Yang-Mills theory, lattice gauge theory and simulations

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Overview

Introduction and physical context

Classical Yang-Mills theory

Lattice gauge theory

Simulating the Glasma in 2+1D

Lattice gauge theory

Motivation

Motivation

Recap: Yang-Mills equations in temporal gauge ($A_0 = 0$)
Equations of motion

$$\partial_0 \pi^i = \partial_j F^{ji} + ig \left[A_j, F^{ji} \right]$$
$$\partial_0 A_i = \pi^i$$

Gauss constraint

$$\partial_i \pi^i + ig \left[A_i, \pi^i \right] = 0$$

Assuming we have consistent initial conditions $A_i(t_0, \vec{x})$, $\pi^i(t_0, \vec{x})$, which satisfy the constraint, can we perform the "time evolution" from t_0 to $t > t_0$ numerically without violating the constraint?

Motivation

Standard method: finite differences

Discretize Minkowski space **M** as a hypercubic lattice Λ with spacings a^μ.

$$\Lambda = \{x \in \mathbf{M} \,|\, x = \sum_{\mu=0}^{3} n_\mu \hat{a}^\mu, \quad n_\mu \in \mathbb{Z}\}, \quad \hat{a}^\mu = a^\mu \hat{e}_\mu \in \mathbf{M} \text{ (no sum)},$$

and unit vectors $\hat{e}_\mu$, e.g. $\hat{e}_0 = (1,0,0,0)^T$, $\hat{e}_1 = (0,1,0,0)^T$, etc.
Use finite difference approximations for derivatives, e.g. the forward difference

$$\partial_\mu^F \phi(x) \equiv \frac{\phi(x + \hat{a}^\mu) - \phi(x)}{a^\mu} \simeq \partial_\mu \phi(x) + \mathcal{O}(a^\mu),$$

and the backward difference

$$\partial_\mu^B \phi(x) \equiv \frac{\phi(x) - \phi(x - \hat{a}^\mu)}{a^\mu} \simeq \partial_\mu \phi(x) + \mathcal{O}(a^\mu),$$

Yang-Mills theory on a lattice: first attempt

Naive approach: put Yang-Mills fields on the hypercubic lattice Λ

"Recipe" for the finite difference method:

- At each point $x \in \Lambda$ define a field value $A_\mu(x) \in \mathfrak{su}(N_c)$
- Derivatives of A_μ are approximated using finite differences ∂^F_ν or ∂^B_ν
- Integrals over **M** are approximated as sums over Λ

In principle, this recipe yields a finite difference approximation of the Yang-Mills equations

Problem: what about gauge symmetry?

Yang-Mills theory on a lattice: first try

Naive approach: put Yang-Mills fields on the hypercubic lattice Λ

Gauge field in the continuum:

$$A_\mu : \mathbf{M} \to \mathfrak{su}(N_c)$$

Gauge field on the lattice:

$$A_\mu : \Lambda \to \mathfrak{su}(N_c)$$

Discretized version of gauge transformation?

Consider a "lattice gauge transformation" $\Omega(x) : \Lambda \to \mathrm{SU}(N_c)$ acting on the gauge field A_μ:

$$A'_\mu(x) \equiv \Omega(x) \left(A_\mu(x) + \frac{1}{ig} \partial^F_\mu \right) \Omega^\dagger(x)$$

Yang-Mills theory on a lattice: first attempt

Naive lattice gauge transformation:

$$A'_\mu(x) \equiv \Omega(x) \left(A_\mu(x) + \frac{1}{ig} \partial^F_\mu \right) \Omega^\dagger(x)$$

$\Rightarrow A'_\mu$ is not traceless or hermitian, i.e. not an element of $\mathfrak{su}(N_c)$!

First term $\Omega(x) A_\mu(x) \Omega^\dagger(x)$ is traceless and hermitian.

