Lectures on Numerical Relativity #3

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Outline

- What is wrong with the ADM form of equations?
- Analogy: rewriting E&M equations
- Hyperbolic formulations
- BSSN formulation
- Next lectures (tentative plan)
  - Harmonic formulations (?)
  - Initial data (August 3rd, 17th and 31st)

ADM Formalism

- Adopt the point of view of the Cauchy Problem: (Classical) 4D gravitational field is the time history of the geometry of a spacelike 3-hypersurface.
- To construct solutions, solve the initial-value problem, and integrate the dynamical eqns. along the prescribed coordinate system.
- If matter is present, its initial value/evolution eqns. must also be taken into account.
- 3+1 line element is written as

$$ds^2 = -\alpha^2 dt^2 + \gamma_{ij}(dx^i + \beta^i dt)(dx^j + \beta^j dt)$$

  where γ_{ij} is the 3-metric of the hypersurface and α and β^i are the lapse and shift functions respectively.
- Define the Extrinsic curvature, along the normal vector, $n^\mu = -\alpha \nabla^\mu t$,

$$K_{ij} = -\frac{1}{2}\mathcal{L}_n \gamma_{ij}$$

- Take $\{\gamma_{ij}, K_{ij}\}$ as dynamical variables.
- Via various projections, Einstein field eqns (in 4D) becomes 4 elliptic (constraint) equations plus 12 hyperbolic (evolution) equations.

ADM Formalism in vacuum

- Constraint equations

$$R + K^2 - K_{ij}K^{ij} = 0$$
$$D_j(K^{ij} - \gamma^{ij}K) = 0$$

where R is 3-dim Ricci scalar, D_i the covariant derivatives associated with the 3-dim metric, γ_{ij}, and K is trace of K_{ij}.

- Evolution equations

$$\begin{aligned}(\partial_t - \mathcal{L}_\beta)\gamma_{ij} &= -2\alpha K_{ij} \\ (\partial_t - \mathcal{L}_\beta)K_{ij} &= -D_i D_j \alpha + \alpha(R_{ij} + KK_{ij} - 2K_{ik}K^k{}_j)\end{aligned}$$

- *Free* evolution. (Cf. (partially) constrained evol.)
  - Solve constraints at $t = 0$.
  - Solve evolution equations for $t > 0$. Monitor (violations on) constraint equations to assess the quality of simulations.

ADM: Why is it not working?

- Most popular formalism used in 3D NR simulations in the '70 through '90s.
- Note that there are a number of exmaples in lower-D, e.g., 1D (spherical symm) or 2D (axi-symm) where the ADM form of equatoins has been successfully used especially when (partially) constrained evolution strategy was used.
- However, there haven't been serious attempts made with constrained evolutions in *3D* yet. Probably this is due to the fact that computational cost (at the moment) is too expensive for 3D simulations.
- When used in the context of *free* evolutions, 3D simulations using the ADM form of equations frequently crashed the code. One asks if the *instability* due to numerical issues in the code or some inherent problems at the continuum level?
- Need to obtain long term stable simulations forced people to look for alternative formulations of Einstein equations. There are several directions taken.

- Fully first order hyperbolic formulations:
  - Attractive in the sense that various mathematical theorems on well-posedness, existence, and uniqueness has been studied.
  - KST system, etc. but there is *no* successful simulations to date in 3D that match the success of BSSN and GH formualtions.
- Modifications on the ADM system.
  - BSSN formulations
    - Promote e.g. conformal connection function, $\tilde{\gamma}^{ij}\tilde{\Gamma}^k_{ij}$, to an *independent* variables and use momentum constraint equation to achieve stability.
    - Separating out conformal and traceless components fo the ADM system.
  - Adding constraint enforcing terms into the ADM eqn.
  - Partially constrained evolutions.
- Fully second order system
  - First used in the context of generalized harmonic formulation.

