The State of the Art in Numerical Relativity

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http://laplace.physics.ubc.ca/~matt/Doc/Talks/miami04.pdf

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

Caveats & Apologies

- 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
  - 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 (except briefly in context of adaptive techniques)

Caveats & Apologies

- 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 see talks by Lindblom and Pfeiffer)
  - Finite element methods (which have been used with considerable success, particularly for the determination of initial data, by Doug Arnold and collaborators)
- 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!

Caveats & Apologies

- Will only briefly discuss initial value problem (see talk by Pfeiffer)
- Will not discuss issues related to hyperbolicity/well-posedness of various formulations of Einstein's equations (see talk by Reula)
- Will not discuss the problem of imposing boundary conditions on a finite computational domain; i.e. solving the initial/boundary value problem for Einstein's equations. (see talk by Sarbach)
- Needless to say, these are all very important issues in numerical relativity, and the subject of much current research!

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 (see talk by Lindblom); boundary conditions further complicate matters
- Expect constrained versus free evolution to be intensively studied in near future

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 shocks in vacuum (as long as evolution system remains linearly degenerate)
  - 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 use in the context of terrestrial detection of gravitational radiation

ADM / 3+1 Formalism

(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

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

  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.

$$\begin{aligned} \mathcal{L}_t \gamma_{ij} &= \mathcal{L}_\beta \gamma_{ij} - 2\alpha K_{ij} & (3) \\ \mathcal{L}_t K_{ij} &= \mathcal{L}_\beta K_{ij} - D_i D_j \alpha + \alpha\left(R_{ij} + K K_{ij} - 2K_{ik}K^k{}_j\right) - \\ &\quad 8\pi\alpha(S_{ij} - \frac{1}{2}\gamma_{ij}(S - \rho)) & (4) \end{aligned}$$

- 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 (coordinate invariance) 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
$$\tilde{A}^{ij} = \tilde{A}^{ij}_{\mathrm{TT}} + \tilde{A}^{ij}_{\mathrm{L}}$$
$$\tilde{D}_j\tilde{A}^{ij} = 0$$
$$\tilde{A}^{ij}_{\mathrm{L}} = 2\tilde{D}^{(i}W^{j)} - \frac{2}{3}\tilde{\gamma}^{ij}\tilde{D}_k W^k \equiv (\tilde{\ell}W)^{ij}$$
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" $\tilde{A}^{ij}_{\mathrm{TT}}$ as
$$\tilde{A}^{ij}_{\mathrm{TT}} = \tilde{T}^{ij} - (\tilde{\ell}V)^{ij}$$
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
$$\begin{aligned}\tilde{\Delta}\psi &= -\frac{1}{8}\tilde{A}_{ij}\tilde{A}^{ij}\psi^{-7} - 2\pi\psi^5\rho = -\frac{1}{8}(\tilde{\ell}X)_{ij}(\tilde{\ell}X)^{ij} - 2\pi\psi^5\rho \\ (\tilde{\Delta}_\ell X)^i &= 8\pi\psi^{10}j^i\end{aligned}$$

- Note decoupling and linearity of momentum constraint.

Puncture Method for Black Hole Initial Data
(Brandt & Brügmann 2003)

- Consider vacuum constraints with previously mentioned simplifying assumptions
$$\tilde{\Delta}\psi + \frac{1}{8}(\tilde{\ell}X)_{ij}(\tilde{\ell}X)^{ij} = 0$$
$$(\tilde{\Delta}_\ell X)^i = 0$$
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 2003)

- 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 2003)

