Post-Newtonian Initial Data with Waves: Progress in Evolution

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Abstract. In Kelly et al. \cite{1}, we presented new binary black-hole initial data adapted to puncture evolutions in numerical relativity. This data satisfies the constraint equations to 2.5 post-Newtonian order, and contains a transverse-traceless “wavy” metric contribution, violating the standard assumption of conformal flatness. We report on progress in evolving this data with a modern moving-puncture implementation of the BSSN equations in several numerical codes. We discuss the effect of the new metric terms on junk radiation and continuity of physical radiation extracted.

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1. Introduction

The astounding success of numerical relativity in simulating the merger of comparable-mass black-hole binaries in recent years stemmed from a number of numerical approaches to initial data, evolution formulations, gauge conditions, and even grid structures. However, many active groups have converged on a simple combination of methods called the “moving puncture” prescription \[2, 3\].

To initialise the numerical fields for a puncture evolution, most groups use the puncture prescription of Brandt & Brügmann [4] with Bowen-York extrinsic curvature [5]. In this scheme, the three-metric $\gamma_{ij}$ is conformally flat:

$$\gamma_{ij} = \psi_4 \eta_{ij},$$  

and the conformal factor $\psi$ must satisfy the Hamiltonian constraint

$$\Delta \psi + \frac{1}{8} K^{ab} K_{ab} \psi^{-7} = 0,$$

where the conformal extrinsic curvature $K_{ij}$ already satisfies the momentum constraint for holes with arbitrary momentum and spin. The zero-momentum constraint can be solved exactly to yield the Brill-Lindquist solution for a pair of holes at a point of time-symmetry \[6\]

$$\psi = 1 + \frac{m_1}{2|\vec{x} - \vec{x}_1|} + \frac{m_2}{2|\vec{x} - \vec{x}_2|}.$$  

Here the $m_A$ are “bare” or “puncture” masses, residing at positions $\vec{x}_A$ on the numerical grid. However, to solve Eq. (2) in general requires numerical methods, and the infinities encountered at the puncture locations are problematical. Brandt & Brügmann’s insight was that the divergent parts of $\psi$ could be formally factored out, leaving a well-behaved, simply connected sheet on which to solve their modified constraint.

With the Brandt-Brügmann prescription, only a single elliptic equation has to be solved, and several fast solvers have been developed to perform this operation to extremely high precision. The physical mass $M_A$ of each black hole after solution will be greater than its puncture mass $m_A$.

However, the restriction of this data is that it is, by construction, conformally flat. We know that the Kerr metric, the archetypal stationary solution of Einstein’s vacuum equations, is not conformally flat unless it has vanishing spin. It would seem that requiring conformal flatness of an astrophysically realistic binary (which has significant orbital angular momentum by construction) is unrealistic. In practice, when evolving puncture binary data, we see early bursts of unphysical high-frequency radiation propagate through the domain; see Fig. [7], as an example of this radiation at different initial separations.

2. Post-Newtonian Metric in the ADM-TT Gauge

In the 1970s, Ohta et al. \[8 \ 9 \ 10\] derived conditions for the post-Newtonian metric of an $N$-particle system in the transverse-traceless ADM (ADM-TT) gauge. The structure of this metric was given to 2.5 PN order by Schäfer [17]:

$$\gamma_{ij} = \psi_{PN}^4 \eta_{ij} + \delta_{TT}^{ij},$$  

where $\psi_{PN}$ is the conformal factor to 2.5 PN order.
where the post-Newtonian conformal factor $\psi$ is expanded as

$$\psi_{\text{PN}} = 1 + \frac{1}{8} \left( \frac{1}{c^2} \phi_{(2)} + \frac{1}{c^4} \phi_{(4)} + \cdots \right). \quad (5)$$

In this expression, $\phi_{(2)}$ alone yields the Brill-Lindquist potential term (3) for two stationary, nonspinning particles, while the leading corrections in $\phi_{(4)}$ depend explicitly on the separation of the particles, and on their momenta. Note that the three-metric $\gamma_{ij}$ is no longer conformally flat, due to the presence of a transverse-traceless term $h_{T T}$. This satisfies an outgoing wave condition:

$$h_{T T} = -\square_{\text{ret}}^{-1} \delta_{TT}^{ij} \left[ \sum_{A=1}^{N} \frac{P_A P_{AI}}{m_A} \delta(x - x_A) + \frac{1}{4} \phi_{(2)}^{(i) \phi_{(2)}^{(j)}} \right]. \quad (6)$$

