Survey of Numerical Approximations of Black Hole Spacetimes

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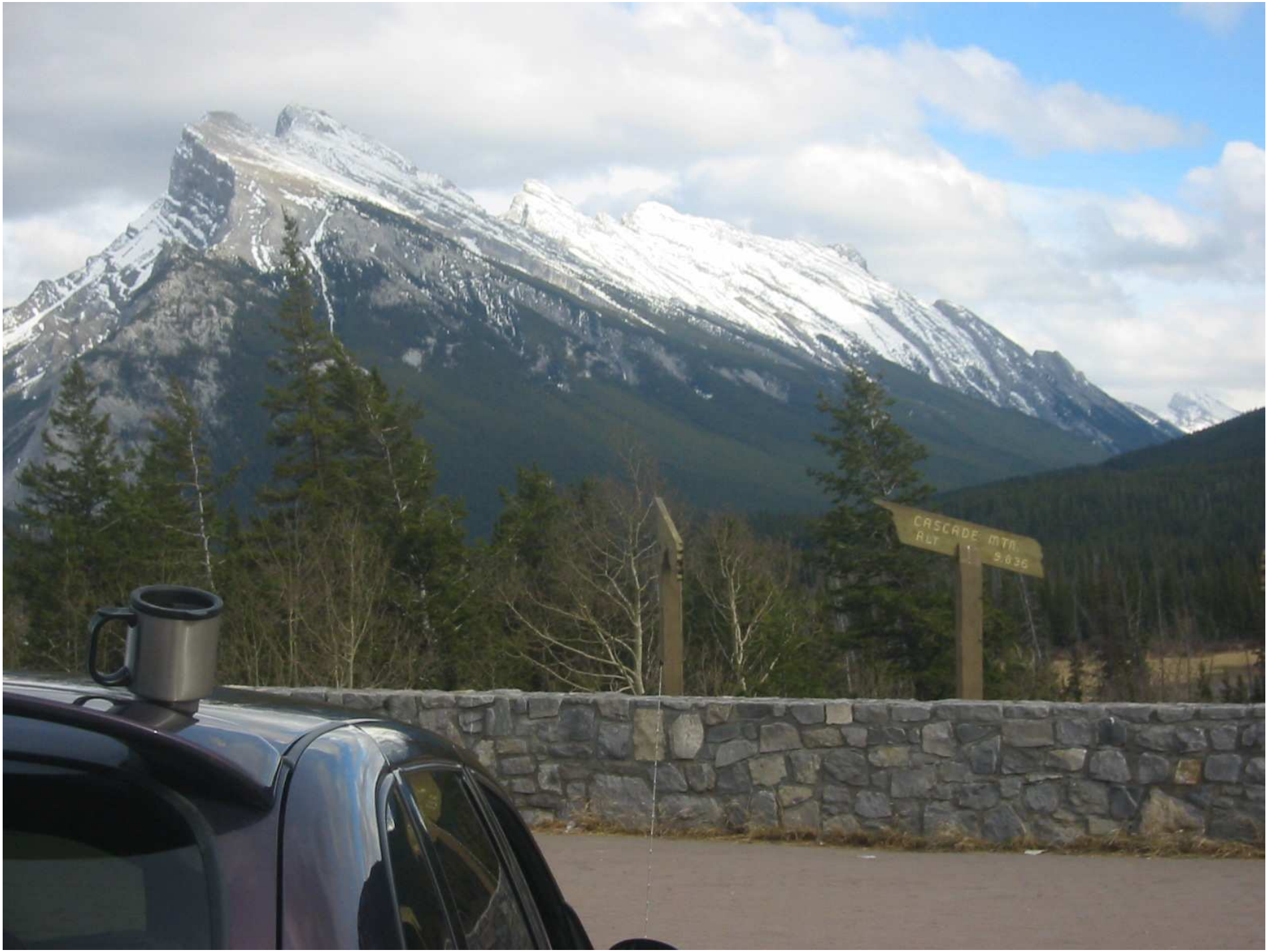
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Recent Review Articles

- 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.

Overview

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

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 are "more stable" than free evolution
- Substantial evidence that at least some free evolution schemes admit non-physical modes, and that these tend to grow exponentially; boundary conditions further complicate matters
- Expect constrained versus free evolution to be continued in the future, though developments with, e.g., generalized harmonic approaches, may make such studies less pressing

Nature of Black Hole Computations

- 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 intrinsic in all BH calculations; for example in binary BH collisions, must resolve dynamics on the scale of the BH horizon, as well as many wavelengths of characteristic 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.

