Numerical Relativity and Variational Integrators

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History of numerical relativity:

1970's: Pioneers Ken Eppley, Larry Smarr (--> NCSA)

1980's: Growing field

1990's: LIGO! LISA! Gravitational waves!
- Realistic 3D simulations needed for binary black hole collisions, binary neutron star collisions, supernova explosions, etc.
Late 1990's: Binary Black Hole Grand Challenge Project

- 5 year, $5M flop?
- Numerical relativity is harder than we thought.

Why? One reason is stability. We need to simulate 2 BH's for time $t \sim 1000 \text{ GM}/c^3$. Naïve codes will simulate 1 BH for about $t \sim \text{ few GM}/c^3$ before crashing. After years of tweaking, current codes can achieve about $t \sim 100 \text{ GM}/c^3$ for 2 BH's (~ one orbital period).

Numerical relativity codes crash due to a subtle instability. We're just now beginning to understand the nature of this instability.
Structure of GR

Spacetime formulation

basic variables: 4D metric $g_{\mu\nu}$

action:

$$S[g] = \int d^4 x \sqrt{-g} R$$

equations of motion:

$$G_{\mu\nu} = 0$$

But we want to specify initial data and evolve forward in time, to see what happens. We need a formulation in which space and time are split.
3+1 (Hamiltonian) formulation:

--due to Dirac (late 50's) and Arnowitt, Deser, Misner (1960's)

basic variables: \( g_{ij}, P^{ij}, \alpha, \beta^i \)

3D metric

~extrinsic curvature

lapse function

shift vector

time

proper time = \( \alpha dt \)

\( \beta^i dt \)
3+1 (Hamiltonian) formulation:

action: \[ S[g, P, \alpha, \beta] = \int dt \left( \int d^3 x \, P^{ij} \dot{g}_{ij} - H \right) \]

Hamiltonian: \[ H = \int d^3 x \left( \alpha C + \beta^i C_i \right) \]

Hamiltonian constraint:
\[ C = 2 \, P^{ij} P_{ij} - P^2 - \sqrt{g} \, R / 2 \]

Momentum constraint:
\[ C_i = -2 \, D_j P^j_i \]
### 3+1 (Hamiltonian) formulation:

**Einstein's theory is both **underdetermined** and **overdetermined**.**

It is underdetermined because the equations of motion do not determine the values of the constraint multipliers (lapse and shift).

It is overdetermined because the variables that *are* determined (metric and extrinsic curvature) are also subject to constraints.
The underdetermined property just means that the equations do not tell us how the coordinate system should be extended into the future. We must decide that for ourselves.

The overdetermined property is not a problem, *analytically*. As long as the initial data satisfy the constraints, they will continue to satisfy the constraints under Hamiltonian evolution.
But the overdetermined property *is* a problem numerically. Codes to date use *free evolution*: solve the constraints initially for $g_{ij}$ and $P^{ij}$, then evolve freely with Hamilton's equations.
Analytically, data on the constraint hypersurface will always stay there. Numerical errors move the solution off the constraint hypersurface where exponentially growing, “constraint violating” modes take over.

We need a way to keep the numerical solution on the constraint hypersurface.
Variational integrator approach to numerical modeling
(Marsden et al)

Standard approach:

Continuum action

\( \text{vary} \)

Continuum equations of motion

\( \text{discretize} \)

Discrete equations of motion

VI approach:

Continuum action

\( \text{discretize} \)

Discrete action

\( \text{vary} \)

Discrete equations of motion
Example: Hamiltonian mechanics

\[ S[p, x] = \int_{t_1}^{t_2} dt \left[ p \dot{x} - H(x, p) \right] \]

Second order discretization with x's at temporal nodes and p's at temporal zone centers

\[ S[p, x] = \sum_{n=1}^{N} \Delta t \left[ p^n \frac{(x^n - x^{n-1})}{\Delta t} - H(x^n, p^n) \right] \]

\[ x^n = \frac{x^n + x^{n-1}}{2} \]
vary with respect to $x^1, x^2, ..., x^{N-1}, p^1, p^2, ..., p^N$

with $x^0$ and $x^N$ held fixed.

\[
\frac{x^{n+1} - x^n}{\Delta t} = \left( \frac{\partial H}{\partial p} \right)^{n+1}, \quad n = 0, 1, ..., N-1
\]

\[
\frac{p^{n+1} - p^n}{\Delta t} = -\left( \frac{\partial H}{\partial x} \right)^{n+1}, \quad n = 1, 2, ..., N-1
\]

Note:

\[
F^n = F(x^n, p^n) = F((x^n + x^{n-1})/2, p^n)
\]

Therefore:

\[
F^n = F(x^n, p^n) = F((x^n + 2x^{n-1} + x^{n-2})/4, (p^n + p^{n+1})/2)
\]
Specific example: two harmonic oscillators with nonlinear coupling.
Why have I focused on the energy? Because energy conservation for a mechanical system is analogous to the preservation of constraints in general relativity.

