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Supercomputers against strong coupling in gravity with curvature and torsion

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Abstract Many theories of gravity are spoiled by strongly coupled modes: the high computational cost of Hamiltonian analysis can obstruct the identification of these modes. A computer algebra implementation of the Hamiltonian constraint algorithm for curvature and torsion theories is presented. These non-Riemannian or Poincaré gauge theories suffer notoriously from strong coupling. The implementation forms a package (the ‘Hamiltonian Gauge Gravity Surveyor’ – HiGGS) for the xAct tensor manipulation suite in Mathematica. Poisson brackets can be evaluated in parallel, meaning that Hamiltonian analysis can be done on silicon, and at scale. Accordingly HiGGS is designed to survey the whole Lagrangian space with high-performance computing resources (clusters and supercomputers). To demonstrate this, the space of ‘outlawed’ Poincaré gauge theories is surveyed, in which a massive parity-even/odd vector or parity-odd tensor torsion particle accompanies the usual graviton. The survey spans possible configurations of teleparallel-style multiplier fields which might be used to kill-off the strongly coupled modes, with the results to be analysed in subsequent work. All brackets between the known primary and secondary constraints of all theories are made available for future study. Demonstrations are also given for using HiGGS – on a desktop computer – to run the Dirac–Bergmann algorithm on specific theories, such as Einstein–Cartan theory and its minimal extensions.

1 Introduction

The modern frontier in the search for alternatives to general relativity (GR) is characterised by a very large number of competing models [1–3]. These models are problematic by dint of their heterogeneity: differences in the mathematical formulation hinder comparison between different classes (e.g. mimetic [4,4] and MOND [5,6] theories). This seems intractable, but we expect the number of classes to grow only in proportion to the community. A more serious problem presents when a class contains a large number of parameters,
e.g. the couplings in a Lagrangian. Critical theoretical properties, such as the number and health of propagating degrees of freedom (d.o.f) may be sensitive to these parameters in ways which are hard not only to characterise in general, but even to calculate in detail for a given parameter choice.

This scenario commonly arises in the Hamiltonian analysis, used routinely to determine the d.o.f.s of a proposed theory [7–11]. If the coupling parameters eliminate some velocity ψ from the motivated Lagrangian L, then the total Hamiltonian H_T must be modified to express the constraint \[ \pi_\psi \sim \partial_\psi L \approx 0. \] That constraint is only preserved if \[ \pi_\psi \sim \{ \pi_\psi, H_T \} \approx 0, \] which either vanishes identically or constitutes a new constraint, ad infinitum. Each constraint subtracts d.o.f.s from the countable fields \( \psi \) naively present in \( L \). The full chain of constraints is systematically elucidated by means of the Dirac–Bergmann algorithm [7,10,12], the fundamental computational unit of which is the Poisson bracket. In theories constructed from the higher-spin representations of the Lorentz group, including most tensor theories of gravity, a single covariant bracket can be surprisingly cumbersome for manual evaluation [13,14]; less so, as we will find, for computer assistance. Through the algorithm, the d.o.f and symmetry structure depend not only on eliminated velocities, but also on all brackets between all constraints, which themselves may be contingent on the couplings in ways that are, ab initio, unknowable.

The strong coupling problem is commonly diagnosed in the Hamiltonian picture. It is usually preferred that two gravitational d.o.f propagate [15,16]. Additional d.o.f may be tolerated unless ghostly or tachyonic, but they must kept under close theoretical and phenomenological control (e.g. by large [19] – or small [20,21] – masses, screening [22] or other measures). Frequently we start with many fields \( \psi \) (ten in the case of GR), so that reduction to two d.o.f is an achievement in the linearised Hamiltonian picture: strongly coupled modes may increase this number when we come to perform the nonlinear analysis [23]. Strong coupling can be imagined as a finely-tuned suppression of the kinetic coefficients \( 1 \) in a mode’s linear wave equation [24]. The nonlinear operators are generally still present, however, and describe a non-perturbative dynamics which may be unacceptable, having for example an elliptic or parabolic character. The linearisation in this case refers to some motivated exact vac-

\[ L_G = -\frac{1}{2\kappa} R + \frac{1}{\kappa} \lambda^{\mu\nu} T_{\mu\nu} + \frac{1}{\kappa} \phi^{\mu\rho} Q_{\mu\rho} . \]
The multipliers \( \lambda^{\rho\sigma}_\mu \) and \( \tilde{\lambda}^{\rho\sigma}_\mu \) constrain the geometry to be torsion-free and metric, while the dynamics are those of curvature. At the time of writing, the attention of the community is drawn to the remarkable non-uniqueness of (1) as a realisation of GR in this broader, non-Riemannian context. By cycling multipliers onto the torsion–non-metricity triad, and identifying suitable dynamical terms, one can construct the flat, metric teleparallel equivalent of GR (TEGR) from pure torsion [48], and the flat, torsion-free symmetric alternative (STEGR) from pure non-metricity [49]. With (1), these points in the space of non-Riemannian theories define the geometrical trinity of gravity [47].

There is now activity to determine a preferred vertex of the trinity, and the viability of the surrounding non-Riemannian landscape. Various considerations must be balanced in a very large parameter space [50–53]. As we mentioned previously, the PGT may be thought of as the sector of the landscape in which the PGT may be thought of as the sector of the landscape were probed at the turn of the millenium [23]: Riemannian landscape. Critically however, the challenge of regard PGT is feared to be representative of the broader non-coupling phenomena are known to be abundant [8, 55–57], beginning with Kibble [58], Utiyama [59], and also Sciama [60].

The linear Hamiltonian structure of PGT is particularly well developed [8, 61–63]. In the nonlinear structure, strong coupling phenomena are known to be abundant, and in this regard PGT is feared to be representative of the broader non-Riemannian landscape. Critically however, the challenge of the Hamiltonian analysis has prevented this structure from being mapped in any comprehensive detail. A few islands in the landscape were probed at the turn of the millenium [23]: minimal extensions to the Einstein–Cartan theory in which a single extra massive spin-parity \((J^{P}) = 1^+, 1^−\) or \(2^−\) torsion particle is present. In each case respectively, \(1^−\), \(1^+\) and \(2^+\) modes were suggested to be strongly coupled. Since then, the PGT sector of the landscape has been treated with a sense of ‘hic sunt dracones’ – i.e. avoided as potentially dangerous – with apparently the only safe configurations being exclusive activation of the \(0^+\) or \(0^−\) scalar torsion particles [46, 64, 65].

In light of our comments above, one can even afford to remain agnostic on the pathology of this strong coupling\(^5\). It would seem, however, given the recent, promising developments in the non-Riemannian approach [47, 50–53], that the extent of the phenomenon should still be understood, and general tools be developed to that end.

In this paper we present a computer algebra implementation of the nonlinear Hamiltonian analysis for a generalisation of the full PGT, in which one may covariantly disable arbitrary irreps of the torsion and curvature by means of Lagrangian multiplier fields. This generalisation was put forward as an anti-strong-coupling measure in [14], and its Hamiltonian structure is elucidated in the companion paper [67]. In the conventions of (1), we may write generalised PGT as

\[
L_G = \frac{\delta_0}{2\kappa} R + \frac{1}{k} \sum_{\nu\sigma} \left( \hat{a}_I R^{\mu\nu} + \hat{a}_I \lambda^{\mu\nu}_{\sigma} \right) \hat{P}^{\sigma}_{\mu\nu} \xi \xi R^{\kappa\pi} \xi \xi \\
+ \frac{1}{k} \sum_{M=1}^3 \left( \hat{\beta}_M T^{\mu}_{\nu\sigma} + \hat{\beta}_M \lambda^{\mu}_{\nu\sigma} \right) M \hat{P}^{\nu\sigma} \pi \xi \xi T^{\kappa\pi} \xi \xi \\
+ \frac{\lambda^{\rho\sigma}_\mu}{k} Q^{\mu}_{\rho\sigma},
\]

where the usual ‘quadratic’ PGT is spanned by the ten parameters \(\hat{a}_0, \{\hat{a}_I\}, \{\hat{\beta}_M\}\). The projections \( J \hat{P}^{\mu\nu}_{\sigma\kappa} \xi \xi \) and \( M \hat{P}^{\nu\sigma}_{\kappa\pi} \xi \xi \) extract the SO\(^2\)(1, 3) field strength irreps. The core of the implementation is (version 1.0.0 of [68]) the Hamiltonian Gauge Gravity Surveyor (HiGGS), a Mathematica package grounded in the popular open-source xAct tensor manipulation suite [69–74].

The HiGGS package is suitable for targeted use on a desktop computer. Since it is parallelised on Poisson brackets, HiGGS also scales to clusters and supercomputers. Development in this direction is with the aim of surveying the constraint structure of the non-Riemannian landscape at scale. Modules from HiGGS, in particular those concerned with bracket evaluation, can be used as a back-end in searching the parameter space for desirable canonical features – as such features become better understood with time.

For the moment, we perform a brute-force ‘calibration’ survey. In this run, which takes a little over 1h, the \(1^+, 1^−\) and \(2^−\) Einstein–Cartan extensions are modified with all possible configurations of curvature- and torsion-disabling multipli-

\(^3\) Note some differences in our convention, regarding the dimensionality and density status of these [47].

\(^4\) It is perhaps telling that the initial value problem is known to be well-posed in specific cases where precisely these modes are activated [42].

\(^5\) It is important to understand that the main historical objection to the strongly coupled modes of the PGT has been their ghostly character, as inferred by an inspection of the signs of squared momenta in the Hamiltonian. These signs are fixed by the unitarity requirements of the desired, linearly active modes in each case, and in each case they are negative [23]. This ‘catch-22’ is particular to the PGT, but, as cogently explained in [66], there are principled reasons to be suspicious of strongly coupled surfaces, which appeal to neither the non-perturbative dynamics, nor the causality arguments mentioned above. Generically, a background which is strongly coupled had better not be one which is also seen in nature, since it cannot have been reached by any smooth trajectory through the phase space.
ers: 192 generalised Poincaré gauge theories in total. During the run HiGGS obtains, for every theory, all the primary and secondary constraints which can be inferred from a knowledge of the literature, and then computes simple covariant expressions for the nonlinear Poisson brackets between all constraint pairs. All brackets identified in this survey can be found in the supplemental materials [75].

Examples are also provided of how to use HiGGS to calculate constraint velocities when implementing the Dirac–Bergmann algorithm. Focus is on the minimal Einstein–Cartan extensions with strong coupling, and the viable $0^+$ and $0^−$ extensions. The unmodified Einstein–Cartan theory is also studied, and HiGGS is used to show that it propagates only the two graviton polarisations. Finally, we will use the results of the initial survey to show how multipliers might conceivably be used to suppress strongly coupled fields. Note that the major undertaking of fully analysing the results, isolating and confirming any viable multiplier configurations, is left to future work.

The remainder of this paper is structured as follows. In Sect. 1.1 we introduce the strong coupling problem in gravity. In Sect. 1.2 we briefly set out our conventions for PGT, using the non-geometric, gauge-theoretic formulation. In Sect. 2 we describe the HiGGS implementation, including general tools for the canonical manipulation curvature and torsion, up to Poisson brackets and higher-level functionality for the theory-specific calculation of constraints and velocities. Solutions for scaling the Hamiltonian analysis to high-performance computing (HPC) resources are also described. In Sect. 3 we present examples of the algorithm, and the results of our initial survey. Conclusions follow in Sect. 4.

1.1 Strong coupling

In an appendix to [66] Beltrán Jiménez and Jiménez-Cano elegantly demonstrate the strong coupling problem by considering the single degree of freedom

$$q\ddot{q} + (1 − q)\dot{q} = 0,$$

(3)

where (just within this section) we work in units that hide dimensionful constants. The field in this case modulates its own acceleration, and so we may expect some strange effects in the vicinity of $q = 0$. In fact $q = 0$ is an exact solution, which confirms only itself through naïve attempts at perturbative expansion. In reality, the full nonlinear treatment reveals it to be an unacceptable separatrix in the phase space of the theory.

The system in Eq. (3) has the very mild disadvantage of not being Hamiltonian, as the authors note, and so we would like to construct a more physically motivated, oscillatory alternative. Using this new system, we also wish to issue a fundamental complaint against strong coupling which does not rely on non-hyperbolic instabilities, as mentioned in the previous section. Similarly, we will not try to relate ‘strong coupling’ here with a scale, or with the running of couplings, which naturally mediate this and similar effects in the powerful framework of low-energy effective theories. Most of the examples referenced in the previous section are ultimately embedded in such a framework. Our example will also still be finite-dimensional, but the key objections are presumed to carry over into field theories.

Consider the system comprising two coupled oscillators

$$L = \frac{1}{2}q_1^2 − \frac{1}{2}q_1^2(q_1 − 1)^2 + \frac{1}{2}q_1^n q_2^2 − \frac{1}{2}q_2^2,$$

(4)

for some integer $n ≥ 1$. The system has field equations

$$\ddot{q}_1 + q_1(q_1 − 1)(2q_1 − 1) − \frac{n}{2}q_1^{n−1}q_2^2 = 0,$$

$$q_1^n q_2 + nq_1^{n−1}\dot{q}_1 q_2 + q_2 = 0.$$

(5)

It is comparatively easy to get as far as the field equations when proposing a novel gravity theory: the next step is typically to identify some desirable exact background solutions. From Eq. (5) we can immediately suggest the static vacua of the double potential in the first oscillator; either $q_1 = q_2 = 0$, or $q_1 = 1$ with $q_2 = 0$. The first of these solutions may naturally be compared with the empty Minkowski background.

In the second solution, the first oscillator adopts a vacuum expectation value.

During early work on the new gravity theory, it might therefore seem economical, or computationally convenient, if the first of these solutions were the physically realised vacuum. Conventional wisdom holds that the stability of a vacuum can be tested by computing the particle spectrum of the nearby quantum field theory. The Lagrangian must be systematically inverted so as to obtain the saturated propagator: the absence of ghost or tachyon modes is then a necessary condition for the background to be stable [76–78]. When we perform the equivalent analysis on the theory in Eq. (4), we can algebraically integrate out the second oscillator to give

$$L = \frac{1}{2}\dot{q}_1^2 − \frac{1}{2}\dot{q}_1^2, \quad q_2 = 0.$$

(6)

This suggests a single stable mode. If instead we attempt a Hamiltonian analysis of the perturbative theory, we obtain

$$H = \frac{1}{2}p_1^2 + \frac{1}{2}q_1^2 + \frac{1}{2}q_2^2 + u\varphi,$$

(7)

with canonical coordinates $q_1$ and $p_1 = \dot{q}_1$, and multiplier $u$ enforcing the primary constraint $\varphi ≡ p_2 = 0$. The consistency of this primary (the vanishing of its velocity) is satisfied.
by the secondary $\chi \equiv q_2 \approx 0$, whose own consistency determines that the multiplier $u$ should vanish. Both constraints are second class, the final number of d.o.f is indeed one and the second oscillator is strongly coupled. An analysis of the partially integrated theory in Eq. (6) would lead to the same (erroneous) conclusion: the canonical trajectories will circle the desired vacuum in a stable fashion, as hoped. Extending this analysis to include the full double-well potential in Eq. (4), but without reintroducing the second oscillator, produces the phase portrait shown in the top frame of Eq. (1). The linear theory consistently describes the centre of the violet region, and by crossing the hyperbolic separatrix one may reach the second, perhaps more speculative, vacuum in gold. The turquoise region is traced by more energetic orbits.

