Developing an explicit Hamiltonian variational integrator

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Abstract. Hamiltonian picture of a dynamical system is mathematically described, breaking down the total physical path described by an N-dimensional coordinate vector into sub-trajectories. Discretization of the extremized action integral is performed by applying the trapezoid rule to approximate the integral and forward and backward difference methods used to approximate the time derivatives of the path. Applying the Hamilton-Jacobi theory to the extremized and discretized action integral partial derivatives with respect to both the position and momentum were taken. Considering consecutive sub-trajectories, a two-step integration scheme was derived. Split Hamiltonian notation from a 2014 paper by Dr. Pihajoki was briefly discussed and an extended phase space leapfrog algorithm was introduced. In an attempt to derive a similar scheme, intersecting sub-trajectories were then introduced using half-steps in the time evolution of the system and a second integration scheme was derived. The derived schemes were compared to the leapfrog algorithm for separable and non-separable Hamiltonian systems. Results showed that the schemes derived had the properties expected from variational integrators but were only applicable to separable Hamiltonian systems. Further steps which could be applied to the method used in this project to develop an explicit non-separable Hamiltonian integration scheme were discussed.

1. Introduction

Variational Symplectic integrators whilst not differing from the mainstream integration schemes in terms of their simplicity to be used in many different systems, offer properties that are not always present. The main advantages are the conservative properties of the discrete variational integrators where the constants of motion are preserved throughout a large number of time steps. Noether's theorem allows these properties to be explained in a simple manner. Symmetries that are present in a function, to be precise the action functional which will be discussed in later sections, translate to conserved quantities in the equations of motions derived from that function. For example, time-shift symmetry corresponds to conservation of energy, and rotational symmetry to the conservation of angular momentum. A very technical description of these is went through in [1]. Because of such properties, these integrators have been widely used in many different areas of science requiring integration schemes to be used over exponentially long periods of time. Namely orbital dynamics [2] and statistical mechanics [3].

This project aims to apply the Hamiltonian formalism of classical mechanics and build on work done by Dr. Tsang [4], in which he explored variational Symplectic integrators in terms of the Lagrangian formalism. Motivation to do so will become clearer in the following sections but to briefly go over it, it is related to the fact that the Lagrangian equations are typically second-order meaning they are much harder to deal with when the exact equation is unknown. Dealing with it in general terms, the time-step evolution algorithm that comes out at the end is implicit, meaning the computational time and costs become too large

to be ignored when applying it. By definition, Hamilton's equations of motion are first order, whilst that does not mean they are necessarily known, the number of them doubles. Whilst there are more equations to deal with, they become much easier to approximate using simple methods such as the trapezoid rule, which is used extensively in this project, without having the error grow too large.

Once the Hamiltonian formalism is applied to the method used by Dr. Tsang, the aim will be to derive explicit algorithms directly mapping the time evolution of Hamiltonian systems and apply it to a few chosen ones. The code to apply the algorithms was written and results visualized using Python.

In the following sections, the theory behind this project will be covered, the approach taken to derive the integration algorithms will be described in detail and finally, the meaning and importance of the work and the results will be discussed.

2. Background theory

In the following sub-sections, the notation and the system will be described in terms of the Lagrangian formalism already done by Dr. Tsang. Also, theories and concepts used extensively in this project will be described to lay the foundation for the work that has been done in this project. These include a description of a system known as the action, Hamilton's principle, Euler-Lagrange equations, the Hamilton-Jacobi principle, and Legendre transforms.

2.1 Hamilton's principle and the system in the Lagrangian formalism

The Lagrangian of a system is defined as the kinetic energy of a system minus the potential energy of the system. In general, the Lagrangian has $2N$ variables, the position of a particle and the velocity of that particle inside a given system. A separable Lagrangian is defined when there are two distinct expressions for each energy containing the position and velocity variables separately. One can also define the Lagrangian with what is known as a velocity-dependent potential although, this applies to some very specific cases one of which is the electromagnetic forces on moving charges [5].

In this project a dynamical system with N degrees of freedom is considered. It is assumed that the system at any time t can be described by a velocity phase space, $[\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t)]$, where $\boldsymbol{q}$ is the N-dimensional coordinate vector and $\dot{\boldsymbol{q}}$ is the N-dimensional velocity vector. Hamilton's principle states that the physical trajectories that hypothetical particles inside this system will follow are the solutions $\boldsymbol{q}(t)$ which extremize the action integral [6]. So, the mathematical picture of the system can be built by writing the definition of an action integral

$$S[\boldsymbol{q}(t)] = \int_{t_0}^{t_f} L(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t)dt\,. \tag{1}$$

The action is considered extremized if for any variation of the trajectory the integral is equal to zero. The long derivation of applying the variation to equation (1) can be found in [7], for purposes of this project only the final form is considered

$$\delta S = \int_{t_0}^{t_f} \left(\left[\frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial q^i} - \frac{d}{dt} \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial \dot{q}^i} \right] \delta q^i \mathrm{dt} \right) + \delta q^i \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial q^i} \Bigg|_{t_0}^{t_f} = 0 \tag{2}$$

where the upper index on q^i indicates a vector quantity. It should also be noted that the time dependance of the position and velocity vectors have been dropped only for notational simplicity and both vectors are still considered time dependant. By setting variation of $\boldsymbol{q}$ to be zero at the boundaries, the "boundary term"

outside of the integral can also be set equal to zero. What follows from equation (2) are known as the Euler-Lagrange equations, which effectively are second-order ordinary differential equations which describe the dynamics of the system

$$\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \boldsymbol{q}} - \frac{d}{dt}\frac{\partial L(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{\boldsymbol{q}}} = 0\,. \tag{3}$$

They can be said to be analogous to Newton's laws of motion but have the added benefit of being generalized meaning same equations can be applied to a system in any generalized coordinates, general case being the velocity phase-space.

