Math 470

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Abstract

In this project we explore geometric properties of numerical integrators applied to Hamiltonian ordinary differential equations; we study the n-body problem, chosen for it's wealth of symmetries and chaotic behavior. We combine symplectic numerical schemes [4] with projections onto invariant manifolds, which we obtain with well known symmetry methods for dimensionality reduction [6]. Using backward error analysis we show that the projections violate symplecticity; postulating that projection methods may give rise to an attractor - a subset of the preserved manifold, we investigate the Lyapunov spectrum of our modified equations but find evidence that for $n \geq 3$ the projection methods make the equations *more* chaotic.

Contents

1 Lie Symmetries for Solving DEs

1.1 Preliminaries.

This section draws largely from [10],[6].

We start by considering first order differential equations of the form

$$\frac{dy}{dx} = \omega(x, y) \qquad , \qquad \mathbb{R} \supset D \to \mathbb{R} \tag{1}$$

A **symmetry** of an ode (1) is a diffeomorphism $\Gamma : \mathbb{R}^2 \to \mathbb{R}^2$ with $(x, y) \mapsto (\hat{x}, \hat{y})$ such that the differential equation is preserved.

$$\frac{d\hat{y}}{d\hat{x}} = \omega(\hat{x}, \hat{y})$$

we can simplify the above equation to obtain

*The **symmetry condition*** (2). We derive a formula by taking the total derivative with respect to x, the quotient

$$\frac{d\hat{y}}{d\hat{x}} = \frac{dx\partial_x\hat{y} + dy\partial_y\hat{y}}{dx\partial_x\hat{x} + dy\partial_y\hat{y}} = \frac{D_x\hat{y}}{D_x\hat{x}} = \frac{\partial_x\hat{y} + \frac{dy}{dx}\partial_y\hat{y}}{\partial_x\hat{x} + \frac{dy}{dx}\partial_y\hat{x}} = \omega(\hat{x}, \hat{y}) \tag{2}$$

It is clear that the set of symmetries $\{\Gamma : \mathbb{R}^2 \to \mathbb{R}^2 | (2) \text{ holds}\}$ is closed under composition and inverses, and thus forms a group. Lie groups are continuous groups which are also smooth manifolds. An *invariant point* is mapped to it's self by every lie symmetry. An *invariant solution*

of some symmetry Γ is mapped to it's self by Γ, so $S_1 = \{(x, f(x)) : x \in \mathbb{R}\}$ is invariant iff $\Gamma(x, f(x)) = (x', f(x'))$.

Given a group G acting on the plane $\mathbb{R}^2$, the symmetries S of a differential equation, this can be written $G \curvearrowright S$ or $G \to \mathrm{Sym}(S) \subset \mathrm{Diffeomorphisms}(\mathbb{R}^2 \to \mathbb{R}^2)$. The *orbit* of an element (x, y) is the set of elements $G \cdot (x, y) = \{(\hat{x}, \hat{y}) : \exists \Gamma \in G | \Gamma(x, y) = (\hat{x}, \hat{y})\}$.

The action of a one parameter (denoted by ϵ) lie group for sufficiently small ϵ can be approximated by the Taylor expansion

$$\Gamma_\epsilon : (x, y) \mapsto (\hat{x}, \hat{y})_\epsilon \text{ s.t. } \begin{cases} \hat{x} = x + \epsilon \xi(x, y) + O(\epsilon^2) & : \quad \frac{d\hat{x}}{d\epsilon} = \xi(\hat{x}, \hat{y}) \\ \hat{y} = y + \epsilon \eta(x, y) + O(\epsilon^2) & : \quad \frac{d\hat{y}}{d\epsilon} = \eta(\hat{x}, \hat{y}) \end{cases} \tag{3}$$

Locally, the orbit $(\hat{x}(\epsilon), \hat{y}(\epsilon))$ of a lie group action is a parameturized smooth surface - in this case it is a curve since we only consider a one-parameter lie group.

We introduce the **characteristic** $\mathcal{Q}(x, y, y') = \eta(x, y) - y'\xi(x, y)$ and the **reduced characteristic** $\overline{\mathcal{Q}}(x, y; \omega(x, y)) = \eta(x, y) - \omega(x, y)\xi(x, y)$ as a tool to help us talk about invariant solutions concisely. An *invariant point* is mapped to it's self by every symmetry, so we require that $\xi(x, y) = \eta(x, y) = 0$. The condition for an *invariant solution* is weaker, we do not require that every point on the solution is invariant, only that the action of the infinitesimal lie group generator is along the solution; in other words, given the solution curve $y = f(x)$ the solution is invariant under the lie symmetry parameturized by ϵ if and only if $\overline{\mathcal{Q}}(x, f(x)) \equiv 0$.

([6] p19 thought 21 and 31 for linearized characteristic)

The n-th **jet-space** J^n of an ode $\dot{y}(t) = \omega(t, y, y', y'', \cdots, y^{(n)})$ is the $n + 2$ dimensional Euclidean space spanned by t, y and the first n derivatives of y, i.e. it is spanned by the variables $(t, y, y^{(1)}, y^{(2)}, \cdots, y^{(n)})$. Each solution curve $y(t)$ defines a curve parameturzied by t in the jet space called the **lift**. The ode defines a hyper-surface S on the jet-space. The map which brings each solution curve to it's lift is injective, and the image of the solution set in the jet-space is S. The extension of the action Γ to all derivatives of order n or less is the n-th **prolongation** of Γ; Γ maps solution curves to solution curves, thus it's prolongation maps S to it's self.

1.2 Lie Groups and Algebras.

A **group** G is a set together with a binary operation $* : G \to \mathrm{End}(G)$ or $* : G \times G \to G$. Axioms : identity, asociativity, closed under composition and inverses.

A **Lie Group** is an infinite group which is also a **differentiable manifold**. We restrict our attention to manifolds embedded in an ambient space $\mathbb{R}^n$. Therefore a Lie Group is a differentiable manifold $\mathcal{M} \subset \mathbb{R}^n$ with a binary operation $* : \mathcal{M} \to \{f : \mathcal{M} \to \mathcal{M} : f \text{ is a bijective diffeomorphism}\}$. The binary operation $*$ takes an element $g \in \mathcal{M}$ to a *bijective diffeomorphism* f_g of the manifold G. We can think about a lie group abstractly as a group G with a map $F : G \to \mathcal{M} \times \mathrm{diff}(\mathcal{M})$. So $F(g) = \{m_g, f_g\}$, the image of $g \in G$ is a point $m_g \in \mathcal{M}$ and a diffeomorphism $f_g : \mathcal{M} \to \mathcal{M}$. The identity of the lie group is $F(\mathbb{1}_G) = \{p, \mathbb{1}_{\mathrm{diff}(\mathcal{M})}\}$. Sometimes we wish to only consider the group properties of some specific lie group, to consider only the group structure (without the manifold), in which case we can view the lie group as, more fundamentaly, a continuous group which admits a faithful and continuous (or is it sensible to use differentiable) representation on the bijective diffeomorphisms of some differentiable manifold. We have set ourselves up to define the lie algebra.

A **Lie Algebra** $\mathfrak{g}$ of a lie group G is the tanjent space at the identity $T_p\mathcal{M}$ together with an alternating bi-linear map $\mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, $(a, b) \mapsto [a, b]$ called the **lie bracket**, the lie bracket operator

is induced by the group binary operation $*$.

1.3 Canonical Coordinates

Canonical Coordinates are a coordinate system $(r(x,y), s(x,y)) = \Phi(x,y)$ such that $\Phi \circ \Gamma_\epsilon(x,y) = (\hat{r}, \hat{s}) = (r(\hat{x}, \hat{y}), s(\hat{x}, \hat{y})) = (r, s + \epsilon)$; The necessary and sufficient condition for a coordinate system to be canonical with respect to some lie symmetry (in the plane) is

$$\left.\frac{d\hat{r}}{d\epsilon}\right|_{\epsilon=0} = 0, \quad \left.\frac{d\hat{s}}{d\epsilon}\right|_{\epsilon=0} = 1 \tag{4}$$

if we can find functions $r(x,y)$ and $s(x,y)$ such that (4) holds, then we can integrate the differential equation (1) directly by quadrature. Using the chain rule we see that (4) becomes

$$\xi\,\partial_x r + \eta\,\partial_y r = 0 \quad , \quad \xi\,\partial_x s + \eta\,\partial_y s = 1 \tag{5}$$

we impose the extra condition that the jacobian of the change of coordinates is non-degenerate

$$|D\Phi| = r_x s_y - r_y s_x \neq 0$$

Curves of constant r are locally invariant under the orbits of the lie group, by definition their tangents coincide $\frac{dr}{d\epsilon} = 0$, hence r is refered to as an *invariant canonical coordinate*.

