A Numerical Approach to Binary Black Hole Coalescence

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The nature of binary black hole coalescence is the final, uncharted frontier of the relativistic Kepler problem. In the United States, binary black hole coalescence has been identified as a computational “Grand Challenge” whose solution is the object of a coordinated effort, just reaching its half-way point, by more than two-score researchers at nearly a dozen institutions. In this report I highlight what I see as the most serious problems standing between us and a general computational solution to the problem of binary black hole coalescence:

- the computational burden associated of the problem based on reasonable extrapolations of present-day computing algorithms and near-term hardware developments;
- some of the computational issues associated with those estimates, and how, through the use of different or more sophisticated computational algorithms we might reduce the expected burden; and
- some of the physical problems associated with the development of a numerical solution of the field equations for a binary black hole system, with particular attention to work going on in, or in association with, the Grand Challenge.

1 Introduction

In its simplest form, the relativistic Kepler problem involves the orbital evolution of two black holes in an asymptotically flat universe with no-incoming-radiation boundary conditions. Consider a binary black hole system at early times when we can speak, in the sense of the correspondence principle, of large orbital angular momentum and orbital energy close to zero. The evolution of such a system can be regarded in three parts:

1. At early times the evolution is adiabatic: the black holes circle each other and the orbits change on timescales long compared to the orbital period.

2. As the separations become smaller the orbit evolves more quickly and the adiabatic approximation breaks down. Shortly thereafter the black holes plunge together and coalesce to form a single, large and highly dynamical black hole.

3. Finally, the descendant black hole radiates away its perturbation and settles down to a stationary state that evolves no further.
The intermediate period of binary evolution described above, beginning when the binary separation is on order $13M$ for equal mass black holes and ending with the emergence of a single perturbed black hole, is of great interest to three communities of scientists:

- to the relativist it represents the missing link in the solution of relativistic Kepler problem, a regime both strongly non-linear and highly dynamical, without whose understanding the initial binary cannot be matched to the final stationary black hole spacetime;

- to the astrophysicist it represents a period of strong gravitational-wave radiation, whose detection may yield the most direct evidence for the existence of black holes, a new determination of the Hubble Constant, and clues to the density and mass distribution of black holes in the universe;

- finally, to the computational physicist it represents a complex physical system whose numerical solution exceeds the capabilities of the present day combination of computing algorithms and hardware and will challenge those of the next generation.

Both the initial period of adiabatic evolution and the final era of black hole “ring-down” can be understood quantitatively using perturbative techniques. The details of the intermediate period — when the evolution is non-adiabatic and the black holes coalesce — is not understood quantitatively and does not appear amenable to approximate treatment short of a fully numerical solution.

In view of the significant computational challenges and great scientific interest in the solution to this outstanding problem of physics, the United States National Science Foundation has funded a “Computational Grand Challenge Team” with the goal of developing, in five years, a general, extensible computational solution to the problem of binary black hole coalescence. The leading investigators of that team are

- Richard Matzner and James Brown (University of Texas, Austin);

- Stuart Shapiro (Center for Astrophysics and Relativity);

- Charles R. Evans and James York (University of North Carolina, Chapel Hill).

- Saul Teukolsky (Cornell University);

- Faisal Saied, Paul Saylor, Edward Seidel, Larry Smarr (National Center for Supercomputing Applications and University of Illinois, Champaign-Urbana);
In addition, close and fruitful collaborations have been struck between members of this Grand Challenge Team, Wai-Mo Suen (Washington University, St. Louis) and Nigel Bishop (University of South Africa).

In this report I highlight what I see as the most serious problems standing between us and a general computational solution to the problem of binary black hole coalescence. In doing so, I hope to convey a real sense of where we are and, more importantly, where we are heading. In §2 I give a conceptual overview of how we formulate the evolution of a vacuum spacetime as an initial value problem. With this as background, in §3 I discuss the computational burden associated with binary black hole coalescence, based on reasonable extrapolations of present-day computing algorithms and near-term hardware developments. In §4 I discuss some of the computational issues associated with those estimates, and how, through the use of different or more sophisticated computational algorithms we might reduce the expected burden. Finally, in §5 I survey some of the physical problems associated with the numerical solution of the field equations for a binary black hole system, focusing on work going on in association with the Grand Challenge.