However, the second term is neither:

$$\begin{aligned} \frac{1}{ig} \Omega(x) \partial^F_\mu \Omega^\dagger(x) &= \frac{1}{iga^\mu} \Omega(x) \left(\Omega^\dagger(x + \hat{a}^\mu) - \Omega^\dagger(x) \right) \\ &= \frac{1}{iga^\mu} \left(\Omega(x) \Omega^\dagger(x + \hat{a}^\mu) - \mathbf{1} \right) \end{aligned}$$

The finite difference approximation of the derivative ∂_μ in the gauge transformation is a problem.

Yang-Mills theory on a lattice: first attempt

As we saw previously, gauge symmetry guarantees us that the equations of motion (here in temporal gauge $A_0 = 0$)

$$\partial_0 \pi^i = \partial_j F^{ji} + ig\left[A_j, F^{ji}\right]$$
$$\partial_0 A_i = \pi^i$$

conserve the Gauss constraint

$$\partial_i \pi^i + ig\left[A_i, \pi^i\right] = 0$$

If we cannot properly formulate gauge symmetry in the discretized version, then there is no guarantee that the discretized Gauss constraint will not be violated.

Yang-Mills theory on a lattice: first attempt

Second problem with this approach: how exactly should one approximate a term like

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig\,[A_\mu, A_\nu] \quad ?$$

Should we use forward differences ∂_μ^F, backward differences ∂_μ^B or some other higher order finite difference scheme?

$\Rightarrow$ A lot of freedom in choosing the specific discretization. Should we just guess?

Can we construct a "consistent" discretization of Yang-Mills theory that has a conserved Gauss constraint without much guesswork?

Yang-Mills theory on a lattice: first attempt

The naive finite difference approach to solving the Yang-Mills equations on a lattice fails when considering gauge symmetry.

We need two "ingredients" to come up with a numerical method that retains some notion of gauge symmetry:

- Different degrees of freedom (other than A_μ), whose gauge transformation law does not involve derivatives of the gauge transformation matrices $\Omega(x)$: gauge links
- A method for deriving "consistent" discretized equations of motion with a conserved Gauss constraint: method of variational integrators

Variational integrators

Variational integrators: basic idea

Variational integrators are a specific numerical integrators that follow from a variational principle.

Usual finite difference approach:

- Vary action S to obtain equations of motion (EOM)
- Replace derivatives in EOM with finite difference approximations to obtain discrete EOM
- Solve discrete EOM on a computer

Variational integrator approach:

- Discretize action S first (replace derivatives with finite differences, integrals with sums, etc) to obtain discretized action S'
- Vary discrete action S' to obtain discrete EOM
- Solve discrete EOM on a computer

Variational integrators: basic idea

Variational integrators: "discretize first, then vary"

Advantage of a variational integrator: if the discretized action S' has some of the symmetry properties of the continuum action S, then the discrete EOM will also respect these symmetries.

Example: if some symmetry of the action S leads to some conservation law (Noethers theorem), then the discrete analogue of that symmetry for S' leads to a discretized version of that conservation law

In the context of Yang-Mills theory: a discretized version of the Yang-Mills action with gauge symmetry leads to discrete equations of motion that conserve a discrete version of the Gauss constraint

Example: planetary motion

Consider a simple mechanical (i.e. not field theoretical) model: the motion of planets around the sun

Trajectory of a planet (mass)

$$\vec{r}(t) = (x(t), y(t))^T$$

Action (mass $m = 1$)

$$S[\vec{r}(t)] = \int_{-\infty}^{\infty} dt \left(\frac{1}{2} (\partial_0 \vec{r})^2 - V(|\vec{r}(t)|) \right)$$

with potential (all constants set to one)

$$V(r) = -\frac{1}{r}$$

Example: planetary motion

Vary the action to derive the equations of motion

$$\delta S[\vec{r}(t), \delta\vec{r}] = \int_{-\infty}^{\infty} dt \left(-\partial_0^2 \vec{r} - \nabla V(\vec{r}(t))\right) \cdot \delta\vec{r}$$

Introduce momentum

$$\vec{p}(t) \equiv \partial_0 \vec{r}(t)$$

Equations of motion

$$\partial_0 \vec{p}(t) = -\nabla V(\vec{r}(t))$$
$$\partial_0 \vec{r}(t) = \vec{p}(t)$$

