Introduction to Numerical Relativity
Lectures 3 & 4
Formalism & Other Continuum Matters

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Spring School in
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KIAS, Seoul, Korea

March 16, 2006

http://laplace.physics.ubc.ca/∼matt/Doc/Talks/...

Recent Review Articles

- Luis Lehner, 2001.*Numerical Relativity: A Review*, Class. Quant. Grav., 18, R25.

- Thomas W. Baumgarte and Stuart L. Shapiro, *Numerical Relativity and Compact Binaries*, 2003. Phys. Rep, 376, 41.

- Greg Cook, 2000 *Initial Data for Numerical Relativity*, Living Rev. Rel., 5, 1.

- Kimberley C.B. New, 2002.*Gravitational Waves from Gravitational Collapse*, Living Rev. Rel., 6, 2.

- Carsten Gundlach, 2003. *Critical Phenomena in Gravitational Collapse*, Phys. Rep, 376, 339.

- Beverly K. Berger, 2002.*Numerical Approaches to Spacetime Singularities*, Living Rev. Rel., 1, 7.

Overview

- The Nature of Numerical Relativity
- ADM / 3+1 Formalism
- Initial Value Problem
- Recently Developed/Used Formalisms for Evolving Einstein's Equations
- Coordinate Conditions
- Black Hole Excision and Apparent Horizon Location

Caveats

- Will focus on "main stream" numerical relativity, which itself is primarily concerned with the prediction of gravitational waveforms from interactions and collisions of compact objects (black holes (BH) and neutron stars (NS))

- In particular, will not discuss (today)
  - Cosmological solutions (e.g. approaches to the singularity)
  - Nature of black hole interiors, black hole singularities
  - Numerical relativity in higher dimensions (e.g. black strings)
  - Critical phenomena

Caveats

- Will restrict attention to "space + time" (a.k.a. 3+1/ADM) approach to numerical relativity

- Will not discuss
  - Characteristic (null) approaches
  - Approaches based on conformal Einstein equations (Friedrich 1981)

- Will largely restrict attention to finite-difference approaches to the discretization of the field equations

- This excludes
  - Spectral methods (but note significant ongoing effort by Caltech/Cornell collaboration)

- Will also thus not discuss relative merits of the various approaches to discretization, but note that at least some pursuing spectral techniques are confident that we'll all be in their camp eventually! Many of those of us *not* in that camp (including HO Kreiss, it should be noted) are *not* so convinced

The Nature of Numerical Relativity

- As with many other areas of computational science, basic job is the solution of a system of non-linear, time-dependent, partial differential equations using numerical methods

- Field Equations

$$G_{\mu\nu} = 8\pi T_{\mu\nu}$$

  are generally covariant, giving rise to separation of equations into those of evolution type, plus constraints

- Determination of initial data is already highly non-trivial due to the constraints, particularly to set "astrophysically realistic" conditions

- Tensorial nature of field equations, plus constraints, plus coordinate freedom invites development of multitude of "formalisms":
  - Specific choice of dynamical variables (i.e. those quantities that will be advanced in time via evolution equations)
  - Specific form of field equations (e.g. multiples of constraints can be added to evolution equations)
  - Specific choices of coordinates, or classes of coordinate systems

The Nature of Numerical Relativity

- Mathematical (as well as empirical) evidence shows that choice of formalism can have significant impact on continuum well-posedness, as well as ability to compute a convergent numerical solution

- STABILITY IS THE KEY ISSUE both at the continuum and numerical level
  - Continuum: Well-posedness is always tied to some notion of stability
  - Discrete: Lax equivalence theorem (or variations thereof) suggest that stability and convergence are equivalent given consistency

- Constraints/coordinate freedom lead to many options in how discrete solution is advanced from one time step to the next (Piran 1980)
  - Free evolution: Constraints are solved at initial time, but then all dynamical variables are advanced using evolution equations
  - Partially constrained evolution: Some or all of the constraints are re-solved at each time step for specific dynamical variables, in lieu of use of the corresponding evolution equation
  - Fully constrained evolution: All of the constraints are re-solved at each time step, and all four degrees of coordinate freedom are used to eliminate dynamical variables, leaving precisely two dynamical degrees of freedom to be advanced using evolution equations

The Nature of Numerical Relativity

- 3D work (i.e. computations in three space dimensions plus time) has been biased to free evolution schemes
  - Elliptic PDEs are considered expensive to solve
  - Better formal understanding of treatment of boundaries for equations of evolutionary type, particularly for strongly hyperbolic systems
  - Theory is generally in better shape for hyperbolic systems than for mixed hyperbolic/elliptic
- At the same time, empirical evidence from 1-, 2-, and even some recent 3D calculations indicate that constrained schemes provide more facile route to stability
- Substantial evidence that at least some free evolution schemes admit non-physical modes (e.g. modes that violate the constraints), and that these tend to grow exponentially; boundary conditions further complicate matters
- Expect studies constrained versus free evolution to be continued in the future, though developments with, e.g. generalized harmonic approaches, may make such studies less pressing

The Nature of Numerical Relativity

- Coupling to matter: Introduces all of the complications associated with the numerical treatment of matter field(s)

- Solution properties
  - Don't expect (physical) shocks to (generically) develop in gravitational variables
  - Do expect singularities, and must be avoided in numerical work, unless one is interested in probing singularity structure
  - Large dynamic range in many problems of interest; for example in binary black hole collisions, must resolve dynamics on the scale of the BH horizon, as well as many wavelengths of characteristic gravitational radiation
  - Gravitational waves tend to be a relatively small effect, but must be computed precisely for maximal utility in the context of terrestrial detection of gravitational radiation

ADM / 3+1 Formalism

(Choquet-Bruhat 1956, ADM 1962, York 1979)

