Geometry and Regularity of Moving Punctures

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The puncture method for black holes in numerical relativity has recently been extended to punctures that move across the grid, which has led to significant advances in numerical simulations of black-hole binaries. We examine how and why the method works. The coordinate singularity and hence the geometry at the puncture are found to change during evolution, but sufficient regularity is maintained for the numerics to work. We construct an analytic solution for the stationary state of a black hole in spherical symmetry that matches the numerical result and demonstrates that the numerics are not dominated by artefacts at the puncture but indeed find the analytical result.

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A key issue in numerical black-hole simulations is how the black holes are represented in the calculations. One successful option has been to use "punctures", where the initial data possesses a Brill-Lindquist wormhole topology [1] and each asymptotic end is compactified to a single point (puncture) on R^3 at the price of a coordinate singularity. Punctures are technically appealing, because they represent black holes on R^3 without excision, and it is well understood how to construct puncture initial data for any number of boosted, spinning black holes [2, 3]. Punctures have also proved useful in dynamical evolutions, allowing the first fully three-dimensional mergers of two black holes [4, 5] and the calculation of gravitational waves for the plunge from the innermost stable circular orbit [6]. These early "fixed puncture" evolutions factored the singularity into an analytically prescribed conformal factor, and the gauge conditions prohibited the punctures from moving through the grid.

Recently two groups [7, 8] independently introduced similar methods to deal with the puncture singularities, which allow the punctures to move freely. These methods have met with spectacular success [9, 10, 11, 12, 13, 14], taking the first orbit simulations of black holes [15, 16] to more than four orbits and allowing accurate wave extraction. In analogy with the term "moving excision" we will refer to this method as "moving punctures".

For the "1+log" slicing condition and "Gamma-freezing" shift used in moving-puncture evolutions, however, a number of questions remain unanswered. What happens to the punctures during the evolution? Do they continue to represent compactified infinities? Does the evolution reach a final, stationary state, or do gauge dynamics persist? And, crucially, does the method accurately describe the spacetime, or does it rely on numerical errors near an under-resolved puncture, implying that it may fail when probed at higher resolutions or for more long-term evolutions?

In this letter we address these questions in three stages. First, we argue that the evolution of the punctures can be split approximately into advection across the hypersurface plus a gauge that locally produces black holes in a stationary state. Second, we assume existence of a stationary solution and show that a local expansion for a Schwarzschild puncture matches the numerical data. And third, we explicitly construct stationary slices for Schwarzschild and discuss their global geometry. We claim that the numerical evolution asymptotes to this analytical result and therefore accurately describes the spacetime, even in the neighborhood of the seemingly under-resolved punctures.

Let r be the distance to one of the punctures. Internal asymptotically flat ends are characterized by 3-metrics of the form $g_{ij} = \psi^4 \tilde{g}_{ij}$, where $\tilde{g}_{ij}$ is finite and the conformal factor ψ diverges as $\psi \sim 1/r$. The method of [7] introduces a regular conformal factor $\chi = \psi^{-4}$ that initially behaves as r^4 near the punctures. The method of [8] is implemented with the conformal factor $\phi = \log\psi$. Ignoring the $\log r$ singularity standard finite-differencing is used near the punctures. Both groups use fourth-order accurate finite differencing. Note that puncture initial data is only C^2 even after the singularity has been absorbed into the conformal factor.

The evolution method is based on the Baumgarte-Shapiro-Shibata-Nakamura (BSSN) formulation. For the lapse we consider "1+log" slicing and for the shift the "Gamma-freezing" condition of [17],

$$(\partial_t - \beta^i\partial_i)\alpha = -2\alpha K, \quad (1)$$

$$\partial_t^2 \beta^i = \frac{3}{4}\partial_t\tilde{\Gamma}^i - \eta\partial_t\beta^i, \quad (2)$$

with damping parameter η (see [18, 19] for variants).

Puncture evolutions use the standard 3+1 decomposition, and the equations can be brought into the form

$$(\partial_t - \mathcal{L}_\beta)u = F, \quad (3)$$

where u is a state vector and F a source term independent of the shift. In this context we do not have to consider the BSSN variable $\tilde{\Gamma}^i$ since it is derived from $\tilde{g}_{ij}$.

Therefore, all relevant non-gauge quantities and the lapse follow (3). Whatever the condition is that produces the shift, all other quantities are properly advected. Of special importance is the motion of the puncture itself, which is marked by a $\log r$ pole in ϕ or equivalently a zero in χ [7], which are advected by the shift like all other variables. As noted in [4, 17], since the shift can describe arbitrary coordinate motion, any shift vector that does not vanish at the puncture can generate motion of the puncture.