- Hamiltonian constraint becomes

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

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

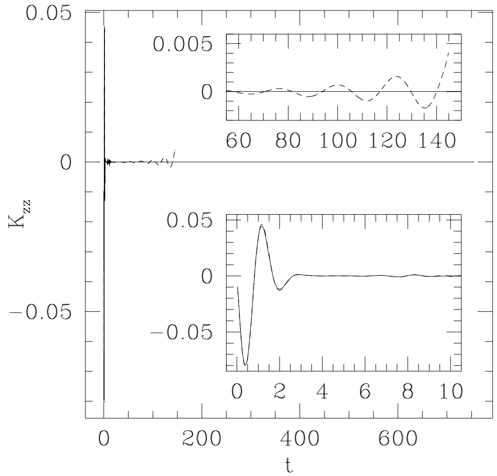
- Get set of evolution equations

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

- 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}

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

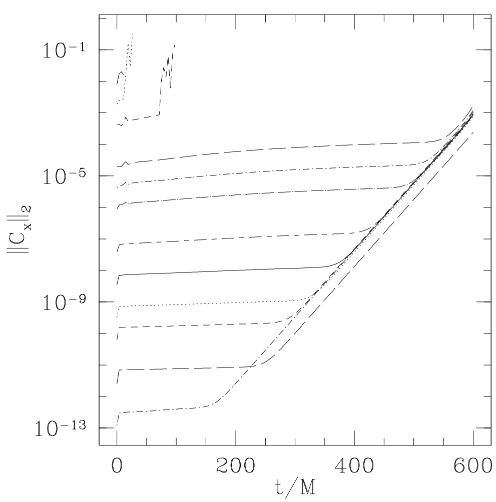
- Redefinitions do not change:
  - Eigenvalues of evolution system
  - Strong hyperbolicity of system
- Redefinitions do change:
  - Eigenvectors, characteristic fields
  - Nonlinear terms in non-principal parts of evolution systems

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 (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 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 $f(\alpha) > 0$

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

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

- Minimal distortion

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

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:

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

- Rewrite as

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

- 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

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

  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)

  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 freely specified 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 massless scalar field pulses.
- 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)

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

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.

- 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

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 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 that 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)

- 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

- Will summarize in the following most of the major recent and current efforts in the 3D simulation of one or more black holes

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

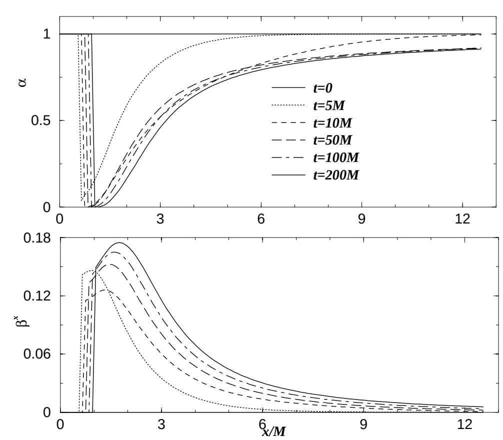
Single Black Hole
(Alcubierre & Brügmann 2001)

- 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)

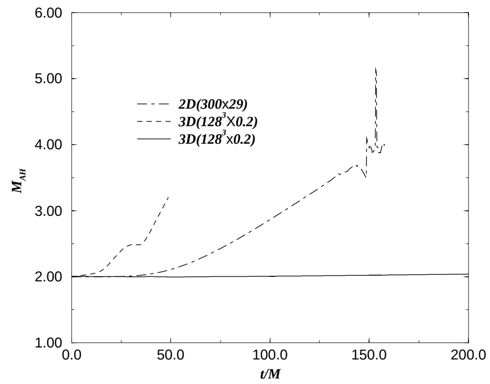
- Approach follows Alcubierre & Brügmann 2001, but focus is on evolution of single black holes distorted with Brill wave
- Initial data
$$ds^2 = \Psi^4\left(e^{2q}\left(d\eta^2 + d\theta^2\right) + \sin^2\theta d\phi^2\right)$$
where $\eta \sim \ln(r)$, and q is the adjustable "Brill wave function"
- 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, $0 \le x, y, z, \le 25.6$, $\Delta x = 0.2$, 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 ($\approx 10^{-3}M_{\mathrm{ADM}}$ 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.

- Coordinate conditions
  - Slicing: "1 + log"

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

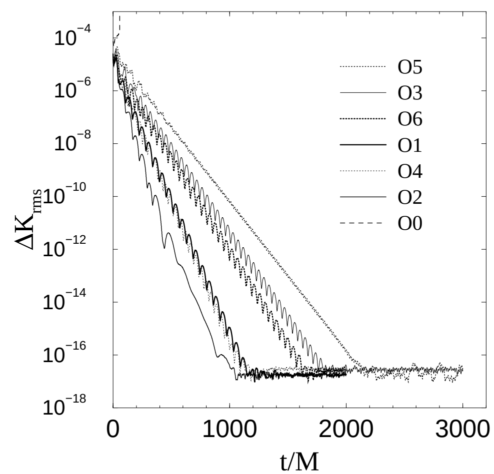
  - Shift: "Gamma driver"

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

  as well as analytic (Kerr-Schild) value

- Computational domain: $-12M \le x, y, z \le 12M$, $h = \Delta x = \Delta y = \Delta z = 0.4M$, 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 $a \rightarrow 1$

