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High-Resolution Mathematical and Numerical Analysis of Involution-Constrained PDEs

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Abstract. Partial differential equations constrained by involutions provide the highest fidelity mathematical models for a large number of complex physical systems of fundamental interest in critical scientific and technological disciplines. The applications described by these models include electromagnetics, continuum dynamics of solid media, and general relativity. This workshop brought together pure and applied mathematicians to discuss current research that cuts across these various disciplines' boundaries. The presented material illuminated fundamental issues as well as evolving theoretical and algorithmic approaches for PDEs with involutions. The scope of the material covered was broad, and the discussions conducted during the workshop were lively and far-reaching.

Mathematics Subject Classification (2010): 58A12, 58J45, 65M99, 74S30, 78M99.

Introduction by the Organisers

The workshop *High-Resolution Mathematical and Numerical Analysis of Involution-Constrained PDEs*, organised by Bruno Després (Paris), Michael Dumbser (Trento), James Kamm (Los Alamos), and Manuel Torrilhon (Aachen), brought together 25 participants from institutes in France, Germany, Italy, the Netherlands, Norway, Russia, Switzerland, and the United States. The topics discussed by these researchers spanned an unusually broad spectrum of mathematics, including theoretical analysis, numerical analysis, and computational studies of involution-constrained PDEs. These topics can be characterized as a subset of the field of mimetic methods for PDEs, with specific focus on the algorithms that satisfy

the involutions constraining the allowable solutions. The workshop began with an overview talk by Jim Kamm, discussing the genesis of the workshop, the scope of its topics, and a brief discussion of numerical approaches to intrinsically satisfy the involution of Eulerian hyperelasticity.

Underpinning any computational approach to the solution of PDEs are theoretical examinations of numerical methods and the underlying structure of the equations. Snorre Christiansen presented the former, while the latter were discussed by Marc Gerritsma, Holger Heumann, and Allen Robinson, each of whom gave specific examples highlighting the relevance of exterior calculus, differential geometry, and algebraic topology in this field.

The Maxwell equations of electromagnetics provide the archetypal physics-based example of involution-constrained PDEs. Here, the involution is the constraint $\nabla \cdot \mathbf{B} = 0$ (where $\mathbf{B}$ is the magnetic induction), which is a necessary condition for physically admissible solutions. A closer examination of the nature of the equations of electromagnetics reveals a deep mathematical structure of the continuous PDEs. Careful algorithmic construction and numerical analysis is required to ensure that this structure is preserved in the corresponding numerical approximations. Topics in to this field were the basis of two presentations given by Alain Bossavit. One important application of electromagnetics is in the modeling of magnetohydrodynamic (MHD) phenomena, which was the focus of the presentations of Dinshaw Balsara, Bruno Després, and James Rossmanith. The MHD equations combine a particular limiting case of the Maxwell equations, combined with the conservation equations for material flow (fluid or solid). The proper formulation of the governing equations here remains an open issue, which has deep implications for both the continuous and discrete mathematics. Solutions of the MHD equations can display extremely complicated structures, the accurate computational approximation of which depends exquisitely on the numerical methods and, in particular, observation of the crucial involution constraint. Such accurate simulation is essential when considering flow instabilities, which not only provide a sensitive indicator of numerical solution quality but also represent a high-consequence physical phenomenon in experimental and industrial facilities, such as the proposed ITER reactor. For the latter application, closely related to MHD is the set of equations used to model the plasma physics relevant to near-wall regions in tokamaks. Aspects of the mathematical and numerical modeling associated with such edge plasma phenomena were addressed in the presentations of Emmanuel Franck, Boniface Nkonga, Ahmed Ratnani, and Eric Sonnendrücker.

The other primary component of the MHD model is given by the balance equations governing material motion. These conservation laws, generically referred to as the equations of hydrodynamics, govern not only fluid behavior but also condensed matter phenomena such as elasticity. Research of the last 30+ years has convincingly demonstrated the important role that high-resolution numerical methods play in the computational solution of these equations, even in the presence of flow discontinuities such as shock waves. The relation of high-resolution methods

to involution-constrained problems of compressible flow was discussed in the presentations of Christiane Helzel and Phil Roe. François Bouchut discussed the particular case of conservation laws applied to shallow water flow on a sphere, Roger Kaeppeli talked about the application of specific involution-conserving schemes to PDEs modeling astrophysical phenomena, and Michael Dumbser presented a new class of high order numerical schemes applicable to general systems of conservation laws. Likewise, the equations for hyperelastic material response are constrained by an involution, which is readily shown, in the Eulerian frame, to be the constraint $\operatorname{curl} \mathsf{G} = 0$ (where G is the inverse deformation gradient). Related topics were discussed by Sergey Gavrilyuk, Gilles Kluth, Ilya Peshkov, and Evgeniy Romenskii.

Preservation of involution constraints is also required during the so-called data transfer process, in which the numerical solution to a set of PDEs is mapped from one computational mesh to another. This aspect is of broad-ranging interest in computational mathematics and was discussed in the presentations of Pavel Bochev and Misha Shashkov.

Summary of Topics Discussed

After the formal presentation program of the workshop, Bruno Després chaired a session in which the week's topics were summarized. Here, we provide groups of presenters, grouped according to the primary perspective or initial motivation of their presented work.

Differential geometry / exterior calculus / algebraic topology - inspired approaches: A. Bossavit, S. Christiansen, M. Gerritsma, H. Heumann, A. Robinson, E. Sonnendrücker.

Regular numerical methods for nonlinear elasticity: B. Després, S. Gavrilyuk, G. Kluth, I. Peshkov, E. Romenskii

High-order numerical methods: M. Dumbser, C. Helzel, J. Rossmanith

New nonlinear solvers: D. Balsara, F. Bouchut, R. Kaeppeli, P. Roe

Large nonlinear systems with preconditioners: E. Franck, B. Nkonga, A. Ratnani

Conservative data-transfer (remapping): P. Bochev, M. Shashkov

Main Results and Important New Developments

There were several discussions during the workshop, each of which engendered energetic exchanges. The following themes were distilled from the discussions.

(1) A key concept is that involutions help one understand the meaning of the equation vis-à-vis the physics.
(2) Workshop participants were interested in *constructive* approaches to the solution of involution-constrained PDEs, i.e., in how to turn theoretical ideas into numerical methods.
(3) An open question in several fields is, "How are we sure that we have the proper involutions?" Examples of this issue are seen in both MHD and nonlinear elasticity.
(4) What is the relation between satisfying involutions and higher order methods? Should one or the other be foremost? Are lower order methods with involution constraints sufficient?

We give below a brief list of a few of the "hot topics" as drawn from the workshop discussions.

The role of exterior calculus: in the numerical methods was subject to spirited debate. Whereas the merit of this formulation for electromagnetics (where it is both physically and mathematically illuminating) is not questioned, the promise of this approach remains elusive for, e.g., hydrodynamics simulations. A key virtue of this approach is that it necessarily involves the separation of topology from geometry in problems, and there was speculation that this formalism might yet prove helpful for nonlinear problems where the numerics necessary to preserve solution structure is not yet known. This hopeful view was counterbalanced by the pragmatic concerns that exterior calculus methods for other equations (1) must be shown to exist and, if so, (2) should be evaluated as to their usefulness.

The role of Riemann solvers: in compressible flow and MHD was a topic of vigorous dialogue. The role of Riemann solvers as a sub-grid model providing "just the right amount" of dissipation was discussed, and the place for approximate multidimensional Riemann solvers was debated.

Appropriate discretization schemes: was a theme that spanned both of the above topics. The concept of the topology of the discretization was a recurring theme, tempered by the notion that one should not overburden a computational mesh into satisfying *ipso facto* certain constraints.

Bruno Després, Michael Dumbser, James Kamm, Manuel Torrilhon

Workshop: High-Resolution Mathematical and Numerical Analysis of Involution-Constrained PDEs

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Abstracts

Multidimensional Riemann Solvers for Divergence-Free MHD

Dinshaw S. Balsara

With easy access to supercomputers, MHD studies have become computationally dominated. Magnetohydrodynamics (MHD) is the most popular and most important approximation for astrophysical, space physics and several terrestrial plasmas. However, there has always been a fundamental inconsistency in the way divergence-free magnetic fields have been evolved on computational meshes, as will be shown below. The only way to patch things up had been to continuously double the dissipation, thereby degrading the quality of the results. Overcoming this inconsistency required a fundamental new invention - multidimensional Riemann solvers (RS) (Balsara 2010, 2012, Balsaraet al. 2013). Below I briefly describe this recent research. I have also started developing a public website, with downloadable codes, that teaches methods in computational astrophysics (http://www.nd.edu/ dbalsara/Numerical-PDE-Course). Several researchers have contributed to the development of numerical MHD (Evans & Hawley 1989, Dai & Woodward 1998, Ryuet al. 1998, Balsara 1998, Falleet al. 1998, Balsara 2004, 2009, Crockett et al. 2005, Ustyugovet al. 2009). Any such listing would be incomplete and I apologize for any incompletions. However, the biggest debate in this field has raged around the treatment of the induction equation (Faraday's law), $\partial\mathbf{B}/\partial t - \nabla\times(\mathbf{v}\times\mathbf{B}) = 0$. Physically, it says that if we have $\nabla\cdot\mathbf{B} = 0$ to begin with, the constraint on the magnetic field, $\mathbf{B}$, is preserved for all time. Faraday's law can be satisfied in discrete form on a computational mesh if the magnetic field components are located at face centers and electric fields at edge centers, please see Fig. 1. The problems are easily apparent if one focuses on the z-component of the electric field in Fig. 1. When the MHD system is written in flux form ($\partial_t\mathbf{U} + \partial_x\mathbf{F} + \partial_y\mathbf{G} + \partial_z\mathbf{H} = 0$), the z-component of the electric field corresponds to the seventh component of the x-flux, $\mathbf{F}_7$, and also to the sixth component of the y-flux, $\mathbf{G}_6$, please see Balsara (2004). Since the x-flux picks up contributions of the waves propagating in the x-direction while the y-flux picks up contributions from the waves propagating in the y-direction, we see that neither of the one-directional fluxes provides an accurate representation of the wave propagation. In a numerical code, this arbitration of the waves is done via a Riemann solver, because the waves can consist of strong shocks which need to be stabilized via appropriate dissipation on a mesh. Furthermore, this dissipation has to be minimized when it is inappropriate. Dai & Woodward (1998), Ryuet al. (1998), Balsara and Spicer (1999) suggested using some combination of the x- and y-directional fluxes that come out of a one-dimensional RS. Londrillo & DelZanna(2004), Gardiner and Stone (2005) suggested doubling the dissipation that comes from each of the one-dimensional RS. Both choices are ill for a simple physical reason - the wave propagation is inherently multidimensional and the RSalso has to be inherently multidimensional.

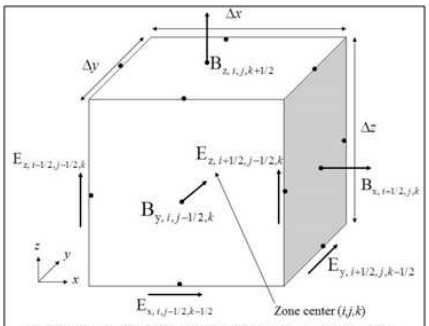

Fig. 1 shows the collocation of face-centered magnetic fields and edge-centered electric fields in a constrained transport method on a Cartesian mesh.

A major innovation was clearly needed! One-dimensional Riemann solvers for numerical MHD had been designed aplenty (Brio & Wu 1988, Roe & Balsara 1996, Cargo & Gallice 1997, Balsara 1998, Gurski 2004, Li 2005, Miyoshi & Kusano 2006). But what was needed was a multidimensional RS. The glaring problem was that an easily-implementable multidimensional Riemann solver was needed.There were some initial studies (Abgrall 1994, Fey 1998), but none of them were suited for implementation in a production code. In Balsara (2010, 2012) and Balsaraet al. (2013) we presented the first truly multidimensional Riemann solvers for hydrodynamics and MHD. Such a RS resides at the vertices of a mesh. It accepts as input all the four states that surround that vertex, see Fig. 2. Fig. 2 shows a space-time diagram for the waves that emanate from that vertex in a multidimensional RS. The multidimensional RS produces two multidimensionallyupwinded fluxes. Note that the RS is approximate with the result that it approximates the best possible evolution of a Monge cone in multiple dimensions. The wave-model is self-similar in space-time, consistent with our physical expectation. It is also consistent with the conservation law and the principle of entropy generation at shocks. The multi-d RS is cost-competitive with one-dimensional RS.The article by Balsara (2012) includes video clips introducing the multidimensional HLLC RS, which makes the topic much more accessible. Fig. 3 shows a comparison of the older method of Gardiner & Stone (2005) vis a vis the methods in Balsara (2010,2012) on a test problem that was proposed by the former authors. From Fig. 3b we see that use of the multidimensional RS enables larger timesteps, more isotropic propagation of the flow features and a reduction of the dissipation that causes smeared solutions in Fig. 3a.

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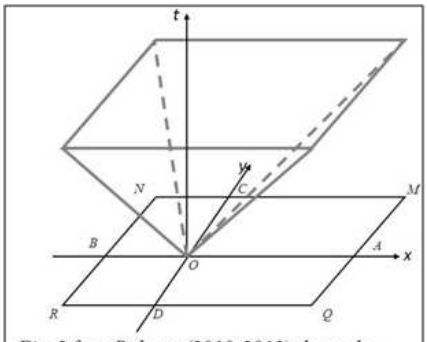
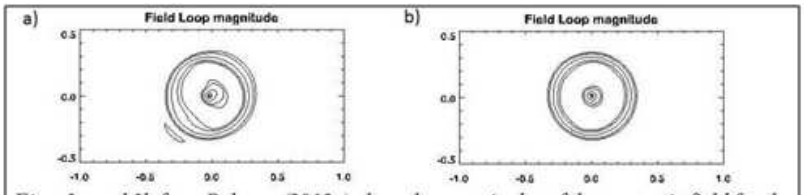


Fig. 2 from Balsara (2010, 2012) shows the wave model that we adopt for the propagation of waves in two space dimensions and one temporal dimension. The four zones, with their corresponding solutions lie in each of the four quadrants of the xy-plane. Points in space-time that are contained within the inverted pyramid, belong to the strongly interacting state where the four states interact strongly with each other.