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

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

- 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

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

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

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

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

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

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

  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 $r \longrightarrow 0$

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

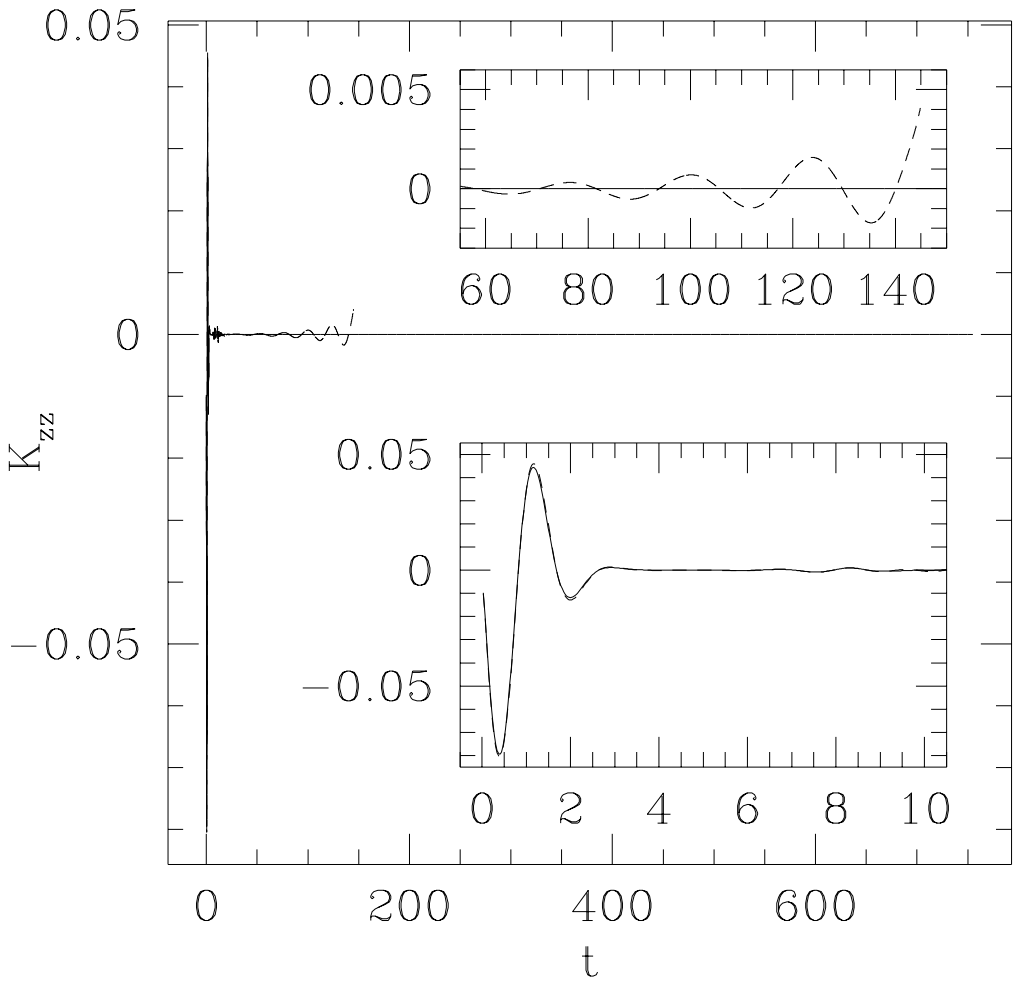
- Get set of evolution equations

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

- 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 $R_{\max}$

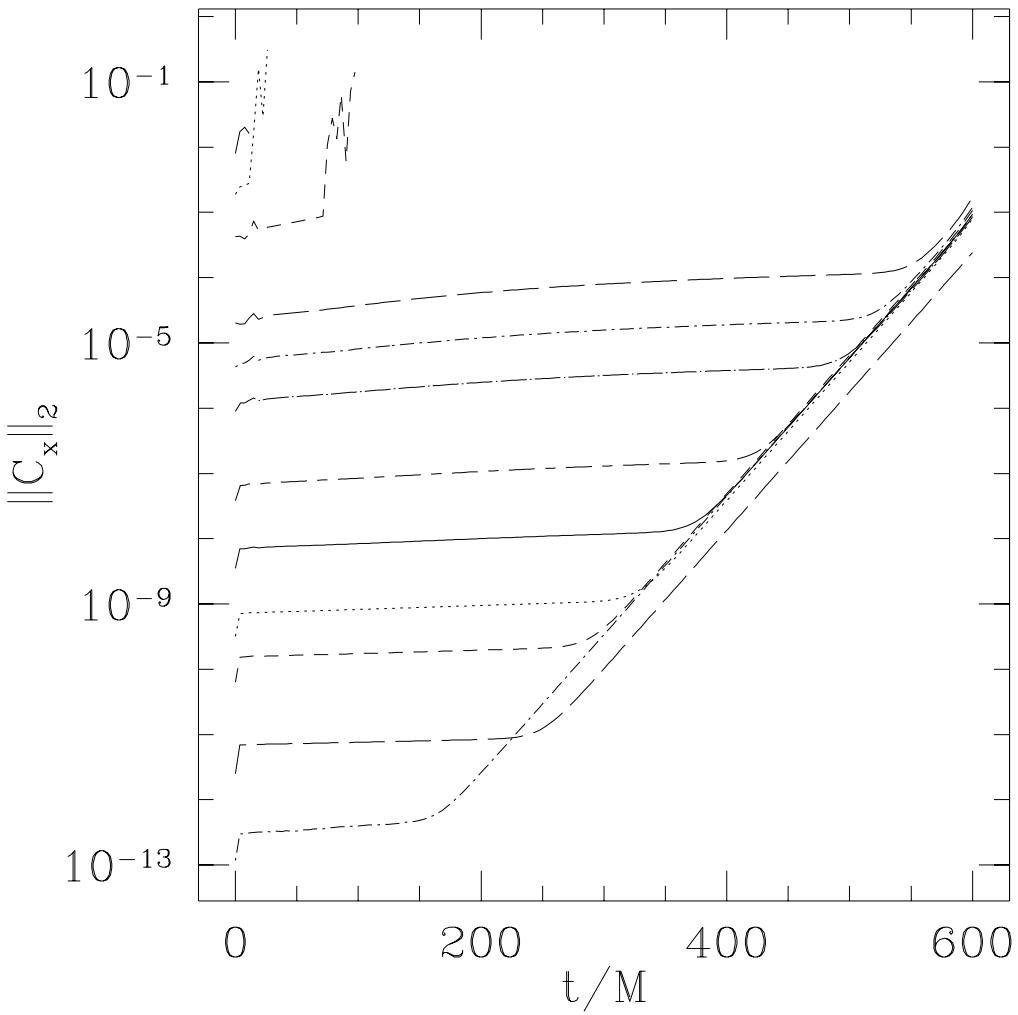
- Search parameter space for particularly long lived evolutions

- 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)

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

- 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

- Harmonic coords. yield wave equations for $g_{\mu\nu}$—can discretize directly in second order form without need for auxiliary vbls.

- Frans will have much more to say about this in his talk later this week

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)

Cost of simulation $\propto$ 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

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)

$$\Theta = D_i s^i - K + s^i s^j K_{ij} = 0 \tag{5}$$

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

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

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.