ADM system: linear analysis

- To see how the ADM system of equations could manifest instability, let us carry out linear perturbative analysis.
- Starting from the ADM system of equations (in vacuum),

$$
\begin{aligned}
(\partial_t - \mathcal{L}_\beta)\gamma_{ij} &= -2\alpha K_{ij} \\
(\partial_t - \mathcal{L}_\beta)K_{ij} &= -D_i D_j \alpha + \alpha(R_{ij} + K K_{ij} - 2K_{ik}K^k{}_j) \\
R + K^2 - K_{ij}K^{ij} &= 0 \\
D_j(K^{ij} - \gamma^{ij}K) &= 0
\end{aligned}
$$

- To make the analysis as simple as possible, let us take geodesic slicing, $\{\alpha = 1, \beta^i = 0\}$. Then equations become

$$
\begin{aligned}
\partial_t \gamma_{ij} &= -2K_{ij} \\
\partial_t K_{ij} &= R_{ij} + K K_{ij} - 2K_{ik}K^k{}_j \\
R + K^2 - K_{ij}K^{ij} &= 0 \\
D_j(K^{ij} - \gamma^{ij}K) &= 0
\end{aligned}
$$

- Consider a linear perturbation of *flat* space,

$$\gamma_{ij} = \delta_{ij} + h_{ij}$$

with $h_{ij} << 1$.

- Then with the quadratic and higher order terms all gone, the equations reduce to

$$\begin{aligned}
\partial_t h_{ij} &= -2K_{ij} \\
\partial_t K_{ij} &= R^{(1)}_{ij} \\
R^{(1)} &= 0 \\
\partial_j (K^{ij} - \delta^{ij} K) &= 0
\end{aligned}$$

where

$$\begin{aligned}
R^{(1)}_{ij} &= -\frac{1}{2}(\nabla^2_{flat} h_{ij} - \partial_j \Gamma_j - \partial_j \Gamma_i) \\
\Gamma_i &\equiv \partial_k h_{ik} - \frac{1}{2}\partial_i h, h \equiv \delta_{ij} h_{ij}
\end{aligned}$$

- Pardon sloppiness with indices, which is ok in linear order.

- HCE:

$$R^{(1)} = \delta_{ij} R^{(1)}_{ij} = -\frac{1}{2}(\nabla^2_{flat} h - 2\partial_i \Gamma_i) = -\frac{1}{2}(\partial_i \partial_i h - 2\partial_i(\partial_k h_{ik} - \frac{1}{2}\partial_i h))$$
$$= -\partial_i \partial_i h + \partial_i \partial_k h_{ik} = -\partial_i(\partial_i h - \partial_k h_{ik})$$

- Define $f_i \equiv \partial_k h_{ik} - \partial_i h$. HCE becomes

$$\partial_i f_i = 0$$

- MCE:

$$\partial_j(K^{ij} - \delta^{ij} K) = \partial_j(K^{ij} - \delta^{ij}\delta_{lk} K_{lk}) = \partial_j(-\frac{1}{2}\partial_t h^{ij} + \delta^{ij}\frac{1}{2}\partial_t h)$$
$$= -\frac{1}{2}\partial_t(\partial_j h_{ij} - \partial_i h) = -\frac{1}{2}\partial_t f_i \quad (1)$$

- Therefore, constraints are

$$\partial_i f_i = 0$$
$$\partial_t f_i = 0$$

- Fourier analysis: Take the following form of a solution, (plane waves moving in the x-direction)

$$
h_{ij} = \hat{h}_{ij} e^{i(\omega t - kx)}
$$
$$
K_{ij} = \hat{K}_{ij} e^{i(\omega t - kx)}
$$

- Then we have, from $\dot{h}_{ij}$ eqn, $\hat{K}_{ij} = -\frac{i\omega}{2}\hat{h}_{ij}$.
- Substituting the above equation to the $\dot{K}_{ij}$ eqn, we obtain,

$$
\begin{aligned}
i\omega \hat{K}_{ij} e^{i(\omega t - kx)} &= R^{(1)}_{ij} \\
\frac{\omega^2}{2}\hat{h}_{ij} e^{i(\omega t - kx)} &= R^{(1)}_{ij} \\
&= -\frac{1}{2}(\partial_l \partial_l h_{ij} - \partial_i \Gamma_j - \partial_j \Gamma_i) \\
&= \frac{1}{2}(k^2 \hat{h}_{ij} e^{i(\omega t - kx)} + \partial_i \Gamma_j + \partial_j \Gamma_i) \\
&= \frac{1}{2}(k^2 \hat{h}_{ij} e^{i(\omega t - kx)} + \partial_i \partial_k h_{jk} + \partial_j \partial_k h_{ik} - \partial_i \partial_j h)
\end{aligned}
$$

