Constraint propagation equations of the 3+1 decomposition of $f(R)$ gravity

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Abstract
Theories of gravity other than general relativity (GR) can explain the observed cosmic acceleration without a cosmological constant. One such class of theories of gravity is $f(R)$. Metric $f(R)$ theories have been proven to be equivalent to Brans–Dicke (BD) scalar–tensor gravity without a kinetic term ($\omega = 0$). Using this equivalence and a 3+1 decomposition of the theory, it has been shown that metric $f(R)$ gravity admits a well-posed initial value problem. However, it has not been proven that the 3+1 evolution equations of metric $f(R)$ gravity preserve the (Hamiltonian and momentum) constraints. In this paper, we show that this is indeed the case. In addition, we show that the mathematical form of the constraint propagation equations in BD-equivalent $f(R)$ gravity and in $f(R)$ gravity in both the Jordan and Einstein frames is exactly the same as in the standard ADM 3+1 decomposition of GR. Finally, we point out that current numerical relativity codes can incorporate the 3+1 evolution equations of metric $f(R)$ gravity by modifying the stress–energy tensor and adding an additional scalar field evolution equation. We hope that this work will serve as a starting point for relativists to develop fully dynamical codes for valid $f(R)$ models.

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1. Introduction
Since its formulation, Einstein’s general theory of relativity (GR) has withstood extensive experimental and observational scrutiny using tests that range from millimeter to solar system scales (see [1] and references therein). The discovery of the late-time cosmic acceleration [2, 3] was a surprise, but one which could be modeled within the minimally extended
framework of ΛCDM [4, 5], GR with a positive cosmological constant. To this day, this simple model remains in very good agreement with data from all competitive probes [6–9], which imply that approximately 70% of the energy density of the universe is made up of a component which does not cluster and has an equation of state with pressure approximately equal to minus the energy density. While the simplest model for this component is indeed the cosmological constant, from the point of view of particle physics, its value implied by the measurements of the cosmological expansion is extremely low and requires a very high level of fine tuning.

A number of alternative models for dark energy have been proposed, most of which suffer from a similar fine-tuning problem to ΛCDM (see the review [10]), but at least provide a set of alternatives against which to test the ΛCDM hypothesis. In this spirit, it is possible to imagine that, rather than proposing the existence of a new, exotic form of energy density, it is the theory of gravity which we use to interpret the cosmological data that must be modified.

There are a number of proposed gravity theories which modify the dynamics at large distances, and metric \( f(R) \) theories of gravity (see, e.g., [11, 12] and references therein) comprise one such class of modifications to GR. This class has attracted considerable attention in recent years, perhaps due to the simplicity of the modifications. Further motivation for the study of \( f(R) \) gravity is reviewed in [12]; for other interesting alternatives see [11] for Gauss–Bonet gravity, [13] for conformal gravity and [14] for Brane-world gravity.

The \( f(R) \) formulation arises from a simple replacement of the Ricci scalar \( R \) in the Einstein–Hilbert action

\[
S = \frac{1}{16\pi} \int \sqrt{-g} \, d^4x \left( R - 2\Lambda \right) + S_m(g_{\mu\nu}, \psi_m),
\]

where \( g \) is the determinant of the metric tensor \( g_{\mu\nu} \), \( \Lambda \) is the cosmological constant, \( S_m \) is the matter term in the action, and \( \psi_m \) collectively denotes the matter fields, by an arbitrary function of the Ricci scalar, i.e.

\[
S = \frac{1}{16\pi} \int \sqrt{-g} \, d^4x f(R) + S_m(g_{\mu\nu}, \psi_m).
\]

Note that throughout this work we adopt geometrized units, where \( G = c = 1 \).

From equations (1) and (2), it is clear that GR is recovered for \( f(R) = R - 2\Lambda \). In metric \( f(R) \) theories, the connection symbols \( ^{(4)}\Gamma^i_{jk} \) are chosen to be the Christoffel symbols associated with the metric tensor, so that the action is a function of only the metric tensor and its derivatives. As a result, in metric \( f(R) \) gravity only the metric tensor is truly dynamical. In Palatini \( f(R) \) gravity, the connections \( ^{(4)}\Gamma^i_{jk} \) are considered independent of the metric tensor, so that the action is a function of both the metric tensor and the connection symbols. Thus, in Palatini \( f(R) \) both \( g_{\mu\nu} \) and \( ^{(4)}\Gamma^i_{jk} \) are dynamical fields (see also [15] for a new class of models which interpolate between the metric and Palatini formulations). In this work, we are concerned with metric \( f(R) \) gravity only.

Early work on \( f(R) \) theories [16–19] was mainly concerned with high-energy corrections to GR and their influence on the early universe (see in particular [19] where the first \( f(R) \) model of inflation was proposed). The discovery of cosmic acceleration [2, 3] renewed the interest in \( f(R) \) models, but now with modifications in the infrared. A number of alternative models to GR have been proposed [20–24]. However, it was later shown that these models neither satisfy local gravity constraints [25–27] nor give rise to a standard matter-dominated era [28, 29].

General conditions for the cosmological viability of \( f(R) \) models were derived in [30] and it was later realized that the so-called Chameleon mechanism—the scalar degree of freedom becomes massive in dense environments and light in diffuse ones—can allow \( f(R) \) gravity to
satisfy solar system constraints [31, 32]. The key consequence of the Chameleon mechanism is that the modification to the metric inside galactic haloes is suppressed: gravity returns to its general-relativistic behavior. The functioning of the Chameleon mechanism has also been confirmed via N-body simulations of large-scale cosmological structure formation in [33–37], where it was shown that predictions for cluster abundance and the matter power spectrum return at small scales to those calculated within the $Λ$CDM framework.

A number of models that satisfy both solar system and cosmological constraints have been proposed in [31, 32, 39–44], and it is now known that for an $f(R)$ theory to be viable, the following four constraints must be met [11]:

(i) $f_{,R} > 0$ for $R \geq R_0$, where $R_0$ is the cosmological value of the Ricci scalar today. This condition is necessary for guaranteeing that the new scalar degree of freedom is not a ghost—a field with negative kinetic energy.

(ii) $f(R) \to R$ for $R \gg R_0$. This condition is necessary for the presence of a matter-dominated era and to evade solar system constraints.

(iii) $f_{,RR} > 0$ for $R \geq R_0$ in the presence of external matter. This condition ensures that the matter-dominated era is the stable solution for cosmology and that the solutions which satisfy solar system constraints are stable.

(iv) $0 < R f_{,RR} / f_{,R} \big|_{r=-2}$, where $r = -R f_{,R} / f$. This condition is necessary for the stability and presence of a late-time de Sitter solution.

The existence of these requirements is a result of the fact that in $f(R)$ gravity the Ricci scalar is a full dynamical degree of freedom, which must behave in a manner similar to the Ricci scalar in GR, where it is controlled through a constraint ($R = -8\pi T$). These conditions ensure that in high-density environments, the so-called high-curvature solutions, where $R \approx 8\pi \rho$, are stable.

An additional constraint that any theory of gravity must satisfy is the existence of stable relativistic (neutron) stars. It was originally pointed out in [45], that many models of $f(R)$ theories reach a curvature singularity at a finite value of the scalar degree of freedom $f_{,R}$ which is not protected by the existence of a potential barrier. This value of the scalar field may be attained in the presence of relativistic matter. This same idea was used in [46] to argue that it is not possible to build spherically symmetric, i.e. non-rotating, relativistic stars in $f(R)$ theories of gravity. These works stimulated further interest, and eventually numerical models of spherical relativistic stars in $f(R)$ gravity were explicitly constructed in [47–49]. There it was shown that building numerical models of neutron stars in $f(R)$ gravity is very sensitive to the treatment of boundary conditions.