2 Spacetime as an initial value problem

Our problem, simply stated, is to evolve forward in time an initial, spacelike hypersurface with two black holes. As posed, the problem distinguishes naturally between space (defined by the initial hypersurface) and time (generally orthogonal to the initial value hypersurface). In the conventional numerical treatment of initial value problems we choose a coordinate system that enforces a distinction between space and time everywhere: we foliate spacetime with spacelike hypersurfaces, of which the earliest is the initial value hypersurface, describe spacetime’s geometry in terms of the intrinsic and extrinsic geometry of these hypersurfaces, and formulate the field equations to allow us, given the intrinsic and extrinsic geometry of one spacelike hypersurface, to find the same for the next. The collection of spacelike hypersurfaces together with their intrinsic and extrinsic geometry completely determine the geometry of a four-dimensional volume of spacetime; in our case, the spacetime of a binary black hole system.
The basic formulation of this $3 + 1$ split of spacetime is due to Arnowitt, Deser and Misner. The spacelike hypersurfaces of the foliation are level surfaces of coordinate time, and three coordinate functions are defined to label points on each hypersurface. There is some ambiguity in the choice of spatial and time coordinates corresponding to the gauge freedom of the theory: this freedom allows us to choose the relation between spatial coordinates on successive hypersurfaces (i.e., lines of constant spatial coordinate may be shifted relative to the hypersurface orthogonal) and also the elapsed proper time along the hypersurface orthogonal joining successive slices.

Figure 1 (adapted from York) illustrates how two successive hypersurfaces of the spacetime foliation are related to each other. In the coordinate system used in the numerical evolution each of these surfaces is a slice of constant coordinate time; the coordinate time difference between the two slices shown is $d\tau$. Focus attention on the bottom slice ($\mathcal{A}$), which is the level surface corresponding to coordinate time $\tau$. The intrinsic geometry of this slice is described by the 3-metric $\gamma_{ij}$, which is the projection of the spacetime 4-metric on $\mathcal{A}$. The tangent to the hypersurface normal at point $\mathcal{P}$ on $\mathcal{A}$ is $n$, and the tangent to the world line of a coordinate-stationary observer at $\mathcal{P}$ is $t$.

The upper hypersurface ($\mathcal{B}$) is the spacelike 3-surface of constant coordinate time $\tau + d\tau$. The elapsed proper time between $\mathcal{A}$ and $\mathcal{B}$ along $n$ is $\alpha(\mathcal{P}) \, d\tau$, where $\alpha$ is the lapse function. The coordinate (gauge) freedom of the theory gives us some freedom in the choice of the lapse. Lying in each spacelike hypersurface is a 3-vector field $\beta$, called the shift, that describes how worldlines of coordinate stationary observers deviate from the hypersurface orthogonal $n$. The choice of three-vector $\beta$ exhausts our coordinate freedom. An exceptionally readable description of the $3 + 1$ decomposition of spacetime is given in York.

Having chosen the $3 + 1$ coordinates, it is necessary to define fields on each hypersurface from which the hypersurface spatial metric and extrinsic curvature can be determined. The Einstein field equations can then be cast in terms of those variables, leading to constraint equations, which do not involve time derivatives of the fields, and evolution equations, which do. Constraint equations must be satisfied by the fields on each hypersurface, while evolution equations involve reference to future surfaces of the foliation and are used to determine the fields on successive hypersurfaces. The identification of field variables, formulation of their equations of motion, and the specification of boundary conditions and initial data are all areas of active research today and are discussed in §5.
Figure 1: In numerical relativity, initial value problems are treated by introducing a coordinate system that distinguishes between space and time; the field equations are then formulated in a way that permits the intrinsic and extrinsic geometry of one slice (the initial data) to determine the same on successive slices. Here is shown the relationship between the spacelike hypersurfaces, which are level surfaces of the coordinate time, their normals, and the spatial coordinates on successive hypersurfaces in the conventional $3 + 1$ decomposition of spacetime. See §2 for details.
3 Computational Burden

Should we tomorrow find ourselves suddenly in command of unlimited computing resources we would be no closer to a numerical solution to binary black hole coalescence than we are today: there remain open questions — regarding the appropriate choice of field variables (and, correspondingly, the equations to be solved), the numerical method of solution and the interpretation of both initial data and the results — that must be settled before we can construct a numerical code that “solves” the black hole binary coalescence problem. Nevertheless, it is instructive to anticipate the ultimate computational burden of a binary black hole coalescence code using present-day techniques.