Figs. 3a and 3b from Balsara (2012a) show the magnitudes of the magnetic field for the field loop advection problem after it has executed one complete orbit around the computational domain. Fig. 3a is based on conventional second order Godunov methods with Gardiner & Stone's (2005) suggestion for doubling the dissipation of the electric field. Fig. 3b presents the results from the multidimensional HLLC Riemann solver-based scheme without any dissipation doubling.

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Perspectives on preservation of physical properties through optimization

Pavel Bochev
(joint work with D. Ridzal, K. Peterson, M. Shashkov)

Discretization reduces an infinite-dimensional problem to a finite algebraic model that can be solved on a computer. This results in *structural* and *qualitative* information losses in the algebraic model. The former lead to unstable, ill-posed discrete equations, whereas the latter cause violations of physical properties such as maximum principles, local bounds, symmetries, and involutions.

For the past 20 years research in compatible discretizations has focused on the preservation of the *formal structures* of mathematical models. Using ideas and tools from vector calculus, algebraic topology and differential forms, researchers were able to develop compatible discretizations that excel in managing structural information losses and lead to stable numerical methods for partial differential equations (PDEs); see [1, 2, 3, 13, 22] and the references therein.

In contrast, development of numerical methods, which preserve qualitative solution properties lags behind despite the importance of this task. Qualitative information losses can be tolerated in single physics codes but not in coupled multiphysics simulations where the outputs from one component provide the inputs for the other components. A standard ad hoc approach that is still widely practiced is to brute force discrete solutions into physically meaningful ranges, thereby reducing solution accuracy in ways that cannot be rigorously quantified.

Direct methods for the preservation of physical properties require special grids and reconstruction operators, or nonlinear modifications of the discrete equations. Typically, such methods tie together the preservation of the desired properties with

geometric conditions on the mesh and/or restrictions on the accuracy. A classic example is the discrete maximum principle (DMP) for the Poison equation, which requires a monotone, or M-stiffness matrix. To ensure this property on triangular elements the sum of the two angles opposing each interior edge should be less than π, and the polynomial degree should be 1 [12, 14, 24]. Extension of DMP to more general triangular or quadrilateral grids requires *nonlinear* schemes [16] such as the nonlinear stabilized finite element method for the Poisson equation [11, 10], the nonlinear extension of the diamond scheme [5], and the nonlinear finite volume scheme in [19]. High-order maximum-principle satisfying and positivity preserving schemes for conservation laws exist in one dimension [27], or on rectangular grids [25, 26]. Their extension even to triangular elements are highly nontrivial [23].

A similar interdependence between mesh, accuracy and preservation of a physical property exists in many of the slope and flux limiters in use today. As a result, many of them do not preserve linear functions on irregular grids [4], which impacts accuracy and robustness. This interdependence is propagated to any algorithm that employs limiters such as advection-based remappers. Because ALE grids are highly unstructured, the alternative to limiters is to rely on sophisticated "repair" procedures [17] or error compensation algorithms [21], which fix the out-of-bound values and maintain positivity, but obscure the sources of the discretization errors.

This talk summarizes our recent efforts to develop an alternative, optimization-based *divide-and-conquer* strategy [7, 6, 9, 8] for the formulation of stable, accurate and physically consistent discretizations. Our main focus is on the application of optimization and control ideas to separate stability and accuracy considerations from the enforcement of the physical properties. Given a mathematical model and a list of desirable physical properties, our approach seeks the corresponding discrete model in the form of a constrained optimization problem in which

- the objective is to minimize the distance, measured in some suitable norm, between the discrete solution and a given *target* solution;
- a discrete model that is *stable and accurate* but is not expected to possess all desired physical properties defines the target solution;
- the optimization constraints *enforce* any desired physical properties that are not already present in the target solution.

This strategy offers a number of important theoretical and computational advantages in the formulation of feature-preserving numerical methods:

- the numerical solution is a global optimal solution from a feasible set defined by the desired physical properties, i.e., it is always the best possible, with respect to the target, approximate solution that also possesses these physical properties;
- the decoupling of the target definition from the preservation of the physical properties allows one to adapt the numerical solution to different problems by choosing the most appropriate target definition and objective function for these problems;

- the enforcement of the desired properties as optimization constraints is impervious to the mesh structure and/or field representations, thereby enabling feature-preserving methods on arbitrary unstructured meshes, including polygonal and polyhedral meshes.

In tis talk we apply the optimization-based strategy to the high-order accurate and feature-preserving remap (constrained interpolation) and transport (advection) of a single scalar conserved quantity ("mass"). The features that we aim to preserve through the use of optimization are (a) the conservation of total mass and (b) physically motivated local bounds on the primitive variable (the density).

The remap task arises in Arbitrary Lagrangian-Eulerian (ALE) methods, where high-order remapping between meshes is critical for the accuracy of the simulation, especially in conjunction with a *continuous rezone* approach, which requires remapping at every time step [21, 17]. The second task, i.e., the stable, accurate and feature-preserving solution of transport equations on general unstructured meshes, remains one of the most challenging numerical problems. This talk exploits the intrinsic connection between transport and incremental remapping [15, 20, 18] to extend the optimization-based remap to conservative, linearity and local bounds preserving transport algorithms.

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Geometric structures underlying mimetic approaches: Towards an extension of the latter to magnetoelasticity

Alain Bossavit

Mimetic methods, in Electromagnetics, replace 3D-space by a finite element mesh and classical differential operators such as grad, rot, div, by matrices that describe the topology of the mesh, in a consistent way (mobilizing some notions of cohomology and differential geometry). They neatly separate "pre-metric" features of the theory from constitutive laws (expressed as Hodge operators, which encapsulate metric properties). The end-result of this process is a system of two interlocked networks, one electric, one magnetic, talking to each other, respectively based on the primal mesh and on its dual.

"Consistent" is the keyword in this brief description. When discretizing, say, rot $A = B$ for a magnetostatics application, simply representing the fields A and B by arrays of node-based vectors, and using the equation to derive relations between components of these vectors, will not do. This would ignore the different physical natures of A and B, meant to be integrated, respectively, along lines (to provide the time-integral of an electromotive forces) and over surfaces (to deliver an induction flux). A differential-geometric approach helps realize that vector fields A and B, there, are just proxies for more fundamental objects, namely differential forms, of degrees 1 and 2 respectively, whose degrees of freedom should be assigned to appropriate integral domains, that is, edges and faces of the finite-element mesh – *not* nodes. It also reveals the real nature of constitutive coefficients such as ϵ, μ, and σ (conductivity): They are in fact *operators*, of the kind known as "Hodge star operator" in differential geometry.

The systematic development of such ideas leads to the discretization *as a whole* of the framework of geometric objects in which Maxwell equations live. Hence a discrete, computer-compatible framework, in which discrete equations can be formulated. These (as implied by the word "mimetic") automatically share with the Maxwell equations such essential properties as electric charge conservation, flux conservation, etc., expressed in terms of discrete entities. All "premetric" features of electrodynamics thus find their discrete equivalents, in a natural way.

Discretizing the constitutive relations (the "metric" aspects of the theory), on the other hand, is less systematic. From the present point of view, this amounts to replacing the Hodge operator by a discrete analogue. This problem is solved in different ways by various mimetic methods ("cell method", "finite integration technique", Galerkin discretization via edge elements, volume elements, etc.). But they all require a convergence proof, which in turn requires a way to compare the solution of the discrete model with the exact solution. In all methods, therefore, one must be able to pass from an array of degrees of freedom to a field: Whitney forms, familiarly known as "edge elements" and "face elements", do this. They are to differential forms what ordinary nodal finite elements are to functions. The discrete framework, once established, can be used as a discretization toolkit thanks to which various, equivalent discretized systems can be built.

Can this methodology be applied to other equations, often coupled with Maxwell's, such as elastodynamics? Analogies help, there. One can present elastodynamics in a way much similar to electromagnetics if strain and stress are considered (with minor departures from the tradition of Mechanics) as, respectively, a vector-valued 1-form ϵ and a twisted covector-valued 2-form σ. Strain ϵ describes the difference between the actual placement and the reference placement of a given material vector (without compatibility conditions being necessarily enforced). Stress σ gives the flux of momentum across a material bivector (and hence, by integration, through any surface). This way, coupled equations for electrodynamics and elastodynamics are (with d for the exterior derivative):

$$-\partial_t d + \mathrm{d}h = j,\ \partial_t b + \mathrm{d}e = 0, \qquad \partial_t p - \mathrm{d}\sigma = f,\ -\partial_t \epsilon + \mathrm{d}v = 0,$$

where p (a twisted covector-valued 3-form) is the momentum density and v (a vector field, but here considered as a vector-valued 0-form) is the material velocity. The current density j and the applied force f are given source terms.

These equations being formally similar, the mimetic machinery can be activated, to produce a finite-dimensional dynamical system that mimics the coupled elasto-electro-dynamic one. But going this way makes one reconsider some basic issues about coupled problems.

In more traditional approaches, a central role is assigned to the concept of "magnetic force" (let's neglect electrostatic forces in this abstract). One is supposed to solve the Maxwell equations first (possibly, at each timestep), then to compute the forces, and finally, adding these forces to the given ones (the f in the above display), to proceed with the evolution of the elastic compartment of the system. But there is an embarrassing variety of *non-equivalent* force formulas in the literature: "Helmholtz force", "Kelvin force", "Maxwell force", etc., to say nothing of the Maxwell tensor: Which is right?

The talk addressed this issue and, by using the virtual power principle, derived the right formula in a few basic cases (isotropic or anisotropic reluctivity, dependent or not on local strain, hard magnets), to conclude as follows: Local force is not a void concept, and the search for the force *field* in magnetized matter is legitimate. But the idea that it could be derived from a knowledge of the electromagnetic field *alone* is wrong. Full knowledge of the coupled constitutive laws is needed.

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Coordinate free finite volume method for the shallow water system over the sphere with arbitrary grid

François Bouchut
(joint work with Robert Eymard, Hassan Fahs)

The shallow water system over the sphere is deduced from the incompressible Euler equations in a shallow three dimensional domain around the sphere. It describes atmospheric or oceanic flows over the earth. For these applications one has to include the topography as a small perturbation of the spherical geometry, and the Coriolis force. The position on the sphere is denoted by $x \in \mathbb{R}^3$, $|x| = R$, and the system is

$$\text{(1)} \qquad \begin{cases} \partial_t h + \nabla_x \cdot (hu) = 0, \\ \partial_t u + u \cdot \nabla_x u + |u|^2 \frac{x}{R^2} + g \nabla_x (h + B) = -2 \left(\frac{x}{R} \cdot \vec{\Omega} \right) \frac{x}{R} \times u, \end{cases}$$

where $h(t,x) \geq 0$ is the width of the layer, $u(t,x)$ is the velocity, $g > 0$ is the gravity, $B(x)$ is the topography, and $\vec{\Omega}$ is the constant angular velocity. The differential operators are the intrinsic ones related to the differential structure of the two-dimensional sphere, they are described for example in [10]. The classical simplified form of the Coriolis force is considered here, while in [10] the full Coriolis force is taken into account.

The special feature of (1) is that the velocity field $u(t,x)$ has to remain *tangent* to the sphere at each point, i.e. $u(t,x) \cdot x = 0$. This involution constraint of geometric nature induces several difficulties at the numerical level:

- For "planar" nonlinear hyperbolic systems, constant initial data give rise to constant (and steady) solutions. It is not the case in spherical geometry. In particular, eventual discontinuities split the solution in *pieces of smooth solutions that are never constant.*
- The notion of constant or piecewise constant value has no meaning for the field u, since u must be *tangent at each point.*
- For u tangent to the sphere at each point, the integral $\int_\Omega u\,dx$ *is tangent at no point* (warning: here we consider the integral of the vector u valued in $\mathbb{R}^3$, and not the integral of its components in a rotating frame).

What is usually done in this context is to use a special coordinate system, that enables to write a quasilinear system with *space variable coefficients.* This is done in [9, 7, 4, 5, 3, 2, 1]. However, this induces some fundamentel limitations:

- Singularities (at the poles), matching of different coordinate systems, which lead to particular treatments (complexity, eventual loss of accuracy, eventual instabilities, increase of computational cost)
- Limitation to a particular grid (and hence difficulty to adapt the grid to data with particular geometry)

In this work I explain how it is possible to formulate intrinsic finite volume methods for the shallow water system over the sphere over arbitrary grid, taking into account the curvature, and the source terms.

The method uses the ideas developed by the "well-balanced" community, and all the source terms are distributed at the interfaces between cells. There a one dimensional solver resolves the waves, taking into account the sources, in a well-balanced and consistent manner. The interest of the approach is that it is possible to prove an entropy inequality satisfied by the scheme, for arbitrary meshes. Numerical tests are performed, including the extension to second-order, using analytic solutions provided in [11, 6, 8].