Black Hole Evolutions

- 3D finite-difference codes universally adopt Cartesian coordinates even if simulating single black hole (possibly with perturbations)

- Principal rationale is that singularities in curvilinear coordinate systems are very difficult to deal with numerically (regularity issues), and is in fact one reason that axisymmetric studies have been largely abandoned

- However, for generic scenarios, Cartesian coordinates make sense unless multiple coordinate patches are to be used

- Current 3D codes typically use BSSN formalism or some variant; i.e. are free evolution codes

- STABILITY is still a key issue, although less so than it was a decade ago

- Codes largely use a single finite difference grid (unigrid codes), with a single resolution $\Delta x = \Delta y = \Delta z = h$, $\Delta t = \lambda h$ (λ is known as the Courant number and typically must be less than one for explicit schemes for stability)

Black Hole Evolutions

- Unigrid design, coupled with computer resource limitations (often memory) restrict computational domain to be quite small, or resolution of near-horizon regions to be quite coarse

- Outer boundary conditions are still largely *ad hoc*; sometimes Dirichlet (perhaps with "blending"), or some form of Sommerfeld (outgoing radiation conditions)

- Spatial compactification offers alternative to conversion of Cauchy problem to mixed initial/boundary value problem (talk by Pretorius)

- Complexity of field equations means that there are literally thousands of floating point operations to be performed per spatial grid point per time step; combined with locality of finite difference operators, makes these codes ideal candidates for parallelization

- Community has invested significant effort in parallelization infrastructure (dating back to the time of the NSF-funded Binary Black Hole Grand Challenge), and Cactus (`www.cactuscode.org`) in particular, has seen widespread use; Pretorius will discuss results generated using another framework—`PAMR/AMRD`—in his talk

Single Black Hole
(Alcubierre & Brügmann 2001)

- Consider Schwarzschild hole in ingoing Eddington-Finkelstein (IEF) coordinates
- Modifications to BSSN
  - Enforce tracelessness of $\tilde{A}_{ij}$ at each time step
  - Use independently evolved $\tilde{\Gamma}^i$ only in terms involving their derivatives, otherwise recompute via $\tilde{\Gamma}^i \equiv \gamma^{jk}\tilde{\Gamma}^i_{jk}$
- Coordinate conditions
  - Slicing: Needed "dynamical" condition for stability, used $\partial_t K = 0$; solve resulting elliptic equation for α at each time step, but keep K constant "by hand"
  - Shift: Experimented with several conditions including "Gamma driver", but also used analytic IEF value

Single Black Hole
(Alcubierre & Brügmann 2001)

- Computational details
  - Crank-Nicholson time differencing, solved (approximately) via iteration
  - Upwind differencing for $\partial_i \beta^i$ (advective) terms, centred otherwise
  - *Excise a cube within horizon*
  - For update on cube faces use RHSs of evolution equations computed from neighboring grid points ($O(\Delta x)$ extrapolation of RHSs)
  - Used grids up to 100^3, outer boundaries $10 - 40M$, 5 to 20 grid points across BH.

- Had to impose octant symmetry for stability

- Were able to evolve essentially forever in certain cases (discrete solutions appeared to be asymptoting to stationary states)

- Calabrese et al 2003 point out that cube excision must be treated carefully; for Schwarzschild, excised cube must have edge length $< 4\sqrt{3}M/9$ or some characteristic directions will be pointing out of the cube.

Single Black Hole
(Alcubierre et al 2001a)

- Approach follows Alcubierre & Brügmann 2001, but focus is on evolution of single black holes distorted with Brill wave

- Initial data

$$ds^2 = \Psi^4 \left(e^{2q} \left(d\eta^2 + d\theta^2 \right) + \sin^2 \theta d\phi^2 \right)$$

  where $\eta \sim \ln(r)$, and q is the adjustable "Brill wave function"

- Coordinate conditions:

$$\partial_t \alpha = -2\alpha(K - K_0)$$

  where K_0 is the initial mean extrinsic curvature

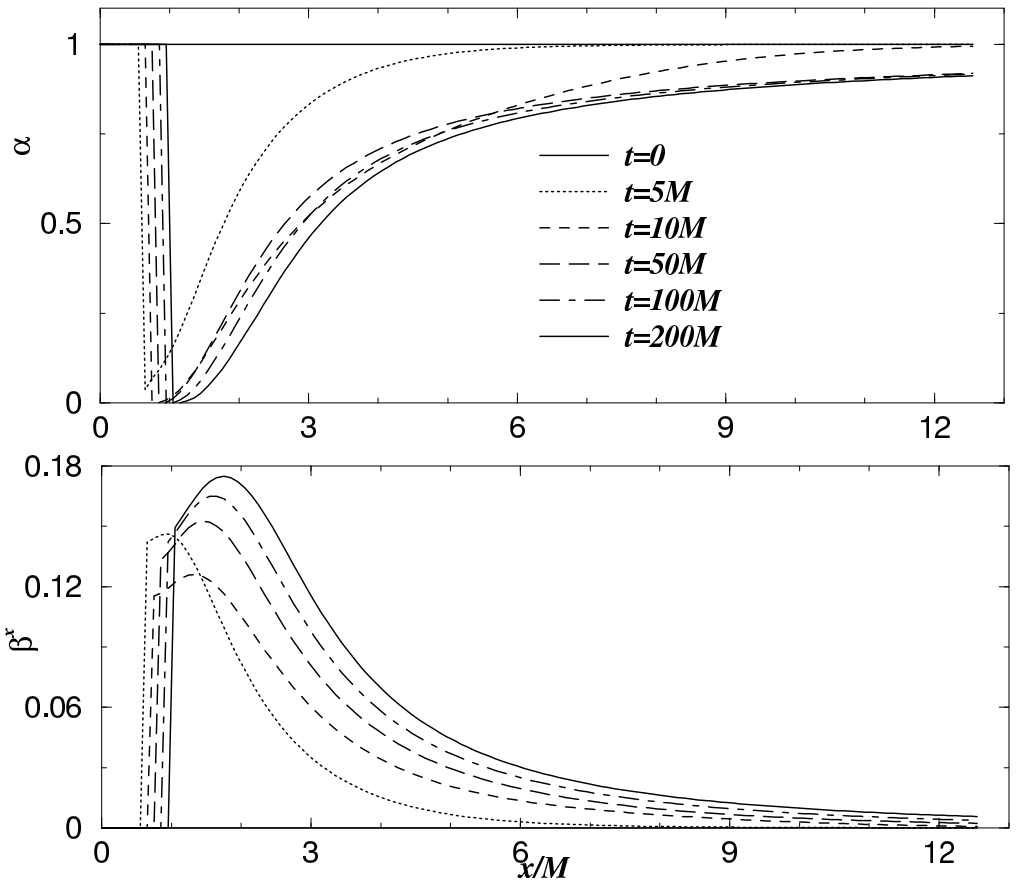
$$\partial_t^2 \beta^i = \frac{0.75}{\Psi^4} \tilde{\Gamma}^i - \frac{3}{M} \partial_t \beta^i$$

