Solving PDEs with constraints

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1 Introduction

Many numerical solvers evolve fields subject to constraints, such as Maxwell equations, $\nabla \cdot \mathbf{B} = 0$ and $\nabla \cdot \mathbf{E} = \rho_e$, in magnetohydrodynamics or the Hamiltonian and momentum constraints in numerical relativity. Even though these constraints are expected to be satisfied by the gauge invariance of the fields, together with the dynamics, discretization error can lead to their violation. Such a drift from the constrain can feed back into the dynamics, producing unphysical forces and unstable growing modes. Classical remedies (constrained transport, projection, hyperbolic cleaning, constraint damping) work well for linear constraints with known structure. They become expensive, hand-tuned or unavailable when constraints are nonlinear, or for unfamiliar field systems where no constraint-preserving formulation is known.

This project will study whether machine learning can control constraint violation inside the time loop of an existing solver. Three approaches will be compared: (1) a neural corrector with hard constraint enforcement, (2) learned constraint-damping terms trained through a differentiable solver, and (3) learned constraint-preserving parameterizations, generalizing the vector-potential idea to systems where none is known.

Work proceeds in stages: benchmark on 2D MHD against exact projection and Dedner cleaning, measuring both constraint violation and accuracy of the physical fields; then extend to nonlinear constraints (lattice Yang–Mills, simplified 3+1 gravity), where ML can offer a real advantage. The goal is corrections that recover the true solution, not merely ones that satisfy the constraint.

2 Example: incompressible fluid dynamics

We start by our original EoM,

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} = -\frac{1}{\rho_0}\boldsymbol{\nabla} p + \nu \nabla^2 \boldsymbol{u} + \mathbf{f} = 0\,, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0\,, \tag{1}$$

where ρ_0 is a constant. After rescaling $\boldsymbol{u} \to \boldsymbol{u}/U$, $p \to p/(\rho U^2)$, $\mathbf{f} \to L\mathbf{f}/(U^2)$, $t \to Ut/L$, $\boldsymbol{\nabla} \to \boldsymbol{\nabla} L$, and defining Reynolds number, Re$= UL/\nu$,

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} = -\boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}}\nabla^2 \boldsymbol{u} + \mathbf{f} = 0\,, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0\,. \tag{2}$$

This provides a closed system where p should be chosen uniquely to enforce divergence-free.

2.1 Chorin decomposition

Let's rewrite this as [1]

$$\partial_t \boldsymbol{u} + \boldsymbol{\nabla} p = \mathcal{F}_i = \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} + \frac{1}{\mathrm{Re}}\nabla^2 \boldsymbol{u} + \mathbf{f}\,. \tag{3}$$

We can then define an auxiliary field $\boldsymbol{u}^*$ that satisfies

$$\partial_t \boldsymbol{u}^* \simeq \frac{c_{n+1}\boldsymbol{u}^* - c_m \boldsymbol{u}^m}{\Delta t} \simeq \frac{\boldsymbol{u}^* - \boldsymbol{u}^n}{\Delta t} = \mathcal{F}_i \,, \tag{4}$$

where c_ℓ are constants that are fixed by the choice of the finite difference scheme, with $\ell = n+1, n, n-1, \ldots$ For example, $c_{n+1} = c_n = 1$ and $c_m = 0$ for $m < n$ in Euler's method, corresponding to the third approximation above. Note that $\boldsymbol{u}^m$ are all divergence free, but $\boldsymbol{u}^*$ is not.

This system allows us to compute $\boldsymbol{u}^*$ for a given numerical scheme. On the other hand, our original discretized equation satisfies

$$\frac{c_{n+1}\boldsymbol{u}^{n+1} - c_m \boldsymbol{u}^m}{\Delta t} = \mathcal{F}_i - \boldsymbol{\nabla} p \Rightarrow \boldsymbol{u}^{n+1} = \boldsymbol{u}^* - c_{n+1}^{-1} \Delta t \, \boldsymbol{\nabla} p \Rightarrow c_{n+1} \frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^*}{\Delta t} = -\boldsymbol{\nabla} p \,. \tag{5}$$

One can then take the divergence of this field to find

$$c_{n+1}^{-1} \Delta t \, \boldsymbol{\nabla}^2 p^{n+1} = \boldsymbol{\nabla} \cdot \boldsymbol{u}^* \,, \tag{6}$$

which allows to compute p^{n+1}.