2.2 The Hamilton-Jacobi theory

Hamilton-Jacoby theory goes into great detail on combining the action integral together with a very powerful idea in mathematics of generating functions. In a way that is very useful for the work done in this project, it describes a function whose partial derivatives with respect to the variables inside of the function itself generate the equations which describe the dynamics of the system. Specifically talking about the action integral, initial and final momenta can be obtained from the partial derivatives of the extremized action integral if the action integral is defined with respect to initial and final positions such that $S = S(\boldsymbol{q}_0, \boldsymbol{q}_f; t_0, t_f)$.

To apply this to the system so far, Dr. Tsang made the following assumptions in his unpublished paper on which this project is built upon [4]: the trajectory is extremized such that $\boldsymbol{q}(t) = \boldsymbol{q}(\boldsymbol{q}_0, \boldsymbol{q}_f; t)$ is a function of time and satisfies the aforementioned Euler-Lagrange equations for any choice of boundary points. Plugging the trajectory into the definition of the action a partial derivative of the action with respect to $\boldsymbol{q}_0$ while keeping $\boldsymbol{q}_f$ fixed can be taken and the resulting forms can be integrated by parts. Since now there are defined, non-zero, boundary points, together with the conclusion from the Hamilton-Jacobi theory, equations for initial and final momenta are generated

$$\frac{S(\boldsymbol{q}_0, \boldsymbol{q}_f; t_0, t_f)}{\partial q_0^i} = -\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\bigg|_{t_0} = -p_i(t_0)\,;\; \frac{S(\boldsymbol{q}_0, \boldsymbol{q}_f; t_0, t_f)}{\partial q_f^i} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\bigg|_{t_f} = p_i(t_f)\,. \tag{4)(5}$$

Whilst so far this just illustrates the same equations already arrived at in the Hamilton-Jacobi theory, it is incredibly useful to write it out in such notation to be able to follow the logic further in this project. Motivation for applying Hamiltonian formalism comes from the fact that when written in discrete notation, (4) gives an implicit step for finding the following position which can then be used in (5) to solve explicitly for the momentum at the following position.

2.3 Defining the piecewise connected trajectories

When thinking in terms of a Lagrangian, since one variable is the position and second one is the derivative of position with respect to time, meaning they are dependent, a path between $\boldsymbol{q}_n$ and $\boldsymbol{q}_{n+1}$ can be fully defined just by the positions at times t_n and t_{n+1} as a single trajectory $\gamma_n \equiv \gamma_n[\boldsymbol{q}_n, \boldsymbol{q}_{n+1}](t)$. A sequence of $N+1$ position points can then be defined by a sequence of N trajectories which are connected in such a way that $\gamma_n[\boldsymbol{q}_n, \boldsymbol{q}_{n+1}](t_n) = \boldsymbol{q}_n$ and $\gamma_n[\boldsymbol{q}_n, \boldsymbol{q}_{n+1}](t_{n+1}) = \boldsymbol{q}_{n+1}$. Assuming that each trajectory uniquely extremizes the action integral, $S[\gamma_n]$, one can now define the total trajectory Γ, which effectively is a set of all the trajectories. This now means that a total action integral which is the sum of all the action integrals over all the smaller sub-trajectories of the whole system can be defined as $S[\Gamma] = \sum_{n=0}^{N-1} S[\gamma_n]$.

Because each action is already by assumption extremized, the total action integral must be also extremized with respect to the position points. Considering for example that the total path only contains

two sub-trajectories and taking the partial derivative of it with respect to the middle point between the two it is seen that the following must be true

$$\frac{\partial S[\Gamma]}{\partial q_{n+1}^i} = \frac{S[\,\gamma_n(\boldsymbol{q}_n, \boldsymbol{q}_{n+1})]}{\partial q_{n+1}^i} + \frac{S[\,\gamma_n(\boldsymbol{q}_{n+1}, \boldsymbol{q}_{n+2})]}{\partial q_{n+1}^i} = 0\,. \tag{6}$$

2.4 Legendre transforms

Legendre transforms are a very powerful mathematical tool which will allows one to look at the same system from the point of view of Hamiltonian mechanics, whilst simultaneously illustrating how this may make the system much easier to deal with and open up new approaches. The full mathematical explanation of Legendre transforms can be found in [8]. For the purposes of this project report only the specific application will be discussed.

For a Lagrangian to a Hamiltonian, the derivation first is started by writing down the differential of the Lagrangian

$$dL(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) = \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial q^i} dq^i + \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial \dot{q}^i} d\dot{q}^i + \frac{\partial L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)}{\partial t} dt\,. \tag{7}$$

Substituting the definition of canonical momentum already shown in equations (4) and (5) and re-arranging the Hamiltonian is generated in terms of the Lagrangian

$$H(\boldsymbol{q}, \boldsymbol{p}, t) = p_i \dot{q}_i - L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)\,. \tag{8}$$

By obtaining a definition of the Lagrangian in terms of the Hamiltonian, the framework of the system in the Hamiltonian formalism can now be set up which is one of the first steps in the work that was done for this project. Important note at this point is that the system can be represented with two independent variables, position and momenta, rather than position and its derivative. In the following section this will be illustrated by applying the stationary-action principle to a new, Hamiltonian, definition of the action to arrive at a new set of equations describing the dynamics of the system.