Single Black Hole
(Scheel et al, 2002)

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

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

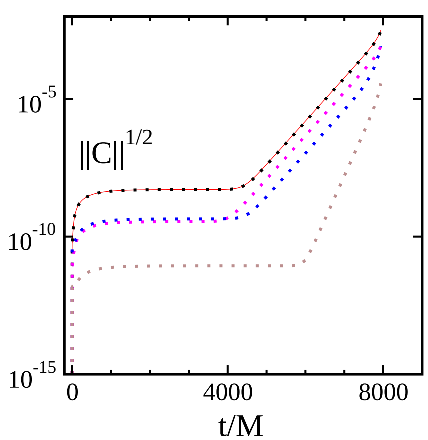
at initial time, plus small perturbations, adopt KST formalism.

- 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

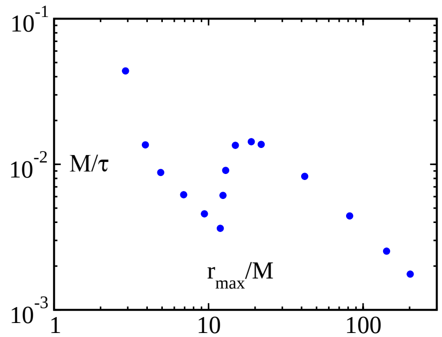
Single Black Hole
(Scheel et al, 2002)

- Computational details: Pseudo-spectral collocation technique, domain is a spherical shell $1.9M \le r \le 11.9M$, 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 $\{\gamma_i j, K_{ij}\}$ and equations
- Modify extrinsic curvature evolution equation

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

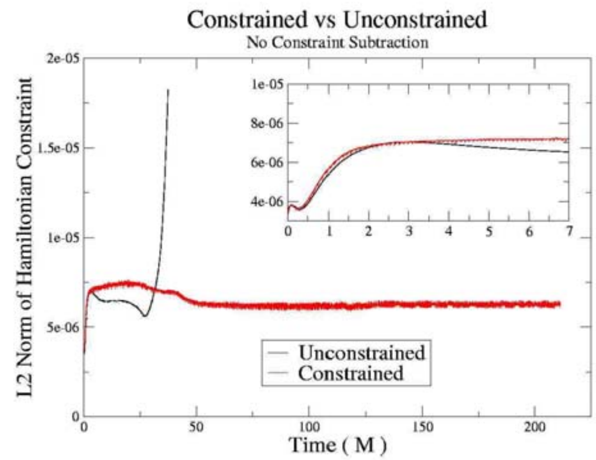
where $\mathcal{C} = 0$ is the Hamiltonian constraint, and the numerical coefficients are determined empirically to maximize evolution time

- 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: $-10M \le x, y, z \le 10M$, $h = M/5$, 100^3 mesh points
- Achieve evolution time $\approx 1000M$

Single Black Hole
(Anderson & Matzner 2003)

- More interestingly, investigated constrained evolution—pre-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

$$t = \bar{t}$$
$$x^i = \bar{x}^i + \xi^i(\bar{t})$$

  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 A_{ij} and modify evolution equation for Γ^i
- Also use densitized lapse q

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

  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), $0 \le x, y, z \le 12M$, $6p^3$ gird points, evolve for 10000M with no signs of instabilities
- Moving hole: computational domain (equatorial symmetry), typical run $-10M \le x, y \le 10M$, $0 \le z \le 7M$, $60 \times 60 \times 30$ grid points
  - Evolution times: $1000 - 6000M$ treatment of outer boundaries likely limiting factor.
- ANIMATION: Rotating motion, K plotted.
- ANIMATION: Inspiral motion, K plotted.

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 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

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

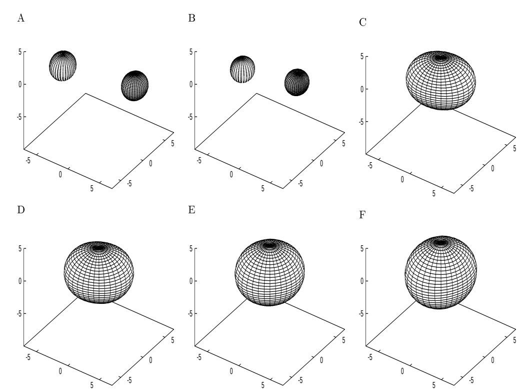
$$\beta^i = \beta^i_1 + \beta^i_2$$

  where $\alpha_1, \alpha_2, \beta^i_1, \beta^i_2$ are computed from boosted KS and dynamically centred at instantaneous location of holes
- Coordinate conditions: Post-merger: Use α, β^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: $-10M \le x, y, z \le 10M$, $h = M/8$, 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