- Choose q to produce highly distorted BH: $M = 1.83$

- Computational domain: Octant symmetry, $0 \leq x, y, z, \leq 25.6$, $\Delta x = 0.2$, 128^3 grid points

Single Black Hole

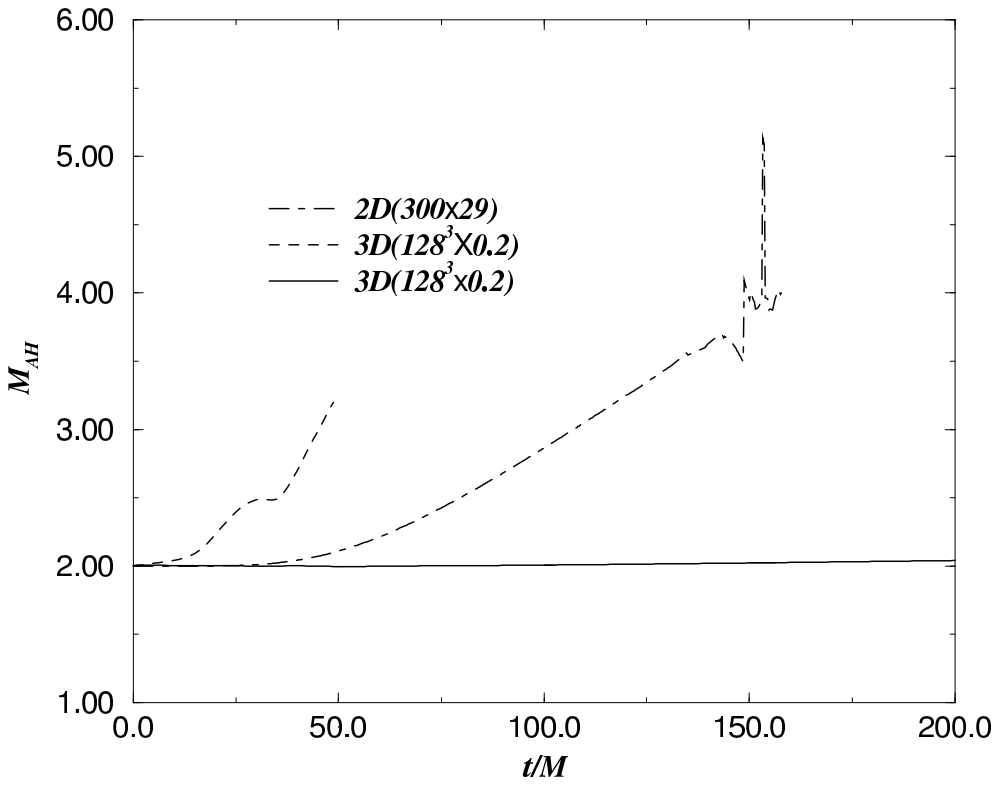
Illustration of Evolution of Lapse & Shift



- Coordinate conditions apparently quickly drive metric to almost static configuration, evolution proceeds beyond $t = 100M$, and waveforms from "perturbation" of BH and subsequent ring-down can be reliably extracted ($\approx 10^{-3} M_{\rm ADM}$ emitted.) Source: Alcubierre et al 2001a

Single Black Hole

Illustration of Evolution of Apparent Horizon Mass



- The solid line shows the development of the apparent horizon mass, $M_{\rm AH}$ during the simulation of a Schwarzschild black hole, while the dashed lines show the AH mass obtained using 2D and 3D codes with no shift and no excision. Source: Alcubierre et al 2001a

Single Black Hole
(Yo, Baumgarte & Shapiro 2002)

- Consider Kerr hole in Kerr-Schild coordinates, adopt BSSN formalism

- Additional constraints

$$\begin{aligned} \mathcal{A} &\equiv \tilde{\gamma}^{ij}\tilde{A}_{ij} = 0 \\ \mathcal{D} &\equiv \det(\tilde{\gamma}_{ij}) - 1 = 0 \\ \mathcal{G}^i &\equiv \tilde{\Gamma}^i - \tilde{\gamma}^{jk}\tilde{\Gamma}^i{}_{jk} = 0 \end{aligned}$$

- Imposed $\mathcal{A}$, $\mathcal{D}$ dynamically by solving for $\tilde{A}_{zz}$, $\tilde{\gamma}_{zz}$ in lieu of corresponding evolution equations

- Modified $\partial_t\tilde{\Gamma}^i$ via

$$\partial_t\tilde{\Gamma}^i = \cdots - \left(\chi + \frac{2}{3}\right)\mathcal{G}^i\partial_j\beta^j$$

  where χ is an adjustable parameter chosen so that the overall factor in RHS of evolution equation $\propto \tilde{\Gamma}^i\partial_j\beta^j$ is negative

Single Black Hole
(Yo, Baumgarte & Shapiro 2002)

- For rapidly rotating holes, also used

$$\partial_t \tilde{\gamma}_{ij} = \cdots - \kappa_1 \alpha \mathcal{C} \tilde{\gamma}_{ij}$$

  where $\mathcal{C} = 0$ is the Hamiltonian constraint, and $k_1 > 0$ is an adjustable parameter