- For the previous eqn, take, for example, $\{i = x, j = x\}$ component.

$$\begin{aligned}
\frac{\omega^2}{2}\hat{h}_{xx}e^{i(\omega t - kx)} &= \frac{1}{2}(k^2\hat{h}_{xx}e^{i(\omega t - kx)} + \partial_x\partial_k h_{xk} + \partial_x\partial_k h_{xk} - \partial_x\partial_x h) \\
&= \frac{1}{2}(k^2\hat{h}_{xx}e^{i(\omega t - kx)} + 2\partial_x^2 h_{xx} - \partial_x^2 h_{xx} - \partial_x^2 h_{yy} - \partial_x^2 h_{zz}) \\
&= \frac{1}{2}(k^2\hat{h}_{yy}e^{i(\omega t - kx)} + k^2\hat{h}_{zz}e^{i(\omega t - kx)}) \\
\omega^2\hat{h}_{xx} &= k^2(\hat{h}_{yy} + \hat{h}_{zz})
\end{aligned}$$

- We can calculate other terms in a similar way. We end up with

$$\omega^2\hat{\mathbf{h}} = k^2 M\hat{\mathbf{h}}$$

where

$$\hat{\mathbf{h}} \equiv (\hat{h}_{xx}, \hat{h}_{xy}, \hat{h}_{xz}, \hat{h}_{yy}, \hat{h}_{yz}, \hat{h}_{zz})^T$$

and

- the matrix $M = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
- Calculate the eigenvalues, λ, and eigenvectors, $\mathbf{v}$.
- For $\lambda = 0$, corresponding eigenvectors

$$\begin{aligned} \mathbf{v}_1 &= (1,0,0,0,0,0) \\ \mathbf{v}_2 &= (0,0,0,1,0,0) \\ \mathbf{v}_3 &= (0,0,0,0,1,0) \end{aligned}$$

- For $\lambda = 1$, corresponding eigenvectors

$$\begin{aligned} \mathbf{v}_4 &= (2,1,1,0,0,0) \\ \mathbf{v}_5 &= (0,1,-1,0,0,0) \\ \mathbf{v}_6 &= (0,0,0,0,0,1) \end{aligned}$$

- What do these solutions mean? Since $\lambda = \frac{\omega^2}{k^2}$, $\lambda = 1$ corresponds to the solutions that travel with speed of light and $\lambda = 0$ corresponds to the solutions that travel with zero speed.
- The presence of the zero speed modes ($\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$) is troublesome. Take $\mathbf{v}_1$. You can easily check that all the $R_{ij}^{(1)}$ components are zero. This means that extrinsic curvature is constant, which also in turn means that metric components grow linearly. This growth is likely lead to an instability. This is already true at the *continuum* level.
- At the discrete level, zero speed modes are also problematic because numerical errors once generated can pile up in place growing without limit, which can lead to instabilities.

Some concepts: briefly

- Well-posed-ness: Quoting Gustafsson, Kreiss, & Oliger,
"Simply stated, the concept of well-posedness means that a well-posed problem should have a solution, that this solution should be unique, and that it should depend continuously on the problem's (initial) data."
- For well-posed evolution systems, the growth of any linear perturbation $\delta u(x,t)$ of a (background) solution $u_0(x,t)$ can be bounded as

$$||\delta u(\cdot,t)|| \leq f(t)||\delta u(\cdot,0)|| \tag{2}$$

where $f(t)$ depends on u_0 but not on $\delta u(x,0)$. In ill-posed system no such bound $f(t)$ exists. Solution depends continously on the initial data for well-posed systems.
- There are different ways to define well-posed-ness. Often expressed as a unique smooth solution that satisfies the estimate

$$||u(\cdot,t)|| \leq K e^{\alpha(t-t_0)}||u(\cdot,t_0)|| \tag{3}$$

In other words, solution $u(x,t)$ is bounded by the above estimate where K and α do *not* depend on initial data at $t = t_0$.