Thus in the linear Lagrangian analysis, as confirmed by the linear Hamiltonian analysis, we retain only one, stable oscillator. Equally in the case of gravity, the particle spectrum analysis may suggest that the environment of the Minkowski vacuum is populated by a very small number of well-behaved species, despite the fact that the theory carries an alarmingly large number of potential spin states in its tensor gauge fields. This is rather suspicious, but it can again be confirmed (quite erroneously) by a linear Hamiltonian analysis [13].

The possibility of the ‘leftover’ modes becoming activated in the strong gravity regime (perhaps near the second vacuum) is sometimes set aside as a complication to be dealt with in further work. We can show however using the paradigmatic model above that on the contrary, this ‘leftover’ mode actually constitutes an existential emergency: it destroys the linear theory. To see this, we obtain from Eq. (4) the nonlinear Hamiltonian

$$H = \frac{1}{2} p_1^2 + \frac{p_2^2}{2 q_1^n} + \frac{1}{2} q_1^2 (q_1 - 1)^2 + \frac{1}{2} q_2^2,$$

(8)

where the second momentum is $p_2 \equiv q_1^n \dot{q}_1$, and the Hamilton equations read

$$\dot{p}_1 = \frac{n p_2^2}{2 q_1^{n+1}} - q_1 (q_1 - 1) (2 q_1 - 1),$$
$$\dot{q}_1 = p_1, \quad \dot{p}_2 = -q_2, \quad \dot{q}_2 = \frac{p_2}{q_1^n}.$$  

(9)

The fatal diagnosis can be made when we graduate from the linear to nonlinear models and lose the primary constraint. There are in general two degrees of freedom, and the physical trajectories turn out to explore volumes of the phase space. The resulting dynamics are absolutely inconsistent with the linear theory. Let us take the ‘least pathological’ case of $n = 2$, so that the sign of $q_1$ never makes a ghost mode out of the second oscillator. The lower four frames in Eq. (1) use Eq. (9) to slice the space at increasing $p_2$, revealing (albeit non-autonomously) the true behaviour of the first oscillator. The second oscillator drives a separatrix straight through the heart of the putative vacuum at $q_1 = 0$. On either side are split two new candidate vacua in red and violet.

Meanwhile, the solution at $q_1 = 1$ is unharmed, because it is not strongly coupled. Hamiltonian analysis of the linear theory near this vacuum will correctly reveal both degrees of freedom, so that this exact solution has some hope of being realised in nature.
The solution at \( q_1 = 0 \) will never be realised. Quantum fluctuations deviating into the energetic flows on either side of the separatrix would tear it apart, and so excite the second oscillator. The second oscillator is not a ghost, nor is it a tachyon, and it destroys the naive vacuum purely because it is strongly coupled there.

Returning to the modified gravity application, we begin to see how the programme of selecting for theories with healthy particle spectra near Minkowski spacetime becomes very dangerous if these spectra turn out to be, in some sense, ‘much sparser than they could be’. Unhappily, we are forced into precisely this ‘sparse’ scenario for the PGT, and for gravitational gauge theories in general, because modes impose conflicting unitarity bounds on the bare couplings. With the exception of the scalar modes, the effect is lethal for all the known ‘sparse’ spectra.

As demonstrated above, the nonlinear Hamiltonian analysis can diagnose the strong coupling problem. We note however a potentially important difference between this paradigmatic example and the effects seen so far in the PGT [13, 23, 46]. In the analysis above, the diagnosis rests on the appearance of a primary constraint in the erroneous, perturbative model. As we will recall in the rest of this paper, the primaries of the PGT are instead well understood, and their constraint structure changes discontinuously and the physical consequence is known to be a theory punctuated by a reducible constraint structure. Rather, it is their commutators, which appear immediately sensitive to the linearisation. In both cases however, the constraint structure changes discontinuously and the physical consequence is known to be a theory punctuated by a reducible constraint structure.

To connect back to the geometric picture? The Minkowskian metric components can be recovered via the contorsion – are provided by the formulae

\[ T_{ij} = 2 h^i_k h^j_l (\partial_k A^l_j - A^l_k | A^l_j |), \]

\[ T^i_{jl} = 2 h^i_k h^j_l (\partial_k A^l_j + A^l_m | A^m_j |). \]

The conversion of these back to the (numerical values) of the geometric components, is done by contraction with the translational gauge field strength tensors – referred to as the curvature and torsion – are provided by the formulatrix

\[ \mathcal{R}^{ij}_{kl} = 2 h^i_k h^j_l (\partial_k A^l_j - A^l_k | A^l_j |), \]

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\[ \mathcal{R}^i_{jk} = 2 h^i_k h^j_l (\partial_k A^l_j + A^l_m | A^m_j |). \]
where our metricity assumption dispenses with the need for the final term in (2), and we use the Planck mass rather than the Einstein constant \( m_p \equiv 1/\sqrt{\kappa} \). Once again, we reiterate that our use of the gauge theory setup over geometric alternatives (including those which use the tetrad and spin-connection over the metric and contorsion) is merely a matter of convenience in the present work.

In this article we will follow [83] by using the following syntax highlighting for code listings: keywords for Mathematica are typeset in green, for xAct in blue and for HiGGS in red. This paper uses the ‘West coast’ signature (+, −, −, −).

2 Implementation

In this section the implementation of the Hamiltonian analysis in the HiGGS package is described. Many aspects of our particular approach will be inefficient: the package is monolithic and expensive in terms of memory and maintenance. At the time of writing, however, HPC is a cheap resource. By carefully tuning only a few aspects of the implementation it is therefore possible to produce a product which surveys the theory space in a matter of hours. It is important to emphasise therefore possible to produce a product which surveys the theory space in a matter of hours. It is important to emphasise with the command BuildHiGGS[]. This paper uses the ‘West coast’ signature (+, −, −, −).

2.1 Geometric setup

We begin by describing the way in which the Riemann–Cartan geometry is implemented in HiGGS. Whilst xAct is perfectly capable of accommodating not only a Riemann–Cartan curvature, but also a torsion tensor, we prefer to adhere to the ‘particle physics’ picture of gravitational gauge theories [8,14,57,79], and set up all the physics on a flat spacetime. The following equivalent xAct commands are issued when the HiGGS environment is initially built (see Eq. (3.1)) with the command BuildHiGGS[]

\[
\text{In[1]}:= \text{DefManifold}[\text{M4}, 4, \text{IndexRange}[[a, z]]]; \text{DefMetric}[-1, \text{G}[-m, -n], \text{CD}, \\{"\text{\"}, "\text{\"} \{\text{\"PartialD} \\}\}], \text{PrintAs} \rightarrow \text{\"}\{\text{\"Gamma}\text{\"}\}, \text{FlatMetric} \rightarrow \text{\"True}, \text{SymCovDQ} \rightarrow \text{\"True};
\]

This sets up a \( D = 4 \) manifold \( \text{M4} \) to represent \( \tilde{M} \), with a flat negative-signature metric \( \text{G}[-m, -n] \) to represent \( \gamma_{\mu\nu} \), and flat covariant derivative \( \nabla_\mu \) represented by \( \text{CD}[-m] \). This offers several advantages, and foremost among these is an easy comparison with the very substantial body of literature on the Hamiltonian structure as mentioned in Eq. (1.2). We will also not be limited by the fact that the non-Riemannian features of \( \text{xAct} \) are (presently) less flexible and comprehensive than those of a simple Minkowskian setup. This is to be expected, given that GR is the preferred effective theory of gravitation.

An essential feature of this setup, which goes beyond the particle picture of the literature, is the conflation of holonomic and non-holonomic tangent spaces: a single collection of indices \( a, b, c \), etc. is ascribed to \( \text{TangentM4} \), and these represent both the Lorentz indices \( i, j, k \) and coordinate indices \( \mu, \nu, \sigma \). This practice might be anathema to the field of differential geometry, but it is acceptable for pragmatic, computational purposes. The coordinates are assumed implicitly to be Cartesian, so that the components of the flat metric \( \gamma_{\mu\nu} \) are Minkowskian (equal to those of \( \eta_{ij} \)), and moreover that a rotational gauge is chosen in which \( e_0 = \hat{e}_0, e_1 = \hat{e}_1, e_2 = \hat{e}_2 \) and \( e_3 = \hat{e}_3 \). As a consequence of this gauge-fixed setup, the covariance of quantities is not guaranteed internally, as it would be if all the features of \( \text{xAct} \) (such as user-defined connections) were fully exploited in HiGGS. It is instead possible to check the covariance by visually inspecting the final results for explicit gauge fields: in practice this turns out to be very easy, and the elimination of bare gauge fields in HiGGS is reliable.

It is important to note that whilst the gauge is fixed to conveniently overload the indices of \( \text{TangentM4} \), the tensor structure of PGT is wholly preserved. This is in contrast, for example, with the seminal paper [61] in which the time gauge imposes \( h_a^0 = 0 \), thereby massively simplifying the various algebraic expressions. On the contrary, the algebraic expressions produced from HiGGS are valid for any gauge, once the various shared indices are interpreted as being either Greek or Roman. Care is taken in the definitions to avoid any ambiguity over this division of indices.

Following on from our discussion of indices, we note that the 1, 2, 3 spacelike indices \( a, b, c \) and \( \alpha, \beta, \gamma \) are also subsumed into \( a, b, c \). These may be extracted by means of the projection operator \( G3[a, b] \), which represents \( \gamma^{ab} \), and lies at the heart of the Arnowitt–Deser–Misner (ADM) split. The ADM or 3+1 split uses a spacelike foliation which is characterised by timelike unit vector \( n_\kappa \), defined as

\[
n_\kappa \equiv h_\kappa^0/\sqrt{g_{00}}, \tag{15}
\]

where we recall that the (gravitational) metric components are recovered by \( g^{\mu\nu} \equiv h^{\mu}_j h^j_\nu \delta^{ij} \). Any vector with local Lorentz indices may then be decomposed into perpendicular and parallel components \( V^i = \mathcal{V}^i + n^i \delta^i + V^i \). An overbar is used to denote the parallel indices. There are then some identities
\[ b^\mu_* h^\alpha_* \equiv \delta^\mu_* \delta^\alpha_* \text{ and } b^\mu_* h^\alpha_* \equiv \delta^\mu_* \delta^\alpha_* \text{, which follow from (15). The} \]
gauge fields \( h^\mu_* \), \( b^\mu_* \) and \( A^\mu_* \) are denoted by \( H[-a,b] \), \( B[a,-b] \) and \( A[a,-b,-c] \). The timelike vector \( n^\mu \) is represented by \( V[a] \), and we see that a variety of identities are then implied within the built HiGGS environment

now that the geometric setup is in place, we introduce the canonical setup [7,8,84]. The canonical momenta are

\[ \pi^\mu_i \equiv \frac{\partial b L_G}{\partial (\partial^0 b^\mu_i)} \quad \pi^0 \equiv \frac{\partial b L_G}{\partial (\partial^0 A^0_j)}. \]  

as with our earlier work [13,14,67], we will neglect the matter Lagrangian \( L_M \). The field strengths in (13a) and (13b) are independent of the velocities for \( b^\mu_* \) and \( A^\mu_* \), so (18) imply 10 primary constraints of the form

\[ \varphi_0^0 \equiv \pi_0^0 \equiv 0, \quad \varphi_{ij}^0 \equiv \pi_{ij}^0 \equiv 0. \]  

from (19) we arrive at the result mentioned above, that the conjugate field \( b^0_* \) is non-physical; the same applies to \( A^0_0 \). by (\( \approx \)), the weak equality is denoted, i.e. not an approximation. The constraints (19) are referred to as the ‘sure’ primary, first class (sPFC) constraints: they are a consequence of Poincaré symmetry, and they apply for all choices of the \( \{ b^\mu_i \}, \{ \beta^\mu_0 \}, \{ \varphi^0_0 \}, \{ \varphi_{ij}^0 \} \). according to (18), HiGGS must support a field momentum for both \( B[a,b] \) and \( A[a,b,c] \). the \( \pi^0_i, \pi^\mu_{ij} \) and the ‘parallel’ \( \pi^0_i, \pi^\mu_{ij} \) are defined as follows

these functions carry information about the part \( b^\mu_* \) of the translational gauge field (which, as we will shortly see, is non-physical), whereas \( n^\mu \) is independent of this quantity. in HiGGS the lapse is \( \text{Lapse}[] \) and we use also the spatial measure \( J[] \) for the quantity \( J \equiv b/N \), where \( b \equiv b^\mu_* \).

some further identities are then

\[ \frac{\partial n_i}{\partial b^\mu_i} = -h_i^\mu, \quad \frac{\partial h_i}{\partial b^\mu_i} = -h_i^\mu, \quad \frac{\partial n_j}{\partial b^\mu_j} = b h_i^\mu, \quad \]  

\[ \frac{\partial J}{\partial b^\mu_j} = h_j^\mu, \quad \frac{\partial N}{\partial b^\mu_j} = N n_j h_j^\mu. \]  

These identities are also incorporated into the HiGGS environment, which prefers to extract – from all derivatives of quantities dependent on the translational gauge field – the form \( \text{CD}[-a][B[-b,-c]] \). it is practical to replace all instances of \( \text{CD}[-a][H[-b,-c]] \) accordingly, since the momentum \( \text{BPI}[-a,-b] \) is defined according to \( B[-a,-b] \), and so we find

the purpose of the parallel momenta is seen above: they are the physical parts not touched by the sPFCs, and defined according to \( \pi^i \equiv \pi^0_i, \pi^\mu_{ij} \equiv \pi_{ij}^\mu \).

we will see in Eq. (2.4) that the specific internal rule \( \text{PiToPi} \) should not often need to be used in practice, and has more general alternative in the \( \text{ToBasicForm[]} \) command which is provided officially by the package. in general, parallel and perpendicular quantities can be accessed with some projections
The flat manifold of course has vanishing Riemannian curvature $R^{\mu \nu \rho \lambda} = 0$, and so we must be careful not to use the $\pi$Act quantities $\text{RiemannCD}[-a,-b,-c,-d]$, $\text{RicciCD}[-c,-d]$ or $\text{RicciScalarCD}[]$. Instead, the field strengths $\mathcal{R}_{ijkl}$ and $\mathcal{T}_{ijk}$ are given by their own tensors, and these expand to give the definitions in Eqs. (13a) and (13b)

\begin{align*}
\text{In[1]} &= \text{quantity} = (\mathcal{R}[-a,-b,-c,-d], \mathcal{R}[a,-a,-c,-d], \mathcal{T}[a,-b,-c], T[a,-b,-c], T[a,-b,b]) \\
\text{Out[1]} &= \left\{ \rho_{acbd}, \rho^{a\,cd}, \rho^{a\,bc}, \omega^{a\,b}, \omega^{a\,b} \right\}
\end{align*}

\begin{align*}
\text{In[2]} &= \text{ScreenDollarIndices[ToCanonical[quantity /. ExpandStrengths]]} \\
\text{Out[2]} &= \left\{ \lambda_{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d} \right\}
\end{align*}

The final set of fields which we introduce are the multip\-liers $\lambda_{ijkl}$ and $\lambda_{ijk}$ — these are precisely the same shape as $\mathcal{R}_{ijkl}$ and $\mathcal{T}_{ijk}$, and we write them

\begin{align*}
\text{In[3]} &= \text{quantity} = (\mathcal{R}[a\,b\,c\,d], \mathcal{R}[a,-a,-c,-d], \mathcal{R}[a,-b,-c\,d], T[a\,b\,c\,d], T[a\,b\,c\,d], T[a\,b\,b]) \\
\text{Out[3]} &= \left\{ \lambda_{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d} \right\}
\end{align*}

The Hamiltonian analysis invites decomposition into irreducible representations of the Lorentz group $SO^+(1,3)$, and (through the ADM split) the special orthogonal group $SO(3)$. The former is useful also in the Lagrangian picture, since the Lagrangian formulation of a theory is typically Lorentz-covariant, it is useful to split field representations into blocks which transform only among themselves. In the Hamiltonian case, the choice of slicing introduces a ‘preferred’ timelike vector — this is not unique, so covariance is not ultimately lost — but the symmetry in the context of the slicing is reduced to the spatial rotations $SO(3)$. In the case of rotations, the irreps of tensor fields correspond to states of definite spin and parity, allowing us to designate the parts as $J^P$.