- Coordinate conditions
  - Slicing: "1 + log"

$$\partial_t \alpha = D_i \beta^i - \alpha K$$

  - Shift: "Gamma driver"

$$\partial_t \beta^i = \lambda \partial_t \tilde{\Gamma}^i$$

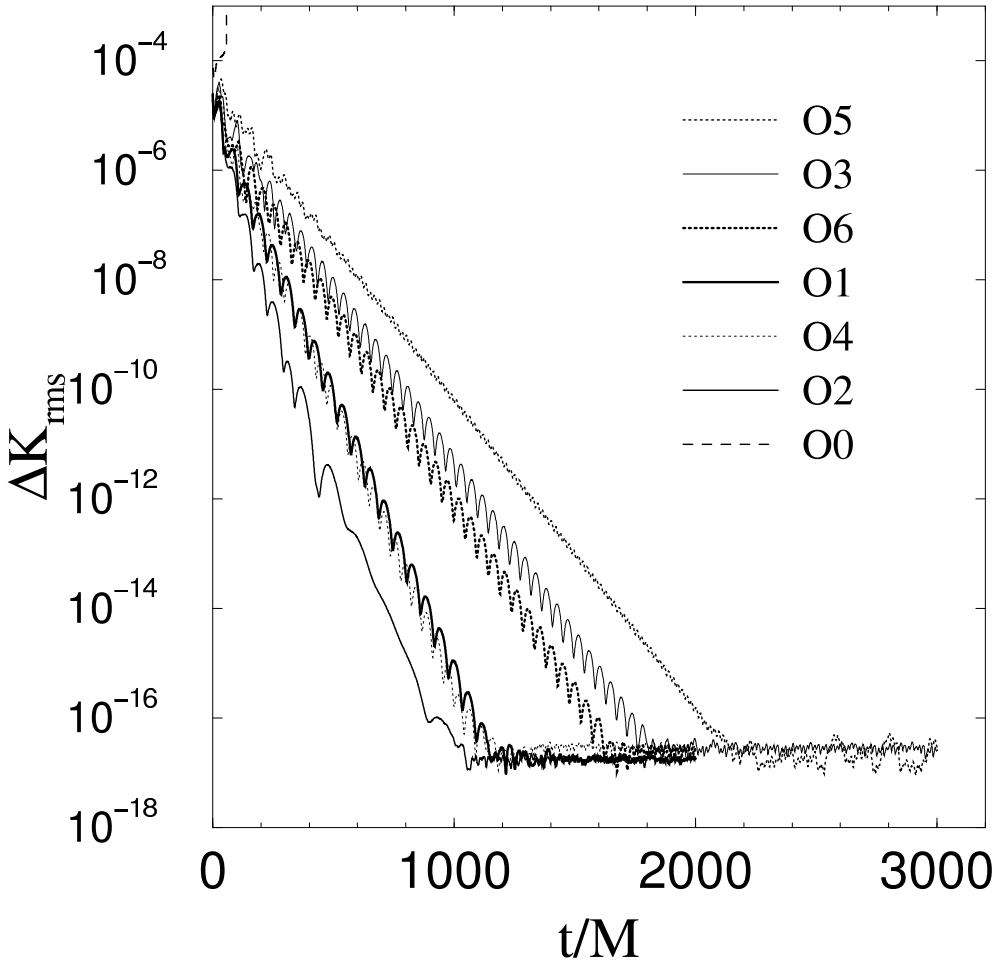
    as well as analytic (Kerr-Schild) value

- Computational domain: $-12M \leq x, y, z \leq 12M$, $h = \Delta x = \Delta y = \Delta z = 0.4M$, 60^3 mesh points

- Finite differencing a la Alcubierre & Brügmann, and excision using both cubical / spherical surfaces

Single Black Hole

Illustration of Long Time Stability



- Plotted is the RMS of the chance in K between consecutive time steps as functions of time for evolutions of Schwarzshild with octant symmetry. Different lines correspond to different choices of coordinates as well as modifications to original BSSN equations mentioned above
  Source: Yo, Baumgarte & Shapiro 2002

- Ran extensive series of experiments, with evolution times typically in range $3000 - 6000M$; in many case seeing no evidence for instability, except as $a \to 1$

Single Black Hole
(Scheel et al, 2002)

- Consider Schwarzschild hole in Painlevé-Gullstrand (PG) coordinates

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

  at initial time, plus small perturbations, adopt KST formalism.

- Were particularly interested in isolating growth of constraint-violating modes (CVMs), so wanted perturbations to be controlled (i.e. not simply due to round-off)

- Used analytic results of Lindblom and Scheel 2002 showing that growth rate of CVMs dependent only on $\{\gamma, \zeta, \hat{z}\}$

- Explored $\{\gamma, \hat{z}\}$ parameter space, other parameters fixed to Generalized Einstein-Christoffel values from KST 2001.

- Coordinate conditions: densitized lapse, shift fixed to PG values

Single Black Hole
(Scheel et al, 2002)

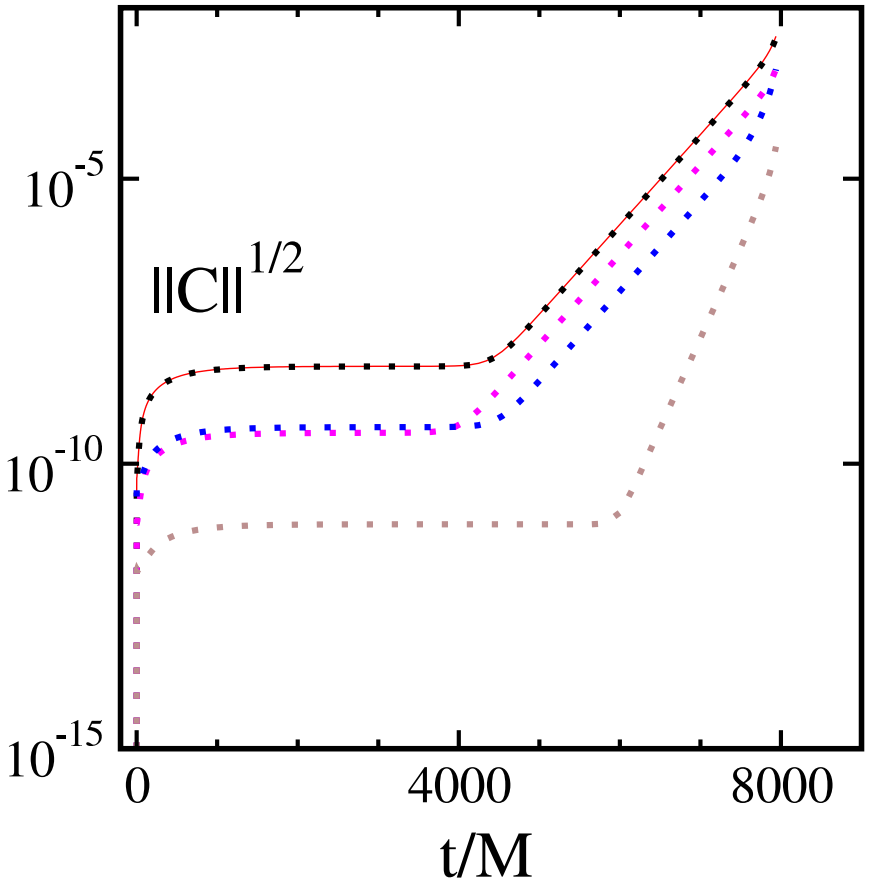
- Computational details: Pseudo-spectral collocation technique, domain is a spherical shell $1.9M \leq r \leq 11.9M$, method-of-lines (MOL) temporal integration using fourth order Runge-Kutta