- Manifold with metric $(M, g_{\mu\nu})$ foliated by spacelike hypersurfaces Σ_t
- Coordinates $x^\mu = (t, x^i)$
- Future directed, timelike unit normal

$$n^\mu = -\alpha \nabla^\mu t$$

where α is the lapse function

- Shift vector β^μ defined via

$$t^\mu = \alpha n^\mu + \beta^\mu$$

$$\beta^\mu n_\mu = 0$$

ADM / 3+1 Formalism

- Hypersurface metric $\gamma_{\mu\nu}$ induced by $g_{\mu\nu}$

$$\gamma_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu$$

- Mixed form of $\gamma_{\mu\nu}$ projects into hypersurface

$$\perp^\mu{}_\nu = \delta^\mu{}_\nu + n^\mu n_\nu$$

- Metric compatible covariant derivative in slices

$$D_\mu \equiv \perp^\nu{}_\mu \nabla_\nu$$

$$D_\mu \gamma_{\alpha\beta} = 0$$

ADM / 3+1 Formalism

- 3+1 line element

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

- Extrinsic curvature (second fundamental form)

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

- 3+1 form of Einstein's equations $G_{\mu\nu} = 8\pi T_{\mu\nu}$ derived by considering various projections of Einstein/Ricci and stress-energy tensors

- Projections of $T_{\mu\nu}$

$$\begin{aligned} \rho &\equiv n^\mu n^\nu T_\mu \nu \\ j_\mu &\equiv -\perp^\alpha{}_\mu n^\beta T_{\alpha\beta} \\ S_{\mu\nu} &\equiv \perp^\alpha{}_\mu \perp^\beta{}_\nu T_{\alpha\beta} \end{aligned}$$

ADM / 3+1 Formalism

- Constraint Equations: From $G_{0i} = 8\pi T_{0i}$, which do not contain 2nd time derivatives of the γ_{ij}
- Hamiltonian Constraint

$$R + K^2 - K_{ij}K^{ij} = 16\pi\rho \tag{1}$$

where R is the 3-dim. Ricci scalar, and $K \equiv K^i{}_i$ is the mean extrinsic curvature.

- Momentum Constraint

$$D_i K^{ij} - D^j K = 8\pi j^i \tag{2}$$

ADM / 3+1 Formalism

- Evolution Equations: From definition of extrinsic curvature, $G_{ij} = 8\pi T_{ij}$, and Ricci's equation.

$$\mathcal{L}_t \gamma_{ij} = \mathcal{L}_\beta \gamma_{ij} - 2\alpha K_{ij} \quad (3)$$

$$\begin{aligned} \mathcal{L}_t K_{ij} &= \mathcal{L}_\beta K_{ij} - D_i D_j \alpha + \alpha \left(R_{ij} + K K_{ij} - 2 K_{ik} K^k{}_j \right) - \\ &\quad 8\pi\alpha (S_{ij} - \frac{1}{2}\gamma_{ij}(S - \rho)) \end{aligned} \quad (4)$$

- Cauchy Problem for Einstein's Equations (vacuum): Prescribe $\{\gamma_{ij}, K_{ij}\}$ at $t = 0$ subject to (1-2), specify coordinates via choice of α and β^i, evolve to future (or past) using (3-4)

- Bianchi identities guarantee that if constraints are satisfied at $t = 0$, will be satisfied at subsequent times; i.e. evolution equations preserve constraints

- Extent to which this is the case in numerical calculations has been a perennial issue in numerical relativity


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Initial Value Problem

(Lichnerowicz 1944, York 1979, Cook 2000, Pfeiffer 2003)

- Key question: Which of the 12 $\{\gamma_{ij}, K_{ij}\}$ do we specify freely at the initial time, and which do we determine from the constraints?

- York-Lichnerowicz approach: Specify dynamical variables only up to overall conformal scalings, and perform decomposition of extrinsic curvature into trace, longitudinal, and transverse pieces.

- Introduce base/background metric, $\tilde{\gamma}_{ij}$, conformal factor ψ

$$\gamma_{ij} = \psi^4 \tilde{\gamma}_{ij}$$

- Decompose K_{ij} into trace/trace-free (TF) parts

$$K_{ij} = A_{ij} + \frac{1}{3}\gamma_{ij} K$$

$$\gamma^{ij} A_{ij} = 0$$

Initial Value Problem

- Define

$$A^{ij} = \psi^{-10}\tilde{A}^{ij}$$

(motivated by $D_j A^{ij} = \psi^{-10}\tilde{D}_j\tilde{A}^{ij}$)

- Split $\tilde{A}^{ij}$ into longitudinal/transverse pieces

$$\tilde{A}^{ij} = \tilde{A}^{ij}_{\mathrm{TT}} + \tilde{A}^{ij}_{\mathrm{L}}$$

$$\tilde{D}_j\tilde{A}^{ij}_{\mathrm{TT}} = 0$$

$$\tilde{A}^{ij}_{\mathrm{L}} = 2\tilde{D}^{(i}W^{j)} - \frac{2}{3}\tilde{\gamma}^{ij}\tilde{D}_k W^k \equiv (\tilde{\ell}W)^{ij}$$

W^i is a vector potential.

- Consider divergence of $\tilde{A}^{ij}$

$$\tilde{D}_j\tilde{A}^{ij} = \tilde{D}_j(\tilde{\ell}W)^{ij} \equiv (\tilde{\Delta}_\ell W)^i$$

$\tilde{\Delta}_\ell \equiv$ vector Laplacian

Initial Value Problem

- In practice, is more convenient to give freely specifiable part of $\tilde{A}^{ij}$ as a symmetric trace free (STF) tensor itself; "reverse decompose" $\tilde{A}^{ij}_{\rm TT}$ as

$$\tilde{A}^{ij}_{\rm TT} = \tilde{T}^{ij} - (\tilde{\ell} V)^{ij}$$

where $\tilde{T}^{ij}$ is STF and V^i is another vector potential.