Example: planetary motion

Action is invariant under rotations

$$\vec{r}' = R\vec{r}, \qquad R = \begin{pmatrix} \cos\omega & -\sin\omega \\ \sin\omega & \cos\omega \end{pmatrix}$$

Action

$$S[\vec{r}'(t)] = \int_{-\infty}^{\infty} dt \left(\frac{1}{2} \left(\partial_0 \vec{r}'\right)^2 - V(|\vec{r}'(t)|) \right) = S[\vec{r}(t)]$$

Consequence: angular momentum is conserved

Example: planetary motion

Action is invariant under infinitesimal rotations

$$\vec{r}' = R\vec{r}, \qquad R = \begin{pmatrix} \cos\omega & -\sin\omega \\ \sin\omega & \cos\omega \end{pmatrix}$$

Expand for small angles ω

$$\vec{r}' = \vec{r} + \Omega\vec{r} + \mathcal{O}(\omega^2), \qquad \Omega = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}$$

Write $\delta\vec{r} = \Omega\vec{r}$ and vary action

$$\delta S[\vec{r}, \delta\vec{r}] = \int_{-\infty}^{\infty} dt \left[\left(-\partial_0 \vec{p} - \nabla V(\vec{r}) \right) \cdot \delta\vec{r} + \partial_0 \left(\vec{p} \cdot \delta\vec{r} \right) \right] = 0$$

Note: $\delta\vec{r}(t)$ does not have compact support

Example: planetary motion

Action is invariant under infinitesimal rotations

$$\delta S[\vec{r}, \delta\vec{r}] = \int_{-\infty}^{\infty} dt \left[\left(-\partial_0 \vec{p} - \nabla V(\vec{r}) \right) \cdot \delta\vec{r} + \partial_0 \left(\vec{p} \cdot \delta\vec{r} \right) \right] = 0$$

Left term vanishes: equations of motion
Right term: yields conservation law (Noether's first theorem)

$$\partial_0 \left(\vec{p} \cdot \delta\vec{r} \right) = 0$$

Use $\delta r = \Omega\vec{r} = \left(-\omega y(t), \omega x(t)\right)^T$ and find

$$\partial_0 L = \partial_0 \left(-p_x(t) y(t) + p_y(t) x(t) \right) = 0.$$

Angular momentum $L = -p_x y + p_y x$ is conserved.

Example: planetary motion

Let's simulate this system numerically!
Naive approach using forward differences: Forward Euler scheme

$$\partial_0 \vec{p}(t) = -\nabla V(\vec{r}) \qquad \Rightarrow \partial_0^F \vec{p}(t) = -\nabla V(\vec{r}(t))$$
$$\partial_0 \vec{r}(t) = \vec{p}(t) \qquad \Rightarrow \partial_0^F \vec{q}(t) = \vec{p}(t)$$

Discrete "time evolution": time step $a^0 = \Delta t$

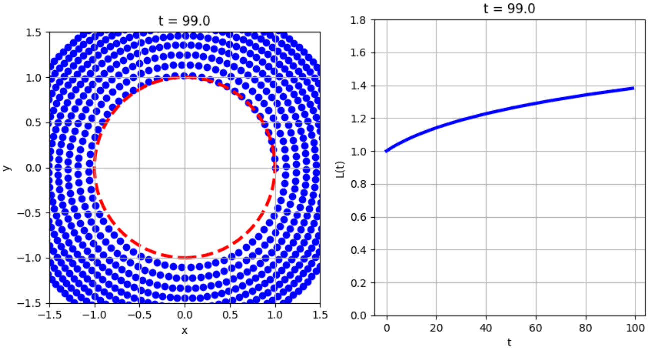
$$\vec{p}(t + \Delta t) = \vec{p}(t) - \Delta t \nabla V(\vec{r}(t))$$
$$\vec{q}(t + \Delta t) = \vec{q}(t) + \Delta t \vec{p}(t)$$

Conserved angular momentum?