3.1 Memory

As discussed in §2, the numerical model of binary black hole coalescence is constructed from an initial, spacelike, three-dimensional slice of spacetime, boundary conditions, and the Einstein field equations. We cannot evolve a slice of infinite volume (nor would we want to if we could); so, we choose the smallest region of spacetime that includes the system of interest and on which we can impose sensible boundary conditions. All simulations proceed by carrying approximate values of field quantities at isolated points within the volume, and the variations of these fields on the important length scales (e.g., black hole mass, radiation wavelength) must be suitably resolved. Together, these constraints determine the primary memory that must be devoted to each timestep in the simulation.

Consider a system of two roughly equal black mass holes with total mass $M$ in a circular orbit of radius $\sim 6M$. The quadrupole order radiation wavelength is on order $100M$, which is substantially greater than the system’s size. To pose sensible outer boundary conditions and extract the radiation from the system we need the outer boundary of the computational volume at least one wavelength away from the system’s center; thus, the computational volume is $\gtrsim 10^6 M^3$. The simulation resolution must be great enough to resolve the individual black hole and the radiation; a resolution of $\Delta x \lesssim M/20$ is a reasonable assumption. Assuming uniform resolution throughout each spatial slice requires that the field variables be maintained at $\gtrsim 10^{10}$ isolated points within the computational volume.

On each slice of constant time are equations governing the evolution of the slice’s spatial metric and its extrinsic curvature. In addition to these fields are several auxiliary quantities that appear frequently enough in the evolution and constraint equations that it is sensible to compute them once on each slice and re-use their stored values when necessary. Thus, there are on order
50 field and auxiliary quantities that must be stored, in double precision, at each of the \(\gtrsim 10^{10}\) points on a given hypersurface, leading to a final estimate of \(\gtrsim 4 \times 10^{12}\) bytes of primary memory for the computational volume. An equivalent amount of secondary storage (e.g., disk storage) is required for each slice of a time evolution that we wish to store for later examination.

### 3.2 Execution speed

A complete simulation involves the evolution of the computational volume from an initial data set of two separate black holes, through their coalescence, to a final data set consisting of a single perturbed black hole. The simulation’s spatial resolution, together with the numerical algorithms used, determines its temporal resolution. The simulations duration and the required temporal resolution determine the number of intermediate spatial slices that must be computed in passing from the initial to the final hypersurface. If we use finite difference methods (cf. §4.1) for solving the partial differential equations that evolve each slice to the next, then the computational work per slice (measured in floating point operations) depends linearly on the slice’s volume and inversely on its spatial resolution. The work per slice and the number of slices then yields the total number of floating point operations required for the full simulation. Insisting that such a simulation take a reasonable amount of time to perform leads to a minimum requirement for the computing speed in floating point operations per second, or flop/s.

Assume that the simulation starts with black holes in a nearly circular orbit at a separation of \(\sim 8M\), and that there are at most two orbits — corresponding to an elapsed time of \(\sim 250M\) — before coalescence. After coalescence the final black hole spacetime will be highly perturbed and the simulation will need to run several (say, five) black hole fundamental mode periods before the perturbations are small enough that the numerical simulation can be matched to a perturbation calculation. The total simulated time is then \(T \gtrsim 500M\). If the field variable characteristics are light cones then the simulation’s time resolution is on order its spatial resolution, or \(\lesssim M/20\), and a complete simulation requires \(\gtrsim 10^4\) timesteps. If the size and spatial resolution of each slice require that field and auxiliary variables be maintained at \(10^{10}\) points at each timestep, then there are \(10^{14}\) updates (of field and auxiliary variables) that occur in the course of a complete simulation. Modern three-dimensional codes require approximately \(5 \times 10^3\) flop/s per update\(^4\); consequently, there are \(\gtrsim 5 \times 10^{17}\) floating operations in a simulation. If we require that each simulation take less than \(\sim 12\) hours of computer time, then the computer must be capable of \(\gtrsim 10^{13}\) flop/s, or 10 Tfpop/s (teraflop/s).
3.3 Conclusions

What do these numbers mean?