- Define $X^i \equiv W^i - V^i$, then

$$\tilde{A}^{ij} = \tilde{T}^{ij} + (\tilde{\ell} X)^{ij}$$

- Constraints become

$$\begin{aligned}
\tilde{\Delta}\psi &= \frac{1}{8}\tilde{R}\psi + \frac{1}{12}K^2\psi^5 - \frac{1}{8}\tilde{A}_{ij}\tilde{A}^{ij}\psi^{-7} - 2\pi\psi^5\rho \\
(\tilde{\Delta}_\ell X)^i &= -\tilde{D}_j\tilde{T}^{ij} + \frac{2}{3}\psi^6\tilde{D}^i K + 8\pi\psi^{10}j^i
\end{aligned}$$

which are 4 quasi-linear, coupled elliptic PDEs for the 4 "gravitational potentials" $\{\psi, X^i\}$

Initial Value Problem

- Common simplifying assumptions:
  - Conformal flatness: $\gamma_{ij} = f_{ij}$, with f_{ij} the flat 3-metric
  - Maximal slice: $K = 0$
  - "Minimal radiation": $\tilde{T}^{ij} = 0$

- Constraints become

$$
\begin{aligned}
\tilde{\Delta}\psi &= -\frac{1}{8}\tilde{A}_{ij}\tilde{A}^{ij}\psi^{-7} - 2\pi\psi^5\rho = -\frac{1}{8}(\tilde{\ell}X)_{ij}(\tilde{\ell}X)^{ij}\psi^{-7} - 2\pi\psi^5\rho \\
(\tilde{\Delta}_\ell X)^i &= 8\pi\psi^{10}j^i
\end{aligned}
$$

- Note that in vacuum ($\rho = j^i = 0$), the momentum constraint is linear and decouples from the Hamiltonian constraint

Puncture Method for Black Hole Initial Data
(Brandt & Brügmann 1997)

- Consider vacuum constraints with previously mentioned simplifying assumptions

$$\tilde{\Delta}\psi + \frac{1}{8}(\tilde{\ell}X)_{ij}(\tilde{\ell}X)^{ij}\psi^{-7} = 0$$

$$(\tilde{\Delta}_\ell X)^i = 0$$

where $\tilde{\Delta}, \tilde{\ell}$ and $\tilde{\Delta}_\ell$ are flat-space operators

- The momentum constraints can be solved analytically (Bowen & York 1980) to produce data corresponding to black holes with specified linear and angular momentum

- These solutions can then be superimposed to generate solutions of momentum constraints representing multiple holes

- Hamiltonian constraint must then be solved numerically, and one must deal with singular behaviour of ψ as $r \to 0$

Puncture Method for Black Hole Initial Data

(Brandt & Brügmann 1997)

- Traditional approach introduced inner boundaries at $r_i = a_i$ around each hole with r_i measured from hole center, then imposed mixed (Robin) conditions to guarantee that final solution *did* describe one or more black holes (i.e. that the solution contained apparent horizons)

- In context of finite difference methods, inner boundaries proved troublesome, particularly in 3D case in cartesian coordinates (not so much of a problem for finite element, spectral approaches)

- Key idea of puncture approach: "Factor out" singular behaviour of ψ via following ansatz for N black holes:

$$\psi = \frac{1}{\alpha} + u = \sum_{i=1}^{N} \frac{M}{2|\vec{r} - \vec{r}_i|} + u$$

where the $\vec{r}_i$ are the locations of the punctures, and $1 + 1/\alpha$ is the Brill-Lindquist conformal factor

Puncture Method for Black Hole Initial Data

(Brandt & Brügmann 1997)

- Hamiltonian constraint becomes

$$\tilde{\Delta} u + \frac{1}{8}\alpha^7 (\tilde{\ell} X)_{ij} (\tilde{\ell} X)^{ij} (1 + \alpha u)^{-7} = 0$$

  with boundary condition

$$\lim_{R\to\infty} u = 1 + O(R^{-1})$$

- Authors showed that by solving this equation *everywhere* on R^3 (i.e. without any points excised), data that is asymptotically flat near punctures is generated, but more importantly, data *do* represent time instants of black hole spacetimes

- Technique has become very popular over the past few years, primarily due to its ease of implementation in 3D Cartesian coordinates

BSSN Formalism

(Shibata & Nakamura 1995, Baumgarte & Shapiro 1998)

- Key ideas: Eliminate mixed second derivatives in R_{ij} via introduction of auxiliary vbls; evolve conformal factor, K separately in spirit of "spin decomposition" of geometric quantities

- Conformal metric

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

$$\phi = \frac{1}{12} \ln \gamma \quad \text{so that} \quad \tilde{\gamma} = 1$$

- TF part of extrinsic curvature (note different scaling relative to initial data approach)

$$\tilde{A}_{ij} = e^{-4\phi} A_{ij}$$

$$\tilde{A}^{ij} = \tilde{\gamma}^{im} \tilde{\gamma}_{jm} \tilde{A}_{ij} = e^{4\phi} A^{ij}$$

