Compatible Discretizations for Multiphysics: A Brief Review and Some Future Challenges*

F. L. Teixeira
ElectroScience Laboratory and Department of Electrical and Computer Engineering
The Ohio State University
Columbus OH, USA
teixeira.5@osu.edu

***Abstract*—We provide a brief discussion on the progress of compatible discretization methods for the simulation of electromagnetics and multiphysics problems. We revisit some of its past success stories and list a few outstanding challenges.**

I. Introduction and Motivation

Numerical solvers for partial differential equations (PDEs) based on finite-elements and finite-differences conventionally rely on a top-down discretization approach, where the starting point is a particular (set of) partial differential equation(s) in component form, with various vector/tensor fields likewise treated in a component-wise fashion. Under the conventional paradigm, each discretization approach along with a (set of) physical equation(s) produce distinct data structures and the resulting picture is a fragmented one, with low interoperability. More importantly, the resulting discretizations often exhibit inconsistencies on irregular grids such as lack of correspondence between computed and true spectra and/or violation of conservation and positivity principles [1]. These inconsistencies are *not* supressed as the mesh is refined and may generate spurious modes, instabilities, and/or convergence issues. This is especially problematic in multiphysics problems where a high degree of geometric flexibility is demanded that may involve irregular, hybrid, and/or overlapped/non-matching meshes [2]. In recent years, compatible discretizations have emerged as a conceptual umbrella to denote discretization methods that seek to avoid such pitfalls [1], [3]. Compatible discretizations are generally designed in a bottom-up fashion, where discrete analogs of the mathematical operators and field quantities are designed from first principles using tools borrowed from algebraic topology and the exterior calculus of differential forms [4]–[9]. Compatible discretizations have a distinct object-oriented flavor because the assembling of discrete operators and model variables (degrees of freedom) into discrete equations is only done at a later stage, providing an increase in portability and reuse of the numerical model.

In this work, we briefly discuss some of the underpinnings of compatible discretizations for multiphysics, its past evolution and a few "success stories", and outline some of the challenges and prospects for the future. Due to limited space, the discussion is necessarily selective and incomplete.

II. An Incomplete Historical Overview

One of the early contributions to compatible discretizations can be traced to the so-called 'Tonti diagrams' [10], outlining the correct commuting diagram properties of (discrete) operators. Another formative work consisted of 'mimetic discretizations' [11]–[13] that yield equations on general meshes conforming to the exactness property of the underlying de Rham complex, and lead to the definition of 'natural' and 'adjoint' discrete operators associated with the exterior derivative d and the codifferential δ [14], respectively, applicable to any PDE.

A. Electromagnetics

The link between compatible discretizations and mixed finite element methods for Maxwell's equations was first established in [15]. This development was instrumental in solving, using vector basis functions, the decade-long problem of spurious modes in finite element solutions of Maxwell's equations. Vector basis functions such as Nédélec (edge or curl-conforming) elements and Raviart-Thomas (face or div-conforming) elements, RWG, and Buffa-Christiansen basis functions can all be recognized as a particular versions of Whitney forms of various degrees, which are interpolants of discrete differential p-forms in n spatial dimensions [5], [16].

B. Elastodynamics

In its various incarnations, Whitney forms have been very successful in electromagnetics. However, they are not sufficient for discretization of some tensor-valued field theories such as elastodynamics. The stable discretization of elastodynamics on irregular grids has been an outstanding problem for many years prior to the application of compatible discretizations. In this case, bundle-valued discrete differential forms [17] or more generalized finite element spaces based on the Koszul complex [18] have proved successful [1].

C. Plasma physics

Multiphysics problems involving Maxwell's equations (for fields) and Newton's force law (for particles), such as in kinetic plasma simulations, are routinely solved by particle-in-cell (PIC) methods [19]. A drawback of conventional PIC algorithms on irregular grids is that they numerically violate charge conservation. A first-principles solution to the

The final published version of this paper appears in *2016 IEEE Antennas and Propagation Society International Symposium Digest*, pp. 1289-1290, June 26 - July 1, Puerto Rico, 2016.

this challenge has eluded researchers for many years. PIC codes require two extra steps to transfer information from the instantaneous field distribution to the particle kinematic update (gather step) and vice-versa (scatter step). This transfer of information may not necessarily satisfy charge continuity exactly and hence lead to spurious charge deposition on the grid. This can be corrected a posteriori using, for example, an extra (elliptic) solver at each time step; however, this degrades the efficiency of the algorithm and sets a limit on mesh refinement since the condition number of such an elliptic system increases with the amount of size disparity among mesh elements. Recently, compatible discretizations were able to solve this longstanding problem and yield exact charge-conserving PIC on irregular meshes based on a consistent representation for particle charges and currents using Whitney forms of appropriate degrees [20].

III. An Incomplete List of Challenges

A. Overlapped/collocated meshes

Spatial and temporal scales can be quite disparate between different physics components in a given multiphysics simulation. As such, the use of a single mesh or synchronous (global) time stepping can be inefficient. When multiple (fully or partially) collocated/non-matching meshes are present, each one solving a different physics component [2], a fundamental problem arises from the need of consistent information exchange between meshes. Since compatible discretizations have already proved useful in providing consistent exchange between mesh-based and ambient-space-based variables [20], they are a promising route to provide consistent mesh-to-mesh information exchange in multiphysics problems as well.

B. Disparate time scales

In multiphysics problems, the presence of disparate timescales calls for for asynchronous or local time-stepping [21]. Causality, stability, and symplecticity of the resulting time-stepping algorithm then becomes a critical issue. One possible strategy here is to describe the physical problem from a four-dimensional standpoint and discretize it using appropriate spatiotemporal mesh elements and differential forms [9], [22], [23].

