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FAST TRACK COMMUNICATION

The applicability of constrained symplectic integrators in general relativity

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Abstract

The purpose of this communication is to point out that a naive application of symplectic integration schemes for Hamiltonian systems with constraints such as SHAKE or RATTLE which preserve holonomic constraints encounters difficulties when applied to the numerical treatment of the equations of general relativity.

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It is well known that the equations of general relativity (GR) can be derived from a variational principle and that they can be cast into Hamiltonian form. The underlying symplectic structure has been studied as early as the 1940s beginning with the work of Bergmann [3, 8], Dirac [9, 10] and ADM [5]. The main motivation then has been to work out a quantization scheme for GR. For various reasons, not the least of them being the peculiar nature of the symplectic structure of GR, these early attempts have not led to any viable theory of quantum gravity.

On the other hand, it has been well established within the numerical mathematics community [12, 13, 16] that the use of so-called symplectic integrators, i.e., numerical ODE solvers which preserve an underlying symplectic structure, can lead to significant improvements in long-time stability, conservation of first integrals and accuracy. These methods have been generalized even to Hamiltonian systems with constraints. There are two particularly noteworthy methods which are called SHAKE [20] and RATTLE [2]. They have been developed within the area of molecular dynamics but since then they have been used successfully in various other applications. However, they only work for holonomic constraints.

Given the success of these methods it is, therefore, natural to apply symplectic numerical methods also to the equations of GR. However, as we will argue in this paper, it is not clear (yet) whether there is any advantage to be gained in this approach.

This paper addresses the question of the applicability of symplectic integrators in GR and it is directed towards both communities, numerical mathematics as well as numerical relativists. This necessarily means that we need to review both the Hamiltonian framework for GR as well as the essence of symplectic integrators. This is reflected in the structure of the paper which consists mostly of sections to introduce the necessary background material. In section 1 we describe finite-dimensional Hamiltonian systems and in section 2 we expand this to include systems with constraints. Section 3 is devoted to a brief exposition of the symplectic structure of GR in the special case of spatially compact spacetimes. In section 4, we describe the essential properties of symplectic integrators for constrained systems. Finally, in section 5 we discuss the consequences of trying to combine these two areas of research.

1. Hamiltonian systems

Before we come to the symplectic structure of GR let us first look at a classical Hamiltonian system with finitely many degrees of freedom such as those occurring in classical mechanics, molecular dynamics, etc. The system is specified by a triple (\mathcal{P}, ω, H) , where \mathcal{P} is a real manifold of even dimension $2n$ which carries a symplectic form ω , i.e., a non-degenerate closed 2-form. The pair (\mathcal{P}, ω) is called the phase space of the system. It is the collection of all states which are accessible to the system and the symplectic form provides a way to locally sort the degrees of freedom into pairs of conjugate variables.

Since ω is non-degenerate it defines at each point $x \in \mathcal{P}$ an isomorphism between the tangent space $T_x \mathcal{P}$ and the co-tangent space $T_x^* \mathcal{P}$. Thus, any function $f \in \mathcal{C}^\infty(\mathcal{P})$ defines a Hamiltonian vector field X_f by the equation

$$X_f \lrcorner \omega + df = 0. \quad (1)$$

From this equation and the closure of ω follows that the Lie derivative

$$L_{X_f} \omega = d(X_f \lrcorner \omega) + X_f \lrcorner d\omega = 0, \quad (2)$$

i.e., the symplectic form, is invariant under the flow generated by a Hamiltonian vector field. Each member of the flow is a canonical transformation. This is true, in particular, for the Hamiltonian vector field X_H generated by the Hamiltonian function $H : \mathcal{P} \rightarrow \mathbb{R}$, the function which specifies the dynamics of the system; the time evolution map ϕ_t generated by X_H which maps an arbitrary initial state $x_0 \in \mathcal{P}$ to the state at time t is a canonical transformation.

Dual to the symplectic form we can introduce a Poisson structure, i.e., Poisson brackets $\{\cdot, \cdot\}$ on \mathcal{P} , by defining for any two functions $f, g \in \mathcal{C}^\infty(\mathcal{P})$

$$\{f, g\} := \omega(X_f, X_g) = L_{X_f} g. \quad (3)$$

This turns the algebra of functions on \mathcal{P} into a Lie algebra with respect to the Poisson bracket, the Jacobi identity being a consequence of the closure of ω . It is well known that there exist preferred so-called canonical coordinates (p_k, q^i) on \mathcal{P} such that locally the symplectic form is

$$\omega = dp_k \wedge dq^k$$

or, equivalently, such that these coordinates have canonical commutation relations