2.2 Leray projection

Leray projection allows to extract the divergence-free component of any vector field, $\boldsymbol{u}$,

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 \tag{7}$$

One can define the projection operator in Fourier space as

$$P_{ij}(\boldsymbol{k}) = \delta_{ij} - \hat{k}_i \hat{k}_j \,, \quad \hat{k}_i = \frac{k_i}{k} \,, \quad \boldsymbol{k} \neq 0. \tag{8}$$

Then, if a field computed numerically, $\boldsymbol{u}^*$, does not satisfy the divergence-free condition, i.e., $\hat{k}_i u_i^*(\boldsymbol{k}) \neq 0$, it can be projected to the physical one by taking Leray projection,

$$u_i(\boldsymbol{k}) = P_{ij}(\boldsymbol{k}) \, u_j^*(\boldsymbol{k}) \,. \tag{9}$$

Indeed, this field automatically satisfies $\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$:

$$\hat{k}_i u_i(\boldsymbol{k}) = \hat{k}_i P_{ij}(\boldsymbol{k}) \, u_j^*(\boldsymbol{k}) = (\hat{k}_j - \hat{k}_j) \, u_j^*(\boldsymbol{k}) = 0 \,. \tag{10}$$

The Leray projection can be generalized to a field with non-zero divergence, determined by a scalar field ρ,

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = \rho \,. \tag{11}$$

Then, in Fourier space, with $\tilde{\boldsymbol{u}} = \mathcal{F}(\boldsymbol{u})$ and $\tilde{\rho} = \mathcal{F}(\rho)$,

$$i \, \boldsymbol{k} \cdot \tilde{\boldsymbol{u}} = \tilde{\rho}. \tag{12}$$

To separate the divergence, we generalise 8 with a scalar a:

$$P_{ij}\tilde{u}_j = \left(\delta_{ij} - a \, \frac{k_i k_j}{k^2} \right) \tilde{u}_j = \tilde{u}_i - a \, \frac{k_i \, (k_j \tilde{u}_j)}{k^2}. \tag{13}$$

Using $k_i k_i = k^2$ and 12, its divergence is

$$i \, k_i P_{ij} \tilde{u}_j = i \left(k_i \tilde{u}_i - a \, \frac{k_i k_i \, k_j \tilde{u}_j}{k^2} \right) = (1-a) \, i \, \boldsymbol{k} \cdot \tilde{\boldsymbol{u}} = (1-a) \, \tilde{\rho}. \tag{14}$$

Hence $P_{ij}\tilde{u}_j$ retains the fraction $(1-a)$ of the divergence, while the remainder $\tilde{u}_i - P_{ij}\tilde{u}_j = a\, k_i k_j \tilde{u}_j/k^2$ carries $a\,\tilde{\rho}$. Requiring the projected part to be solenoidal for arbitrary $\tilde{\rho}$ gives

$$a = 1, \tag{15}$$

which recovers 8. The field therefore splits as

$$\tilde{u}_i = \underbrace{\left(\delta_{ij} - \frac{k_i k_j}{k^2}\right)\tilde{u}_j}_{\tilde{u}_i^s} + \underbrace{\frac{k_i k_j}{k^2}\,\tilde{u}_j}_{\tilde{u}_i^d}, \tag{16}$$

where, using $k_j\tilde{u}_j = -i\,\tilde{\rho}$ from 12,

$$\tilde{u}_i^d = -\frac{i\,k_i\,\tilde{\rho}}{k^2}, \qquad i\,k_i\tilde{u}_i^s = 0, \qquad i\,k_i\tilde{u}_i^d = \tilde{\rho}. \tag{17}$$

The mean mode $\boldsymbol{k} = 0$ is excluded from 16 and requires $\tilde{\rho}(\mathbf{0}) = 0$.

