On constraint preservation in numerical simulations of Yang-Mills equations

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Einstein – Yang-Mills

- Discussion IMA "Hot Topics" June 2002: Douglas Arnold, Alan Rendall and Ragnar Winther.
- Level of difficulty of simulating Yang-Mills between Einstein and (linear) Maxwell.
- Flow preserves non-linear differential constraints.
- Transfer knowledge from charge conservation properties of variational finite element discretization of Maxwell to Einstein.

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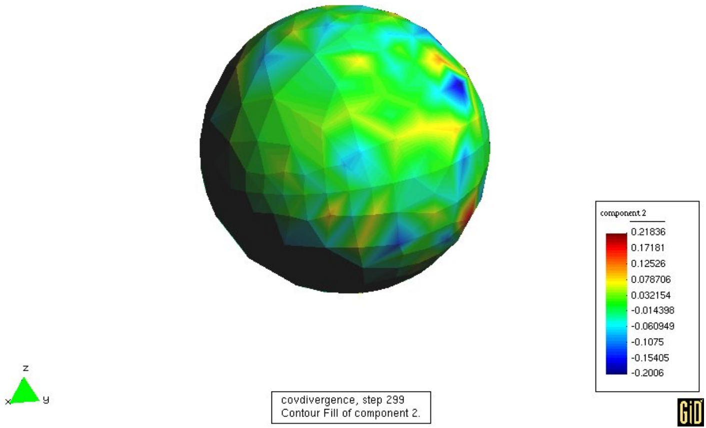
Constraint not preserved



Maxwell's equations

- Evolution equation (vacuum):

$$\partial_t E = \operatorname{curl} H, \tag{1}$$
$$\partial_t H = -\operatorname{curl} E. \tag{2}$$

- Preserved constraints :

$$\operatorname{div} E = 0, \tag{3}$$
$$\operatorname{div} H = 0. \tag{4}$$

- Magnetic potential (temporal gauge):

$$H = \operatorname{curl} A, \tag{5}$$
$$E = -\partial_t A. \tag{6}$$

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Lagrangian formalism

- Second order formulation:

$$\partial_t^2 A = -\operatorname{curl}\operatorname{curl} A. \tag{7}$$

- Lagrangian (Kinetic - Potential energy):

$$\mathcal{L}(A, \dot{A}) = (1/2)\|\dot{A}\|^2_{\mathrm{L}^2} - (1/2)\|\operatorname{curl} A\|^2_{\mathrm{L}^2}. \tag{8}$$

- Stationary points for action:

$$\int_0^T \mathcal{L}(A(t), \partial_t A(t))\mathrm{d}t. \tag{9}$$

Lie algebras and SU2

- A Lie algebra $\mathfrak{g}$ with a compatible scalar product:

$$[u, v] + [v, u] = 0, \quad (10)$$
$$[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0, \quad (11)$$
$$([u, v]|w) + (v|[u, w]) = 0. \quad (12)$$

- SU2:
skew-hermitian, trace-free 2×2 complex matrices.
Choice of basis ($i\times$ Pauli matrices):

$$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad (13)$$

Orthogonal and we have:

$$[e_0, e_1] = e_0 e_1 - e_1 e_0 = 2e_2. \quad (14)$$

Lie algebra valued functions

- Functions $P : \mathbb{R}^n \to \mathfrak{g}$.
- Choose n-tuple $A = (A_1, \cdots, A_n)$ of such functions. "Gauge potential" ($\leftrightarrow$ Christoffel symbols).
- Differential operators on $P : \mathbb{R}^n \to \mathfrak{g}$:

$$\partial_{i,A} P = \partial_i P + [A_i, P]. \tag{15}$$

- Compound operators $\mathrm{grad}_A, \mathrm{curl}_A, \mathrm{div}_A$, i.e. :