The corresponding extrinsic curvature is derived from the conjugate post-Newtonian three-momentum:

$$\pi^{ij} = \psi^{-4}_{\text{PN}} \left[ \frac{1}{c^3} \hat{\pi}^{ij}_{(3)} + \frac{1}{c^5} \left( (\phi_{(2)} \hat{\pi}^{ij}_{(3)})^{TT} + \frac{1}{2} h_{ij}^{TT} \right) + \cdots \right]. \quad (7)$$

Explicit expressions were given for the terms $\phi_{(2)}$, $\phi_{(4)}$ and $\hat{\pi}^{ij}_{(3)}$ by [11], who also suggested a “near zone” approximation for $h_{ij}^{TT}$, by splitting the retarded inverse d’Alembertian in (6) with an inverse Laplacian:

$$h_{ij}^{TT} = -[\Delta^{-1} + (\square_{\text{ret}}^{-1} - \Delta^{-1})] \delta_{TT}^{ij} \left[ \sum_{A=1}^{N} \frac{P_A P_{AI}}{m_A} \delta(x - x_A) + \frac{1}{4} \phi_{(2)}^{(i) \phi_{(2)}^{(j)}} \right] \quad (8)$$

$$= h_{ij}^{TT(NZ)} + h_{ij}^{TT(\text{remainder})} + O(v/c)^5. \quad (9)$$

The explicit form of this near-zone approximation was supplied by [12].

Tichy et al. [13] adapted the ADM-TT-gauge 2.5PN results to puncture initial data for NR. They established that although the ADM-TT metric was not conformally flat, the
behaviour of the metric near the black holes was dominated by the conformal factor, and so fixed-puncture evolution methods should work as for standard puncture data.

A few years later Kelly et al. [1] completed the picture for nonspinning binaries by determining the “remainder” TT term, $h_{ij}^{TT\text{(remainder)}}$ to 2PN order. In the next section, we highlight some of the main properties of the complete solution.

3. Summary of Global Properties of Solution

While the work of [11] and [12] applies to general systems of particles, the “remainder” term presented in [11] applies only to the simplified situation of a binary system ($N = 2$). In such a system, they determined that the structure of the remainder term divides into three segments, according to time of evaluation:

$$h_{ij}^{TT\text{(remainder)}} = h_{ij}^{TT\text{(present)}} + h_{ij}^{TT\text{(retarded)}} + h_{ij}^{TT\text{(interval)}}. \quad (10)$$

For each field point where $h_{ij}^{TT}$ is to be evaluated, the “present” term is evaluated using the particle positions and momenta at $t = 0$, the time at which the simulation will start. The “retarded” term is evaluated using positions and momenta at the retarded time of each source particle relative to the field point. Finally, the “interval” term is an integral over the particles’ paths from the retarded time to the present. Figure 2 illustrates this division.

Each of these segments, moreover, consists of a “kinetic” and a “potential” part, the former depending on the particles’ momenta, the latter on their relative positions.

In this expression, the present-time piece almost completely cancels the near-zone solution of [12]: the kinetic terms cancel exactly, while the slightly more involved potential terms are suppressed by three powers of the field distance $R$:

$$h_{ij}^{TT\text{(NZ+present)}} = \frac{G^2 m_1 m_2 r}{16 R^3} \{ \cdots \} + \mathcal{O}\left(\frac{1}{R^4}\right). \quad (11)$$

The retarded-time piece reduces to the well-known quadrupole solution for a nonspinning binary as $r/R \to 0$. The most involved term, the interval piece, is too difficult to do in
generality, and must be integrated numerically. In Figure 3 we evaluate the full solution $h^{TT}_{ij}$ over time, along the orbital axis of an equal-mass system, assuming a simple inspiral. We see that the waveform is very close to the quadrupole solution.

Figure 4 shows one of the three-metric components for the full solution, with the characteristic quadrupole swirl we expect from an inspiralling binary.

4. Encoding the Binary’s Past Inspiral

To evaluate the retarded-time and time-interval contributions, $h^{TT}_{ij \ (\text{retarded})}$, $h^{TT}_{ij \ (\text{interval})}$, we need a model for the past history of the black holes. Initially, in [1], we employed a hybrid
Post-Newtonian Initial Data with Waves: Progress in Evolution

procedure (here \( M = M_1 + M_2 \) is the total mass of the system, while \( \eta \equiv M_1 M_2 / M^2 \) is the symmetric mass ratio):

(i) obtain separation \( r \) as a function of orbital frequency \( \Omega \) to 2PN order by (numerically) inverting the “puncture adapted” relation from [14]:

\[
M \Omega = \left( \frac{64 M^3 r^3}{(M + 2r)^6} + \frac{1}{c^2} \frac{M^4 \eta}{r^4} + \frac{1}{c^4} \frac{M^5 (-5 \eta + 8 \eta^2)}{8r^5} \right); \tag{12}
\]