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Constraint preservation in Maxwell-Klein-Gordon and related equations

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(joint work with Tore G. Halvorsen)

The Maxwell-Klein-Gordon equation is a nonlinear PDE which couples an electromagnetic field to a scalar (complex valued) one. The scalar field gives a current which the electromagnetic field can see through Maxwell's equations. The electromagnetic field is described by scalar and vector potentials, and these enter the

coefficients of the wave equation that the scalar field should satisfy. The Maxwell-Klein-Gordon equation are Euler-Lagrange equations coming from a variational principle for a certain Lagrangian. This (coupled) evolution equation preserves two constraints on the Cauchy data: at any time, the magnetic field is divergence free, and the divergence of the electric field is the charge density defined by the scalar field (Gauss law). Though similar in appearance, these constraints have quite different interpretations. The first constraint is a Bianchi identity for the vector potential. The second constraint is one of the Euler Lagrange equations. That it is preserved by the flow of the other Euler-Lagrange equations (which are evolution equations) can be deduced from Noether's theorems. These assert that to any group action leaving the Lagrangian unchanged correponds a conservation law, expressing a differential relation between the Euler-Lagrange equations. The MKG Lagrangian is invariant under gauge transformations and the corresponding conservation law gives preservation of Gauss law.

Lattice Gauge Theory is a discretization developed by Kenneth Wilson for the purposes of quantum field theory, which mimicks these structures. In [4] we gave a first analysis from the point of view of numerical analysis. The underlying space of fields is tensorproduct Whitney forms for the vector and scalar potentials, which guarantees that a Bianchi identity holds. A discrete Lagrangian (or at least an action) is constructed, which is invariant under certain discrete gauge transformations. A discrete Noether theorem then guarantees that a discrete Gauss law also holds.

These results can be compared with a pure finite element method, in which the continuous action is restricted to the finite element space. As it turns out the finite element space is not invariant under nontrivial gauge transformations, and simulations show a considerable drift in Gauss law, so that in effect electric charge is not conserved. Nevertheless we could achieve both constraint and energy conservation in a fairly explicit scheme by a non-standard application of Lagrange multipliers [1]. This technique could be generalized [2] to a large class of wave-like equations coming from a variational principle, with an action invariant under some group. Constraint and energy preservation (combined with, in particular, Kato's inequality) gave enough a priori estimates to be able to conclude convergence [3]. In LGT one redefines both the discrete gauge transformations and the discrete action. The latter is then a variational crime compared with the the finite element method.

The LGT formalism was initially developed for cubical grids, for the full Yang-Mills-Higgs equations. In [5] we generalized it to unstructured simplicial grids, interpreting the method as a variational crime on Lie-algebra valued Whitney forms. Also, a discrete Noether's theorem could be developed in this setting, which is sufficiently general to prove discrete charge conservation.

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On of some multidimensional formulations of ideal MHD

Bruno Després

The system of ideal magnetohydrodynamics is

$$\left\{\begin{array}{l} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot \left(\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I} + \frac{|\mathbf{B}|^2}{2\mu_0} \mathbf{I} - \frac{\mathbf{B} \otimes \mathbf{B}}{\mu_0} \right) = 0, \quad \mu_0 = 4\pi, \\ \partial_t (\rho e + \frac{|\mathbf{B}|^2}{2\mu_0}) + \nabla \cdot \left(\rho \mathbf{u} e + p \mathbf{u} + \frac{(\mathbf{u} \wedge \mathbf{B}) \wedge \mathbf{B}}{\mu_0} \right) = 0, \\ \partial_t \mathbf{B} - \nabla \wedge (\mathbf{u} \wedge \mathbf{B}) = 0. \end{array}\right.$$

The entropy law can be used to check the non linear structure

$$\partial_t (\rho S) + \nabla \cdot (\rho S \mathbf{u}) = - \frac{(\mathbf{B}, \mathbf{u})}{\rho T} \nabla \cdot \mathbf{B},$$

where the physical entropy per unit mass is $S\, TdS = d\varepsilon + pd\tau, \varepsilon = e - \frac{1}{2} |\mathbf{u}|^2, \tau = \frac{1}{\rho}$. For perfect gas $S = \log \left(\varepsilon \tau^{\gamma - 1} \right)$ and $p = (\gamma - 1) \rho \varepsilon$. The system is "only" weakly hyperbolic (Powell). But "of course" the involutive constraint must be added: $\nabla \cdot \mathbf{B} = 0$. All this has impact on the stability of numerical methods: see [2, 3] and many other contributions in the literature. These issues show that the interaction of the entropy with the free divergence of the magnetic fields is key tool to analyze the structure of this system. It also questions the possibility of having a re-formulation of ideal MHD such that the entropy law is independent of the divergence of the fields.

We first describe a first formal modification of this system that was proposed in [1]. The magnetic is decoupled in two parts: $\mathbf{B}$ and $\mathbf{C}$

$$\left\{\begin{array}{l} \partial_t \rho + \nabla . \rho \mathbf{u} = 0, \\ \partial_t \mathbf{B} + \nabla (\mathbf{u} \otimes \mathbf{B} - \mathbf{C} \otimes \mathbf{u}) = 0, \\ \partial_t \rho \mathbf{u} + \nabla . (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla P - \nabla . \frac{\mathbf{C} \otimes \mathbf{B}}{\mu} = 0, \\ \partial \rho e + \nabla . \left(\rho \mathbf{u} e + P \mathbf{u} - \frac{1}{\mu} \mathbf{C} (\mathbf{B}, \mathbf{u}) \right) = 0, \end{array}\right.$$

where $\mathbf{C}$ is any free-div vector field. This system is endowed with the entropy law $\partial_t (\rho S) + \nabla \cdot (\rho S \mathbf{u}) = 0$ for all free-div $\mathbf{C}$. The discretization of $\mathbf{C}$ can performed with a specific discretization $\partial_t \mathbf{C} - \nabla \wedge (\mathbf{u} \wedge \mathbf{C}) = 0$.

A second possibility [4] to rewrite the system in a form with an interesting structure is as follows. The Euler-Lagrange mapping writes $\mathbf{x}'(t) = \mathbf{u}, \qquad \mathbf{x}(0) =$

$\mathcal{X}$. The deformation gradient is $\mathbf{F} = \nabla_{\mathcal{X}}\mathbf{x} \Rightarrow D_t\mathbf{F} = \nabla_{\mathcal{X}}\mathbf{u}$ where $D_t = \partial_t + \mathbf{u}\cdot\nabla = \partial_{t|\mathcal{X}}$ is the material (Lagrangian) derivative. For all vector fields $\mathbf{G}$, one has the formula

$$J\nabla_{\mathbf{x}} \cdot \mathbf{G}^t = \nabla_{\mathcal{X}} \cdot \left(\mathbf{G}^t \mathrm{cof}\,(\mathbf{F})\right)$$

where: $J = \det(\mathbf{F}) = \frac{\rho_0}{\rho}$; and $\mathrm{cof}\,(\mathbf{F})$ is the comatrix, that is the matrix of the cofactors; $\mathrm{cof}\,(\mathbf{F}) = \frac{\mathbf{F}^t}{\det(\mathbf{F})}$. This Piola formula is true in the weak sense in nD. So $\nabla_{\mathcal{X}} \cdot (\mathbf{B}^t \,\mathrm{cof}\,(\mathbf{F})) = 0$. It is an additional free-divergence constraint in the variable $\mathcal{X}$. After inspection of the equation one can find the involution relation $D_t\left(\mathrm{cof}\,(\mathbf{F})^{\mathrm{t}}\,\mathbf{B}\right) = 0$, which corresponds to the frozen in law; the magnetic flux across a Lagrangian surface is constant. Define a new vector $\mathbf{C} = \mathrm{cof}\,(\mathbf{F})^{\mathrm{t}}\,\mathbf{B}$ such that $D_t\mathbf{C} = 0$. The magnetic field is function of $\mathbf{C}$ and of the deformation gradient $\mathbf{F}$

$$\mathbf{B} = \mathrm{cof}\,(\mathbf{F})^{-\mathrm{t}}\,\mathbf{C} = \frac{\mathbf{FC}}{\det(\mathbf{F})}.$$

In view of the hyperelastic formulation of material strength it is natural to introduce the potential

$$\varphi^M(\mathbf{F}, S, \rho_0, \mathbf{C}) = \varepsilon_g\left(\frac{\det(\mathbf{F})}{\rho_0}, S\right) + \frac{|\mathbf{FC}|^2}{2\rho_0\mu_0\det(\mathbf{F})}.$$

At the end of the analysis φ^M is the internal energy $e = \frac{1}{2}|\mathbf{u}|^2 + \varphi^M(\mathbf{F}, S, \rho_0, \mathbf{C})$. It is also natural to define the magnetic Piola-Kirchhoff stress tensor $\sigma^M = \rho_0\nabla_{\mathbf{F}}\varphi^M$. One can prove the identity

$$\sigma^M = -\left(p\mathbf{I} + \frac{|\mathbf{B}|^2}{2\mu_0}\mathbf{I} - \frac{\mathbf{B}\otimes\mathbf{B}}{\mu_0}\right)\mathrm{cof}\,(\mathbf{F}).$$

All this analysis allows to write the lagrangian formulation of ideal MHD under the form

$$\begin{cases} D_t\rho_0 = 0, \\ D_t\mathbf{C} = 0, \\ D_t\mathbf{F} = \nabla_{\mathbf{X}}\mathbf{u}, \\ D_t(\rho_0\mathbf{u}) = \nabla_{\mathbf{X}} \cdot \left(\rho_0\nabla_{\mathbf{F}}\varphi^M\right), \\ D_t(\rho_0 e) = \nabla_{\mathbf{X}} \cdot \left(\rho_0\mathbf{u}^t\nabla_{\mathbf{F}}\varphi^M\right). \end{cases}$$

This structure is exactly the one of a lagrangian hyperelastic model in non linear elasticity with the correspondence

$$\begin{cases} \text{Magnetic:} & \varphi^M = \varepsilon_g(\rho, S) + \frac{|\mathbf{FC}|^2}{2\rho_0\mu_0\det(\mathbf{F})}, \\ \text{Hyperelastic:} & \varphi = \psi(i_1, i_2, i_3, S, \rho_0) \end{cases}$$

where $i_1 = \lambda_1+\lambda_2+\lambda_3$, $i_2 = \lambda_1\lambda_2+\lambda_2\lambda_3+\lambda_3\lambda_2$ and $i_3 = \lambda_1\lambda_2\lambda_3$ and λ_j eigenvalue of the Finger Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^t\mathbf{F}$.

Proposition: *Assume $\partial_S\varphi_g \neq 0$ and $\rho_0 > 0$. One has the entropy property $D_tS = 0$ for smooth solutions,* **without any free divergence constraint**. *The proof is more or less elementary.*

It is an open problem to understand the role of this structure in numerical calculations, and to determine wether it could have an influence on the stability of Riemann solvers for ideal MHD.

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High Order One-Step AMR and ALE Methods for Hyperbolic PDE

Michael Dumbser
(joint work with W. Boscheri, A. Hidalgo, O. Zanotti)

In this talk we present two recent extensions of the high order accurate one-step $P_N P_M$ approach first introduced in [13, 14]: one extension concerns the use of space-time adaptive Cartesian meshes (AMR) together with high order time accurate local time stepping (LTS), see [18] and [19]; the other extension concerns high order one-step schemes on moving unstructured meshes using the direct Arbitrary-Lagrangian-Eulerian (ALE) framework, see [20, 5, 21].

The nonlinear system of time-dependent governing PDE is considered to be of the form

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{Q}, \nabla \mathbf{Q}) + \mathbf{B}(\mathbf{Q}) \cdot \nabla \mathbf{Q} = \mathbf{S}(\mathbf{Q}), \tag{1}$$

where $\mathbf{Q}$ is the state vector, $\mathbf{F}$ is the nonlinear flux tensor, $\mathbf{B}(\mathbf{Q}) \cdot \nabla \mathbf{Q}$ is a non-conservative term and $\mathbf{S}(\mathbf{Q})$ is an algebraic source term, that is also allowed to be stiff.

The common building blocks in both numerical approaches (AMR and ALE) are i) a high order non-oscillatory WENO reconstruction operator; ii) a local space-time Galerkin predictor method that evolves the spatial reconstruction polynomials in time within each element by solving local Cauchy problems *in the small*. For this purpose, the PDE is written in a weak variational form in space-time, which also allows a proper high order accurate discretization of stiff source terms, see [16, 17]; iii) the final one-step schemes are derived by integration over space-time control volumes. In the case of ALE the space-time control volumes are moving and the local mesh velocity can be chosen independently of the fluid velocity.

Furthermore, in the context of cell-centered ALE methods, the computation of the mesh velocity requires the solution of multi-dimensional Riemann problems, or something equivalent [4]. Several approaches are possible: i) either a simple arithmetic average of the vertex-extrapolated velocities in all elements adjacent to that vertex, see [8, 24]; ii) or the use of a node-solver as suggested by Després and

Mazeran [11, 12] and Maire et al. [26, 25]; iii) or the use of a multi-dimensional HLL-type Riemann solver, as recently proposed by Balsara in [2, 3].

The non-conservative products are discretized by a path-conservative approach [6, 27, 15, 22, 23] that defines the jump terms on the element boundaries following the theory of Dal Maso, Le Floch and Murat [9]. For a further discussion of the topic see [1] and [7].

In the talk we present applications to the Newtonian equations of viscous and resistive magnetohydrodynamics (MHD) as well as to the ideal and resistive relativistic MHD equations (RMHD). In both numerical approaches presented in this talk, the involution associated with the PDE, namely the divergence constraint on the magnetic field, is taken into account on the discrete level using the hyperbolic generalized Lagrangian multiplied (GLM) approach proposed by Dedner et al. [10].

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Time implicit schemes for the JOREK MHD code: Newton procedure, continuation and preconditioning

Emmanuel Franck
(joint work with M. Hölzl, E. Sonnendrücker)

In the context of the ITER magnetic fusion project it is important to simulate the behavior of edge instabilities in the Tokamak. Indeed these disruptive instabilities can damage wall components due to their extremely high energy transfer rate. Consequently, it is essential to estimate the amplitude of these instabilities and understand how control these.