A non-constant function $\phi(x,y)$ is called a *first integral* of a first order ODE

$$\frac{dy}{dx} = f(x,y)$$

if it's value is constant on any solution $y = y(x)$. Hence it's gradient will be perpendicular to the tanjent vectors of the solution

$$(1, f(x,y)) \cdot \nabla\phi = \phi_x + f(x,y)\phi_y = 0$$

the general solution can be written as level curves of the first integral $\phi(x,y) = c$. Hence we can find the *invariant canonical coordinate* by solving (6) which follows from (5) and the above identity

$$\frac{dy}{dx} = \frac{\eta(x,y)}{\xi(x,y)} \tag{6}$$

once we have found r we use $r(x,y)$ to find $y(r,x)$ or $x(r,y)$, then using

$$1 = \frac{ds}{d\epsilon} = \frac{\frac{dx}{d\epsilon}}{\xi(x,y)} = \frac{\frac{dy}{d\epsilon}}{\eta(x,y)}$$

we can integrate with respect to ϵ to recover

$$(r,x) = \int \frac{dx}{\xi(x, y(r,x))} = \int \frac{dy}{\eta(x(r,y), y)} \tag{7}$$

1.4 Finding symmetries, the linearised symmetry condition.

When looking for symmetries, we are essentially looking for a vector field satisfying the *linearised symmetry condition*(8), which is arrived at by substituting the Taylor expansion of Γ_ϵ (3) into the symmetry condition (2) and equating the order ϵ^1 terms

$$\eta_x + (\eta_y - \xi_x)\omega - \xi_y\omega^2 = \xi\omega_x + \eta\omega_y \tag{8}$$

practically this is useful because (8) is often easier to solve by Anzats than the original symmetry condition (2)

(p39ish of [6]). We can view a lie symmetry as being generated by an **infinitesimal generator** of a lie group in the plane. The infinitesimal generator is defined as follows

$$X = \xi(x,y)\partial_x + \eta(x,y)\partial_y \tag{9}$$

hence the, the canonical coordinates $r(x,y), s(x,y)$ can be rewritten $Xr = 0 \qquad Xs = 1$. A lie symmetry generated by X acts on a the Hilbert space $\mathcal{H}$ of smooth function $F : \mathbb{R}^2 \to \mathbb{R}$ be written in terms of it's generator

$$F(\Gamma_\epsilon(x,y)) = F(\hat{x}, \hat{y}) = F(e^{\epsilon X}\hat{x}, e^{\epsilon X}\hat{y}) = e^{\epsilon X}F(x,y) \tag{10}$$

We can recover Γ_ϵ thanks to the correspondence between a lie symmetry Γ_ϵ and it's tanjent field (ξ, η), which is also the tanjent field of $e^{\epsilon X}$. So $\Gamma_\epsilon = e^{\epsilon X}$

1.5 Noether's Theorem

There is a statement of Noether's theorem in [4] (Hairer & Lubich - geometric numerical integration) at the bottom of page 210. Another statement of Noether's theorem can be found on page 88 of [1] (Arnold, mathematical methods of classical mechanics).

One statement of Noether's theorem [1].

Let M be a smooth manifold and $\mathcal{L} : TM \to \mathbb{R}$ a smooth function on it's tanjent bundle. Let $h^s : M \to M$ be a smooth map and $h^s_* : TM \to TM$ is the canonical extension of h^s to TM (Levi-Civita connection).

Definition A Lagrangian system $(M, \mathcal{L})$ *admits the mapping* h if for any vector $v_q \in TM$

$$\mathcal{L}(v_q) = \mathcal{L}(h_* v_q)$$

Noether's Theorem. If the system $(M, \mathcal{L})$ admits the one parameter lie group of diffeomorphisms $h^s : M \to M$, $s \in \mathbb{R}$, then the Lagrangian of the system of equations corresponding to $\mathcal{L}$ has the first integral $I : TM \to \mathbb{R}$.

In local coordinates, let $M = \mathbb{R}^n$ be coordinate space. Let $q : \mathbb{R}^2 \to M$, $q(s,t) = h^s\phi(t)$, where we denote the time derivative $\partial_t q =: \dot{q}$, q is a solution to Lagrange's equations for any fixed s. Since h^s_* preserved $\mathcal{L}(q, \dot{q})$. Making use of the Euler-Lagrange equations (14) we have

$$\frac{\partial \mathcal{L}}{\partial s} = \frac{\partial \mathcal{L}}{\partial q}\frac{\partial q}{\partial s} + \frac{\partial \mathcal{L}}{\partial \dot{q}}\frac{\partial^2 q}{\partial t \partial s} = \left(\frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{q}}\right)\frac{\partial q}{\partial s} + \frac{\partial \mathcal{L}}{\partial \dot{q}}\left(\frac{\partial}{\partial t}\frac{\partial q}{\partial s}\right) = \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\frac{\partial q}{\partial s}\right) = 0 \tag{11}$$

integrating with respect to dt we obtain the first integral (12)

$$I(q, \dot{q}) = \frac{\partial \mathcal{L}}{\partial \dot{q}}\frac{\partial q}{\partial s} = \text{cnst. wrt } t \tag{12}$$

1.5.1   A basic example of Noether's theorem applied to a Lagrangian system

We start with a simple version of the theorem, applied to Lagrangian systems for many bodies [8].

$$\mathcal{L}(q, \dot{q}) = T - U \tag{13}$$

motion is described by the Euler-Lagrange equation which occurs when the action $\int_{t_0}^{t_f} \mathcal{L}(q, \dot{q})dt$ is stationary

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial q} \tag{14}$$

with the added condition, typical of many body and other systems

$$\dot{p} = \frac{\partial \mathcal{L}}{\partial q} \qquad\qquad p = \frac{\partial \mathcal{L}}{\partial \dot{q}} \tag{15}$$

One parameter lie groups of symmetries lead to conserved quantities. Each symmetry $\Gamma_\epsilon :$ $(q, \dot{q}) \mapsto (q(\epsilon), \dot{q}(\epsilon))$ which preserves the Lagrangian $\frac{\partial}{\partial \epsilon}\mathcal{L}(q(\epsilon, t), \dot{q}(\epsilon, t)) = 0$ implies a conserved quantity. To see this we take the partial derivative

$$\frac{\partial}{\partial \epsilon}\mathcal{L}(q, \dot{q}) = \frac{\partial q}{\partial \epsilon}\frac{\partial \mathcal{L}}{\partial q} + \frac{\partial \dot{q}}{\partial \epsilon}\frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial q}{\partial \epsilon}\frac{\partial p}{\partial t} + p\frac{\partial^2 q}{\partial t \partial \epsilon} = \frac{\partial}{\partial t}\left(p\frac{\partial q}{\partial \epsilon}\right) = 0 \tag{16}$$

Example As an illustration, consider the free particle Lagrangian, $U(q, \dot{q}) = C$, then the Lagrangian admits the symmetry

$$\Gamma_\epsilon : (p, q) \mapsto (\hat{p}, \hat{q}) = (p, q + v\epsilon) \qquad \Rightarrow \begin{cases} \partial_\epsilon \hat{p} = 0 \\ \partial_\epsilon \hat{q} = v \end{cases}$$

where v is some (constant wrt t and ϵ) translation vector v. We verify that $\partial_\epsilon \mathcal{L} = 0$

$$\partial_\epsilon \mathcal{L} = \frac{\partial q}{\partial \epsilon}\frac{\partial \mathcal{L}}{\partial q} + \frac{\partial^2 q}{\partial \epsilon \partial t}\frac{\partial \mathcal{L}}{\partial (\partial_t q)} = v\frac{\partial \mathcal{L}}{\partial q} + \frac{\partial v}{\partial t}\frac{\partial \mathcal{L}}{\partial (\partial_t q)} = -v\nabla U + 0 \cdot \frac{\partial \mathcal{L}}{\partial(\partial_t q)} = 0$$

hence applying (16) we find that the momentum of such a system is conserved

$$\partial_t\left(p\frac{\partial q}{\partial \epsilon}\right) = \partial_t(pv) = 0 \Rightarrow \partial_t p = 0 \tag{17}$$

Example Another example is conservation of angular momentum, in the single body problem. Here we take $q = (x, y, z)$ and $p = \mu\dot{q}$ where mu is the (reduced) mass. The Lagrangian here is given in Cartesian coordinates

$$\mathcal{L}(q, \dot{q}) = T - U = \frac{\dot{q}^2}{2\mu} - U(|q|) \tag{18}$$

we show that the angular momentum operator $L^2 = (\vec{r} \times \vec{p})^2$ is a symmetry of the Lagrangian. Using the identity (I derived it from an equation in Townsend [11]) $\vec{r} \times \vec{p} = \vec{r}^2\vec{p}^2 - (\vec{r} \cdot \vec{p})^2$ we derive conservation of momentum, [**see also if you can find how conservation of momentum in the z direction works, try the generator** $-y\partial_x + x\partial_y$ **...**]

2 Celestial mechanics, the N-Body problem.

In this section we introduce the n-body problem in Euclidean space starting with 2 bodies, then 3 and then n. We look at the symmetries of the Lagrangian and find the first integrals in each case.

2.1 The Kepler Problem

The Hamiltonian for the two body problem is

$$H(p,q) = E = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} - \frac{Gm_1m_2}{|q_2 - q_1|} \tag{19}$$

with $\xi := |q_2 - q_1|$ and $\eta := -Gm_1m_2$ we obtain with $\xi_1 = q_{21} - q_{11}$ and $\xi_2 = q_{22} - q_{12}$, so $\xi = \sqrt{\xi_1^2 + \xi_2^2}$.

$$\nabla H_{kepler}(p,q) = \begin{pmatrix} \frac{p_{11}}{m_1} & \frac{p_{12}}{m_1} & \frac{p_{21}}{m_2} & \frac{p_{22}}{m_2} & \frac{\eta}{\xi^3}\xi_1 & \frac{\eta}{\xi^3}\xi_2 & -\frac{\eta}{\xi^3}\xi_1 & -\frac{\eta}{\xi^3}\xi_2 \end{pmatrix} \tag{20}$$

We compute the the hessian $D^2 H$, see (...resources, places in document and outside...)