- Conformal connection functions

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

BSSN Formalism

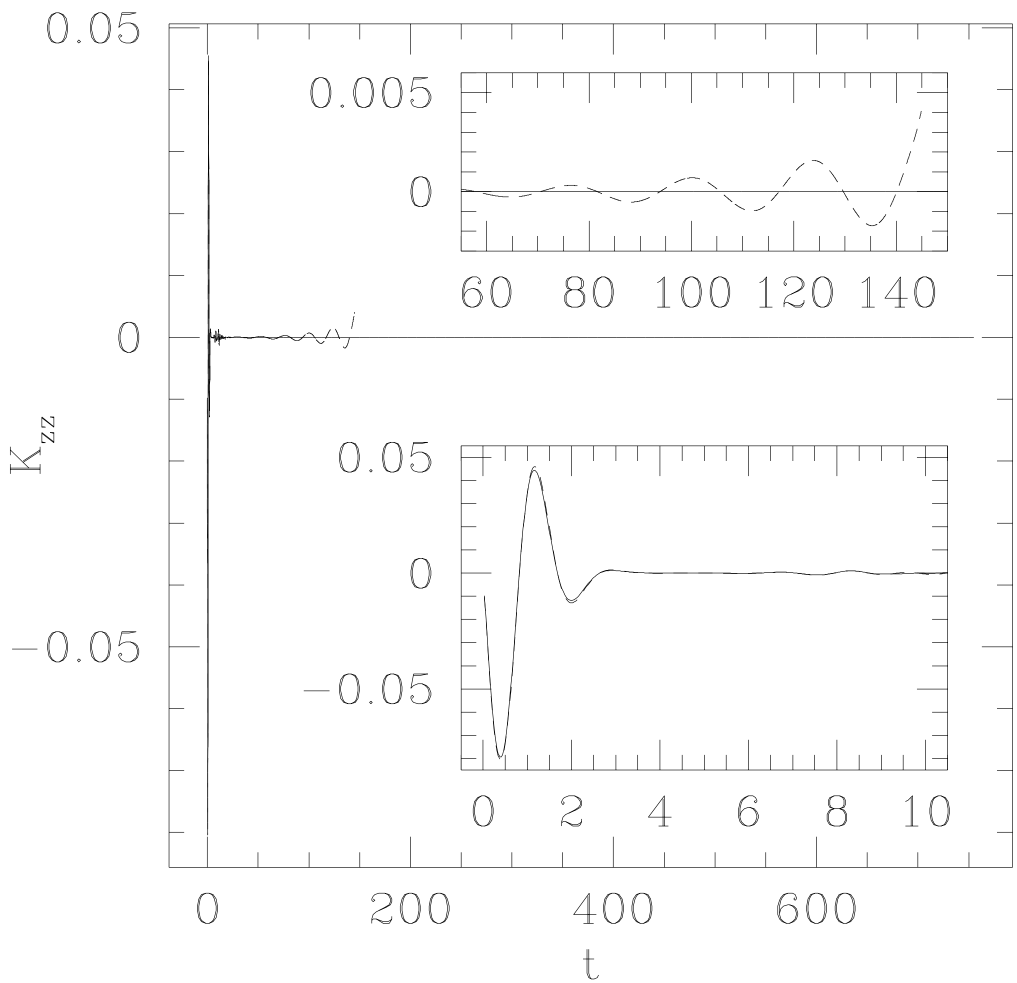
- Get set of evolution equations

$$
\begin{aligned}
\partial_t \phi &= \frac{1}{6}\alpha K + \beta^i \partial_i \phi + \frac{1}{6}\partial_i \beta^i \\
\partial_t K &= -\gamma^{ij} D_j D_i \alpha + \alpha(\tilde{A}_{ij}\tilde{A}^{ij} + \frac{1}{3}K^2) + 4\pi\alpha(\rho + S) + \beta^i \partial_i K \\
\partial_t \tilde{\gamma}_{ij} &= -2\alpha \tilde{A}_{ij} + \beta^k \partial_k \tilde{\gamma}_{ij} + 2\tilde{\gamma}_{k(i}\partial_{j)}\beta^k - \frac{2}{3}\tilde{\gamma}_{ij}\partial_k \beta^k \\
\partial_t \tilde{A}_{ij} &= e^{-4\phi}((-D_i D_j \alpha)^{\mathrm{TF}} + \alpha(R_{ij}^{\mathrm{TF}} - 8\pi S_{ij}^{\mathrm{TF}})) + \alpha(K\tilde{A}_{ij} - 2\tilde{A}_{il}\tilde{A}^l{}_j) + \\
&\quad \beta^k \partial_k \tilde{A}_{ij} + 2\tilde{A}_{k(i}\partial_{j)}\beta^k - \frac{2}{3}\tilde{A}_{ij}\partial_k \beta^k \\
\partial_t \tilde{\Gamma}_i &= -2\tilde{A}^{ij}\partial_j \alpha + 2\alpha(\tilde{\Gamma}^i{}_{jk}\tilde{A}^{kj} - \frac{2}{3}\tilde{\gamma}^{ij}\partial_j K - 8\pi\tilde{\gamma}^{ij}S_j + 6\tilde{A}^{ij}\partial_j \phi) \\
&\quad \beta^j \partial_j \tilde{\Gamma}^i - \tilde{\Gamma}^j \partial_j \beta^i + \frac{2}{3}\tilde{\Gamma}^i \partial_j \beta^j + \frac{1}{3}\tilde{\gamma}^{mi}\partial_m \partial_j \beta^j + \tilde{\gamma}^{mj}\partial_m \partial_j \beta^i
\end{aligned}
$$

- Crucially, momentum constraint is used to eliminate $\partial_j \tilde{A}^{ij}$ in the derivation of $\partial_t \tilde{\Gamma}_i$

BSSN Formalism

Comparison with Standard ADM



- Evolution of the extrinsic curvature component K_{zz} at the origin using harmonic slicing and $\beta^i = 0$. Solid line computed using the BSSN equations, dotted lines with standard ADM. (Source: Baumgarte & Shapiro 1998)

- As a result of this work, the BSSN approach was rapidly and widely adopted in 3D numerical relativity

- Additional modifications leading to better numerical performance have also been introduced, some will be mentioned below

KST Formalism

(Kidder, Scheel & Teukolsky 2001)

- Performed systematic investigation of impact of constraint addition, definition of dynamical variables on hyperbolicity of field equations and efficacy for numerical calculations

- Constraints:

$$
\begin{aligned}
\mathcal{C} &\equiv \frac{1}{2}(R - K_{ij}K^{ij} + K^2) - 8\pi\rho = 0 \\
\mathcal{C}_i &\equiv D_j K^j{}_i - D_i K - 8\pi j_i = 0
\end{aligned}
$$