Two Black Hole Grazing Collision
(Alcubierre et al 2001b)

- Initial data: "Puncture type", corresponding to black holes in mutual orbit:

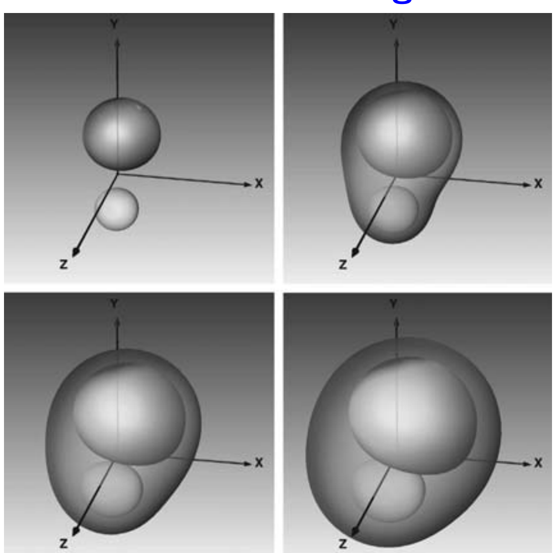
$$
\begin{array}{ll}
R_1 = (0, +1.5m, 0) & R_2 = (0, -1.5m, 0) \\
P_1 = (+2m, 0, 0) & P_2 = (-2m, 0, 0) \\
S_1 = (-m^2/2, 0, -m^2/2) & S_2 = (0, m^2, -m^2)
\end{array}
$$

- Use BSSN formalism, essentially as described in Baumgarte & Shapiro 1998, $O(h^2)$ spatial differencing, iterative Crank Nicholson time stepping, approximate Sommerfeld outer boundary conditions
- Coordinate conditions: Solve maximal slicing condition at $t = 0$, use "1 + log" slicing thereafter, $\beta^i = 0$
- *NO excision*

Two Black Hole Grazing Collision
(Alcubierre et al 2001b)

- Computational domain: $-19m \le x, y, z, \le 19M$, $h = 0.2M$, 387^3 grid points
- Evolution extended to $t \sim 30 - 40M$ (about twice as long as Brandt et al 2000)
- Waveforms were extracted, with an estimated 1% of ADM mass emitted as gravitational radiation
- As is case with Brandt et al computations, not clear that initial data really represents two distinct holes

Two Black Hole Grazing Collision



- The merger of the apparent horizon for the grazing collision described above. Shown are marginally trapped surfaces at times $2.5M$, $3.7M$, $5.0M$ and $6.2M$, where $M \sim 3.22m$ is the ADM mass of the spacetime and m is the initial bare mass of each black hole. Source: Alcubierre et al 2001b

Neutron Star Collisions

- Despite the complications of relativistic hydrodynamics, this type of calculation is somewhat further advanced than the BH case, primarily because BH singularities are not an issue until late phases of evolution (assuming that collision *does* lead to BH formation)
- As with BH case, Cartesian coordinates are universally adopted for 3D work, and finite difference approaches currently dominate
- Neutron star matter typically treated as a perfect fluid; stress tensor $T_{\mu\nu}$ given by

$$T_{\mu\nu} = (\rho + \rho\epsilon + P)u_\mu u_\nu + P g_{\mu\nu}$$

where ρ, ϵ, P, u_μ are baryon rest-mass density, specific internal energy, pressure and fluid four velocity

Neutron Star Collisions

- Initial conditions: Polytropic equation of state (EOS)

$$P = K\rho^\Gamma \qquad \Gamma = 1 + \frac{1}{n}$$

  where K, n are the polytropic constant, index

- During evolution, use Γ-law EOS

$$P = (\Gamma - 1)\rho\epsilon$$

- $\Gamma = 2$ typical choice (stiff EOS)
- Computational treatment of fluid
  - Shocks major issue
  - Artificial viscosity and simple upwinding schemes were traditional choices
  - In past few years, high resolution shock capturing (HRSC) methods (higher order Gudonov techniques) have become popular in numerical relativity

Neutron Star Collisions
(Shibata, Taniguchi & Uryu 2003)