$$D^2 H = \left(\begin{array}{cccc|cccc} 1/m_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/m_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/m_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/m_2 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \frac{-\eta}{\xi^3} + \frac{\eta}{\xi^5}\xi_1^2 & \frac{\eta}{\xi^5}\xi_1\xi_2 & \frac{\eta}{\xi^3} - \frac{\eta}{\xi^5}\xi_1^2 & \frac{-\eta}{\xi^5}\xi_1\xi_2 \\ 0 & 0 & 0 & 0 & \frac{\eta}{\xi^5}\xi_1\xi_2 & \frac{-\eta}{\xi^3} + \frac{\eta}{\xi^5}\xi_2^2 & \frac{-\eta}{\xi^5}\xi_1\xi_2 & \frac{\eta}{\xi^3} - \frac{\eta}{\xi^5}\xi_2^2 \\ 0 & 0 & 0 & 0 & \frac{\eta}{\xi^3} - \frac{\eta}{\xi^5}\xi_1^2 & \frac{-\eta}{\xi^5}\xi_1\xi_2 & \frac{-\eta}{\xi^3} + \frac{\eta}{\xi^5}\xi_1^2 & \frac{\eta}{\xi^5}\xi_1\xi_2 \\ 0 & 0 & 0 & 0 & \frac{-\eta}{\xi^5}\xi_1\xi_2 & \frac{\eta}{\xi^3} - \frac{\eta}{\xi^5}\xi_2^2 & \frac{\eta}{\xi^5}\xi_1\xi_2 & \frac{-\eta}{\xi^3} + \frac{\eta}{\xi^5}\xi_2^2 \end{array} \right) \tag{21}$$

The angular momentum

$$L(p,q) = \sum q_i \wedge p_i = \begin{vmatrix} q_{11} & p_{11} \\ q_{12} & p_{12} \end{vmatrix} + \begin{vmatrix} q_{21} & p_{21} \\ q_{22} & p_{22} \end{vmatrix} = q_{11}p_{12} - q_{12}p_{11} + q_{21}p_{22} - q_{22}p_{21} \tag{22}$$

so

$$\nabla L(p,q) = \begin{pmatrix} -q_{12} & q_{11} & -q_{22} & q_{21} & p_{12} & -p_{11} & p_{22} & -p_{21} \end{pmatrix} \tag{23}$$

and the hessian is

$$D^2 L(p,q) = \left(\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \tag{24}$$

it is evident that $D^3 L = 0$

2.2   N bodies.

We use the notation

$$\xi_{ij} := q_j - q_i \qquad {}_k\xi_{ij} := {}_kq_j - {}_kq_i \qquad\qquad \xi_{ij} \in \mathbb{R}^3 \quad , \quad {}_k\xi_{ij} \in \mathbb{R}$$

Each point-mass is described by 6 dimensions of phase space, so this is a $6n$ dimensional ODE. The Lagrangian is

$$\mathcal{L}(q,\dot{q}) = T - U = \sum_i \frac{1}{2}m_i\dot{q}_i^T\dot{q}_i - \sum_{i<j}\frac{Gm_im_j}{\sqrt{\xi_{ij}^T\xi_{ij}}} \tag{25}$$

taking the partial derivative with respect to ${}_kq_i$ (rem $k \in \{x,y,z\}$) we get

$$\frac{\partial L}{\partial\,{}_kq_i} = \sum_{\substack{j=1\\j\neq i}}^n \frac{Gm_im_j}{\left(\xi_{ij}^T\xi_{ij}\right)^{3/2}}\,{}_k\xi_{ij} \tag{26}$$

2.2.1   Symmetries of the n-body problem.

Energy, total momentum, total angular momentum.

The Lagrangian is invariant with respect to the lie group of **translations** in any direction $x_i \in \{x,y,z\}$, this is an abelian group of symmetries of the form $\Gamma_s : (q,\dot{q}) \mapsto (q+vs,\dot{q})$, we show that the Lagrangian is invariant

$$\frac{\partial\mathcal{L}(q(t,s),\dot{q}(t,s))}{\partial s} = \frac{\partial\mathcal{L}}{\partial q}\frac{\partial q}{\partial s} = \sum_{k\in\{x,y,z\}} v_k\left(\sum_{i=1}^n \frac{\partial\mathcal{L}}{\partial\,{}_kq_i}\right) = \sum_{k\in\{x,y,z\}} v_k\left(\sum_{i=1}^n\left[\sum_{\substack{j=1\\j\neq i}}^n \frac{Gm_im_j}{\left(\xi_{ij}^T\xi_{ij}\right)^{3/2}}\,{}_k\xi_{ij}\right]\right)$$

$$= \sum_{k\in\{x,y,z\}} v_k\left(\sum_{i,j} \frac{Gm_im_j}{\left(\xi_{ij}^T\xi_{ij}\right)^{3/2}}\left[{}_k\xi_{ij} + {}_k\xi_{ji}\right]\right) = 0$$

By Noether's theorem (12) we have

$$\frac{\partial L}{\partial\dot{q}}^T \vec{v} = \text{cnst.} \Rightarrow \sum_i m_iq_i = \text{cnst.} \tag{27}$$

This is a statement of conservation of total linear momentum an n-3 dimensional first integral.

Our system is conservative, autonomous: the Lagrangian $L(q,\dot{q},t)$ does not depend explicitly on time translations

$$\frac{\partial\mathcal{L}}{\partial t} = 0$$

therefore the **energy** is conserved

$$\frac{\partial\mathcal{L}}{\partial\dot{q}}\frac{\partial q}{\partial t} = \sum_i m_i\dot{q}_i^T\dot{q}_i = 2T = \text{cnst.} \tag{28}$$

The Lagrangian is invariant with respect to total **rotations**, rotations about any axis can be expressed as compositions of rotations about the x, y and z axes. It is sufficient to show that the

Lagrangian is invariant under rotations about the z axis. The generator or rotations about the z axis is the operator (29)

$$\sum_i \left({}_yq_i \frac{\partial}{\partial\, {}_xq_i} - {}_xq_i \frac{\partial}{\partial\, {}_yq_i} \right) \tag{29}$$

applying this to the Lagrangian of the system we obtain

$$\sum_i \left(\sum_{\substack{j \\ j\neq i}} \left[{}_yq_i \frac{Gm_im_j}{(\xi_{ij}^T\xi_{ij})^{3/2}} {}_x\xi_{ij} - {}_xq_i \frac{Gm_im_j}{(\xi_{ij}^T\xi_{ij})^{3/2}} {}_y\xi_{ij} \right] \right) = \\ \sum_{i<j\leq n} \left(\frac{Gm_im_j}{(\xi_{ij}^T\xi_{ij})^{3/2}} \left[{}_yq_i\,{}_x\xi_{ij} - {}_xq_i\,{}_y\xi_{ij} + {}_yq_j\,{}_x\xi_{ji} - {}_xq_j\,{}_y\xi_{ji} \right] \right) = 0 \tag{30}$$

From this we obtain the conservation law

$$\text{cnst.} = \frac{\partial\mathcal{L}}{\partial\dot{q}} \sum_i \left({}_yq_i \frac{\partial q}{\partial\, {}_xq_i} - {}_xq_i \frac{\partial q}{\partial\, {}_yq_i} \right) = \sum_i \left({}_xp_i\,{}_yq_i - {}_yp_i\,{}_xq_i \right) \tag{31}$$

Hence the **angular momentum** in the z direction is conserved $L_z = \text{cnst}$. We can apply the same argument for L_x and L_y. Thus we have found three more first integrals.

3 Numerical Integration, Theory

3.1 Symplectic Manifolds and Symplectic Transformations

[pointers for research in this section : [2],[4],[3]]

A **Symplectic Manifold** is an even dimentional manifold which admits a **symplectic form** - a closed non-degenerate (skew-symmetric) 2-form $\omega^2 : TM \otimes TM \to \mathbb{R}$. Non-degenerate means that for each vector $\rho_p \in T_pM \quad \exists\rho_p' : \omega_p(\rho,\rho') \neq 0$.

A **Symplectic Transformation** is a map which preserves the symplectic form, in $\mathbb{R}^{2d}$ this is a map g such that $\omega(\xi,\eta) = \omega(g'(\xi), g'(\eta))$. The canonical symplectic form can be written as an anti-symmetric matrix $\omega(\xi,\eta) = \xi^T J\eta$ where the matrix J is

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \in \mathbb{R}^{2d\times 2d} \qquad \text{note that} \quad J^{-1} = -J = J^T = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \tag{32}$$

The **flow** of a system $\dot{y} = f(y)$ is a function ϕ_t which time evolves the system by t; it is the map

$$\psi_t : y_0 \mapsto y(t) \qquad \text{if} y_0 = y(0) \tag{33}$$

With regard a hamiltonian system, $\dot{y} = J^{-1}\nabla H(y = (p,q))$. When the system is autonomous (or conservative $H = cnst$) then we can express the time evolution operator in terms of the hamiltonian equation by exponentiation

$$\psi_t(y) = e^{J^{-1}\nabla Ht}(y) \tag{34}$$

We refer to the maps $\Phi : y_n \mapsto y_{n+1}$ as the **numerical flow** or **discrete flow**.

3.2   Lagrangian systems are Hamiltonian systems.

We show that Lagrangian systems are Hamiltonian, by constructing a Hamiltonian system from a Lagrangian one (Hamiltonian systems however are not generally Lagrangian). Lagrangian systems are characterised by

$$\mathcal{L}(q, \dot{q}) = T - U \qquad \mathcal{L} : TM \to \mathbb{R}$$

the manifold M is called the configuration manifold, in local coordinates $q = q_1, ..., q_d$ is a basis for U_α - one of the coordinate charts in the atlas $\phi_\alpha : U_\alpha \hookrightarrow M$. From the Lagrangian we define the 'conjugate' momentum to be

$$p_k := \frac{\partial L}{\partial \dot{q}_k}$$

thus we define our Hamiltonian function

$$H(p, q) = p^T \dot{q}(p, q) - \mathcal{L}(q, \dot{q})$$

An important distinction between Lagrangian and Hamiltonian systems is that the phase space of a Lagrangian system is always the tanjent bundle of some configuration manifold, whereas Hamiltonian systems are defined on arbitrary symplectic manifolds. In other words, the q in a Lagrangian represents postition and the p has to do with change in $\dot{q}$; whereas I think in Hamiltonian systems p and q are more abstract...?