$$L(t) = -p_x(t) y(t) + p_y(t) x(t)$$

Example: planetary motion

Animation of simulation data: trajectory $\vec{r}(t)$ and angular momentum $L(t)$ as a function of time t from Forward Euler scheme



Trajectory unstable, no conserved angular momentum

Example: planetary motion

Variational integrator approach: formulate discretized action with rotational symmetry built in

$$S[\vec{r}(t)] = \Delta t \sum_t \left(\frac{1}{2} \left(\partial_0^F \vec{r}(t) \right)^2 - V(|\vec{r}(t)|) \right)$$

Invariance:

$$V(|\vec{r}'(t)|) = V(|R\vec{r}(t)|) = V(|\vec{r}(t)|)$$

$$\partial_0^F \vec{r}'(t) = R\partial_0^F \vec{r}(t), \quad \Rightarrow \quad \left(\partial_0^F \vec{r}'(t) \right)^2 = \left(\partial_0^F \vec{r}(t) \right)^2$$

Example: planetary motion

Discrete action to be "varied":

$$S[\vec{r}(t)] = \Delta t \sum_t \left(\frac{1}{2} \left(\partial_0^F \vec{r}(t) \right)^2 - V(|\vec{r}(t)|) \right)$$

The action is now a function of the positions $\vec{r}(t)$ at the discrete times $t_0, t_1, t_2, \ldots$

The "variation" $\delta S[\vec{r}, \delta r]$ is now just the total differential dS.

I will keep using the $\delta S[\vec{r}, \delta r]$ notation anyways, even though I'm not using functional derivatives.

Example: planetary motion

Useful formulae for finite differences

The product rule(s)

$$\begin{aligned}
\partial_0^B(f(t)g(t)) &= (f(t)g(t) - f(t-\Delta t)g(t-\Delta t))\,/\Delta t \\
&\quad + f(t-\Delta t)g(t)/\Delta t - f(t-\Delta t)g(t)/\Delta t \\
&= \partial_0^B f(t)g(t) + f(t-\Delta t)\partial_0^B g(t)
\end{aligned}$$

and

$$\partial_0^F(f(t)g(t)) = \partial_0^F f(t)g(t) + f(t+\Delta t)\partial_0^F g(t)$$

Switching between forward/backward differences

$$\partial_0^F f(t) = \partial_0^B f(t+\Delta t)$$

Example: planetary motion

Variation of the discrete action

$$\delta S[\vec{r},\delta\vec{r}] = \Delta t \sum_t \left(\partial_0^F \vec{r}(t)\cdot\partial_0^F \delta\vec{r}(t) - \nabla V(|\vec{r}(t)|)\cdot\delta\vec{r}(t)\right)$$
$$= \Delta t \sum_t \Big[\left(-\partial_0^B\partial_0^F \vec{r}(t) - \nabla V(|\vec{r}(t)|)\right)\cdot\delta\vec{r}(t)$$
$$+ \partial_0^F \left(\partial_0^F \vec{r}(t)\cdot\delta\vec{r}(t)\right)\Big] = 0$$

Second term vanishes, because $\delta r(t)$ has "compact support". Introduce $\vec{p}(t) = \partial_0^F \vec{r}(t)$. The discrete EOM then read

$$\partial_0^B \vec{p}(t) = -\nabla V(|\vec{r}(t)|)$$
$$\partial_0^F \vec{r}(t) = \vec{p}(t)$$

Note: use of backward difference in first EOM

Example: planetary motion

Infinitesimal rotation with angle ω

$$\vec{r}' = \vec{r} + \Omega\vec{r} + \mathcal{O}(\omega^2) = \vec{r} + \delta\vec{r} + \mathcal{O}(\omega^2), \qquad \Omega = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}$$

Variation of action due to rotation

$$\delta S[\vec{r}, \delta\vec{r}] = \Delta t \sum_t \Big[\Big(-\partial_0^B \partial_0^F \vec{r}(t) - \nabla V(|\vec{r}(t)|) \Big) \cdot \delta\vec{r}(t) + \partial_0^F \Big(\partial_0^F \vec{r}(t) \cdot \delta\vec{r}(t) \Big) \Big] = 0$$