- Had previously focused on equal mass case, now consider unequal masses
- Had found in equal mass simulations that accretion disk formed as a result of merger then collapse to BH was not very massive; suggested that equal-mass collision was not a likely progenitor for gamma ray bursts (GRBs) (Most GRB models invoke a BH with accretion disk $\sim 0.1 - 1M_\odot$)
- Argued that unequal mass interaction more likely to lead to massive disk
- Use formalism closely related to BSSN

Neutron Star Collisions
(Shibata, Taniguchi & Uryu 2003)

- Coordinate conditions
  - Approximate maximal slicing

$$\partial_\tau \ln\alpha = \Delta \ln\alpha + (D_i \ln\alpha)(D^i \ln\alpha) + \cdots + f_\alpha K g(\rho)$$

    where f_α is an $O(1)$ constant, and the last term is chosen to drive solution to $K = 0$. Discretized version typically applied about 30 times per time step.
  - Dynamical shift condition

$$\partial_t^2 \beta^i = \Delta_f \beta^i + \frac{1}{3}\gamma^{ik}\partial_k\partial_j\beta^j - \tilde{S}^j$$

    where Δ_f is the flat-space Laplacian and $\tilde{S}^j$ are source functions. Produces β^i similar to that of "approximate minimal distortion"

Neutron Star Collisions
(Shibata, Taniguchi & Uryu 2003)

- Initial conditions: Start with stars in quasiequilibrium circular orbits (assume helical Killing vector), irrotational velocity fields; solve coupled set of elliptic equations for hydrodynamic/geometric variables via pseudo-spectral technique
- Computational domain (typical case): $-20M \le x, y \le 20M$, $0 \le z \le 20M$ (equatorial symmetry), $633 \times 633 \times 317$ grid points; initially each star is resolved by about 40 grid points
- ANIMATION: Unequal mass irrotational binary: no black hole formation
- ANIMATION: Unequal mass irrotational binary: black hole formation
  Source of animations: `http://esa.c.u-tokyo.ac.jp/~shibata/anim.html`
- Find $\sim 0.5\%$ of ADM mass, $\sim 6 - 8\%$ of initial angular momentum radiated away.
- Calculations of similar scale, using very similar techniques have recently been carried out by Miller, Gressmann and Suen 2003.

Construction of Stable FD Schemes for NR

(Calabrese et al 2003)

- Approaches to finite differencing in NR have often been *ad hoc*, with much trial and error particular with regards to boundaries, both outer and inner (e.g. excision boundaries); again stability is key issue

- Authors apply techniques from numerical analysis of hyperbolic equations to problem of 3D propagation of scalar field on Schwarzschild background

- Basic idea: Symmetric hyperbolic systems can be shown to be well posed (stable) by defining an energy function (via a spatial integral), and showing that it can be bounded as a function of the initial/boundary data; integration by parts plays key role here

- Stable FD schemes for such systems can be constructed so that similar energy estimates hold at the discrete level

- Four steps in construction

  1. Equations are semi-discretized (time remains continuous) on finite-domain with cubical region interior to BH excised; scalar product Σ between any two grid function defined, which in turn allows definition of semi-discrete energy, E; Σ and discrete spatial difference operator, D, must be carefully constructed so that summation by parts (SBP) holds

Construction of Stable FD Schemes for NR

2. At discrete level, boundary terms at edges and vertices of grid that remain after SBP contribute to E at any given resolution; BC's have to be imposed on incoming characteristic modes along "effective" normal vectors so as not to destroy energy estimate; technique used is to project RHSs of evolution equations onto subspace of grid functions that satisfy discrete BCs
3. To minimize growth of error, add sub-truncation-order dissipation terms (a la Kreiss & Oliger 1973, but suitably modified near boundaries) and rewrite/rearrange discrete equations to ensure that optimal continuum energy estimates hold at discrete level
4. Stability of fully discrete scheme ensured by use of temporal integration scheme such as 3rd or 4th order Runge-Kutta that satisfies local stability condition or that preserves energy estimate

- ANIMATION $z = 0$ cut of initially off-centre Gaussian pulse of scalar field propagating on Schwarzschild background

- ANIMATION $z = 0$ cut of scalar field with $l = 2$ angular structure propagating on Schwarzschild background
  Source of animations:
  `http://relativity.phys.lsu.edu/movies/scalarfield`