$$\{p_i, p_k\} = 0, \quad \{q^i, q^k\} = 0, \quad \{p_i, q^k\} = \delta_i^k.$$

The flow generated by a function $H \in \mathcal{C}^\infty(\mathcal{P})$ induces a change in a function f which is given by

$$\dot{f} = \{H, f\}.$$

In particular, the rate of change in the canonical variables can be used to obtain a coordinate expression for the flow

$$\dot{q}^i = \{H, q^i\}, \quad \dot{p}_k = \{H, p_k\}.$$

Hamiltonian systems frequently arise from Lagrangian systems by performing a Legendre transformation. The most common case is where the Lagrangian system is defined by an action functional

$$\mathcal{A} = \int \mathcal{L}(q, \dot{q}) dt$$

over a Lagrangian function $\mathcal{L} : TQ \rightarrow \mathbb{R}$ on the tangent bundle of a configuration manifold Q . A Legendre transformation is then used to define a Hamiltonian system on the cotangent bundle T^*Q of the configuration space. A detailed description of these structures can be found, e.g., in [1, 4, 23].

In many cases the Legendre transformation is well-defined and invertible and the Hamiltonian system is valid without any restrictions, i.e., it is unconstrained. In some cases, however, when the Lagrangian function is degenerate, the Legendre transformation is not a local diffeomorphism. This implies that not all the possible states in T^*Q are available to the Hamiltonian system, i.e., that there are constraints which have to be imposed.

This situation has been analysed in detail by Dirac [9, 10] (see also [15]) who developed a theory of Hamiltonian systems with constraints.

2. Constraints in Hamiltonian systems

From the geometric point of view a constraint in a phase space (\mathcal{P}, ω) is a sub-manifold \mathcal{C} of \mathcal{P} which comprises the states which are accessible to the system. The symplectic form ω restricts to a closed 2-form $\bar{\omega}$ on \mathcal{C} . In general, $\bar{\omega}$ will not be regular. Let

$$G_x = \{U \in T_x\mathcal{C} : \bar{\omega}(U, V) = 0, \forall V \in T_x\mathcal{C}\}.$$

At each $x \in \mathcal{C}$ this is a subspace of $T_x\mathcal{C}$ and we assume that the dimension of G_x is constant as x varies over \mathcal{C} . Then $G = \bigcup G_x$ is a sub-bundle of $T\mathcal{C}$ (and hence also of $T\mathcal{P}$) which defines a distribution in $T\mathcal{C}$. It is easily seen that this distribution is integrable: let X, Y be two sections of G , so that $X \lrcorner \bar{\omega} = Y \lrcorner \bar{\omega} = 0$. Then, the closure of $\bar{\omega}$ implies

$$[X, Y] \lrcorner \bar{\omega} = L_X(Y \lrcorner \bar{\omega}) - Y \lrcorner L_X \bar{\omega} = -Y \lrcorner d(X \lrcorner \bar{\omega}) - Y \lrcorner (X \lrcorner d\bar{\omega}) = 0.$$

Therefore, there exist maximal integral surfaces \mathcal{G} tangent to G which foliate \mathcal{C} . Under certain technical assumptions (for the details see [23] and references therein) the space of leaves $\mathcal{P}' = \mathcal{C} \setminus \mathcal{G}$ is a differentiable manifold. Furthermore, there exists a closed 2-form ω' on \mathcal{P}' which pulls back to $\bar{\omega}$ under the canonical projection and which is regular. Thus, the pair (\mathcal{P}', ω') is a phase space on its own.

This is all that can be said from ‘inside \mathcal{C} ’, i.e., without taking into account that \mathcal{C} is in fact a sub-manifold of \mathcal{P} . Doing this, one obtains information about how the embedding of \mathcal{C} in \mathcal{P} affects the structure inside \mathcal{C} . Let us first define

$$T_x\mathcal{C}^\perp = \{U \in T_x\mathcal{P} : \omega(U, V) = 0, \forall V \in T_x\mathcal{C}\}.$$

then, clearly, $G_x = T_x\mathcal{C} \cap T_x\mathcal{C}^\perp$. Let r be the co-dimension of \mathcal{C} in \mathcal{P} , then we have $\dim T_x\mathcal{C} = 2n - r$ and $\dim T_x\mathcal{C}^\perp = r$. Furthermore, let $f \in \mathcal{C}^\infty(\mathcal{P})$ be constant on \mathcal{C} , so that the restriction of df to \mathcal{C} vanishes. Then at all $x \in \mathcal{C}$ we have for any $V \in T_x\mathcal{C}$

$$\omega_x(X_f, V) = -V(f) = 0$$

i.e., $X_f(x) \in T_x \mathcal{C}^\perp$. Let C_A be r independent functions which vanish on \mathcal{C} near x so that \mathcal{C} may locally be regarded as the zero set of these functions. Clearly, any function which is locally constant on \mathcal{C} is functionally dependent on the C_A . Hence, the Hamiltonian vector fields $X_A := X_{C_A}$ evaluated at x generate an r -dimensional vector space which, therefore, coincides with $T_x \mathcal{C}^\perp$.