3 Example: MHD with large conductivity

3.1 Ideal MHD

Let us first consider the case of ideal MHD, i.e., the dynamics of charged/ionized fluids with infinite conductivity. Ohm's law provides the freeze-in condition for the electric field,

$$\boldsymbol{E} \simeq -\boldsymbol{u}\times\boldsymbol{B}\,, \quad \boldsymbol{u}\cdot\boldsymbol{E} = 0\,., \tag{18}$$

which is equivalent to setting $E^\mu = U_\nu F^{\mu\nu} = 0$. On the other hand, Maxwell equation,

$$\partial_t \boldsymbol{E} = \boldsymbol{\nabla}\times\boldsymbol{B} - \boldsymbol{J}\,, \tag{19}$$

can be reduced to the following expression, under the assumption that the displacement current is negligible compared to the term $\sigma\boldsymbol{E}$ that appears in $\boldsymbol{J}$ from Ohm's law,

$$\boldsymbol{J} = \boldsymbol{\nabla}\times\boldsymbol{B}\,. \tag{20}$$

Let us now consider relativistic Gauss' law, taking $\gamma \to 1$ [2],

$$\boldsymbol{\nabla}\cdot\boldsymbol{E} = J^0 = \gamma(\rho_e + \sigma\boldsymbol{u}\cdot\boldsymbol{E}) = \rho_e/\gamma + \boldsymbol{u}\cdot\boldsymbol{J}\,, \tag{21}$$

where ρ_e is the charge density in the fluid rest frame. Taking divergence of Eq. (18), we find a closed expression for ρ_e:

$$\boldsymbol{\nabla}\cdot\boldsymbol{E} = -\boldsymbol{\nabla}\cdot(\boldsymbol{u}\times\boldsymbol{B}) = -\boldsymbol{B}\cdot\boldsymbol{\omega} + \boldsymbol{u}\cdot\boldsymbol{J} = \rho_e/\gamma + \boldsymbol{u}\cdot\boldsymbol{J} \Rightarrow \rho_e = -\gamma\,\boldsymbol{B}\cdot\boldsymbol{\omega}\,, \tag{22}$$

where $\boldsymbol{\omega} = \boldsymbol{\nabla}\times\boldsymbol{u}$ is the vorticity. Therefore, in ideal MHD, the charge density cannot be arbitrarily set to zero under the assumption of quasineutralitiy and it needs to be consistent with the evolution of ideal MHD.

The induction equation is

$$\partial_t\boldsymbol{B} = -\boldsymbol{\nabla}\times\boldsymbol{E} = \boldsymbol{\nabla}\times(\boldsymbol{u}\times\boldsymbol{B}) = (\boldsymbol{B}\cdot\boldsymbol{\nabla})\boldsymbol{u} - \boldsymbol{B}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) - (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{B}\,. \tag{23}$$

Finally, the Lorentz force is

$$f^0_{\rm Lor} = \boldsymbol{E}\cdot\boldsymbol{J} = -(\boldsymbol{u}\times\boldsymbol{B})\cdot\boldsymbol{J} = \boldsymbol{u}\cdot(\boldsymbol{J}\times\boldsymbol{B})\,, \tag{24}$$

$$f^i_{\rm Lor} = J^0 E_i + (\boldsymbol{J}\times\boldsymbol{B})_i = -(\rho_e + \boldsymbol{u}\cdot\boldsymbol{J})(\boldsymbol{u}\times\boldsymbol{B})_i + (\boldsymbol{J}\times\boldsymbol{B})_i\,. \tag{25}$$

We note that the contribution from ρ_e to the Lorentz force cannot be arbitrarily neglected. This is, however, usually done in MHD systems under the assumption of small fluid perturbations, such that $\boldsymbol{E} \sim \mathcal{O}(\boldsymbol{u})$, $J^0 \sim \mathcal{O}|u|$ and, hence, $J^0|\boldsymbol{E}| \sim \mathcal{O}(u^2)$.

In general, for ideal MHD systems, the electric field should satisfy

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = J^0 = -\boldsymbol{B} \cdot \boldsymbol{\omega} + \boldsymbol{u} \cdot \boldsymbol{J}\,, \tag{26}$$

which is automatically satisfied when the electric field is not a dynamical variable.

3.2 Resistive MHD

This can be generalized to a system with large but finite conductivity. Then, Ohm's law is [2]

$$\boldsymbol{E} = \eta\,(\boldsymbol{J} - \rho_e \boldsymbol{u}) - \boldsymbol{u} \times \boldsymbol{B}\,, \tag{27}$$

where $\eta = 1/\sigma$ is small. Note that setting $\eta = 0$ recovers the ideal MHD limit.