The Gamma-freezing shift condition generates a shift that manages two feats, stabilizing the black holes against slice stretching, and moving the punctures. Considering that in actual runs those two effects appear to happen independently of each other, i.e., the black holes move while maintaining approximate stationarity in comoving coordinates, we propose that the shift can be split into two pieces, $\beta^i = \beta^i_{adv} + \beta^i_{sls}$, where β^i_{sls} counters slice-stretching and β^i_{adv} is responsible for the motion of the punctures. If we have *exact* stationarity, then the defining properties of the two components of the shift can be expressed as (here the linearity of the Lie derivative is essential),

$$(\partial_t - \mathcal{L}_{\beta_{adv}})u = 0, \quad \mathcal{L}_{\beta_{sls}} u + F = 0. \tag{4}$$

An alternative picture is that in the early phase of a binary inspiral simulation the vector $(\frac{\partial}{\partial t})^a$ should be an approximate helical Killing vector, up to a rigid rotation. We can choose either corotation, or vanishing rotation at infinity, which would imply that the punctures' coordinate speeds equal their physical speeds as seen from infinity. A helical Killing vector alone would not counter slice stretching of the individual black holes, so near each puncture the approximate Killing vector will also approximate the stationary Killing vector of a single black hole.

In general, for orbiting black holes with gravitational waves eq.s (4) can hold only approximately, but they should be an excellent approximation in the immediate vicinity of the punctures. Furthermore, if the shift is regular at a puncture with a leading constant plus higher order terms,

$$\beta^i = b^i_0 + O(r), \quad \beta^i_{adv}\big|_{r=0} = b^i_0, \quad \beta^i_{sls}\big|_{r=0} = 0, \tag{5}$$

then (4) implies trivial advection of the puncture without further approximations, i.e., $u = u(x + b_0 t)$. The reason is that $\mathcal{L}_{b_0} u = b^i_0 \partial_i u$, since for the constant vector b^i_0 all other terms in the Lie derivative of any tensor in u vanish, and b^i_0 does not appear in any other terms.

We conclude that, assuming approximate stationarity, the question of numerical stability of the moving puncture process can be approached by splitting it into a standard advection problem and a stability analysis of a stationary puncture solution. The main open issue is whether there exists a regular, stationary solution for a single puncture that the method can find. Since the key novel features of this stationary solution already occur for a non-moving, spherically symmetric puncture (computed with the moving puncture method), we focus on this case here and leave the general case to future work.

Consider initial data for a single puncture with mass M at $t = 0$, with $\alpha = 1$, $\beta^i = 0$, $\tilde{g}_{ij} = \delta_{ij}$, $\tilde{A}_{ij} = 0$, $K = 0$, and $\phi_0 = \log(1 + \frac{M}{2r})$. When inserted into the BSSN and gauge equations, the data evolves and develops certain powers of r at the puncture [17]. If a regular, stationary state is reached, then all variables should possess power series expansions at $r = 0$ that satisfy (4). The following ansatz is consistent with (4) and the constraints for the single, non-moving puncture case in spherical symmetry:

$$\begin{aligned}
\psi^{-2} &= e^{-2\phi} = p_1 r + p_2 r^2 + O(r^2), && (6)\\
\tilde{g}_{ij} &= \delta_{ij} + O(r^2), && (7)\\
\tilde{A}_{ij} &= (A_0 + A_1 r)(\delta_{ij} - 3 n_i n_j) + O(r^2), && (8)\\
K &= K_0 + K_1 r + O(r^2), && (9)\\
\alpha &= a_0 + a_1 r + O(r^2), && (10)\\
\beta^i &= (b_1 r + b_2 r^2) n^i + O(r^3). && (11)
\end{aligned}$$

Here $r = (x^2 + y^2 + z^2)^{1/2}$ is the coordinate radius of quasi-isotropic Cartesian coordinates (x, y, z). Note that r is continuous but not differentiable and the radial normal vector $n^i = x^i/r$ is discontinuous at $r = 0$. Note also that in this context $\partial_i O(r^0) = O(r^{-1})$.

The evolution equations and the constraints result in 8 independent equations for the 10 coefficients $(p_1, p_2, A_0, A_1, K_0, K_1, a_0, a_1, b_1, b_2)$, with M and η free parameters. The shift condition (2) does not give an additional condition for a stationary solution. A first result is that $a_1 \neq 0$ and $K_0 \neq 0$ are required for nontrivial stationarity; a more regular solution is not consistent with the equations. For consistency $a_0 = 0$, that is the lapse has collapsed at the puncture if we assume exact stationarity, or for approximate stationarity the lapse has to be correspondingly small. Further simple relations are $b_1 = 2K_0$ and $b_2 = -3A_0 a_1$ from the evolution equations for the lapse and the metric.