At this writing (November 1995), the “fastest” general-purpose supercomputer in the world (as measured by its performance on the LINPACK benchmark) is the Fujitsu “Numerical Wind Tunnel”, installed at the National Aeronautics Laboratory in Japan. Its realized peak performance is $170 \times 10^9$ flop/s, or 170 Gflop/s, compared to a “theoretical” peak performance of 236 Gflop/s. Of those computers generally available for academic research, the fastest is the 512 node IBM SP2, installed at the Cornell Theory Center, with a realized peak performance of 88.4 Gflop/s and a theoretical peak performance of 136 Gflop/s. The National Center for Supercomputing Applications (NCSA) numerical relativity group reports a realized speed of 14.6 Gflop/s on a Thinking Machines CM-5 (whose theoretical peak performance is 63 Gflop/s). If we assume this latter ratio to be typical of the realized to theoretical performance for the next generation parallel-processing computers, then we anticipate the need for a two order of magnitude increase in the computing performance, on computers with terabyte primary storage, before generic three-dimensional binary black hole coalescence calculations, made using current methodology, are tractable.

4 Computing algorithms

The conclusion of the previous section — that a two order-of-magnitude increase in available computing speed is required to make binary black hole coalescence calculations tractable — comes accompanied by the important caveat that no change in either the computational algorithms or problem formulation affects significantly the assumptions that underly it.

The estimate of the computing burden of a generic binary black hole coalescence calculation is most sensitive to the simulation’s spatial resolution: if, without loss of accuracy or significant increase in the cost of the computation per update, the spatial resolution can be reduced by a factor of two in each dimension, the memory burden is reduced by a factor of 8 and the required computational speed by a factor of 16. Algorithm changes can affect the attainable accuracy as a function of the resolution; so, as we hope for faster computers we not neglect the search for more efficient (in the sense accuracy for a given resolution) computing algorithms. In this section I describe two different methods for solving partial differential equations on computers and comment on the strengths, weaknesses, and promise of each.

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A computer’s theoretical peak performance may be interpreted as that performance it is guaranteed never to exceed.
4.1 Numerical solution of partial differential equations

Computers don’t do calculus: differential equations are solved numerically by converting them to a set of algebraic equations that are solved by the more elementary operations of addition, subtraction, multiplication and division. There is a range of methods used to approximate partial differential equations by algebraic ones; however, the practice of numerical relativity has focused almost exclusively on the finite difference approximation.

Finite differencing

In a finite difference approximation the derivatives in the differential equations are replaced by approximations formed from field variable values at discrete points. For example, an approximation to the second derivative of $u$ might be written as

$$\frac{d^2 u}{dx^2}(x_i) \rightarrow \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{(\Delta x)^2}, \quad (1)$$

where the $x_i$ are discrete points and $\Delta x = x_{i+1} - x_i$. Clearly the points $x_i$ do not need to be spaced equally; similarly, the algebraic approximations for different derivatives can be made arbitrarily complex and accurate to high order in the spacing. With a choice of points and a “differencing scheme” for converting derivatives to ratios of finite differences, any set of differential equations can be converted to a set of algebraic equations that can be solved using standard methods of linear algebra.

In a finite difference approximation, the solution to the approximate equations converges upon the solution to the exact equations as a finite power of the resolution $h \sim |x_i - x_{i-1}|$. The exponent is called the order of the differencing scheme; for example,

$$\frac{[u(x_{i+1}) - u(x_i)](x_i - x_{i-1})}{(x_{i+1} - x_i)(x_{i+1} + x_{i-1})} + \frac{[u(x_i) - u(x_{i-1})](x_{i+1} - x_i)}{(x_i - x_{i-1})(x_{i+1} + x_{i-1})} = \frac{du}{dx}(x_i) + O(h^2) \quad (2)$$

is a second-order difference approximation to $du/dx$ at $x_i$ for unevenly spaced points $x_i$. For problems with smooth solutions, the difference between the solutions to the differential and difference equations is, for small $h$, proportional to $h^N$, where $N$ is related to the order of the least accurate differencing scheme used to approximate the system and its boundary conditions.