3.3   Hamiltonian systems and Symplecticity.

The following proofs and theorems draw heavily from [4].

    Theorem (Poincaré). Let $H(p, q)$ be twice continuously differentiable on $U \subset \mathbb{R}^{2d}$. Then for each fixed t, the flow ψ_t is a symplectic transformation. To see this we observe that $D\psi_t \equiv \frac{\partial \psi_t}{\partial y_0}$ at $t = 0$ is trivially the identity map

$$\left. \frac{\partial \psi_t}{\partial y_0} \right|_{t=0} = \mathbb{1} \quad \Rightarrow \quad \left. \frac{\partial \psi_t}{\partial y_0}^T J \frac{\partial \psi_t}{\partial y_0} \right|_{t=0} = J \tag{35}$$

we take the time derivative of the symplectic form applied to the Jacobian

$$\frac{d}{dt} \left(\frac{\partial \psi_t}{\partial y_0}^T J \frac{\partial \psi_t}{\partial y_0} \right) = \left(\frac{\partial^2 \psi_t}{\partial t \partial y_0} \right)^T J \frac{\partial \psi_t}{\partial y_0} + \frac{\partial \psi_t}{\partial y_0}^T J \left(\frac{\partial^2 \psi_t}{\partial t \partial y_0} \right) \tag{36}$$

by the equality of mixed partials we obtain (37) from the equation of motion

$$\frac{\partial^2 \psi_t}{\partial t \partial y_0} = \frac{\partial}{\partial y_0} \frac{\partial \psi_t}{\partial t} = \frac{\partial}{\partial y_0} J^{-1} \nabla H(\psi_t) = J^{-1} D^2 H \frac{\partial \psi_t}{\partial y_0} \tag{37}$$

substituting (37) into (36) we get (38), which evaluates to zero since $J^{-T} = J$ and $J^2 = -\mathbb{1}$.

$$\frac{d}{dt} \left(\frac{\partial \psi_t}{\partial y_0}^T J \frac{\partial \psi_t}{\partial y_0} \right) = \frac{\partial \psi_t}{\partial y_0}^T D^2 H J^{-T} J \frac{\partial \psi_t}{\partial y_0} + \frac{\partial \psi_t}{\partial y_0}^T J J^{-1} D^2 H \frac{\partial \psi_t}{\partial y_0} = 0 \tag{38}$$

It follows from (38) and (35) that the flow is symplectic (39).

$$\frac{\partial \psi_t}{\partial y_0}^T J \frac{\partial \psi_t}{\partial y_0} = J \tag{39}$$

$\square$

We define what it means to be **locally hamiltonian** and then prove a slightly weaker version of the converse of Pointcaré's above theorem, that symplectic systems are locally hamiltonian. A system $y' = f(y) \mid f : U \subset \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is said to be locally hamiltonian if for each $y_0 \in U$ there exists an open neighbourhood $N_{y_0} \subset \mathbb{R}^{2d}$ containing y_0 and some function $H_{y_0} : N_{y_0} \to \mathbb{R}$ such that $f(y) = J^{-1}\nabla H(y) \quad \forall y \in N_{y_0}$. Locally hamiltonian systems defined over simply connected domains are globally hamiltonian; more precisely if the vector field (or one form) of the system is exact and locally hamiltonian, then the system is globally hamiltonian.

Lemma. *(Integrability Lemma) [4] Let $D \subset \mathbb{R}^{2n}$ open, $f : D \to \mathbb{R}^{2d}$ differentiable and such that the Jacobian $f'(y)$ is symmetric, $\frac{\partial f_j}{\partial k} = \frac{\partial f_k}{\partial j}$. For every $y_0 \in D$ there exists a real valued differentiable function H defined in a neighbourhood of $y_0 \in N_{y_0} \subset D$, with $H : N_{y_0} \to \mathbb{R}$ such that $f = \nabla H$. In other words the differential form $f_1(y)dy_1 + \cdots f_{2d}(y)dy_{2d} = dH$ is a total differential (dH is exact, but it is only defined locally on some simply connected domain aka trivial deRham cohomology).*

Proof. Consider a ball $N_{y_0} \subset D$ around y_0, assume $y_0 = 0$ and let

$$H(y) = \int_0^1 (y)^T f(ty) dt + \text{cnst}.$$

taking the partial derivatives we obtain

$$\begin{aligned}
\frac{\partial H}{\partial y_k} &= \int_0^1 f_k(ty) + ty^T \frac{\partial f}{\partial y_k}(ty) dt \\
&\overset{\text{symmetry}}{=} \int_0^1 f_k(ty) + t \sum_i y_i \frac{\partial f_k}{\partial y_i} dt = \int_0^1 f_k(ty) + t D f_k(ty) y \\
&= \int_0^1 \frac{d}{dt}\left(t f_k(ty)\right) dt = f_k(y)
\end{aligned} \tag{40}$$

thus $dH = \sum f_k dy_k$

$\square$

Theorem. *Symplectic systems are locally hamiltonian (the converse follows from Pointcaré's theorem above). Consider the ode $\frac{dy}{dt} = f(y)$ with $f : U \subset \mathbb{R}^{2d} \to \mathbb{R}^{2d}$, the system is symplectic.* The flow is ϕ_t and by commutativity of the differential operators ∂_t and ∂_{y_0} we have (41)

$$\partial_t \frac{\partial \phi_t}{\partial y_0} = \frac{\partial}{\partial y_0} \frac{\partial \phi_t}{\partial t} = \frac{\partial}{\partial y_0} f\left(y(t) = \phi_t(y_0)\right) = Df \frac{\partial \phi_t}{\partial y_0} \tag{41}$$

by the integrability lemma, we need only show that JDf is symmetric to establish the existence of H, since the flow generated by f is symplectic by assumption we have (42)

$$0 = \partial_t \left(\frac{\partial \phi_t}{\partial y_0}^T J \frac{\partial \phi_t}{\partial y_0}\right) = \left(\frac{\partial^2 \phi_t}{\partial t \partial y_0}\right)^T J \frac{\partial \phi_t}{\partial y_0} + \frac{\partial \phi_t}{\partial y_0}^T J \left(\frac{\partial^2 \phi_t}{\partial t \partial y_0}\right) \tag{42}$$

substituting (41) into the RHS of (42) we obtain (43)

$$0 = \frac{\partial \phi_t}{\partial y_0}^T \left(Df^T J + JDf\right) \frac{\partial \phi_t}{\partial y_0} \overset{J=-J^T}{\implies} Df^T J^T = (JDf)^T = JDf \tag{43}$$

Thus JDf is symmetric, by the integrability lemma $\exists H$ such that in some neighbourhood of y_0 (and for sufficiently small time t) $\nabla H = f$

$\square$

Theorem (see also Thm 2.8 p187 in [4]). *Symplectic bijections of the manifold M, map hamiltonian systems to hamiltonian systems. The converse it also true: bijective diffeomorphisms on a symplectic manifold which map hamiltonian flows to hamiltonian flows are symplectic.*

Proof ($\Rightarrow$) Let $\psi : M \to M$, $\psi : y \mapsto z$ be a bijective symplectic diffeomorpism. Then the hamiltonian flow $\dot{y} = J^{-1}\nabla_y H(y)$ is mapped to $\dot{z} = J^{-1}\nabla_z K(z)$, where $K \circ \psi(y) = H(y)$. We note that since ψ is bijective there exists an inverse and that, by the inverse function theorem $D(\psi^{-1})\big|_{\psi(p)} = (D\psi)^{-1}\big|_{\psi(p)} : T_{\psi(p)}M \to T_pM$. We make an important observation (44)

$$\nabla K(z) = \nabla_z H \circ \psi^{-1}(z) = \left(\nabla_y H^T \frac{\partial \psi^{-1}}{\partial z_1}, \cdots, \nabla_y H^T \frac{\partial \psi^{-1}}{\partial z_{2d}}\right)^T = D\psi^{-T}\nabla H \tag{44}$$

by definition of symplecticity we have (45)

$$D\psi^T J D\psi = J \overset{()^{-1}}{\iff} D\psi^{-1} J^{-1} D\psi^{-T} = J^{-1} \iff J^{-1} = D\psi J^{-1} D\psi^T \tag{45}$$

with the two above observations we see that

$$\dot{z} = D\psi \dot{y} = D\psi J^{-1}\nabla H \overset{(44)}{=\!=} D\psi J^{-1} D\psi^T \nabla K = J^{-1}\nabla K \tag{46}$$

($\Leftarrow$) Conversely we see that if ψ maps hamiltonian flows to hamiltonian flows, $\psi : y \mapsto z$ so by assumption we start from (46), which holds for any hamiltonian flow H and thus

$$D\psi J^{-1} D\psi^T = J^{-1} \iff D\psi^T J D\psi = J$$

the form is preserved.

$\square$

Corollary *Liouville's Theorem: It follows that the volume is preserved.* $\det(J) = 1$ thus

$$\det\left(D\psi_t^T J D\psi_t\right) = \det(D\psi_t)^2 = 1 \Rightarrow \det(D\psi_t) = \pm 1$$

$D\psi_t$ is continuous wrt t and $D\psi_{t=0} = \mathbb{1}$ thus $\det(D\psi_t) \equiv 1 \quad \forall t$

$\square$

3.4   Symplectic Geometry

In this section (for now) I will make some statements without proving them, and the content will be in my own words and only exists for the benefit of my understanding, so it's likely not to be too coherent... I'm just using this section to offload some thoughts I have while playing with the ideas on paper that are in the textbook (Arnold [1] and Koszul Zou intro to symp geo [7])

Symplectic manifolds have a non degenerate two forms ω^2 which can be represented in some basis as a matrix J, so $\omega^2(\xi,\eta) = \xi^T J\eta$. We can write this form as

$$\omega^2 = d\mathbf{p} \wedge d\mathbf{q} = dp_1 \wedge dq_1 + \cdots + dp_d \wedge dq_d$$

since the symplectic form is preserved then so are the wedges of the symplectic form so $\omega^2 \wedge \omega^2 = 2\sum_{i<j} p_i \wedge q_i \wedge p_j \wedge q_j$, furthermore, the volume form is preserved since $\omega^2 \wedge \cdots \wedge \omega^2$ (d times) is $(d!) \cdot dp_1 \wedge dq_1 \wedge \cdots \wedge dp_d \wedge dq_d = dV$, thus hamiltonian flows preserve volume in phase space. (notation here gets confusing cause d is overloaded.)