The vector fields X_f for locally constant f need not be tangent to \mathcal{C} . We will be interested mostly in two cases: when either none or all of the vector fields are tangent to \mathcal{C} .

In the first case we have $G_x = T_x \mathcal{C} \cap T_x \mathcal{C}^\perp = \{0\}$, so that $\bar{\omega}$ is regular and $\mathcal{P}' = \mathcal{C}$. Then $(\mathcal{C}, \bar{\omega})$ is a symplectic sub-manifold of (\mathcal{P}, ω) , i.e., it is a phase space in its own right. Note that $Q_{AB} := \omega(X_A, X_B) = \{C_A, C_B\}$ is a non-singular $r \times r$ -matrix when evaluated on \mathcal{C} . In this case, the constraint functions C_A are called *second-class constraints*.

Since $(\mathcal{C}, \bar{\omega})$ is a phase space there also exists a Poisson bracket on \mathcal{C} corresponding to $\bar{\omega}$ defined for functions on \mathcal{C} . Denoting the inverse of Q_{AB} by Q^{AB} , so that $Q_{AB} Q^{BC} = \delta_A^C$, we can express the Poisson bracket $\{\bar{f}, \bar{g}\}$ between two functions \bar{f} and \bar{g} on \mathcal{C} in terms of Poisson brackets on \mathcal{P} as follows. Choose extensions of \bar{f} and \bar{g} to \mathcal{P} , i.e., functions f and g on \mathcal{P} which restrict to \bar{f} and \bar{g} on \mathcal{C} . Then, on \mathcal{C} the following equation holds:

$$\{\bar{f}, \bar{g}\} = \{f, g\} - \{f, C_A\} Q^{AB} \{C_B, g\}. \tag{4}$$

Here, the left-hand side is the Poisson bracket on $(\mathcal{C}, \bar{\omega})$ and it is defined only on \mathcal{C} while the right-hand side is well defined even on \mathcal{P} . It makes sense for arbitrary functions f and g . It is easy to see that it vanishes if f or g are taken as constraints. Since two extensions of \bar{f} coincide on \mathcal{C} they differ by constraints. This shows that it is irrelevant which extensions for \bar{f} or \bar{g} are used. The expression on the right-hand side satisfies the defining properties of a Poisson structure so we may also regard it as defining a new Poisson bracket $\{\cdot, \cdot\}_D$ on \mathcal{P} , which is adapted to the existence of the constraint surface. This new Poisson bracket is called Dirac bracket [10]. Note that we can now express the Poisson bracket on \mathcal{C} in terms of Dirac's bracket

$$\{\bar{f}, \bar{g}\} = \{f, g\}_D,$$

which in turn enables us to discuss the Poisson structure of constrained system in terms of quantities on the original phase space.

The second case of interest is characterized by the fact that all the Hamiltonian vector fields X_A corresponding to constraint functions are tangent to \mathcal{C} . Therefore, we have $T_x \mathcal{C}^\perp \subset T_x \mathcal{C}$ and $G_x = T_x \mathcal{C}^\perp$. This implies that

$$\{C_A, C_B\} = \omega(X_A, X_B) = L_{X_A} C_B$$

which vanishes on \mathcal{C} . It has been useful to introduce the notion of 'weak equality' of two functions f and g if and only if they restrict to the same function on \mathcal{C} . Thus,

$$f \approx g \iff f - g = \mu^A C_A$$

for appropriate functions $\mu^A \in \mathcal{C}^\infty(\mathcal{P})$. Hence, in the present case we may write

$$\{C_A, C_B\} \approx 0.$$

In this case, the functions C_A which define the constraint hypersurface are in involution. They are called *first-class constraints*.

Since $G_x \neq \{0\}$ the restriction of the symplectic form $\bar{\omega}$ is degenerate and $(\mathcal{C}, \bar{\omega})$ is a pre-symplectic manifold. Factoring out the leaves of the foliation we obtain the reduced phase space (\mathcal{P}', ω') , sometimes called the space of the true degrees of freedom.