$$\mathrm{grad}_A P = (\partial_{1,A} P, \cdots, \partial_{n,A} P), \tag{16}$$

$$(\mathrm{curl}_A E)_{ij} = \partial_{i,A} E_j - \partial_{j,A} E_i, \tag{17}$$

$$\mathrm{div}_A E = \sum_i \partial_{i,A} E_i. \tag{18}$$

Curvature of gauge potentials

- A gauge potential $A = (A_1, \cdots, A_n)$ on $\mathbb{R}^n$ representing a Lie algebra valued one-form.
- Curvature of A is the Lie algebra valued two-form (Cartan's formula):

$$\mathcal{C}(A) = \operatorname{curl} A + (1/2)[A, A]. \tag{19}$$

More explicitely ($\leftrightarrow$ Riemannian curvature tensor):

$$\mathcal{C}(A)_{ij} = \partial_i A_j - \partial_j A_i + [A_i, A_j]. \tag{20}$$

- Then:

$$\operatorname{curl}_A \operatorname{grad}_A P = [\mathcal{C}(A), P], \tag{21}$$

or more explicitely:

$$(\operatorname{curl}_A \operatorname{grad}_A P)_{ij} = [\mathcal{C}(A)_{ij}, P]. \tag{22}$$

Lagrangian, Euler-Lagrange equation

- Lagrangian (Kinetic - Potential energy):

$$\mathcal{L}(A, \dot{A}) = (1/2)\|\dot{A}\|_{\mathrm{L}^2}^2 - (1/2)\|\mathcal{C}(A)\|_{\mathrm{L}^2}^2. \quad (23)$$

- Stationary points for action:

$$\int_0^T \mathcal{L}(A(t), \partial_t A(t))\mathrm{d}t. \quad (24)$$

- Euler-Lagrange equation:

$$\forall A' \quad \langle \partial_t^2 A(t), A' \rangle = -\langle \mathcal{C}(A(t)), \mathrm{D}\mathcal{C}(A(t))A' \rangle. \quad (25)$$

Galerkin space of gauge potentials

- Simplicial mesh. Nédélec's edge elements X_h are most successful for Maxwell's equations.
- Y_h scalar continuous piecewise affine functions. Then:

$$\mathrm{grad} : Y_h \to X_h. \tag{26}$$

and in trivial topology (exact sequence property):

$$\forall u \in X_h \ \ \mathrm{curl}\, u = 0 \Rightarrow \exists v \in Y_h \ \ \mathrm{grad}\, v = u. \tag{27}$$

- Lie algebra valued forms can be obtained by:

$$X_h \otimes \mathfrak{g}, \quad Y_h \otimes \mathfrak{g}. \tag{28}$$

- An element of $X_h \otimes \mathfrak{g}$ is specified by one element of $\mathfrak{g}$ for each edge of the mesh.

Semidiscretization

- Stationary point $A : \mathbb{R} \to X_h \otimes \mathfrak{g}$ for action:

$$\int_0^T \mathcal{L}(A(t), \partial_t A(t)) \mathrm{d}t. \qquad (29)$$

- Euler-Lagrange equation (ODE) $\forall A' \in X_h \otimes \mathfrak{g}$:

$$\langle \partial_t^2 A(t), A' \rangle = -\langle \mathcal{C}(A(t)), \mathrm{D}\mathcal{C}(A(t))A' \rangle. \qquad (30)$$

- Using:

$$\mathcal{C}(A(t)) = \operatorname{curl} A + (1/2)[A, A], \qquad (31)$$

$$\mathrm{D}\mathcal{C}(A(t))A' = \operatorname{curl}_A A'. \qquad (32)$$

Numerical result I

- Component 0 of Gauge potential on sphere: a one-form represented by a vector field.
- Movie