2.2.1 Lorentz group

We do not often encounter the Lorentz decomposition in the course of Hamiltonian calculations, but it is implemented across the higher-rank tensors, for example the ‘human-readable’ decomposition into familiar irreps such as the Weyl

\begin{align*}
\mathcal{W}_{ijkl} &\equiv \mathcal{R}_{ijkl} - \frac{1}{2} (\eta_{ik} \mathcal{R}_{jl} - \eta_{il} \mathcal{R}_{jk} - \eta_{jk} \mathcal{R}_{il} \\
&+ \eta_{jl} \mathcal{R}_{ik}) + \frac{1}{6} \mathcal{R},
\end{align*}

the Ricci and the Ricci scalar

\begin{align*}
\mathcal{R}_{ij} &\equiv \mathcal{R}^{l}_{ilj}, \quad \mathcal{R} \equiv \mathcal{R}^{l}_{ll},
\end{align*}

and the tensor torsion, defined as the remainder of $\mathcal{T}^i_{jk}$ after removing the vector (i.e. torsion contraction) and pseudovector components

\begin{align*}
\mathcal{T}_i &\equiv \mathcal{T}^j_{ij}, \quad \mathcal{T}^j_{il} \equiv \epsilon_{ijkl} \mathcal{T}^{kl},
\end{align*}

— see e.g. \cite{23,46,85}. These components may be accessed as follows

\begin{align*}
\text{In[4]} &= \text{ScreenDollarIndices[ToCanonical[quantity /. ExpandStrengths]} \\
\text{Out[4]} &= \left\{ \lambda_{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d} \right\}
\end{align*}

It should be emphasised again that rules such as ExpandStrengths, PadmaActivate and PiToPi should not often be needed, and are subsumed under the ToBasicForm[] command.

2.2 Irreducible decompositions

The Hamiltonian analysis invites decomposition into irreducible representations of the Lorentz group $SO^+(1,3)$, and (through the ADM split) the special orthogonal group $SO(3)$. The former is useful also in the Lagrangian picture, since the Lagrangian formulation of a theory is typically Lorentz-covariant, it is useful to split field representations into blocks which transform only among themselves. In the Hamiltonian case, the choice of slicing introduces a ‘preferred’ timelike vector — this is not unique, so covariance is not ultimately lost — but the symmetry in the context of the slicing is reduced to the spatial rotations $SO(3)$. In the case of rotations, the irreps of tensor fields correspond to states of definite spin and parity, allowing us to designate the parts as $J^P$.

More commonly, we might need access to the complete, orthonormal $SO^+(1,3)$ operators which appear in (14). These may be associated with the couplings $\{\hat{\alpha}_1\}$, $\{\hat{\beta}_M\}$, $\{\hat{\alpha}_I\}$, $\{\hat{\beta}_M\}$ as follows, for the purposes of constructing a Lagrangian\footnote{Note that $HGGS$ does not define a Planck mass $m_p$; all scales are absorbed into the couplings $\text{Bet1, Bet2, Bet3}$, which are really $m_p^2\hat{\beta}_1$, etc., and likewise for the multiplier coefficients and $\text{Alp0}$.}

\begin{align*}
\text{In[5]} &= \text{ScreenDollarIndices[ToCanonical[TLambda [a,-b,-c]. \text{StrengthLambdasSO13Activate}]} \\
\text{Out[5]} &= \left\{ \lambda_{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d}, \lambda^{a\,b\,c\,d} \right\}
\end{align*}
\[ \begin{align*}
\text{In[1]:=} & \quad \text{quantity} = \{\text{Alp1}\cdot\text{PR1[-i,-k,-l,-m,a,b,c,d]} + \text{Alp2}\cdot\text{PR2[-i,-k,-l,-m,a,b,c,d]} + \text{Alp3}\cdot\text{PR3[-i,-k,-l,-m,a,b,c,d]} + \text{Alp4}\cdot\text{PR4[-i,-k,-l,-m,a,b,c,d]} + \text{Alp5}\cdot\text{PR5[-i,-k,-l,-m,a,b,c,d]} + \text{Alp6}\cdot\text{PR6[-i,-k,-l,-m,a,b,c,d]}\}\cdot\text{R[-a,-b,-c,-d]} \\
\text{Out[1]=} & \quad \left(\hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}\right)_{\text{abcd}}
\end{align*} \]

\[ \begin{align*}
\text{In[2]:=} & \quad \text{quantity} = \text{ScreenDollarIndices[ToCanonical[quantity /. \text{PActivate} /. \{\text{Alp1} \to 1, \text{Alp2} \to 1, \text{Alp3} \to 1, \text{Alp4} \to 1, \text{Alp5} \to 1, \text{Alp6} \to 1\}]]} \\
\text{Out[2]=} & \quad \left(\hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}\right)_{\text{abcd}}
\end{align*} \]

\[ \begin{align*}
\text{In[3]:=} & \quad \text{ScreenDollarIndices[ContractMetric[ToCanonical[T[i,k,l] \cdot (\text{Bet}\cdot\text{PT}[{-i,-k,-l,-m,a,b,c,d]} + \text{cAlp6}\cdot\text{R[i,k,l,m]} - \text{PR6[-i,-k,-l,-m,a,b,c,d]} + \text{R[-a,-b,-c,-d]} + \text{cAlp2}\cdot\text{PT2[-i,-k,-l,-m,a,b,c,d]} + \text{cBet2}\cdot\text{PT2[-i,-k,-l,-m,a,b,c,d]} + \text{cAlp6}\cdot\text{PR6[-i,-k,-l,-m,a,b,c,d]} + \text{R[-a,-b,-c,-d]} + \text{Tlambda[-a,-b,-c]} \cdot \text{PActivate}] /\text{PActivate}]]} \\
\text{Out[3]=} & \quad \left(\hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}\right)_{\text{abcd}}
\end{align*} \]

From this we see how to access the \( J^P \) and \( M_{ij}^{kl} \) projections.

### 2.2.2 Rotation group

The SO(3) projections are similarly defined, but of course refer to the vector \( n_i \), not just the Lorentzian metric \( \eta_{ij} \). The parallel momenta can be decomposed in this way: for the translational case

\[ \hat{\pi}_{kl} = \hat{\pi}_{kl} + n_k \hat{\pi}_{\perp l}, \quad (23a) \]

\[ \hat{\pi}_{kl} = \frac{1}{3} \eta_{kl} \hat{\pi} + \hat{\pi}_{kl} + \hat{\pi}_{\perp l}, \quad (23b) \]

where the second term in (23a) is the \( 1^- \) vector mode, and the terms in (23b) are respectively the \( 0^+ \) scalar, skew-symmetric \( 1^+ \) vector and symmetric-traceless \( 2^+ \) tensor modes. The rotational case is similarly decomposed as

\[ \hat{\pi}_{klm} = \hat{\pi}_{klm} + 2n_k \hat{\pi}_{\perp l m}, \quad (24a) \]

\[ \hat{\pi}_{klm} = \frac{1}{3} \eta_{klm} \hat{\pi} + \hat{\pi}_{klm} + \hat{\pi}_{\perp l m}, \quad (24b) \]

\[ \hat{\pi}_{klm} = \frac{1}{6} \eta_{klm} \hat{\pi} + \hat{\pi}_{\perp l m} + \frac{1}{3} \eta_{klm} \hat{\pi}_{\perp l m}, \quad (24c) \]

where (24a) are the \( 0^+, 1^+ \) and \( 2^+ \) modes and (24b) are the \( 0^-, 1^- \) and \( 2^- \) modes. Accordingly, we access these as follows

\[ \begin{align*}
\text{In[4]:=} & \quad \text{ScreenDollarIndices[ToCanonical[(\text{API}\cdot\text{R[-a,-b,-c]} + \text{BPI}\cdot\text{R[-a,-b]}) /. \text{PToP03}]]} \\
\text{Out[4]=} & \quad \left(\hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}, \hat{\pi}_{\text{ijklm}}\right)_{\text{abcd}}
\end{align*} \]

The parallel parts of the field strengths can also be decomposed, since they are canonical, but we neglect the perpendicular parts which depend on the unphysical fields \( b^0_1 \) and \( A^{ij}_0 \), and also on non-canonical velocities. The field strength decomposition is

\[ R_{ijkl} = R_{ijkl} + 2n_k \langle R_{l \perp j} \rangle, \quad (25a) \]

\[ T_{ijkl} = T_{ijkl} + 2n_k \langle T_{l \perp j} \rangle, \quad (25b) \]

We notice that \( R_{ijkl} \) and \( R_{ij \perp j} \) both share all six \( J^P \) representations present in the rotational momentum. In the parallel case, these are denoted by the \( 0^+ \) scalar \( R \), \( 1^+ \) dual vector \( R_{[ij]} \), 2\(^+\) symmetric-traceless tensor \( \overline{R}_{[ij]} \), 0\(^-\) pseudoscalar \( P R_{0,i} \), 1\(^-\) vector \( \overline{R}_{i} \) and 2\(^-\) tensor \( T \overline{R}_{i \perp j} \). In general, the \( (\cdot) \) brackets indicate the symmetric-traceless operation. The perpendicular irreps are denoted as the \( 0^+ \) scalar \( \overline{R}_{ij \perp k} \), 1\(^+\) dual vector \( \overline{R}_{ij \perp k} \), 2\(^+\) symmetric-traceless tensor \( R_{ij \perp k} \), 0\(^-\) pseudoscalar \( P R_{0,i} \), 1\(^-\) vector \( \overline{R}_{i} \) and 2\(^-\) tensor \( T \overline{R}_{i \perp j} \). The situation for the torsion is slightly different, because of the reduced number of components. The parallel \( T_{ijkl} \) contains the 0\(^-\) pseudoscalar \( P T \), 1\(^+\) dual vector \( T_{[ij]} \), 1\(^-\) vector \( \overline{T}_{i} \) and 2\(^-\) tensor \( T_{ij \perp k} \). The perpendicular \( T_{i \perp j} \) contains the 0\(^+\) scalar \( T_{ij} \), 1\(^+\) dual vector \( T_{[ij]} \), 1\(^-\) vector \( T_{i \perp j} \) and 2\(^+\) tensor \( T_{(ij) \perp} \) just as with the translational momentum.
In HiGGS, only the canonical, parallel parts of these tensors are decomposed. The multipliers share the same tensor structure, and both their parallel and perpendicular parts are decomposed: this is because all multiplier fields are assumed to be canonical. The resultant decomposition is

\[ \text{ToCanonical}[(\mathcal{R}[-a,-b,-c,-d], \mathcal{R}[-a,-b,-c]) /. \text{StrengthDecompose} /. \text{StrengthLambdaDecompose}] \]

\begin{align*}
\{ & \mathcal{R}_{ab} = \mathcal{R}_{ab}, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \\
& \mathcal{R}_{ab} c = \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c, \mathcal{R}_{ab} c \}.
\end{align*}

Note above that it is sometimes necessary to repeatedly apply routines in order to recover the desired form. In principle, the HiGGS commands are constructed so as to be idempotent, but broadly in Mathematica and \textit{xAct} repeated commands are sometimes helpful when multiple functions are nested.

\section{2.3 Derivatives}

While the gauge-fixed Minkowskian setup initially makes for easy development, it sometimes means that we have to ‘reinvent the wheel’ in order to access machinery for which there is already a very sophisticated implementation in \textit{xAct}. A clear example of this is given by the way in which HiGGS
handles gauge-covariant derivatives in the Poincaré gauge theory. Generalising from (12), we recall from \([8, 14, 79, 80]\) that for some matter field \(\phi\) we have
\[
D_i \phi \equiv h_{i}^{\mu} \left( \partial_{\mu} + \frac{1}{2} A_{\mu}^{kl} \Sigma_{kl} \right) \phi, \quad D_{\mu} \phi \equiv h_{\mu}^{i} \cdot D_{i} \phi, \tag{26}
\]
where \(\Sigma_{ij}\) are the Lorentz group generators specific to the representation of \(\phi\). This construction could be implemented using the \(xAct\) command \(\text{DefCovD[]}\), in such a way that the \(\Sigma_{ij}\) generators are automatically calculated for tensorial representations of the kind that arise in the Hamiltonian analysis of the matter-free theory. In particular, the derivative \(D_{\mu}\) is geometrically interpreted as \(\nabla_{\mu}\phi\) as it appears in (10). Rather than following this route, \(HiGGS\) defines a pair of first derivatives (broadly corresponding to the two definitions in (26)) for every canonical quantity which might be of interest. This process is not very efficient or flexible, but it is sufficient when explicit covariant derivatives are scarce. Indeed, the most common occurrence of the gauge covariant derivative is through its commutator
\[
2D_{[i} D_{j]} \phi = \left( \frac{1}{2} R_{ij, kl} \Sigma_{kl} - T_{ij} D_k \right) \phi, \tag{27}
\]
in the form of the field strengths; as we saw in Sect. 2.1, these have a separate implementation. Explicit gradients will tend to arise mostly at the end of the calculations for which \(HiGGS\) is designed. Gradients of the field strengths cannot usually be fed back into the algorithm anyway, since they would require an implementation of the second order Euler–Lagrange equations in order to be processed.