- Ill-posed problem:

$$u_t = -u_{xx}$$

- For initial data

$$u(x,0) = e^{i\omega x}\hat{f}(x)$$

  the solution is given by

$$u(x,t) = e^{i\omega x + \omega^2 t}\hat{f}(x)$$

- One cannot find α that is independent of ω.
- In numerical simluations, we need well-posedness in order to prevent uncontrolable growth of numerical errors. If the system of equations being used is not well-posed at a continuum level, there is no way that the discretized system would magically fix the instability problem.

- Hyperbolicity refers to algebraic conditions on the *principal* part of the equations which imply well posedness for the Cauchy problem.
- There are several different notions of hyperbolicity. Regarding quasilinear systems, strong hyperbolicity is one of the more general notions of hyperbolicity that implies well posedness of the Cauchy problem.
- In the context of first-order systems with constant coefficients in one-space dim, let
$$A = \begin{pmatrix} a_{11} & ... & a_{1m} \\ a_{21} & ... & a_{2m} \\ ... & ... & ... \\ a_{m1} & ... & a_{mm} \end{pmatrix} \text{ and } u = \begin{pmatrix} u^1(x,t) \\ u^2(x,t) \\ ... \\ u^m(x,t) \end{pmatrix}$$
Consider the initial value problem
$$\begin{aligned} \partial_t u &= A \partial_x u \\ u(x,0) &= f(x) \end{aligned}$$
- Theorem: Well-posed iff the eigenvalues, λ of A are real and there is a complete system of eigenvectors.

- Definition: Strongly hyperbolic if the eigenvalues are real and there exist a complete system of eigenvectors; weakly hyperbolic if the eigenvalues are real.
- Roughly, strong hyperbolicity $\leftrightarrow$ well posedness.
- Weakly hyperbolic system is ill-posed.
- Note that well-posedness and hyperbolicity is necessary condition, not sufficient condition for a stable numerical evolution. But certainly helps(!) to start with system of equations that are well-posed.

- Is ADM system of equations well-posed?
- Two theorems by Nagy, Ortiz, and Reula, roughly:
  - Theorem 1: For a fixed (densitized) lapse and shift, ADM system of equations is weakly hyperbolic, i.e., ill-posed.
  - Theorem 2: For a fixed (densitized) lapse and shift, BSSN-type system of equations, where (1) new variables, $f^\mu \equiv \gamma^{\nu\sigma}\Gamma^\mu_{\nu\sigma}$ are introduced and (2) Momentum constraint equations are used in the evolution equatons of f^μ, is strongly hyperbolic, i.e., well-posed.
  - $Q \equiv \gamma^b \alpha$, $\gamma \equiv \det(\gamma_{ij})$, b is constant.
  - Detailed proofs are involved and go beyond the scope of thie series.
- However, note in general, *dyanmic* lapse and shift conditions are used in real-life simulations.
- Also, well-posedness does not in itself automatically gaurantee well-behaved numerical simulations.

Analogy with E&M

- To help us to see how one might go about to find a system of equations that is better-behaved, let us go back to the E&M case.
- Remember Maxwell's equations.

$$\begin{aligned} \partial_t A_i &= -E_i - D_i \Phi \\ \partial_t E_i &= -D^j D_j A_i + D_i D^j A_j - 4\pi J_i \\ D^i E_i &= 4\pi \rho_e \end{aligned}$$

- Take time derivative of the first equation above, we get

$$-\partial_t^2 A_i + D^j D_j A_i - D_i D^j A_j = D_i \partial_t \Phi - 4\pi J_i .$$

- Note that the mixed derivative term, $D_i D^j A_j$ prevents write the equation in a manifestly hyperbolic form.
- How to eliminate the mixed derivative term?

