Journal of Computational Physics 313 (2016) 455–477

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Optimization-based mesh correction with volume and convexity constraints

Marta D'Elia [a,*], Denis Ridzal [a], Kara J. Peterson [a], Pavel Bochev [a], Mikhail Shashkov [b]

[a] Center for Computing Research, Sandia National Laboratories,[1] MS-1320, Albuquerque, NM 87185-1320, USA
[b] X-Computational Physics, XCP-4, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

ARTICLE INFO

Article history:
Received 11 March 2015
Received in revised form 11 February 2016
Accepted 11 February 2016
Available online 24 February 2016

Keywords:
Lagrangian motion
Incremental remap
Semi-Lagrangian transport
Departure volume correction
Volume fraction
Passive tracer transport

ABSTRACT

We consider the problem of finding a mesh such that 1) it is the closest, with respect to a suitable metric, to a given source mesh having the same connectivity, and 2) the volumes of its cells match a set of prescribed positive values that are not necessarily equal to the cell volumes in the source mesh. This volume correction problem arises in important simulation contexts, such as satisfying a discrete geometric conservation law and solving transport equations by incremental remapping or similar semi-Lagrangian transport schemes. In this paper we formulate volume correction as a constrained optimization problem in which the distance to the source mesh defines an optimization objective, while the prescribed cell volumes, mesh validity and/or cell convexity specify the constraints. We solve this problem numerically using a sequential quadratic programming (SQP) method whose performance scales with the mesh size. To achieve scalable performance we develop a specialized multigrid-based preconditioner for optimality systems that arise in the application of the SQP method to the volume correction problem. Numerical examples illustrate the importance of volume correction, and showcase the accuracy, robustness and scalability of our approach.

Published by Elsevier Inc.

1. Introduction, motivation and background

Mesh motion is at the core of many numerical methods for time dependent flow and structure problems. Examples include Lagrangian hydrodynamics methods [1], in which the mesh evolves with time in order to track deformations of the problem domain, and the related Arbitrary Lagrangian–Eulerian [2] methods, which incorporate a mesh rezoning step to mitigate excessive mesh deformations and mesh tangling. Another important example are semi-Lagrangian methods for advection problems [3,4], including schemes utilizing incremental remapping [5,6] as a transport algorithm. Such methods perform a single Lagrangian step and then remap the resulting solution back to a fixed Eulerian mesh.

Despite individual differences all such methods require computation of the mesh motion under a velocity field $\boldsymbol{u}$. Most of them approximate the deformed Lagrangian mesh by 1) solving numerically the kinematic relation $d\boldsymbol{x}/dt = \boldsymbol{u}$ to estimate

* Corresponding author.
E-mail addresses: mdelia@sandia.gov (M. D'Elia), dridzal@sandia.gov (D. Ridzal), kjpeter@sandia.gov (K.J. Peterson), pbbochev@sandia.gov (P. Bochev), shashkov@lanl.gov (M. Shashkov).

[1] Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

http://dx.doi.org/10.1016/j.jcp.2016.02.050
0021-9991/Published by Elsevier Inc.

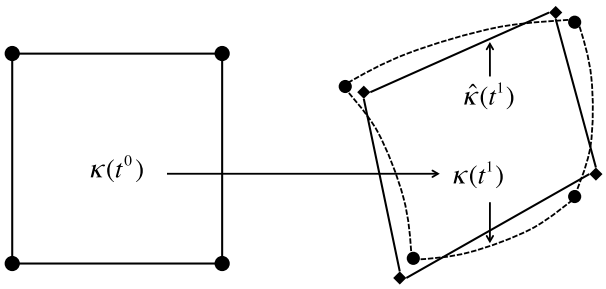

Fig. 1. A non-divergent velocity field deforms an initial cell $\kappa(t^0)$ into a cell $\kappa(t^1)$ having the same volume. Approximation of vertex positions by numerical time integration (diamonds) and their subsequent linking by straight lines yields an approximate deformed cell $\widehat{\kappa}(t^1)$ with a different volume.

the new cell vertex positions, and 2) connecting them by straight lines. Consequently, the cells in the deformed mesh incur two types of errors: one due to the approximation of the vertex trajectories and another due to the approximation of the deformed cell edges by straight lines. The former can be viewed as a time discretization error, while the latter can be interpreted as a spatial error.