(ii) obtain transverse momentum \( p \) as a function of \( \Omega \) to 2PN order from Schäfer & Wex [15]:

\[
p(\Omega) = M \eta \left[ (M \Omega)^{1/3} + \frac{(15 - \eta)}{6} (M \Omega) + \frac{(441 - 324 \eta - \eta^2)}{72} (M \Omega)^{5/3} \right]; \tag{13}
\]

(iii) obtain orbital phase \( \Phi \) (and hence frequency \( \Omega \equiv d\Phi/dt \)) as a function of time to 2PN order using the explicit relation from [16]:

\[
\Phi(t) = \Phi(t_c) - \frac{1}{\eta} \left[ \Theta^{5/8} + \left( \frac{3715}{8064} + \frac{55}{96} \eta \right) \Theta^{3/8} - \frac{3\pi}{4} \Theta^{1/4} + \cdots \right], \tag{14}
\]

where \( \Theta \equiv \eta (t_c - t)/5M \), and \( t_c \) is the (nominal) merger time.

This method has several drawbacks. For one thing, it is quite limited in post-Newtonian order. For another, the components are in inconsistent gauges. Finally, we have no prescription for an instantaneous radial momentum, necessary for low-eccentricity inspiral.

A conceptually simpler approach is to get all the needed information from a single source. Following recent practice in initial parameters for numerical evolutions of punctures [17], we can evolve the binary system inspiral through Hamiltonian evolution of the PN equations of motion. This has been shown by Husa et al. [17] to result in extremely low eccentricity, at least for nonspinning data. For more generic spinning binaries, the situation is more complicated, but promising; see, for instance, [18].

Although we need much more information for the new data, the Hamiltonian evolution method should perform just as well as for simple punctures: the puncture positions and momenta required are all from earlier times, and hence larger separations with lower velocities, where post-Newtonian methods are guaranteed to work. The only drawback is that potentially a lot of data must be stored about the past history of the binary to calculate the retarded and interval terms: and the larger the numerical grid, the further back in time we must reach.

5. Numerics

In the geometric units \( (G = c = 1) \) commonly used for vacuum numerical relativity, time, length, and mass can be scaled by a single number. For this purpose we use \( M = M_1 + M_2 \), the total mass of the binary system.

The numerical implementation of the wavy PN data has taken place in three independent codes, the Cactus-based LazEv code [19] [20], the BAM code [21] [22] [23], and the Paramesh-based Hahndol code [24] [25]. Some of the code was auto-generated using a Mathematica
script supplied by Gerhard Schäfer. For simplicity, the time-derivatives of $h_{ij}^{TT}$ appearing in the 2.5PN extrinsic curvature calculation (7) are carried out using simple second-order-accurate centred differencing (this is easily accurate enough, as the time spacing used is much smaller than the spatial discretisation of the numerical grid).

To calculate the two retarded times for each field point (one for each black hole), we use a Newton solver. Interval terms are then calculated by integrating from these retarded times to the present using Romberg integration.

Before discussing the evolution of the data, we note two numerical properties of the initial data. The first is that, as expected, the Hamiltonian constraint violation for the complete solution is better than for a partial solution: the left panel of Fig. 5 demonstrates this with the Hamiltonian constraint evaluated for the complete solution with and without the “interval” term.

On the other hand, it seems that leaving out the $h_{ij}^{TT}$ terms entirely yields even lower constraint violations, as seen in the right panel of Fig. 5. The reason for this is unclear, but may have to do with the greatly increased number of numerical evaluations in the $h_{ij}^{TT}$ terms. Given the observed behaviour of the black-hole (horizon) masses described in the next section, it seems that the bulk of the constraint violation “falls back” into the hole, with little escaping to the field zone to pollute the waveforms. We discuss the residual constraint violation further in Sec. 7.

6. Early Evolution Results

Initial evolutions have been carried out for equal-mass nonspinning binaries, with initial separations between $6M$ and $10M$. All evolutions show a combination of desirable and undesirable effects, which we illustrate with figures from $10M$-separation evolutions at low central resolution ($3M/128$ near the punctures) with the Goddard Hahndol code. We will often compare with the results of a more traditional moving puncture evolution of Bowen-York puncture data, with initial separation of $11M$, using parameters from [17]. For this data, we solved the Hamiltonian constraint numerically using Marcus Ansorg’s TwoPunctures spectral code [26]. In both cases, we tracked apparent horizons before and after merger with Jonathan Thornburg’s AHFinderDirect code [27].
6.1. Eccentricity and Horizon Masses

The first thing we note is the presence of strong eccentricity in the puncture tracks of the holes – see Fig. 6. This eccentricity appears to be around 10%, far greater than that of the traditional evolution, and persists until around 100M before merger.