To see this more clearly...reformulate mechanics with $t$ promoted to the status of a dynamical variable:

$$S[x, p, t, \pi, \alpha] = \int_\sigma d\sigma \left[ p \dot{x} + \pi \dot{t} - \alpha C \right]$$

$$\alpha = \frac{dt}{d\sigma}$$

$$C \equiv \pi + H(x, p)$$

Like general relativity, this formulation of mechanics is both underdetermined and overdetermined. Hey, let's apply the VI construction to this action!
Discretize and vary...we get more than we bargained for!

\[
\frac{x^{n+1} - x^{n}}{\Delta \sigma} = \left( \alpha \frac{\partial C}{\partial p} \right)^{n+1}, \quad \frac{p^{n+1} - p^{n}}{\Delta \sigma} = - \left( \alpha \frac{\partial C}{\partial x} \right)^{n+1}
\]

\[
\frac{t^{n+1} - t^{n}}{\Delta \sigma} = \alpha^{n+1}, \quad \frac{\pi^{n+1} - \pi^{n}}{\Delta \sigma} = 0
\]

\[C^{n+1} = 0\]

Unlike the continuum theory, the discrete theory is neither underdetermined nor overdetermined. Rather, the equations of motion determine the lapse (time step) during the evolution and keep the constraint satisfied!
**Specific example:**
two harmonic oscillators with nonlinear coupling.
Let's apply the VI construction to general relativity:

\[ S[g, P, \alpha, \beta] = \int dt \, d^3x \left( P^{ij} \dot{g}_{ij} - \alpha C - \beta^i C_i \right) \]

\[ C = 2 P^{ij} P_{ij} - P^2 - \sqrt{g} \, R/2 \]

\[ C_i = -2 D_j P^j_i \]

Discretize and vary

Slow down, let's look at some test cases first.
Example: GR with plane symmetry described by the model

$$g_{ij} = \begin{pmatrix} g(x) & 0 & 0 \\ 0 & h(x) & 0 \\ 0 & 0 & h(x) \end{pmatrix}$$

$$P^{ij} = \begin{pmatrix} P(x) & 0 & 0 \\ 0 & Q(x) & 0 \\ 0 & 0 & Q(x) \end{pmatrix}$$

$$S[g, h, P, Q, \alpha, \beta] = \int dt \ dx \left( P \dot{g} + 2 Q \dot{h} - \alpha C - \beta^1 C_1 \right)$$

$$C = \frac{1}{\sqrt{g h}} \left[ P^2 g^2 - 4 P Q g h + h h'' - \frac{h h' g'}{2 g} - \frac{(h')^2}{4} \right]$$

$$C_1 = -2 g P' - g' P + 2 h' Q$$
Solutions are cosmologies with a *big crunch*.

Lapse after the second timestep.

Lapse after 5, 10, 15, etc timesteps. The lapse “collapses” as the singularity is approached.
Log of the L2 norm of the Hamiltonian constraint, for solutions of varying numerical accuracy.

With free evolution, the constraint violation would continue to grow exponentially.
Lessons:

- The form of the VI equations depends on the choice of cell centered or node centered data in space and in time, for each variable. This choice is very important!

- The “P-dot” equations range over discrete times $n = 1, \ldots, N-1$. The other equations have range $n = 0, \ldots, N-1$. What's up with that?
Before we begin the generic evolutionary step with \( n=1 \), the \( n=0 \) subset of the equations of motion must be solved. This subset includes the “g-dot” equations, Hamiltonian constraint, and momentum constraints. The “g-dot” equations give the definitions of the momenta (extrinsic curvature) in terms of the velocities (g-dot).

The \( n=0 \) equations are a discrete expression of the initial value problem of general relativity. We must first solve these equations to obtain coordinates and momenta that lie on the constraint hypersurface. These data are evolved forward in time starting with the discrete equations at \( n=1 \).
Do the $n=0$ equations always have a solution?