The temporal and spatial errors yield approximate Lagrangian cells whose volumes do not match the volumes of the exact Lagrangian cells; see Fig. 1 for an illustration with a non-divergent velocity field. Unfortunately, volume approximation errors may have an outsized influence on the accuracy of numerical methods relying on mesh motion. In particular, a scheme may fail to preserve constant solutions even though temporal and spatial errors in the approximation of the Lagrangian cell are better than first-order accurate.

To understand this phenomenon let us examine the Lagrangian motion of a single mesh cell $\kappa(t)$, representing a fluid parcel with material density ρ, under a non-divergent velocity field $\boldsymbol{u}$. Let $\kappa(t^0)$ denote the initial position of the fluid parcel and $\kappa(t)$ be the exact Lagrangian parcel at time $t > t^0$, and let the volume and mass of κ at time t be defined as

$$|\kappa(t)| = \int_{\kappa(t)} dV \quad \text{and} \quad M_\kappa(t) = \int_{\kappa(t)} \rho dV\,.$$

Because non-divergent Lagrangian flows preserve volume and mass there holds

$$\frac{d}{dt}|\kappa(t)| = 0 \quad \text{and} \quad \frac{d}{dt}M_\kappa(t) = 0. \tag{1}$$

Suppose now that $\rho = const$ and $\kappa(t)$ moves from its initial position at time t^0 to a new position at time $t^1 = t^0 + \Delta t$, then by (1)

$$\rho(t^1) = \frac{M_\kappa(t^1)}{|\kappa(t^1)|} = \frac{M_\kappa(t^0)}{|\kappa(t^0)|} = \rho(t^0) = const.$$

On the other hand, since $\kappa(t^1)$ is not known exactly, except for some trivial velocity fields, a numerical scheme uses an approximation $\widehat{\kappa}(t^1)$ for which $|\widehat{\kappa}(t^1)| \neq |\kappa(t^1)|$; see Fig. 1. As a result, the material state $\widehat{\rho}$ in the approximate Lagrangian fluid parcel $\widehat{\kappa}(t^1)$ is given by

$$\widehat{\rho}(t^1) = \frac{M_\kappa(t^1)}{|\widehat{\kappa}(t^1)|} \neq \frac{M_\kappa(t^0)}{|\kappa(t^0)|} = \rho(t^0). \tag{2}$$

In other words, the constant density is not preserved. Yet, many Lagrangian and semi-Lagrangian methods rely on relationships such as (2) to approximate densities, tracer mixing ratios, material volume fractions and other quantities of interest. This effectively renders such methods unable to represent exactly *constant* solutions despite the fact that $\widehat{\kappa}(t^1)$ can be an accurate approximation of the exact fluid parcel $\kappa(t^1)$.

This example illustrates the consequences of violating the broader notion of a *Discrete Geometric Conservation Law* [7] (D-GCL) for a given numerical scheme. D-GCL stipulates that computation of geometric quantities in the deformed mesh configuration must be done in a way that allows the associated numerical scheme to reproduce constant states for any mesh motion.

One possible pathway for achieving a D-GCL for (2) is to enforce equality of deformed cell volumes at all time steps to their initial volumes in the undeformed configuration. This can be done by further deforming $\widehat{\kappa}(t^n)$ to a *corrected* cell $\kappa^*(t^n)$ such that

$$|\kappa^*(t^n)| = |\kappa(t^0)| \quad \forall n\,. \tag{3}$$

The corrected cell must be valid and can be subject to further mesh quality conditions such as convexity. In addition, we require that $\kappa^*(t^n)$ remain close to $\widehat{\kappa}(t^n)$ at all time steps, because the latter approximates the unknown exact Lagrangian