Construction of Stable FD Schemes for NR

- Similar techniques have now been applied by LSU group to several other problems:
  - Sarbach & Lehner 2003: Investigation of possibility of naked singularity formation in spherically symmetric bubble spacetimes
  - Calabrese & Neilsen 2003: 2D (axisymmetric) simulations of massless scalar field propagation on boosted Schwarzschild background using multiple coordinate patches / FD meshes
  - Tiglio et al 2003: 3D simulation of Schwarzschild hole with excision (also includes dynamics lapse condition, and dynamical choice of "constraint-multipliers" added to evolution equations in attempt to control constraint violating modes)

- Expect that this work will have major impact on FD numerical relativity

The Need for Mesh Adaptivity in Numerical Relativity

- Problems of interest, particularly those involving black holes, span orders of magnitude in spatio temporal scales

- Example: Inspiralling collision of two BHs
  - Individual BHs: $\sim M$
  - Orbital scale: $\sim 10M$
  - Wave zone, where waveforms can be reliably read off: $\sim 100M$
  - Temporal scales: $\sim M - \sim 1000M$

- Slow rate of progress in 3D finite difference NR is *in part* attributable to use of "unigrid" codes (those characterized by a single discretization scale, h.

The Need for Mesh Adaptivity in Numerical Relativity

- Moore's Law: Computational power doubles roughly every 1.5 years; 10 years $\sim$ 7 doublings resulting in about a factor of 100 in resources (CPU speed, memory)
- 3+1-D problem, execution time scales like h^{-4}, 100 fold increase buys about a factor of 3 in resolution!
- Much effort has been expended over the past decade and more to incorporate mesh refinement techniques in NR; basic idea is to allow h to be a function of space and time, so that resolution can be adapted to solution features
- Specific algorithm due to Berger & Oliger 1984 has had most impact in this area.

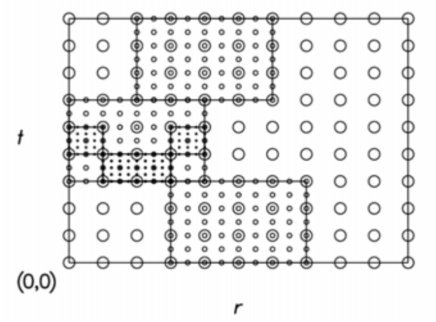
Adaptive Mesh Refinement (AMR)
(Berger & Oliger 1984)

- Employ hierarchy of locally uniform finite difference meshes, organized into levels, $l = 0, 1, 2, \cdots, l_{\max}$ with discretization scales satisfying

$$h_l \equiv \rho_l h_{l+1}$$

where ρ_l are integers. Typically for 3D applications, $\rho_l = \rho = 2$

- 1+1 example: $l_{\max} = 2, \rho = 2$



Adaptive Mesh Refinement (AMR)
(Berger & Oliger 1984)

- Refine in time as well as in space, take coarse time steps first in order to provide boundary conditions on fine grids (at fine-coarse interfaces, a.k.a. AMR boundaries) via interpolation
- Remesh *dynamically*, typically using estimate of local error in solution
- Example: Consider two-level explicit finite difference scheme at discretization scale h; write time-advance update as

$$u^{n+1} = Q^h u^n$$

where Q^h is the one-time-step update operator

- Then

$$\left(Q^h Q^h - Q^{2h}\right) u^n$$

provides an estimate of the local solution error

Adaptive Mesh Refinement (AMR)
(Berger & Oliger 1984)

- Shortcomings:
  - Have to deal with AMR boundaries, additional stability considerations often arise
  - Only "optimally efficient" (in computational complexity sense) if solution features are volume filling
  - Assumes locality of influence (i.e. designed for hyperbolic systems), algorithm requires modification if elliptic equations must also be solved, some successful strategies exist (Pretorius 2002)

Potential Speed-up using AMR
(Pretorius 2003)

- Case analysis for equal-mass BH merger
- Assumptions
  - Finest level grids cover each BH, diameter $2M$
  - Linear filling factor of $1/2$ (i.e. at each level, only $1/8$ of the volume requires subsequent refinement)
  - 2:1 refinement ratio ($\rho = 2$)
  - Outer boundary at $L_X M$
  - Evolution to $t = L_T M$
  - Courant factor $\equiv \Delta t / \Delta x = 1/2$
  - Finest level $l_{\max} = \log_2(L_X)$ is sufficiently large that

$$\sum_{n=0}^{l_{\max}-1} \left(\frac{1}{2}\right)^n \sim 2$$

Potential Speed-up using AMR
(Pretorius 2003)

- Speed-up:
$$\frac{T_{\rm UNI}}{T_{\rm AMR}} \approx \frac{C_{\rm UNI}}{2C_{\rm AMR}} (L_X)^3 \approx (L_X)^3$$
where $T \equiv$ run time, $C \equiv$ computational cost per grid point
- For $L_X = 100$, we have a potential speed-up of order 10^6, equivalent to 30 yrs of Moore's Law!