To our knowledge a stability analysis of non-rotating equilibrium models of neutron stars in the context of $f(R)$ theories has not been carried out yet. One may expect that the stability properties of relativistic stars in viable $f(R)$ gravity are the same as those in GR, because of condition (iii) above. However, given the subtleties that arise in obtaining relativistic stellar configurations in $f(R)$ theories due to the effective scalar degree of freedom, it is natural to expect that the back-reaction of the scalar field will affect the stability, too. In addition, it would be interesting to explore the existence and stability of rotating neutron stars and how $f(R)$ gravity affects the criterion for the onset of the bar mode, r-mode and other non-axisymmetric instabilities [50–55]. Furthermore, it is intriguing to study gravitational radiation arising from compact stars, both in isolation and in binary systems. Included in this list are neutron star–neutron star [56], black hole–black hole [57], black hole–neutron star [58–76] and white-dwarf–neutron-star binaries [77, 78].

Some of these studies can be carried out analytically via perturbation theory, and some require direct numerical simulations. One of the main points we make in this work is
that current numerical relativity techniques (see the texts by Baumgarte and Shapiro [79] and Alcubierre [80] and references therein), i.e. the solution of the Einstein equations by computational means, should be able to handle the equations of $f(R)$ gravity straightforwardly. In particular, the minimum requirement is to modify the stress–energy tensor and add a new scalar field evolution equation. However, to achieve long-term stable numerical integration of any set of partial differential equations, well-posedness of the Cauchy (or initial value) problem must be guaranteed.

Unlike GR, the field equations of metric $f(R)$ gravity in the so-called Jordan frame are fourth order (see section 2). Nevertheless, these theories can be cast in second-order form, by promoting $f,R$ (the derivative of $f(R)$ with respect to $R$) to an effective dynamical scalar degree of freedom. Alternatively, metric $f(R)$ gravity can be reduced to second-order form by a transformation of the $f(R)$ action to a Brans–Dicke (BD) [81] action with $\omega = 0$ [25]. This means that $f(R)$ gravity is equivalent to BD gravity without a kinetic term. Exploiting this equivalence and the 3+1 decomposition approach of [82], it was demonstrated in [83] that metric $f(R)$ gravity admits a well-posed initial value problem. As in 3+1 GR, to solve the initial value problem, first one solves the 3+1 constraint equations to obtain initial data and then uses the 3+1 evolution equations to advance the initial data in time. For this approach to yield a consistent solution of the covariant (4D) field equations, the 3+1 evolution equations must preserve the constraints of the theory. To prove this, one has to derive the evolution equations of the constraints, which are often referred to as the constraint propagation equations, and show that if the constraint equations are initially satisfied, they must be satisfied for all times. To our knowledge this has never been demonstrated for a 3+1 formulation of $f(R)$ gravity and in this work we show that this is indeed the case.

To date there are two methods for deriving 3+1 constraint propagation equations. One approach is to take the time derivative of the constraint equations in 3+1 form and then replace the time derivatives of all dynamical variables by using the evolution equations for these variables. We call this the 3+1 or ‘brute force’ method. This is a rather tedious approach and to our knowledge, it has been performed in GR only for vacuum spacetimes in [84]. A pedagogical example that explains the ‘brute force’ method is given in section II of [84], and more involved applications involving Maxwell’s equations can be found in [85].

The other approach, which is more elegant, takes the advantage of the Bianchi identities. We call this the Frittelli method [86] (see also [80]).

However, the equations derived in [86] were not cast in pure 3+1 language. Here and throughout this paper by ‘pure 3+1 language’ we mean that a given equation is written solely in terms of scalars and purely spatial objects and their derivatives. Yoneda and Shinkai [87, 88] have derived the Arnowitt–Deser–Misner (ADM) constraint propagation equations in pure 3+1 language but they did not indicate how they arrived at their result.

In this work, we employ the Frittelli approach to derive the constraint propagation equations of $f(R)$ gravity and cast the resulting equations in pure 3+1 language. We show that the mathematical form of the constraint propagation equations is the same as that of the standard ADM formulation of GR. We also demonstrate that this result holds true both in the Jordan and the Einstein frames of metric $f(R)$ gravity, as well as for the BD-equivalent version of metric $f(R)$ gravity. Finally, we compare our equations with published results of the constraint propagation equations derived using the 3+1 approach and show that the expressions obtained via both approaches agree.

While none of our results are surprising, they serve to prove that $f(R)$ gravity is self-consistent. Moreover, it is revealing to demonstrate how previous results from GR can be extended to alternative theories of gravity and the consistency between alternative approaches. Finally, obtaining the extended constraint propagation equations in pure 3+1 form may prove
useful for performing 3+1 numerical simulations, where constraint preservation can be used as a check on the integration.

This paper is organized as follows. In section 2, we review the field equations of generic metric $f(R)$ models. In section 3, we provide a simple pedagogical argument (see also [79, 89]) to demonstrate the basic idea of constraint preservation in the context of GR. In section 4, we review the 3+1 decomposition of the BD-equivalent metric $f(R)$ equations. In section 5, we employ the Frittelli method and use the results of section 4 to derive the 3+1 metric $f(R)$ constraint propagation equations. In section 6, we cast our generalized evolution equations of the constraints in pure 3+1 language. In section 7, we argue that the 3+1 constraint propagation equations of $f(R)$ gravity in both the Jordan and Einstein frames can be cast in the same form as that in the 3+1 BD-equivalent version of $f(R)$ theories. Finally, we summarize our work in section 8.

2. $f(R)$ field equations

As in GR, the fundamental quantity in $f(R)$ gravity is the spacetime metric tensor $g_{\alpha\beta}$,
\[
d s^2 = g_{\alpha\beta} d x^\alpha d x^\beta, \tag{3}\]
where $d s$ is the line element, and $x^\alpha$ denote the spacetime coordinates. Here and throughout this paper, the Greek indices run from 0 to 3, while the Latin indices run from 1 to 3.

The goal of the theory is to determine the metric given a mass–energy distribution. Because of the existence of an additional scalar degree of freedom in the gravitational field sector, it is possible to formulate the field equations of $f(R)$ theory in many ways, depending on the amount of mixing between these two fields. We will discuss three such formulations: the Jordan frame, the Einstein frame, and the BD-equivalent formulation.

The Jordan frame and Einstein frame formulations have different metrics as dynamical variables. The two metric tensors are related via a conformal transformation
\[
\tilde{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}, \tag{4}\]
where $\Omega$ is the conformal factor, and $g_{\mu\nu}$ here denotes the metric in the Jordan frame. Note that equation (4) is equivalent to a transformation of units [90].

In this section, we review the field equations of $f(R)$ gravity in both the Jordan and Einstein frames, as well as those of the BD-equivalent form of $f(R)$ gravity.

2.1. Jordan frame

The action (2) is called the Jordan frame action. An action is said to be in the Jordan frame, if the dynamical metric tensor in the action is the metric whose geodesics particles follow, i.e., the physical metric. The Jordan frame is the one in which the definition of the matter stress–energy tensor is
\[
T^{(m)}_{\mu\nu} = -\frac{2}{\sqrt{-g}} \frac{\delta S_m}{\delta g^{\mu\nu}}, \tag{5}\]
where $\delta S_m/\delta g^{\mu\nu}$ is the functional derivative of $S_m$ with respect to $g^{\mu\nu}$. For example, it is in this frame that the stress–energy tensor of a perfect fluid has the form
\[
T^{(m)}_{\mu\nu} = (\rho + P)u^\mu u^\nu + P g_{\mu\nu}, \tag{6}\]
where $\rho$ is the total energy density of the fluid, $P$ is the fluid pressure, and $u^\mu$ is the fluid four-velocity.

\[\text{5 For various Hamiltonian formulations of } f(R) \text{ gravity see [38].}\]
Varying the action (2) with respect to the metric yields the \( f(R) \) field equations \([11, 12]\) in the Jordan frame
\[
\Sigma_{\mu\nu} = 8\pi T_{\mu\nu}^{(m)},
\]
where \( T_{\mu\nu}^{(m)} \) is the matter stress–energy tensor and
\[
\Sigma_{\mu\nu} = FR_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} - \nabla_\mu \nabla_\nu F + g_{\mu\nu} \Box F,
\]
with \( F \equiv f, R \). Note that for brevity we have dropped the argument of both \( f(R) \) and \( F(R) \).
Clearly, GR is recovered for \( f = R - \frac{2}{\Lambda} \), in which case equations (7) and (8) yield
\[
\Sigma_{\mu\nu} = G_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi T_{\mu\nu}^{(m)},
\]
where \( G_{\mu\nu} \) is the Einstein tensor.