Let us now consider time evolution. Given a Hamiltonian $H \in \mathcal{C}^\infty(\mathcal{P})$ for a system with constraints we need to ask for compatibility of the time evolution generated by H with

the constraints: when the system is started out on \mathcal{C} then it should remain on \mathcal{C} , i.e., the Hamiltonian vector field X_H should be tangent to \mathcal{C} or, expressed in terms of Poisson brackets, the weak equality

$$\{H, C_A\} \approx 0 \tag{5}$$

should hold for all constraints C_A . Clearly, for the behaviour of the constrained system only the restriction \tilde{H} of the Hamiltonian function to \mathcal{C} is relevant and the extensions of \tilde{H} to \mathcal{P} (of which H is one) are all *a priori* equivalent. However, we may try to find a compatible extension \tilde{H} for which the Hamiltonian vector field $X_{\tilde{H}}$ is tangent to \mathcal{C} . Writing $\tilde{H} = H + \lambda^B C_B$ we find

$$0 \approx \{\tilde{H}, C_A\} = \{H, C_A\} + \lambda^B \{C_B, C_A\} + \{\lambda^B, C_A\} C_B \approx \{H, C_A\} + \lambda^B Q_{BA}.$$

This equation tells us that we can find a compatible extension only if Q_{AB} is invertible, i.e., only if the constraints are second class. Only in this case we can express the dynamics of the constrained system entirely in terms of the original phase space \mathcal{P} .

In the case of first class constraints $Q_{AB} \approx 0$ so that either all extensions or none satisfy the compatibility condition (5). If it is satisfied then H is constant along the Hamiltonian vector fields X_A generated by the constraints C_A . Hence, it descends to a well-defined function on \mathcal{P}' . Furthermore, for its Hamiltonian vector field X_H we have

$$[X_H, X_A] \lrcorner \omega = -d(\{H, C_A\}).$$

Since for any weakly vanishing function $f \approx 0$ one has $df = d\lambda^A C_A + \lambda^A dC_A$ for suitable functions λ^A this implies that for any $x \in \mathcal{C}$ and $Y \in T_x \mathcal{C}$

$$\omega([X_A, X_H], Y) = \bar{\omega}([X_A, X_H], Y) = \lambda^B Y(C_B) = 0.$$

Thus, $[X_A, X_H] \in T_x \mathcal{C}^\perp$ so that

$$L_{X_A} X_H \in G_x.$$

This implies that X_H is projectable onto \mathcal{P}' . One can also easily see that its projection is the Hamiltonian vector field for the projected Hamiltonian with respect to the symplectic form ω' .

Let us now illustrate the two cases with two examples.

2.1. Example 1: a particle restricted to a hypersurface

Consider a free particle in a Riemannian manifold (Q, g_{ab}) whose motion is restricted to a hypersurface $S \subset Q$. Let $C_0 = F$ be a function whose zero set locally defines S . In local coordinates q^a on Q the action for this situation is given by

$$\mathcal{A} = \int \left(\frac{1}{2} m g_{ab}(q) \dot{q}^a \dot{q}^b - \lambda F(q) \right) dt$$

This leads to the Hamiltonian $H = \frac{1}{2m} g^{ab} p_a p_b + \lambda F(q)$. Requiring that $\{H, C_0\} \approx 0$ gives us (using the notation $F_a = \nabla_a F$)

$$C_1 := p^a F_a \approx 0,$$

so we need to include C_1 as a constraint. Since $\{C_0, C_1\} = -F_a F_b g^{ab} \neq 0$ we can solve the equations

$$\{H + \lambda_0 C_0 + \lambda_1 C_1, C_i\} \approx 0 \quad \text{for } i = 0, 1$$

for λ_0 and λ_1 and obtain

$$\lambda_0 = 0, \quad \lambda_1 = \frac{1}{m} \frac{p^a p^b F_{ab}}{F^a F_a}$$

with $F_{ab} = \nabla_a \nabla_b F$. Hence, the final Hamiltonian is

$$H = \frac{1}{2m} p^a p_a - \frac{1}{m} \frac{p^a p^b F_{ab}}{F^a F_a} C_0.$$

It is straightforward to check that its Hamiltonian vector field annihilates both constraints.

2.2. Example 2: relativistic particle

We consider a particle in a Lorentzian spacetime (Q, g_{ab}) . In this case, the action for the worldline $q^a(\tau) \in Q$ of the particle is given by

$$\mathcal{A} = m \int \sqrt{g_{ab} \dot{q}^a \dot{q}^b} d\tau.$$

The distinguishing feature of this action is its invariance under reparametrization, $\tau \mapsto \tau' = T(\tau)$. The conjugate momentum is

$$p_a = \frac{m}{\ell} \dot{q}^b g_{ab},$$

where we abbreviate $\ell = \sqrt{g_{ab} \dot{q}^a \dot{q}^b}$. Obviously, we obtain the relation

$$C(p, q) := g^{ab} p_a p_b - m^2 = 0, \tag{6}$$

i.e., the momenta cannot attain all possible values. Hence, the states of the system are confined to the sub-manifold $\mathcal{C} \subset T^*Q$ defined by (6). From this constraint we obtain the further relation