- Find quite sensitive dependence of instability growth on $\hat{z}$, less so for γ, and considerable dependence on location of outer boundary.

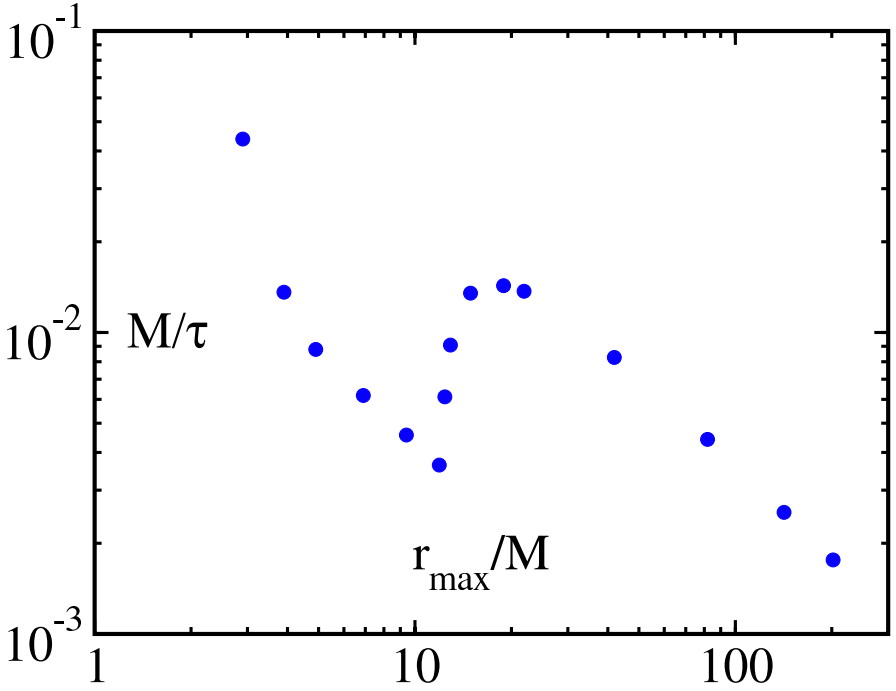
- For appropriately tuned parameters, could achieve evolution times $> 8000M$, again using fixed coordinate conditions

- Not clear what would happen if outer boundary were moved to ∞

Constraint Growth & Outer Boundary Impact



- Solid curve shows the evolution of the integral norm of all the constraints for the most stable set of evolution parameters. Dotted curves show the individual contributions from the various constraints.



- Instability growth as a function of the location of the outer boundary of the computational domain for the evolution parameter values $\gamma = -12$, $\hat{z} = -0.425$

  Source: Scheel et al 2002

Single Black Hole
(Anderson & Matzner 2003)

- Consider Schwarzschild hole in IEF coordinates
- Adopt standard ADM variables $\{\gamma_{ij}, K_{ij}\}$ and equations
- Modify extrinsic curvature evolution equation

$$\partial_t K_{ij} = \cdots - \alpha \mathcal{C}(0.464\,\gamma_{ij} + 0.36\,K_{ij})$$

  where $\mathcal{C} = 0$ is the Hamiltonian constraint, and the numerical coefficients are determined empirically to maximize evolution time

- Coordinate conditions: lapse (*not* densitized), shift fixed to IEF values
- Computational details: Spherical excision surface, fourth order spatial discretization, appropriately one-sided near excision surface, variable order MOL temporal integration
- Typical computational domain: $-10M \leq x, y, z \leq 10M$, $h = M/5$, 100^3 mesh points
- Achieve evolution time $\approx 1000M$

Single Black Hole
(Anderson & Matzner 2003)