Based on the understanding that we are always dealing with arbitrarily-indexed (possibly mixed) tensorial representations, \(HiGGS\)'s two preferred forms of the derivative are \(D_{\mu} \phi_{\alpha\beta\cdots}\) and \(\delta_{\alpha\beta\cdots} \delta_{\mu}^{\nu} \nabla_{\nu} \phi_{\alpha\beta\cdots}\). The former is straightforward\(^7\), and the latter is the parallel projection of the gradient on all indices. Picking a couple of \(SO(3)\) irreps at random, we find for example

\[
\text{In[]} := \text{quantity} = \{\text{DPIPA2m[-z,-a,-b,-c], CD[-z][PIPA2m[-a,-b,-c], DRP2p[-z,-a,-b], CD[-z][RP2p[-a,-b]]}\}
\]
\[
\text{Out}[] = \{\{h_{\mu}^{i} \cdot \nabla \nabla_{i} \phi_{abc}, h_{\mu}^{i} \cdot \nabla \nabla_{i} \phi_{abc}\} - \delta_{\mu}^{\nu} \nabla_{\nu} \phi_{abc}\}
\]

\[
\text{In[]} := \text{quantity} = \text{ScreenDollarIndices}[\text{ContractMetric[ToCanonical[quantity /. DIPActivate /. DIPDeactivate]]}]
\]
\[
\text{Out}[] = \{\{\text{Dh} \cdot \nabla \nabla_{i} \phi_{abc}, \text{Dh} \cdot \nabla \nabla_{i} \phi_{abc}\} - \delta_{\mu}^{\nu} \nabla_{\nu} \phi_{abc}\}
\]

One cannot generally pass from \(D_{\mu} \phi_{\alpha\beta\cdots}\) to a parallel derivative, unless only the spacelike indices are involved, e.g. \(D_{\mu} \phi_{\alpha\beta\cdots}\). Since \(HiGGS\) tries to achieve parallel derivatives wherever possible, this serves as one of the internal checks on the canonical status of a quantity, making sure that any unacceptable time derivatives would appear explicitly in the output. Accordingly, continuing from above

\(^7\) Note that we use an accent to indicate an arbitrary number of indices, following from \([67, 86]\).
We see in the penultimate expression above the two parallel derivatives. If an expression containing gradients is covariant, velocity-independent and parallel, then the various other terms should cancel among themselves. As we have mentioned, covariance also requires that gauge fields do not explicitly appear, but are implicit in covariant quantities. Overall, the work of packaging an expression into a canonical, covariant form, parallel if possible and free from unphysical fields, is done by the \texttt{ToNesterForm[]} command, which we introduce in Eq. (2.4).

As a final comment on the use of derivatives, we recall that the formulae Eqs. (13a) and (13b) imply a pair of Bianchi identities [8,85] as follows

\begin{align}
\epsilon_{\rho\mu\lambda\nu} D_{\mu} (b_j^l b_j^l R_{ij}^l) & \equiv \epsilon_{\rho\mu\lambda\nu} b_k^l b_j^l R_{kl}^l , \quad (28a) \\
\epsilon_{\rho\mu\lambda\nu} D_{\lambda} (b_k^l b_j^l R_{kl}^l) & \equiv 0 . \quad (28b)
\end{align}

These can be verified using the tools already introduced, but the process will be easier with the \texttt{ToBasicForm[]} and \texttt{ToNesterForm[]} commands.

### 2.4 Low-level functions

Throughout Sects. 2.1 and 2.2 we have used many rules, such as \texttt{DpRPDeactivate}, \texttt{DPiPActivate}, etc., which – whilst they are not confined to \texttt{xAct ‘HiGGS ‘Private} and so are available to the user – should not often be needed within a \texttt{HiGGS} science session. Instead these rules are wrapped into two ‘official’ functions: \texttt{ToNesterForm[]}, which strives to collect expressions,\(^8\) and \texttt{ToBasicForm[]}, which expands them. Naturally \texttt{ToNesterForm[]} is the more complicated of the two. It is, in some sense, the extension of the \texttt{ToCanonical[]} command from \texttt{xAct} into \texttt{HiGGS}.

\(^8\) The chosen naming refers to the fact that the irrep conventions and notation of collected expressions tends to align most closely with those of a collection of articles – very useful during development – for which Nester is a common author, see e.g. [23,45,46,55,82,87–92].

#### 2.4.1 Module: ‘ToBasicForm’

We begin by breaking some expressions which we know to be covariant, using \texttt{ToBasicForm[]}

```
{In}:= quantity = ToBasicForm[{T[i,-j,-k], PiPB0p[], PiPA1p[-i,-j]};
{Out}=
```

The gradient of a more complicated irrep such as \texttt{DpPiPA2m[-i,-j,-k]} would span many pages after an application of \texttt{ToBasicForm[]}, rendering manual evaluation of brackets impractical, yet we will see in Eq. (3) that there is nothing to stop these terms arising in the analysis.

Now is a convenient time to verify the second Bianchi identity in (28b). Setting up the derivative, and using the gauge-fixed \(\epsilon_{\mu\nu\sigma\lambda} \) which follows from \(\gamma_{\mu\nu} \) – \texttt{epsilonG[a,b,c,d]} – we find

```
{In}:= quantity2 = ToBasicForm[epsilonG[r,m,l,n]*CD[-1][B[k,-m]*B[q,-n]*R[i,j,-k,-q]] + A[i,-x,-1]*B[k,-m]*B[q,-n]*R[i,-x,-k,-q] + A[j,-x,-1]*B[k,-m]*B[q,-n]*R[i,-x,-k,-q]);
```
Evidently, this quantity vanishes, and so what we are seeing is a side-effect of the HiGGS geometric setup: xAct does not know that CD[-1][] is the partial derivative, so we need a final step

\[ \text{ToBasicForm}[] \]

\[
\text{quantity2} = (\text{ToCanonical}[(1/2)*(#1^2 - 1)^{-1}*(#1 - 1)^{-1}*(#1 - 6)^{-1}*(#1 - 1)] & )
\]

\[ \text{ToNesterForm}[] \]

ToBasicForm[] is not a sophisticated function, it essentially imposes a list of internal rules on its argument, and the expansion of SO(3) field strength irreps, as with those of momenta, would be perfectly straightforward to implement in the source if and when needed.

When ToNesterForm[] is passed a non-covariant quantity, it is unable to return a covariant result. Nonetheless, it tries, returning for the innocuous gradient \( \partial_\mu \)

\[ \text{quantity2} = (\text{ToCanonical}[(1/2)*(#1^2 - 1)^{-1}*(#1 - 1)^{-1}*(#1 - 6)^{-1}*(#1 - 1)] & )
\]

As with this case, it is usually easy to identify nonphysical expressions which indicate a human error, through the appearance of bare gauge fields. If needed, this covariance check is easy to automate through an output search with the Mathematica Head[] function for an unwanted HiGGS quantity, such as A or B. We can also observe in the output above part of the route taken by ToNesterForm[]. Gauge field gradients are converted, where possible, to field strengths and covariant derivatives. The residual spin connection terms are then extensively manipulated in an attempt to cancel them. Leftover asymmetric derivatives of the translational gauge field can sometimes be ascribed to covariant quantities through (17), for example the following gradient cannot be expressed through the torsion alone

\[ \text{quantity2} = (\text{ToCanonical}[(1/2)*(#1^2 - 1)^{-1}*(#1 - 1)^{-1}*(#1 - 6)^{-1}*(#1 - 1)] & )
\]

Note that whilst the results are covariant, we do not get back the same form from ToNesterForm[] as that which was provided to ToBasicForm[], instead we recover the SO(3) expansion. The reason for this is that reducible quantities such as \( T[-a, -b, -c] \) are usually quickly broken up during the course of the Hamiltonian analysis: the output of ToNesterForm[] is tuned so as to be useful in that context. Moreover, we note that this operation will not now work in reverse, since input such as \( \text{TP2m}[-a, -b, -c]/\text{ToBasicForm} \) will not return a broken expression. There is no special reason behind this:

\[ \text{ToBasicForm}[] \]

\[ \text{quantity2} = (\text{ToCanonical}[(1/2)*(#1^2 - 1)^{-1}*(#1 - 1)^{-1}*(#1 - 6)^{-1}*(#1 - 1)] & )
\]

2.4.2 Module: ‘ToNesterForm’

Let us now undo the breaking, using ToNesterForm[]. In general, much of the functionality of ToNesterForm[] has to do with fully incorporating the known primary and secondary constraints of the theory during the course of simplification — so as to leave no extra conditions for the user to worry about. Before a theory has been defined (see Sect. 2.5) using DefTheory[], we will have to suppress this activity by passing the option "ToShell" → False, yielding

\[ \text{quantity} = \text{ToNesterForm}[\text{quantity}, \text{ToShell} \rightarrow \text{False}] \]

\[ \text{In[] := quantity = ToNesterForm[quantity, \text{ToShell} \rightarrow \text{False}] \}
\]

\[ \text{Out[] :=} \]

\[
\{\text{\( \frac{1}{2}\) e}^\mu_\nu \text{e}^\nu_\rho \text{e}^\rho_\lambda \text{\( \nabla^\mu \nabla^\nu \nabla^\rho \nabla^\lambda \))},
\text{\( \frac{1}{2}\) \text{\( \nabla^\mu \nabla^\nu \nabla^\rho \nabla^\lambda \))}
\]

\[ \text{Note that the above result could equally be written as the single term \( -D_\mu V[-q, -y] \), but ToNesterForm[] takes the opportunity to separate out the antisymmetric part. Before moving on, we return to verify the first Bianchi identity in (28b). We can access the canonical (i.e. velocity-}

\[ \text{In[] := quantity = ToNesterForm[quantity, \text{ToShell} \rightarrow \text{False}] \}
\]

\[ \text{Out[] :=} \]

\[
\{\text{\( \frac{1}{2}\) e}^\mu_\nu \text{e}^\nu_\rho \text{e}^\rho_\lambda \text{\( \nabla^\mu \nabla^\nu \nabla^\rho \nabla^\lambda \))},
\text{\( \frac{1}{2}\) \text{\( \nabla^\mu \nabla^\nu \nabla^\rho \nabla^\lambda \))}
\]

Note that whilst the results are covariant, we do not get back the same form from ToNesterForm[] as that which was provided to ToBasicForm[], instead we recover the SO(3) expansion. The reason for this is that reducible quantities such as \( T[-a, -b, -c] \) are usually quickly bro-
independent) part of this identity by projecting Eq. (28b) with $b^\mu\gamma$ or equivalently using in place of $\epsilon^{i\mu\nu\lambda}$ the foliation equivalent $\epsilon^{i\mu\nu\lambda\perp}$. This is given in HiGGS by

\[ \text{Eps}[i,j,k], \]

with a natural extension of the formula when multiplier fields are admitted. The formula (29) may appear no more daunting than a commonplace action variation, but in practice $A$ and $B$ are frequently local tensors rather than nonlocal scalars. Locality signifies that the underlying functionals contain Dirac distributions, themselves subject to the total derivatives of the generalised Euler–Lagrange equations. The full ramifications of covariantly removing these Dirac gradients are detailed in [14,67], and some special cases are discussed in electrodynamics on the lightcone [93] and noncritical string theory [94]. Currently, HiGGS is able to accommodate the first order Euler–Lagrange formalism in PoissonBracket[]. First order brackets, evaluated by inserting the spatial dependence into (29), produce four terms of the form

\[ \left\{ A(x_1), B(x_2) \right\} = \int d^3x \left[ J_1(x)\delta^3(x-x_1)\delta^3(x-x_2) + J_2^a(x)\delta^3(x-x_1)\partial_a\delta^3(x-x_2) + J_3^{a\beta}(x)\partial_a\delta^3(x-x_1)\partial_{\beta}\delta^3(x-x_2) + J_4^{a\beta\gamma}(x)\partial_a\delta^3(x-x_1)\partial_{\beta}\delta^3(x-x_2) \right], \]

where the $J_1$, $J_2^a$, $J_3^{a\beta}$ and $J_4^{a\beta\gamma}$ can be determined by certain formulae. Note that by our conventions in [13,14,67], we will in future denote by $\delta^3$ the equal-time Dirac function $\delta^3(x_1 - x_2)$. Without any special instructions, PoissonBracket[] returns a List of the four Dirac coefficients in (30). This behaviour is tied into calls to PoissonBracket[] from within Velocity[], which we introduce in Sect. 2.5. Note that PoissonBracket[] contains calls to ToNesterForm[], and so works to exhaust transformations which can be applied to the output by virtue of the known primary and secondary constraints. In this sense, it depends on the theory introduced by DefTheory[] and so for the time being we must again pass the option "ToShell" → False. We begin with a very simple bracket, whose output can be understood in terms of our previous ToNesterForm[] result for DpV[-a,-b]

\[ \text{In}[] := \text{PoissonBracket}[\text{PiP2p}[-a,-b], \text{TP1p}[-c,-d], "\text{ToShell}" \rightarrow \text{False}], \]

\[ \text{Out}[] = \left\{ \begin{array}{c} \text{\varepsilon}_{nab} \cdot \varepsilon^{cd} \times \\
\frac{1}{4} (\partial n)_{ab} \cdot \varepsilon^{cd} - \frac{1}{4} (\partial n)_{db} \cdot \varepsilon^{ac} + \frac{1}{4} (\partial n)_{bc} \cdot \varepsilon^{ad} + \\
\frac{1}{4} (\partial n)_{cb} \cdot \varepsilon^{ad} - \frac{1}{4} \partial_{n} \cdot \varepsilon^{bd} - \\
\frac{1}{4} (\partial n)_{da} \cdot \varepsilon^{bc} - \frac{1}{4} (\partial n)_{ac} \cdot \varepsilon^{bd} + \frac{1}{4} (\partial n)_{ca} \cdot \varepsilon^{db} - \\
\frac{1}{4} \partial_{ad} \cdot \varepsilon^{bc} - \frac{1}{4} \partial_{bc} \cdot \varepsilon^{ad} - \frac{1}{4} \partial_{ad} \cdot \varepsilon^{bc} + \\
\frac{1}{3} \partial_{ab} \cdot \varepsilon^{cd} \left[ 0,0,0 \right] \end{array} \right\}, \]

The bracket is not ‘surfacial’, in the sense that the latter three entries vanish and the nonvanishing part of the bracket is a compact, covariant expression. If the latter three coefficients are nonvanishing however, explicit covariance in this expression will be lost, as we can see by modifying the previous example
In such ‘surficial’ cases the default output of \texttt{PoissonBracket[]} will not be helpful for visual inspection. To resolve this we can recall, again from [14], that (30) can be alternatively expressed as

\[
\int d^3x \{ A_{\mu}(x_1), B_{\nu}(x_2) \}_{\Sigma}(x_2) = \mathcal{J}_{\mu}(x_1) \mathcal{C}_{\nu}(x_1) + \mathcal{J}_{\nu}(x_1) \mathcal{C}_{\mu}(x_1) + \mathcal{J}_{\mu}(x_1) \mathcal{D}_{\nu}(x_1) + \mathcal{J}_{\nu}(x_1) \mathcal{D}_{\mu}(x_1).
\]  

(31)

The three-component \texttt{List} output corresponding to (31) can be produced by passing the option "Surficial" \texttt{→} True. Trying again with this option, we obtain

\[
\{v_{r \alpha \beta}, v_{\gamma \alpha \beta} \} = \frac{1}{2} \mathcal{L}_{\mu}(x_1) \mathcal{D}_{\nu}(x_1) + \frac{1}{2} \mathcal{L}_{\mu}(x_1) \mathcal{D}_{\nu}(x_1) + \frac{1}{2} \mathcal{L}_{\mu}(x_1) \mathcal{D}_{\nu}(x_1).
\]

We see that the result is indeed covariant, and fairly simple. We will come back to this ‘surficial’ case in Sect. 3.2, where we attempt to recover the historical results in [23,46].

