simply combining with existing systems.

On the other hand, the particle systems is understood as the intepolation from the grid counterpart. To exploit the divergence-free field better and gain lower interpolation errors proportional to the cell width, higher-order interpolation strategies are needed. However, since velocity lies in $\Omega^1(W)/\,\mathrm{d}\Omega^0(W)$, higher-order schemes may conflict with the interpolated and recorded velocity fields at the dual position. A more generalized understanding of the physical entities corresponding to velocity fields in space is required.

With an improved understanding of the state space, my objective is to extend controllability principles beyond linear time-invariant systems to encompass nonlinear dynamical systems. Differential flatness pertains to the flatness with respect to finite-order derivatives. Within continuous-time finite-dimensional flat systems, it becomes possible to algebraically compute state and input trajectories based on the output and its discrete-time derivatives. This algebraic approach allows us to invert system without resorting to numerical integration. The port Hamiltonian system, characterized by its differential structure, exhibits differential flatness. Leveraging this property, we can design effective transfer strategies for achieving efficient control.

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