Taking the divergence of Eq. (27), together with Gauss' law Eq. (21), we get

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = -\boldsymbol{\nabla} \cdot (\eta \rho_e \boldsymbol{u}) - \boldsymbol{B} \cdot \boldsymbol{\omega} + \boldsymbol{u} \cdot \boldsymbol{J} = \rho_e + \boldsymbol{u} \cdot \boldsymbol{J} \Rightarrow \rho_e + \boldsymbol{\nabla} \cdot (\eta \rho_e \boldsymbol{u}) = -\boldsymbol{B} \cdot \boldsymbol{\omega}\,, \tag{28}$$

which now provides a differential equation that ρ_e should satisfy.

The induction equation and the Lorentz force become

$$\partial_t \boldsymbol{B} = \boldsymbol{\nabla} \times (\boldsymbol{u} \times \boldsymbol{B} - \eta \boldsymbol{J} + \eta \rho_e \boldsymbol{u})\,, \tag{29}$$

$$f^0_{\rm Lor} = \boldsymbol{E} \cdot \boldsymbol{J} = \boldsymbol{u} \cdot (\boldsymbol{J} \times \boldsymbol{B}) + \eta \boldsymbol{J}^2 - \eta \rho_e \boldsymbol{u} \cdot \boldsymbol{J}\,, \tag{30}$$

$$f^i_{\rm Lor} = J^0 E_i + (\boldsymbol{J} \times \boldsymbol{B})_i = (\rho_e + \boldsymbol{u} \cdot \boldsymbol{J})(\eta \boldsymbol{J} - \eta \rho_e \boldsymbol{u} - \boldsymbol{u} \times \boldsymbol{B}) + (\boldsymbol{J} \times \boldsymbol{B})_i\,. \tag{31}$$

$$f^i_{\rm Lor} = \gamma \rho_e (\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B}) + \gamma \sigma \big[(\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B}) \times \boldsymbol{B}) + \boldsymbol{E}(\boldsymbol{u} \cdot \boldsymbol{E})\big]\,, \tag{32}$$

$$f^0_{\rm Lor} = \gamma \rho_e \boldsymbol{u} \cdot \boldsymbol{E} + \gamma \sigma \boldsymbol{E} \cdot \big(\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B}\big)\,. \tag{33}$$

3.3 Displacement current

More interesting is the case when the displacement current cannot be neglected. In this case, Ampère's law does no longer act as a constrain equation ensuring that $\boldsymbol{J} = \boldsymbol{\nabla} \times \boldsymbol{B}$, but instead provides a dynamical equation to advance $\boldsymbol{E}$,

$$\partial_t \boldsymbol{E} = \boldsymbol{\nabla} \times \boldsymbol{B} - \boldsymbol{J}\,. \tag{34}$$

Therefore, $\boldsymbol{J}$ is not in generally known and it needs to be computed via Ohm's law

$$\boldsymbol{J} = \rho_e \boldsymbol{u} + \sigma\,(\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B})\,. \tag{35}$$

This also implies that $\boldsymbol{E}$, and hence, $\boldsymbol{\nabla} \cdot \boldsymbol{E}$, is not fixed by Ohm's law, which was providing an equation for ρ_e as a function of the other fields in previous cases. In this case, ρ_e is required to follow the continuity equation,

$$\partial_\mu J^\mu = \partial_t J^0 + \boldsymbol{\nabla} \cdot \boldsymbol{J} = 0\,, \tag{36}$$

which is equivalent to

$$\partial_t J^0 + \boldsymbol{\nabla} \cdot (\rho_e \boldsymbol{u}) + \sigma \big[J^0 + \boldsymbol{B} \cdot \boldsymbol{\omega} - \boldsymbol{u} \cdot (\boldsymbol{\nabla} \times \boldsymbol{B})\big] = 0\,. \tag{37}$$

4 Divergence cleaning in MHD

In [3, 4, 5, 6] it was pointed out that numerical errors arising from the imprecise treatment of the divergence equations of the $\boldsymbol{B}$ and $\boldsymbol{E}$ can be mitigated with the use of Generalized Lagrange Multiplayer (GLM) method,

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