$$p^a dp_a = 0 \tag{7}$$

which holds on \mathcal{C} . The restriction of ω to \mathcal{C} has a kernel which we can determine as follows. Let $X = X^a \partial/\partial q^a + Y_b \partial/\partial p_b$ then we search for non-vanishing X on \mathcal{C} with

$$0 = X \lrcorner \omega = Y_b dq^b - X^a dp_a$$

which in view of (7) implies $Y_b = 0$ and $X^a = \alpha p^a$ for an arbitrary function α on \mathcal{C} . Thus, every vector field in the kernel of $\bar{\omega}$ has the form

$$X = \alpha p^a \frac{\partial}{\partial q^a}.$$

Since the kernel is one-dimensional the vector fields are proportional to each other and their integral curves coincide as sets. It is not difficult to show that these vector fields generate exactly the reparametrization along the integral curves, i.e., they generate gauge transformations.

The Hamiltonian vector field of the constraint C is also in the kernel of $\bar{\omega}$,

$$X_C = 2p^a \frac{\partial}{\partial q^a},$$

so that it is tangent to \mathcal{C} . It generates the flow

$$\phi_\lambda(p_a, q^a) = (p_a, q^a + 2\lambda p^a).$$

The Hamiltonian function can be determined from the Lagrangian in the usual way:

$$H = p_a \dot{q}^a - m\ell = \frac{m}{\ell} g_{ab} \dot{q}^a \dot{q}^b - m\ell = 0.$$

Clearly, this Hamiltonian is compatible with the constraints. In fact, it vanishes on \mathcal{C} which is consistent with the fact that it generates gauge transformations.

Thus, we have the following picture. The system does not specify individual points $(p_a, q^a) \in \mathcal{C}$ as its states but instead one should regard the collection of all points which lie on the same integral curve of the gauge vector fields X as one state. They must be considered as equivalent because they are related by some gauge transformation. Hence, the states of the system are global entities, an entire worldline considered as a point set, i.e., without a distinguished parametrization.

Since the Hamiltonian vanishes on \mathcal{C} it is functionally dependent on the constraint and it also generates a gauge transformation. So, in this sense there is no distinguished time evolution in this system which would map from one state to another as it is the case in many ‘normal’ systems.

If one is interested in the structure of an individual worldline then one can proceed by fixing an initial point on the line and then, using the Hamiltonian vector field of H , the integral curve through that point can be found. However, the result will be a curve together with a special parameter which is determined by the choice of the Hamiltonian. The system of a relativistic particle is very similar to the situation in GR to which we will now turn.

3. The symplectic structure of GR

We now come to a brief introduction to the symplectic structure of GR. We follow loosely the exposition in [6]. Other treatments can be found in, e.g., [7, 11, 22, 23]. Let Σ be a three-dimensional compact closed manifold¹. We consider globally hyperbolic spacetimes of the form $M = \Sigma \times \mathbb{R}$. We choose a global time function $t : \Sigma \times \mathbb{R} \rightarrow \mathbb{R}$ and a vector field t^a such that the hypersurfaces Σ_t of constant t are diffeomorphic to Σ and such that $t^a \partial_a t = 1$. We assume that the hypersurfaces Σ_t are spacelike and that the vector field t^a is future directed and timelike. Let n_a be the future directed co-normal of the hypersurfaces and denote by ${}^4g_{ab}$ resp. g_{ab} the spacetime metric resp. the metric on Σ_t .

We can perform a $(3 + 1)$ -decomposition of the geometrical quantities in the usual way [22] by writing $t^a = \alpha n^a + \beta^a$, thereby introducing the lapse function α and the shift vector β^a . Thus, we can express the 4-geometry in terms of (families of) three-dimensional quantities. In this way, the Einstein–Hilbert action

$$\int_{\Sigma \times \mathbb{R}} {}^4R \sqrt{-{}^4g} \, d^4x \tag{8}$$

can be expressed up to boundary terms as the following action:

$$\mathcal{A} = \int_{\mathbb{R}} \mathcal{L}(g, \dot{g}; \alpha, \beta) \, dt \tag{9}$$

where the Lagrangian is

$$\mathcal{L}(g, \dot{g}; \alpha, \beta) = \int_{\Sigma} \alpha (R + K^{ab} K_{ab} - K^2) \sqrt{g} \, d^3x. \tag{10}$$

Here, we have used the scalar curvature R of the metric g_{ab} on Σ_t , the extrinsic curvature K_{ab} and its trace $K = K_c{}^c$ of Σ_t within the spacetime M . Due to the relationship

$$2\alpha K_{ab} = \dot{g}_{ab} - (L_{\beta}g)_{ab}$$

between the extrinsic curvature and the Lie derivative $\dot{g}_{ab} := (L_t g)_{ab}$ of the metric the Lagrangian is considered as a functional of g_{ab} , its time derivative \dot{g}_{ab} as well as the lapse and