- Auxiliary variables:

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

- Additional constraints:

$$
\begin{aligned}
\mathcal{C}_{kij} &\equiv d_{kij} - \partial_k \gamma_{ij} = 0 \\
\mathcal{C}_{klij} &\equiv \partial_{[k} d_{l]ij} = 0 \quad \Rightarrow \quad \partial_k \partial_l \gamma_{ij} = \partial_{(k} d_{l)ij}
\end{aligned}
$$

KST Formalism

- Evolution equations:

$$
\begin{aligned}
\hat{\partial}_0 \gamma_{ij} &\equiv -2\alpha K_{ij} \\
\hat{\partial}_0 d_{kij} &\equiv -2\alpha \partial_k K_{ij} - 2K_{ij}\partial_k \alpha \\
\hat{\partial}_0 K_{ij} &\equiv F[\,\partial_a d_{bcd},\ \partial_a \partial_b \alpha,\ \partial_a \alpha,\ \cdots]
\end{aligned}
$$

where $\hat{\partial}_0 \equiv \partial_t - \mathcal{L}_\beta$

- Introduce densitized lapse, Q

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

where σ is the densitization parameter, Q, β^i considered arbitrary gauge functions *independent* of the dynamical vbls.

KST Formalism

- System 1: Add constraints via 4 parameters $\{\gamma, \zeta, \eta, \chi\}$
- New evolution system: (γ here not to be confused with $\det \gamma_{ij}$)

$$
\begin{aligned}
\hat{\partial}_0 K_{ij} &= (\cdots) + \gamma\alpha\gamma_{ij}\mathcal{C} + \zeta\alpha\gamma^{mn}\mathcal{C}_{m(ij)n} \\
\hat{\partial}_0 d_{kij} &= (\cdots) + \eta\alpha\gamma_{k(i}\mathcal{C}_{j)} + \chi\alpha\gamma_{ij}\mathcal{C}_k
\end{aligned}
$$

- Hyperbolicity analysis: Compute characteristic speeds, eigenvectors of principal part of evolution system as function of $\{\sigma, \gamma, \zeta, \eta, \chi\}$
- Find two cases yielding strong hyperbolicity; in both instances must have $\sigma = 1/2$; one case has two free parameters, other has one
- Show that constraints evolve as per the evolution equations; same characteristic speeds; constraint evolution is strongly hyperbolic when evolution scheme is

KST Formalism

- System 2: Start with System 1, but redefine dynamical variables K_{ij}, d_{kij} using 7 additional parameters $\{\hat{a}, \hat{b}, \hat{c}, \hat{d}, \hat{e}, \hat{k}, \hat{z}\}$

- Generalized extrinsic curvature: P_{ij}

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

- Generalized metric derivative: M_{kij}

$$M_{kij} = M_{kij}[\, d_{kij},\ \gamma^{mn}d_{kmn},\ \gamma^{mn}d_{mnk},\ \gamma_{ij},\ \{\hat{a}, \hat{b}, \hat{c}, \hat{d}, \hat{e}, \hat{k}\}]$$

- Redefinitions do not change:
  - Eigenvalues of evolution system
  - Strong hyperbolicity of system

- Redefinitions do change:
  - Eigenvectors, characteristic fields
  - Nonlinear terms in non-principal parts of evolution systems

KST Formalism

- Recover several previously studied systems (Fritelli & Reula 1996, Einstein-Christoffel (Anderson & York 1999)) with appropriate choices of the 12 parameters.

- System 3: Sub-case of System 2; generalized Einstein-Christoffel system with free parameters $\{\eta, \hat{z}\}$

- Study numerical evolution of Schwarzschild hole using spectral method and Painlevé-Gullstrand coordinates

$$ds^2 = -dt^2 + \left(dr + \sqrt{\frac{2M}{r}}dt\right)^2 + r^2 d\Omega^2$$

(fixed gauge) on domain from inside horizon to some $R_{\max}$

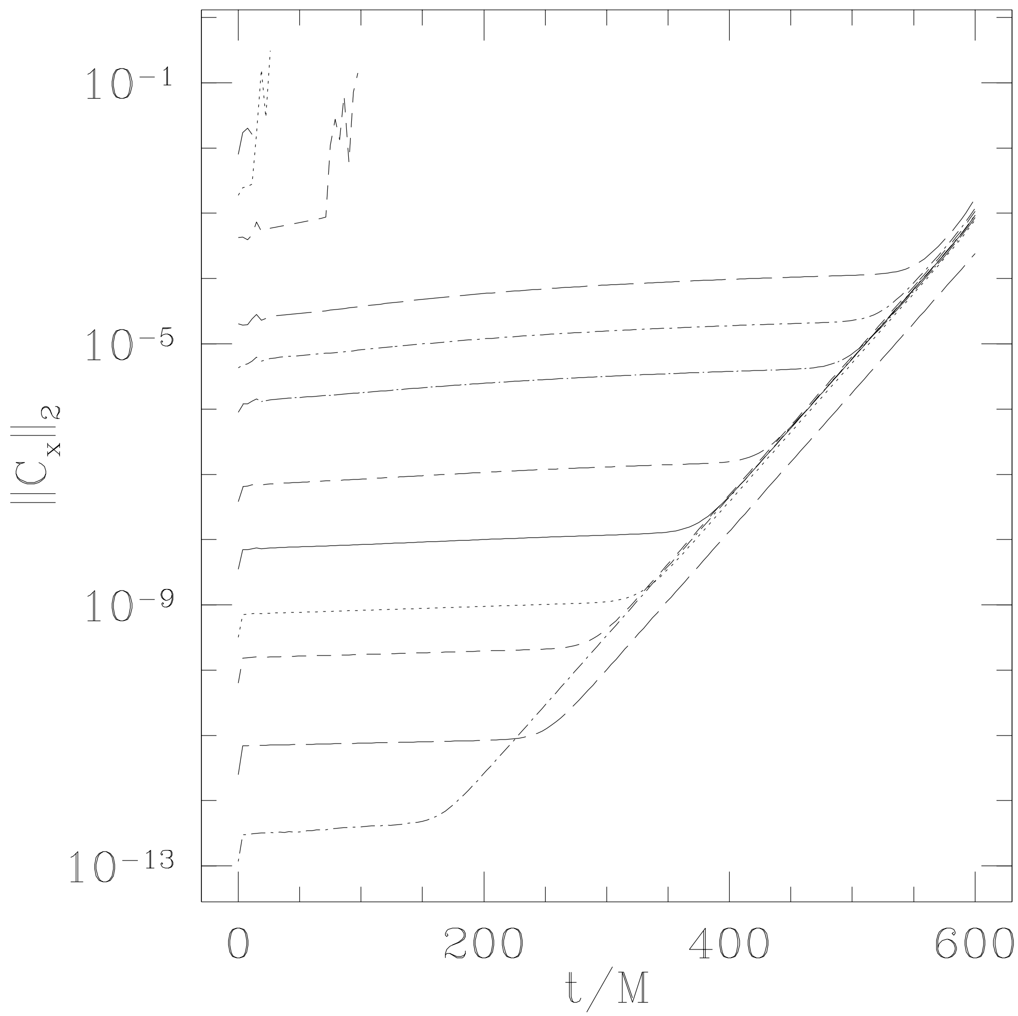
- Search parameter space for particularly long lived evolutions