3. Method

3.1 Stationary-action principle on the Hamiltonian

Using the new definition of the Lagrangian in terms of the Hamiltonian one can now write down a new definition of the action integral. By also recognizing that $\dot{q}^i = dq^i/\mathrm{d}t$ the form can be immediately changed to one that does not contain any time derivatives,

$$S = \int_{t_0}^{t_f} p^i dq^i - H(\boldsymbol{q}, \boldsymbol{p}, t) dt\,. \tag{9}$$

By applying the stationary-action principle (also known as principle of least action) to this system the aim is to first derive the equations of motion in terms of the Hamiltonian. This will allow to find what variables the system depends on. When applying the variations, it is said that p^i and q^i are replaced with functions $p^i + \delta p^i$ and $q^i + \delta q^i$ respectively. Plugging these into equation (12) the following is obtained

$$\delta S = \int_{t_0}^{t_f} \delta p^i dq^i + p^i \delta\big(dq^i\big) - \left(\frac{\partial H(\boldsymbol{q}, \boldsymbol{p}, t)}{\partial q^i} \delta q^i\,\mathrm{d}t + \frac{\partial H(\boldsymbol{q}, \boldsymbol{p}, t)}{\partial p^i} \delta p^i\,\mathrm{d}t\right). \tag{10}$$

The second term, $p_i \delta(dq_i)$, can be re-written as $p_i d(\delta q_i)$ using the logic that the variation in the change in q^i equals the change in the variation in q^i [9]. Doing this re-arrangement is crucial as now it allows for the same term to be integrated by parts

$$\int_{t_0}^{t_f} p^i d(\delta q^i) = p^i \delta q^i \Big|_{t_0}^{t_f} - \int_{t_0}^{t_f} dp^i \delta q^i \,, \tag{11}$$

giving two terms on the right hand side which can be reffered to as the "boundary term" and a "bulk term" respectively. For this initial derivation it is assumed that the q variation at the end points is zero and hence the boundary term dissappears leaving the bulk term which can be placed inside the integral in equation (10). After some re-arranging of the obtained equation, what comes out is the final form of the variation in the action

$$\delta S = \int_{t_0}^{t_f} \left(\delta p^i \left(\frac{dq^i}{dt} - \frac{\partial H(\boldsymbol{q}, \boldsymbol{p}, t)}{\partial p^i} \right) - \delta q^i \left(\frac{dp^i}{dt} + \frac{\partial H(\boldsymbol{q}, \boldsymbol{p}, t)}{\partial q^i} \right) \right) dt = 0 \,. \tag{12}$$

From which it can now be seen, that to fulfill the requirement of the principle of least action, the terms inside the brackets must independently be equal to zero and hence the following pair of equations must be true

$$\frac{dq^i}{dt} = \frac{\partial H(\boldsymbol{q}, \boldsymbol{p}, t)}{\partial p^i} \,, \qquad \frac{dp^i}{dt} = -\frac{\partial H(\boldsymbol{q}, \boldsymbol{p}, t)}{\partial q^i} \,, \tag{13) (14}$$

which are known as Hamilton's equations of motion. These equations now show that the dynamics of the system, in the Hamiltonian formalism, do not solely depend on the position but also on the momentum. From this, a new path which contains both position and momenta as the variables can be defined, giving extra equations to work with mathematically. Comparing the Euler-Lagrange equations, equation (3), to the Hamiltonian equivalent illustrates how the system goes from N second-order differential equations to $2N$ first-order differential equations simply by using a different formalism.

3.2 Partial derivatives of the new action integral

Starting with the definition of the action in terms of the Hamiltonian (10), next step is to take the derivative of it with respect to the initial position to confirm that section 2.2 still applies. This then takes the following form

$$\frac{\partial S(\boldsymbol{q}_0, \boldsymbol{q}_f, \boldsymbol{p}_0, \boldsymbol{p}_f; t_0, t_f)}{\partial q_0^i} = \int_{t_0}^{t_f} \left(p^i \, \partial(dq^i) - \partial H(\boldsymbol{q}, \boldsymbol{p}, t) dt \right) \frac{1}{\partial q_0^i} . \tag{15}$$

Applying the previously mentioned logic to the $p^i \, \partial(dq^i)$ term and switching the partial derivative and derivative signs around, it again allows integration by parts giving the following

$$\int_{t_0}^{t_f} p^i d(\partial q^i) = p^i \, \partial q^i \Big|_{t_0}^{t_f} - \int_{t_0}^{t_f} dp^i \, \partial q^i \,. \tag{16}$$

After plugging (19) into (18) and after re-arranging, the following is obtained

$$\frac{\partial S(\boldsymbol{q}_0, \boldsymbol{q}_f, \boldsymbol{p}_0, \boldsymbol{p}_f; t_0, t_f)}{\partial q_0^i} = \int_{t_0}^{t_f} \left(-dp^i \, \partial q^i - \partial H(\boldsymbol{q}, \boldsymbol{p}, t) dt \right) \frac{1}{\partial q_0^i} + \frac{p^i \, \partial q^i}{\partial q_0^i} \Bigg|_{t_0}^{t_f} . \tag{17}$$

Hamilton's equations derived previously show that the $-dp^i \, \partial q^i$ term is indeed just equal to $\partial H(\boldsymbol{q}, \boldsymbol{p}, t) dt$ making the integral equal to zero and leaving only the boundary part of the equation. Because for the purposes of this derivation the action is still defined only in terms of the values at initial and final time

steps, $S(\boldsymbol{q}_0, \boldsymbol{q}_f, \boldsymbol{p}_0, \boldsymbol{p}_f; t_0, t_f)$, following relationships $\partial q^i / \partial q_0^i \big|_{t_0} = \delta_i^j$ and $\partial q^i / \partial q_0^i \big|_{t_f} = 0$ must be true. Applying these to the boundary term left in equation (21) the result of taking the derivative of the action with respect to the initial position generates the initial momentum

$$\frac{\partial S(\boldsymbol{q}_0, \boldsymbol{q}_f, \boldsymbol{p}_0, \boldsymbol{p}_f; t_0, t_f)}{\partial q_0^i} = \left. \frac{p^i \, \partial q^i}{\partial q_0^i} \right|_{t_0} = -p^i(t_0) \, . \tag{18}$$