Equation (7) is fourth order due to the term \( \nabla_\mu \nabla_\nu F \). However, if we take the trace of equation (7), we obtain
\[
3 \Box F + FR - 2 f = 8\pi T^{(m)},
\]
where \( T^{(m)} = g^{\mu\nu} T_{\mu\nu}^{(m)} \) and
\[
\Box F = \frac{1}{\sqrt{-g}} \partial_\mu (\sqrt{-g} g^{\mu\nu} \partial_\nu F).
\]
Equation (10) can be used to promote \( F(R) \) to an effective dynamical scalar degree of freedom (often referred to as ‘scalaron’), thus recasting the theory in second-order form.

Equation (7) can also be written in the following form \([40]\):
\[
G_{\mu\nu} = 8\pi (T_{\mu\nu}^{(m)} + T_{\mu\nu}^{(f)}),
\]
where \( T_{\mu\nu}^{(f)} \) can be thought of as a ‘dark energy’ stress–energy tensor, given by
\[
8\pi T_{\mu\nu}^{(f)} = \frac{1}{2} g_{\mu\nu} (f - R) + \nabla_\mu \nabla_\nu F - g_{\mu\nu} \Box F + (1 - F) R_{\mu\nu}.
\]
This form of the field equations of the theory is interesting because the Bianchi identities \( \nabla_\mu G_{\mu\nu} = 0 \) together with \( \nabla_\mu T_{\mu\nu}^{(m)} = 0 \) imply that
\[
\nabla_\mu T_{\mu\nu}^{(f)} = 0,
\]
i.e. the dark energy tensor \( T_{\mu\nu}^{(f)} \) is conserved.

### 2.2. Einstein frame

To obtain the Einstein frame action of \( f(R) \) gravity, i.e. an action linear in a Ricci scalar \( \hat{R} \) associated with a metric \( \hat{g}_{\mu\nu} \), all we have to do is perform a conformal transformation on the metric
\[
\hat{g}_{\mu\nu} = F g_{\mu\nu},
\]
i.e. the conformal factor \( \Omega \) in equation (4) is \( \Omega^2 = F \). For the transformation to be physical, \( F \) must satisfy \( F > 0 \). Note that this condition is in accord with the first condition for cosmological viability of \( f(R) \) gravity listed in section 1.

If we introduce a new field \( \phi \) such that
\[
\phi \equiv \sqrt{\frac{3}{16\pi}} \ln F,
\]
then the \( f(R) \) Jordan action transforms to \([11]\)
\[
S_E = \frac{1}{16\pi G} \int d^4x \sqrt{-\hat{g}} \hat{R} + S_\phi + S_m(F^{-1}(\phi)\hat{g}_{\mu\nu}, \psi_m),
\]
where
\[ S_\phi = \int \sqrt{-\tilde{g}} \left[ -\frac{1}{2} \tilde{g}^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - V(\phi) \right] \] (18)
is the scalar field term in the action, and the scalar field potential is defined as
\[ V(\phi) = \frac{FR - f}{16\pi F^2} . \] (19)

The dynamical metric tensor in the Einstein frame is not the physical \((g_{\mu\nu})\) but the conformal one \((\tilde{g}_{\mu\nu})\). However, the matter still follows the geodesics of the physical (Jordan) metric. Variation of the matter action with respect to \(\tilde{g}_{\mu\nu}\) yields
\[ \tilde{T}^{(m)}_{\mu\nu} = -\frac{2}{\sqrt{-\tilde{g}}} \frac{\delta S_m}{\delta \tilde{g}^{\mu\nu}} = \frac{1}{F} \tilde{T}^{(m)}_{\mu\nu} , \] (20)

which is no longer independent of the scalar field \(\phi\).

Variation of the action (17) with respect to \(\phi\) yields the scalar field equation
\[ \tilde{\square} \phi - V,\phi - \frac{1}{2} \int \sqrt{-\tilde{g}} \left[ \frac{1}{2} \tilde{g}^{\alpha\beta} \partial_\alpha \phi \partial_\beta \phi + V(\phi) \right] = 0 , \] (21)

where \(\tilde{T}^{(m)} = \tilde{g}^{\mu\nu} \tilde{T}^{(m)}_{\mu\nu}\) and
\[ \tilde{\square} \phi = \frac{1}{\sqrt{-\tilde{g}}} \partial_\mu (\sqrt{-\tilde{g}} \tilde{g}^{\mu\nu} \partial_\nu \phi) . \] (22)

Equation (21) implies that the scalar field is directly coupled to matter.

Finally, variation of the action (17) with respect to \(\tilde{g}^{\mu\nu}\) yields
\[ \tilde{G}_{\mu\nu} = 8\pi \left( \tilde{T}^{(m)}_{\mu\nu} + \tilde{T}^{(\phi)}_{\mu\nu} \right) , \] (23)

where the scalar field stress–energy tensor is
\[ \tilde{T}^{(\phi)}_{\mu\nu} = \partial_\mu \phi \partial_\nu \phi + \tilde{g}_{\mu\nu} \left[ \frac{1}{2} \tilde{g}^{\alpha\beta} \partial_\alpha \phi \partial_\beta \phi + V(\phi) \right] . \] (24)

Note that in the Einstein frame \(\tilde{\nabla}_\mu \tilde{T}^{(m)}_{\mu\nu} \neq 0\); instead we have
\[ \tilde{\nabla}_\mu \tilde{T}^{(m)}_{\mu\nu} = \tilde{\nabla}_\mu \left( \tilde{T}^{(m)}_{\mu\nu} + \tilde{T}^{(\phi)}_{\mu\nu} \right) = 0 , \] (25)

where \(\tilde{\nabla}_\mu\) is the covariant derivative associated with \(\tilde{g}_{\mu\nu}\). It can also be shown that [11]
\[ \tilde{\nabla}_\nu \tilde{T}^{(m)}_{\mu\nu} = -\frac{1}{\sqrt{\tilde{g}}} \tilde{T} \tilde{\nabla}_\nu \phi , \quad \tilde{\nabla}_\nu \tilde{T}^{(\phi)}_{\mu\nu} = \frac{1}{\sqrt{\tilde{g}}} \tilde{T} \tilde{\nabla}_\nu \phi . \] (26)

### 2.3. Equivalence with BD gravity

Another way to cast \(f(R)\) gravity in second-order form is to express the theory as a BD theory. To show that \(f(R)\) gravity is equivalent to BD gravity with a potential, the following action was considered in [25]:
\[ S = \frac{1}{16\pi} \int \sqrt{-g} \, d^4x \left[ f(\chi) + f_{,\chi} (\chi)(R - \chi) \right] + S_m . \] (27)

Varying the action with respect to \(\chi\) yields
\[ f_{,\chi\chi} (\chi)(R - \chi) = 0 . \] (28)