- Find evidence for exponentially growing "constraint violating" mode, that appears *not* to be due to the numerics.

- Some dependence of longevity of runs on $R_{\max}$, but only up to a point

KST Formalism

Illustration of Constraint Violating Instability



- Momentum constraint $\mathcal{C}_X$ vs time for evolutions of a Painlevé-Gullstrand slicing of a Schwarzschild black hole using the Generalized Einstein-Christoffel system with $\eta = 4/33$ and $\hat{z} = -1/4$ Angular and temporal resolutions are fixed, and the various lines show several radial resolutions. Outer boundary is at $11.9M$; if it is moved out to $40M$ run time extends to $\sim 1300M$ for the same accuracy. (Source: Kidder, Scheel & Teukolsky 2001)

Coordinate Conditions

HOW DO WE DEFINE/DETERMINE GOOD COORDINATE SYSTEMS/CONDITIONS FOR USE IN NUMERICAL RELATIVITY?

- Desirable features: (not exhaustive, some may not be consistent with others)
  - Cover region(s) of spacetime of interest
  - Avoids physical singularities
  - Remain non-singular/non-pathological
  - Simplify equations of motion
    - Eliminate variables from update scheme
    - Cast equations into particularly nice form (e.g. harmonic coordinates)
  - Simplify physics
    - Traditional use of coord. freedom, e.g. spherical coords. for spherical problems
    - Co-rotating coords for binary inspiral, absorb bulk dynamics into coord. system, more dynamic range available for secular dynamics
    - Symmetry seeking coordinates (Garfinkle & Gundlach 1999)
    - Known asymptotic states (e.g. Kerr BH) have unique/recognizable representation
    - Maintains linearity between "dynamical vbls." and "physical vbls."

Coordinate Conditions

- Desirable features:
  - Computationally efficient (elliptic conditions are generally avoided)
  - Compatible with hyperbolicity, well-posedness (STABILITY!)
  - Facilitates well posed-discrete problem (STABILITY!)
  - Compatible with excision techniques
- IMPORTANT NOTE: When things get sufficiently non-linear/time-dependent, coordinate choices will only go so far in optimizing calculation; physics of situation, which varies from scenario to scenario, and which is not known *a priori* dictates, e.g., what discretization scale is necessary

Coordinate Conditions: Traditional Choices

- Geodesic (Gaussian-normal) Coordinates:

$$\alpha = 1 \qquad \beta^i = 0$$

  See e.g. May and White 1966. Singularity *seeking*, but *may* have some utility in context of excision techniques. Provide substantial simplification of 3+1 equations.

- Normal Coordinates:

$$\beta^i = 0$$

  Historically has been widely used, particularly in initial phases of code development due to simplification of evolution equations—many early codes had difficulty with "shift" / "advective" terms.

Coordinate Conditions: Traditional Choices

- Maximal Slicing:

$$K = 0 \quad \Rightarrow \quad D_i D^i \alpha = \alpha(K_{ij}K^{ij} + 4\pi(\rho + S))$$

Estabrook et al 1973. Volume of hypersurfaces maximized with respect to continuous deformations within spacetime. Widely used due to singularity avoidance, compatibility with York IVP approach, simplifying property

Need to solve elliptic equation at every time step—often considered computationally too expensive

Harmonic Coordinates

- Coordinate functions x^μ are harmonic

$$\nabla^\alpha \nabla_\alpha x^\mu = 0$$

- In 3+1 context yield following for lapse and shift

$$\begin{aligned}
(\partial_t - \beta^j \partial_j)\alpha &= -\alpha^2 K \\
(\partial_t - \beta^j \partial_j)\beta^i &= -\alpha^2 \left(\gamma^{ij}\partial_j \ln\alpha + \gamma^{jk}\Gamma^i{}_{jk}\right)
\end{aligned}$$

- Appeal is that field equations reduce to non-linear wave equations, widely used in early hyperbolic formulations (e.g. Choquet-Bruhat 1952)

- Used in 3D by Landry & Teukolsky 2000 in preliminary study of neutron star coalescence

Harmonic Coordinates

- Also used in 3D by Garfinkle 2002 to study generic singularity formation in spacetimes with topology $T^3 \times R$ with scalar field matter source.