¹ We concentrate here on the case of spatially closed spacetimes because we are interested in the intrinsic Hamiltonian framework. Issues concerning boundary conditions such as in the case of asymptotically flat spacetimes or even in the quasi-local regime are somewhat cumbersome to formulate or are not even resolved yet [21].

shift. Note that \mathcal{L} does not contain any time derivatives of α or β^a which indicates that it is singular. In fact, computing the variations of \mathcal{L} with respect to α and β^a yields

$$C \equiv \frac{\delta \mathcal{L}}{\delta \alpha} = \sqrt{g}(R - K^{ab}K_{ab} + K^2), \quad C_a \equiv \frac{\delta \mathcal{L}}{\delta \beta^a} = 2\sqrt{g}\nabla_b(K^b{}_a - \delta_a^b K). \quad (11)$$

The vanishing of these expressions as required by the Euler–Lagrange equations yields constraints on the possible configurations.

In a similar way, we compute the momentum conjugate to g_{ab} as

$$p^{ab} \equiv \frac{\delta \mathcal{L}}{\delta \dot{g}_{ab}} = \sqrt{g}(K^{ab} - K g^{ab}). \quad (12)$$

Note that this and the constraint expressions are tensor-valued densities of weight 1.

Finally, we determine the Hamiltonian from the formula

$$H(g, p) = \int_{\Sigma} \dot{g}_{ab} p^{ab} d^3x - \mathcal{L} \quad (13)$$

and find (up to boundary terms)

$$H(g, p) = \int_{\Sigma} \alpha \sqrt{g} \left[-R + \frac{1}{g}(p^{ab} p_{ab} - \frac{1}{2} p^2) \right] + \beta^b [-2\nabla_a p^a{}_b] d^3x. \quad (14)$$

Thus, we have the following situation. As the configuration space Q we take the space of Riemannian metrics on Σ . The tangent space $T_g Q$ consists of all symmetric covariant second rank tensor fields δg_{ab} on Σ . The cotangent space $T_g^* Q$ is defined as the space of functionally differentiable 1-forms on $T_g Q$, i.e., linear real-valued maps which are of the form

$$T_g Q \ni \delta g_{ab} \mapsto \int_{\Sigma} p^{ab} \delta g_{ab}$$

where p^{ab} is a tensor-valued density of weight 1. The phase space \mathcal{P} of general relativity (in the context of spatially closed spacetimes) is the cotangent bundle $T^* Q$ over the space Q of Riemannian metrics over Σ . Points of \mathcal{P} are represented as pairs (g_{ab}, p^{ab}) and tangent vectors to \mathcal{P} are represented as pairs $(\delta g_{ab}, \delta p^{ab})$. Being a cotangent bundle \mathcal{P} carries a canonical symplectic form and hence also a Poisson structure.

The symplectic form between two tangent vectors to \mathcal{P} is defined by

$$\omega_{(g,p)}((\delta_1 g, \delta_1 p), (\delta_2 g, \delta_2 p)) = \int_{\Sigma} \delta_1 p^{ab} \delta_2 g_{ab} - \delta_2 p^{ab} \delta_1 g_{ab} d^3x \quad (15)$$

and the corresponding Poisson bracket between two functions F and G on \mathcal{P} is

$$\{F, G\} = \int_{\Sigma} \frac{\delta F}{\delta p^{ab}} \frac{\delta G}{\delta g_{ab}} - \frac{\delta F}{\delta g_{ab}} \frac{\delta G}{\delta p^{ab}} d^3x. \quad (16)$$

The constraints expressions (11) yield functions on \mathcal{P} by integration over Σ :

$$C_f = \int_{\Sigma} f C d^3x, \quad C_v = \int_{\Sigma} v^a C_a d^3x,$$

where f and $\mathbf{v} = v^a$ are arbitrary test (vector) fields on Σ . Using the Poisson bracket we can easily see that the constraint functions satisfy the Poisson commutation relations

$$\begin{aligned} \{C_f, C_g\} &= -C_f \nabla_g - g \nabla f, \\ \{C_f, C_v\} &= -C_{v(f)}, \\ \{C_v, C_w\} &= -C_{[v,w]}. \end{aligned} \quad (17)$$

Therefore, the Poisson brackets among all constraints are again constraints, i.e., *the constraints are first class*. The constraint functions C_f and C_v generate transformations on \mathcal{C} which

correspond to gauge transformations, thus mapping a state (g_{ab}, p^{ab}) to an ‘equivalent’ state. The constraints C_v generate three-dimensional diffeomorphisms within Σ . The constraints C_f , however, generate transformations between different hypersurfaces Σ_t which can be interpreted as the ‘evolution’ of the intrinsic and extrinsic geometries of Σ within the spacetime M along the vector field $t^a = fn^a$.