Similarly taking the derivative with respect to the final position gives

$$\frac{\partial S(\boldsymbol{q}_0, \boldsymbol{q}_f, \boldsymbol{p}_0, \boldsymbol{p}_f; t_0, t_f)}{\partial q_f^i} = \left. \frac{p^i \, \partial q^i}{\partial q_f^i} \right|_{t_f} = p^i(t_f) \, , \tag{19}$$

and it can be clearly seen that the Hamilton-Jacobi theory still applies. It should be noted that for the purposes of this write-up, in the derivations above, the partial derivative operator can be seen treated as another function which can be kept outside the brackets. Performing the same derivation with more mathematical formality in these cases give the same results, it is recognized that not in all cases that can be said to be true.

Since the action is now also a function of the momentum, one can take partial derivatives with respect to the initial and final values of the momentum. Performing the same process for these partial derivatives as the ones with respect to the position the following are generated

$$\frac{\partial S(\boldsymbol{q}_0, \boldsymbol{q}_f, \boldsymbol{p}_0, \boldsymbol{p}_f; t_0, t_f)}{\partial p_0^i} = 0 \, ; \frac{\partial S(\boldsymbol{q}_0, \boldsymbol{q}_f, \boldsymbol{p}_0, \boldsymbol{p}_f; t_0, t_f)}{\partial p_f^i} = 0 \, . \tag{20)(21}$$

In this section both sets of partial derivatives were performed for an ideal Hamiltonian case, meaning it was assumed that the action integral was already known.

3.3 New path and partial derivatives of the discretized action

In practice, the ideal case rarely applies, meaning the action must be discretized, in other words approximated. A discretized action can be constructed by firstly approximating the trajectory between the two 'boundary points' in the sequence and then the integral must be approximated by means of some quadrature method, in this project one mostly explored was the trapezoid rule.

Viewing the system from a Hamiltonian point of view, the path can no longer be described purely by the positions but also need to include the second variable, the momentum. So, a single trajectory becomes $\gamma_n \equiv \gamma_n[\boldsymbol{q}_n, \boldsymbol{q}_{n+1}, \boldsymbol{p}_n, \boldsymbol{p}_{n+1}](t)$ and a similar sequence as in section 2.3 can be defined, such that $\gamma_n[\boldsymbol{q}_n, \boldsymbol{q}_{n+1}, \boldsymbol{p}_n, \boldsymbol{p}_{n+1}](t_n) = (\boldsymbol{q}_n, \, \boldsymbol{p}_n)$ and $\gamma_n[\boldsymbol{q}_n, \boldsymbol{q}_{n+1}, \boldsymbol{p}_n, \boldsymbol{p}_{n+1}](t_{n+1}) = (\boldsymbol{q}_{n+1}, \, \boldsymbol{p}_{n+1})$ now giving both the position and momenta at the respective time steps. The total action then becoming the sum of the action integrals along each newly defined sub-trajectory

$$\mathrm{S}[\Gamma] \equiv \sum_{n=0}^{N-1} S[\gamma_n(\boldsymbol{q}_n, \boldsymbol{q}_{n+1}, \boldsymbol{p}_n, \boldsymbol{p}_{n+1})]. \tag{22}$$

Employing the trapezium rule for the approximation the following form is obtained

$$\begin{aligned} S_d \left[\gamma_n^d [\boldsymbol{q}_n, \, \boldsymbol{q}_{n+1}, \boldsymbol{p}_n, \boldsymbol{p}_{n+1}] \right] \\ \approx \sum_{n=0}^{N-1} \Bigg(& \frac{q_{n+1} - q_n}{\Delta t} p_n - H(\boldsymbol{q}_n, \boldsymbol{p}_n) + \frac{q_{n+1} - q_n}{\Delta t} p_{n+1} \\ & - H(\boldsymbol{q}_{n+1}, \boldsymbol{p}_{n+1}) \Bigg) \frac{\Delta t}{2}, \end{aligned} \tag{23}$$

where the integral is replaced by a sum, and the velocity is treated as a differential of the position which is hence approximated using forward and backward difference methods respectively. Effectively each sub-trajectory contains the action evaluated at two consecutive points, with the velocity treated as a constant. For the point n that corresponds to a forward difference where for point $n+1$ it is backward difference. Additionally, the newly added subscripts on S_d and γ_n^d show that the action and the path are discretized. Considering the total path to be made up of N sub-trajectories such that

$$S_d[\Gamma] = \sum_{n=0}^{N-1} \partial S_d[\gamma_n^d(\boldsymbol{q}_n, \boldsymbol{q}_{n+1}, \boldsymbol{p}_n, \boldsymbol{p}_{n+1})], \tag{24}$$

the same logic as in section 2.3 can be applied, in this case also including the momentum. Since the action is extremized on the sub-trajectory, the total trajectory extremizes the action if the total action is extremized with respect to the points $(\boldsymbol{q}_n, \boldsymbol{p}_n)$. Next step becomes to take partial derivatives of the total discretized action using the previously mentioned approximation. To make the derivations practical and the integration scheme easier to see, six consecutive sub-trajectories were considered making sure that all evaluations around each point of interest were included. Performing the derivations for the whole set of sub-trajectories, setting them equal to zero as per equation (6) and re-arranging them the first two-step integration scheme is obtained