- Harmonic *slicing* (or variants) has also been used in several other 3D computations over the past few years, as will be discussed below

- Disadvantages:
  - Harmonic slices may tend to be singularity *seeking* instead of singularity avoiding
  - Harmonic coordinates may be susceptible to coordinate singularities (coordinate shocks, Alcubierre 1997)

Generalized Harmonic Coordinates

- Introduce specified source functions, H^μ

$$\nabla^\alpha \nabla_\alpha x^\mu = H^\mu$$

  H^μ to be chosen, for example, to stave off coordinate singularities

- Open question: What are good choices for the H^μ for scenarios of current interest, such as binary inspiral?

- Implementation note: Harmonic coords. yield wave equations for $g_{\mu\nu}$—can discretize directly in second order form (Pretorius in progress) without need for auxiliary vbls.

- Leads to economical storage requirements, particularly relative to many of the first-order hyperbolic approaches used in conjunction with finite-differencing.

Bona-Masso Slicings
(Bona et al 1995)

- Considered slicing conditions invariant under $x^i \to \tilde{x}^i$ on each hypersurface—condition must be expressed in terms of "slicing scalars" and their proper time derivatives

- Restricting to first order scalars get

$$(\partial_t - \beta^i \partial_i) \ln \alpha = -\alpha f(\alpha) K$$

with $f(\alpha) \geq 0$

Bona-Masso Slicings

- $f = 0$: Geodesic slicing (with $\alpha = 1$ initially)

- $f = \infty$: Maximal slicing

- $f = 1$: Harmonic slicing

- $f = 2/\alpha$: "1 + log" slicing; for case $\beta^i = 0$, can integrate slicing equation to get
$$\alpha = 1 + \ln \gamma$$

- Empirically, "1 + log" slicing has singularity avoidance properties similar to maximal and is inexpensive computationally

- Has been used extensively in 1D and 3D black hole work, as will be seen below

Minimal Strain / Minimal Distortion
(Smarr & York 1978)

- Consider hypersurface "strain" and "distortion" tensors

$$\Theta_{ij} \equiv -\frac{1}{2}\alpha K_{ij} + \mathcal{L}_\beta \gamma_{ij}$$
$$F_{ij} \equiv \gamma^{1/3}\mathcal{L}_n\left(\gamma^{-1/3}\gamma_{ij}\right)$$

  and extremize

$$\int_\Sigma \Theta_{ij}\Theta^{ij} dV$$
$$\int_\Sigma F_{ij}F^{ij} dV$$

  w.r.t. β^i

- In both instances, get system of elliptic equations for β^i

Minimal Strain / Minimal Distortion

- Minimal strain

$$D_i D^i \beta^j + D_i D^j \beta^i - 2 D_i (\alpha K^{ij}) = 0$$

- Minimal distortion

$$D_i D^i \beta^j + \frac{1}{3} D^j D_i \beta^i + R^j{}_i \beta^i - 2 D_i (\alpha (K^{ij} - \frac{1}{3} K)) = 0$$

  As name suggests, this choice tends to minimize distortion of spatial coords. during an evolution, as well as the rate of change of metric vbls.

- Both have been used for 2D, 3D black hole and neutron star work, but generally deemed too expensive computationally, complex to implement

- Provided motivation for conditions that approximated behaviour of those choices, but which were more efficient

Driver (Dynamical) Conditions

(Balakrishna et al 1996)

- Sought *active* enforcement of coordinate conditions, motivated by secular "drifts" when conditions were "passively" enforced

- K driver:

$$\partial_t K + cK = 0 \qquad c > 0 \qquad \Rightarrow \qquad K \to 0 \quad \text{exponentially}$$

- Rewrite as

$$D_i D^i \alpha - K_{ij} K^{ij} \alpha - \beta^i D_i K - 4\pi(S + \rho)\alpha - cK \equiv L[\alpha] = 0$$

- Convert *elliptic* PDE to *parabolic* one

$$\partial_t \alpha = \epsilon L[\alpha]$$

- For properly chosen ϵ and c (non-trivial problem), α "diffuses" to maximal solution, and idea can be applied to other elliptics (e.g. minimal distortion/strain)

Driver Conditions

- Alcubierre & Brügmann 2001 constructed coordinate condition closely related to minimal distortion based on conformal connection $\tilde{\Gamma}^i \equiv \gamma^{jk}\tilde{\Gamma}^i{}_{jk}$; instead of $\tilde{\Gamma}^i = 0$, impose

$$\partial_t \tilde{\Gamma}^i = 0 \qquad \tilde{\Gamma}^i(0, x^i) = 0$$

- Yields complicated elliptic equation for β^i, write schematically as

$$L[\beta^i] = 0$$

- Then solve

$$\partial_t \beta^i = \epsilon L[\beta^i] \qquad \epsilon > 0$$

- Alcubierre et al 2001a also tried hyperbolic version

$$\partial_t^2 \beta^i = \Psi^{-4} \epsilon_1 \partial_t \tilde{\Gamma}^i - \epsilon_2 \partial_t \beta^i \qquad \epsilon_1, \epsilon_2 > 0$$

where Ψ is the time-independent Brill-Linquist conformal factor

Black Hole Adapted Coordinates

- Kerr-Schild form of Kerr Metric

$$
\begin{aligned}
ds^2 &= (\eta_{\mu\nu} + 2Hl_\mu l_\nu)\, dx^\mu dx^\nu \\
\eta_{\mu\nu} &= \mathrm{diag}(-1, 1, 1, 1) \\
\eta^{\mu\nu} l_\mu l_\nu &= g^{\mu\nu} l_\mu l_n u = 0 \\
H &= \frac{Mr}{r^2 + a^2 \cos^2\theta}
\end{aligned}
$$

where a is the angular momentum parameter

- 3+1 form

$$
\begin{aligned}
\alpha &= (1 + 2H)^{-1/2} \\
\beta^i &= 2Hl_i \\
\gamma_{ij} &= \eta_{ij} + 2Hl_i l_j
\end{aligned}
$$

Black Hole Adapted Coordinates

- For $a = 0$ reduces to ingoing Eddington-Finkelstein coordinatization of Schwarzschild.