- First way to eliminate the mixed derivative term is by choosing a gauge condition (Lorentz gauge).

$$\partial_t \Phi = -D^i A_i$$

- However, in GR, fixing the gauge *a priori* is not in general a good idea because one doesn't know if that fixed gauge is optimal for the problem at hand. It is more desirable to have a freedom to choose gauge conditions that are dynamics-dependent.
- Second way is bring Maxwell's equation into an explicitly hyperbolic form by taking the time derivative of $\dot{E}$ equation instead of $\dot{A}$. We get,

$$\partial_t^2 E_i = D_i D^j(-E_j - D_j \Phi) - D_j D^j(-E_i - D_i \Phi) - \partial_t J_i$$

- Using the constraint equations, we obtain,

$$-\partial_t^2 E_i + D_j D^j E_i = \partial_t J_i + 4\pi D_i \rho_e$$

- Some difficulties might arise in the situations where matter terms are not so smooth.

- Third way to re-writing the Maxwell's equation is by introducing an *auxiliary* variable

$$\Gamma = D^i A_i.$$

- Then $\dot{E}$ equation becomes

$$\partial_t E_i = -D_j D^j A_i + D_i \Gamma - 4\pi J_i$$

- We should consider evolution equation for Γ as well.

$$\partial_t \Gamma = \partial_t D^i A_i = D^i \partial_t A_i = -D^i E_i - D_i D^i \Phi = -D_i D^i \Phi - 4\pi \rho_e$$

First Order Hyperbolic Formulations

- Back to GR and discussion on the ADM system of equations.
- Ill-posedness of ADM system of equations (at least in the context where it has been studied) combined with the painful empirical observations of many that using the ADM system of evolutions in free evolution strategy produced countless code crashes and unstable evolutions, forced people to look for better formulations.
- Many people started to look at the fully first order formulations and suggested a number of either strongly or symmetric hyperbolic first-order reduction of the ADM system that assure well-posedness of the systems.

KST Formalism

- Kidder, Scheel & Teukolsky, 2001 performed systematic investigation of impact of constraint addition, definition of dyamical variables on hyperbolicity.
- Introduce new variables:

$$d_{kij} \equiv \partial_k \gamma_{ij}$$

- This implies we get additional constraint equations to satisfy:

$$C_{kij} \equiv d_{kij} - \partial_k \gamma_{ij} = 0$$

- Taking derivatives of d_{kij},

$$C_{klij} \equiv \partial_{[k} d_{l]ij} = 0$$

which implies

$$\partial_k \partial_l \gamma_{ij} = \partial_{(k} d_{l)ij} \quad (4)$$

which is used to replace second derivatives of 3-metric.

- Basic evolution equations become:

$$
\begin{aligned}
(\partial_t - \mathcal{L})\gamma_{ij} &\equiv -2\alpha K_{ij} \\
(\partial_t - \mathcal{L})d_{kij} &\equiv -2\alpha\partial_k K_{ij} - 2K_{ij}\partial_k\alpha \\
(\partial_t - \mathcal{L})K_{ij} &\equiv F[\partial_a d_{bcd}, \partial_a\partial\alpha, \partial_a\alpha, ...]
\end{aligned}
$$

- Densitized lapse, Q, is introduced

$$Q \equiv \ln(\alpha\gamma^{-\sigma})$$

- Starting from the above equations, KST considered two kinds of systems.
- System 1: Adding multiples of constraints.

$$
\begin{aligned}
C &\equiv \frac{1}{2}(R - K_{ij}K^{ij} - K^2) = 0 \\
C_i &\equiv \nabla_a K^a_i - \nabla_i K = 0
\end{aligned}
$$

- New evolution system: (4 free parameters $\{\gamma, \zeta, \eta, \chi\}$)

$$
\begin{aligned}
(\partial_t - \mathcal{L}_\beta) K_{ij} &= (\ldots) + \gamma\alpha\gamma_{ij} C + \zeta\alpha\gamma^{mn} C_{m(ij)n} \\
(\partial_t - \mathcal{L}_\beta) d_{kij} &= (\ldots) + \eta\alpha\gamma_{k(i} C_{j)} + \chi\alpha\gamma_{ij} C_k
\end{aligned}
$$