$$\frac{\partial S_d[\Gamma]}{\partial q_n^i} \rightarrow p_{n+1} = p_{n-1} - 2\frac{\partial H_n}{\partial q_n^i}\Delta t, \tag{25a}$$

$$\frac{\partial S_d[\Gamma]}{\partial q_{n+1}^i} \rightarrow p_{n+2} = p_n - 2\frac{\partial H_{n+1}}{\partial q_{n+1}^i}\Delta t, \tag{25b}$$

$$\frac{\partial S_d[\Gamma]}{\partial p_n^i} \rightarrow q_{n+1} = q_{n-1} + 2\frac{\partial H_n}{\partial p_n^i}\Delta t, \tag{25c}$$

$$\frac{\partial S_d[\Gamma]}{\partial p_{n+1}^i} \rightarrow q_{n+2} = q_n + 2\frac{\partial H_{n+1}}{\partial p_{n+1}^i}\Delta t. \tag{25d}$$

It can immediately be noticed that whilst it is indeed explicit, given only one initial set of variables, to start the scheme the variables at the previous time-step must also be known. This can be overcome in practice by different methods, one used is simply setting the first two time-steps to be equal with a sufficiently small time-step. To obtain make the scheme resemble the mapping of $(\boldsymbol{q}_n, \boldsymbol{p}_n) \rightarrow (\boldsymbol{q}_{n+1}, \boldsymbol{p}_{n+1})$ more formally-half points were introduced. In this way the path becomes $\gamma_n^d\left(\boldsymbol{q}_n, \boldsymbol{q}_{n+\frac{1}{2}}, \boldsymbol{p}_n, \boldsymbol{p}_{n+\frac{1}{2}}\right)$ and performing all the same steps gives

$$\frac{\partial S_d[\Gamma]}{\partial q_n^i} \rightarrow p_{n+\frac{1}{2}} = p_{n-\frac{1}{2}} - 2\frac{\partial H_n}{\partial q_n^i}\Delta t, \tag{26a}$$

$$\frac{\partial S_d[\Gamma]}{\partial q^i_{n+\frac{1}{2}}} \rightarrow p_{n+1} = p_n - 2\frac{\partial H_{n+\frac{1}{2}}}{\partial q^i_{n+\frac{1}{2}}}\Delta t, \tag{26b}$$

$$\frac{\partial S_d[\Gamma]}{\partial p_n^i} \rightarrow q_{n+\frac{1}{2}} = q_{n-\frac{1}{2}} + 2\frac{\partial H_n}{\partial p_n^i}\Delta t, \tag{26c}$$

$$\frac{\partial S_d[\Gamma]}{\partial p^i_{n+\frac{1}{2}}} \rightarrow q_{n+1} = q_n + 2\frac{\partial H_{n+\frac{1}{2}}}{\partial p^i_{n+\frac{1}{2}}}\Delta t. \tag{26d}$$

3.4 Leapfrog algorithm

In a 2014 paper [10] Dr Pihajoki discusses how for systems for which the Hamiltonian can be separated into a sum of distinct functions for the kinetic energy and potential energy, $H(\boldsymbol{q}, \boldsymbol{p}) = V(\boldsymbol{q}) + T(\boldsymbol{p})$, Hamilton's equations of motion (16) and (17) can be directly integrated. By doing so the solutions can be combined to obtain two forms of a second order leapfrog algorithm known as the Störmer–Verlet method. In Dr. Pihajoki's paper the algorithm is presented in the following form

$$\boldsymbol{q}_{n+\frac{1}{2}} = \boldsymbol{q}_n + \frac{h}{2}\nabla_{\boldsymbol{p}} T(\boldsymbol{p}_n), \quad (27a) \qquad \boldsymbol{p}_{n+\frac{1}{2}} = \boldsymbol{p}_n - \frac{h}{2}\nabla_{\boldsymbol{q}} V(\boldsymbol{q}_n), \quad (27d)$$

$$\boldsymbol{p}_{n+1} = \boldsymbol{p}_n - h\nabla_{\boldsymbol{q}} V\left(\boldsymbol{q}_{n+\frac{1}{2}}\right), \quad (27b) \qquad \boldsymbol{q}_{n+1} = \boldsymbol{q}_n + h\nabla_{\boldsymbol{p}} T\left(\boldsymbol{p}_{n+\frac{1}{2}}\right), \quad (27e)$$

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_{n+\frac{1}{2}} + \frac{h}{2}\nabla_{\boldsymbol{p}} T(\boldsymbol{p}_{n+1}), \quad (27c) \qquad \boldsymbol{p}_{n+1} = \boldsymbol{p}_{n+\frac{1}{2}} - \frac{h}{2}\nabla_{\boldsymbol{q}} V(\boldsymbol{q}_{n+1}), \quad (27f)$$

where $\nabla_{\boldsymbol{p}} = (\partial/\partial\, p_1, \ldots, \partial/\partial\, p_n)$ and h is the time-step. This algorithm offers a fully explicit integration scheme, except for its downfall of being only applicable to seperable Hamiltonians. In the same paper Dr. Pihajoki goes further to introduce the idea of an extended phase space as a way to deal with inseparable Hamiltonians. By extending the phase space such that $(\boldsymbol{q}, \boldsymbol{p})$ becomes $(\boldsymbol{q}, \tilde{\boldsymbol{q}}, \boldsymbol{p}, \tilde{\boldsymbol{p}})$ the number of equivalent Hamilton's equations is also doubled. By defining the new extended Hamiltonian as such

$$\tilde{H}(\boldsymbol{q}, \tilde{\boldsymbol{q}}, \boldsymbol{p}, \tilde{\boldsymbol{p}}) = H_1(\boldsymbol{q}, \tilde{\boldsymbol{p}}) + H_2(\tilde{\boldsymbol{q}}, \boldsymbol{p}), \quad (28)$$