Finite difference approximations are relatively simple and straightforward to program. They are also flexible: the choice of grid points and their spacing can conform to irregular boundaries or be concentrated in areas where increased resolution is needed. On the other hand, finite difference methods are
sensitive to coordinate singularities: accurate difference operators for points on
or near the origin or polar axis of a spherical coordinate system are difficult to
construct and generally. The implementation of boundary conditions that are
not algebraic in the evolving fields (e.g., a Sommerfeld out-going wave bound-
ary condition) often involves introducing grid points “beyond the boundary”
that are not evolved, but are reset at each timestep so that the differencing
scheme, applied at the boundary, leads to an appropriate approximation. Fi-
nally, there are a variety of finite difference schemes, whose errors scale with
resolution identically but whose performance, at boundaries and coordinate
singularities, differ greatly. An acceptable choice of differencing scheme near
these singularities is generally problem specific and requires fine-tuning.

The large computational burden of the binary black hole coalescence calcu-
lation is due primarily to the high spatial resolution required in each spacelike
slice. High resolution is not required everywhere in the slice, however, but
only where the field variables are changing on short lengthscales. Near the
black holes, resolution on sub-$M$ scales is necessary to resolve the spacetime
curvature accurately; however, far from the holes (in the larger part of the
computational volume) the shortest lengthscale is a radiation wavelength and
a much coarser resolution will provide the same level of accuracy. If we give
up the convenience of uniform resolution, the computational burden of a fi-
nite difference calculation can be reduced dramatically by allowing the spatial
resolution to vary so that the approximation is equally accurate everywhere.

This is the idea behind adaptive mesh refinement: in any region resolve
only so far as is necessary to attain the desired local accuracy. Adaptive mesh
refinement is being pursued aggressively within the collaboration by physicists
and computer scientists at the University of Texas and Syracuse University.
In the present example, high ($M/20$) resolution is needed only near the black
holes: for most of the volume of each spatial slice resolution of order $M$ to
$10M$ may be more appropriate. Adaptive mesh refinement might then lead
to a reduction in the memory required per spatial slice of a factor $10^4$ over
a monolithic grid, and a reduction in the speed requirements by a factor $10^5$
(less the increased cost per time step).

Collocation pseudo-spectral methods

In finite differencing the differential equations are approximated by algebraic
ones that are then solved numerically. A complementary approach approxi-
mates not the equations, but their solution. In a collocation pseudo-spectral
approximation, the solution $u$ is written as a sum over a set of basis functions
\( \phi_n \) with unknown coefficients:

\[
u(x) \simeq \sum_{n=0}^{N} c_n \phi_n(x).
\]  \hspace{1cm} (3)

In two or more dimensions it is typical to choose a separate basis in each dimension and express \( u(x) \) as a sum over products of the basis functions in each dimension: e.g.,

\[
u(x,y) \simeq \sum_{m,n=0}^{M,N} c_{mn} \phi_m(x)\psi_n(y).
\]  \hspace{1cm} (4)

Algebraic equations for the \( N \) coefficients \( c_n \) of the approximate solution are found by insisting that the approximate solution satisfy exactly the equations and boundary conditions at an equal number of collocation points \( x_i \). The basis functions and collocation points are typically chosen to exploit a discrete orthogonality relation: for example, the basis might be a finite subset of Chebyshev polynomials \( \phi_n = T_n \) on the domain \( x \in [-1XSAS, 1] \) and the collocation points \( x_k = \cos(\pi k/N) \) so that

\[
\sum_{k=1}^{N} T_i(x_k)T_j(x_k) = \begin{cases} 
0 & i \neq j \\
N/2 & i = j \neq 0 \\
N & i = j = 0
\end{cases}
\]  \hspace{1cm} (5)

For problems with \( C_\infty \) solutions a collocation pseudo-spectral approximation is extremely efficient: with a suitable basis the asymptotic rate of convergence of the approximate to the real solution is exponential, which is faster than can be achieved with any finite difference approximation. The choice of appropriate basis is not difficult, either: a Fourier decomposition in variables where periodic boundary conditions hold and a Chebyshev decomposition elsewhere is usually sufficient. The computation cost per coefficient (or collocation point) grows more rapidly than linearly; however, for Fourier and Chebyshev expansion bases that growth is no faster than \( \log N \). In the asymptotic regime, then, the marginal return of accuracy on an investment of computing resources is greater for a solution found using a collocation pseudo-spectral approximation than for one found using a finite difference approximation.