Thus, if \(f_{,\chi\chi} (\chi) \neq 0\) (in agreement with condition (iii) in section 1), then
\[ \chi = R . \] (29)
Hence, equation (27) recovers the Jordan frame $f(R)$ action (2). If we now let $\phi = f, \chi (\chi)$, equation (27) can be written as follows:

$$S = \frac{1}{16\pi} \int \sqrt{-g} \, d^4x [\phi R - V(\phi)] + S_m,$$

(30)

where the potential is given by

$$V(\phi) = \chi(\phi)\phi - f(\chi(\phi)).$$

(31)

Action (30) is the same as the original BD action with a potential and without the kinetic term $(\omega/2)g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi$, i.e. the BD parameter is $\omega = 0$. Varying the action (30) with respect to the metric yields the BD-equivalent $f(R)$ field equations [12]

$$G_{\mu\nu} = \frac{8\pi}{\phi} \left( T_{\mu\nu}^{(m)} + T_{\mu\nu}^{(\phi)} \right),$$

(32)

where

$$8\pi T_{\mu\nu}^{(\phi)} = \nabla_\mu \nabla_\nu \phi - g_{\mu\nu} \left( \Box \phi + \frac{1}{2} V(\phi) \right).$$

(33)

Taking the trace of equation (32) we can replace $R$ in equation (29) to obtain

$$3 \Box \phi + 2 V(\phi) - \phi \frac{dV}{d\phi} = 8\pi T.$$

(34)

Equations (32) and (34) are the BD-equivalent $f(R)$ field equations.

3. Constraint preservation in a spacetime context

In this section, we review the concept of constraint preservation using the standard Einstein equations in 4D covariant form, i.e. we do not invoke machinery of the 3+1 decomposition of spacetime. The reason for doing so is that so far we have written the most popular representations of metric $f(R)$ field equations in a GR-like form

$$G_{\mu\nu} = 8\pi \bar{T}_{\mu\nu},$$

(35)

where $\bar{T}_{\mu\nu}$ is an ‘effective’ stress–energy tensor that is conserved, i.e. $\nabla_\mu \bar{T}_{\mu\nu} = 0$. Thus, it is instructive to first consider the Einstein equations in their familiar 4D covariant form.

For the Einstein equations with a cosmological constant, we have $\bar{T}_{\mu\nu} = T_{\mu\nu}^{(m)} - \Lambda g_{\mu\nu}/8\pi$. Since the Einstein equations are second-order partial differential equations, the evolution of the 4-metric $g_{\alpha\beta}$ in time can be determined by specifying $g_{\alpha\beta}$ and $\partial_t g_{\alpha\beta}$, everywhere on a three-dimensional spacelike hypersurface that corresponds to a given initial time $t$.

Equation (35) can provide us with expressions for $\partial_t^2 g_{\alpha\beta}$, which we can use to evolve the metric in time. There are ten metric components and there are ten field equations in (35). Hence, it appears that we have the exact number of equations for the ten degrees of freedom of the metric. However, the Bianchi identities $\nabla_\beta G^{\alpha\beta} = 0$ give

$$\partial_t G^{\alpha0} = -\partial_\beta G^{\alpha\beta} - G_{\beta(4)}^{\beta(4)} \Gamma^\alpha_{\beta\mu} - G^{\beta(4)}_{\beta(4)} \Gamma^{\mu}_{\beta\mu},$$

(36)

where we set $\partial_t \equiv \partial_0$ and $^{(4)}\Gamma^{\mu}_{\beta\mu}$ are the Christoffel symbols associated with $g_{\alpha\beta}$. Since no term on the right-hand side of equation (36) contains third time derivatives or higher, the four quantities $G^{\alpha0}$ cannot contain second time derivatives. Thus, the four equations

$$G_{\mu0} = 8\pi \bar{T}_{\mu0}$$

(37)

do not provide any information on the dynamical evolution of the metric. They are instead a set of constraints that $g_{\alpha\beta}$ and $\partial_t g_{\alpha\beta}$ have to satisfy. The only truly dynamical equations are the six remaining equations

$$G_{ij} = 8\pi \bar{T}_{ij}.$$

(38)
The apparent mismatch between the number of metric components and the number of evolution equations is immediately resolved once we invoke the coordinate freedom of GR. The theory is four dimensional, and hence we can always choose four conditions to specify a coordinate system. For example, we can choose the four \( g_{0\beta} \) components and assign them certain values, or demand that they satisfy a given set of four partial differential equations. This way we are left with six independent metric components, for which we have the exact number of evolution equations (38).

However, solving equation (38) does not guarantee that the full set of the Einstein equations (35) will be satisfied. For that to be true, equation (37) has to be satisfied for all times. In other words, if one solves equation (38) starting with initial data that satisfy equation (37), one has to prove that the constraints are preserved.

To demonstrate that this is indeed the case, we make use of the Bianchi identities in the following form:

\[ \nabla_\beta E^{\alpha\beta} = 0, \] (39)

or

\[ \partial_\xi E^{\alpha 0} = -\partial_1 E^{\alpha 1} - \mathcal{E}^{\beta\mu(4)} \Gamma^\alpha_{\mu\beta} - \mathcal{E}^{\alpha\beta(4)} \Gamma^\mu_{\beta\mu}, \] (40)

where

\[ \mathcal{E}^{\alpha\beta} \equiv G^{\alpha\beta} - 8\pi \bar{T}^{\alpha\beta}. \] (41)

If we let \( C = E^{00} \) and \( C^i = E^{i0} \), equation (40) can be rewritten as

\[ \partial_\xi C = -\partial_1 C^1 - C \left( 2^{i(4)} \Gamma^0_{i00} + C^{(4)} \right) \Gamma^1_{00} - \left( 3^{i(4)} \Gamma^0_{i0} + C^{(4)} \right) \Gamma^1_{ij} \] (42)

\[ \partial_\xi C^i = -C^{(4)} \Gamma^i_{00} - 2C^{i(4)} \Gamma^0_{i0} - C^{(4)} \Gamma^\beta_{0\beta}, \] (43)

where we have used equation (38), \( E^{ij} = 0 \), to obtain the result. Thus, if the constraints are initially satisfied, then \( C = C^1 = 0 \) initially and from equation (42) the time derivative of the constraints will be zero and hence the constraints will remain zero for all times. Since this conclusion resulted from setting \( E^{ij} = 0 \), the previous statement is equivalent to saying that the evolution equations preserve the constraints, a result that is well known.

4. 3+1 decomposition of \( f(R) \) gravity

Well posedness of the Cauchy problem in metric \( f(R) \) gravity has been demonstrated in [83] using the BD-equivalent \( f(R) \) formulation. In this section, we focus on the BD version of \( f(R) \) gravity and review the salient features of its 3+1 decomposition that will be useful in our proof of constraint preservation.

The form of the field equations of the theory is that of equation (35), where

\[ \tilde{T}_{\mu\nu} = \frac{1}{\phi} \left( T^{(m)}_{\mu\nu} + T^{(\phi)}_{\mu\nu} \right). \] (44)

The 3+1 decomposition of spacetime is a decomposition of spacetime into space and time. To do this, one assumes that the four-dimensional spacetime manifold can be foliated by a one-parameter family of nonintersecting spacelike hypersurfaces. The parameter of this family of hypersurfaces is taken to be the coordinate time. The spacetime metric is then rewritten as [91]

\[ ds^2 = -\alpha^2 dt^2 + \gamma_{ij}(dx^i + \beta^i dt)(dx^j + \beta^j dt), \] (45)

where \( \alpha \) is the lapse function, \( \beta^i \) is the shift vector, and \( \gamma_{ij} \) is the 3-metric on the spacelike hypersurfaces, induced by \( g_{\alpha\beta} \). The lapse function and the shift vector are gauge quantities;
they dictate how to build the coordinate system and can be freely specified. The relation between $\gamma_{ij}$ and $g_{\alpha\beta}$ is

$$
\gamma_{\alpha\beta} = \delta_{\alpha\beta} + n^\alpha n_\beta,
$$

(46)

where $\gamma_{\alpha\beta} = g^{\alpha\mu} g_{\beta\mu}$, $\delta_{\alpha\beta}$ is the Kronecker delta, and $n^\alpha$ is the future-directed timelike unit vector normal to the $t = \text{const.}$ hypersurfaces. The tensor $\gamma_{\alpha\beta}$ is the operator that projects tensors onto spacelike hypersurfaces.