3.5 Survey of Classical Integration methods

3.5.1 Types of integrators

Def : a **symmetric** method is one that is time reversible: if you propagate a point forward n timesteps then backward n time-steps using the same method you end up in the same spot. Formally, the numerical flow ϕ_h is symmetric ....[**EXPOUND**]

"Numerical experiments indicate that symmetric methods applied to integrable and near-integrable reversible systems share similar properties to symplectic methods applied to (near-)integrable Hamiltonian systems: linear error growth, long-time near-conservation of first integrals, existence of invariant tori. The present chapter gives a theoretical explanation of the good long-time behaviour of symmetric methods. The results and techniques are largely analogous to those of the previous chapter - the extent of the analogy may indeed be seen as the most surprising feature of this chapter." ([4] intro to chapter XI)

Def : a method $\phi_h : y_n \mapsto y_{n+1}$ is **symplectic** if the numerical flow is symplectic. Rem, the numerical flow can be approximated by a series expansion $\phi_h(y) = y + hf(y) + h^2 d_2(y) + O(h^3)$. We say that a method is symplectic to kth order if the first k terms of the modified equation of the numerical flow are symplectic? - or do we say this when the numerical flow is actually symplectic; I'm pretty sure it's just when the first k terms are syplectic.

3.5.2 Explicit Euler

This is the most straight forward method. For the ODE $y' = f(y,t)$ the explicit euler method is defined

$$y_{n+1} = \phi_h(y_n, n \cdot h) = y + hf(y_n, n \cdot h) \tag{47}$$

3.5.3 Strömer Verlet

The (explicit one-step) Strömer Verlet method is a symplectic integrator, who's numerical flow is given below for the n-body problem $\phi_h : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$

$$
\begin{aligned}
p_{n+1/2} &= p_n - \frac{h}{2}\frac{\partial H}{\partial q}(q_n) \\
q_{n+1} &= q_n + h\frac{\partial H}{\partial p}(p_{n+1/2}) \\
p_{n+1} &= p_n - \frac{h}{2}\left(\frac{\partial H}{\partial q}(q_n) + \frac{\partial H}{\partial q}(q_{n+1})\right)
\end{aligned}
\tag{48}
$$

In section 4.2 we show that the numerical flow belonging to this scheme is symplectic up to order $O(h^2)$.

3.5.4 Explicit Midpoint rule

Estimate the midpoint, use gradient at this point to find multiplied by the stepsize h to determine where to next.

3.6 Kepler Projection Methods Experiment.

3.6.1 Aim

To find some numerical evidence for or against the hypothesis, to generate ideas for where to go next, to gain intuitive understanding of which numerical integrators work better for this type of problem, do error analysis.

3.6.2 Theory / Hypothesis

The setup is the two body or Kepler problem with point masses m_1, m_2 the hamiltonian is the usual one with parameters $p_{11}, p_{12}, p_{21}, p_{22}, q_{11}, q_{12}, q_{21}, q_{22}$. The total mass is denoted M, and the reduced mass μ, the reduced velocity is an $\mathbb{R}^2$ vector and is denoted v and the reduced distance r.

The Kepler problem is given by the ode

$$\dot{y} = (\dot{p}, \dot{q}) = J^{-1} \nabla H(p, q) \tag{49}$$

where $J = \left[\begin{array}{c|c} 0 & \mathbb{1} \\ \hline -\mathbb{1} & 0 \end{array} \right]$ is the canonical symplectic form and H is the Kepler hamiltonian.

We can solve it analytically, see [12] page 129.

There is a theorem which states that syplectic flow which conserve all first integrals (invariants) of a Hamiltonian system (Find the theorem and name it, state it formally and possibly prove it!) must be exact, i.e. there is a unique syplectic flow which conserves all first integrals. The projection methods' numerical flow conserves all invariants, is not exact and hence is not symplectic.

Our ode (49) can either be viewed as an 8 dimensional beast or, when put into the inertial CM frame we can reduce the dimensions to 4, in which case it is the same ode as of a single reduced mass orbiting a central potential in the plane. We do not reduce the dimensions for the integration schemes for we wish to use similar integrators for the n-body problem. With every integration step we project onto the the $L-E$-manifold, the intersection of the energy and angular momentum first integrals. In the following numerical experiments, we are looking for evidence of an attracting sub-manifold of the $L-E$-manifold. This is the main hypothesis : the numerical flow of projection methods creates attractors.

3.6.3 Method

We use the following methods to try and gauge what is going on.

The acceleration of a point mass travelling in a circle is $a_c = v^2/|r|$ (inwards), the centripetal acceleration of the reduced mass is $GM/|r|^2$. We define the **k-factor** as the quantity $k(p, q) = v^2 - \frac{GM}{|r|}$. Hence, when the orbit is circular this quantity goes to zero $k \to 0$. If the orbit is elliptical and highly eccentric, we should observe this quantity oscillating wildly up and down with each orbit, the k-factor for the exact flow, for such an orbit should be a periodic and un-damped. We use this quantity to see if an integration scheme is pulling the orbit into a circular one.

Another quantity we are interested in is the **angle** between the first-integral level surfaces L and E onto which we are projecting. Using the euclidean metric induced by the (p, q) coordinate system we define the angle between these manifolds at a point p as the arc-cosine of the absolute value of the dot product of their area-forms. Taking the absolute value gives us the acute angle. The dot product of the area forms are the same as the dot product of their Hodge-duels which are parallel to the gradients of the first integral functions. So the acute angle of surfaces $H = cnst$ and $L = cnst$ with area forms ω_H, ω_L resp. are given by

$$\theta_p = \arccos |\omega_H(p) \cdot \omega_L(p)| = \arccos | \star \omega_H(p) \cdot \star \omega_L(p)| = \arccos \left| \frac{\nabla H \cdot \nabla L}{|\nabla H||\nabla L|} \right|_p \tag{50}$$

The projection methods used are given in detail above.

The

Error analysis. For the syplectic integrators we can do some backward error analysis, comparing the truncated modified vector field with the exact one. And second since there is an analytic solution to the Kepler problem we can just compare our results with the exact solution and obtain the global error of each method.

3.6.4 Results, Observations, Remarks, Speculation.

For reference the k-factor is

$$v^2 - \frac{GM}{r} \quad : \quad M = m_1 + m_2 \tag{51}$$

The experiments which generated the pngs in gallary exp kepler where set in the following starting configurations (initial conditions). **Configuration 1**

```
p1,p2,q1,q2 = [0.4,0.0] , [-0.4,0.0] , [0,-1] , [0,1]
y = [p1,p2,q1,q2] # supervector
m1,m2 = 1.0 , 1.4
E = -0.563
L = 0.800
```

The integration constants use are `STEPS` and the time-step is h = `H` specified in the graphs in title of energy plots.

Starting configuration, same energy and ang momentum as in configuration 1, the program puts us automatically into CM frame. We are in same starting position but not same starting momentum.

```
p1,p2,q1,q2 = [0.3 , 0.07] , [-0.5 , 0] , [0,-1] , [0,1]
y = [p1,p2,q1,q2] # supervector
m1,m2 = 1.0 , 1.4
E = -0.563
L = 0.800
```

Configuration 3

```
p1,p2,q1,q2 = [0.8 , 0.0] , [-0.8 , 0] , [0,-1] , [0,1]
y = [p1,p2,q1,q2] # supervector
m1,m2 = 1.0 , 1.4
E =
L =
```

Configuration 4

```
p1,p2,q1,q2 = [0.4,0.1] , [-0.4,-0.1] , [0,-1] , [0,1]
y = [p1,p2,q1,q2] # supervector
m1,m2 = 1 , 1.4
E =
L =
```

3.6.5 Remarks

Exp Euler The method performed poorly in general. However when integrated with very small time steps, it did conserve the angles between invariant level sets slightly better than when combined with a projection method. There was no drift in the mean although the amplitude did increase.

When combined with a projection, the angles between invariant level sets tend to orthonormalize and the k-factor goes to zero, which means the orbit becomes circular after a long time.

Strömer Verlet The Strömer Verlet scheme on it's own perserves all six of the quantities for a long time. Of special interest is that the plots of the k-factor and the angles between invarient level sets are preserved over long time periods even with large steps, this is expected because the roughly elliptic orbits of the modified equation (**??**) are integrated exactly and are not pulled toward circular orbits. The same goes for the angles betweent he invarient level sets, these are preserved very well over long time periods as demonstrated the figure `invarients_config4_stromer_verlet_None_h=0.05_STEPS=100000.png`.

Upon inspection of the plots (see fig 2, see also many more plots online) we observe that in every starting configuration, no matter the integrator, the projection methods invariable maximized the orthogonality of the invariant level sets (energy and angular momentum) who's intersection constitutes the invariant manifold onto which we are projecting.