**NO!**

The problem posed by the $n=0$ equations is a *discrete* version of the original *thin sandwich problem* of general relativity. The thin sandwich problem says: Given the spatial metric on two nearby time slices (that is, given $g$ and $g$-dot) solve the Hamiltonian and momentum constraints for the lapse and shift.

\[
C \equiv 2 \, P^{ij} \, P_{ij} - P^2 - \sqrt{g} \, R/2 = 0
\]

\[
C_i \equiv -2 \, D_j \, P^j_i = 0
\]

\[
P_{ij} \equiv (\dot{g}_{ij} - D_i \beta_j - D_j \beta_i)/(2 \alpha)
\]

It is know that this mathematical problem is *not* well posed. In general, there is no solution.
Even in the plane symmetric model of general relativity, it is not possible to solve the $n=0$ equations for the shift vector. In that case the Hamiltonian constraint can be solved for the lapse function, so that's all I did.

**How do we proceed?** There is a recent restatement of the thin sandwich problem that leads to a well-posed system: the *conformal thin sandwich problem*. The conformal thin sandwich problem uses a “conformal—t raceless splitting” of the spatial metric and extrinsic curvature:

- Split $g_{ij}$ into a conformal factor $\phi$ and a conformal metric $h_{ij}$.
- Split $P^{ij}$ into its trace $\tau$ and trace—f ree part $A^{ij}$. 
The conformal thin sandwich construction can be described in terms of a canonical transformation (we'll need this to rewrite the action):

*old coordinates*: \( g_{ij} \)

*old momenta*: \( P^{ij} \)

*new coordinates*: \( \tau \equiv \frac{2}{3} \phi^{-6} P, \quad h_{ij} \equiv \phi^{-4} g_{ij} \)

*new momenta*: \( -\phi^6 \equiv \frac{\sqrt{g}}{\sqrt{h_0}}, \quad A^{ij} \equiv \phi^4 \left( P^{ij} - \frac{1}{3} g^{ij} P \right) \)

(where \( \sqrt{h_0} \) is fixed)
The conformal thin sandwich equations:

\[ A_{ij} = \frac{\ddot{h}_{ij}}{4\alpha} + \cdots \]

\[ \bar{D}^i \bar{D}_i \alpha = \frac{3 \dot{\tau}}{2 \ g \ \phi^2} + \cdots \]

\[ \bar{D}^i \bar{D}_i \phi = \cdots \]

\[ (\bar{\Delta}_L \beta)_i = \cdots \]

Coordinate-dot equations (define the momenta)

Hamiltonian constraint

Momentum constraints

\( \bar{D}^i \bar{D}_i \) and \( \bar{\Delta}_L \) are conformal Laplacian operators for scalars and vectors. They are generically well defined, invertible.
The initial data is specified by giving the coordinates $h_{ij}$ and $\tau$ on two neighboring time slices. The conformal thin sandwich equations are solved for the lapse $\alpha$, shift $\beta_i$, and momenta $\phi$ and $A_{ij}$.

So here's what we need do:
- Express the action in terms of the new canonical variables.
- Discretize.
- Vary.

*The n=0 equations will be well defined!*
Questions:

Q: So the $n=0$ equations are well posed. How about the $n=1, 2,...$ equations?

A: I don't know, but I suspect they are well defined too.

Q: How do we fix spatial boundary conditions? Should we excise black holes?

A: I don't know, I haven't looked into these issues yet.
More Questions:

Q: Should we be willing to give up our freedom to choose the lapse and shift?

A: This is an important issue. Researchers have spent a great deal of effort trying to find good “gauge conditions” for the lapse and shift. Good conditions should keep the spatial slices away from black hole singularities, and keep the coordinates untangled and smooth. With the VI approach, we give up the freedom to choose the lapse and shift (the equations are not underdetermined) in order to keep the constraints satisfied (the equations are not overdetermined).

I have thought about this issue a great deal. If we find it necessary to keep control over the lapse and shift, there are several promising options.
**Summary:**

The variational integrator approach to numerical modeling yields a discretization of general relativity that explicitly preserves the constraints. To insure that the discrete equations are well—posed, we must express the canonical variables in terms of the conformal—traceless splitting of the spatial metric and extrinsic curvature. The hope is that this approach will suppress the exponentially growing “constraint violating modes” that limit the run times of current numerical relativity codes.