2.5 High-level functions

As we mentioned in Sect. 2.4, much of the work done by \texttt{ToNesterForm[]} has to do with the imposition of the theory shell so as to simplify the argument. The particular shell used is not specifically that of primary vs secondary constraints, but it is restricted to the constraints of which we have prior knowledge from the literature, and does not include new constraints discovered in the course of a \texttt{HiGGS} session. In particular, we rely on the so-called if-constraint structure which was discovered by Blagojević and Nikolić in [61]. Depending on the Lagrangian parameters in (14), the number and type of primary constraints may be radically different: these contingent primaries are called primary if-constraints (PiC). There are similarly secondary (SiC) and tertiary (TiC) quantities, etc. Returning to [67], the PiCs of the theory (14) take the form

\[
\alpha_{\phi} \equiv \left( \frac{1}{J} \mathcal{A}_{\phi} + 2 \mathcal{A}_{\phi} \mathcal{M}_p \mathcal{T} - 8 \mathcal{A}_{\phi} \mathcal{M}_p \mathcal{T} \right) \mathcal{A}_{\phi} \mathcal{A}_{\phi} \mathcal{A}_{\phi} \mathcal{A}_{\phi} \mathcal{A}_{\phi} \mathcal{A}_{\phi}
\]

(32a)

\[
\alpha_{\psi} \equiv \left( \frac{1}{J} \mathcal{A}_{\psi} - 2 \mathcal{A}_{\psi} \mathcal{M}_p \mathcal{T} \right) \mathcal{A}_{\psi} \mathcal{A}_{\psi} \mathcal{A}_{\psi} \mathcal{A}_{\psi} \mathcal{A}_{\psi} \mathcal{A}_{\psi}
\]

(32b)

where we defined e.g. \( \mathcal{A}_{\phi} \equiv \sum_{\phi} M_{\phi} \mathcal{A}_{\phi} \), with the matrix \( M_{\phi} \mathcal{M}_p \mathcal{T} \) \( M_{\phi} \mathcal{M}_p \mathcal{T} \). In the handling of PiCs, it is extremely useful to refer to the functions

\[
\mu(x) = \begin{cases} x^{-1}, & \text{for } x \neq 0 \\ 0, & \text{for } x = 0. \end{cases}
\]

(33)

and we note that the PiC functions defined in Eqs. (32a) and (32b) are only constrained when \( \mu(x) = 1 \) or \( \mu(x) = 1 \). The structure of Eqs. (32a) and (32b) is quite useful in that it allows momenta to substituted for parallel field strengths. These substitutions are among those performed every time \texttt{ToNesterForm[]} is called, unless the option "ToShell" \texttt{→} False is passed as above in Sect. 2.4.

2.5.1 Module: ‘DefTheory’

In order to discover these PiCs, we must first set up the shell using \texttt{DefTheory}[]. Let us consider the simple example of Einstein–Cartan theory, i.e. the substantial restriction of (14) to the simple Einstein–Hilbert term

\[
L_G = -\frac{1}{2} \mathcal{A}_0 \mathcal{M}_p \mathcal{T}.
\]

(34)
We implement the theory (34) by passing to the DefTheory[] command the system of equations which deactivates all the \( \{ \hat{a}_A \}, \{ \hat{p}_E \}, \{ \bar{a}_A \}, \{ \hat{p}_E \} \), while leaving \( \hat{A}_0 \) untouched. We want to store our knowledge of the shell once it has been obtained, and so we pass the label "Export" to "EinsteinCartan", which will be used to construct a filename. The input is

```math
\begin{align*}
\text{In[1]:=} & \text{DefTheory[]} \{ \text{Alp1} == 0, \text{Alp2} == 0, \text{Alp3} == 0, \text{Alp4} == 0, \text{Alp5} == 0, \text{Alp6} == 0, \\
& \text{Bet1} == 0, \text{Bet2} == 0, \text{Bet3} == 0, \text{cAlp1} == 0, \text{cAlp2} == 0, \text{cAlp3} == 0, \text{cAlp4} == 0, \text{cAlp5} == 0, \text{cAlp6} == 0, \text{cBet1} == 0, \\
& \text{cBet2} == 0, \text{cBet3} == 0 \}, \text{"Export"} \rightarrow \text{"EinsteinCartan", \"Order\"} \rightarrow \text{Infinity};
\end{align*}
```

** DefTheory: Found the following primary if-constraints:

\[
\phi_\alpha \equiv \mathcal{J}^{-1} \hat{\pi}_\alpha = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_i \equiv \mathcal{J}^{-1} \hat{\pi}_i = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_m \equiv 3 \hat{a}_\alpha \mathcal{J}^{-1} \hat{\pi}_m = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

\[
\phi_{ij} \equiv \mathcal{J}^{-1} \hat{\pi}_{ij} = 0
\]

** DefTheory: Found the following secondary if-constraints:

** DefTheory: Found the following parallel if-constraints:

** DefTheory: Found the following singular if-constraints:

** DefTheory: The super–Hamiltonian is:

\[
\mathcal{H}_\pi = -\frac{\mathcal{J} \mathcal{J}^{-1} \hat{\pi} \mathcal{J}^{-1} \hat{\pi}}{2} = 0
\]

In the output above we can see the listing of the PiCs. It is clear from (34) and also from the form of the constraints in Eqs. (32a) and (32b), why we get this specific list. All the coefficients associated with the SO\(^+\)(1, 3) irreps of \( R_{ijkl} \) and \( T_{ijkl} \) are vanishing, and so all the PiCs functions become constraints. Moreover, these constraints are very simple in their form: they are all pure momenta, with the single exception being in the case of the \( 0^+ \) roton constraint, which contains a constant

\[
\varphi_\perp = 3 \hat{a}_0 m p^2 + \frac{1}{\mathcal{J} \hat{\pi}_\perp} \approx 0.
\]

Following this listing of the PiCs, there are references to perpendicular, parallel and singular SiCs, none of which are present in the Einstein–Cartan theory. We will return to these in Sect. 3.3, but for now we note that they follow from the imposition of multipliers in (14), and their presence is fully understood in [67], just as the presence of the PiCs of the basic Poincaré gauge theory is understood in [61,63]. This is the intended scope of DefTheory[]: to elucidate not only the primary constraints, but all of that part of the constraint structure which is already known from the literature. Every if-constraint identified by DefTheory[] is used during the DefTheory[] call in the construction of very large internal rule sets $StrengthPShellToStrengthPO3$, $PiPShellToPiPPO3$, $TheoryCDPiPToCDPiPO3$ and $TheoryPiPToPiPO3$. These rules are applied – by default – during ToNesterForm calls. Most of the if-constraints that can arise, as detailed in [67], are of the form \( \frac{1}{4} \hat{\pi}_\mu + \ldots \approx 0 \) or \( \frac{1}{4} \hat{\pi}_\mu + \ldots \approx 0 \), and so the shell is defined by replacing all possible instances of the momenta in favor of other quantities. There are also the ‘parallel’ SiCs, which deactivate irreps within the canonical parts of the field strength tensors in Eqs. (25a) and (25b) – these are straightforwardly implemented.

Following the listing of the if-constraints, the output above details the structure of the canonical Hamiltonian, which
from \cite{67} is written

\[ \mathcal{H}_C \equiv N \mathcal{H}_\perp + N^a \mathcal{H}_a - \frac{1}{2} A^{ij}_0 \mathcal{H}_{ij} + \partial_a \mathcal{P}^a. \]  

(36)

This Dirac form \cite{62,95} is useful because it expresses part of the Hamiltonian as a linear combination of the nonphysical fields \( N, N^a \) and \( A^{ij}_0 \). The physical (and canonical) coefficients of these undetermined fields are

\[ \mathcal{H}_\perp \equiv \hat{\pi}_i T^i_{\perp k} + \frac{1}{2} \hat{\pi}_{ij} R_{ij \perp k} - J L_G - n^k D_a \pi_k^a, \]  

(37a)

\[ \mathcal{H}_a \equiv \pi_i^β T^i_{αβ} + \frac{1}{2} \pi_{ij}^β R_{ij αβ} - b^k D_β \pi_k^β, \]  

(37b)

\[ \mathcal{H}_{ij} \equiv 2 \pi_i^a b_j{\alpha} + D_a \pi_{ij}^a, \]  

(37c)

and they form the ‘sure’ secondary FC constraints (sSFCs)

\[ \mathcal{H}_\perp \approx 0, \quad \mathcal{H}_a \approx 0, \quad \mathcal{H}_{ij} \approx 0. \]  

(38)

We see that these 10 constraints are divided up under SO(3) to give the final four entries in the output above, with \( \mathcal{H}_{ij} = \mathcal{H}_{ij \perp} + 2n_{[i} \mathcal{H}_{j \perp j]} \). The (linearised) values returned for \( \mathcal{H}_\perp \) and \( \mathcal{H}_a \) seem sensible in the context of the constraint in (35) – we can see from this that HiGGS has begun imposing the PiC shell. What about the angular super-momentum? Let us verify by hand that the answer is correct. The first term in (37c) vanishes on the PiC shell, because HiGGS has told us that \( \hat{\pi} \approx \hat{\pi}_{\perp \perp} \approx \hat{\pi}_{\perp k} \approx 0 \). For the second term, we find from (35) after a few lines that

\[ \pi_{kl}^β \approx -2\hat{\alpha}_0 m_p^2 J n_k h_t^l, \]  

(39)

from which we determine

\[ \mathcal{H}_{kl} \approx -2\hat{\alpha}_0 m_p^2 J \left[ h_{\alpha} (\hat{\alpha}_0 b_m{\alpha} n_k h_t^l) + D_a \left( n_k h_t^l \right) \right] \]

\[ = -2\hat{\alpha}_0 m_p^2 J \left( T_{k \perp l} + 2n_k T_{l} \right). \]  

(40)

These are indeed the \( 1^+ \) and \( 1^- \) parts of the torsion, as HiGGS is claiming.

\[ ^9 \text{Note that } \mathcal{P}^a \equiv b^a_0 \pi_i^a + \frac{1}{2} A^{ij}_0 \pi_{ij}^a. \]

2.5.2 Module: ‘StudyTheory’ and ‘Velocity’

The greater part of the analysis – i.e. that which is not necessarily encoded in the literature – is requested by means of the StudyTheory[] command. We will see in Sect. 2.6 that this command is just a high-level wrapper for parallelising Poisson matrices and constraint velocities, and also for DefTheory[] as discussed in Sect. 2.5.1. We will see how to use StudyTheory[] for a batch of theories in Sect. 2.3. For now we note that having called DefTheory[] above, we can pass the option "Import" → True to the command

\[ \text{In}[] := \text{JobsBatch} = \{("EinsteinCartan", \{Alp1 == 0, Alp2 == 0, Alp3 == 0, Alp4 == 0, Alp5 == 0, Alp6 == 0, Bet1 == 0, Bet2 == 0, Bet3 == 0, cAlp1 == 0, cAlp2 == 0, cAlp3 == 0, cAlp4 == 0, cAlp5 == 0, cAlp6 == 0, cBet1 == 0, cBet2 == 0, cBet3 == 0\}); \]

\[ \text{JobsBatch-\text{StudyTheory}-("Import" \Rightarrow True); \}

and – since the calculation is expensive – run it through a Wolfram Language package file. The evaluation of the Poisson matrix is fairly straightforward, and made up from calls to PoissonBracket[] as discussed in Sect. 2.4.3. It is better then to turn to Velocity[].

The linearised velocity of (e.g.) some PiC \( B \varphi \bar{c} \) is calculated using the formula

\[ B \varphi \bar{c}(x_1) = \int d^3 x_2 \left\{ B \varphi \bar{c}(x_1), \mathcal{H}_T(x_2) \right\}, \]  

(41)

where from (36) we need evaluate only the commutator with \( \mathcal{H}_\perp \), which is re-expressed in \cite{67} on the PiC shell as

\[ \mathcal{H}_\perp \equiv \frac{1}{64} \sum_A c_A^\mu (\hat{\alpha}_A^{\perp l}) \varphi_{\perp l} A^\varphi \bar{c}^\mu \]

\[ + \frac{1}{16m_p^2} \sum_E c_E^\mu (\hat{\alpha}_E^{\perp l}) E^\varphi \bar{c}^\mu \bar{e}^\varphi + \frac{1}{2} \hat{\alpha}_0 m_p^2 R \]

\[ - \sum_I \left( \alpha_I \hat{R}_{l}^{ij} + \alpha_I \hat{\lambda}_{l}^{ij} \right) \left( \hat{A}_{ij}^{\perp l} \right)^T \left( \hat{R}_{nm}^{\perp} \right)^{\perp} + \hat{\lambda}_M \hat{T}_{l}^{ij} \left( \hat{M}_{ijkl}^{\perp} \right)^T \left( \hat{R}_{nm}^{\perp} \right)^{\perp} \]

\[ - n^k D_a \pi_k^a. \]  

(42)

A particular problem now is that (42) has a quadratic structure. If we apply PoissonBracket[] to evaluate a velocity for some PiC \( B \varphi \bar{c}, \mathcal{H}_\perp \), we will actually be calling ToBasicForm[] directly on \( \mathcal{H}_\perp \). This will generally result in a very expensive computation, which we avoid in Velocity[] by manually applying the Leibniz rule. Accordingly in the HiGGS source there is a collection of prepared formulae for generic expressions such as
which collectively act as a template for each velocity. For each SO(3) index $A$ shown in the sum in the second equality in (43), we need the four portions of a single Poisson bracket, as given in (30) and returned as a List by a call to PoissonBracket[]. Accordingly, the whole of (42) is broken into blocks, each of four terms, which follow from a single bracket, and these are evaluated in parallel as discussed in Sect. 2.6.

As we mentioned in Sect. 2.4.3, the formula (30) is not explicitly covariant, and hence the appearance in (43) of partial derivatives. Ultimately, a call to ToNesterForm[] is needed to restore explicit covariance to the quadratic expression (43). This setup is not so good: the use of block formulae restricts us to calculating velocities over the given $\mathcal{H}_\perp$ – it is also susceptible to human error, and concludes with an expensive simplification process. We propose that any future iterations of HIGGS implement velocities based on two extensions to PoissonBracket[]:

1. The operands should be expressed as sums of products of covariant quantities, and the Leibniz rule be used to distribute the operation.
2. The operation should return the covariant form given in (31), so that covariance is maintained at all steps.

An improvement of PoissonBracket[] along these lines should be straightforward to implement, and would also be equally emenable to parallelisation: we defer its development to future work.

2.5.3 Module: ‘ViewTheory’

The final module ViewTheory[] is used to produce a human-readable summary of the results from StudyTheory[]. Since we already have a summary of the literature constraint structure from the DefTheory[] call in Sect. 2.5.1, we pass for brevity our earlier theory name with the option "Literature" -> False, producing

```mathematica
In[1]:= ViewTheory["EinsteinCartanVelocities", "Literature" -> False];

** DefTheory: Incorporating the binary at svy/EinsteinCartanVelocities.thr.mx
```

We see how the results are stored in the theory binary at svy/EinsteinCartan.thr.mx. There are four non-vanishing Poisson brackets, all between the translational and rotational pairs of the same SO(3) irrep, $\psi$ vs $\psi_\perp$, $\hat{\psi}_\perp$ vs $\psi_\perp$, $\hat{\psi}_\perp$ vs $\hat{\psi}_\perp$, and $\phi_\perp$ vs $\phi_\perp$. These are the conjugate pairs, whose commutators are proportional to mass parameters in the theory [61] – here mediated by the Einstein–Hilbert term $\hat{\alpha}_0$. The involved PICs are second class (SC).