- KST did hyperbolicity analysis computing characteristic speeds, eigenvectors of principal part of evolution system as function of $\{\sigma, \gamma, \zeta, \eta, \chi\}$.
- Found two cases that make the system strongly hyperbolic. In both cases, $\sigma = \frac{1}{2}$.
- System 2: Start with System 1, but redefine dynamical variables K_{ij}, d_{kij} using 7 additional parameters $\{\hat{a}, \hat{b}, \hat{c}, \hat{d}, \hat{e}, \hat{k}, \hat{z}\}$.
- Define generalized extrinsic curvature: P_{ij}

$$
P_{ij} \equiv K_{ij} + \hat{z}\gamma_{ij} K
$$

- Define generalized derivatives of metric: M_{kij}

$$
M_{kij} \equiv \frac{1}{2}\{\hat{k} d_{kij} + \hat{e} d_{(ij)k} + \gamma_{ij}[\hat{a} d_k + \hat{b} b_k] + \gamma_{k(i}[\hat{c} d_{j)} + \hat{d} b_{j)}]\}
$$

where $d_k \equiv \gamma^{ab} d_{kab}$, $b_k \equiv \gamma^{ab} d_{abk}$, $M_k \equiv \gamma^{ab} M_{Kab}$, and $W_k \equiv \gamma^{ab} M_{abk}$.

- The redefinitions do change eigenvectors, characteristic fields, but not eigenvalues and strong hyperbolicity of system.

BSSN System of Equations

- Shibata & Nakamura 1995, Baumgarte & Shapiro 1998.
- Ideas: (1) eliminate mixed derivatives in R_{ij} by introducing an auxiliary variable, $\tilde{\Gamma}$ (2) Conformal, traceless (CT) split in the spirit of York initial value formalism.
- Conformal decomposition of 3-metric: (introducing a new variable ϕ)

$$\tilde{\gamma}_{ij} = e^{-4\phi}\gamma_{ij}$$

and impose $\tilde{\gamma} = 1$.

- Split K_{ij} into trace of extrinsic curvature, K, and traceless part, $\tilde{A}_{ij}$.

$$\begin{aligned} K_{ij} &= A_{ij} + \frac{1}{3}\gamma_{ij}K \\ \tilde{A}_{ij} &= e^{-4\phi}A_{ij} \end{aligned}$$

- Note $\tilde{\gamma}^{ij} = e^{4\phi}\gamma^{ij}$, $\tilde{A}^{ij} = e^{4\phi}A^{ij}$
- Introduce an auxiliary varible:

$$\tilde{\Gamma}^i \equiv \gamma^{jk}\tilde{\Gamma}^i_{jk} = -\partial_j\tilde{\gamma}^{ij}$$

- Note that Ricci tensor can now be written as

$$R_{ij} = R^{\phi}_{ij} + \tilde{R}_{ij}$$

where

$$\tilde{R}_{ij} = -\frac{1}{2}\tilde{\gamma}^{lm}\tilde{\gamma}_{ij,lm} + \tilde{\gamma}_{k(i}\partial_{j)}\tilde{\Gamma}^{k} + \tilde{\Gamma}^{k}\tilde{\Gamma}_{(ij)k} + \tilde{\gamma}^{lm}(2\tilde{\Gamma}^{k}_{l(i}\tilde{\Gamma}_{j)km} + \tilde{\Gamma}^{k}_{im}\tilde{\Gamma}_{klj})$$

and

$$R^{\phi}_{ij} = -2\tilde{D}_i\tilde{D}_j\phi - 2\tilde{\gamma}_{ij}\tilde{D}^l\tilde{D}_l\phi + 4\tilde{D}_i\phi\tilde{D}_j\phi - 4\tilde{\gamma}_{ij}\tilde{D}^l\phi\tilde{D}_l\phi$$

- Note that the principar part is now hyperbolic with all the other derivatives (especially mixed derivatives) absorbed into $\tilde{\Gamma}$ terms.
- Cf. original ADM system

$$R_{ij} = \frac{1}{2}\gamma^{kl}(\gamma_{kj,il} + \gamma_{il,kj} - \gamma_{kl,ij} - \gamma_{ij,kl}) + (...)$$

- Baumgarte and Shapiro used weak gravitational field initial data to compare BSSN formalism with ADM system of equations.
    - ADM evolution crashed very early while BSSN evolution remianed stable.
- Due to superior stability property of BSSN for this case, a large number of groups adopted this formalism quickly and now became a sort of standard formalism. BSSN is being used by most groups doing binary black hole merger simulations.