Comments on a recent article by Ruhoff, Præstegaard and Perram on Constrained Dynamics

By Werner M. Seiler

Institut für Algorithmen und Kognitive Systeme
Universität Karlsruhe, 76128 Karlsruhe, Germany
Werner.Seiler@informatik.uni-karlsruhe.de

We discuss the results of an article by Ruhoff *et al.* (RPP96) on the numerical simulation of constrained systems. We point out that some of them are well-known. But we also show that in the Hamiltonian formalism their approach has a number of interesting features and how these can be at least partially explained.

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1. Introduction

Recently, Ruhoff *et al.* (RPP96) presented a new approach to the numerical integration of constrained systems. This classical problem is of great practical importance in many fields like robotics, vehicle or molecular dynamics.

Designing a method to numerically integrate a constrained system consists of two steps: (i) choosing the equations of motion (due to the constraints one has much freedom here) and (ii) choosing a numerical method to solve them. Obviously, these two steps are not independent, as the numerical method depends decisively on the way one treats the constraints in the equations of motion.

We discuss in this short note how Ruhoff *et al.* dealt with both aspects. We point out that within the Lagrangian formalism they rediscovered only well-known results but that within the Hamiltonian formalism their approach has a number of interesting features. We will give here only a brief survey of some of them; a detailed discussion with proofs will appear elsewhere (Sei97).

2. Constrained Dynamics

Ruhoff *et al.* considered a special case of constrained dynamics: a regular system with imposed holonomic constraints. This should not be confused with the constrained systems considered by Dirac (Dir64), namely *singular* or *degenerate* systems where the Legendre transformation is not one-to-one.

For such systems there exist two basic strategies. Either one finds minimal coordinates eliminating the constraints or one keeps all coordinates and and must then construct the constraint forces. Within the Lagrangian formalism this leads to the Euler-Lagrange equations of second and first kind, respectively (Gol80; Kuy93). In the engineering literature one often speaks of a *state space* and a *descriptor form*, respectively, of the equations of motion.

The confusion with the Dirac theory arises, because one way to derive the Euler-Lagrange equations of the first kind consists of the artificial introduction of a singular Lagrangian by adding the constraints with some multipliers to the original Lagrangian L_0. Ruhoff *et al.* modified this procedure (following (dLPP90)) by adding the time derivatives of the constraints.

This approach can already be found in the literature, although only in connection with anholonomic constraints where it is known as *vakonomic mechanics* (AKN88; Koz83). In the holonomic case, it was also studied (independently of Ruhoff *et al.*) under the name *impetus-striction formalism* by Dichmann *et al.* (DM96; DMP96; MP95). They were especially interested in its application to infinite-dimensional systems like elastica or fluids.

For anholonomic systems the vakonomic approach yields equations of motion which are not equivalent to those derived for example with the Principle of d'Alembert. For holonomic constraints $\phi_\alpha(q) = 0$ the situation is simpler. Comparing the Lagrangians $L' = L_0 + \mu^\alpha \phi_\alpha$ (which represents the usual way to derive the Euler-Lagrange equations of the first kind) and $L^* = L_0 + \lambda^\alpha \dot{\phi}_\alpha$ (which corresponds to the approach of Ruhoff *et al.*), we see that after a proper identification of the multipliers ($\mu^\alpha = -\dot{\lambda}^\alpha$) they differ only by a total derivative. Thus they lead to identical equations of motion.

Apparently, Ruhoff *et al.* did not notice this fact. What they called "constrained Lagrangian approach" yields in fact the well-known Euler-Lagrange equations of the first kind; they only derived them in a different way. Most works on the numerical simulation of constrained systems are based on these equations.

One of the central results of (RPP96) is the statement that this approach was superior (at least with respect to efficiency) to using the Euler-Lagrange equations of the second kind. This is rather well-known and indeed many programs for the automatic generation of equations of motion of mechanical systems are based on such a constrained approach.

But it is also well-known that one has to make a trade-off here. In the unconstrained formulation the dimension of the configuration space is smaller and hence one has less equations of motion. However, these are typically more complicated; for example the mass matrix is usually no longer constant and less sparse. In general, it depends on many factors which formulation is more efficient.

In a comparison one should also take into account that there exist more efficient ways to evaluate the unconstrained equations of motion than the straightforward use of the Euler-Lagrange equations applied by Ruhoff *et al.* Recursive schemes (see e.g. (Hol80)) also achieve a complexity linear in the number n of links. A discussion of some of these approaches can be found in (Fea87).