Therefore, the assumption that there exists a stationary solution with some minimal regularity at the puncture implies specific predictions for kinks and discontinuities in our variables. To test the predictive power of the ansatz, we compare it to the numerical results for a Schwarzschild puncture evolved to $t = 50M$, at which time the data appears to have reached a stationary state to within a few percent in all variables. For a central resolution of $M/128$ the run is well within the convergent regime. When zooming into the data at this resolution, Fig. 1, *we do find the kinks and discontinuities consistent with the ansatz*. Although closer inspection shows some numerical artefacts near the puncture (in particular in $\tilde{A}_{ij}$ and the derivatives), they remain localized and comparatively small. All equations are satisfied to within ± 0.05 for $M = 1$, that is the numerical data is approximated well by the ansatz.

The most intriguing implication of the power series expansion is that *the singularity in the conformal factor changes* during evolution. With $a_0 = 0$,

$$\partial_t \phi = \beta^i \partial_i \phi + \frac{1}{6} \partial_i \beta^i + O(r) \simeq b_1 r \partial_r \phi + \frac{b_1}{2}. \qquad (12)$$

For the conformal factor of the initial data, we have $r\partial_r \phi_0 \simeq -1$, and $\partial_t \phi_0 \simeq -b_1/2$. With $b_1 \neq 0$ we are forced to conclude that the evolution of the conformal factor will stop only when $r\partial_r \phi \simeq -1/2$. In other words,

$$\psi_0 = O(1/r) \quad \text{evolves into} \quad \psi = O(1/\sqrt{r}), \qquad (13)$$

which is built into (6). The puncture still marks a coordinate singularity, but since the areal radius of the sphere $r = 0$ is $R_0 = \lim_{r \to 0} r\psi^2 = 1/p_1$, the slice no longer reaches the other asymptotically flat end of the Brill-Lindquist wormhole, but ends at a finite areal radius, $R_0 \approx 1.3M$, with p_1 determined numerically.

We now show by explicit construction in the proper distance gauge (which is regular through the horizon), that such stationary slices exist globally. The proper distance coordinate is denoted as l, $\partial_l f = f'$, α is the Killing lapse, β the Killing radial shift component and R the areal radius (the Schwarzschild radial coordinate). On any spherical slice through the Schwarzschild solution one finds $R' = \alpha$ and $\alpha^2 - \beta^2 = 1 - 2M/R$. Using these, the equation for the stationary 1+log slices of Schwarzschild, i.e., $\beta\alpha' = 2\alpha K$, becomes

$$R'' = \frac{2R'}{R} \frac{\frac{3M}{R} - 2 + 2R'^2}{\frac{2M}{R} - 1 + R'^2 - 2R'}. \qquad (14)$$

It is clear that the right-hand side of (14) is singular whenever $2M/R - 1 + R'^2 - 2R' = 0$. It can also be shown that any solution of (14) that is suitably asymptotically flat, i.e., $R \approx l$, must pass through such a singular point. The only way of resolving this difficulty is for the numerator of (14) to simultaneously vanish at the "singular" point. We have two options: either (a) $R' = 0$, or (b) $3M/R - 2 + 2R'^2 = 0$. Let us discuss them separately. In the case (a) we have $R' = 0, R = 2M$. Therefore the slice passes through the bifurcation sphere. This is the standard moment of time symmetry slice through the Schwarzschild solution, which obviously satisfies the stationary 1+log equation because $\beta \equiv 0$ and $K \equiv 0$. In case (b), the case we are really interested in, we can solve the pair of simultaneous equations to give $R' = \sqrt{10} - 3, R \approx 1.54M$. This solution corresponds to *two* slices in the Schwarzschild solution. These are mirror images of each other, one in the upper half plane, one in the lower. These slices do not continue into the left quadrant of the extended Schwarzschild solution. Rather they asymptote to a cylinder in the upper (lower) quadrant of fixed radius. This agrees with the numerical observation that the singularity in the conformal factor

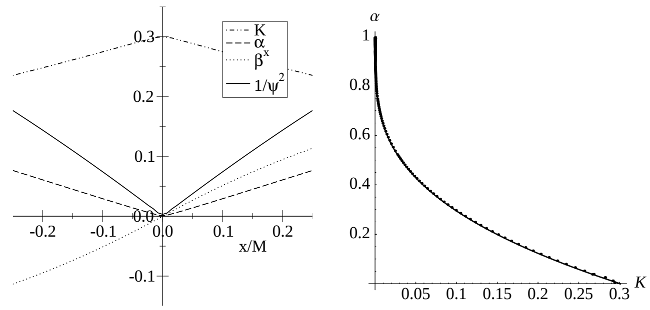

FIG. 1: Numerical evolutions of a spherically symmetric puncture result in specific kinks at the puncture (left). Plotting α as a function of K shows how well the numerical data (dots) matches the analytic stationary solution (right). At the puncture, $\alpha \approx 0.0$ and $K \approx 0.3$.