2D Axisymmetric AMR
(Pretorius 2002, Choptuik et al 2003b)

- Added Berger & Oliger AMR capability to previously developed axisymmetric code (Choptuik et al 2003a) that incorporates a massless scalar field as the matter source
- Axisymmetric code adopts 2+1+1 formalism (Geroch 1971, Maeda et al 1980), but for rotation-free case, is equivalent to standard ADM approach
- Metric & Stress Tensor: (cylindrical coordinates)

$$ds^2 = -\alpha dt^2 + \psi^4 \left[(d\rho + \beta^\rho dt)^2 + (dz + \beta^z dt)^2 + \rho^2 e^{2\rho\bar\sigma} d\phi^2 \right]$$

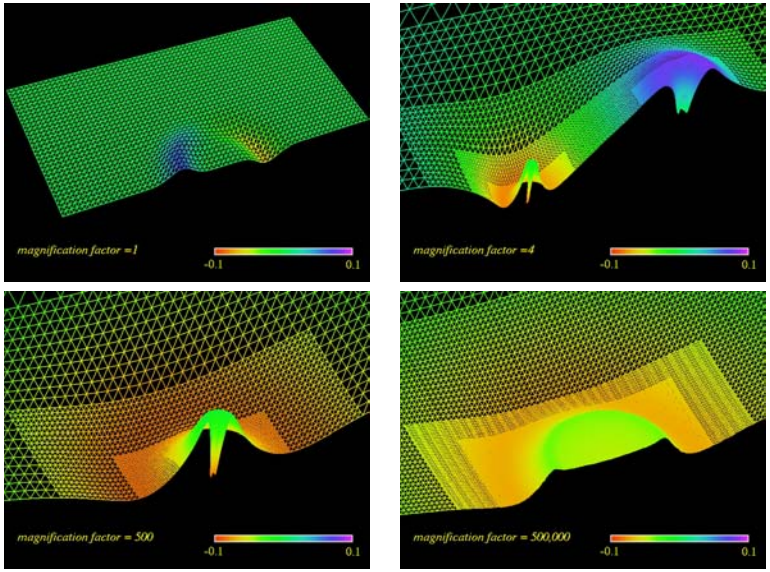
$$T_{\mu\nu} = 2\Phi_{,\mu}\Phi_{,\nu} - g_{\mu\nu}\Phi_{,\sigma}\Phi^{,\sigma}$$

- Introduce conjugate variables, $\bar\Omega \sim \partial_t \bar\sigma$, $\Pi \sim \partial_t \Phi$

2D Axisymmetric AMR
(Pretorius 2002, Choptuik et al 2003b)

- System of PDEs
  - Evolution equations for $\Phi, \Pi, \bar\sigma, \bar\Omega$, and optionally ψ, solved using $O(h^2)$ centred differencing techniques; iterative Crank Nicholson update
  - Coupled elliptic equations for $\alpha, \beta^\rho, \beta^z, \psi$, solved using $O(h^2)$ FD methods and multigrid
- Study critical collapse (black hole threshold behaviour) of massless scalar field
- Consider parameterized families of initial data representing gaussian spherical shells of scalar field, family parameter is overall amplitude factor, which is then tuned to machine precision
- ANIMATION: Near critical solution displayed in logarithmic radial coordinate
- ANIMATION: Same evolution, but in original cylindrical coordinates, and with continuous "zoom-in" on critical region

Illustration of Adaptive Remeshing



- Calculation used 24 2:1 levels of refinement. Figures show every other grid line.