We must thus conclude that Ruhoff *et al.* presented only well-known material for the Lagrangian formalism. The situation is different in the Hamiltonian formalism. Adding the time derivative of the constraints yields different momenta compared with the standard approach.

Ruhoff *et al.* compared mainly the unconstrained and the constrained formulations. But actually their most important numerical result is the comparison of the constrained Lagrangian and Hamiltonian formulations. They showed that the constraint and the energy errors for the Hamiltonian version are several orders of magnitude smaller. As the execution times of the Lagrangian version are only slightly smaller, this is a striking result demanding an explanation.

Ruhoff *et al.* partially explained it by noting that the Lagrangian multipliers are determined such that the constraints for the accelerations are satisfied, whereas the equations for the Hamiltonian multipliers ensure the preservation of the momentum constraints. We will now indicate a somewhat different view.

Denoting by $p = \partial L_0/\partial \dot{q}$ the momenta of the classical approach, the ansatz of Ruhoff *et al.* yields as canonically conjugate momenta

$$p^* = p + \lambda^\alpha \frac{\partial \phi_\alpha}{\partial q} \,. \tag{2.1}$$

This equation is the key for understanding the new approach. Instead of considering p^* as momenta derived from a modified Lagrangian L^* one may interpret (2.1) as part of a canonical transformation $(q,p) \leftrightarrow (q^*,p^*)$ where $q^* = q$ for those points satisfying the position constraints $\phi_\alpha(q) = 0$.

The position constraints $\phi_\alpha(q) = 0$ generate via the Dirac algorithm (Dir64) the momentum constraints $\psi_\alpha(q,p) = \{\phi_\alpha, H_0\} = 0$ where H_0 is the Hamiltonian for the regular Lagrangian L_0. In the approach of Ruhoff *et al.* the canonical transformation is used backwards. The multipliers λ^α are determined such that for a point (q^*,p^*) with $\phi_\alpha(q^*) = 0$ the transformed point (q,p) satisfies not only $\phi_\alpha(q) = 0$ but also $\psi_\alpha(q,p) = 0$.

A closer look at the equations of motion of Ruhoff *et al.* reveals that they contain the momenta p^* only in the form $p^* - \lambda^\alpha \partial\phi_\alpha/\partial q$, i.e. they always apply this canonical transformation. Thus we may say that these equations of motion possess a kind of built-in projection on the momentum constraints and that it is thus not surprising that these are preserved with high accuracy. But (RPP96) offers no explanation why this should influence so drastically the position and the energy errors. We will discuss this important point in the next section.

3. Differential Algebraic Equations

The Euler-Lagrange equations of the second kind are often preferred to those of the first kind because of the numerical difficulties in integrating the latter ones. They represent a system of *differential algebraic equations* and naive approaches to their integration often suffer under a drift off the constraint manifold. This problem received much attention in the last twenty years (BCP96; HW96). The simulation of constrained systems has always been a central topic here; see e.g. the recent survey (Sim95) and the classical articles (FL91; GLG85).

There exist two basic possibilities to handle the problem of the drift. One can use the above mentioned freedom in setting up the equations of motion to obtain a differential algebraic equation which is less sensitive to numerical errors. This is usually called *stabilization* (ACR94). Or one can design special numerical methods preserving at last some of the constraints.

Obviously, the two possibilities can be combined; Ruhoff *et al.* are in fact doing this. Their new method to derive the Hamiltonian equations of motion can be seen as a stabilization. Its effect does not only show in the smaller absolute values of the constraint residuals but also in their growth. We integrated as a simple example a 1-link pendulum with the constrained Lagrangian and the constrained Hamiltonian formalism (in the terminology of (RPP96)). In the Lagrangian approach the position errors grow quadratically in time; in the Hamiltonian one only linearly. The momentum errors always grow linearly.

Much more important is however the effect on the integration error which is not considered at all by Ruhoff *et al.* Small constraint residuals alone are rather useless, if this error is too large. We estimated it by comparing with the numerical solution of the state space form for a ten times smaller step size. One finds that in the Lagrangian formalism the error grows cubically in time, whereas the Hamiltonian formalism shows a slightly worse than linear growth. The absolute values are again several orders of magnitude better.