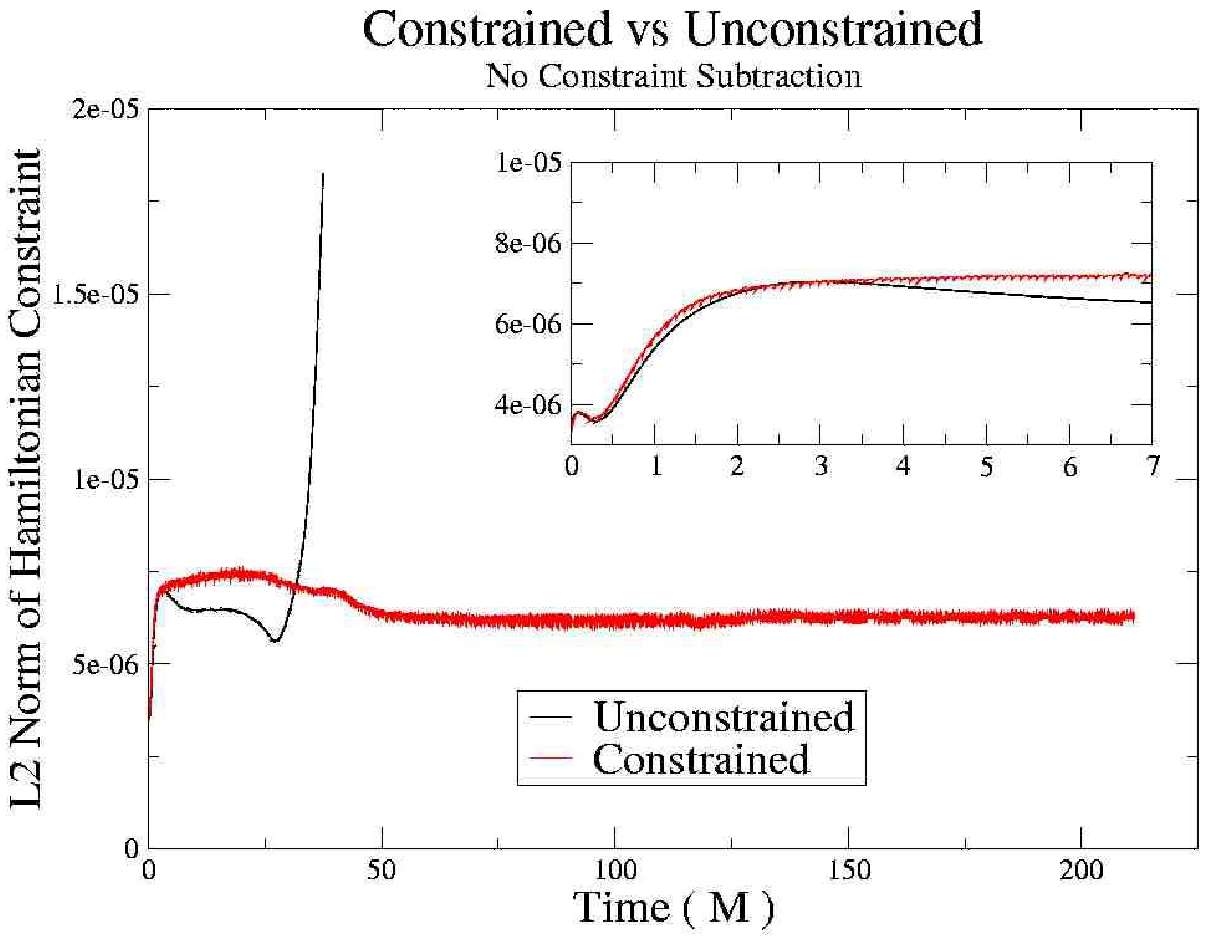
- More interestingly, investigated constrained evolution—re-solution of constraints at each time step or every few steps)

- After initial explicit time advance of dynamical variables $\{\gamma_{ij}, A_{ij}\}$, view those values as conformal trial functions $\{\tilde{\gamma}_{ij}, \tilde{A}_{ij}\}$

- Then solve constraint equations for potentials ψ, X^i, and dress conformal quantities to get new $\{\gamma_{ij}, K_{ij}\}$ (for BCs, use $\psi = 1$, $X^i = 0$ at both inner and outer boundaries)

- Demonstrated evolution times in excess of $200M$ even without "constraint subtraction"

Single Black Hole



- The ℓ_2 norm of the Hamiltonian constraint violation for constrained and unconstrained simulation of a Schwarzschild black hole with excision. Neither simulation used any constraint subtraction. The simulations were performed at a resolution of $M/5$ on a domain size of $\pm M$.

  Source: Anderson & Matzner 2003

"Moving" Single Black Hole
(Sperhake et al 2003)

- Consider single Schwarzschild black hole in IEF coords., but then adopt coordinate transformation

$$\begin{aligned} t &= \bar{t} \\ x^i &= \bar{x}^i + \xi^i(\bar{t}) \end{aligned}$$

  with ξ^i chosen to produce circling or spiraling motion of hole in computational domain

- Adopt BSSN approach and following Yo et al 2002, dynamically enforce tracelessness of $\tilde{A}_{ij}$ and modify evolution equation for $\tilde{\Gamma}^i$

- Also use densitized lapse q

$$q = \gamma^{-n/2}\alpha$$

  and find best results for $n = 1$

- Coordinate conditions: analytic shift, analytic lapse or compute dynamically via "1 + log" condition

"Moving" Single Black Hole
(Sperhake et al 2003)

- Outer boundary conditions: set to analytic values
- Computational details: Use $O(h^2)/O(h^3)$ extrapolations of evolution equation source terms/dynamical variables for updating excision boundary values as well as for "populating" previously undefined sites, used both cubical and spherical excision with similar results
- Static hole: computational domain (octant symmetry), $0 \leq x, y, z \leq 12M$, 60^3 gird points, evolve for 10000M with no signs of instabilities
- Moving hole: computational domain (equatorial symmetry), typical run $-10M \leq x, y \leq 10M$, $0 \leq z \leq 7M$, $60 \times 60 \times 30$ grid points
  - Evolution times: $1000 - 6000M$ treatment of outer boundaries likely limiting factor.
- ANIMATION: Rotating motion, K plotted.
- ANIMATION: Inspiral motion, K plotted.

Head on Black Hole Collisions
(Sperhake et al 2005)

- Group has now successfully extended work to case of head on collisions; again use black hole excision as well as "fixed mesh refinement" to enhance dynamical range

- Buttonhole Pablo for more information.