To simulate this phenomena, we use a 3D reduced MHD code in cylindrical geometry named Jorek. The full model is the resistive MHD equations:

$$
(1) \qquad \begin{cases} \partial_t \rho + \nabla.(\rho \mathbf{v}) = \nabla.(D_{||}\nabla_{||}\rho + D_\perp \nabla_\perp \rho) \\ \rho \partial_t \mathbf{v} + \rho \mathbf{v}.\nabla \mathbf{v} + \nabla(\rho T) = \mathbf{J} \times \mathbf{B} + \nu \triangle \mathbf{v} \\ \rho \partial_t T + \rho \mathbf{v}.\nabla T + (\gamma - 1)\rho T \nabla \mathbf{v} = \nabla.(K_{||}\nabla_{||} T + K_\perp \nabla_\perp T) \\ \partial_t \mathbf{B} = \nabla \times (\mathbf{v} \times \mathbf{B}) - \nabla \times \eta \mathbf{J} \\ \nabla.\mathbf{B} = \mathbf{0} \end{cases}
$$

with ρ the density, $\mathbf{v}$ the velocity, T the temperature, $\mathbf{B}$ the magnetic field, $\mathbf{J} = \nabla \times \mathbf{B}$ the current and $D_{||}$, $D_\perp$, $K_{||}$, $K_\perp$ are anisotropic diffusion tensors.

To obtain the reduced MHD models ([10]-[11]) discretized in the code, we define the fields with a formulation of $\mathbf{v}$ and $\mathbf{B}$ based on potentials (useful to preserve the involution constraint $\nabla \cdot \mathbf{B} = 0$). It is defined by $\mathbf{B} = \frac{F_0}{R}\mathbf{e}_\phi + \frac{1}{R}\nabla\Psi \times \mathbf{e}_\phi$ and $\mathbf{v} = -R\nabla u \times \mathbf{e}_\phi + v_{||}\mathbf{B}$ with u the electrical potential, Ψ the poloidal magnetic flux and the parallel velocity $v_{||}$. Plugging these formulations of the fields in the equations and projecting the momentum equation in the toroidal direction and in the poloidal plane we obtain the reduced models.

The poloidal plane is discretized using cubic Bezier finite elements and the toroidal plane is discretized using Fourier expansion. For the time discretization we use an implicit method based on an inexact Newton procedure [5]-[6] coupled with a Crank Nicholson scheme. The linear system is preconditioned with a left preconditioning. The preconditioning operator P corresponds to the approximation of the Jacobian where the coupling terms between the Fourier modes are neglected. In the nonlinear phase where the modes are strongly coupled this method is not very efficient. We propose different ways to obtain better preconditioning.

The first way is to use a continuation method to compute an adapted initial guess for the Newton procedure. We consider the nonlinear system $R(\mathbf{U}) = 0$ hard to solve. The idea is to replace this system by the system $F(\mathbf{U}, \alpha) = 0$ more easy to solve with $F(\mathbf{U}, \alpha = 0) = R(\mathbf{U})$. To obtain a well-conditioned system we propose to use $F(\mathbf{U}, d) = R(\mathbf{U}) + \alpha D(\mathbf{U})$ with D a diffusion operator. The algorithm is

- **Algorithm**
- Set $\alpha_0 = \alpha_{max}$ and $R_0 = R(\mathbf{U}^0)$
- For $i = 1, 2, 3....$ do
  - Set $F_0 = F(\mathbf{U}^i, \alpha_i)$
  - For $n = 1, 2, 3..n_{max}$ do
    - Compute residual $R(\mathbf{U})$
    - if $||R(\mathbf{U})|| \leq \epsilon_1 ||R_0||$ then done
    - Compute homotopy map $F(\mathbf{U}, \alpha_i)$
    - if $||F(\mathbf{U})|| \leq \epsilon_2 ||F_0||$ then exit loop
    - Inexact Newton step: find $\delta\mathbf{U}$ such as $||A\delta\mathbf{U} + F|| \leq \eta F$.
    - $\mathbf{U} = \mathbf{U} + \delta\mathbf{U}$ and end for
  - set $\alpha_{i+1} < \alpha_i$

The second is to use a preconditioning method based on a splitting + parabolization procedure [1]-[2]-[3]-[4]. Indeed the hyperbolic coupling terms unlike parabolic equations cannot be efficiently solved with multigrid methods. The idea is to use a right preconditioning where operator P is obtained by splitting the diffusion terms and the hyperbolic coupling terms which are parabolized. For example we study the implicit scheme for wave equation:

$$\left\{ \begin{array}{l} \partial_t u = \partial_x v \\ \partial_t v = \partial_x u \end{array} \right. \longrightarrow \left\{ \begin{array}{l} u^{n+1} = u^n + \Delta t \partial_x v^{n+1} \\ v^{n+1} = v^n + \Delta t \partial_x u^{n+1} \end{array} \right.$$

Assuming that the matrix associated to the previous linear system is

$$\left(\begin{array}{cc} D_1 & U \\ L & D_2 \end{array} \right) = \left(\begin{array}{cc} I & -\Delta t \partial_x \\ -\Delta t \partial_x & I \end{array} \right)$$

Using a Schur decomposition we obtain

$$\left(\begin{array}{cc} D_1 & U \\ L & D_2 \end{array} \right) = \left(\begin{array}{cc} I & -\Delta t \partial_x \\ 0 & I \end{array} \right) \left(\begin{array}{cc} P_{schur} & 0 \\ 0 & I \end{array} \right) \left(\begin{array}{cc} I & 0 \\ -\Delta t \partial_x & I \end{array} \right)$$

The first and third matrices are triangular so easily to invert and $P_{schur} = D_1 - UD_2^{-1}L = (1 - \Delta t^2 \partial_{xx})$ is well-conditioned. To finish we can solve $P\delta\mathbf{U} = -R(\mathbf{U})$ with P the preconditioning operator using the operators P_{schur} and D_1 preconditioned with multigrid methods. This method will be applied to the reduced MHD introducing in Jorek using some algebraic manipulations on the equations and some approximation to compute the Schur complement.

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Hyperbolicity in hyperelasticity and applications to high velocity impact problems

Sergey Gavrilyuk
(joint work with Nicolas Favrie, Serge Ndanou)

The equations of motion for hyperelastic materials are hyperbolic, if the specific energy e is a rank-one convex function of the deformation gradient $\mathbf{F}$ (see, for example, [1]). In statics, the condition of rank-one convexity is also called "strong ellipticity" condition [2], [3]. This condition is not easy (almost impossible) to check even in the case of isotropic elastic materials, where the specific energy depends only on the invariants of the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ or the left Cauchy-Green deformation tensor $\mathbf{B} = \mathbf{F}\mathbf{F}^T$.

An alternative approach to the hyperbolicity study was proposed in [4], [5]. It consists in rewriting the equations of isotropic elastic materials into a symmetric t-hyperbolic in the sense of Friedrichs system. Such a transformation allows us to assure hyperbolicity of the governing equations and to calculate the eigenvalues in terms of symmetric matrices. This approach is also not direct. Indeed, to perform such a transformation, we need to present the internal energy as a function of $\mathbf{F}$, the cofactor matrix $cof\mathbf{F}$, the solid density ρ and the specific entropy η. We obtain then additional compatible equations for $cof\mathbf{F}$ and ρ, and symmetrize this augmented system. The convexity of the energy with respect to the augmented variables will guarantee the hyperbolicity of the governing equations. This approach is quite opaque. Indeed, in practice, we have the energy obtained from experimental data. It is given in terms of the singular values of $\mathbf{F}$ and the entropy η. However, there is no rational way to "play" with this energy by transforming it to a convex function of augmented arguments.

In the numerical treatment of mathematical models of elastic-plastic solids one usually uses a splitting procedure : the "elastic" step is followed by the "plastic"

relaxation step [6], [7], [8], [9]. It is necessary to assure the hyperbolicity condition at each "elastic" step. Indeed, the hyperbolicity is necessary for the wellposdness of the Cauchy problem and the corresponding numerical Godunov-type methods.

We will consider the Eulerian formulation of the hyperelasticity for isotropic solids. These equations are invariant under rotation group $SO(3)$. The consequence of that are immediate : for hyperbolicity it is sufficient to consider only 1D case. Indeed, the normal characteristic direction can always be transformed by rotation to the one of Cartesian basis vectors (we have to use three composed rotations defined by the Euler angles between the Cartesian basis and a natural local basis on characteristic surface). So, the problem to assure the hyperbolicity of the one-dimensional system for arbitrary strains and shears becomes the basic one. This 1D problem stays complex because the number of unknowns involved in such a formulation is large (14 scalar partial differential equations for $\mathbf{F}$, ρ, η and the velocity field $\mathbf{v}$).

We will concentrate on a particular class of elastic materials described by a stored energy e in separable form :

$$e = e^h\left(|\mathbf{G}|, \eta\right) + e^e\left(\mathbf{g}\right).$$

Here $\mathbf{G} = \mathbf{B}^{-1}$ is the Finger tensor, $\mathbf{g} = \mathbf{G}\,|\mathbf{G}|^{-1/3}$, and $|\mathbf{G}|$ is the determinant of $\mathbf{G}$. The choice of the Finger tensor is more natural for the Eulerian description of isotropic solids. The energy $e^h\left(|\mathbf{G}|, \eta\right)$ is the hydrodynamic part of the energy, depending only on the determinant of $\mathbf{G}$ and the entropy η, and $e^e\left(\mathbf{g}\right)$ is the shear elastic energy. The shear part of the energy is unaffected by the volume change. Such a decomposition into purely volumetric and isochoric deformation is, in particular, useful for description of nearly incompressible isotropic hyperelasticity. This implies that the Cauchy stress tensor is also in separable form :

$$\sigma = -p\mathbf{I} + \mathbf{S},$$

where p is the pressure calculated only by the hydrodynamic part of the energy, $\mathbf{I}$ is the identity tensor, and the deviatoric part $\mathbf{S}$ is calculated only by the shear energy. Under a classical hypothesis about the pressure behavior (the hydrodynamic sound speed should be positive), we reduce the problem of hyperbolicity to a simpler one : show that a symmetric 3x3 matrix (determined in terms of e^e) is positive definite on a one-parameter family of unit-determinant deformation gradient compact surfaces. Some explicit forms of the stored energy are formulated which guarantee the hyperbolicity of equations for the motion of hyperelastic materials. This talk is partially based on the paper [10]. Numerical applications to the high velocity impact problems are also discussed.

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Discrete representation of momentum as a covector-valued volume form

Marc Gerritsma

The use of differential forms in which to write physical models and the use of k-cochains to represent such physical models at the discrete level has led to a whole new class of *mimetic* or *structure-preserving* scheme in which the connection with the underlying geometry is explicitly employed, [1, 2, 3, 4, 6, 8, 9, 10, 12, 13, 16, 17, 18, 19]. This approach leads to methods in which fundamental properties of the continuous equations are retained at the discrete level. Despite the success of this approach, the use of differential forms is not sufficient for continuum models such as elasticity and fluid mechanics. In [15] incompressible fluids were simulated with differential forms and conservation of mass could be satisfied up to machine precision. But conservation of momentum, i.e. force balance over volumes, could not be guaranteed.

Momentum – or better still – *momentum density* should be represented by a covector-valued twisted volume form, see [5, 11]. In this description momentum μ is given by $\mu = m^{(1)} \otimes \text{vol}$, where $m^{(1)}$ is a straight 1-form which remains unchanged if the orientation of ambient space is reversed and vol is the twisted volume form which changes sign if the orientation of ambient space is changed.

Differential k-forms can be integrated over k-dimensional point sets and these integrals can be interpreted as k-cochains, but bundle-valued forms such as momentum do not admit integration. These covector-valued volume forms form the dual space of vector fields on the domain Ω, $\mathfrak{X}(\Omega)$. Let $\mu \in \Lambda^1(\Omega) \otimes \Lambda^3(\Omega)$ and $\mathbf{v} \in \mathfrak{X}(\Omega)$, then this duality pairing is given by, [11]

$$\langle \mu, \mathbf{v} \rangle = \left\langle m^{(1)} \otimes \text{vol}, \mathbf{v} \right\rangle := \int_\Omega \left\langle m^{(1)}, \mathbf{v} \right\rangle \text{ vol} \,,$$

where in the integral $\left\langle m^{(1)}, \mathbf{v} \right\rangle$ denotes the *point-wise* duality pairing between a covector, $m^{(1)}$ and a vector $\mathbf{v}$.

This nodal duality pairing suggests that we treat the vector field $\mathbf{v}$ as a *vector-valued* 0-form, i.e. as vectors defined in the nodes of the primal mesh. Likewise, the 1-form $m^{(1)}$ should be associated to nodes on the primal mesh. The precise way in which these geometric concepts are represented on a cell-complex is an active area of research. The time rate of change of momentum should equal the divergence of the stress tensor. A geometric description of the stress tensor can be found in an appendix in the book by Frankel, [7] and in [14]. A discrete representation of the stress tensor in elasticity is given in Yavari, [21]. For an initial attempt for fluid dynamics, see Toshniwal et al., [20].

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High-Order Constrained Transport Methods for the 3D Ideal Magnetohydrodynamic Equations

Christiane Helzel
(joint work with James A. Rossmanith, Bertram Taetz)

In my talk, I presented our recent work [1, 2] on the construction of high-order unstaggered constrained transport methods for the ideal magnetohydrodynamics equations (MHD).