A related phenomenon may be seen in the evolution of apparent horizon masses for the pre-merger binary – see Fig. 7. The apparent horizon mass $M_{AH}$ of a hole is related to the area of the apparent horizon. We locate the former numerically using the AHFinderDirect code [27]. We calculate the proper area $A_{AH}$ of this 2-surface, and derive from this the irreducible mass $M_{irr} \equiv \sqrt{A_{AH}/16\pi}$. The horizon mass is then related to $M_{irr}$ by inverting the Christodoulou formula [28]:

$$M_{AH}^2 = \frac{2M_{irr}^2}{\hat{a}^2} \left[ 1 - \sqrt{1 - \hat{a}^2} \right],$$

where $\hat{a} \equiv |\vec{S}|/M^2$ is the dimensionless spin of the hole. Note that for zero-spin holes, the horizon mass $M_{AH}$ is identical to the irreducible mass $M_{irr}$.

In Fig. 7 we see that while the standard horizon masses quickly settle down to a stable value, varying insignificantly over the 1100M of pre-merger evolution, the unsolved wavy data masses decay at a much slower rate, and with a periodic saw-tooth feature over time. If this is not merely an artifact of the horizon-finding algorithm or implementation, then the holes are losing mass steadily over the course of the inspiral. As discussed in [30], this could be associated with the nature of the residual constraint violation on the initial time-slice. This would lead to a considerable ambiguity in what the “correct” horizon mass is. The initial momenta (as well as the entire past history in the $h^{TT}$ terms) depend sensitively on the hole’s mass; an incorrect mass might result in considerable eccentricity.
6.2. Waveforms

The main quantity of interest from these evolutions must be the gravitational radiation extracted. In the left panel of Fig. 8 we show the real part of the dominant \((\ell = 2, m = 2)\) waveform mode \(R\psi_4\), as extracted on the coordinate sphere \(R = 45M\). We note that indeed the physical waveform is present from \(t = 0\), with less junk radiation than is present in the standard solved data.

Unfortunately a poor choice in the structure of the numerical grid in the radiation zone led to noisy extraction for both traditional and new data. Note that a high-accuracy waveform would be extracted at (or extrapolated to) \(R \rightarrow \infty\); however, this was not possible with the numerical grid used for these initial evolutions. Coupled with the relatively low resolution used, we estimate waveform amplitude errors of up to \(\sim 8\%\) at the peak; thus our numerical results are qualitative in nature at this point. Higher-accuracy extraction and analysis methods will be appropriate in future evolutions, when the mass and eccentricity issues described above have been resolved.

6.3. Final State

The final state of the post-merger black hole, which we analyse using the AHFinderDirect code [27], is qualitatively similar to that of the standard solved data. The final spin, as estimated by values of the Coulomb scalar on the surface of the apparent horizon [29], is around \(\hat{a} \equiv S_z/M^2 \approx 0.68625\). Using (15), we estimate the total horizon mass \(M_{\text{AH}}\) of the remnant hole. Figure 9 shows \(\hat{a}\) and \(M_{\text{AH}}\) for the standard and wavy merger remnants.
From these early evolutions, we see that the new wavy PN data appears to achieve at least some of our goals: it does evolve stably in the moving puncture recipe, without any special tweaks in gauge or evolution equations. Moreover, the early waveforms do indeed show more reasonable start-up behaviour than those of a standard puncture evolution, with a physically reasonable non-zero value and a diminished nonphysical pulse.

Nevertheless, some aspects of the numerics are not satisfactory, most notably the high orbital eccentricity and the slowly settling horizon masses of the pre-merger holes. These two phenomena may be simply related, as our experience in working with standard puncture data
has shown us that small errors in tuning masses will lead to eccentricity. It is conceivable that the residual Hamiltonian constraint violation of the wavy data causes this mass defect; similar effects have been studied recently in [30].

Resolving the mass issue may necessitate the introduction of a numerical elliptic solver to remove the residual constraint violation. To do this completely is not straightforward, as the ADM-TT gauge used here will change the form of the Hamiltonian constraint; moreover, the momentum constraint will in general need to be solved too.

Looking beyond these issues, we may consider the introduction of spin to our data. Though explicit post-Newtonian solutions of the constraint equations with spin are not yet available, we note that the leading-order momentum contributions to the conformal extrinsic curvature are just the Bowen-York momentum terms. It is conceivable that the leading-order spin contributions are given by the corresponding Bowen-York terms also.

Finally, we note that we have not addressed the initial conditions of the lapse function and shift vector. It is known that in standard puncture evolutions with the popular “1+log” slicing conditions, these settle down at late times to a “trumpet” form [31, 32]. Until these late-time forms can be incorporated into the full initial data, we cannot expect to eliminate gauge pulses in our waveforms.

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