The field equations can then be decomposed into a set of evolution equations and a set of constraint equations by using $\gamma_{\alpha\beta}$ and $n^\alpha$.

Projecting equation (35) twice with the projection operator yields the evolution equations

$$
E_{\mu\nu} \equiv (G_{\alpha\beta} - 8\pi \bar{T}_{\alpha\beta}) \gamma_{\mu\alpha} \gamma_{\nu\beta} = G_{\alpha\beta} \gamma_{\mu\alpha} \gamma_{\nu\beta} - 8\pi \bar{S}_{\mu\nu} = 0,
$$

(47)

where

$$
\bar{S}_{\mu\nu} \equiv \bar{T}_{\alpha\beta} \gamma_{\mu\alpha} \gamma_{\nu\beta} = S_{\mu\nu} + S_{\mu\nu}^{(\phi)},
$$

(48)

Using equation (33), we can write $S_{\mu\nu}^{(\phi)}$ in equation (49) as follows:

$$
S_{\mu\nu}^{(\phi)} = \frac{1}{8\pi} \left[ D_\mu \nabla_\nu \phi - \gamma_{\mu\nu} \left( \Box \phi + \frac{1}{2} V(\phi) \right) \right],
$$

(50)

where $D_\mu$ is the covariant derivative associated with $\gamma_{\mu\nu}$.

Contracting equation (35) twice with $n^\alpha$ yields the Hamiltonian constraint

$$
H \equiv (G_{\alpha\beta} - 8\pi \bar{T}_{\alpha\beta}) n^\alpha n^\beta = G_{\alpha\beta} n^\alpha n^\beta - 8\pi \bar{\rho} = 0,
$$

(51)

where

$$
\bar{\rho} \equiv \bar{T}_{\alpha\beta} n^\alpha n^\beta = \rho + \rho^{(\phi)},
$$

(52)

Using equation (33) we also obtain

$$
\rho^{(\phi)} = \frac{1}{8\pi} \left[ n^\mu n^\nu \nabla_\mu \nabla_\nu \phi + \left( \Box \phi + \frac{1}{2} V(\phi) \right) \right].
$$

(53)

Contracting equation (35) once with $n^\alpha$ and projecting once with $\gamma_{\alpha\beta}$ yields the momentum constraints

$$
M_\mu \equiv - (G_{\alpha\beta} - 8\pi \bar{T}_{\alpha\beta}) n^\alpha \gamma_{\mu\beta} = -G_{\alpha\beta} n^\alpha \gamma_{\mu\beta} - 8\pi j_\mu - 8\pi j_{\mu}^{(\phi)} = 0,
$$

(55)

where

$$
j_\mu \equiv -T_{\alpha\beta}^{(\mu)} n^\alpha \gamma_{\mu\beta}, \quad j_{\mu}^{(\phi)} \equiv -T_{\alpha\beta}^{(\phi)} n^\alpha \gamma_{\mu\beta},
$$

(56)

and where from equation (33) we find

$$
j_{\mu}^{(\phi)} = \frac{1}{8\pi} n^\alpha \gamma_{\mu\beta} \nabla_\alpha \nabla_\beta \phi.
$$

(57)

We can now write equation (35) as a linear combination of the evolution and the constraint equations:

$$
G_{\alpha\beta} - 8\pi \bar{T}_{\alpha\beta} = (G^{\mu\nu} - 8\pi \bar{T}^{\mu\nu}) \gamma_{\mu\alpha} \gamma_{\nu\beta} = (G^{\mu\nu} - 8\pi \bar{T}^{\mu\nu}) \gamma_{\mu\alpha} - n^\alpha n_\mu)(\gamma_{\nu\beta} - n^\beta n_\nu),
$$

(58)
where we used equation (46) in the second line to replace the Kronecker deltas. By use of equations (47), (51) and (55), equation (58) becomes

\[ G^{\alpha \beta} - 8\pi \bar{T}^{\alpha \beta} = L^{\alpha \beta} + 2n^{\mu} M^\mu + Hn^\alpha n^\beta. \]  

This last equation has been derived by Frittelli, (see equation (9) in [86]) for GR. Here, we have shown that this equation is valid in \( f(R) \) gravity, too, provided that appropriate definitions of \( H \) and \( M' \) are given.

As was shown in [86], setting \( E^{\alpha \beta} = 0 \) yields the evolution equations of the original ADM formulation [91], whereas setting \( E^{\alpha \beta} = \gamma^{\alpha \beta} H \) yields the evolution equations of the standard ADM formulation [79, 80, 92]. Following the parametrization of [86] we set \( E^{\alpha \beta} = \lambda \gamma^{\alpha \beta} H \), so that in the ADM language \( \lambda = 0 \) corresponds to the original ADM formulation, while \( \lambda = 1 \) to the standard ADM formulation, except that here we deal with \( f(R) \) 3+1 formulations.

It is now evident from equation (59) that if \( M^\mu = H = 0 \) and \( E^{\alpha \beta} = \lambda \gamma^{\alpha \beta} H \), then the \( f(R) \) equations are satisfied.

By introducing the extrinsic curvature \( K_{ij} \),

\[ K_{ij} = -\frac{1}{2} \mathcal{L}_n \gamma_{ij}, \]  

where \( \mathcal{L}_n \) stands for the Lie derivative along the timelike unit vector \( n^\alpha \), using the Gauss, Godazzi and Ricci equations (see e.g. equations (2.68), (2.73), (2.82) in [79]), and adopting the usual coordinate basis where

\[ n^\mu = (\alpha^{-1}, -\alpha^{-1} \beta^i), \]  

one can derive the evolution and constraint equations in 3+1 form, which (for \( \lambda = 0 \)) are presented in [83] and we do not repeat them here.

A subtlety that must be addressed for our purpose and which is pointed out in [82, 83] is that to remove the time derivatives of the scalar field \( \phi \) from the sources \( S(\phi)_{\mu \nu, \rho} \) one introduces the gradients of \( \phi \) as new dynamical variables

\[ \Pi^I = \mathcal{L}_n \phi = n^\mu \nabla_\mu \phi, \]  

\[ Q_\mu = D_\mu \phi. \]  

The \( \Box \phi \) operator in the sources \( S(\phi)_{\mu \nu, \rho} \) can be removed by use of equation (34). Furthermore, equation (34) in combination with equation (62), which can be written as

\[ \alpha \Pi = \partial_t \phi - \beta_i Q_i, \]  

can be used to derive the evolution equation for \( \Pi \). Eventually, one finds [82]

\[ \mathcal{L}_n \Pi = \Pi K + Q^i D_i (\ln \alpha) + D_i Q^i - \Box \phi, \]  

where \( K = \gamma^{ij} K_{ij} \).

To promote \( Q_i \) to a dynamical variable, we take a time derivative of \( Q_i \) and using equation (64) we obtain

\[ \partial_t Q_i = \mathcal{L}_n Q_i + D_i (\alpha \Pi), \]  

where

\[ \mathcal{L}_n Q_i = \beta^\sigma \partial_\sigma Q_i + Q_i \partial_\sigma \beta^\sigma. \]  

The introduction of new variables \( Q_i \) introduces an extra constraint, which the evolution equations have to satisfy

\[ C_i \equiv Q_i - D_i \phi = 0. \]  

In addition to this, the ordering constraint

\[ C_{ij} \equiv D_i Q_j - D_j Q_i = 0 \]  

has to be satisfied, too.