The ideal MHD equations can be written in the form

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho\mathbf{u}\\ E\\ \mathbf{B}\end{pmatrix}+\nabla\cdot\begin{pmatrix}\rho\mathbf{u}\\ \rho\mathbf{u}\mathbf{u}+\left(p+\frac{1}{2}\|\mathbf{B}\|^2\right)\mathbb{I}-\mathbf{B}\mathbf{B}\\ \mathbf{u}\left(E+p+\frac{1}{2}\|\mathbf{B}\|^2\right)-\mathbf{B}\left(\mathbf{u}\cdot\mathbf{B}\right)\\ \mathbf{u}\mathbf{B}-\mathbf{B}\mathbf{u}\end{pmatrix}=0, \qquad \nabla\cdot\mathbf{B}=0, \tag{1}$$

where ρ, $\rho\mathbf{u}$ and E are the total mass, momentum and energy densities, and $\mathbf{B}$ is the magnetic field. The thermal pressure, p, is related to the conserved quantities through the ideal gas law

$$p=(\gamma-1)\left(E-\frac{1}{2}\|\mathbf{B}\|^2-\frac{1}{2}\rho\|\mathbf{u}\|^2\right), \tag{2}$$

where $\gamma=5/3$ is the ideal gas constant.

Our goal is to construct finite volume methods for the MHD equations, which satisfy the divergence free condition for the magnetic field in some appropriate discrete sense. In our approach, this is done by solving, in addition to the MHD equations, an evolution equation for the magnetic potential. Starting with the last line of the MHD equations (1), which can be rewritten in the form

$$\partial_t\mathbf{B}+\nabla\times(\mathbf{B}\times\mathbf{u})=0, \tag{3}$$

we set $\mathbf{B}=\nabla\times\mathbf{A}$, with the magnetic potential $\mathbf{A}\in\mathbb{R}^3$, and obtain

$$\nabla\times\{\partial_t\mathbf{A}+(\nabla\times\mathbf{A})\times\mathbf{u}\}=0.$$

From this, we obtain an evolution equation for the magnetic potential, which has the form

$$\partial_t\mathbf{A}+(\nabla\times\mathbf{A})\times\mathbf{u}=-\nabla\phi, \tag{4}$$

where ϕ is an arbitrary scalar function. In our constrained transport method, we solve the MHD equations (1) as well as the system (4) during each time step. At the end of each time step, the magnetic field is updated by taking the curl of the

magnetic potential. In a method of line approach, we solve both systems during each stage of the Runge-Kutta method and also update **B** during each stage.

Such an approach to discretize the MHD equations was first introduced by Rossmanith [4]. There, he first restricted his considerations to the spatially two-dimensional case, where the evolution equation for **A** reduces to a scalar transport equation of the form

$$\partial_t A^3 + u^1 \partial_x A^3 + u^2 \partial_y A^3 = 0.$$

Thus, in the two-dimensional case, standard methods for hyperbolic problems (not in divergence form) can be used to discretize the evolution equation for the magnetic potential. In [4], a version of the wave propagation algorithm of LeVeque [3] was used. Note that limiting is more subtile in this context. Rossmanith developed a limiting strategy, which suppresses spurious oscillations in derivatives of the magnetic potential and thus in approximations of the magnetic field.

More recently, Rossmanith, Taetz and myself developed related constrained transport methods for the three-dimensional MHD equations, see [1, 2]. In order to get a closed set of evolution equations for the magnetic potential **A**, one needs to consider (4) together with an additional constrained, i.e., the gauge condition. A discussion of different gauge conditions can be found in [1]. Our numerical methods are based on discretizations of (4) with the Weyl gauge, which means we set $\nabla\phi = 0$. In this case the resulting evolution equation for the magnetic vector potential is *weakly hyperbolic*, which requires a special numerical treatment. In [1], we used different operator splitting methods to discretize the weakly hyperbolic system for the magnetic potential on Cartesian grids. In [2], we developed an unsplit method for the weakly hyperbolic system. This unsplit method was used on Cartesian grids as well as on logically rectangular mapped grids.

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Differential Involutions, Discrete Differential Forms and Constraint Preserving Discretizations on Unstructured Meshes

Holger Heumann

A stationary, linear, first order differential equation with homogeneous righthand side is an *involution* of some given hyperbolic conservation law if the solution of the conservation law is also a solution of that *involution* equation for all times [5, p. 375]. Very often, these involutions are considered to be a very important

structural feature of the conservation law, e.g. the vanishing divergence of the magnetic field for Maxwell equations. As a consequence much effort has been devoted to devising finite volume schemes that compute numerical solutions that are, at least approximately, solution of some discrete version of the involution as well.

An important model problem for the numerical treatment of conservation laws with involutions, that has attracted considerable attention in the literature [9, 14, 2, 23, 6, 19, 22, 16, 21, 7], is the magnetic advection problem for the magnetic field $\mathbf{B}$

$$\partial_t \mathbf{B} + \operatorname{curl}(\mathbf{u} \times \mathbf{B}) = 0\,, \tag{1}$$

with its involution $\operatorname{div} \mathbf{B} = 0$. For many existing methods for rectangular meshes it can be shown [10, Section 2.2.3] that they build on finite difference flavored techniques. They combine central finite difference stencils in one coordinate direction with averaging stencils [19] in the other directions to approximate the partial derivatives in (1). The obvious commuting property of such stencils ensures that a discrete divergence vanishes for all times. It remains to specify the concrete choice of the so-called numerical flux or potential, and we refer to [16, 17, 18] for extensive numerical studies of such methods.

The magnetic advection problem (1) is also a transport equation in the following sense: If $\mathbf{X}(t, \mathbf{x}) := \mathbf{X}_t(\mathbf{x})$ denotes the flux induced by the velocity $\mathbf{u}$ and M denotes an arbitrary 2-dimensional manifold then (1) is equivalent to:

$$\int_M \mathbf{B}\, d\mathbf{S} = \int_{\mathbf{X}_t(M)} \mathbf{B}\, d\mathbf{S} \left(:= \int_M \mathbf{X}_t^* \mathbf{B}\, d\mathbf{S} \right) .$$

The magnetic flux through an advected surface remains constant. This, a standard result in differential geometry [15, p. 142] (see also [12, Section 2]), was exploited first in [3] and then later in [11, 20] to derive numerical methods that ensure that the continuous involution holds exactly for the numerical solution. The reason of this astonishing feature, is the insight that curl and div are dual to the boundary operator on manifolds and we would like to refer to [1, 4, 24, 13, 8] and the many references therein for a detailed introduction into numerical methods inspired by the geometric language of differential forms. The beneficial ingredient that this theory provides for our problem are polynomial spaces V_h of piecewise smooth vector fields on structured and unstructured meshes that have a well defined curl or div. Further, there exist so-called canonical interpolation operators that map smooth vector fields onto the vector fields in V_h and that commute with the derivatives curl or div. The Lagrangian methods in [11] exploit additionally, that the canonical interpolation operators commute with the pullback. The staggered, finite difference approach in [9] falls also in this class of methods.

In this talk we will show, that the schemes of this second class of methods, not only preserve the divergence exactly but are also conservative. Further we will present a new approach for the derivation of finite volume methods, which yield numerical solutions to (1) that fulfill a certain discretization of the involution. The derivation will apply both for structured and unstructured meshes [10, p. 30-35].

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Structure preserving schemes

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(joint work with S. Mishra)

Standard numerical schemes for solving conservation laws are in a mature stage of development. These schemes permit the robust and accurate simulation of complex physical phenomena modeled by nonlinear systems of time-dependent PDEs

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{f} = 0,$$

where $\boldsymbol{u}$ is the vector of conserved variables and $\boldsymbol{f}$ the flux tensor.

However, beside the conserved quantities these equations also possess certain associated structures that are analytically preserved in the form of so-called involutions. A prominent example of such a structure is the divergence free constraint of the magnetic field. This a reflection of the physical fact that magnetic monopoles are not observed in nature. A second example is the conservation of angular momentum in (magneto-) hydrodynamics, which is a direct consequence of the symmetry of the momentum flux tensor. The conservation of angular momentum plays crucial role in e.g. climate modeling and astrophysics. Thirdly, the conservation of (pseudo-) vorticity is of great importance in e.g. weather forecast and aerodynamics.

Standard numerical schemes fail in maintaining these structures at the discrete level. The degree of failure is proportional to the scheme's truncation error for smooth solutions, but it may become $O(1)$ for discontinuous ones. Hence, the fidelity with respect to the physics may be spoiled in numerical simulations.

We will focus on two non-standard extensions aiming at preserving a discrete version of certain structures in the context of hydrodynamics. The first extension deals with the conservation of angular momentum and the second with the conservation of (pseudo-) vorticity. We discuss the requirements on a numerical scheme to maintain these structures discretely. It turns out that realizing certain symmetry properties of the flux tensor and the differential operators discretely is crucial.

We then derive explicit finite volume schemes, which preserve the named structures. To achieve this we start from the recent work by Mishra and Tadmor [1, 2, 3], where a framework for designing genuinely multi-dimensional constraint preserving finite volume schemes was developed. The schemes are based on reformulating standard edge centered numerical fluxes in terms of vertex centered potentials. The vertex centered potentials are then exploited to preserve the structures in a discrete manner. We obtain high-resolution shock-capturing schemes,

which conserve mass, linear momentum and total energy, *and*, at the same time, also angular momentum. Within the potential based framework we also derive a predictor-corrector scheme, which conserves angular momentum *and* pseudo-vorticity. The later scheme can be identified as the rotated Richtmyer scheme [4]. We conclude, that the potential based framework can be used to formulate schemes that preserve a variety of structures of the underlying continuum equations at the discrete level.

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Perspectives on the Workshop on High-Resolution Mathematical and Numerical Analysis of Involution-Constrained PDEs

James Kamm

This workshop is focused on involution-constrained PDEs, which are pervasive in many areas of computational physics. Involutions provide a critical constraint for physically admissible solutions, yet satisfying these constraints in numerical methods presents an ongoing mathematical challenge. A primary motivation for this workshop is captured in the statement of Gawlik et al. [11]:

> Naive discretizations of physical theories can, in general, fail to respect the physical and geometric structure of the system at hand.

Indeed, some sophisticated discretizations fail in this regard, as well. An additional motivation is that ongoing demand for accurate physical simulations of increasingly complicated phenomena and continuing advances in theory and numerics (and computing platforms) make this an opportune time to review mathematical achievements, to discuss current efforts, and to pursue new research objectives.

The archetype here is given by Maxwell's equations of electromagnetism, with the involution that the divergence of the magnetic inductance must remain zero at all time if it vanishes initially. The equations for dynamic hyperelasticity in the Eulerian frame have the involution that the curl of the inverse deformation gradient must vanish for all time. A conceptually similar, although more intricate, situation obtains in general relativity (see, e.g., [21] and references therein).

Four important threads are woven through the fabric of this workshop.

1. *Analytical and numerical developments in PDE theory.* Theoretical work gives the foundational justification of and insight into modern numerical methods, as discussed, e.g., in the monograph of Dafermos [9], the analysis of Christiansen et al. [8], the work of Mishra & Tadmor ([19] and its precursors), and others.
2. *Advances in mimetic differencing methods and algorithms.* Mimetic methods have had a profound influence on numerical algorithms. Applied mathematicians, starting in the 1970s and continuing through the 1990s in, e.g., the work of Hyman, Shashkov, and Steinberg (e.g., [16]), among others, have embraced these concepts. The 2004 IMA workshop produced a notable manuscript [2].
3. *The topological vs. the geometric in continuum and discrete theories.* Tonti's seminal work [22] emphasized the distinction between topology (intrinsic structure, independent metric) and geometry (qualities dependent on the underlying metric) in physics. These ideas led to the application of exterior calculus, differential geometry, and algebraic topology to involution-constrained PDEs. Salient reviews of these concepts are given, e.g., by Bochev [6] and Gerritsma [12].
4. *The development of discrete differential geometry/exterior calculus.* Recent work extending continuum concepts of exterior calculus, differential geometry, and algebraic topology to the discrete context is both important and promising; see, e.g., the works of Arnold et al. [3] and Hirani [15]. These ideas have been applied extensively by the electromagnetics community, e.g., in the significant works of Bossavit (e.g., [7] and many others), Hiptmair [14], and Gross & Kotiuga [13]. They are less well developed but evolving for solid dynamics; see, e.g., the work by Arnold et al. [4], Eastwood [10], and Angoshtari & Yavari [1].

One application invoking the first two of these issues is the numerical approach proposed by Kamm & Walter [18] for Eulerian-frame hyperelastic flow. These authors suggested the application of the Flux Distribution method of Torrilhon & Fey [23] (see also [24, 5]) as a means by which to ensure that the involution constraint is preserved numerically. Plohr & Plohr [20] show that the governing mass, momentum, and energy conservation equations for this case can be written

$$\rho_t + (\rho u^j)_j = 0\,, \tag{1}$$

$$(\rho u^i)_t + (\rho u^i u^j - \mathsf{S}^{ij})_j = 0\,, \tag{2}$$

$$(\rho E)_t + (\rho E u^j - u_i \mathsf{S}^{ij})_j = 0\,, \tag{3}$$

where ρ is the mass density, u^i is the ith velocity component, $E := (1/2)u_k u^k + \varepsilon$ is the specific total energy with ε the specific internal energy, and S^{ij} is the (i,j)-element of the Cauchy stress tensor. Cartesian coordinates are assumed, and repeated indices are summed. Compatibility conditions augment these equations:

$$(\mathsf{G}^\alpha_i)_t + (\mathsf{G}^\alpha_j u^j)_i = 0 \qquad \text{and} \qquad \epsilon^{ijk}\,\mathsf{G}^\alpha_{j,k} = 0\,, \tag{4}$$

where $\mathsf{G}^\alpha_i := \partial X^\alpha/\partial x^i$ is the (α, i)-element of the inverse deformation gradient (IDG), with $\boldsymbol{X}$ the (undeformed) material coordinate and $\boldsymbol{x}$ the (deformed) current coordinate.[1] This set of equations is closed by the hyperelastic relation, which, for

[1] Wagner [25] provides an insightful discussion of these equations.

a homogeneous and isotropic material, can be written as:

$$\mathsf{S}^{ij} = \rho\, \mathsf{F}^{i}_{\alpha}\, (\partial\psi/\partial \mathsf{E}_{\alpha\beta})|_{\varepsilon}\, \mathsf{F}^{j}_{\beta}\,, \tag{5}$$

where $\mathsf{F} := \partial \boldsymbol{x}/\partial \boldsymbol{X} = \mathsf{G}^{-1}$ is the deformation gradient and $\psi(\varepsilon, \mathsf{E})$ is the free energy, with $\mathsf{E} := (1/2)(\mathsf{G}^{-\mathsf{T}}\mathsf{G}^{-1} - \mathsf{I})$ the Lagrangian strain tensor.