changes from $1/r$ to $1/\sqrt{r}$. These three are the only asymptotically regular solutions of the stationary 1+log equation, up to isometries. It is easy to show that the actual slice exponentially approaches a cylinder of radius R_0, i.e., $R \approx R_0 + A \exp Bl$ as $l \to -\infty$, where

$$B = 2{R_0}^{-1} (3M - 2R_0) (2M - R_0)^{-1}.$$

The value of the lapse at the horizon, which can be used as a simple horizon-finding or merger-time criterion, is evaluated numerically as $\alpha(R = 2M) \approx 0.376$. It is also possible to produce an algebraic solution in terms of an implicit equation for the lapse and Schwarzschild radius, which we omit for brevity. Suffice it to say that the lapse equation gives

$$3 \sinh^{-1}(3) = \log\left(128(2 - \frac{R_0}{M})\right) + 3 \log\left(\frac{R_0}{M}\right) + \sqrt{10} - 3,$$

from which one can determine $R_0 \approx 1.31241M$.

For comparison we have also studied harmonic and maximal slicing. With harmonic slicing (which can be generalized to the Kerr spacetime [20, 21]), one again finds a moment of time symmetry slice and two mirror copies of a slice that puncture evolutions driven toward stationarity should approach. The slices hit the singularity at $R = 0$, K blows up as $R \to 0$, and at the horizon $\alpha(R = 2M) = 1/2$. Fixed-puncture evolutions have used 1+log slicing without the shift term in (1). Stationary slices must then be maximal [22, 23], of the "odd lapse" type, $\alpha^2 = 1 - \frac{2M}{R} + \frac{C^2}{R^4}$. For $C = 3\sqrt{3}M^2/4$ such slices will again approach a cylinder, of constant $R_0 = 3M/2$.

Let us close with a discussion. The key result about the geometry of moving punctures is that for a Schwarzschild black hole the numerical evolutions approach a stationary slice that neither reaches an internal asymptotically flat end nor hits the physical singularity, as might be expected for a stationary slice with non-negative lapse [24]. Rather, the slice ends at a throat at finite Schwarzschild radius, but infinite proper distance from the apparent horizon. This changes the singularity structure of the "puncture". It is still a puncture in that there is a coordinate singularity at a single point in the numerical coordinates, but it does not correspond to an asymptotically flat end. In the coarse of Schwarzschild evolutions we have found that the throat does collapse to the origin. Where one would have expected an inner and an outer horizon, we find only one zero in the norm of $(\frac{\partial}{\partial t})^a$, corresponding to the outer horizon. An under-resolved region does develop in the spacetime (it is the region between the throat and the interior spacelike infinity), but we are pushed out of causal contact with it. The throat itself has receded to infinite proper distance from the outer horizon. Matter fields or gravitational radiation will be trapped between the inner horizon and the throat, because unlike the gauge their propagation is limited by the speed of light; this issue is left to future work.

The main result about regularity is contained in the specific kinks and discontinuities discovered in both the power series and the numerical data, which are implied by our stationary solution. The construction of an explicit power series solution in r for a single Schwarzschild puncture can be repeated for a single puncture with Bowen-York linear momentum, which imposes a certain dipole structure. Preliminary results indicate that the shift can acquire the constant leading term responsible for the motion of the punctures, and that there are no new fundamental regularity issues. The power series ansatz matches nicely the numerical data for a Schwarzschild puncture. Even as an approximate match, the presence of specific kinks and discontinuities has the important consequence that the question of how well a particular finite difference scheme can handle the moving puncture coordinate singularity is reduced to how well the finite differencing can handle derivatives of r and n_i. This is a rather simple question compared to the complexity of the equations. The fourth-order schemes (both centered and upwind) in use are actually known to be reasonably successful in this context, the lack of differentiability not withstanding. Incidentally, the introduction of χ results in $O(r^2)$ terms and not $O(r^4)$ as expected, but this still results in significantly cleaner data then the $\log r$ method. Perhaps most importantly, our analysis suggests a concrete remedy if the remaining numerical issues at the puncture create problems in simulations of black-hole binaries, namely to resort to finite differencing that is expertly adapted to the discontinuities at hand.

Our results suggest several directions for future research directly relevant to the binary black-hole problem, such as perturbations of the stationary solutions (including constraint violating perturbations to check constraint stability of evolutions systems), the clarification of numerical issues, and the construction of initial data adapted to the stationary solutions, e.g. of asymptotically cylindrical data. Furthermore, in the Schwarzschild case we can use local properties of the stationary solutions to directly read off spacetime properties from a numerical solution, e.g., the mass is calculated from the puncture value of K. It is important to determine if such algorithms can be extended to two moving, spinning black holes.

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