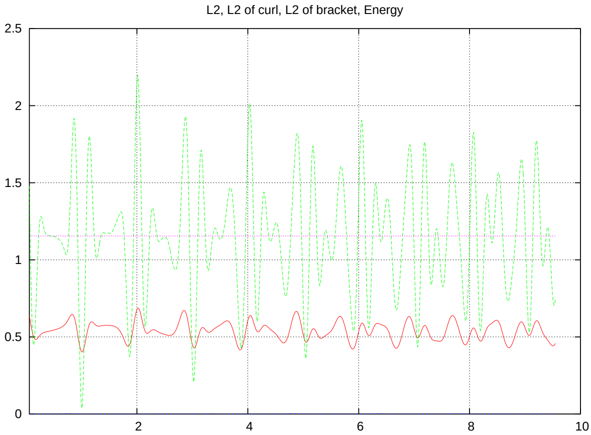
Numerical result II

- Component 0 of curvature:
  a two-form represented by a scalar field.
- Movie

Numerical result III

- Component 2 of Gauge potential.
  Arizes through non-linear coupling
  of component 0 and component $1([e_0, e_1] = 2e_2)$.
  Approximateley ten times smaller than component 1.
- Movie

Numerical result IV



Divergence preservation

- div $H = 0$. Analogue is Bianchi identity:

$$\mathrm{d}_A \mathcal{C}(A) = 0. \tag{33}$$

  Not a problem because $\mathcal{C}(A)$ represented exactly.

- div $E = 0$. Analogue is Gauss law:

$$\mathrm{div}_A \, \partial_t A = 0. \tag{34}$$

  Big problem.

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Variational interpretation

- Gauss law obtained by testing with $A' = \operatorname{grad}_A P$ at each t:

$$\langle \partial_t^2 A, \operatorname{grad}_A P \rangle = -\langle \mathcal{C}(A), \operatorname{curl}_A \operatorname{grad}_A P \rangle . \quad (35)$$
$$= -\langle \mathcal{C}(A), [\mathcal{C}(A), P] \rangle = 0 . \quad (36)$$

- Gives the conserved quantity:

$$\langle \partial_t A, \operatorname{grad}_A P \rangle . \quad (37)$$

  Weak form of $\operatorname{div}_A \partial_t A = 0$.

- Problem: grad_A maps $Y_h \otimes \mathfrak{g}$ out of $X_h \otimes \mathfrak{g}$.
  Maxwell: discrete weak divergence preservation.
  Yang-Mills: $\operatorname{grad}_A P$ is not a valid test function.

Noether interpretation

- Gauge transformations. Given Lie group valued function $Q : \mathbb{R}^n \to G$:

$$A \mapsto QAQ^{-1} - (\operatorname{grad} Q)Q^{-1} \qquad (38)$$

- Group of tranformations that leave Lagrangian invariant.
  By Noether's theorem we obtain the Gauss law.
- Galerkin space $X_h \otimes \mathfrak{g}$ is not invariant.

Numerical example A

- Gauss law is violated.
- Component 2 of P such that:

$$\forall P' \quad \langle P, P' \rangle = \langle \partial_t A, \operatorname{grad}_A P' \rangle. \tag{39}$$

- Movie

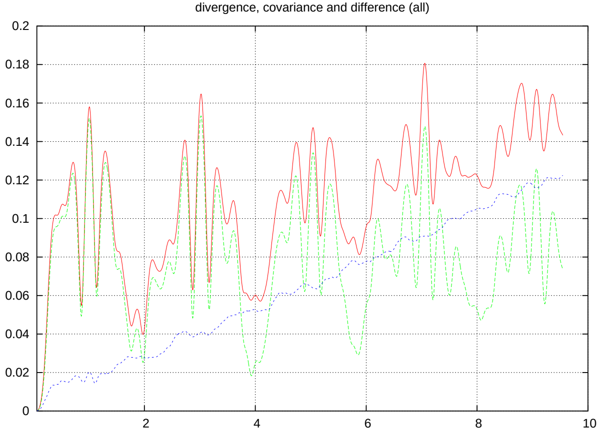
Numerical example B

- Divergence of $\partial_t A$ is polluted (noise is as big as signal).
- Component 2 of P such that:

$$\forall P' \quad \langle P, P' \rangle = \langle \partial_t A, \operatorname{grad} P' \rangle. \tag{40}$$