Thus, constraint preservation means that the evolution equations must preserve all the constraints of the 3+1 decomposition, i.e. equations (51), (55), (68), and (69).
5. Constraint propagation equations of 3+1 $f(R)$ gravity

The backbone of the Frittelli approach is to express the field equations in the form of equation (59) and plug it in the Bianchi identities in order to derive the evolution equations for the constraints, assuming that the evolution equations are satisfied $E^\mu_\nu = \lambda \gamma^\mu_\nu H$. So far we have extended the Frittelli approach to general metric $f(R)$ gravity. Since the form of equations (59) is the same as in [86], the derivation of the 3+1 BD-equivalent $f(R)$ constraint propagation equations is precisely the same as that in [86], which is valid for GR, and to which the interested reader is referred for more details. Here, we only sketch the derivation and write the result.

The Bianchi identities are

$$ \nabla_\mu (G^{\mu\nu} - 8\pi T^{\mu\nu}) = 0. \quad (70) $$

or, equivalently, after substituting equation (59) into equation (70)

$$ \nabla_\mu (E^{\mu\nu} + 2n^{(\mu} M^{\nu)}) + H n^\mu n_\nu = 0. \quad (71) $$

To find the evolution of the Hamiltonian constraint we contract equation (71) with $n^\alpha$ and after some algebra we find

$$ 0 = -E^{\mu\nu} D_\nu n_\mu - 2n^\nu M^{\mu} \nabla_\nu n_\mu - D_\mu M^{\nu} - n^\nu \nabla_\nu H - H D_\mu n^\nu. \quad (72) $$

To find the evolution of the momentum constraint we project equation (71) with $\gamma_{\alpha\beta}$ and after some algebra we find

$$ 0 = D_\mu E^{\mu\alpha} + n^\nu E^{\mu\nu} \nabla_\mu n_\nu + n^\nu \nabla_\mu M^{\alpha} - n^\alpha M^{\nu} n^\mu \nabla_\mu n_\nu + \gamma_{\alpha\beta} M^\mu D_\mu n^\nu + H n^\mu \nabla_\mu n^\alpha. \quad (73) $$

The proof that our equations are correct will be provided below when we cast the constraint propagation equations in pure 3+1 language and compare our result with published results in the literature obtained via the 3+1 approach.

Using the following identities

$$ \gamma^{\mu\nu} H D_\mu n_\nu = H D_\mu n^\mu, \quad (74) $$

$$ n^\alpha \gamma^{\alpha\nu} H \nabla_\mu n_\nu = H n^\alpha \nabla_\mu n^\alpha, \quad (75) $$

and substituting $E^{\mu\nu} = \lambda \gamma^{\mu\nu} H$ into equations (72) and (73) we find that the evolution of the constraints is given by

$$ n^\nu \nabla_\mu H = -2n^\nu M^{\mu} \nabla_\mu n_\nu - D_\mu M^{\mu} - (1 + \lambda) H D_\mu n^\mu, \quad (76) $$

$$ n^\nu \nabla_\mu M^{\nu} = -\lambda \gamma^{\mu\alpha} D_\mu H + n^\nu M^\mu n^\nu \nabla_\mu n_\alpha - M^{\nu} D_\mu n^\alpha - M^{\nu} D_\mu n^\nu - (1 + \lambda) H n^\mu \nabla_\mu n^\nu. \quad (77) $$

These last two equations have the same mathematical form (except for a factor of 2; see footnote 5) as those derived in [86] that applied to the case of GR, i.e. $f(R) = R$. Here, we have proven that the form of the Hamiltonian and momentum constraint propagation equations is the same for both vacuum ($T^{(m)}_{\mu\nu} = 0$) and non-vacuum spacetimes ($T^{(m)}_{\mu\nu} \neq 0$), and that it is independent of the $f(R)$ function, because we have absorbed all terms that depend on these quantities in the definition of the Hamiltonian and momentum constraints (see equations (51) and (55)).

We deal with the evolution of constraints (68) and (69), in the following section.

6 We note here that equation (11) in [86], differs from our equation (73) by a factor of 2 in the term $H n^\mu \nabla_\mu n^\nu$. We believe that this discrepancy is simply due to a typographical error.
6. $f(R)$ constraint propagation equations in pure 3+1 language

Note that equations (76) and (77) involve both spacetime and purely spatial objects. This is not a form that easily yields a comparison between the constraint propagation equations obtained in the Frittelli approach with those obtained in the 3+1 approach, nor it is convenient for integration in a 3+1 numerical implementation that could serve as a check of the numerical integration of the evolution equations of the dynamical variables. For this reason, we now cast these equations in pure 3+1 language. To our knowledge such a calculation has never been published before; hence it is instructive to include it here.

Alternative expressions for the extrinsic curvature are (see e.g. equations (2.49), (2.52) in [79])

\begin{equation}
D_{(\alpha}n_{\beta)} = -K_{\alpha\beta}
\end{equation}

and

\begin{equation}
K_{\alpha\beta} = -\nabla_{\alpha}n_{\beta} - n_{\alpha}a_{\beta},
\end{equation}

where $a_{\alpha} = n^{\beta}\nabla_{\beta}n_{\alpha}$ is the acceleration of normal observers, also equal to (see equation (2.22) in [93])

\begin{equation}
a_{\beta} \equiv D_{\beta} \ln \alpha.
\end{equation}

From equation (78) it can be shown that

\begin{equation}
D_{\rho}n^{\rho} = -K \quad \text{and} \quad D_{\rho}n_{\alpha} = -K_{\beta}^{\alpha}.
\end{equation}

By use of equations (78), (79) and (80), equations (76) and (77) can be written as

\begin{equation}
n^{\mu}\nabla_{\mu}H = -D_{\mu}M^{\mu} + (1 + \lambda)H K - 2M^{\mu}D_{\mu} \ln \alpha,
\end{equation}

\begin{equation}
n^{\mu}\nabla_{\mu}M^{\nu} = -\mu\gamma^{\mu\nu}D_{\mu}H + n^{\rho}M^{\mu}D_{\mu} \ln \alpha + M^{\mu}K + M^{\mu}K_{\mu}^{\nu} - (1 + \lambda)H D^{\nu} \ln \alpha.
\end{equation}

The identities, $\nabla_{\alpha}H = \partial_{\alpha}H$, $\gamma^{\mu\nu}D_{\mu}H = \gamma^{\mu\nu}\partial_{\mu}H$, $M^{\nu}D_{\alpha} \ln \alpha = M^{\nu}\partial_{\alpha} \ln \alpha$, $\nabla_{\mu}M^{\nu} = \partial_{\mu}M^{\nu} + \Gamma^{\nu}_{\mu\rho}M^{\rho}$, can be used to replace the covariant derivatives that occur above. Furthermore, the timelike unit vector ($n^{\mu}$) can be replaced by equation (61). Equations (81) and (82) can then be written as

\begin{equation}
\partial_{t}H = \beta^{i}\partial_{i}H - 2M^{i}\partial_{i}\alpha - \alpha D_{i}M^{i} + (1 + \mu)\alpha H K,
\end{equation}

\begin{equation}
\partial_{t}M^{j} = -\mu\gamma^{ij}\partial_{i}H + \beta^{i}\partial_{i}M^{j} - (\gamma^{ij}\Gamma^{k}_{ij}M^{k})
\end{equation}

\begin{equation}
+ (\gamma^{ij}\Gamma^{k}_{ij}M^{k} + n^{i}M^{j}\partial_{i}\alpha + \alpha M^{j}K + \alpha M^{i}K_{j}^{i} - (1 + \mu)\gamma^{ij}H \partial_{i}\alpha),
\end{equation}

where we have focused on the spatial indices of $M^{\mu}$, since $M^{\mu}$ is purely spatial.