What about the remaining PICs $\hat{\psi}_\perp$ vs $\hat{\psi}_\perp$? These 0$^-$ and 2$^-$ irreps$^{10}$ are not represented in the translational sector. Previous analyses tell us that their relevant commutators will be with their own secondaries [61]. Accordingly, we turn to the velocities, which are also provided in the above

$^{10}$ Note that the velocity of $\hat{\psi}_\perp$ is not simplified: HIGGS inherits this inability from xAct, as no efficient algorithm is known for simplifying multi-term symmetries [74] such as that of the 2$^-$ sector.

```mathematica
{\{\varphi_\perp, \varphi_\perp\} = \{-\frac{2}{3} \hat{\alpha}_0 \varphi_\perp, \frac{1}{3} \hat{\alpha}_0 \varphi_\perp\}}
```

```mathematica
{\{\varphi_\perp, \varphi_\perp\} = \{-\frac{2}{3} \hat{\alpha}_0 \varphi_\perp, \frac{1}{3} \hat{\alpha}_0 \varphi_\perp\}}
```
output. Unlike the if-constraints, the linearised sSFC Hamiltonian constraints are not automatically implemented when \(\text{"ToShell"} \rightarrow \text{True} \) is passed: we therefore note that since \(R^5 \approx T^i_j \approx 0\), from the output of \text{DefTheory[]} above, both rotational and translational (Hamiltonian) multipliers for the \(0^+\) and \(1^-\) sectors will also vanish at linear order. The same is true of the translational \(1^+\) and \(2^+\) Hamiltonian multipliers, but the rotational counterparts will be linearly proportional to \(R^5 \) and \(T^i_j \). Returning to the ‘lonely’ \(0^+\) and \(2^-\) sectors, we can go right ahead and calculate the expected brackets mentioned above. We first find

\[
\{\phi_n, \phi_T\} = \{0, 0, 0\}
\]

As expected, this commutator survives at linear order: one could determine also the \(0^-\) multiplier, but it is enough to notice that both \(\tilde{T}^i_j\) and its linearised secondary \(\tilde{\chi}^{(b)}\) are SC. Moving on, we find

\[
\{\phi_{ijkm}, \phi_{lmn}\} = \\
\begin{bmatrix}
-3 \phi^l_{in} \phi^m_{jk} \phi^k_{il} + 3 \phi^m_{in} \phi^k_{jl} \phi^l_{jk} - 3 \phi^k_{in} \phi^l_{jm} \phi^m_{jl} + 3 \phi^l_{jm} \phi^m_{il} \phi^k_{jm} - 3 \phi^m_{il} \phi^k_{jm} \phi^l_{jm} + 8 \phi^k_{jm} \phi^l_{jm} \\
16 \frac{\tilde{T}^i_j}{j} - 16 \frac{\tilde{T}^i_j}{j} \\
9 \phi^l_{jm} \phi^m_{ij} + 9 \phi^m_{in} \phi^k_{ij} \phi^l_{jm} + 9 \phi^k_{in} \phi^l_{jm} \phi^m_{ij} - 8 \phi^k_{jm} \phi^l_{jm} \\
32 \frac{\tilde{T}^i_j}{j} - 32 \frac{\tilde{T}^i_j}{j} \\
32 \frac{\tilde{T}^i_j}{j} - 32 \frac{\tilde{T}^i_j}{j} \\
0, 0, 0
\end{bmatrix}
\]

The same, then, is true of \(\tilde{T}^i_j\) and its linearised secondary \(\tilde{\chi}^{(b)}\), and so the algorithm terminates.

What can HiGGS tell us about the physics of Einstein–Cartan theory? The PGT contains \(2 \times (24 + 16) = 80\) naive d.o.fs in its gauge fields. The non-physicality of the lapse and shift (the Poincaré gauge symmetry), remove \(2 \times 10\) d.o.fs through the sure, primary (sPFC) constraints; a further \(20\) d.o.f are removed via the sSFCs. We further learn from HiGGS about the number and class (all SC) of the if-

\footnote{The \((b)\) symbol denotes linearisation near Minkowski spacetime.}

constraints. The final d.o.f count is thus

\[
\frac{1}{2}(80 - 2 \times 10 - 2 \times 10)
\]

\(- (1 + 1 + 3 + 3 + 3 + 3 + 5 + 5)
\]

\(- (1 + 1 + 5 + 5)) = 2,
\]

i.e. the massless graviton.

2.6 Parallelisation and HPC

The current version of HiGGS is not only designed for the local or desktop operations conducted in Sects. 2.1–2.5. The intended use is the evaluation of quantities useful to the Hamiltonian analysis, in an environment where multiple parallel kernels are available. As mentioned in Sect. 1, there are
some generic features of the Hamiltonian analysis which lend themselves very well to parallelisation.

Naïvely, we notice that once the primary constraints have been identified, the resulting constraint chains (i.e. the recursive consistency conditions of each primary) can notionally be evaluated in parallel. This seems a natural route down which to parallelise, but in reality chains might seem to continue indefinitely in a kernel with knowledge only of the primary constraint shell. Velocities are the most expensive quantities, and so it seems prudent to pause after each is calculated, to see if the corresponding acceleration is strictly necessary. However, when we parallelise over chains we also find that the velocities, accelerations and jerks rapidly desynchronise: this is to be expected given the varying complexities of the SO(3) irreps which underlie each chain. Accordingly, pre-velocity checks would require e.g. a centralised knowledge of the complete shell to be kept on the master kernel, to which sub-kernels could refer as needed. We could even imagine a setup where one sub-kernel is interrupted in mid-evaluation on the basis of a report from another.

While it is tempting to develop something sophisticated along these lines, the route turns out not to be practical. In practice, the number of chains is typically very few per theory (and strictly not more than ten in the case of the Poincaré gauge theory without multipliers). The desynchronisation effect is then so severe that most kernels would sit idle whilst waiting for the highest-spin chain to complete. More importantly, the question of whether chain A need continue based on a new constraint from chain B, is not a trivial problem in computer algebra. In the case of the PiCs, each constraint has as one term a unique part of the momentum: as mentioned in Sect. 2.5.1 this lends itself to a replacement rule which reliably implements the PiC shell, but in more general cases it is less clear how to proceed.

Ultimately, the experience of [23,46] suggests that evaluation of the accelerations is not usually necessary anyway. Once the brackets between the PiCs are known, it is often possible to determine from a visual inspection whether any chains are worth continuing. Velocities are expensive because they are less easy for computers to use. Once covariantised however, such constraints often comprise straightforward tensor equations which humans can readily manipulate. This suggests a pragmatical division of labour in which HiGGS returns an organised structure of covariantised brackets – formerly the primary Poisson matrix (PPM) [13,14,23] – and velocities for human inspection. If velocities are expensive because they require multiple brackets, we can break them up accordingly, along with the quadratic covariantisation steps: in this way we can reduce chain desynchronisation.

The final structure of a HiGGS survey is as follows;

1. A list of theories is passed to StudyTheory[] in the master kernel. This function runs DefTheory[], for each theory, in its own parallel sub-kernel. The literature knowledge of the constraint shell of each theory is cached as a binary.

2. Within the same StudyTheory[] call, the master kernel imports the shells and prepares a combined List of brackets which need to be evaluated for the Poisson matrices. The List elements are delegated to all available parallel sub-kernels – as many of which are launched as necessary. Brackets are transferred to the next available sub-kernel using the Wolfram Symbolic Transfer Protocol (WSTP). The WSTP overhead is marginal, since each sub-kernel only needs to transfer data after its PoissonBracket[] call.\(^{12}\)

3. Within the same StudyTheory[] call, the master kernel decomposes each linearised velocity into blocks dependent on a single bracket. For the velocity of some PiC \(B \varphi \), the blocks are;

\[
\begin{align*}
\{ B \varphi \}, & \quad \forall A : \nu(\hat{\alpha}^{\perp \perp}) = 1, \\
\{ B \varphi \}, & \quad \forall E : \nu(\hat{\beta}^{\perp \perp}) = 1, \\
\{ B \varphi, R \}, & \quad \{ B \varphi, T \}, \\
\{ B \varphi, J \}, & \quad \{ B \varphi, -n^k D_a \varphi \}. 
\end{align*}
\]

\(^{12}\) The use of Print[] for debugging and development purposes means that this is not strictly true, and there is also an overhead from the system timing wrappers which we use to produce plots. These features are not actually needed when running a survey.
The blocks are delegated to the sub-kernels again using WSTP. After the PoissonBracket[] call, each sub-kernel pre-processes its block using ToNesterForm[] before passing the result back to the master kernel.

4. Within the same StudyTheory[] call the blocks are recombined into velocities, and all results are cached in a final binary.

We illustrate this process in Fig. 2. In the parallel HiGGS environment of any node, one has at any one time a collection of theories, each of which has associated with it a complex and growing structure of constraints and commutators. This environment suggests an object-oriented approach. While Mathematica allows for object-oriented programming using e.g. Association[] (see also [96]), the scope of HiGGS is simple enough that we can retain a procedural approach. In fact, the shell structure of any one theory is referenced fairly infrequently, matching the rate of PoissonBracket[] calls. This means that while WSTP is necessary for the scheduling of evaluations, the information needed to switch between theories within a sub-kernel can be sourced by using relay system of binary files. Consequently, very minimal use is made by HiGGS of DistributeDefinitions[] to transfer theory-specific data between kernels. In a more serious implementation of the Dirac–Bergmann algorithm, we would envisage more extensive use of WSTP and the object-oriented approach.

How efficient is the above approach? Pending an implementation of the Leibniz rule, the efficacy of Fig. 2 as it applies to the whole constraint algorithm is hard to gauge. The full run is only implemented in Sect. 3.2 for a handful of previously studied theories (without multipliers). Averaged over those cases, and for the non-fundamental reasons outlined above, a minority of the Velocity[] calls contain serial tasks which turn out to dominate the workload. The truly parallel fraction of the workload (including the initial evaluation of all constraint brackets) is then as low as $\frac{1}{1 - p + \frac{p}{n}}$, most of which is devoted to the calculation of Poisson brackets, there is a clear benefit from parallelisation.

3 Examples

Having introduced the implementation in Sect. 2, we now give some basic examples. These will include a reproduction of the analysis in [23,46] and a simple HPC survey which extends those same ‘minimal’ theories with the use of multipliers.

3.1 Preparing a science session

To prepare a science session, we begin by loading the package into a fresh Mathematica kernel

\[
\text{In}[] := \text{<<xAct'HiGGS';}
\]

If the HiGGS sources have been correctly placed with respect to the xAct directory tree, a copyright greeter should be displayed, indicating that the context xAct‘HiGGS’ and its dependency contexts xAct‘xTensor’, xAct‘xPerm’, xAct‘xCore’, xAct‘xTras’ have been loaded.

However, loading the package does not yet introduce the physics: the kernel is still in a fresh xAct session, without even a differential manifold. To construct the very many physical definitions needed for science we must build the package using the command

\[
\text{In}[] := \text{BuildHiGGS[];}
\]

This begins an execution in xAct‘HiGGS’Private’ of xAct/HiGGS/HiGGS_sources.m, most of which is taken up with symbol definitions, and in particular calls to DefTensor[] and MakeRule[]. To shorten the process, the most expensive definitions (including those for SO$^+(1,3)$ projection operators) have been stored in binary files under xAct/HiGGS/bin/build/*.mx – those binaries are

---

13 See however an xAct implementation of the 3 + 1 Baumgarte–Shapiro–Shibata–Nakamura (BSSN) formulation of the bimetric gravity field equations [98].
imported at this time\textsuperscript{14}. In an active front end, the output cells displaying the progress of this build process are periodically deleted, and should finally be replaced by the following message (adjusting for memory).

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
CPU per node $n$ & Wallclock time $\langle t(n) \rangle /s$ & Speedup $S(n)$ & Efficiency $5 \times S(n)/n$ \\
\hline
32 & 550 ± 100 & 2.97 ± 85 & 0.46 ± 13 \\
28 & 565 ± 68 & 2.88 ± 92 & 0.51 ± 13 \\
24 & 590 ± 100 & 2.73 ± 76 & 0.57 ± 16 \\
20 & 640 ± 120 & 2.53 ± 73 & 0.63 ± 18 \\
16 & 720 ± 160 & 2.26 ± 71 & 0.71 ± 22 \\
12 & 835 ± 81 & 1.95 ± 46 & 0.81 ± 19 \\
8 & 1110 ± 310 & 1.46 ± 52 & 0.91 ± 32 \\
\hline
\end{tabular}
\caption{Approximate benchmarks for parallel brackets. The spin-parity $1^+$ theory in (49) is augmented with all configurations of the multipliers $\{\hat{\alpha}, \hat{\alpha}_4, \hat{\alpha}_6, \hat{\beta}_1, \hat{\beta}_3\}$ – see (14) – and all the Poisson brackets are obtained. Either four or five theories are allocated per node, wall-clock time $\langle t(n) \rangle$ is averaged over all 14 nodes, but apparent $\sigma$ remains uniformly high (i.e. suspicious) due to a paucity of expensive brackets. For survey structure and specifications of the Peta4 cluster, see Sect. 3.3}
\end{table}

\textit{Out$\{\}$:= ** BuildHiGGS: The HiGGS environment is now ready to use and is occupying 63184600 bytes in RAM.}

The context \texttt{xAct\ '/HiGGS'} should now be populated with many physical quantities, and as a result the session alone is very memory-intensive. We can view some of these quantities through the \texttt{xAct} variables \texttt{\$Tensors} and \texttt{\$ConstantSymbols}. From this point we may perform the various operations in Sect. 2, or proceed directly to science.

3.2 Yo–Nester unit tests

As a first application, and to verify that HiGGS has been correctly calibrated, we recapitulate the historical analysis in [23,46].