A similar picture emerges, if one studies the energy error for this conservative system. Ruhoff *et al.* showed already that its absolute values are considerably smaller for the Hamiltonian approach. But the growth rates are also different: quadratical in the Lagrangian formalism and about $\sqrt{t}$ in the Hamiltonian one. For the constrained Lagrangian approach we gave a theoretical explanation for these error growth rates in (Sei96) using perturbation techniques.

As special numerical method Ruhoff *et al.* proposed a simple post-processing, namely orthogonal projection, of the results obtained by a conventional integrator. This belongs to the oldest and simplest techniques for preserving constraints (or invariants). Shampine (Sha86) studied it for one-step methods; Eich (Eic93) extended his results to multi-step methods. In contrast to (RPP96) these works also contain proofs of convergence and error estimates. Eich furthermore discusses the effect of the projections on the truncation error. A general overview of projection techniques can be found in (EFLR90).

However, opposed to (RPP96) most of the numerical literature studies only projections on the position constraints $\phi_\alpha = 0$. The constraints for the momenta and velocities, respectively, are often ignored. But as Fig. 7 of (RPP96) clearly shows, preservation of these can be very important. Unfortunately, Ruhoff *et al.* offered no explanation for this observation. They only stated that without a correction the momenta grow; but this could be an effect specific to their test problem and/or the numerical method they applied.

Alishenas (AO94) analyzed this effect with perturbation techniques. He showed for the Lagrangian formalism that projections on the velocity constraints reduce the growth of the errors. Without projections the integration error increases cubically in time. Velocity corrections reduce this to quadratic growth, whereas position corrections have no effect on the growth. For the Hamiltonian formalism we confirmed recently Alishenas' results theoretically and numerically (Sei96).

In order to apply these results to the constrained Hamiltonian approach we must study the relation between the orthogonal projections of (AO94; Sei96) and the "canonical projection" (2.1) used by Ruhoff *et al.* For an orthogonal projection one makes an ansatz precisely of the form (2.1). If one compares how the multipliers λ^α are determined, one discovers that the canonical transformation discussed in the last section *is* an orthogonal projection!

Thus we can indeed apply the results of (AO94; Sei96) for analyzing the approach of Ruhoff *et al.*, as they automatically use in each time step of the numerical integration orthogonally projected momenta. When Ruhoff *et al.* applied additional momentum corrections, they only improved the numerical result of the first projection, i. e. effectively they solved the arising linear system for the multipliers λ^α iteratively in order to obtain an even smaller momentum constraint residual. That this is sometimes necessary only further emphasizes the importance of the momentum constraints.

4. Conclusion

Ruhoff *et al.* proposed an interesting new approach for setting up *Hamiltonian* equations of motion for a regular system with imposed holonomic constraints. Compared with the standard approach based on the Euler-Lagrange equations of the first kind, it leads to significantly smaller errors. This holds not only for the constraint residuals but also for the integration and the energy error. Furthermore, all errors grow considerably slower.

In order to understand this numerical stability one must realize the importance of the momentum constraints which are often neglected. One has considerable freedom in writing the equations of motion of a constrained system. While the various formulations are physically equivalent, their numerical stability can be very different. (RPP96) belongs to the few works that try to exploit this freedom in order to obtain efficient and stable numerical simulation schemes. Other attempts can be found in (Sim93; Sei95; Sei96).

Within the Lagrangian formalism the approach of Ruhoff *et al.* coincides with the usual one based on the Euler-Lagrange equations of the first kind. The use of (orthogonal) projection methods for these equations is quite common. They can be made more efficient by combining the projections with the numerical integration of the underlying differential equations. This reduces the necessary linear algebra compared with the simple post-processing applied in (RPP96).

The restriction of Ruhoff *et al.* to Lagrangians which are quadratic in the velocities is unnecessary. Obviously, they imposed this condition only to ensure that they can explicitly compute the multipliers. For more general Lagrangians these are determined by a nonlinear system. However, a closer look at the equations of motion reveals that all terms containing derivatives of the multipliers cancel. For a numerical evaluation of the equations of motion it suffices to have numerical values for the multipliers which can be easily computed. Thus this approach can be applied to much more general systems, too.

Especially for the long term integration of Hamiltonian systems *symplectic integrators* (SSC94) are very popular, as they maintain many qualitative features of the exact solution. The approach of Ruhoff *et al.* is of considerable interest in this context, as for example the composition methods of Reich (Rei96) are closely related to it. This will be discussed in more detail in (Sei97).

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