- Movie

Numerical example C



Saddlepoint

- Try to enforce:

$$\langle \partial_t A, \operatorname{grad}_A P \rangle = 0, \tag{41}$$

- Reformulate as first order sys (A and $E = -\partial_t A$), incremental form ($\partial_t \langle E, \operatorname{grad}_A P\rangle = 0$) and Lagrange multipliers. Use cancellation:

$$\langle \partial_t A, [\partial_t A, P] \rangle = 0. \tag{42}$$

Gives:

$$\dot{A} = -E, \tag{43}$$

$$\langle \dot{E}, E' \rangle + \langle E', \operatorname{grad}_A P \rangle = \langle \mathcal{C}(A), \operatorname{curl}_A E' \rangle, \tag{44}$$

$$\langle \dot{E}, \operatorname{grad}_A P' \rangle = 0. \tag{45}$$

- Energy and constraint preserving ODE.

A Brezzi Inf-Sup condition

- grad_A maps $Y_h \otimes \mathfrak{g}$ out of $X_h \otimes \mathfrak{g}$, but not orthogonally, for small sets of A.
- Theorem: (3D problems) For each set $\mathfrak{A}$ of gauge potentials A which is compact in L^3 there is a constant $C > 0$ and $\bar{h}$ such that for all $h < \bar{h}$, all $A \in \mathfrak{A}$:

$$\inf_{P \in Y_h \otimes \mathfrak{g}} \sup_{A' \in X_h \otimes \mathfrak{g}} \frac{\langle A', \mathrm{grad}_A P \rangle}{\|A'\|_{\mathrm{L}^2} \|P\|_{\mathrm{H}^1}} \geq 1/C. \qquad (46)$$

- Proof: For $A = 0$ it is trivial, for fixed $A \in \mathrm{L}^3$ $[A, \cdot] : \mathrm{H}^1 \to \mathrm{L}^2$ is compact by Sobolev injection theorems and approximation, finally covering property.
- Interpretation: L^3 control of trajectories gives weak divergence control in addition.

Time discretization of constraint

- Staggered scheme with saddlepoint:

$$\begin{aligned}
\frac{A^i - A^{i-1}}{\tau} &= -E^{i-1/2},\\
\langle F^i, E' \rangle + \langle E', \mathrm{grad}_{A^i} P^i \rangle &= \langle \mathcal{C}(A^i), \mathrm{D}\mathcal{C}(A^i) E' \rangle,\\
\langle F^i, \mathrm{grad}_{A^i} P' \rangle &= 0,\\
\frac{E^{i+1/2} - E^{i-1/2}}{\tau} &= F^i
\end{aligned}$$

- Discrete constraint preserving in the following sense: For any solution of above system the following quantities are preserved:

$$\langle \frac{A^{i+1} - A^{i-1}}{2\tau}, \mathrm{grad}_{A^i} P' \rangle. \quad (47)$$

Numerical results

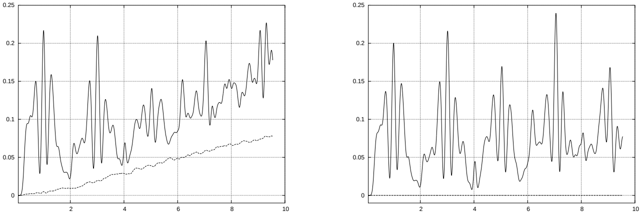


Figure: L^2 norms squared of divergence (plain) and charge (dashed) of E^i.

Div-Curl lemma

- Even though $\operatorname{div}_A \partial_t A \neq 0$ we have Galerkin control over $\langle \partial_t A, \operatorname{grad}_A P \rangle$ for large space of functions P (but finite dimensional).
- A div-curl lemma: (SIAM J. Numer. Anal.)
  Edge elements, no time.
  Suppose A'_h, A_h are weakly converging in L^2 to A' and A, as $h \to 0$.
  Suppose A'_h is "Galerkin divergence free" and $\operatorname{curl} A_h$ is relatively compact in H^{-1} (e.g. bounded in L^2).
  Then $A'_h \cdot A_h \to A' \cdot A$ in the sense of distributions:

$$\forall \phi \in C_c^\infty \quad \int (A'_h \cdot A_h)\phi \to \int (A' \cdot A)\phi. \qquad (48)$$