3.7 Projection Methods

Note on notation: in the following subsections we use $2d$ and n interchangeably to denote the dimension of the hamiltonian system. I hope this does not cause confusion, (Note to self: refactor and homogenise notation when writing final draft if this work ends up being something I'm proud of)

3.7.1 First method. The *Naive* Projection Method

$$p = y(0) \qquad y' = \nabla\beta \tag{52}$$

then the projection is defined

$$\rho_E(p) = y(t) \qquad \text{such that } t \text{ satisfies} \quad \beta(y(t)) = E \tag{53}$$

We can approximate the flow of this system to first order by Taylor expantion

$$y(t) = p + \nabla\beta(p)t + O(t^2) \tag{54}$$

since $\beta(\rho_E(p)) = E$ by definition we can use the approximation (54) we find an approximate solution for the projection onto the manifold $\beta = E$ by solving the following equation (55) for λ

$$E = \beta(\rho_E(p)) \approx \beta(p + \lambda\nabla\beta(p)) \approx \beta(p) + D\beta(p)\lambda\nabla\beta(p) = \beta(p) + \lambda\left(\nabla\beta(p)\right)^T \nabla\beta(p) \tag{55}$$

using (55) to estimate λ, the approximate projection operator is

$$\widetilde{\rho}_E(p) := p + \lambda\nabla\beta(p) \qquad \text{with} \qquad \lambda := \frac{E - \beta(p)}{\nabla\beta \cdot \nabla\beta\big|_p} \tag{56}$$

Given a set of s first integrals $\{\beta_i\}_{i=1}^s$ we modify the numerical flow to preserve the quantities $\beta_i = E_i$. Given $\Phi_h : y_n \mapsto y_{n+1}$

$$\widetilde{\Phi}_h(y_n) := \tilde{y}_{n+1} = y_{n+1} + \sum_{i=1}^s \lambda_{E_i} \nabla\beta_i(y_{n+1}) = y_{n+1} + \sum_{i=1}^s \frac{E_i - \beta_i(y_{n+1})}{\nabla\beta_i(y_{n+1})^2} \nabla\beta_i(y_{n+1}) \tag{57}$$

instead you can evaluate iteratively $f(y'_{n+1})$.

Implementation of the naive projection method for the kepler problem.

```
def naive_projection(y,first_integrals=[(get_energy,nabla_H),
                                        (get_total_angular_momentum,nabla_l)]):
    # apply each projection one after the other
    for i,j in first_integrals:
        fint,nabla_fint = i,j(y)
        lambda_i = fint(Y0) - fint(y)
        lambda_i /= supervec_norm(nabla_fint)
        y = y + lambda_i*nabla_fint

    return
```

3.7.2 Naive Symmetric Method.

I got this method from [5] page 1003, algorithm 3.2.

Given the invariant level surfaces given by our first integrals $\{y : \beta_i(y) = c_i \forall i \leq m\}$ we define the function $g : \mathbb{R}^{2d} \to \mathbb{R}^m$ such that $g(y) = (\beta_1(y) - c_1, \cdots, \beta_m - c_m)$. Hence the invariant manifold is given by $\{y : g(y) = 0\}$. We denote the Jacobian $G := g'$. The algorithm [5] is essentialy the same as the naive one only this time we over-shoot by double instead of landing on the manifold.

- $\hat{y}_n = y_n + G^T(y_n)$

3.7.3 Better algorithm for projection methods of first integrals. The *Parallel* projection method.

The above method has a weakness, while it is successful in preserving the energy manifold, it in-fact takes us off of the other invariants (in our example linear momentum is not conserved, which is a quantity that even the explicit Euler integrator doesn't have any trouble with). Our problem now is that we have a set of level sets $\{\beta_i(y) = c_i\}_{i=1}^s$ where the β_i are first integrals and c_i are constants, and we wish to preserve all of them. We solve this by modifying the projection (57) so that we for each projection ρ_{E_i} we are projection onto the level set $\beta_i = c_i$ along the intersection of the other conserved level sets, so $\beta_j(p) = \beta_j(\rho_{E_i}(p))$. In this section explore one algorithm that does this.

We wish to find an easy to implement projection $\widetilde{\rho}_E^{(2)}$ which projects the point p onto the manifold $\beta_i = c_i$ while conserving $\beta_j(p) \forall j \neq i$. We modify the projection operator $\widetilde{\rho}_E$ from equation (56) (re-written):

$$\widetilde{\rho}_{E_i}(p) = p + \lambda\nabla\beta_i(p) \qquad \text{with} \qquad \lambda := \frac{E - \beta_i(p)}{\nabla\beta_i(p) \cdot \nabla\beta_i(p)}$$

We refine the projection iteratively with respect to it's components, each of which is associated with a first integral. We start by initializing our set $\{\nabla\beta'_1, \cdots, \nabla\beta'_s\} := \{\nabla\beta_1, \cdots, \nabla\beta_s\}$, we start with

$j = 1$. For each $i \neq j$ we redefine the set, projecting each vector with the operator $\hat{P}_{j,\{\nabla\beta_1', \cdots, \nabla\beta_s'\}}$ which we write $\hat{P}_j$ for short; defined as follows

$$\hat{P}_j : \nabla\beta_i' \mapsto \nabla\beta_i' - \alpha_{ij}\nabla\beta_j' \qquad \text{with} \qquad \alpha_{ij} = \frac{\nabla\beta_j \cdot \nabla\beta_i'}{\nabla\beta_j \cdot \nabla\beta_j'} \tag{58}$$

This formula is derived from $\nabla\beta_j \cdot (\nabla\beta_i - \alpha_{ij}\nabla\beta_j') = 0$, we can also find it by finding the optimal a_{ij} which minimizes $(\nabla\beta_i - a_{ij}\nabla\beta_j')^T(\nabla\beta_i - a_{ij}\nabla\beta_j')$.

Applying the operators $\{\hat{P}_1, \hat{P}_2, \cdots, \hat{P}_s\}$ one by one to the set $\{\nabla\beta_1, \cdots, \nabla\beta_s\}$ iteratively (we remark that $\hat{P}_j$ is defined with respect to the set $\{\nabla\beta_i'\}_{i=1}^s$, here each time the next $\hat{P}_{j+1}$ operator is applied to the set we use the output of the previous operator to define it, hence the method is recursive and lends it's self to for loops)

Now we find the proper coefficient λ_i' in order to land near-to (on up to first order expansion) the conserved manifold - i.e. the intersection of each of the first integrals $\beta_i(y_n) = \beta_i(y_0)$. Since $\lambda_i \nabla\beta_i$ reaches the desired tanjent space, want the $\lambda_i \nabla\beta_i$ component of $\lambda_i' \nabla\beta_i'$ to be the same size. Hence λ_i' must satisfy (59) and thus (60)

$$(\lambda_i'\nabla\beta_i')^T (\lambda_i\nabla\beta_i) = \lambda_i^2 \nabla\beta_i^T \nabla\beta_i \quad \Rightarrow \quad \lambda_i' := \lambda_i \frac{\nabla\beta_i^T \nabla\beta_i}{\nabla\beta_i^T \nabla\beta_i'} \tag{59}$$

by substituting in the value of λ_i from equation (56) we obtain

$$\lambda_i'(p) = \frac{E_i - \beta_i(p)}{\nabla\beta_i^T \nabla\beta_i'} \tag{60}$$

Hence we can express our new operator in a notationally condense form using the expressions from equations (60), (**??**)

$$\widetilde{\rho}^{(2)}(p) = \sum_{i=1}^s \widetilde{\rho}_{E_i}^{(2)}(p) \approx p + \sum_{i=1}^s \left(\lambda_i'\nabla\beta_i'\right) \tag{61}$$

To summarise, this projection (61) can be thought of as concatenation of many projections $\widetilde{\rho}_{E_i}$ which project onto the desired level set $\beta_i(p) = E_i$ while preserving all other conserved quantities to first order.

For the actual implementation of the algorithm there is a fear that the denominator of the expression for λ_i will vanish - that $\nabla\beta_i^T \nabla\beta_i' = 0$ i.e. that $\nabla\beta_i$ and $\nabla\beta_i'$ are perpendicular, this may arise in the case where two level sets of invariants are parallel or almost parallel at a point p. If this were to happen our projection operator might become really big, which is not what we want, the aim of this approximate projection is to apply small rectifications to our solutions at every time-step (or perhaps every few steps). Thus we may consider adding a small but non-zero term $\epsilon|E_i - \beta_i(p)|$ to the denominator of λ_i' (62). (choice of epsilon to be determined experimentally), Note that $\nabla\beta_i^T \nabla\beta_i' \geq 0$ I THINK, THIS HAS YET TO BE PROVEN, BUT WILL PROBABLY NEVER GET ROUND TO IT BECAUSE THERE ARE MORE PRESSING MATTERS TO ATTEND TO! since we define $\nabla\beta'$ by projection $\nabla\beta$ onto a surface. I just added a try catch for overflow. Also this paragraph, is the only thing that needs to change in this subsection.

$$\widetilde{\rho}^{(3)} : p \mapsto p + \sum_{i=1}^s \left(\frac{E_i - \beta_i(p)}{\nabla\beta_i^T \nabla\beta_i' + \epsilon|E_i - \beta_i(p)|}\nabla\beta_i'\right) \tag{62}$$

In practice we can substitute the ϵ on the denominator with a conditional statement.

A weakness of this algorithm is that it does not work when the function $\nabla\beta = 0_V$, i.e. when the level set is defined at an extrema of the first integral. However this happens very rarely **(according to something I read, find it and cite it!)**.