The Hamiltonian (14) turns out to be a combination of constraints

$$H(g, \pi) = C_\alpha + C_\beta. \tag{18}$$

Hence, it generates gauge transformations, namely the evolution of Σ along the general evolution vector $t^a = \alpha n^a + \beta^a$. This implies that we have a similar situation here as in the case of the relativistic particle. A particular given state (g_{ab}, p^{ab}) on \mathcal{C} is equivalent to states $(\hat{g}_{ab}, \hat{p}^{ab})$ which are obtained by such transformations. Each equivalence class corresponds to the same single spacetime.

The fact that GR is a completely constrained system is the Hamiltonian way of reinstating general covariance of the theory. Any time evolution in the Hamiltonian sense would map equivalence classes to equivalence classes, i.e., a spacetime to an entirely different spacetime which would not make any sense. Instead the Hamiltonian formulation of GR specifies the general covariant geometry of a single spacetime eliminating any allusion to a notion of time.

4. Symplectic integrators

Let (\mathcal{P}, ω, H) be a (finite-dimensional) Hamiltonian system possibly with constraints. The flow generated by H maps initial states x_0 to later states $x_t = \phi_t(x_0)$. The map $\phi_t : \mathcal{P} \rightarrow \mathcal{P}$ is a canonical map, the ‘time- t ’ map. It is obtained by finding the integral curves of the Hamiltonian vector field of H , i.e., by solving a system of ODE when expressed in canonical coordinates.

There are many methods to solve systems of ODE by numerical means. Some of them have the special property that they preserve the structure defining the Hamiltonian system. We may regard a numerical method as a map $\Phi_h : \mathcal{P} \rightarrow \mathcal{P}$ which maps a state x_n to the next state x_{n+1} and we call such a method a symplectic integrator (of order p) if Φ_h is a canonical transformation for every h which approximates the exact Hamiltonian flow for a Hamiltonian function H in the sense that

$$\Phi_h(x) = \phi_h(x) + \mathcal{O}(h^{p+1}) \tag{19}$$

for all $x \in \mathcal{P}$. In [14] it is shown that a symplectic integrator of order p is backward stable, i.e., that there exists a Hamiltonian function $\tilde{H}_h - H = \mathcal{O}(h^{p+1})$ and Φ_h is the time- h map of the Hamiltonian vector field corresponding to \tilde{H}_h . This means that a symplectic method can be regarded as the exact time- h map for a slightly perturbed Hamiltonian system.

When constraints are present the symplectic integrators can be generalized to numerical methods which preserve the symplectic structure and the constraint hypersurface simultaneously [12, 17]. Examples of such methods are the well-known algorithms SHAKE [20] and RATTLE [2] developed within the context of molecular dynamics. They are implemented schematically as follows. Consider the Hamiltonian system (\mathcal{P}, ω, H) together with constraints C_A and let $x_0 = (p_0, q_0)$ be a point on the constraint hypersurface \mathcal{C} . We seek a method to compute the next point $x_h = (p_h, q_h)$ after time h on \mathcal{C} according to the Hamiltonian H . One considers the extended Hamiltonian

$$\tilde{H} = H + \lambda^A C_A$$

which generates the equations of motion on \mathcal{C}

$$\dot{p} = -\frac{\partial H}{\partial q} - \lambda^A \frac{\partial C_A}{\partial q}, \quad \dot{q} = \frac{\partial H}{\partial p} + \lambda^A \frac{\partial C_A}{\partial p}. \tag{20}$$

These have the approximate solutions

$$\begin{aligned} p_h &= \left(p_0 - h \frac{\partial H}{\partial q}(x_0) \right) - h\lambda^A \frac{\partial C_A}{\partial q}(x_0) + \mathcal{O}(h^2), \\ q_h &= \left(q_0 + h \frac{\partial H}{\partial p}(x_0) \right) + h\lambda^A \frac{\partial C_A}{\partial p}(x_0) + \mathcal{O}(h^2). \end{aligned} \quad (21)$$

However, the multipliers λ_A are not yet known. They are determined by requiring that the point $x_h = (p_h, q_h)$ lies on \mathcal{C} . Thus, one puts

$$\hat{p} = p_0 - h \frac{\partial H}{\partial q}(x_0), \quad \hat{q} = q_0 + h \frac{\partial H}{\partial p}(x_0)$$

and notes that

$$\begin{aligned} C_B(x_h) &= C_B(\hat{x}) - h \frac{\partial C_B}{\partial p}(\hat{x}) \frac{\partial C_A}{\partial q}(x_0) \lambda^A + \frac{\partial C_B}{\partial q}(\hat{x}) \frac{\partial C_A}{\partial p}(x_0) \lambda^A + \mathcal{O}(h^2) \\ &= C_B(\hat{x}) - h\lambda^A \{C_B, C_A\}(\hat{x}) + \mathcal{O}(h^2). \end{aligned}$$

Thus, one can find the multipliers λ^A by iteratively solving the linear equation

$$C_B(\hat{x}) - h\lambda^A \{C_B, C_A\}(\hat{x}) = 0. \quad (22)$$

At each step λ^A are used to update \hat{x} , thus entering a new iteration until the constraints $C_B(\hat{x}) = 0$ are satisfied to a desired accuracy at which point one puts $x_h = \hat{x}$.