The theory in which the $0^+$ mode is active, as considered in [46], is given by imposing the following constraints on (14)

$$\hat{\alpha}_1 = \hat{\alpha}_2 = \hat{\alpha}_3 = \hat{\alpha}_4 = \hat{\alpha}_5 = 2\hat{\beta}_1 + \hat{\beta}_2 = \hat{\beta}_1 + 2\hat{\beta}_3 = 0, \quad \hat{\alpha}_6 \neq 0, \quad \hat{\alpha}_0 \neq 0.$$  \hfill (47)

All the constraint couplings $\{\sqrt{I}\}$ and $\{\bar{\beta}_M\}$ are of course assumed to vanish, since they are only recently proposed in [14,67]. No other ‘simple’ linear identities are assumed among the couplings, and this avoids collision with other theories. The other theory in [46], in which the $0^-$ mode is instead allowed to propagate, is defined by

$$\hat{\alpha}_1 = \hat{\alpha}_2 = \hat{\alpha}_4 = \hat{\alpha}_5 = \hat{\alpha}_6 = 2\hat{\beta}_1 + \hat{\beta}_2 = \hat{\beta}_1 + 2\hat{\beta}_3 = 0.$$  \hfill (48)

In [23] the analysis was extended to ‘higher-spin’ modes. The theory with only the $1^+$ mode propagating is

$$\hat{\alpha}_1 = \hat{\alpha}_2 = \hat{\alpha}_3 = \hat{\alpha}_4 = \hat{\alpha}_6 = \hat{\beta}_1 = \hat{\beta}_2 = 0, \quad \hat{\alpha}_0 \neq 0, \quad \hat{\alpha}_3 = 0, \quad \hat{\beta}_3 \neq 0.$$  \hfill (49)

The theory with only the $1^-$ mode propagating is

$$\hat{\alpha}_1 = \hat{\alpha}_2 = \hat{\alpha}_3 = \hat{\alpha}_4 = \hat{\alpha}_6 = \hat{\beta}_1 = \hat{\beta}_2 = 0, \quad \hat{\alpha}_0 \neq 0, \quad \hat{\alpha}_5 \neq 0, \quad \hat{\beta}_2 \neq 0.$$  \hfill (50)

and the theory with only the $2^-$ mode propagating is

$$\hat{\alpha}_2 = \hat{\alpha}_3 = \hat{\alpha}_4 = \hat{\alpha}_5 = \hat{\alpha}_6 = \hat{\beta}_1 = \hat{\beta}_2 = \hat{\beta}_3 = 0, \quad \hat{\alpha}_0 \neq 0, \quad \hat{\alpha}_1 \neq 0.$$  \hfill (51)

There is also tested in [23] a pair of more complex theories in which the $0^-$ and $2^-$ modes are both active at the same time. These are given respectively by

$$\hat{\alpha}_1 = \hat{\alpha}_3 = \hat{\alpha}_4 = \hat{\alpha}_5 = \hat{\alpha}_6 = \hat{\beta}_1 = \hat{\beta}_2 = \hat{\beta}_3 = 0, \quad \hat{\alpha}_0 \neq 0, \quad \hat{\alpha}_2 < 0.$$  \hfill (52)

and

$$\hat{\alpha}_2 = \hat{\alpha}_4 = \hat{\alpha}_5 = \hat{\alpha}_6 = \hat{\beta}_1 = \hat{\beta}_2 = \hat{\beta}_3 = 0, \quad \hat{\alpha}_0 \neq 0.$$  \hfill (53)

The seven configurations Eqs. (47)–(53) can of course be processed in parallel. We set up a list called \texttt{JobsBatch}, which stores the coupling conditions and assigns a string label to each theory.

\begin{verbatim}
In[]:= jobsBatch={};
In[]:= jobsBatch=AppendTo{"spin_0p", {Alp1 == 0, Alp2 == 0, Alp3 == 0, Alp4 == 0, Alp5 == 0, 2Bet1 + Bet2 == 0, Bet1 + 2 Bet3
\end{verbatim}

\textsuperscript{14} Note that the HiGGS binaries were compiled on a 64-bit machine: they can, if needed, be recompiled on alternative architecture via minor changes to the source as indicated in \texttt{xAct/HiGGS/HiGGS.nb}.**
constraint chain.

created to store a summary of our prior knowledge of each

129 GB memory and eight available 2

perform the run on a dedicated data processing server with

ries such as bina-

The option "Import" → True assumes that DefTheory[] has already been run on all seven cases. In that case binaries such as svy/spin_0p.thr.mx etc., will have been created to store a summary of our prior knowledge of each constraint chain.

Even in the case of the small batch in JobsBatch, the calculation is barely viable using sub-HPC resources. We perform the run on a dedicated data processing server with 129 GB memory and eight available 2.90 GHz Intel® Xeon® E5-2690 0 CPU cores, corresponding to a maximum of eight parallel Mathematica kernels. This computation lasts ~14h, but as mentioned in Sect. 2.6 almost all of this time is spent on the inefficient evaluation of velocities.

Once the calculations of the StudyTheory[] call are complete, we recall from Sect. 2.5.3 that the results are displayed in human-readable form via the ViewTheory[] command. We will not provide full analysis here, but focus on the exemplar 1+ case. Skipping the breakdown of PiCs and neglecting the velocities, all the nonlinear brackets are

In[] := JobsBatch~StudyTheory~("Import" -> True);

This information (which by itself is obtained within the first minutes of the StudyTheory[] run) encodes the whole nonlinear primary Poisson matrix (PPM) of the theory: it may be compared with the expressions carefully obtained in [23]. We see that the brackets \( \{ \psi_{ij}^{+}, \psi_{k}^{+} \} \), \( \{ \psi_{ij}^{+}, \psi_{k}^{+} \} \), \( \{ \psi_{ij}^{+}, \psi_{k}^{+} \} \), \( \{ \psi_{ij}^{+}, \psi_{k}^{+} \} \), \( \{ \psi_{ij}^{+}, \psi_{k}^{+} \} \) and \( \{ \psi_{ij}^{+}, \psi_{k}^{+} \} \) are strictly nonlinear: they vanish in the linear theory for which the 1+ mode is moving. The effect of this discontinuity in the constraint structure, when moving from the linear to the nonlinear theory, is well described in [23].
that the three extra d.o.f of the massive $1^\perp$ mode are nonlinearly activated: HiGGS thus tells us that a vector torsion mode is strongly coupled.

The results of the remaining cases in JobsBatch are provided in the supplemental materials [75]. We find that, up to terms which vanish due to multi-term symmetries (i.e. which cannot be eliminated in the xAct architecture), the nonlinear brackets agree with those found in [23,46]. There is a possible exception in the case of the general bracket $[\hat{\phi}_{ij}, \dot{\phi}_{ij}]$, which we find to be ‘surficial’ in ways illustrated already by the bracket in Sect. 2.4.3. This subtlety appears only to touch the scalar mode results in [46]; it seems worthwhile to investigate – in future work – if and how this might affect the final d.o.f counting. For brevity we will omit the velocities here, since even the covariantised, linear expressions can still be very cumbersome. Examples are provided in Sect. 1 for the minimal $1^+$ case above: these illustrate how gradients of the field strengths can arise as the algorithm progresses, necessitating a future extension of HiGGS to the second-order Euler–Lagrange formalism.

3.3 Simple HPC survey

The purpose of this section is to further extend our knowledge of the theories examined in Sect. 3.2, by running HiGGS on basic HPC resources, so as to chart the effects of introducing multiplier fields. The findings of this survey, and any viable multiplier configurations, will be presented in future work. The starting point will be the ‘minimal’ Poincaré gauge theories set out in Eqs. (47)–(53). Of these, we know that (47) and (48) are the traditional cases in which massive $0^+$ and $0^-$ scalars propagate safely alongside the usual $2^+$ graviton. Of the cases with active higher-spin modes, we know that (52) and (53) propagate both $0^-$ and $2^-$ modes, and may be safe.

The minimal ‘problem’ cases are Eqs. (49)–(51). These are ostensibly simple linearised theories which propagate extra $1^+$, $1^-$ and $2^-$ modes respectively, but which appear to suffer from mode activation in the fully nonlinear regime. This mode activation is identified by counting the canonical degrees of freedom in the Hamiltonian analysis: its association with a particular $J^P$ sector is not shown explicitly, but inferred by examining the unconstrained PiC functions in each case. These are as follows;

- In the minimal $1^+$ theory (49), $\dot{\hat{\phi}}_{ij}$, $\dot{\phi}_{ij}^\perp$ and $\tilde{\phi}$ are unconstrained, the $1^+$ mode is thought to be activated.
- In the minimal $1^-$ theory (50), $\varphi$, $\varphi^\perp$ and $\varphi_{jk}^\perp$ are unconstrained, the $1^-$ mode is thought to be activated.
- In the minimal $2^-$ theory (51), $\psi_{ij}^\perp$ and $\psi_{ijk}$ are unconstrained, the $2^-$ mode is thought to be activated.

In [67] a potential avenue was outlined for preventing mode activation by means of the multiplier fields set out in (14). For any conventional Poincaré gauge theory, there are $2^6 \times 3^2 = 1536$ possible multiplier configurations. Any pair of configurations differs, if not by the constrained $J^P$ sectors, then by the ‘singular’ or ‘parallel’ nature of a constrained sector. These differences may have quite unpredictable consequences in the analysis. In order to efficiently explore the space of multiplier configurations, it is therefore important to have all the commutators between the known constraints to hand.

3.3.1 Scope of survey

By adding various multipliers, there are $3 \times 2^6 \times 3^2 = 1536$ separate theories which can be constructed from the minimal PGTs. However, some of these can be ruled out immediately on phenomenological grounds. In [67] we focussed on the modification of (49) by allowing $\tilde{\beta}_i \neq 0$. In the Lagrangian picture, this maps to a pair of constraints on the $1^-$ part of the torsion tensor, suppressing velocities or equating them to gradients. The main phenomenological constraint on the minimal extensions is the requirement that they contain the Einstein–Cartan dynamics, for which the gravitational field still is described by the Riemann–Cartan curvature. For this reason, we suspect that it will generally be safer to impose the $\{\tilde{\beta}_M\}$ than the $\{\tilde{\alpha}_i\}$.

How dangerous is it to suppress parts of the rotational sector? To get an idea, we consider the two d.o.fs in Einstein–Cartan gravity might be manifest in a gravitational wave-type solution. Rather than studying the Einstein–Cartan waves directly, we instead introduce novel solutions to the special (purely quadratic, i.e. $\hat{\phi}_0 = 0$) PGT from [13,14,80,81] which describe null pp–waves on the Minkowski background [99]. The wave solutions are formulated in the Brinkmann gauge, rather than the more popular transverse-traceless (TT) setup [100]. To introduce the Brinkmann gauge we start with a Cartesian coordinate system, and the rotation gauge is first chosen as in the HiGGS environment, so that the local Lorentz and coordinate bases are aligned. We then define ‘perpendicular’ and ‘null’ vectors as

15 The few velocities which are known from [46] corroborate our results, however we note that ToNesterForm[] actually fails to fully covariantise the velocity of $\varphi_{ij}$ in the simple $0^+$ case. This ‘bug’ is not known to occur elsewhere, and certainly not during the evaluation of nonlinear brackets: the main feature of HiGGS. We suggest that a fully nonlinear ‘Leibniz rule’ implementation of velocities, as recommended above, would greatly reduce the risk of such effects by demanding less of ToNesterForm[] in each call.

16 The uncertainty in these cases is based on the fact that the rank of the PPM may still change on non-Minkowskian surfaces in the phase space. As mentioned in Sect. 1, whether this is actually a physical problem should be determined by closer analysis.
encounter the Lagrangian constraints
\[ e_1 \equiv \hat{e}_0, \quad e_x \equiv \hat{e}_1, \quad e_y \equiv \hat{e}_2, \quad e_z \equiv \hat{e}_3, \]
\[ e_{\perp} \equiv \cos(\theta)e_x + \sin(\theta)e_y, \quad e_{\pm} \equiv e_i + e_j. \quad (54) \]

We will denote the ‘wave coordinate’ as \( \tau \equiv t - z \); the wave amplitude is taken in all solutions to be a smooth and compact scalar function \( A \equiv A(\tau) \). The Brinkmann gauge is complementary to the TT gauge in the sense that it confines waves to the time and longitudinal components of the metric perturbation. The wave will therefore alter the definition of the unit timelike vector \( n^i \), which defines the foliation, and unit spacelike vector \( l_i \), which defines the direction of travel, but not the polarisation vector \( e_{\perp} \). Restricting to the case of weak waves, we will then have \( n_i \equiv h_i^0/\sqrt{|g|^{00}} = (e^i)_0 + O(A), l_i \equiv h_i^j/\sqrt{|g|^{jj}} = (e^i)_j + O(A) \) and \( e_{\perp} \equiv \cos(\theta)(e^i)_j + \sin(\theta)(e^j)_i. \) While the Brinkmann gauge is opposed to the TT gauge at the level of the metric, this turns out to be somewhat reversed at the level of the field strengths. Accordingly, it is useful to define the ‘TT symmetric-traceless’ operation on the indices of a general TT tensor \( X_{ij} \) as \( X_{ij}^{(TT)} \equiv X_{ij} - \frac{1}{2} \epsilon^{i0k} \eta_{lj} + \frac{1}{2} \epsilon^{j0k} \eta_{lk} \), where we recall the original ‘symmetric-traceless’ operator \( X_{ij}^{(ST)} \equiv X_{ij} - \frac{1}{2} \epsilon^{i0k} \eta_{lj} \) from [13].

The new exact solution which concerns us describes a wave in the Riemann–Cartan curvature, with vanishing torsion and two d.o.fs quantified by a polarisation vector. It has the components
\[ R_{(ij)} = A \epsilon^{(ij)} + O(A^2), \quad (55) \]
\[ R_{(ij)\perp} = A \epsilon^{(ij)} + O(A^2), \quad (56) \]
\[ T R_{(ij)\perp} = A \epsilon^{(ij)} l_j + O(A^2), \quad (57) \]
\[ T R_{(ij)\perp} = -A \epsilon^{(ij)} l_j + O(A^2). \quad (58) \]

These components turn out to be identical [99] to those of the Riemann tensor in the presence of the vacuum pp-waves known from GR. Recall that Eqs. (49)–(51) were initially set up as a modifications of Einstein–Cartan theory. Since the Einstein–Cartan theory differs from GR only by a contact torsion interaction, and since the linear 1+, 1− and 2+ modes are massive, it would seem strange if the the null pp-wave solution Eqs. (55)–(58) is not also mandatory in the minimal extensions. Referring back to [67], we find that we should then always take \( 1 \equiv 0 \), since we would otherwise encounter the Lagrangian constraints
\[ 1 \neq 0 \Rightarrow R_{(ij)} + R_{(ij)\perp} \approx T R_{(ij)\perp} - T R_{(ij)\perp} \approx 0, \quad (59) \]

which both force the wave amplitude \( A \rightarrow 0 \). This already halves the volume of our parameter space, and so we make no attempt exhaustively determine the various other phenomenological constraints.

Other limitations on the allowed multipliers come from the linearised particle spectrum. For the 1+ theory with \( \tilde{a}_0 = 0 \) only the group \( \tilde{a}_0, \tilde{a}_1, \tilde{a}_2, \tilde{a}_3, \beta_1, \beta_2, \beta_3 \) does not immediately constrain \( \tilde{\chi}_{+} \). Similarly for the 1− theory the space is \( \{ \tilde{a}_2, \tilde{a}_3, \tilde{a}_6, \tilde{\beta}_1, \tilde{\beta}_2, \tilde{\beta}_3 \} \). For the 2− theory, we consider the group \( \{ \tilde{a}_3, \tilde{a}_5, \tilde{a}_6, \tilde{\beta}_1, \tilde{\beta}_2, \tilde{\beta}_3 \} \). Rightly, we ought to allow \( \tilde{a}_4 \neq 0 \) in this case, especially since the momentum \( \tilde{P}_{\perp} \) of the (anticipated) strongly coupled 2+ mode would then be disabled: just for this initial survey, however, the complexity of the 2− calculations is such that restricting to \( \tilde{a}_4 = 0 \) results in a significant economy.