Implementation of this algorithm in python for the kepler problem.

```python
def parallel_projection(y,first_integrals=[(get_energy,nabla_H),
                                           (get_lin_mom_x,nabla_lin_x),
                                           (get_lin_mom_y,nabla_lin_y)]):
    global overflow_count

    # first compute the gradients
    fivag = [(i(y),i(Y0),j(y)) for i,j in first_integrals]
    finty,fint0,beta = [j for i,j,k in fivag],[i for i,j,k in fivag],[k for i,j
                                             ,k in fivag]
    beta_prime = [j[:] for j in beta] # copy of the gradients to be modified


    # for each j, project all the i's out of the j surface
    for j in range(len(fivag)):
        for i in range(len(fivag)):
            if j != i:
                try:
                    beta_i_prime = beta_prime[i] - supervec_dot(beta[j],
                                                     beta_prime[i]) /
                                                     supervec_dot(beta[j
                                                     ],beta_prime[j]) *
                                                     beta_prime[j]
                    beta_prime[i] = beta_i_prime
                except OverflowError("overflow, probably the manifolds have
                                                    small angle"):
                    overflow_count+=1

    y_proj = y[:]
    # project along each axis
    for e0,ey,b_i_p,b_i in zip(finty,fint0,beta_prime,beta):
        try:
            lambda_i = (e0 - ey) / supervec_dot(b_i_p,b_i)
            y_proj += lambda_i * b_i_p
        except OverflowError("overflow in computing lambda_i"):
            overflow_count+=1

    return y_proj
```

3.7.4 Standard Projection Method

See algorithm 4.2 on page 110 of [4].

[explain the implementation of this thing : by means of newton iterations the projection numerically optimizes the closest distance to the conserved manifold and projects onto it.]

3.7.5 Modified differential equation, turn the manifold into an attractor?? by modifying the equation.

By modifying the equation and turning the conserved manifold (intersection of first integral level sets) into an attractor, we hope that the flow and the numerical flow of the modified equation in

regions near the attracting manifold will mirror the numerical flow of other methods combined with the projection methods described above.

[answer the question - why would you use my methods instead of the standard projection methods? Because the numerical flow of the modified equation is closer to my methods than it is to the standard projection method.]

[Describe how the equation is modified]

3.7.6 Infidelity of the projections, 'difference flow' (made up term).

Discuss and motivate the formula you found for this flow which represents your best guess of how the flow is affected, the following differential equation is something I derived which I think describes the 'error flow' induced by the projections. I hope to be able to use this to show that some exact solutions are stable under projection and other are not, as further evidence for the existence of an invariant manifold.

$$\dot{y} = D^2\beta\nabla\beta - \frac{\nabla\beta^T D^2\beta\nabla\beta}{\nabla\beta^T\nabla\beta}\nabla\beta : TM \to TM : M = \{x \in \mathbb{R}^{2d} : \beta(x) = \text{cnst}\} \tag{63}$$

generalised

$$\dot{y} = \sum_{i=1}^{n} D^2\beta_i\nabla\beta_i - \frac{\nabla\beta_i^T D^2\beta_i\nabla\beta_i}{\nabla\beta_i^T\nabla\beta_i}\nabla\beta_i : TM \to TM : M = \left\{x \in \mathbb{R}^{2d} : \begin{cases} \beta_1(x) = \text{cnst} \\ \cdots \\ \beta_n(x) = \text{cnst} \end{cases}\right\} \tag{64}$$

I hypothesise that this flow is qualitatively similar to the projected flow vector field minus the exact flow vector field.

We turn the conserved manifold into an attractor by modifying the differential equation, although this does not preserve the syplectic form, I haven't seen it mentioned anywhere...

3.8 Second order Conservation of invariants via method of Local co-ordinates.

I remember reading a theorem that said if the flow is syplectic (= locally hamiltonian) and all the invariants are preserved, then it is exact, therefore must this method be non-syplectic? If this is the case is it true then our flow does not preserve any syplectic form and therefore even if we stay on a manifold the volume will not be preserved, it may become squished.

3.8.1 Implementation of projection Algorithm. (See documentation on site, link to github repo readme / documentation)

To start off we implement this for the Kepler problem. I have already done this for a single conserved quantity. I will take a small step and implement the projection method for two conserved quantities - Energy and Angular momentum.

The gradients vector fields of an energy first integral is just the gradient of the hamiltonian. The gradient of the total angular momentum first integral is given by FALSE

$$\nabla L(p_{11}, p_{12}, p_{21}, p_{22}, q_{11}, q_{12}, q_{21}, q_{22}) = \begin{pmatrix} -q_{12} & q_{12} & -q_{22} & q_{21} & p_{12} & -p_{11} & p_{22} & -p_{12} \end{pmatrix} \tag{65}$$

Figure out whether the symplectic two form being preserved is the same as all the Pointcaré symmetries being preserved - what does this even mean

4 Backward Error Analysis

Backward error analysis dates back to the 1960s, it is very useful for studying the qualitative behaviour of numerical methods, and when statements over very long time intervals are needed. For formal analysis the modified equation - a formal series in powers of h (the step size) has to be truncated. The error induced by such a truncation can be made exponentially small, and the results remain valid on exponentially long time intervals. See introduction of chapter IX of [4], page 337.

We start with a differential equation

$$\frac{d}{dt}y = \dot{y} = f(y) \tag{66}$$

and a numerical flow $\phi_h : y_n \mapsto y_{n+1}$ which we assume can be expanded as follows

$$\phi_h(y) = y + hf(y) + h^2 d_2(y) + h^3 d_3(y) + O(h^4) \tag{67}$$

our goal is to find a modified equation who's exact flow is the numerical flow of our original equation. We wish to find an equation for which the curve $\widetilde{y}(t)$ is a solution, which is exactly a solution to the numerical flow so that $\widetilde{y}(hn) = \phi_h^n(y_0)$. Assuming $\dot{\widetilde{y}}$ is analytic in $\widetilde{y}$ we write the modified equation in Taylor form

$$g(\widetilde{y}) := \frac{d}{dt}\widetilde{y} = \dot{\widetilde{y}} = f(\widetilde{y}) + hf_2(\widetilde{y}) + h^2 f_3(\widetilde{y}) + h^3 f_4(\widetilde{y}) + O(h^4) \tag{68}$$

To find the relationship between coefficients of the modified equation (68) and those of our numerical flow (67) Taylor expand $\widetilde{y}(t+h)$ about $\widetilde{y}(t)$. Equating the exact flow of the modified equation the numerical flow for a single step we obtain

$$
\begin{aligned}
\widetilde{y}(t+h) &= \widetilde{y}(t) + h\dot{\widetilde{y}}(t) + \frac{h^2}{2!}\ddot{\widetilde{y}}(t) + O(h^3) \\
&= \widetilde{y}(t) + hg(\widetilde{y}) + \frac{h^2}{2!}g^{(1)}(\widetilde{y})g(\widetilde{y}) + O(h^3) \\
&= \widetilde{y}(t) + hf(\widetilde{y}) + h^2 d_2(\widetilde{y}) + h^3 d_3(\widetilde{y}) + O(h^3) = \phi_h(\widetilde{y}(t))
\end{aligned}
\tag{69}
$$

Equating like powers of h we obtain a recurrence relation for finding f_n in terms of $\{f_i\}_{i<n}$. We obtain the following recurrence relations:

$$f_2(y) = d_2(y) - \frac{1}{2}f^{(1)}f(y) \tag{70}$$

$$f_3(y) = d_3(y) - \frac{1}{6}\left(f^{(2)}(f,f)(y) + f^{(1)}f^{(1)}f(y)\right) - \frac{1}{2}\left(f^{(1)}f_2(y) + f_2^{(1)}f(y)\right) \tag{71}$$

$$
\begin{aligned}
f_4(y) = d_4 &- \frac{1}{2}\left(f_3^{(1)}f + f_2^{(1)}f_2 + f^{(1)}f_3\right) \\
&- \frac{1}{6}\Big(f_2^{(2)}(f,f) + f^{(2)}f_2 f + f^{(2)}ff_2 \\
&\qquad + f_2^{(1)}f^{(1)}f + f^{(1)}f_2^{(1)}f + f^{(1)}f^{(1)}f_2\Big) \\
&- \frac{1}{24}\Big(f^{(3)}(f,f,f) + f^{(2)}f^{(1)}(f,f) + 2f^{(2)}(f,f^{(1)}f) \\
&\qquad + f^{(1)}f^{(2)}(f,f) + f^{(1)}f^{(1)}f^{(1)}f\Big)
\end{aligned}
\tag{72}
$$

etc.

Rem. if $y \in \mathbb{R}^n$ then $f : \mathbb{R}^n \to \mathbb{R}^n$ and $f^{(1)} : \mathbb{R}^{n\otimes 2} \to \mathbb{R}^n$ and so $f^{(k)} : \mathbb{R}^{n\otimes k} \to \mathbb{R}^n$.
For any hamiltonian system

$$
(\dot{p}, \dot{q}) = J^{-1}\nabla H(p,q) \qquad \leftrightarrow \qquad \dot{y} = f(y)
\tag{73}
$$

we calculate the first and second derivatives of $f = J^{-1}\nabla H$

$$
f^{(1)} = J^{-1}D^2 H \qquad\qquad f^{(2)} = DJ^{-1}D^2 H \quad \left|\left[DJ^{-1}D^2 H\right]_{q_k} = \frac{\partial}{\partial q_k}J^{-1}D^2 H\right.
\tag{74}
$$

thus for equation (70) we get

$$
f^{(1)}f(y) = J^{-1}D^2 H J^{-1}\nabla H(p,q)
\tag{75}
$$

we compute the components of (75)

$$
\left[f^{(1)}f\right]_{p_k} = \left[J^{-1}D^2 H J^{-1}\nabla H(p,q)\right]_{p_k} = \sum_{i=0}^{d}\frac{\partial^2 H}{\partial p_i \partial q_k}\frac{\partial H}{\partial q_i} - \sum_{i=0}^{d}\frac{\partial^2 H}{\partial q_i \partial q_k}\frac{\partial H}{\partial p_i}
\tag{76}
$$

and

$$
\left[f^{(1)}f\right]_{q_k} = \left[J^{-1}D^2 H J^{-1}\nabla H(p,q)\right]_{q_k} = -\sum_{i=0}^{d}\frac{\partial^2 H}{\partial p_i \partial p_k}\frac{\partial H}{\partial q_i} + \sum_{i=0}^{d}\frac{\partial^2 H}{\partial q_i \partial p_k}\frac{\partial H}{\partial p_i}
\tag{77}
$$