Due to the special structure of holonomic constraints and their associated ‘hidden’ constraints the SHAKE and RATTLE algorithms differ in the details of this iteration procedure but the general structure of the algorithms is as indicated here. The main point about them is that they make the tacit assumption that *the matrix $Q_{AB} = \{C_A, C_B\}$ is invertible at every \hat{x}* . This implies that these algorithms *work only for second class constraints*. In fact, the above calculation is nothing but a variant of the calculation to find an extension of $H|_{\mathcal{C}}$ whose Hamiltonian vector field is tangent to \mathcal{C} .

5. Conclusion

We have seen in section 3 that GR is a fully constrained theory with first-class constraints. All the Hamiltonians (14) are combinations of constraints generating gauge-transformations. So, strictly speaking, there is no time evolution. However, within computational gravity one uses numerical methods to compute the geometry and hence the physics of one particular spacetime. In terms of the Hamiltonian framework this can be understood as follows.

Fix initial data, i.e., a point (g_{ab}, p^{ab}) on the constraint surface \mathcal{C} and specify a particular Hamiltonian by fixing lapse function and shift vector. This Hamiltonian generates a gauge flow which maps the initial point to points which correspond to hypersurfaces at a ‘later’ coordinate time. This ‘evolution’ is clearly symplectic and it preserves the constraints. Hence, one can try to use symplectic integrators for the task of determining the geometry of the spacetime in a particular gauge.

Suppose that we have arranged a spatial discretization of the infinite-dimensional system which results in a finite-dimensional Hamiltonian system. This means that the discretization results in a system of ODE which is Hamiltonian with respect to the discretized symplectic form and which preserves the discretized constraints. This can be achieved by an appropriate discretization of the action and then performing a Legendre transformation². Let Δ be a parameter which measures the discretization error. The discretization should be consistent

² It is an interesting and open question as to how much structure of the continuous Hamiltonian system can be carried over to the discrete system.

with the continuous system in the sense that we recover the latter from the former in the limit $\Delta \rightarrow 0$.

Following the implementation of a symplectic integrator we determine the equations of motion from an extended Hamiltonian $H + \lambda^A C_A$. Note that the index A ranges over four times the number of degrees of freedom used in the discretization. As demonstrated in section 4 the method relies on the invertibility of the matrix $Q_{AB} = \{C_A, C_B\}$.

Now two things may happen. Either the Poisson brackets of discretised constraints vanish on the constraint surface, i.e., they are also first class with respect to the discretized symplectic structure. Then the matrix Q_{AB} is not invertible and the symplectic integrator algorithm fails.

The other possibility is that the Poisson brackets of the discretized constraints do not vanish which means that the matrix Q_{AB} could be invertible so that multipliers λ^A could be found. However, consistency requires that in the limit of vanishing Δ one recovers the continuous system from the discrete one. And this in turn implies that in that limit the conditioning of the matrix Q_{AB} will become increasingly bad so that the linear equation (22) cannot be reliably solved anymore. Therefore, the continuum limit $\Delta \rightarrow 0$ will result in increasingly inaccurate discrete approximations to the real solution in contrast to expectations.

These consequences are observed in numerical implementations of the Einstein equations which make use of symplectic integration techniques [18].

The question of how to treat Hamiltonian systems with first class constraints numerically appears to be an open issue within the theory of symplectic integrators. At the moment there is no straightforward remedy to these shortcomings. One possibility to circumvent the consequences could be to change the system. Recall that we have chosen a Hamiltonian by fixing lapse function and shift vector arbitrarily but independently of the evolution. One way to proceed might be to couple the choice of these gauge functions to the Hamiltonian system. This could break the general covariance in such a way that the resulting system has only second class constraints. However, exactly how to proceed remains largely unclear (see [19] for a recent approach).

Another issue of relevance here is the relationship between holonomic constraints with their hidden constraints on the one hand and the first class/second class classification of constraints. Is it possible to find gauge conditions i.e., a 3 + 1 split and a choice of spatial coordinates, which give second class constraints, and can be regarded as holonomic constraints in an appropriate generalized sense? These issues need further clarifications.

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