The aim is then to obtain covariant expressions for all the possible commutators among all known if-constants for all \( 3 \times 3 \times 3 = 192 \) theories stipulated above. The current HiGGS setup is supposed to be able to do this, and produce binaries of the results suitable for use in a database. The requisite calculations would take years on a single desktop computer core, so we distribute them over 14 nodes of the Peta4 supercomputer – the CPU cluster component of the heterogeneous CSD3 facility. Each node has two 2.60GHz Intel® Xeon® Skylake 6142 CPUs, each having 16 cores with 6GB of memory apiece, amounting to 448 processors. As described in Sect. 2.6, HiGGS runs on a master kernel within each node. The master kernel delegates the analysis of a (randomly allocated) batch of theories, and has a total of 32 parallel sub-kernels at its disposal.

The node count of 14 is a service-level restriction on Peta4 rather than limitation of the implementation. We can see from a visual inspection that not all theories are equally expensive: some multiplier configurations engender more constraints and more brackets, while others more heavily involve the higher-spin sectors. An examination of the stack trace from each node suggests that the most time-consuming cases are those for which a multiplier is used to constrain a J+ sector which was thought to be nonlinearly activated. This is an interesting observation in the context of the strong coupling considerations. In particular, delays occur when new ‘parallel’ or ‘singular’ SiCs of the form
\[ A \chi^\parallel_{\nu} \equiv A \bar{P}_{\nu m} \bar{\mu} R_{nm} \bar{\mu} \approx 0, \quad (60) \]
\[ E \chi^\parallel_{\nu} \equiv m_\nu 2 E \bar{P}_{\nu m} \bar{\tau} R_{nm} \bar{\tau} \approx 0, \quad (61) \]
\[ A \chi^\pm_{\nu} \equiv A \bar{\nu} \frac{8 A A_{\nu}}{\bar{\alpha} A} \bar{\alpha}_{\nu} \bar{\alpha} A \bar{\mu} \bar{\nu} R_{jk} \bar{\tau} \approx 0, \quad (62) \]
\[ E \chi^\pm_{\nu} \equiv E \bar{\nu} \frac{4 B E}{\bar{B} E} \bar{\mu} \bar{\nu} \approx m_\nu 2 E \bar{P}_{\nu m} \bar{\tau} R_{nm} \bar{\tau} \approx 0, \quad (63) \]
are introduced. It is known from manual calculations in [14] that these secondaries (specifically their field strength terms) fail to commute with many other constraints, and can produce brackets of surprising complexity.

Physics binaries (HiGGS extension *.thr*.mx files) of all nonlinear brackets identified in this survey, along with plaintext stack traces and clocking times, can be found in the supplemental materials [75].

3.3.2 Results and prospects for new physics

In this final section, we make some preliminary observations on the new data provided by the ‘calibration’ survey [75] – the bulk of this analysis being reserved for future work. We focus on the $1^+$ and $1^-$ modes.

The investigation in [23] seems to identify the source of strong coupling as follows. In the linear theory without multipliers, rotational PiCs $A\phi^i_v$ may be paired off with conjugate PiCs $E\phi^i_v$, so as to determine $A\hat{u}^i_v$ and $E\hat{u}^i_v$ and so terminate both chains. Unpaired PiCs generate SiCs, whose consistency conditions fix the original PiC Hamiltonian multipliers – all within the same $J^P$ sector.

As the theory becomes nonlinear, the PiC structure does not, of course, change. However there are generally more PiC-PiC commutators which emerge, and which do not fail to commute with many other constraints, and can produce predictable, linear commutators with the conjugate $J^P$ sectors of the $\phi^{ij}_{kl}$ and $\phi^{ij}_{kl}$. For the case of translational multipliers (as discussed in Sect. 3.3.1, we suspect these to be safer), an approach might be to use the consistencies of the constrained $\phi^{ij}_{kl}$ irreps to solve for a large number of $\{E\hat{u}^i_v\}$ in the linear theory. This would force the rotational sector into developing the maximum number of SiCs ab initio. Assuming nonlinear commutators between the SiCs and rotational PiCs proliferate as usual, one then expects to solve for all the remaining Hamiltonian multipliers as before, with a generally SC system whose SiCs are not contingent on nonlinear effects.

The ‘calibration’ survey covers the simple extension of (49) by the condition $\beta_2 \neq 0$, and we used the resultant brackets when exploring this mechanism in [67]. That theory does not appear to be strongly coupled, but it is also unlikely to be unitary. We close this section by suggesting another option. In [23] the basic PGT with only $\alpha_0 \neq 0$ and $\alpha_5 \neq 0$ was briefly considered, in which both $1^+$ and $1^-$ modes were strongly coupled. This theory contains all the translational PiCs$^{18}$ $\phi$ and $\phi^\perp$, $\psi$, $\sigma^\perp$ and $\chi^\perp$. The rotational PiCs are only conjugate in the $1^+$ and $2^+$ sectors, so the linear theory produces SiCs $\chi^\perp_{\perp 1 1}$, $\chi^\perp_{\perp 1 \perp}$, $\chi^\perp_{\perp \perp}$ and $T\chi^\perp_{\perp \perp}$. In the nonlinear case, all 12 d.o.f in the rotational and translational sectors are assumed to solve exactly for each others’ Hamiltonian multipliers: no SiCs are produced and the total d.o.f rises by two massive vectors $1/2(1 + 5 + 3 + 3) = 3 + 3$.

However by imposing $\beta_1 \neq 0$, we can obtain all the translation Hamiltonian multipliers except for in the $0^+$ sector – which remains under traditional conjugacy. In this way, an extra $\chi^\perp_{\perp 1 1}$ is forced in both regimes, and its natural conjugacy (comparing to the experience of the $0^+$ in [67]) will be $\phi^\perp_{(ij)_\perp}$. A similar structure develops in the $2^-$ sector. Denoting consistency conditions with arrows, we arrive at

\begin{equation}
\begin{aligned}
\tilde{\chi}^\perp_{\perp 1 1} & \rightarrow \tilde{\psi}^\perp_{\perp 1 1} \\
T\chi^\perp_{ijk} & \leftarrow T\phi^\perp_{ijk} \\
\chi^\perp_{\perp 1 1} & \rightarrow \tilde{\psi}^\perp_{\perp 1 1} \\
T\chi^\perp_{ijk} & \leftarrow T\phi^\perp_{ijk} \\
\end{aligned}
\end{equation}

where solid arrows indicate that a Hamiltonian multiplier is determined, and dashed arrows indicate that a secondary

\[\text{Recall from Sect. 2.2 that we inherit the SO(3) irrep notation from Eqs. (23a), (23b), (24a), and (24b), but just replace the underlying symbol.}\]
must be constructed. Four-step consistency chains such as in (59) are not seen in the original PGT. If the overall SC structure is indeed preserved in the nonlinear theory, it would seem that the additional 3 + 3 d.o.f beyond GR are present both in the linear and nonlinear regimes, i.e. their strong coupling is removed on the Minkowski background. Regardless of strong coupling, these vector modes are traditionally problematic in combination because the unitarity of either one of them restricts the other to become a ghost: they enter into the Hamiltonian with equal and opposite signs, both parameterised by \( \tilde{\alpha}_5 \) [23]. The use of partial multipliers also allows us to fix this problem, e.g. by suppressing one vector with an additional \( \beta_2 \neq 0 \).

The resulting theory would allow for the PGT, defined by Poincaré gauge bosons and the geometry-constraining multipliers native to non-Riemannian theories, to propagate non-scalar unitary modes beyond GR without the usual risk of strong coupling on the Minkowski background. These modes could, for example, be made heavy so as to introduce extra contact interactions to the Einstein–Cartan model: the overall phenomenological differences with GR would then be very interesting to study. We defer this again to further work.

4 Conclusions

In this paper we have presented the package HiGGS, written for the tensor manipulation suite \texttt{xAct} and the computer algebra software \texttt{Mathematica}. The HiGGS package performs calculations – such as Poisson brackets – which frequently arise in the Hamiltonian (canonical) analysis of modified gravity theories with curvature and/or torsion. The current iteration of the package is tailored to the generalised Poincaré gauge theory in Eq. (14): given an action of that class, HiGGS can identify primary and secondary constraints, and calculate arbitrary field velocities. For more original torsionful actions, HiGGS may still be used to evaluate brackets, and canonicalise expressions by irreducible decomposition.

Parallelisation is a core feature of HiGGS. We have argued that those aspects of the Dirac–Bergmann Hamiltonian constraint algorithm which can become cumbersome during manual evaluation, are actually very well suited to parallel computing. On a laptop or desktop computer, HiGGS can take advantage of available cores to shorten the analysis of a given theory. Parallelisation is done within the HiGGS environment. This capability meshes well with the problem of surveying large numbers of action configurations using high-performance computing (HPC), since it avoids the need to educate general-purpose job scheduling tools (such as \textit{SLURM} [101] or \textit{TORQUE} [102]) about the physical details of the Hamiltonian constraint structure. In our example HPC survey, all job-scheduling decisions were made from within the \textit{HiGGS} environment, to whole-node granularity.

The HPC survey we have performed here – whose results will be discussed further in future work – targets minimal extensions to the Einstein–Cartan theory in which a single extra massive spin-parity \( 1^+ \), \( 1^- \) or \( 2^- \) torsion particle is present, i.e. extending the two usual graviton polarisations by three or five extra degrees of freedom (d.o.f). These minimal extensions were believed [103–105] to be ghost free according to the linearised analysis. Subsequent nonlinear Hamiltonian analysis [23] suggested that the linear regime strongly couples extra modes of spin-parity \( 1^- \), \( 1^+ \) or \( 2^- \) respectively, so that these modes spoil the theories’ viability. Based on the hypothesis that multiplier fields could selectively suppress these modes – in the style of teleparallel gravity – our survey lists all the commutators among all the known primary and secondary ‘if-constraints’ (i.e. constraints which may arise due to a choice of Lagrangian couplings), for the various possible multiplier configurations. Our level of analysis at least matches that of mode activation\(^{20}\) in [23], where the primary Poisson matrices of the minimal Einstein–Cartan extensions are obtained. We note that some of these results (which are available in the supplemental materials [75]) have already been used in [67].

While the HiGGS package may be of use to researchers in the ways described above, we must observe some of its many limitations;

- The \texttt{PoissonBracket[]} module automatically expands its operands, rather than first taking advantage of the Leibniz rule wherever those operands are products of covariant factors. This can result in costly attempts by \texttt{ToNesterForm[]} to covariantise arbitrarily complex brackets.
- The \texttt{Velocity[]} module is directly associated with the canonical Hamiltonian in (42) of the generalised Poincaré gauge theory in (14). This could easily be avoided (i.e. in favour of user-defined Hamiltonian) with Leibniz rule functionality in \texttt{PoissonBracket[]}.
- The \texttt{PoissonBracket[]} module is incapable of processing the second-order Euler–Lagrange formulation. The lack (to our knowledge) of a general formula in Poincaré gauge theory for the second-order bracket was also a limiting factor for our previous analysis in [13].

\(^{19}\) We point out that multipliers can occasionally be be used in this way, consistent with our hypothesis of switching off bad modes, but in general the way in which they turn out to address the strong coupling phenomenon (through mechanisms such as in Eq. (59)) is rather more subtle, and has nothing whatever to do with ‘suppressing the strongly coupled modes’.

\(^{20}\) We do not, however, perform the extra step in [23] of considering the problem of constraint bifurcation using the Poisson matrix pseudo-determinant.
grounds upon which to dismiss a rich class of theories. In general, HiGGS relies quite heavily on the gauge-covariant derivatives $D_\mu$ or $\nabla_\xi$. The xAct suite already has a very sophisticated functionality to accommodate the definition of such derivatives, which is not exploited by the HiGGS implementation.

In general, HiGGS relies very heavily on the $\text{SO}^+ (1, 3)$ and (particularly) the $\text{SO}(3)$ decompositions of tensorial fields. However, these are manually defined in the implementation, for each decomposed field. A clear case is made for a general decomposition tool, more closely integrated with the existing functionality in xAct's SymManipulator.

Notwithstanding the Lagrangian structure implied by Velocity[], inclusion of new dynamical variables constitutes a different problem. Extension to the metric affine gauge theory (MAGT) structure would be a straightforward, if time-consuming, exercise. More work would likely be needed for the inclusion of (e.g. fermionic) matter fields.

The background assumed by HiGGS when the option "ToOrder" $\rightarrow 0$ or "ToOrder" $\rightarrow 1$ is passed to modules such as ToNesterForm[], is Minkowski spacetime with vanishing background torsion. There are, however, obvious motivations for considering curved backgrounds, such as de Sitter or Schwarzschild. Moreover in [13, 14, 80, 81] it is argued that non-minimal gravitational gauge theories, which are detached from the geometrical trinity, only become viable in an attractor background of constant axial torsion.

Whether these limitations are best addressed by improving the HiGGS implementation, or beginning ab initio with an improved understanding of the challenges posed by canonical computer algebra, remains to be seen. For the moment, we hope at least to have shown that modified gravity is now ready for computer algebra assistance at scale. In this sense we build on the recent work of Lin, Hobson and Lasenby [77, 86], who used computer algebra to systematically obtain all ghost and tachyon-free cases of the linearised Poincaré gauge theory, and did so with far more limited resources than were brought to bear in this paper. A future is then suggested in which vague concerns – viz, a potential for strong coupling demonstrated among a handful of cases – are no longer valid grounds upon which to dismiss a rich class of theories.

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Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: The associated software was released prior to submission of this article under the GNU General Public License; it is and will remain publically available and open-source.]

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Appendix A: Linear velocities of the simple spin-1⁺ case

In this appendix we provide the linearised velocities of the PiCs appearing in the simple 1⁺ extension to Einstein–Cartan theory:

\[
\begin{align*}
\frac{d}{dt} \phi_{ij} & = \dot{\phi}_{ij} = \frac{\partial \phi_{ij}}{\partial t} + \frac{\partial \phi_{ij}}{\partial x^\alpha} \dot{x}^\alpha + \frac{\partial \phi_{ij}}{\partial x^\beta} \dot{x}^\beta + \frac{\partial \phi_{ij}}{\partial x^\gamma} \dot{x}^\gamma \\
\frac{d}{dt} \phi_{\alpha} & = \dot{\phi}_{\alpha} = \frac{\partial \phi_{\alpha}}{\partial t} + \frac{\partial \phi_{\alpha}}{\partial x^\beta} \dot{x}^\beta + \frac{\partial \phi_{\alpha}}{\partial x^\gamma} \dot{x}^\gamma
\end{align*}
\]

This manuscript has no associated data or the data will not be deposited. [Authors’ comment: The associated software was released prior to submission of this article under the GNU General Public License; it is and will remain publically available and open-source.]
\[
\frac{d}{dt} \psi_{ij} = \left( \frac{\partial}{\partial x^a} \phi_{ji} \right) N + \frac{3}{4} \left( \frac{\partial}{\partial x^a} \phi_{ik} \right) k \frac{1}{3} \frac{\partial}{\partial x^a} \phi_{jk} N - \frac{2}{3} \frac{\partial}{\partial x^a} \phi_{jkl}.
\]

These expressions are expressed on the PGT shell, but not on the sSFC shell. We note in particular the general presence of momentum gradients, which arise at the end of the HiGGS run. In non-minimal theories (i.e., those with PGTs which depend on the field strengths), we can expect gradients of the field strengths to also appear. These are second derivative quantities, even in the first-order formulation of gravity that is PGT: they cannot be further processed by HiGGS, which uses a first-order Euler–Lagrange implementation.

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