- Dynamical variables well behaved across horizon

- Have been used extensively in recent years in studies of single black hole evolutions, as well as in construction of 2-BH initial data and evolutions thereof (Brandt et al 2000)

- Open question: Can this system be effectively generalized for use in generic BH interactions?

Black Hole Excision Techniques

(Unruh c1982)

- Motivation 1: Simulation of BH spacetimes need to avoid physical singularities
- Traditionally, coord. freedom was used for this purpose (e.g. maximal slicing), but coordinate pathologies generally arose on a dynamical timescale
- Lead to violation of principle of simulation linearity (A. Brandt's Golden Rule of Numerical Analysis)

$$\text{Cost of simulation} \propto \text{Amount of physical process simulated}$$

- Typically in BH calcs., dynamical vbls. and/or their gradients would grow without bound, while "physical dynamics" was perfectly bounded.
- Resulted in disheartening and persistent era wherein exponential increase in computer power yielded approximately linear increase in physical time for which BH spacetimes could be simulated

Black Hole Excision Techniques

- Motivation 2: BH simulations need to abide by the "Golden Rule" (eventually at least!)

- Unruh's first suggestion: Given that BH interiors are causally disconnected from the exterior universe, excise insides of BHs from the computational domain (was originally greeted with considerable scepticism in the NR community, but has since transmuted into an "obvious" idea that verges on dogma)

- Unruh's second suggestion: Since event horizons require knowledge of the complete spacetime, use the apparent horizons as surfaces within which to excise

- Idea was championed and explored by Thornburg in his graduate work, but first successful implementation (in spherical symmetry) was due to Seidel & Suen 1992, and is now used extensively in 3D black hole work

Excision: Mathematical/Computational Considerations

- Free evolution schemes particularly those where α, β^i are either specified functions or satisfy evolution equations themselves have advantage

- Key idea is that equations of motion themselves are applied at excision surface—i.e. *no* boundary conditions *per se* are required

- Hyperbolic formulations even more advantageous due to identification of characteristics, and fact that all disturbances propagate along characteristics

- Especially natural for spectral methods, since evaluation of EOM (derivatives) is independent of location within computational domain

- In principle, "No BC" approach should also work for finite difference codes, but generally require modification of difference equations at/near excision surface

Excision: Mathematical/Computational Considerations

- Constrained evolution: Excision has also been employed in this case, primarily in 1D (spherical) and 2D (axisymmetric) situations

- ANIMATION Spherical example: Choptuik, Hirschmann & Marsa 1999. Einstein Yang-Mills collapse—tuning to a "colored" black hole.

- ANIMATION Axisymmetric example: Pretorius 2002. Head-on collision of two black holes, each generated via collapse of a massless scalar field pulse

- Inner (excision) boundary poses a problem for elliptics
  - Dynamical vbls. Can use corresponding evolution equation at/near excision surface.
  - Gauge vbls. Not clear what can be done here, Pretorius' work shows inconsistency of constrained evolution w.r.t. evolution equations, once trapped surfaces have been detected and excised.

- Open Question: Is is possible to devise appropriate BC's for elliptic coordinate conditions to generate consistent evolution?

- Driver conditions may provide one route.

Finding Apparent Horizons / Marginally Trapped Surfaces

- On any hypersurface, Σ_t, consider closed 2-surface, S with outward pointing normal, s^μ, $s^\mu s_\mu = 1$. Then
$$k^\mu = s^\mu + n^\mu$$
is tangent field to outgoing null geodesics emanating from S

- Marginally trapped surface (MTS) has vanishing expansion, Θ
$$\Theta = \nabla_\mu k^\mu = 0$$

- In 3+1 language, find (York 1979)
$$\Theta = D_i s^i - K + s^i s^j K_{ij} = 0 \qquad (5)$$

Finding Apparent Horizons

- Adopting spherical coordinates on S, and some origin interior to S, consider

$$\varphi(r, \theta, \phi) = r - \rho(\theta, \phi) \tag{6}$$

  where r is the coordinate distance from the origin.

- MTS is then defined by the level surface $\varphi = 0$

- Substitution of (6) in (5) yields 2nd order elliptic equation for φ (in S) that can be solved in a variety of ways

- Finite difference approach: (Huq et al 2002, Thornburg 2003); solve non-linear elliptic equation for φ directly using finite difference approximation, global Newton iteration, and sparse solver (such as incomplete LU-conjugate gradient)

Finding Apparent Horizons

- Spectral methods: (Nakamura et al 1984/1985); expand ρ in spherical harmonics

$$\rho(\theta,\phi) = \sum_{l=0}^{l_{\rm max}} \sum_{m=-l}^{l} a_{lm} Y_{lm}(\theta,\phi)$$

and then use iterative algorithm to determine coefficients a_{lm} that solve MTS equation.

  - Variation (Libson et al 1994), convert root-finding to minimization of

$$\int \Theta(a_{lm})^2$$

- Curvature flow: (Tod 1991); convert elliptic problem to parabolic one by deformation of trial surface S via

$$\frac{\partial x^i}{\partial \tau} = -s^i \Theta$$

Finding Apparent Horizons

- Level flow: (Shoemaker et al 2000). Extends curvature flow by tracking collection of level surfaces; can detect change in topology of apparent horizon.

- Many implementations of AH locators now, and some benchmarks, no clear winners in terms of efficiency

- Also not clear how vital AH location is for excision strategies, may be able to choose appropriately parametrized surfaces that are "suitably trapped" (e.g. Pretorius 2002), and thus obviate need for AH detection at each time step (or even every few time steps)

- Locators certainly continue to be useful for, e.g., detecting (approximately) when black holes have formed in collapse computations

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