Larry Kidder and I have been investigating the use of collocation pseudo-spectral methods in numerical relativity applications. Our first investigations have focused on solving the initial value problem for a single black hole with Brill waves, a problem also studied using finite difference methods. On typical problems we find exponential convergence of the solution with spectral
bases involving greater than 5 angular and 5 radial Chebyshev polynomials. Comparing spectral and finite difference methods on the same problem, a spectral expansion using 20 radial and 20 angular basis functions (400 collocation points) achieved the same level of accuracy as a finite difference calculations using 400 radial and 105 angular subdivisions ($4 \times 10^4$ grid points); furthermore, the accuracy of the spectral calculation could be increased to machine precision (8 orders of magnitude better than the best finite difference calculation reported) with a basis of 70 radial and 70 angular (Chebyshev) functions. Finally, while the finite difference calculations were performed on the NCSA Cray Y-MP and Cray 2, the $20 \times 20$ spectral solution took 30 s, and the most highly resolved spectral calculation ($70 \times 70$) less than 10 minutes, on a Sun SPARCstation II.

Investigation of collocation pseudo-spectral methods for vacuum gravity have only just begun and their ultimate usefulness remains to be demonstrated. Despite their great promise, however, they are not a useful tool for this Grand Challenge application, which is committed to having a working solution by the end of 1998. To meet this goal, the collaboration must focus its efforts on increasing the efficiency of solutions based on the more mature (in this application) finite difference approximation.

5 Issues of physics

5.1 Radiation and the outer boundary

A principal goal of the Grand Challenge project is to determine the gravitational radiation arising from the coalescence of a binary black hole system. The appropriate boundary conditions (no incoming radiation) are most naturally posed at past null infinity and the radiation is naturally identified at future null infinity; however, the initial data for the numerical evolution is a spacelike hypersurface of finite volume. Consequently, boundary conditions must be posed and the radiative component of the fields identified at the boundary of this slice — at finite distance from the binary system and not at past and future null infinity. For the outer boundary of the spacelike slice, then, we must formulate boundary conditions to be applied at a finite distance from the origin that, as nearly as possible,

1. do not introduce any spurious radiation (either as incoming radiation from past null infinity or as reflections from the boundary) into the computational volume, and

2. allow us to determine the radiation waveforms, radiated power, etc., from the interior fields.
Two approaches to this outer boundary condition problem — which have come to be referred to as “radiation extraction” and “Cauchy-characteristic matching” — are under investigation. In radiation extraction it is assumed that the spacetime exterior to the worldtube enclosing the computational volume is well-approximated by a perturbation of an exact, stationary spacetime (e.g., Minkowski, Schwarzschild or Kerr spacetimes). Using the appropriate perturbation equations (e.g., the Zerilli equation for an approximately Schwarzschild exterior) the metric perturbations determined at the edge of the computational volume are readily “propagated” to large distances where the asymptotic radiation fields (in, e.g., TT gauge), radiated power, etc., can be determined. At the same time, boundary conditions corresponding to no incoming radiation from the exterior spacetime are imposed on the boundary of the interior volume.

In radiation extraction the worldtube boundary of the evolving spacelike hypersurfaces are assumed to match onto a perturbation of an exact, stationary spacetime. In the Cauchy-characteristic matching method (under development at Pittsburgh and Penn State) the worldtube is joined to a foliation of the exterior spacetime by null hypersurfaces that extend to future null infinity. The generators of these null hypersurfaces are the future-directed null geodesics orthogonal to the worldtube boundary of the spacelike-hypersurface foliation. By choosing a compactified radial coordinate on the null hypersurfaces, future null infinity becomes a sphere at finite radial coordinate (see figure 2). The spacelike interior foliation and the null exterior foliation are evolved together using the field equations; in this way, radiation generated in the interior that reaches the worldtube boundary appears immediately at future null infinity.