the new and old variables are mixed. When the new set of Hamilton's equations are integrated directly, the actions are obtained. Dr. Pihajoki develops this further to arrive at two equivalent extended phase space leapfrog algorithms

$$\boldsymbol{q}_{n+\frac{1}{2}} = \boldsymbol{q}_n + \frac{h}{2}\nabla_{\boldsymbol{p}} H_2(\tilde{\boldsymbol{q}}_n, \boldsymbol{p}_n), \quad (29a) \qquad \tilde{\boldsymbol{q}}_{n+\frac{1}{2}} = \tilde{\boldsymbol{q}}_n + \frac{h}{2}\nabla_{\tilde{\boldsymbol{p}}} H_1(\boldsymbol{q}_n, \tilde{\boldsymbol{p}}_n), \quad (30a)$$

$$\tilde{\boldsymbol{p}}_{n+\frac{1}{2}} = \tilde{\boldsymbol{p}}_n - \frac{h}{2}\nabla_{\tilde{\boldsymbol{q}}} H_2(\tilde{\boldsymbol{q}}_n, \boldsymbol{p}_n), \quad (29b) \qquad \boldsymbol{p}_{n+\frac{1}{2}} = \boldsymbol{p}_n - \frac{h}{2}\nabla_{\boldsymbol{q}} H_1(\boldsymbol{q}_n, \tilde{\boldsymbol{p}}_n), \quad (30b)$$

$$\tilde{\boldsymbol{q}}_{n+1} = \tilde{\boldsymbol{q}}_n + h\nabla_{\tilde{\boldsymbol{p}}} H_1\left(\boldsymbol{q}_{n+\frac{1}{2}}, \tilde{\boldsymbol{p}}_{n+\frac{1}{2}}\right), \quad (29c) \qquad \boldsymbol{q}_{n+1} = \boldsymbol{q}_n + h\nabla_{\boldsymbol{p}} H_2\left(\tilde{\boldsymbol{q}}_{n+\frac{1}{2}}, \boldsymbol{p}_{n+\frac{1}{2}}\right), \quad (30c)$$

$$\boldsymbol{p}_{n+1} = \boldsymbol{p}_n - h\nabla_{\boldsymbol{q}} H_1\left(\boldsymbol{q}_{n+\frac{1}{2}}, \tilde{\boldsymbol{p}}_{n+\frac{1}{2}}\right), \quad (29d) \qquad \tilde{\boldsymbol{p}}_{n+1} = \tilde{\boldsymbol{p}}_n - h\nabla_{\tilde{\boldsymbol{q}}} H_2\left(\tilde{\boldsymbol{q}}_{n+\frac{1}{2}}, \boldsymbol{p}_{n+\frac{1}{2}}\right), \quad (30d)$$

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_{n+\frac{1}{2}} + \frac{h}{2}\nabla_{\boldsymbol{p}} H_2(\tilde{\boldsymbol{q}}_{n+1}, \boldsymbol{p}_{n+1}), \quad (29e) \qquad \tilde{\boldsymbol{q}}_{n+1} = \tilde{\boldsymbol{q}}_{n+\frac{1}{2}} + \frac{h}{2}\nabla_{\tilde{\boldsymbol{p}}} H_1(\boldsymbol{q}_{n+1}, \tilde{\boldsymbol{p}}_{n+1}), \quad (30e)$$

$$\tilde{\boldsymbol{p}}_{n+1} = \tilde{\boldsymbol{p}}_{n+\frac{1}{2}} - \frac{h}{2}\nabla_{\tilde{\boldsymbol{q}}} H_2(\tilde{\boldsymbol{q}}_{n+1}, \boldsymbol{p}_{n+1}), \quad (29f) \qquad \boldsymbol{p}_{n+1} = \boldsymbol{p}_{n+\frac{1}{2}} - \frac{h}{2}\nabla_{\boldsymbol{q}} H_1(\boldsymbol{q}_{n+1}, \tilde{\boldsymbol{p}}_{n+1}). \quad (30f)$$

When given an initial value problem, setting $\tilde{\boldsymbol{q}}_0 = \boldsymbol{q}_0$ and $\tilde{\boldsymbol{p}}_0 = \boldsymbol{p}_0$ these algorithms give identical time-evolutions which are equal to the original and physical momentum phase space of the system. For the purposes of this write-up, scheme (29) will be referred to as the Pihajoki-Störmer-Verlet method (PSVM). Dealing with more complex Hamiltonians or even setting the two Hamiltonians to be slightly different introduces the need for Lie algebra which will not be discussed further.

3.5 Intersecting sub-trajectories

So far, the total path was considered as a combination of consecutive sub-trajectories. In an attempt to arrive at an equivalent form of the PSVM by using the methodology used so far in this project, the idea of intersecting sub-trajectories was considered. Introducing half-points into the system allows for the total path to be defined as

$$S_d[\Gamma] = \sum_{n=0}^{N-1} S_d\left[\gamma^d_{n-\frac{1}{2}}\left(\boldsymbol{q}_{n-\frac{1}{2}}, \boldsymbol{q}_{n+\frac{1}{2}}, \boldsymbol{p}_{n-\frac{1}{2}}, \boldsymbol{p}_{n+\frac{1}{2}}\right)\right] + S_d[\gamma^d_n(\boldsymbol{q}_n, \boldsymbol{q}_{n+1}, \boldsymbol{p}_n, \boldsymbol{p}_{n+1})]. \quad (31)$$

Since the action is now effectively evaluated four times each time-step, central difference method was deemed the most appropriate to use in the approximations.