Using $D_{i}M^{j} = \gamma^{ij}\partial_{j}M_{k} + \gamma^{ij}\Gamma^{k}_{ij}M_{k}$, and the expressions for the Lie derivatives of the constraints along $\alpha n^{\mu}$

\begin{equation}
\mathcal{L}_{\alpha n}H = \partial_{t}H - \beta^{i}\partial_{i}H,
\end{equation}

\begin{equation}
\mathcal{L}_{\alpha n}M^{j} = \partial_{t}M^{j} - \beta^{i}\partial_{i}M^{j} + M^{i}\partial_{i}\beta^{j}
\end{equation}

we write equations (83) and (84) as

\begin{equation}
\mathcal{L}_{\alpha n}H = -2M^{i}\partial_{i}\alpha - \alpha\gamma^{ij}\partial_{j}M_{k} + \alpha\gamma^{ij}\Gamma^{k}_{ij}M_{k} + (1 + \mu)\alpha H K,
\end{equation}

\begin{equation}
\mathcal{L}_{\alpha n}M^{j} = -\lambda\gamma^{ij}\partial_{i}H + A_{i}^{j}M^{i} + \alpha M^{j}K - (1 + \lambda)\gamma^{ij}H \partial_{i}\alpha + \gamma^{ij}M^{i}\partial_{i}\beta_{k} - M^{j}\beta^{k}\gamma^{jm}\partial_{i}\gamma_{m},
\end{equation}

where

\begin{equation}
A_{i}^{j} \equiv -\gamma^{ij}\Gamma^{k}_{ij} + \gamma^{ij}\Gamma^{k}_{ij}M^{k} - \alpha^{-1}\beta^{k}\partial_{k}\alpha + \alpha K_{i}^{j}.
\end{equation}
We now need to express the Christoffel symbols associated with the spacetime metric $g_{\mu\nu}$, that appear in equation (89), in terms of the 3-metric $\gamma_{ij}$ and the gauge variables. We do this as follows:

$$^{(4)}\Gamma^{j}_{i0} = \frac{1}{2} g^{j\rho} (\partial_{i} g_{0\rho} + \partial_{\rho} g_{i0} - \partial_{\rho} g_{i0})$$

$$= \frac{1}{2} g^{j\rho} \partial_{i} g_{00} + \frac{1}{2} g^{j\ell} (\partial_{i} g_{\ell 0} + \partial_{0} g_{i\ell} - \partial_{\ell} g_{i0}).$$

(90)

Using the relations between $g_{\mu\nu}$ and $\alpha, \beta^i, \gamma_{ij}$ [93]

$$g_{00} = -\alpha^2 + \beta_{\ell} \beta^{\ell}, \quad g_{0i} = \beta_{i}, \quad g^{ij} = \gamma^{ij} - \alpha^{-2} \beta^{i} \beta^{j},$$

(91)

equation (90) eventually becomes

$$^{(4)}\Gamma^{j}_{i0} = -\alpha^{-1} \beta^i \partial_i \alpha + \frac{1}{2} \alpha^{-2} \beta^{j} \beta^{i} \partial_i \beta^{\ell} - \frac{1}{2} (\alpha^{-2} \beta^{j} \beta^{i} \beta^{\ell} \partial_i \beta^{\ell} - \gamma^{ij} \partial_i \beta^{\ell} - \gamma^{ij} \partial_0 \gamma_{\ell \ell})$$

$$- \frac{1}{2} (\gamma^{ij} \partial_0 \beta^{i} + \alpha^{-2} \beta^{j} \beta^{i} \partial_i \gamma^{\ell j} - \alpha^{-2} \beta^{j} \beta^{i} \partial_i \beta^{j}),$$

(92)

where we have also used the following identities:

$$\beta^i = \gamma^{ij} \beta^j, \quad \partial_k \gamma^{ij} = -\gamma^{is} \gamma^{jm} \partial_k \gamma^{sm}.$$

(93)

The next object that appears in equation (89), and which we cast in 3+1 language is $\beta^k (^{(4)}\Gamma^{j}_{i0})^{ik}$. We can write this as

$$\beta^k (^{(4)}\Gamma^{j}_{i0})^{ik} = \frac{1}{2} \beta^k g^{j\rho} (\partial_i g_{k\rho} + \partial_{k} g_{i\rho} - \partial_{\rho} g_{i\rho})$$

$$= \frac{1}{2} \beta^k g^{j\rho} (\partial_i g_{k0} + \partial_{k} g_{i0} - \partial_{\rho} g_{i0}) + \frac{1}{2} \beta^k g^{j\ell} (\partial_i g_{k\ell} + \partial_{k} g_{i\ell} - \partial_{\ell} g_{i0}).$$

(94)

By virtue of equations (91) and (93), equation (94) finally becomes

$$\beta^k (^{(4)}\Gamma^{j}_{i0})^{ik} = -\alpha^{-2} \beta^{k} \beta^{i} \partial_i \beta^{j} + \frac{1}{2} \alpha^{-2} \beta^{k} \beta^{i} \partial_k \beta^{j}$$

$$- \frac{1}{2} (\gamma^{ij} \partial_i \beta^{k} + \alpha^{-2} \beta^{j} \beta^{i} \partial_k \gamma^{\ell j} - \alpha^{-2} \beta^{j} \beta^{i} \partial_k \beta^{j}),$$

(95)

or equivalently

$$\beta^k (^{(4)}\Gamma^{j}_{i0})^{ik} = -\alpha^{-2} \beta^{k} \beta^{i} \partial_i \beta^{j} + \frac{1}{2} \alpha^{-2} \beta^{k} \beta^{i} \partial_k \beta^{j}$$

$$- \frac{1}{2} \alpha^{-2} \beta^{k} \beta^{i} \partial_0 \gamma_{\ell j} + \beta^k (^{(4)}\Gamma^{j}_{i0})^{ik} - \alpha^{-2} \beta^{j} \beta^{k} \partial_i \gamma^{\ell j},$$

(96)

where $\Gamma^{j}_{i0}$ stand for the Christoffel symbols associated with the 3-metric.

By use of equations (92) and (96), equation (89) becomes

$$A^j_i = -\frac{1}{2} \gamma^{ij} \partial_i \beta^{\ell} - \frac{1}{2} \gamma^{ij} \partial_\ell \beta^{i} + \frac{1}{2} \gamma^{ij} \partial_i \beta^{\ell} + \beta^k (^{(4)}\Gamma^{j}_{i0})^{ik} + \alpha K^{j}_i.$$  

(97)

From the evolution equation of the 3-metric, equation (60), we have

$$\frac{1}{2} \gamma^{ij} \partial_0 \gamma_{\ell j} = -\alpha K^{j}_i + \frac{1}{2} \gamma^{ij} \partial_i \beta^{\ell} + \frac{1}{2} \gamma^{ij} \partial_\ell \beta^{i} - \gamma^{ij} \Gamma^{\ell j}_i \beta^{\ell}.$$ 

(98)

Substitution of equation (98) into equation (97) yields

$$A^j_i = -\gamma^{ij} \partial_i \beta^{\ell} + \gamma^{ij} \partial_\ell \beta^{i} + 2 \alpha K^{j}_i.$$  

(99)

Finally, substituting equation (99) into equation (88) yields the desired result:

$$\mathcal{L}_{\alpha} M^j = -\lambda \gamma^{ij} \partial_i H + 2 \alpha K^{j}_i M^j + \alpha M^j K - (1 + \lambda) \gamma^{ij} H \partial_\alpha.$$  

(100)

Equations (87) and (100) are the Hamiltonian and momentum constraint propagation equations in pure 3+1 language, where the Lie derivatives are given in equations (85) and (86).

We have already established that the form of the constraint propagation equations is the same for both vacuum and non-vacuum spacetimes and is independent of the form of the function $f(R)$. Thus, to validate our equations we can use the known results that apply to the case of GR and have been derived by using the 'brute force' method.