Radiation extraction and Cauchy-characteristic matching can be compared in several ways. Both methods attempt to impose only outgoing-wave boundary conditions (a strict implementation of no-incoming radiation boundary conditions requires the ability to control past null infinity, which involves the entire past history of the initial data slice). Radiation extraction is simpler to implement — it involves only perturbations about flat, Schwarzschild or Kerr spacetimes — while Cauchy-characteristic matching involves the field equations in all their partial-differential glory, along with a complicated matching between the Cauchy and characteristic evolution codes. On the other hand, perturbative treatments are only satisfactory when the fields are perturbative, while the Cauchy-characteristic method allows boundary conditions on the spatial slice to be posed where the geometry is strongly dynamical (as long as the exterior fields are never so axisymmetric that the hypersurface generators cross); additionally, the boundary conditions come from future null infinity and not a finite distance approximation. Finally, while Cauchy-
Figure 2: In Cauchy-characteristic matching each finite volume spacelike slice is joined to a null hypersurface that extends to future null infinity where the outgoing radiation is readily determined. See §5.1 for more details.
characteristic matching has been demonstrated for non-trivial vacuum gravity simulations\textsuperscript{2-4}, radiation extraction is the more mature technology\textsuperscript{9-11}.

5.2 Apparent Horizon Boundary Conditions

A numerical computation deals only with finite quantities; consequently, the spatial computational volume must avoid approaching too closely any spacetime singularities. In evolving a black hole spacetime it has been conventional to choose an initial slice that passes through the black hole throat, thus avoiding the singularity. As the initial slice is evolved, the lapse coordinate gauge freedom is exploited to “freeze” the evolution at and near throat, thus avoiding the interception of the singularity.

There is a price paid in avoiding the singularity in this manner, however: as time progresses the volume of the spatial slice grows exponentially near the throat as it is stretched to connect the evolving space far from the black hole to the unevolved space close to the throat. With the exponential stretching comes an unavoidable exponential growth in the computational resources devoted to the physically uninteresting transition between the evolved and unevolved regions. The net result is that, even if all other numerical pitfalls are overcome, the inability to resolve the stretching throat destroys the accuracy of the simulation more rapidly than a single orbital period of a binary black hole system.

The rapid change of the metric and extrinsic curvature near the throat reflect the singularity avoiding gauge choice and not anything of physical interest. Furthermore, because this region lies inside the event horizon it can have no physical effect on the spacetime outside the horizon. This suggests a different approach to the evolution of a the exterior black hole spacetime: use the horizon as a boundary, posing down-going radiation boundary conditions on it. Of course, the event horizon is not suitable for this purpose since it is known only after the development of the spacetime is complete; however, apparent horizons, even though gauge dependent, have all the requisite properties and can be identified on a spatial slice.

Apparent horizon boundary conditions have been pioneered by the Washington University/NCSA\textsuperscript{14,15} and the Cornell/Center for Astrophysics and Relativity\textsuperscript{16} groups.

5.3 Gauge and physics

Having chosen a spacetime slicing, the apparent horizon is a causal surface in the sense that nothing physical propagates outward from it. It is this property that makes it possible to conceive of evolving the volume outside the horizon
without reference to the volume inside, as discussed in §5.2. While physical effects propagate at the speed of light (or less for “tail” terms or simulations involving matter fields), non-physical (gauge) fields can propagate superluminally. If we are to use the apparent horizon as a boundary surface we must be certain that none of the characteristics of the (gauge dependent) fields we are evolving are superluminal.

The conventional formulation of the Einstein field equations in the 3 + 1 spacetime decomposition determines equations of motion for the spatial metric \((\gamma_{ij})\) and the intrinsic curvature of the hypersurface \((K_{ij})\) of each spacelike hypersurface. These coupled, non-linear differential equations are not hyperbolic; consequently, in this formulation there is no rigorous domain of dependence or region of influence for the fields at a point in spacetime and no assurance that the (gauge dependent) fields \(\gamma_{ij}\) and \(K_{ij}\) at a point outside an apparent horizon do not depend on the fields inside the horizon.

Recent work, carried out independently by several different groups but motivated by its significance for numerical relativity calculations, has led to a number of new formulations of the Einstein field equations that are explicitly hyperbolic. In the most general of these formulations the equations of motion for the fields (now the extrinsic curvature and its Lie derivative along the time axis \(t\), cf. fig. 1) are hyperbolic independent of the choice of spatial gauge, and the only non-zero characteristic speed is \(c\).

While the significance of this hyperbolic formulation of the Einstein field equations extends far beyond its numerical relativity application, its importance to numerical relativity is difficult to overstate. Since, in this formulation, the characteristics are well-defined and light-like, apparent horizon boundary conditions can now be rigorously and confidently imposed in black hole spacetimes. Because all fields are either Lie-dragged along the time axis or propagate along light cones, imposition of boundary conditions on the outer-boundary of a spacelike slice (or matching to an exterior Cauchy evolution) is greatly simplified. As might be expected (since the only non-zero propagation speed is \(c\)), the perturbative reduction of the field equations lead directly to gauge-invariant quantities, simplifying greatly radiation extraction. Finally, a hyperbolic formulation of the field equations gives numerical relativity direct access to an extensive, but hitherto unusable, body of mature work on the numerical evolution of hyperbolic systems.