For the purpose of illustrating the algebra, part of the sum relevant to the derivations is showcased in (32). With each evaluation of the action integral having the approximation already discussed applied to it, the following form is obtained

$$\begin{aligned} S_d[\Gamma] = \Bigg(\ldots + 2\left(\left(\frac{q_n - q_{n-1}}{\Delta t}\right) p_{n-\frac{1}{2}} - H_{n-\frac{1}{2}}\right) + 2\left(\left(\frac{q_{n+\frac{1}{2}} - q_{n-\frac{1}{2}}}{\Delta t}\right) p_n - H_n\right) \\ + 2\left(\left(\frac{q_{n+1} - q_n}{\Delta t}\right) p_{n+\frac{1}{2}} - H_{n+\frac{1}{2}}\right) + 2\left(\left(\frac{q_{n+\frac{3}{2}} - q_{n+\frac{1}{2}}}{\Delta t}\right) p_{n+1} - H_{n+1}\right) \\ + \cdots \Bigg) \frac{\Delta t}{2}. \end{aligned} \quad (32)$$

Taking partial derivatives of (32) the following scheme is obtained

$$\frac{\partial S_d[\Gamma]}{\partial q^i_n} \to p_{n+\frac{1}{2}} = p_{n-\frac{1}{2}} - \frac{\partial H_n}{\partial q^i_n}\Delta t, \quad (33a) \qquad \frac{\partial S_d[\Gamma]}{\partial p^i_n} \to q_{n+\frac{1}{2}} = q_{n-\frac{1}{2}} + \frac{\partial H_n}{\partial p^i_n}\Delta t, \quad (33c)$$

$$\frac{\partial S_d[\Gamma]}{\partial q^i_{n+\frac{1}{2}}} \to p_{n+1} = p_n - \frac{\partial H_{n+\frac{1}{2}}}{\partial q^i_{n+\frac{1}{2}}}\Delta t, \quad (33b) \qquad \frac{\partial S_d[\Gamma]}{\partial p^i_{n+\frac{1}{2}}} \to q_{n+1} = q_n + \frac{\partial H_{n+\frac{1}{2}}}{\partial p^i_{n+\frac{1}{2}}}\Delta t. \quad (33d)$$

Whilst it is almost identical to the first scheme obtained, a factor of two is absent from the partial derivatives of the Hamiltonians. The effect this has on the results will be presented and discussed in the following sections.

4. Results

4.1 Single pendulum test case

Firstly, each algorithm was applied to a one-dimensional single pendulum system. Implementation was done from scratch in Python together with the plotting of the results. Constants of the pendulum were chosen to be $m = 1, l = 10$ and initial values of $q_0 = \pi/4$ and $p_0 = 0$. For schemes 1 and 2 since in both cases extra set of values at half-steps was needed, they were set equal to the same initial values. Additionally, the time-step chosen was $\Delta t = 0.001$.

Figure 1 illustrates the relative error values of the consecutive sub-trajectory scheme (26) (scheme 1) together with the intersecting sub-trajectory scheme (33) (scheme 2) and the PSVM (29). From the results it can be clearly seen that schemes 1 and 2 are effectively the same, with the only difference being in how many oscillations the schemes go through in the same time period, which is due to the factor of two. Averaging the Hamiltonian values obtained throughout the integration scheme showed low uncertainties with $\pm 8.23 * 10^{-4}\%$ for scheme 1 and $\pm 1.93 * 10^{-3}\%$ for scheme 2. With the PSVM as expected showing much better results at a $\pm 2.40 * 10^{-5}\%$ uncertainty. In the following section the same schemes were applied to an inseparable Hamiltonian system.

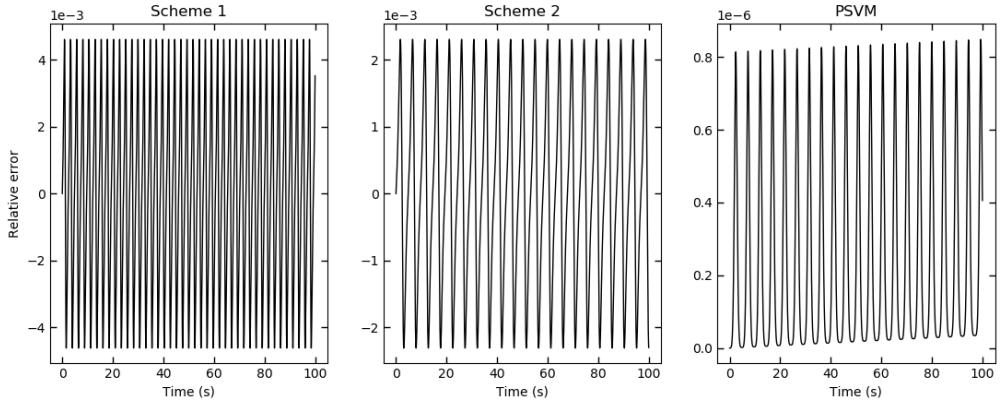

Figure 1. Relative errors in the Hamiltonian values from each of the three discussed integration schemes. Schemes 1 and 2 show periodic oscillations around the initial value with a small error. Stormer-Verlet scheme shows a similar oscillation above the initial value and illustrates near preservation of energy.

4.2 Simple inseparable Hamiltonian test case

In a recent paper submitted November 2021 [11], extended phase space was explored further together with a symmetric projection method to derive a symplectic integration scheme for non-separable Hamiltonian systems. One of the test cases used was a simple Hamiltonian of the form

$$H(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{2}(\boldsymbol{q}^2+1)(\boldsymbol{p}^2+1)\,. \tag{34}$$

Schemes discussed already in this project were applied to (34) to test if the behaviour is similar to the single pendulum case. Initial values were set to $q_0 = -3$ and $p_0 = 0$, and the same time period was considered with a $\Delta t = 0.001$ time-step. Figure 2 illustrates relative Hamiltonian error results obtained.