For this reason, we now compare our results with results published in [84, 87] that apply for $f(R) = R$, i.e. for the Einstein equations. In these two papers, the evolution equations of
the constraints were presented assuming $T_{\mu\nu} = 0$. In [84], the 3+1 approach was employed to derive the constraint propagation equations. For direct comparison with these published results, we also derive the evolution equations for $H = 2H$ and the evolution for $M_i$ which were used in [84, 87] instead.

Using
\[ \mathcal{L}_\alpha M_i = M_1 \mathcal{L}_\alpha \gamma_{ij} + \gamma_{ij} \mathcal{L}_\alpha M_j \]
\[ = -2\alpha K_{ij} M_j + \gamma_{ij} \mathcal{L}_\alpha M_j \]
(101)
and replacing $H = \frac{\mathcal{H}}{2}$ in (87) and (100), we obtain the following alternative form for the constraint propagation equations:
\[ \mathcal{L}_\alpha \mathcal{H} = -4M^i \partial_i \alpha - 2\alpha \gamma^{ij} \partial_i M_j + 2\alpha \gamma^{ij} T^k_{ij} M_k + (1 + \lambda)\alpha \mathcal{H} K, \]
(102)
\[ \mathcal{L}_\alpha M_i = -\frac{1}{2} \lambda \partial_i \mathcal{H} + \alpha M_i K - (1 + \lambda) \frac{1}{2} \mathcal{H} \partial_i \alpha. \]
(103)
For $\lambda = 1$, equations (102) and (103) become precisely the same as the expressions in [84], when the quantities, $C_{kij} = \partial_k \gamma_{ij} - D_{kij}$, defined in [84], satisfy $C_{kij} = 0$. In that work, $C_{kij}$ are constraints that arise from the introduction of the auxiliary variables $D_{kij} \equiv \partial_k \gamma_{ij}$, which were used to reduce the ADM formulation to first order. Also, a straightforward calculation shows that the expressions above are equivalent to the corresponding expressions in [87]. From equations (102) and (103), it is again evident that the constraints remain satisfied ($H = M_i = 0$), if they are initially satisfied.

We now turn our attention to the evolution equations of $C_i$ and $C_{ij}$. To derive the evolution of $C_i$ and $C_{ij}$, we simply take a time derivative of $C_i$ and $C_{ij}$, use the commutation relation $\partial_t \partial_i \alpha = \partial_t \gamma_{ij}$ and replace the time derivative of variables via equations (64) and (66) to find that
\[ \partial_t C_i = \beta^s C_{s i} \]
(104)
and
\[ \partial_t C_{ij} = \mathcal{L}_\beta C_{ij}, \]
(105)
where
\[ \mathcal{L}_\beta C_{ij} = \beta^s \partial_i C_{s j} + C_{s j} \partial_i \beta^s + C_{j i} \partial_j \beta^s. \]
(106)

Equations (104) and (105) imply that if the constraints $C_i, C_{ij}$ are initially satisfied, then the evolution equations will preserve the constraints.

We stress again that equations (102)–(105) are valid not only for vacuum, but also for non-vacuum spacetimes, as well as for any viable $f(R)$ model. This is a new result that to our knowledge has not been pointed out previously and is not trivial to prove, if one employs the 3+1 or ‘brute force’ method to derive the constraint propagation equations. Here, we proved this without the prior knowledge of the evolution equations of the dynamical variables $K_{ij}, \gamma_{ij}$, on the basis of the Frittelli approach.

Finally, we note that the agreement between our expressions and results obtained by the ‘brute force’ approach confirms that equation (73) is correct (see footnote 5).

7. Constraint propagation in the Jordan and Einstein frames

The form of the $f(R)$ field equations both in the Jordan frame (see equations (10) and (12)) and in the Einstein frame (see equations (21) and (23)) is the same as the BD formulation of $f(R)$ gravity. For this reason, it is evident from our discussion in section 5 that the form of the constraint propagation equations in these two frames must be the same as those in the BD formulation, provided that we define the Hamiltonian and momentum constraints analogously.
to equations (51) and (55) with one important caveat: the foliation in the Einstein frame must be based on the conformal (Einstein) metric and not the physical (Jordan), i.e. the induced 3-metric on spacelike hypersurfaces must be \( \tilde{\gamma}_{ab} = \tilde{g}_{ab} + \tilde{n}_a \tilde{n}_b \), where the normal timelike vector now satisfies \( \tilde{g}_{ab} \tilde{n}^a \tilde{n}^b = -1 \) and not \( g_{ab} \tilde{n}^a \tilde{n}^b = -1 \). Note that this last condition is only a mathematical requirement for the 3+1 machinery to remain the same. Physical conclusions must still be drawn based on the Jordan metric.

Finally, we note that if one applies the general recipe for a 3+1 decomposition (see section 4) to more general scalar–tensor theories of gravity considered in [83], then the constraint propagation equations will be the same as our equations (102)–(105). This is because the covariant (Jordan frame) formulation of these theories obtains the same form as equations (32) and (34) that we considered here, which lead to the same decomposition (59).

8. Summary and discussion

We have extended the ADM constraint propagation equations, using the Frittelli method [86], to generic metric \( f(R) \) gravity represented as a BD theory. For a direct comparison with published results, we wrote our general evolution equations of the constraints (defined via equations (51) and (55)) in the same form as the original equations given in [86]. This mathematical form, given by equations (76) and (77), combines both spacetime and purely spatial objects. To make transparent the connection between these equations and the language of the 3+1 decomposition of spacetime, we cast equations (76) and (77) in the pure 3+1 form, i.e. in a form that involves only scalar and purely spatial objects and their derivatives (see equations (102) and (103)). The 3+1 form is the mathematical form the evolution equations of the constraints would take on, if one had employed a ‘brute force’ 3+1 approach for performing this derivation. The brute force approach requires the prior knowledge of the exact 3+1 equations and is much more involved.

The main result of this work is that the mathematical form of the constraint propagation equations is the same for both vacuum and non-vacuum spacetimes, as well as for any (viable) form of the function \( f(R) \), provided that \( T^{(m)}_{\mu\nu} \) and \( T^{(\phi)}_{\mu\nu} \) (see section 4) are absorbed properly in the definition of the constraints. We have also argued that the mathematical form of the evolution of the constraints for 3+1 \( f(R) \) gravity in the Jordan frame remains the same as that of the BD-equivalent 3+1 \( f(R) \) gravity. This result holds true in the Einstein frame, too, if the spacetime foliation is chosen based on the Einstein metric \( \tilde{g}_{\mu\nu} \) and not the physical (Jordan) metric \( g_{\mu\nu} \). Finally, a comparison between our equations and previous GR results, using the 3+1 approach, shows that all expressions for the constraint propagation equations agree.

We end this work by pointing out that the 3+1 BD-equivalent \( f(R) \) equations can be incorporated in current numerical relativity codes with only minor additional effort. For example, the minimum requirement for studying vacuum spacetimes in viable \( f(R) \) models is to include the contribution of the scalar field stress–energy tensor \( T^{(\phi)}_{\mu\nu} \) (see section 4) and implement a scalar field solver in the form of equations (64)–(66). As in GR, it is almost certain that the stability of numerical implementations of the fully nonlinear equations of \( f(R) \) gravity will be sensitive to the formulation used. Given that the structure of the \( f(R) \) constraint propagation equations is fundamentally the same as that of the ADM formulation, we believe that dynamical \( f(R) \) simulations will benefit from formulations such as the Baumgarte–Shapiro–Shibata–Nakamura (BSSN; [94, 95]) approach or the generalized harmonic decomposition [96]. If these formalisms fail, other approaches such as those proposed in [85, 97, 98] may prove useful. We hope that this work will serve as a starting point for relativists to develop fully dynamical codes for viable \( f(R) \) models.
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