### 5.4 Assembling the pieces

As discussed in the introduction, binary black hole coalescence is only one part of a larger problem — the relativistic Kepler problem. In the context
of this larger problem, a numerical solution to black hole coalescence takes as its initial conditions the results of a perturbative treatment of binary inspiral, and its end-results become the initial conditions for a perturbative treatment of black hole ringdown. In this way an initial black hole binary system, whose components are so widely separated that they can be regarded as isolated, is associated with a final black hole of given mass and angular momentum (and also gravitational radiation from the inspiral, coalescence and ringdown).

When the binary component separation is large then one can speak sensibly of the component masses and spins as well as the system’s orbital energy and angular momentum. When the component separation is small, however, these familiar quantities are no longer available to us: as the orbit tightens the distinctions between the binary component masses and the system’s total mass, or between the spin and orbital angular momentum, or between the total mass, the orbital energy, and the energy in the radiation, become blurred and lose their meaning.

This is as it should be — the final state is, after all, a quiescent black hole characterized only by its mass and angular momentum; nevertheless, it complicates our ability to place the initial data in an astrophysical setting. As discussed in §3, the combination of high computational burden and limited resources will require that we start each binary black hole simulation at most two or three “orbits” before coalescence. At these late times the binary evolution is far from adiabatic, spacetime is highly dynamical, the separation of the black holes is small compared to the system’s total mass, and it is meaningless to talk of separate black hole masses and spins, distinguish between total and orbital angular momentum, or orbital energy, total mass and radiation.

In fact, the situation is not as grim as one might suppose. In fact, what we are interested in is not some impossible definition of component masses and spins during the system’s penultimate orbit; rather, it is the masses, spins, and orbital characteristics of the data’s astrophysical antecedent: the system that evolved from large separation, where component masses and spins, and orbital energy and angular momentum, have sensible cognates, to the very compact state that is the initial data of our binary black hole coalescence calculation.

One approach to this problem, being explored by Kidder and Finn at Northwestern University, is to evolve binary systems, using post-Newtonian perturbation techniques, from wide to compact separation and compare, in a common gauge, the results of these perturbation calculations with conventional binary black hole initial data sets. In this way perturbation calculations can be used to characterize, at least in a rough sense, the antecedents of binary black hole initial data sets.
6 Conclusions

The nature of binary black hole coalescence is the final, uncharted frontier of the relativistic Kepler problem. In the United States, binary black hole coalescence has been identified as a computational “Grand Challenge” whose solution is the object of a coordinated effort, just reaching its half-way point, by more than two-score researchers at nearly a dozen institutions.

The computational burden associated with binary black hole coalescence can be estimated. Using current numerical algorithms a simulation of binary black hole coalescence, beginning one or two orbits before coalescence and ending when the final black hole is weakly perturbed, requires terabyte computer primary memory and multi-terabyte secondary storage. In order that such a simulation take less than 12 hours of computing time, the computer must be capable of a sustained performance of \( \gtrsim 10^{12} \) floating point operations per second. In both memory and time these requirements exceed the capabilities of present day computers by several orders of magnitude and will stretch the capabilities of the next generation. If we are to be able to solve for the coalescence of a black hole binary numerically new and more efficient computational methods must be developed for this problem.

Even with faster computers and new, more efficient computational methods, there are still open questions of physics associated with the problems formulation remain to be settled: Can black holes be excised from the computational domain by exploiting the apparent horizon as a Cauchy horizon? Can perturbative methods be used to extract radiation and pose out-going wave boundary conditions at finite distance from the binary system, or must an interior Cauchy evolution be matched to a characteristic surface exterior evolution that extends to future null infinity? How do we relate two black holes, deep in their common potential and no more than a few orbits prior to coalescence, to a binary system with well-defined component masses and spins and orbital energy and angular momentum? The questions of physics raised by the goal of completing the solution to the relativistic Kepler problem make the journey itself as interesting and exciting as the destination.

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