- First term vanishes (EOM)
- Second term under the sum must vanish, but $\delta r(t)$ does not have compact support

Example: planetary motion

In order to get $\delta S[\vec{r}, \delta\vec{r}] = 0$, the discrete conservation law must hold:

$$\partial_0^F \left(\partial_0^F \vec{r}(t) \cdot \delta\vec{r}(t) \right) = 0$$

$\Rightarrow$ discrete angular momentum

$$L(t) = -\partial_0^F x(t) y(t) + \partial_0^F y(t) x(t) = -p_x(t) y(t) + p_y(t) x(t)$$

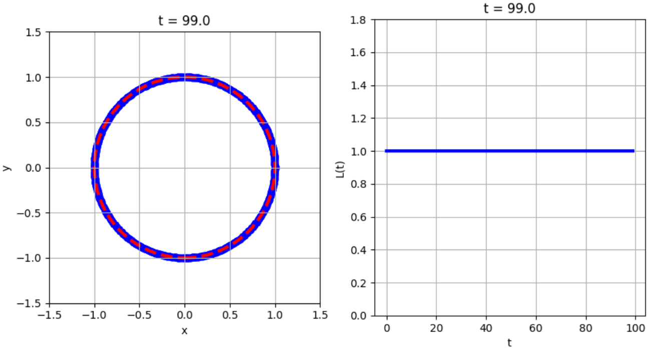
is conserved

$$\partial_0^F L(t) = 0$$

Everything completely analogous to the continuous model!

Example: planetary motion

Animation of simulation data: trajectory $\vec{r}(t)$ and angular momentum $L(t)$ as a function of time t from variational integrator



Trajectory stable, conserved angular momentum (up to numerical precision)

Example: planetary motion

Not all symmetries of the original (continuous) problem can be easily built into a discretized model.

Example: energy conservation

Energy conservation follows from the invariance under time translations $t' = t + \epsilon$.

$$\partial_0 E = \partial_0 \left(\frac{1}{2} \left(\partial_0 \vec{r}(t) \right)^2 + V(|\vec{r}(t)|) \right) = 0$$

Discretizing the time coordinate breaks this symmetry and energy is not exactly conserved in the simulation.

Example: two-body problem

One more example: **the two body problem** $(m_1 = m_2 = 1)$

$$S\left[\vec{r}_1(t), \vec{r}_2(t)\right] = \int dt \left(\frac{1}{2} \left(\partial_0 \vec{r}_1\right)^2 + \frac{1}{2} \left(\partial_0 \vec{r}_2\right)^2 - V(|\vec{r}_1(t) - \vec{r}_2(t)|) \right)$$

Equations of motion from $\delta S = 0$:

$$\begin{aligned} \vec{p}_1 &\equiv \partial_0 \vec{r}_1 \\ \vec{p}_2 &\equiv \partial_0 \vec{r}_2 \\ \partial_0 \vec{p}_1 &= -\nabla_{(1)} V(|\vec{r}_1 - \vec{r}_2|) \\ \partial_0 \vec{p}_2 &= -\nabla_{(2)} V(|\vec{r}_1 - \vec{r}_2|) \end{aligned}$$

Example: two-body problem

$$S\left[\vec{r}_1(t), \vec{r}_2(t)\right] = \int dt \left(\frac{1}{2} \left(\partial_0 \vec{r}_1\right)^2 + \frac{1}{2} \left(\partial_0 \vec{r}_2\right)^2 - V(|\vec{r}_1(t) - \vec{r}_2(t)|) \right)$$

Symmetries and conservation laws:

- Invariance under rotations: $\vec{r}_i' = R\vec{r}_i$
  $\Rightarrow$ angular momentum conservation

$$\partial_0 L(t) = 0$$

- Invariance under spatial translations $\vec{r}_i' = \vec{r} + \vec{\epsilon}$
  $\Rightarrow$ linear momentum conservation

$$\partial_0(\vec{p}_1 + \vec{p}_2) = 0$$

- Invariance under time translations $t' = t + \epsilon$
  $\Rightarrow$ energy conservation

$$\partial_0 E = \partial_0 \left(\frac{1}{2} \vec{p}_1^2 + \frac{1}{2} \vec{p}_2^2 + V(|\vec{r}_1 - \vec{r}_2|) \right) = 0$$

Example: two-body problem

Discretized action for the two-body problem

$$S\left[\vec{r}_1(t), \vec{r}_2(t)\right] = \Delta t \sum_t \left(\frac{1}{2}\left(\partial_0^F \vec{r}_1\right)^2 + \frac{1}{2}\left(\partial_0^F \vec{r}_2\right)^2 - V(|\vec{r}_1(t) - \vec{r}_2(t)|) \right)$$

Symmetries and conservation laws:

- Invariance under rotations: $\vec{r}_i' = R\vec{r}_i$
  $\Rightarrow$ angular momentum conservation

$$\partial_0^F L(t) = 0$$

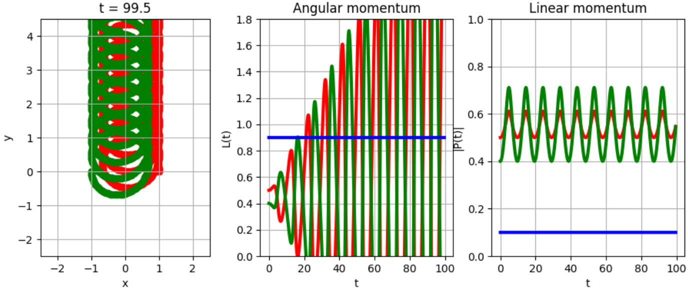
- Invariance under spatial translations $\vec{r}_i' = \vec{r} + \vec{\epsilon}$
  $\Rightarrow$ linear momentum conservation

$$\partial_0^F (\vec{p}_1(t) + \vec{p}_2(t)) = 0$$

- ~~Invariance under time translations $t' = t + \epsilon$~~
  ~~$\Rightarrow$ energy conservation~~

Example: two-body problem

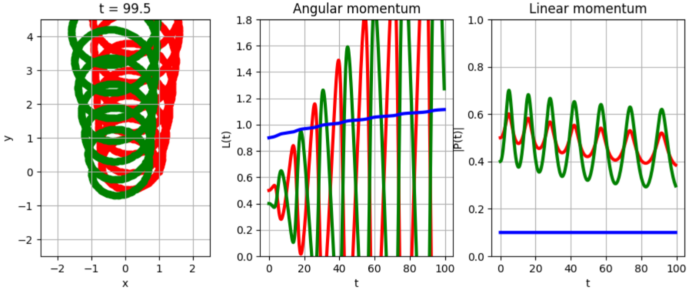
Motion of two bodies using variational integrator



Discrete angular momentum and linear momentum exactly conserved.

Example: two-body problem

Comparison: simple forward Euler scheme



Discrete angular momentum not conserved. Linear momentum happens to be conserved.

Variational integrators: summary

- The method of variational integrators removes a lot of guesswork when deriving numerical schemes to solve initial value problems.
- Discretized actions can "keep" symmetries of their respective continuum analogues
- Symmetries of discretized actions lead to discretized conservation laws (Noether's theorem - discrete version)

Yang-Mills on the lattice and gauge symmetries

We will construct a discretized action for Yang-Mills theory, which "keeps" gauge symmetry.

$\Rightarrow$ Conserved Gauss constraint when solving Yang-Mills equations numerically

Variational integrators: summary

Literature:

- J. E. Marsden and M. West, "Discrete mechanics and variational integrators", Acta Numerica, 2001
- Adrián J. Lew, Pablo Mata A, "A Brief Introduction to Variational Integrators", chapter 5 of Peter Betsch (editor), "Structure-preserving Integrators in Nonlinear Structural Dynamics and Flexible Multibody Dynamics", CISM International Centre for Mechanical Sciences 2016, Springer, Cham