Two Black Hole Grazing Collision
(Brandt et al 2000)

- Initial data: Spinning holes, equal bare mass m, positioned at $(\pm 5m, \pm m, 0)$, initial boost speed $c/2$, impact parameter $2m$, orbital angular momentum, L, in z direction

- Adopt traditional ADM/3+1 formalism, dynamical variables $\{\gamma_{ij}, K_{ij}\}$

- Considered three cases
  - Both holes have $a = 0.5m$ anti-aligned with L
  - Both holes have $a = 0$
  - Both holes have $a = 0.5m$ aligned with L

- Superimpose two separately boosted Kerr-Schild (KS) datasets, e.g.

$$\gamma_{ij} = \delta_{ij} + 2B_1 \left(H l_i l_j\right)_1 + 2B_2 \left(H l_i l_j\right)_2$$

  where B_1 (B_2) are attenuation/blending functions that are 1 everywhere but in the vicinity of BH 2 (1), where they are 0

Two Black Hole Grazing Collision
(Brandt et al 2000)

- Could take ansatz as conformal background and then resolve constraints but argue that ansatz actually solves constraints to within level of truncation error in discrete evolution scheme

- Coordinate conditions: Pre-merger

$$\alpha = \alpha_1 + \alpha_2 - 1$$

$$\beta^i = \beta_1^i + \beta_2^i$$

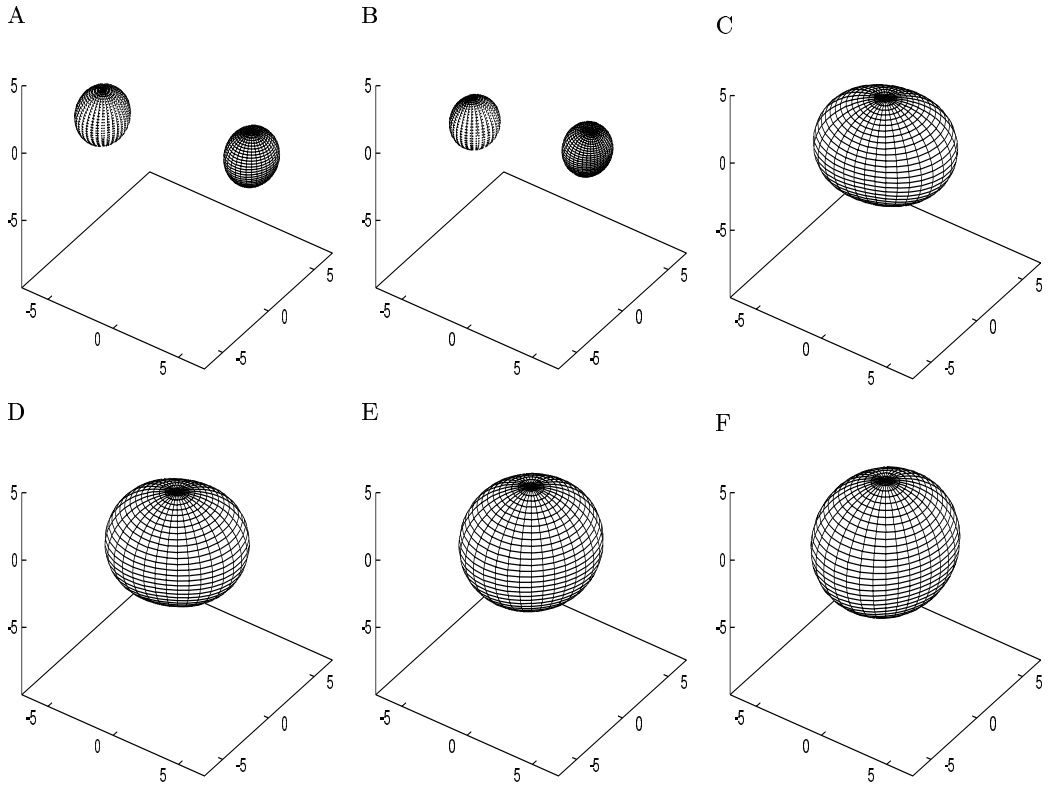
  where $\alpha_1, \alpha_2, \beta_1^i, \beta_2^i$ are computed from boosted KS and dynamically centred at instantaneous location of holes

- Coordinate conditions: Post-merger: Use $\alpha,\ \beta^i$ for single BH based on $M = M_1 + M_2,\ J = J_1 + J_2 + L$

Two Black Hole Grazing Collision
(Brandt et al 2000)

- Use excision technique and locate apparent horizon at each time step using a combined direct finite difference solver and a flow method
- Outer boundary conditions: Dirichlet for γ_{ij}, "blended" Dirichlet for K_{ij}
- Computational domain: $-10M \leq x, y, z \leq 10M$, $h = M/8$, 160^3 grid pts.
- Find similar results for all 3 runs; common apparent horizon forms promptly $(t \sim 2M)$, evolutions end at $t \sim 15M$
- Calculations suggest that $> 2\%$ of total ADM mass may be radiated as gravitational waves, but must be viewed as very rough estimate

Two Black Hole Grazing Collision



- Time history of apparent horizon locations for grazing collision of two equal mass black holes (bare mass m), each with $a = 0.5m$ anti-aligned with the orbital angular momentum. Times corresponding to (A)-(F) are $t = 0$, $2.6m$, $5.1m$, $8.8m$, $13.8m$ and $18.8m$. After the merger the horizon oscillates through a fraction of a cycle

  Source: Brandt et al 2000

Orbiting Black Holes
(Brügmann, Tichy & Jansen 2003)

- Key advance: Construction and use of co-moving coordinate system in conjunction with fixed mesh refinement technique

- Initial data: Puncture data for 2 equal mass BHs, no spin, on quasi-circular orbit based on approximate helical Killing vector

- Use modified form of BSSN equations (Alcubierre et al 2001a), with simple excision technique described in Alcubierre & Brügmann 2001, and spherical excision surfaces that are fixed in time

- Slicing condition

$$\partial_t \alpha = -2\alpha K \Psi^4$$

where Ψ is the time-independent Brill-Lindquist conformal factor ($1/\alpha$ in the puncture approach)

Orbiting Black Holes
(Brügmann, Tichy & Jansen 2003)

- Initialize shift so that if BHs were point particles in a circular orbit, coordinate system would be exactly co-moving; involves introduction of angular and radial velocities ω, $\dot{r}$

- Periodically recompute $\omega(t)$, $\dot{r}(t)$ and adjust shift to keep "centers" of BHs (as determined by asymmetry of α along excision boundaries) near the punctures

- Impose Sommerfeld outer boundary conditions generalized to rigid rotation

- Use fixed mesh refinement with up to 7 levels of 2:1 refinement, use single (fine grid) time step; yields small $\Delta t/\Delta x$ near the outer boundary which is crucial due to superluminal shifts at large distances from the holes

- Evolutions last more than one orbit, and no common apparent horizon is detected for sufficiently large initial separations

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