3D Fixed Mesh Refinement

(Schnetter et al 2003)

- Approach very similar to Berger & Oliger, except that refinements are specified in advance based on *a priori* knowledge of solutions features, and *do not* move in time
- Algorithm is simplified since there is no need for truncation error estimation and the concomitant regridding process
- Implemented as a "Driver thorn" for Cactus, which in principle should facilitate use by large number of extant and future Cactus applications (i.e. will work in parallel)

3D Fixed Mesh Refinement

(Schnetter et al 2003)

- Presented series of test calculations, each using a single level of $2:1$ refinement (i.e. one coarse grid, one fine grid)
  - Wave equation in flat space
  - Minkowski spacetime with small perturbations ("robust stability test")
  - "Gauge wave" (Minkowski in time/space-dependent coordinates)
  - Schwarzschild BH with excision
- For most part find that adaptive runs have similar accuracy, convergence properties as unigrid runs at finest resolution
- Not surprisingly, find that special attention must be paid to refinement boundaries for stability

3D AMR

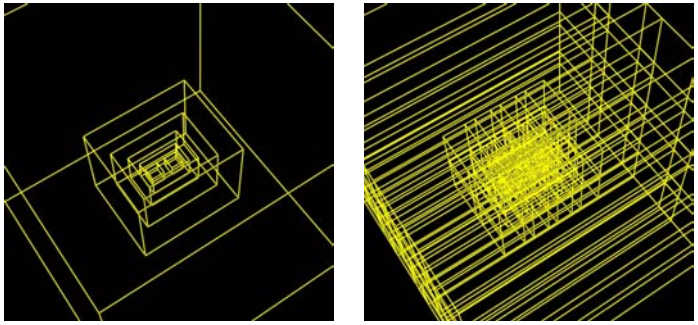
(Pretorius in progress)

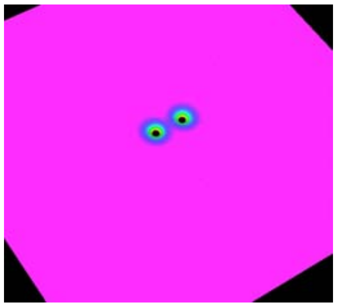
- Has implemented Message Passing Interface (MPI)-based library to support parallel adaptive mesh refinement of Berger & Oliger type
- Also incorporates support for multigrid solution of elliptic PDEs
- Currently studying 3D critical scalar collapse using a generalized harmonic code

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

  with the H^μ chosen to avoid coordinate singularities
- Has included apparent horizon detection and excision
- Uses spatially compactified coordinates that facilitate setting precise outer boundary conditions (asymptotic flatness), but which induce reflections that preclude accurate long-time integrations
- Typical calculation: Two blobs of scalar field, set up to promptly collapse to form BHs, track subsequent BH dynamics

Illustration of 3D AMR - Head on BH Collision





- Upper left: Bounding boxes delineating different levels
- Upper right: Bounding boxes showing parallel distribution
- Lower left: $z = \mathrm{const.}$ slice of lapse

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
- Use excision, with 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 Sommerfield 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
- Evolutions last more than one orbit, and no common apparent horizon is detected for sufficiently large initial separations
- Computations still crash eventually, but clearly this is an exciting advance.

Conclusions & Open Issues

- 3D Numerical relativity has seen SUBSTANTIAL progress in past few years
  - Improved theoretical understanding of hyperbolic forms of Einstein's equations
  - Improved stability of free evolution schemes based on such forms
  - Positive identification of unphysical (constraint violating) modes in free evolution schemes, and the beginning of developments aimed at controlling them
  - Improved theoretical understanding of boundary conditions, and beginnings of effective numerical implementations thereof
  - Improved theoretical understanding of construction of astrophysically realistic initial data for binary inspiral, and development of very efficient and accurate codes for the solution of the IVP
  - Beginnings of development of effective coordinate conditions for scenarios such as binary inspiral
  - Introduction of "provably stable" FD techniques
  - Development of effective numerical strategies for black hole excision
  - Widespread use of parallel computation
  - Beginnings of application of adaptive mesh refinement to 3D problems

Conclusions & Open Issues

- Open Issues
  - SEE PREVIOUS LIST!
  - Constrained vs free evolution: given relatively glacial progress in solving even the problem of simulating Schwarzschild, is view that elliptic equations are simply too expensive misguided, particularly when methods with optimal scaling (i.e. linear cost in the number of grid points) exist?
  - Computational demands
    - Time scale for “production” 3D runs is still weeks or even months; many problems not identified until large-scale, long-time computations are attempted—adaptivity and/or spectral techniques should help
    - Parameter space exploration adds additional “dimensionality” to any problem of significant interest and is easy to forget about when doing development work
  - Analysis
    - When 3D NR begins to produce results of physical interest, how will the physics be extracted/understood? Huge amount of data will be generated and efficient and effective analysis tools will become just as important (if not more so) than the underlying code itself
    - Advanced interactive visualization/analysis systems likely to play a crucial role, and continued development on this front is needed

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