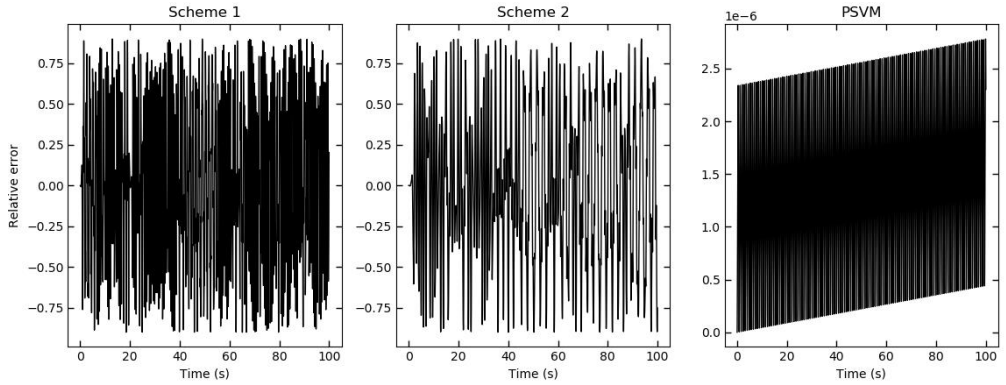

Figure 2. Relative Hamiltonian error value results obtained by implementing the schemes to (31). Schemes 1 and 2 still show oscillation around the true value but with a very high error, indicating that they are not applicable for such systems. PSVM on the other hand shows identical behaviour to the single pendulum test case.

The expected behaviour of PSVM in a non-separable system showcases that the implementation was done correctly and that indeed (29) and (30) are applicable to such systems. Schemes derived in this project appear to break down when implemented to a non-separable Hamiltonian. Reasons for this and further steps to be taken to improve them will be discussed in the discussion. Uncertainties in the Hamiltonian values

were again calculated for consistency purposes showing the following results: uncertainty in scheme 1 $\pm 1.11 * 10^{-1}\%$; uncertainty in scheme 2 $\pm 1.74 * 10^{-1}\%$; PSVM had an uncertainty of $\pm 1.44 * 10^{-4}\%$.

5. Discussion

Positive single pendulum and negative non-separable Hamiltonian system results show that following the methodology in this project allowed for separable Hamiltonian integration schemes to be derived, but further development is needed to derive non-separable Hamiltonian integration schemes. Oscillations seen in figure 1 perfectly illustrate a property of discrete variational integrators which come from discretizing the action. In the discretization, a time step must be introduced allowing one to relate discrete and continuous mechanics. This means that using these integrators the Hamiltonian will not be exactly preserved, but by error analysis methods it can be shown that it will be "nearly preserved" for exponentially long times [12]. This can be seen in figure 1 for all the schemes and in figure 2 for the PSVM. To add on, PSVM showed a linear take-off from the initial Hamiltonian value in both tested systems, same phenomena can be seen in [13] where the Störmer-Verlet method was tested on a Toda lattice, a Hamiltonian system used to describe one dimensional crystal lattices. It is interesting to note that whilst in the non-separable case the maximum uncertainty in the Hamiltonian is too large for both schemes 1 and 2, indicating clearly that they cannot be considered good integration schemes for the system; the averages still give the initial Hamiltonian value within reason. Further testing and a larger number of results should be obtained to investigate if this is consistent. Nevertheless, it can be argued that for a separable Hamiltonian system the derived schemes performed admirably well. Work on the project not included in this report included considering the whole path to be made up of only two sub-trajectories. In those cases, problems with definitions of values at the boundaries made the integration schemes give varying results which were not immediately realised to be wrong.

The fact that schemes derived are not applicable to non-separable Hamiltonians stems from the fact that partial derivatives of the Hamiltonian were treated as if it was separable. When taking the partial derivatives, the Hamiltonian should have been treated in the following manner

$$\frac{\partial \mathrm{H}}{\partial p_0} = \frac{\partial \mathrm{H}}{\partial q}\frac{\partial q}{\partial p_0} + \frac{\partial \mathrm{H}}{\partial p}\frac{\partial p}{\partial p_0} \ . \tag{35}$$

Application of (32) to the method would serve as a solid basis for further work in this area. To go in parallel with treating the Hamiltonians differently, higher order quadrature methods used for approximations are a promising way of making the integration schemes more accurate. As trapezium rule treats the paths as straight lines when parabolas are likely to be a more physical representation.

6. Conclusions

Hamiltonian formalism was applied to a dynamical system via Legendre transforms from a Lagrangian formalism. The total action of the system was approximated using trapezoid rule and defined as a sum of sub-trajectories containing information about the variable values of two consecutive points. Partial derivatives were taken with respect to the variables inside the action to derive two similar Hamiltonian integration schemes. The schemes were applied to separable and non-separable Hamiltonian systems showing to be applicable to the first but not to the latter. Discrete variational integrator properties were seen in both set of results. The fact that a paper on the topic was published so recently, shows that this is a very active field of research in the numerical analysis field. Whilst the methodology used in both [10] and [11] perform the derivations with much more mathematical formality, method used in this project attempts to capture the logic in a more intuitive way, without introducing complicated topics such as Lie Algebra. The limitations of the method were recognized as a low order integral approximation, as well as the partial

derivatives of the Hamiltonians being treated as separable functions. Future work could develop the mathematics further by using equation (35) in the derivations of the integration schemes.

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