The involution constraining this motion is given by the curl constraint in (4): if the curl of the IDG vanishes at the initial time, then it remains zero for the entire motion. The Flux Distribution approach applies naturally to the satisfaction of the involution. At the core of this method is the use of fluxes in the entire neighborhood of a computational cell to obtain discrete spatial differencing operators that enforce the constraint locally, exactly, and independent of how the fluxes are computed. Jeltsch & Torrilhon [17] give a detailed description for the 2D shallow water equations. Although the application of this approach to conservation laws for hyperelasticity has not been implemented, it presents a clear example of high-resolution method for the solution of involution-constrained PDEs.

The workshop provided an open forum in which research related to each of these subjects was presented and vigorous discussions among mathematicians were held.

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Discretization of compressible hyperelasticity on unstructured mesh.

Gilles Kluth
(joint work with Bruno Després)

In this talk, we summarize mathematical properties of the system of hyperelasticity and we present its discretization : we extend hydrodynamic cell-centered lagrangian finite volume schemes by using a multiplicative discretization of the deformation gradient [1]. Finally, we discuss about the introduction of plasticity in this system.

The mathematical structure of the system of hyperelasticity is very rich [2]. Firstly, PDEs are involution-constrained. In the Lagrangian coordinates, PDEs on the deformation gradient F give the involutions

$$\forall i,j,k \qquad \frac{\partial F_{ij}}{\partial X_k} = \frac{\partial F_{ik}}{\partial X_j}$$

which are compatibility conditions for existence of the motion. In the Eulerian coordinates, PDEs on the inverse deformation gradient [3] give

$$\forall i,j,k \qquad \frac{\partial F^{-1}_{ij}}{\partial x_k} = \frac{\partial F^{-1}_{ik}}{\partial x_j}$$

which are the compatibilty conditions for existence of the inverse motion, and PDEs on the cofactor [4] of the inverse deformation gradient give

$$\sum_k \frac{\partial}{\partial x_k}\left(\frac{F_{ki}}{\det(F)}\right) = 0$$

which is known as the Piola identity. Secondly, the hyperelastic system is thermodynamically compatible : its potential structure is constructed so as that the entropy production is null for smooth thermomechanical process. Thirdly, the hyperelastic system satifies the frame-indifference principle. For instance, it is naturally invariant by applying rotation. Finally, the hyperbolicity is given by the positivity of the accoustic tensor, or the rank-one convexity of the internal energy. A proof is given in [1].

Numerically, we extend hydrodynamic cell-centered Lagrangian finite volume schemes [5, 6, 7]. By construction of the approximate Riemann solver, these schemes satisfy the thermodynamic principle. Thus the extension consist in generalizing scalar solver (pressure) with tensorial one (stress tensor). Moreover, we use a multiplicative discretization of the deformation gradient, and show that doing this we obtain exactly the true deformation on meshes with simplices , and obtain a difference of order 2 in the timestep on general mesh.

The aim of this work was to pave the way for finite plasticity. Modern works [9, 10] have extended these Lagrangian schemes to plasticity based on hypoelasticity. Other modern Eulerian works [12, 11] introduced plastic models of Maxwell relaxation type in the hyperelastic system [13]. In [8], we introduced a nonlinear elastic model with threshold (Hencky type model) to simulate plasticity during loads. Here we present a sketch model that we would like to study in the case of shock waves.

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Numerical Strategies for MHD and Reduced MHD: Toroidal geometries

Boniface Nkonga
(joint work with G. Huysmans, M. Becoulet and J. Costa)

One of the major difficulties in the numerical simulations of MHD instabilities in tokamak plasmas is the multiple time scales the system. Typical values of the linear growth of ELM (Edge Localazed Modes) instability is of the order of 0.05ms and non-linear stage of ELM crash about 0.2ms [14]. However the typical time scale of RMP(Resonant Magnetic Perturbations) penetration into pedestal plasma is related to the resistive time scale, which is usually largest time scale in tokamaks. For low ITER relevant resistivity ($\eta \simeq 10^{-9}$, corresponding to $S \simeq 10^9$) characteristic time could reach 10^6 Alfven times ($\simeq 0.1s$) [15]. Vertical kicks used for ELM triggering are also possibly linked to the edge currents generation and, hence, again local pedestal resistive time scales should be resolved together with shorter ELM instability scale. Multi ELM cycles will also involve confinement time scale ($\simeq 1s$) needed for re-heating after the ELM crash. Additional complications in the simulations of MHD instabilities in tokamaks result from the very high magnetic Reynolds numbers ($S \simeq 10^6 - 10^9$) leading to the very thin current layers and structures and the large anisotropy of the directions parallel and perpendicular to the magnetic field. For example the typical ratio of parallel and perpendicular energy conductivities $\frac{\kappa_\parallel}{\kappa_\perp} \simeq 10^8$ to 10^{10}.

The finite element method is the often used technique for the computer-based MHD simulations when applied to fusion devices and hinges [12, 9, 10, 11, 13] on the assumption that the discretized domain and the field of the model are represented both by the mean of piecewise polynomials functions. Eventually, this representation can also insure the continuity of derivatives with Bell, Powell-Sabin or B-splines elements. However, as target flows can be dominated by advection, we need numerically dissipation to enforce stability and robustness. Moreover, this dissipation should be design to preserve the background equilibrium (non-constant in space) and also to be consistent with the inherent anisotropy of the flow structure. The strategy considered is design in the Taylor-Galerkin framework.

According to Lax-Wendroff technique [1, 2] the solution is expanded in time using higher order (2 or 3) Taylor formula. Then, using the partial differential equation under concern, space derivatives are substituted to time derivatives. The current strategy is based on TG2/TG3 semi-implicit Taylor-Galerkin methods proposed in [4]. After linearization and simplifications, the stabilized semi-discrete (in time) approximation may be written in the following compact form

$$(1)\quad \frac{\delta\omega}{\delta t} + \theta\left(L(\partial_x, \omega^{n+1}) - L(\partial_x, \omega^n)\right) - \frac{\delta t\xi}{2}\partial^2_{A^*}\omega^{n+1} = -L(\partial_x, \omega^n) + \frac{\delta t\beta}{2}\partial^2_{A^*}\omega^n$$

where the state vector ω contains the density, the velocity, the pressure, the temperature and the magnetic field formulated with the potential vector in order to achieve divergence free constraint. This potential formulation introduces higher order derivatives and can need, for well posedness of the weak formulation, smooth trial functions that are at least C1. Numerical dissipations are second order derivatives in the characteristic lines associated to the linearized matrix A^* : $\partial^2_{A^*}\omega = \nabla\cdot(A^* \otimes A^*\partial_x\omega)$. The linearized Jacobian A^* is derived from L and particularly the ideal MHD component such as to insure that $\partial^2_{A^*}\omega$ is a self-adjoint operator inducing stabilization, ξ and β are free parameter of the stabilization. This strategy turn out to be a generalization of the "Harned and Kerner" method [8]. When applied to Reduce MHD equations, significant stability improvement is obtained with with almost the same numerical accuracy. Work is underway to implement and assess the performance of the full MHD equations in vector potential formulation.

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Non-Stationary Multiscale Irreversible Deformation and Involution Constraints

Ilya Peshkov
(joint work with Evgeny Romenski)

We would like to present our recent results on formulation of the equations governing motion of a generalized (i.e. fluid or solid) continua and discuss the role of involution constraints like $\nabla \times \mathbf{A} = \mathbf{B}$ in the multiscale continual modelling of irreversible deformation.

The base of our research is the elastoplastic model of hyperelastic type with relaxation terms describing plastic deformation derived by Godunov and Romenski in [1]. Our current understanding of irreversible deformation is saying that this model can be used in order to describe elastoplastic deformation of solids as well as flows of viscous fluids (whether Newtonian or non-Newtonian). In the Eulerian framework, the model is:

$$
\begin{aligned}
&\frac{\partial \rho v_i}{\partial t} + \frac{\partial (\rho v_i v_k + \rho a_{mi} E_{a_{mk}})}{\partial x_k} = 0, \\
&\frac{\partial a_{ik}}{\partial t} + \frac{\partial a_{im} v_m}{\partial x_k} = -v_j \left(\frac{\partial a_{ik}}{\partial x_j} - \frac{\partial a_{ij}}{\partial x_k} \right) - \frac{\phi_{ik}}{\tau}, \\
&\frac{\partial \rho s}{\partial t} + \frac{\partial \rho s v_k}{\partial x_k} = \eta.
\end{aligned}
\tag{1}
$$

Here, $\mathbf{v} = (v_1, v_2, v_3)^{\mathsf{T}}$ is the velocity, $\mathbf{A} = [a_{ij}]$ is the inverse of the elastic deformation gradient $\mathbf{E} = \mathbf{A}^{-1}$ (i.e. we use the multiplicative decomposition of the overall deformation gradient $\mathbf{F} = \mathbf{EP}$ onto the elastic $\mathbf{E}$ and plastic part $\mathbf{P}$), s is the entropy, $\rho = \rho_0 \det \mathbf{A}$ is the mass density, ρ_0 is the reference mass density, $E = E(I_1, I_2, I_3, s)$ is the internal energy, where I_i are the invariants of the tensor

$\mathbf{G} = \mathbf{A}^{\mathsf{T}}\mathbf{A}$, i.e. $I_1 = \mathrm{tr}\sqrt{\mathbf{G}}$, $I_2 = \mathrm{tr}\mathbf{G}$, $I_3 = \det\sqrt{\mathbf{G}} = \rho/\rho_0$, τ is the strain dissipation (due to microstructure rearrangement) characteristic time, the tensorial function ϕ_{ik} sets the "direction" of the strain dissipation, $\eta = E_{a_{ik}}\phi_{ik}/\tau$ is the entropy production source term due to the strain dissipation ϕ_{ik}/τ.

The most critical constitutive function here is τ. It has a clear physical meaning in case a material is in the condensed state (solid or liquid) – it is the time that particles live in a certain place in the microstructure (e.g. in elastic solids, particles live infinite time in a certain place in the microstructure and $\tau = \infty$). In turn, in the definition of τ we use another critical function σ_Y that is the yield limit. It also plays a role of the switcher between solid-like and fluid-like motion. Namely, σ_Y is a function of the temperature $T = E_s$ and $\sigma_Y > 0$ in case of a solid, and $\sigma_Y = 0$ in case of a fluid. At the first sight, it may seem that the equality $\sigma_Y = 0$ results in the absence of tangential stresses in fluids at all. It is really so if $\tau = 0$ (i.e. instantaneous microstructure rearrangement), but if $\tau > 0$ then, in a relaxed media, the actual (current) yield limit σ_{AY} depends on the deformation rate and it is always greater then σ_Y. As the deformation rate tends to zero then $\sigma_{AY} \to \sigma_Y$ and the tangential stresses eventually disappear.

It also may seem that the plan to describe fluid flows in terms of strains will fail, but the fact is that the inverse elastic strain tensor $\mathbf{A}$ (or $\mathbf{E}$), used as a state variable, is always remains small and thus it is an appropriate state variable for fluid-like motions. Remark that the overall deformation gradient $\mathbf{F}$ and the plastic strain tensor $\mathbf{P}$ potentially can grow unlimitedly in fluid flow applications.

Therefore, model (1) is a pure hyperbolic alternative to the Navier-Stokes model for viscous fluids. Though, the application range of (1) is wider, e.g. it also can be applied to flows of non-Newtonian liquids if the strain dissipation time τ is chosen in an appropriate way.

According to our approach, the internal energy for a viscous fluid should have the following form:

$$E = E^{class}(\rho, s) + E^{visc}(\rho, I_2, I_3, s),$$

where E^{class} is a classical internal energy for fluids and E^{visc} is the term that is responsible for the generation of viscous stresses (see the momentum Eq. in (1)).

Then, we extend the model in order to take into account more microscopic details. The true source of irreversible deformation of a real material (whether solid or fluid) are the microscopic slips. We shall rather use the notion of defects. In case of fluids, slips produce microscopic vortices and thus defects can be associated directly with these eddies. We believe that such microscopic events as generation, migration, interaction and self organizing behaviour of defects is quit important in case of highly unsteady non-equilibrium processes as turbulence in fluids or damage/fracture of solids. Therefore, model (1) should be extended in order to take dynamics of defects into account.

The extension is closely connected with involution constraints of system (1). The non-conservative term on the r.h.s. of the second Eq. in (1) is $(\nabla \times \mathbf{A})\mathbf{v}$.

Since the tensor $\nabla \times \mathbf{A}$ satisfies to an extra conservation law:

$$\frac{\partial b_{ij}}{\partial t} + \frac{\partial}{\partial x_k}\left(v_k b_{ij} - v_j b_{ik} + \varepsilon_{jmk}\phi_{im}\right) = 0, \tag{2}$$

where we denote $\mathbf{B} = [b_{ij}] = \nabla \times \mathbf{A}$, then the introduction of $\mathbf{B}$ as a new state variable allows to treat the non-conservative term as a classical (with no spatial derivatives) source term $\mathbf{Bv}$. Therefore, system (1) jointly with Eq. (2) forms a system of non-homogeneous conservation laws. Though, the extended model have an involution constraint, i.e. the two state variables $\mathbf{A}$ and $\mathbf{B}$ have a differential connection $\mathbf{B} = \nabla \times \mathbf{A}$. The numerical method capable to solve system (1), (2) and preserving the connection $\mathbf{B} = \nabla \times \mathbf{A}$ is unknown.