C. Multiphysics at very high energies

In high-energy physics, the interaction picture between the electromagnetic field and the fermionic fields involves the Dirac equation. Fermionic fields defy a lattice description with local coupling that gives the correct energy spectrum in the limit of zero lattice spacing and the correct chiral invariance [24]. This is associated to the well-known 'fermion-doubling' problem [25]. Compatible discretizations offer an explanation of the source of this difficulty by generalizing the Dirac operator $\gamma^\mu \partial_\mu$ where γ^μ are Euclidean gamma matrices, to the operator $d - \delta$, which admits a natural discretization on a mesh. Once squared, both operators recover the D'Alambert operator $\Box$, i.e. $(\gamma^\mu \partial_\mu)^2 = -\Box$ and $(d-\delta)^2 = -\Box$; however, they act on different spaces (spinors versus inhhomogeneous differential forms, resp.) [26] and so it remains to be seen whether the longstanding fermion doubling problem can be solved by exploiting such connection.

Acknowledgement

Support from NSF grant 1305838 is acknowledged.

References

[1] D. N. Arnold et al., eds., *Compatible Spatial Discretizations*. IMA Volumes in Mathematics and its Applications, Springer-Verlag, 2006.

[2] X. Jiao and M. T. Heath, "Common-refinement-based data transfer between non-matching meshes in multiphysics simulations," *Int. J. Num. Meth. Eng.*, vol. 61, pp. 2402-2427, 2004.

[3] D. White, J. Koning, and R. Rieben, "Development and application of compatible discretizations of Maxwell's equations," in *Compatible Discretization of Partial Differential Equations*, Springer-Verlag, 2006.

[4] D. H. Adams, "R-torsion and linking numbers from simplicial Abelian gauge theories," arXiv:9612009 [hep-th], 1996.

[5] F. L. Teixeira and W. C. Chew, "Lattice electromagnetic theory from a topological viewpoint," *J. Math. Phys.*, vol. 40, no. 1, pp. 169-187, 1999.

[6] S. Sen et al., "Geometric discretization scheme applied to the Abelian Chern-Simons theory," *Phys. Rev. E*, vol. 61, no. 3, pp. 3174–3185, 2000.

[7] P. W. Gross and P. R. Kotiuga, *Electromagnetic Theory and Computation: A Topological Approach*, Cambridge University Press, 2004.

[8] B. He and F. L. Teixeira, "On the degrees of freedom of lattice electrodynamics," *Phys. Lett. A*, vol. 336, no. 1, pp. 1–7, 2005.

[9] F. L. Teixeira, "Lattice Maxwell's equations," *PIER*, vol. 148, pp.113-128, 2014.

[10] E. Tonti, "The reason for analogies between physical theories," *Appl. Math. Model.*, vol. 1, pp. 37–50, 1976.

[11] J. M. Hyman and M. Shashkov, "Mimetic discretizations for Maxwell's equations," *J. Comp. Phys.*, vol. 151, pp. 881–901, 1999.

[12] F. Brezzi and A. Buffa, "Innovative mimetic discretizations for electromagnetic problems," *JCAM*, vol. 234, pp. 1980–1987, 2010.

[13] K. Lipnikov et al., "The mimetic finite difference method for the 3d magnetostatic field problems on polyhedral meshes.," *J. Comp. Phys.*, vol. 230, pp. 305–328, 2011.

[14] B. He and F. L. Teixeira, "Differential forms, Galerkin duality, and sparse inverse approximations in finite element solutions of Maxwell equations,' *IEEE Trans. Ant. Propagat.*, vol. 55, pp. 1359-1368, 2007.

[15] A. Bossavit, "Whitney forms: A new class of finite elements for three-dimensional computations in electromagnetics," *IEE Proc. A*, vol. 135, pp. 493–500, 1988.

[16] F. L. Teixeira, "Geometrical aspects of the simplicial discretization of Maxwell's equations," *PIER*, vol. 32, pp. 171–188, 2001.

[17] A. Yavari, "On geometric discretization of elasticity," *J. Math. Phys.*, vol. 49, p. 022901, 2008.

[18] V. W. Guillemin and S. Sternberg, *Supersymmetry and Equivariant de Rham Theory*. Berlin: Springer, 1999.

[19] D. L. Bruhwiler et al., "Particle-in-cell simulations of plasma accelerators and electron-neutral collisions," *Phys. Rev. ST Accelerators and Beams*, vol. 4, p. 10132, 2001.

[20] H. Moon et al., "Exact charge-conserving scatter-gather algorithm for particle-in-cell simulations on unstructured grids: A geometric perspective," *Comput. Phys. Comm.*, vol. 194, pp. 43-53, 2015.

[21] L. D. Angulo et al., "Causal-path local time-stepping in the discontinuous Galerkin method for Maxwells equations," *J. Comp. Phys.*,, vol. 256, pp. 678-695, 2014.

[22] J. Erickon et al., "Buliding space-time meshes over arbitrary spatial domains," *Eng. Computers*, vol. 290, pp. 342-353, 2005.

[23] J. Salamon et al., "Geometric representations of Whitney forms and their generalization to Minkowski spacetime," arXiv:1402.7109, 2014.

[24] D. H. Adams, "Fourth root prescription for dynamical staggered fermions," *Phys. Rev. D*, vol. 72, 114512, 2005.

[25] I. F. Herbut, "Time reversal, fermion doubling, and the masses of lattice Dirac fermions in three dimensions," *Phys. Rev. B*, vol. 83, 245445, 2011.

[26] F. L. Teixeira, "Differential forms in lattice field theories: An overview," *ISRN Math. Phys.*, 487270, 2013.