Recall that the tensor $\mathbf{B}$ has a physical meaning of density of defects (e.g. see [1]). Thus, the resulting defect based model is presented by system (3) below. We use the notations $\mathbf{B}$ and $\mathbf{D} = [d_{ij}]$ for the defect density and rate of defect density, $\mathbf{f} = (f_1, f_2, f_3)^{\mathsf{T}} = \nabla \cdot \mathbf{B}$ and $\mathbf{g} = (g_1, g_2, g_3)^{\mathsf{T}} = \nabla \cdot \mathbf{D}$. Also, the strain dissipation tensor ϕ_{ik}/τ and the energy E should be chosen in a consistent way with the rate of defect density so that $\phi_{ik}/\tau = E_{d_{ik}}$.

An internal energy function $E(\mathbf{A}, \mathbf{B}, \mathbf{D}, s)$ for the extended model may be constructed in the following way

$$\begin{aligned}
&\frac{\partial \rho v_i}{\partial t} + \frac{\partial(\rho v_i v_k - \rho b_{mk} E_{b_{mi}} - \rho d_{mk} E_{d_{mi}} + \rho a_{mk} E_{a_{mi}})}{\partial x_k} = 0,\\
&\frac{\partial a_{ik}}{\partial t} + \frac{\partial a_{im} v_m}{\partial x_k} = -\varepsilon_{kml} v_m b_{il} - E_{d_{ik}},\\
&\frac{\partial b_{ij}}{\partial t} + \frac{\partial}{\partial x_k}\left(v_k b_{ij} - v_j b_{ik} + \varepsilon_{jmk} E_{d_{im}}\right) = -v_j f_i,\\
&\frac{\partial d_{ij}}{\partial t} + \frac{\partial}{\partial x_k}\left(v_k d_{ij} - v_j d_{ik} - \varepsilon_{jmk} E_{b_{im}}\right) = -v_j g_i - J_{ij},\\
&\frac{\partial f_i}{\partial t} + \frac{\partial f_i v_k}{\partial x_k} = 0, \qquad \frac{\partial g_i}{\partial t} + \frac{\partial(g_i v_k + J_{ik})}{\partial x_k} = 0.
\end{aligned} \tag{3}$$

$$E = E^{class}(\rho, s) + E^{visc}(\rho, I_1, I_2, s) + E^{defect}(\rho, \mathbf{B}, \mathbf{D}, s),$$

where the last term is responsible for the generation of stresses due to nucleation, migration and interaction of defects. As can be seen from the momentum equation in system (3), the overall stress tensor $\mathbf{T}$ is given by the formula

$$\mathbf{T} = \rho \mathbf{B}^{\mathsf{T}} E_{\mathbf{B}} + \rho \mathbf{D}^{\mathsf{T}} E_{\mathbf{D}} - \rho \mathbf{A}^{\mathsf{T}} E_{\mathbf{A}}.$$

Conclusion. The quest for the ultimate turbulence model has been ongoing for nearly a century now. But at the moment, there are at least 30 models of turbulence, meaning that the quest is still in progress. In turn, this means that there is still no sufficient understanding of turbulent flows amongst the modeling community. One of the reasons for that is a strong belief that the Navier-Stokes model (NSm) is a genuine model for viscous flows. However, it is clear that the

NSm is just an approximation to real flows. Moreover, it has crucial drawbacks. Namely, (i) the viscous stress tensor is a phenomenological one and was derived from observations on steady flows, while the turbulence is a highly unsteady phenomena; (ii) the NSm is a parabolic type model (i.e. it admits infinite velocity of disturbance propagation), while, by its nature, a flow of a fluid is a pure hyperbolic process (all disturbances propagate at finite velocities); (iii) in addition, the mathematical regularity of the NSm is not clear (it is still one of the six unsolved Millennium Prize Problems that were stated by the Clay Mathematics Institute).

We hope that our results on formulation of defect based pure hyperbolic and pure non-stationary model will help to progress in modelling of such complex highly unsteady phenomena as turbulent flows of viscous fluids and damage/fracture of elastoplastic solids.

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Lagrangian/Eulerian Multiphysics Modeling and deRham Complex Based Algorithms

Allen C. Robinson

Multiphysics hydrodynamic modeling in an arbitrary Lagrangian/Eulerian (ALE) framework leads naturally to numerical algorithms which match the geometric meaning of the operators in the deRham complex. We discuss our experience with exploring and utilizing these concepts in tracking solid kinematics and magnetohydrodynamics (MHD). We are also interested in exploring whether these concepts may be effectively utilized for the coupled non-reduced versions of Maxwell's electrodynamics equations and the equations of continuum mechanics and we describe some thoughts in this regard.

In modeling of solid mechanics, general material response depends on the deformation of material with respect to its initial configuration. The inverse deformation gradient is curl free. We have explored an algorithm of constrained transport type connecting $H(grad)$ and $H(curl)$ spaces for remapping the inverse deformation gradient and compared this with another algorithm which depends on remapping the stretch and rotation individually [1]. The primary difficulties encountered included the speed of the algorithm implementation and the fact that no algorithmic solution was achieved for maintaining both deformation positivity and the discrete curl free property. An algorithm utilizing optimization based remap concepts is currently being explored to overcome this obstacle [2].

Moving down the deRham complex diagram we arrive at the connection between $H(curl)$ and $H(div)$. In our approach for 3D resistive MHD modeling we keep the magnetic flux on faces as the fundamental variable, require that all algorithmic components including the initial magnetic field definition, the magnetic diffusion equations and the remap operators all maintain consistency with a zero discrete

flux divergence on every element. We use an extended version of the constrained transport algorithm first introduced for MHD on Cartesian grids by Evans and Hawley [3]. Our algorithm utilizes the properties of low and extended order face elements on hexes [4].

Moving to more speculative future algorithms, it is interesting to consider if a capability can be developed which continues to maintain the deep natural connection to the physics operators in Maxwell's equations but yet does not remove the displacement current term. Desirables for such an algorithm would be that it could effectively bridge between electro-quasistatic and magneto-quasistatic regimes by reducing to these approximations for time steps that are large relative to $\Delta x/c$ and usefully retain a relevant concept of charge. Such a formulation would give additional insight as well as greater flexibility in defining physically relevant boundary value problems. We discuss a possible formulation and show how a deRham complex based remapping of the electric displacement is achievable by combining ideas from divergence free remap and standard volume based remap algorithms which operate in the $H(div)$ to L^2 transition in the deRham complex. Thus we complete a full algorithmic tour of the deRham complex.

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Lagrangian Origin of Involution-Constrained Hyperbolic Systems of Conservation Laws and Equivalent Eulerian Formulation

Evgeniy Romenski

The goal of this talk is to demonstrate that the presence of time independent constraints is an essential feature of the continuum physics equations. It is known that some equations of mathematical physics can be derived as the Euler-Lagrange equations by the minimization of Lagrangian. As an example one can consider nonlinear elasticity equations in Lagrangian coordinates and Maxwell's equations of electrodynamics [1]. If we formulate governing equations as the first order hyperbolic system in both these examples, then the solution must satisfy time

independent constraints such as zero curl of the deformation gradient for elasticity equations and zero divergences of electric and magnetic field for Maxwell's equations.

We consider Lagrangian of the general form, the density of which is represented as the difference between the kinetic and potential energies:

$$\mathcal{L} = \int \left(\frac{1}{2} \frac{\partial x^i}{\partial t} \frac{\partial x^i}{\partial t} - U \left(\frac{\partial x^i}{\partial \xi^j}, \frac{\partial \theta}{\partial t}, \frac{\partial \theta}{\partial \xi^k}, -\frac{\partial A_m}{\partial t} + \frac{\partial \theta}{\partial \xi^m}, \varepsilon_{mpq} \frac{\partial A_p}{\partial \xi^q} \right) \right) d\xi dt. \tag{1}$$

Here ξ^i are Lagrangian coordinates of the particle with Eulerian coordinates x^i, θ is the scalar potential for the fluid flow through element of the medium, A_m is the vector magnetic potential for electromagnetic field, θ is the scalar electric potential for electromagnetic field, ε_{mpq} is the Levi-Civita symbol.

The minimization of the above Lagrangian gives us the Euler-Lagrange equations of continuous media in the presence of electromagnetic field. Introducing new variables $u^i = \frac{\partial x^i}{\partial t}$ - velocity of the particle, $F^i_j = \frac{\partial x^i}{\partial \xi^j}$ - deformation gradient, $n = \frac{\partial \theta}{\partial t}$ - fluid density, $\eta_k = \frac{\partial \theta}{\partial \xi^k}$ - flux of fluid flow, $d_m = -\frac{\partial A_m}{\partial t} + \frac{\partial \theta}{\partial \xi^m}$ - electric field, $h_m = \varepsilon_{mpq} \frac{\partial A_p}{\partial \xi^q}$ - magnetic field, then rewriting Euler-Lagrange equations in terms of these variables and adding compatibilty conditions one can obtain the system of first order equations:

$$\begin{aligned}
&\frac{\partial u^i}{\partial t} - \frac{\partial}{\partial \xi^j} \left(\frac{\partial U}{\partial F^i_j} \right) = 0, && \frac{\partial F^i_j}{\partial t} - \frac{\partial u^i}{\partial \xi^j} = 0, \\
&\frac{\partial}{\partial t} \left(\frac{\partial U}{\partial n} \right) + \frac{\partial}{\partial \xi^m} \left(\frac{\partial U}{\partial \eta_m} \right) = 0, && \frac{\partial \eta_m}{\partial t} - \frac{\partial n}{\partial \xi^m} = 0, \\
&\frac{\partial}{\partial t} \left(\frac{\partial U}{\partial d_m} \right) - \varepsilon_{mpq} \frac{\partial}{\partial \xi^p} \left(\frac{\partial U}{\partial h_q} \right) = 0, && \frac{\partial h_m}{\partial t} + \varepsilon_{mpq} \frac{\partial d_q}{\partial \xi^p} = 0.
\end{aligned}$$

The solution to the above system must satisfy to the set of steady constraints which is a consequence of the definition of the parameters of state:

$$\frac{\partial F^i_j}{\partial \xi^k} - \frac{\partial F^i_k}{\partial \xi^j} = 0, \quad \frac{\partial \eta_m}{\partial \xi^k} - \frac{\partial \eta_k}{\partial \xi^m} = 0, \quad \frac{\partial h_m}{\partial \xi^m}.$$

An additional steady equation $\frac{\partial}{\partial \xi^p} \left(\frac{\partial U}{\partial h_p} \right) = 0$ follows from the minimization procedure.

Thus, we see that the solution of the Euler-Lagrange equations obtained from the minimization of Lagrangian (1) must satisfy time independent constraints which appear intrinsically as a result of formulation of the equations as the first order system. Note, that an arbitrary number of variables (parameters of state) q_i can be included to the potential energy, evolution in time of which described by the equation $\frac{\partial q_i}{\partial t} = 0$. The most important variable of such a type is S - specific entropy and corresponding equation is $\frac{\partial S}{\partial t} = 0$ (we consider processes without dissipation in which there is no entropy production).

The system of Euler-Lagrange equation together with the compatibility equations can be formulated as a thermodynamically compatible system of hyperbolic

conservation laws in Lagrangian coordinates described in [2]. To do this it is necessary to define generating variables and generating potential L connected with the parameters of state $u^i, F^i_j, n, \eta_k, d_m, h_m$ and potential energy U. Finally we come to the system formulated in [2]

$$\begin{aligned}
&\frac{\partial L_{u_i}}{\partial t} - \frac{\partial p_{ij}}{\partial \xi^j} = 0,\\
&\frac{\partial L_{p_{ij}}}{\partial t} - \frac{\partial u_i}{\partial \xi^j} = 0,\\
&\frac{\partial L_n}{\partial t} + \frac{\partial J_m}{\partial \xi^m} = 0,\\
&\frac{\partial L_{J_m}}{\partial t} + \frac{\partial n}{\partial \xi^m} = 0,\\
&\frac{\partial L_{d_m}}{\partial t} - \varepsilon_{mpq}\frac{\partial b_q}{\partial \xi^p} = 0,\\
&\frac{\partial L_{b_m}}{\partial t} + \varepsilon_{mpq}\frac{\partial d_q}{\partial \xi^p} = 0,\\
&\frac{\partial L_{s_i}}{\partial t} = 0.
\end{aligned}$$

Solution to this system satisfies an additional energy conservation law

$$\frac{\partial}{\partial t}\left(L - u_i L_{u_i} - p_{ij}L_{p_{ij}} - nL_n - J_m L_{J_m} - d_m L_{d_m} - b_m L_{b_m} - s_i L_{s_i}\right)$$
$$-\frac{\partial}{\partial \xi^k}\left(u_i p_{ik} + nJ_k - \varepsilon_{kqm} d_q b_m\right) = 0.$$

It is easy to see that the latter system can be rewritten in the symmetric form and if $L(u_i, p_{ij}, n, J_m, d_m, b_m, s_i)$ is a convex function, then it is a hyperbolic system in the sense of Friedrichs. We emphasize that steady constraints remain the same and in terms of generated potential and variables read as

$$\frac{\partial L_{p_{ij}}}{\partial \xi^k} - \frac{\partial L_{p_{ik}}}{\partial \xi^j} = 0, \quad \frac{\partial L_{J_m}}{\partial \xi^k} - \frac{\partial L_{J_k}}{\partial \xi^m} = 0, \quad \frac{\partial L_{d_m}}{\partial \xi^m} = 0, \quad \frac{\partial L_{b_m}}{\partial \xi^m} = 0.$$

Note that equations written in terms of generating potential L have a coupled structure of equations and each couple is responsible for the description of different processes. The first pair represents nonlinear elasticity, the first and the second pairs can be taken for the description of fluid flow through element of the medium and the third one takes into account electromagnetic field. Thus one or the other model of continuous medium in Lagrangian coordinates can be constructed with the use of this system (see for example Lagrangian equations of magnetohydrodynamics presented in [3]).

In fact if we want to study real processes, then in many cases the Eulerean version of equations is preferable. The Eulerean reformulation of Lagrangian thermodynamically compatible system described above is presented in [2],[4],[5]. Application of this Eulerian master system to design conservative models for different media is presented in [5, 6]. In some cases dissipation leads to the violence of steady

constraints in Eulerian formulation of equations and additional artificial variables should be introduced in order to save the conservative form of equations. In recent years this approach has been successfully applied to the development of two-phase compressible flow models [7].

Summarizing all above we emphasize again that the presence of time independent constraints is an essential feature of hyperbolic conservation laws in continuum physics and advanced numerical methods should take this fact into account.

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Correction Schemes to Satisfy Involutions in Hyperbolic PDEs: MHD and Vlasov Equations

James Rossmanith

(joint work with A. Christlieb, C. Helzel, B. Taetz, Q. Tang)

Partial differential equations (PDEs) with involutions and/or additional conservation properties are ubiquitous in plasma physics applications. Mimetic approaches strive to satisfy these properties through careful numerical constructions that mimic important properties on the continuous level. However, in many systems that model physically interesting problems, it is generally not well understood how to generate appropriate mimetic schemes that satisfy all of the desired properties. Therefore, the philosophy espoused in this work can be summarized as follows: (1) produce a numerical *prediction* to the PDE of interest that in general does not satisfy the desired involution or additional conservation properties; then (2) generate a *correction* that when combined with the prediction produces a numerical approximation that does satisfy the desired involution and/or additional conservation property. The two examples considered here are (1) the divergence-free constraint of the magnetic field in the ideal magnetohydrodynamic (MHD) system and (2) energy conservation in the Vlasov-Poisson system.

The ideal MHD equations are a first order hyperbolic system of conservation laws that can be written in the form

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho\mathbf{u}\\ \mathcal{E}\\ \mathbf{B}\end{bmatrix} = -\nabla\cdot\begin{bmatrix}\rho\mathbf{u}\\ \rho\mathbf{u}\mathbf{u}+\left(p+\frac{1}{2}\|\mathbf{B}\|^2\right)\mathbb{I}-\mathbf{B}\mathbf{B}\\ \mathbf{u}\left(\mathcal{E}+p+\frac{1}{2}\|\mathbf{B}\|^2\right)-\mathbf{B}\left(\mathbf{u}\cdot\mathbf{B}\right)\\ \mathbf{u}\mathbf{B}-\mathbf{B}\mathbf{u}\end{bmatrix}, \tag{1}$$

$$\nabla\cdot\mathbf{B}=0, \tag{2}$$

where ρ, $\rho\mathbf{u}$ and $\mathcal{E}$ are the total mass, momentum and energy densities, and $\mathbf{B}$ is the magnetic field. The termal pressure, p, is related to the conserved quantities through the ideal gas law

$$p=(\gamma-1)\left(\mathcal{E}-\frac{1}{2}\|\mathbf{B}\|^2-\frac{1}{2}\rho\|\mathbf{u}\|^2\right), \tag{3}$$

where $\gamma=5/3$ is the ideal gas constant. Here $\|\cdot\|$ denotes the Euclidean vector norm.

Since the magnetic field is divergence-free, it can be written as the curl of a magnetic vector potential:

$$\mathbf{B}=\nabla\times\mathbf{A}. \tag{4}$$

Plugging the above relationship into the evolution equation for $\mathbf{B}$ and invoking the Weyl gauge conditions (see Helzel et al. [4]), we obtain the following evolution equation for the magnetic vector potential:

$$\mathbf{A}_{,t}=-N_1(\mathbf{u})\,\mathbf{A}_{,x}-N_2(\mathbf{u})\,\mathbf{A}_{,y}-N_3(\mathbf{u})\,\mathbf{A}_{,z}, \tag{5}$$

with

$$N_1=\begin{bmatrix}0&-u^2&-u^3\\0&u^1&0\\0&0&u^1\end{bmatrix}, N_2=\begin{bmatrix}u^2&0&0\\-u^1&0&-u^3\\0&0&u^2\end{bmatrix}, N_3=\begin{bmatrix}u^3&0&0\\0&u^3&0\\-u^1&-u^2&0\end{bmatrix}. \tag{6}$$

It can be shown that this system is only weakly hyperbolic [4].

The basic predictor-corrector framework described in this work is based on the following algorithm:

(0) Start with $Q^n_{\mathrm{MHD}}=(\rho^n,\rho\mathbf{u}^n,\mathcal{E}^n,\mathbf{B}^n))$ and $Q^n_{\mathrm{A}}=\mathbf{A}^n$ (the solution at t^n).

(1) Independently update the MHD system (1) and the magnetic vector potential equation (6):

$$Q^*_{\mathrm{MHD}}=Q^n_{\mathrm{MHD}}+\Delta t\,\mathcal{L}(Q^n_{\mathrm{MHD}}),$$
$$Q^{n+1}_{\mathrm{A}}=Q^n_{\mathrm{A}}+\Delta t\,\mathcal{H}(Q^n_{\mathrm{A}},\mathbf{u}^n),$$

where $\mathcal{L}$ is a discrete version of the right-hand side of (1), $\mathcal{H}$ is a discrete version of the right-hand side of (6), and $Q^*_{\mathrm{MHD}}=(\rho^{n+1},\rho\mathbf{u}^{n+1},\mathcal{E}^{n+1},\mathbf{B}^*)$. $\mathbf{B}^*$ is the predicted magnetic field that in general does not satisfy a discrete divergence-free constraint.

(2) Replace $\mathbf{B}^*$ by a discrete of the magnetic potential Q_{A}^{n+1}:

$$\mathbf{B}^{n+1} = \nabla \times Q_{\mathrm{A}}^{n+1}.$$

This discrete curl will be defined appropriately so that $\nabla \cdot \mathbf{B}^{n+1} = 0$ for some appropriate definition of the discrete divergence operator.

We describe in this talk recent work on weighted essentially non-oscillatory (WENO) schemes. A finite volume WENO method was developed in Helzel et al. [5]. This method uses a modified version of the non-conservative finite volume method of Castro et al. [1] to solve the weakly hyperbolic system (6). A finite difference WENO version of this approach was developed in Christlieb et al. [3]. This method uses a version of the WENO scheme for Hamilton-Jacobi equations [6] to solve (6). For both the FV-WENO and the FD-WENO schemes, special limiters were designed to control unphysical oscillations in the corrected magnetic field.

In the second part of the talk we describe a high-order semi-Lagrangian discontinuous Galerkin scheme for solving the Vlasov-Poisson system [7]:

$$f_{,t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \mathbf{E} \cdot \nabla_{\mathbf{v}} f = 0, \tag{7}$$

$$\mathbf{E} = -\nabla_{\mathbf{x}} \phi, \quad -\nabla_{\mathbf{x}}^2 \phi = \rho_0 - \rho(t, \mathbf{x}). \tag{8}$$

There are several challenges in solving the Vlasov-Poisson system, including (1) f is a function of as many as 7 independent variables: $(t, \mathbf{x}, \mathbf{v})$, (2) there is a potentially severe time-step restriction due to the possibility of particles with large velocities, v, (3) the distribution function should remain positive $f > 0$ in order to remain physically meaningful, and (4) Vlasov-Poisson is a Hamiltonian system and thus there are an infinite number of quantities that are conserved; in many applications the most important of these are the charge density and the total energy.

In this talk we describe a semi-Lagrangian scheme using the standard operator splitting approach of Cheng and Knorr [2]. Using a high-order discontinuous Galerkin discretization in phase space, we develop positivity-preserving limiters using a modification of the ideas developed by Zhang and Shu [8]. This basic scheme allows for large time-steps, keeps the distribution function positive, and conserves the charge density. The missing ingredient is the conservation of total energy. In this talk we describe some potential strategies for achieving conservation of energy.

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Constrained Data Transfer

Mikhail Shashkov

In this presentation we consider two examples of constrained data transfer.

First example, is conservative interpolation of divergence-free vector field from one mesh to another, [1] The algorithm is based discrete vector calculus and consist of an explicit recovery, postprocessing and interpolation of a potential for the original vector field and a subsequent application of a curl operator to obtain the desired divergence-free discrete vector field on the new mesh. Old and new meshes are neither required to have the same connectivity, nor to be close to each other.

Second example, is the interpolation of the fluid velocity field from the old to new mesh (which has the same connectivity), [2] . Standard interpolation generate a discrepancy between the remapped kinetic energy, and the kinetic energy that is obtained from the remapped nodal velocities which conserves momentum. In most hydro codes, this discrepancy is redistributed to the internal energy of adjacent computational cells which allows for the conservation of total energy. This approach can introduce oscillations in the internal energy field, which may not be acceptable. We describe approach, which eliminates (when it is possible) or reduces the energy discrepancy.

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Handling the divergence constraints in the Vlasov-Maxwell system

Eric Sonnendrücker
(joint work with M. Campos Pinto, N. Crouseilles, S. Salmon)

The evolution of a plasma, which is a gas of charged particles, can be described by the Vlasov-Maxwell equations. The Vlasov equation for a species of particle indexed by s reads

$$\frac{\partial f_s}{\partial t} + \mathbf{v}\cdot\frac{\partial f_s}{\partial \mathbf{x}} + \frac{q}{m}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\frac{\partial f_s}{\partial \mathbf{v}} = 0,$$

where m is the mass of the particles, q their charge and $f \equiv f(\mathbf{x},\mathbf{v},t)$ represents the particle density in phase space at point $(\mathbf{x},\mathbf{v})$ and at time t. It has the structure of a transport equation in phase space which includes the three dimensions of physical space and the three dimensions of velocity space (or momentum in the relativistic case). The self-consistent electromagnetic field can be calculated by coupling with Maxwell's equation with sources that are the charge densities and current calculated from the particles:

$$\begin{aligned} -\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} + \operatorname{curl}\mathbf{B} &= \mu_0\,\mathbf{J}, \\ \frac{\partial \mathbf{B}}{\partial t} + \operatorname{curl}\mathbf{E} &= 0, \\ \operatorname{div}\mathbf{E} &= \frac{\rho}{\epsilon_0}, \\ \operatorname{div}\mathbf{B} &= 0, \end{aligned}$$

with

$$\rho(\mathbf{x},t) = q\int f(\mathbf{x},\mathbf{v},t)\,d\mathbf{v}, \quad \mathbf{J}(\mathbf{x},t) = q\int f(\mathbf{x},\mathbf{v},t)\mathbf{v}\,d\mathbf{v}.$$

It is well known, that the constraints $\operatorname{div}\mathbf{E} = \frac{\rho}{\epsilon_0}$ and $\operatorname{div}\mathbf{B} = 0$ are satisfied at all times, provided they are satisfied at time $t = 0$ and the continuity equation $\frac{\partial\rho}{\partial t} + \operatorname{div}\mathbf{J} = 0$ is satisfied and when the electromagnetic field is a solution of the two first of Maxwell's equations. Moreover, if this continuity equation is not satisfied, Maxwell's equations are ill-posed.

The same is true at the discrete level, and care has to be taken so that the particle distribution f remains consistent with all of Maxwell's equation. One possibility, which was introduced in [4, 5] is to modify Maxwell's equations so that they remain well posed in all case and that a correcting potential p can absorb the error in the continuity equation at each time step.

$$\begin{aligned} -\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} + \operatorname{curl}\mathbf{B} - \nabla p &= \mu_0\mathbf{J}, \\ \frac{\partial \mathbf{B}}{\partial t} + \operatorname{curl}\mathbf{E} &= 0, \\ g(p) + \operatorname{div}\mathbf{E} &= \frac{\rho}{\epsilon_0}, \\ \operatorname{div}\mathbf{B} &= 0. \end{aligned}$$

This implies

$$\frac{\partial g(p)}{\partial t} - c^2 \Delta p = \frac{1}{\epsilon_0}(\frac{\partial \rho}{\partial t} + \text{div } \mathbf{J}),$$

with $g = 0, Id, \partial_t$.

In this talk we are interested in methods that conserve at the discrete level the properties of the continuous equations. In particular denoting curl_h and div_h the discrete curl and div operators. We are looking for methods such that $\text{div}_h \text{curl}_h = 0$ and that also satisfy a discrete continuity equation. All this on the one hand for Particle In Cell (PIC) method [3] and on the other hand for semi-Lagrangian methods [6].

For this we need first a solver that verifies a discrete exact sequence.

$$H^1 \overset{\mathbf{grad}}{\longrightarrow} \mathbf{H}(\mathbf{curl}) \overset{\mathbf{curl}}{\longrightarrow} \mathbf{H}(\text{div}) \overset{\text{div}}{\longrightarrow} L^2.$$

This is provided by many solvers in the framework of discrete exterior calculus introduced recently by Arnold, Falk and Winther [1].

In practice for the PIC method, we use a Maxwell solver based on the following conforming high order discrete spaces: Lagrange, Nedelec, Raviart-Thomas, Disccontinuous Galerkin. The first of the spaces chosen dictates the order of all of them. The it remains to compute the current and charge density from the particles so that a discrete continuity equation is satisfied. This is done in weak form by using a weak form of Ampère's equation and Gauss' law. The discrete continuity then follows naturally by taking care of integrating the source terms exactly by using a Gauss integration of sufficiently high order to be exact for the polynomials considered on each cell.

For the Semi-Lagrangian method, we use a split procedure as in [7] and note that the continuity equation only follows from the advection in x part as long as the advection in v is conservative. The algorithm then consists in a careful computation of the fluxes in relation with the Maxwell solver as in [2].

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