Note that in the equations (76) and (77) we can either think of p_i and q_i as individual components, or in the case of the n body problem in $6d$ dimensions $d = n$ the equations also work with $p_i, q_i \in \mathbb{R}^3$. With reference to the n-body problem we make use of the following identities (78) and (79) to simplify (77)

$$
\frac{\partial^2 H}{\partial p_i \partial q_k} = 0 \quad , \quad \frac{\partial^2 H}{\partial p_i \partial p_k} = \frac{\delta_{ik}}{m_k}\mathbb{1} \quad , \quad \frac{\partial^2 H}{\partial q_i \partial q_k} = \frac{Gm_i m_k}{\left(\xi_{jk}^T \xi_{jk}\right)^{3/2}}\left(\frac{3\xi_{jk}\xi_{jk}^T}{\xi_{jk}^T \xi_{jk}} - \mathbb{1}_{3\times 3}\right) \quad i \neq k
\tag{78}
$$

$$
\frac{\partial^2 H}{\partial q_i^2} = \sum_{\substack{j \\ j\neq i}}\frac{Gm_i m_j}{\left(\xi_{ij}^T \xi_{ij}\right)^{3/2}}\left(\mathbb{1}_{3\times 3} - \frac{3}{\xi_{ij}^T \xi_{ij}}\xi_{ij}\xi_{ij}^T\right)
\tag{79}
$$

Thus (76) and (77) become (80)

$$
\left[f^{(1)}f\right]_{p_k} = \sum_{\substack{i=1 \\ i\neq k}}^{d}\frac{Gm_i m_k}{\left(\xi_{ik}^T \xi_{ik}\right)^{3/2}}\left(\frac{3\xi_{ik}^T \dot{\xi}_{ik}}{\xi_{ik}^T \xi_{ik}}\xi_{ik} - \dot{\xi}_{ik}\right) \quad , \quad \left[f^{(1)}f\right]_{q_k} = \sum_{\substack{i=1 \\ i\neq k}}\frac{Gm_i}{\left(\xi_{ik}^T \xi_{ik}\right)^{3/2}}\xi_{ik}
\tag{80}
$$

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4.1 Algorithm for finding modified equation coefficients.

The following section outlines the algorithms implemented for the calculations needed for the above. The source code is written in python and is available here in the `modified_equations.py` script.

The function `next_gamma` enables us to find an expression for the n-th total derivative of (68) wrt t : $\frac{d^n}{dt^n}g(\widetilde{y})$, in terms of it's self and it's derivatives wrt $\widetilde{y}$. We use the notation $g^{(n)} := \frac{d^n}{d\widetilde{y}}g$. The algorithm is straightforward because $\frac{d}{dt}g^{(n)}(\widetilde{y}(t)) = g \cdot g^{(n+1)}$. We represent the polynomial in g and it's derivatives $g^{(n)}$ with a list who's elments are coefficients of $g^{(n)}$ together with multiplicities, the format is `[ [multiplicity , (coef g**1,coef g**2,...)] , ...]`. For example (81)

$$3 \cdot ggg^{(1)}g^{(2)}g^{(4)} + 2 \cdot gg^{(1)} \longleftrightarrow \texttt{[[3,(2,1,1,0,1)] , [2,(1,1)]]} \tag{81}$$

`next_gamma` works simply by taking an expression such as the RHS of (81) and returning the list representing it's total derivative wrt t.

The function `gamma_to_pihsr` converts expressions in terms of g and it's derivatives into expressions in terms of $\{f, f_1, f_2, ...\}$ and their derivatives by means of convolutions. And the function `expand_taylor_ytilde` takes a natural number n and returns the n-th order polynomial approximation of $\widetilde{y}(t)$, the output of this method is displayed in figure 1

Figure 1: Polynomials recurrence relations.

4.2 Truncated modified equations for integrators

Note on the notation, we make no distinction between $D^2H = \nabla^2 H = \nabla^2 H^T$, these are used interchangeable and denote the Hessian of the Hamiltonian. Reminder : the modified equation is given by $\widetilde{y}$, this gives us

$$\dot{\widetilde{y}} = g(\widetilde{y}) = f(\widetilde{y}) + hf_2(\widetilde{y}) + h^2 f_3(\widetilde{y}) + \cdots$$

see above sections for more context.

4.2.1   Explicit Euler

The numerical flow can be written exactly (82) since $d_2, d_3, ... \equiv 0$

$$\phi_h : (p, q) \mapsto (p, q) + h \left(-\frac{\partial H}{\partial q}, \frac{\partial H}{\partial p} \right) \tag{82}$$

Using the expressions (70) for f_2 and (71) for f_3, and with the hamiltonian expressions (73) and (74) for the first two derivatives of the infinitesimal propagator $J^{-1}\nabla H$ we obtain $f^{(1)}, f^{(2)}$, the terms of the modified equation read

$$f_2 = -\frac{1}{2} J \nabla^2 H J \nabla H = \frac{1}{2} \left(H_{qq} H_p \ , \ H_{pp} H_q \right) \tag{83}$$

$$\begin{aligned} f_3 = \ & -\frac{1}{6} \left(J^{-1} D^3 H \left(J^{-1} \nabla H, J^{-1} \nabla H \right) + J^{-1} D^2 H J^{-1} D^2 H J^{-1} \nabla H \right) \\ & + \frac{1}{4} \left(J^{-1} D^3 H (J^{-1} \nabla H \ , \ J^{-1}) + 2 \left(J^{-1} D^2 H \right)^2 J^{-1} \nabla H \right) \end{aligned} \tag{84}$$

To second order the explicit Euler modified equation reads

$$g(\widetilde{y}) = f(\widetilde{y}) + h \frac{1}{2} \left(H_{qq} H_p, H_{pp} H_q \right) + O(h^2) $$

4.2.2   Strömer Verlet

The Strömer Verlet scheme (48) has numerical flow

$$\phi_h : (p, q) \mapsto (p, q) + h f^h(p, q) + h^2 d_2^h(p, q) + h^3 d_3^h(p, q) + O(h^4)$$

truncated to $O(h^3)$. Naturally the $O(h)$ term is the gradient $J^{-1}\nabla H$; assuming, as it is in the n body problem, that the mixed partials of the hamiltonian evaluate to zero $H_{pq} = H_{qp} = 0$ the $O(h^2)$ and $O(h^3)$ terms read

$$d_2(p_n, q_n) = -\frac{1}{2} \left(H_{qq} H_p \ , \ H_{pp} H_q \right) \qquad d_3(p_n, q_n) = -\frac{1}{4} \left(H_{qqq}(H_p, H_p) + \frac{1}{3} H_{qq} H_{pp} H_q \ , \ 0 \right) \tag{85}$$

The above equations are evaluated at (p, q). For the n body problem these terms are straightforward to compute. Furthermore, we notice that $d_2 = -\frac{1}{2} J^{-1} D^2 H J^{-1} \nabla H = -\frac{1}{2} f^{(1)} f$. **(IMPORTANT! ARE THE EXPANSIONS OF SYMMETRIC NUMERICAL METHODS ODD FUNCTIONS, I THINK I MISUNDERSTAND THIS)**

We calculate the Jacobian (86)

$$\frac{\partial \phi_h(p, q)}{\partial(p, q)} = \frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} = \mathbb{1} + h \begin{pmatrix} 0 & -H_{qq} \\ H_{pp} & 0 \end{pmatrix} - \frac{h^2}{2} \begin{pmatrix} H_{qq} H_{pp} & H_{qqq} H_p \\ 0 & H_{pp} H_{qq} \end{pmatrix} + O(h^3) \tag{86}$$

we show that the flow is symplectic to first order (87) (confusingly this means $O(h^2)$ in the below equation. In fact, due to the symmetry of the Strömer Verlet scheme - symplecticity is preserved to 2nd order $O(h^3)$). For reference there are slightly easier ways of showing symplecticity

in chapter VI of [4], but we use the Taylor expansions to illustrate that symplecticity is broken by the projections.

$$\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}^T J \frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} = J + h\nabla^2 H J^{-T} J + J J^{-1}\nabla^2 H + h^2 \nabla^2 H J \nabla^2 H$$

$$- \frac{h^2}{2}\left[\begin{pmatrix} H_{pp}H_{qq} & 0 \\ H_p^T H_{qqq} & H_{qq}H_{pp} \end{pmatrix} J + J \begin{pmatrix} H_{qq}H_{pp} & H_{qqq}H_p \\ 0 & H_{pp}H_{qq} \end{pmatrix}\right] + O(h^3) \quad (87)$$

$$= J + O(h^3)$$

Using (70), (71), (85) we obtain the modified equations (88), (91)

$$f_2 = 0 \tag{88}$$

in words: (88) is the conjugation of the Hessian of the hamiltonian, acting on the gradient of the hamiltonian. We rewrite (71) for ease of reference.

$$f_3(y) = d_3(y) - \frac{1}{6}\left(f^{(2)}(f, f)(y) + f^{(1)}f^{(1)}f(y)\right)$$

The followin identities (89),(90) come from from the fact that $H_{ppp} = H_{pq} = 0$ that there is only 1 out of 8 quadrants of the tensor $\nabla^3 H$ which is not empty: H_{qqq},

$$J^{-1}\nabla^3 H(J^{-1}\nabla H, J^{-1}\nabla H) = (H_{qqq}(H_p, H_p), 0) \tag{89}$$

$$J\nabla^2 H J \nabla^2 H J \nabla H = J\left[\begin{array}{c|c} H_{pp} & 0 \\ \hline 0 & H_{qq} \end{array}\right] J \left[\begin{array}{c|c} H_{pp} & 0 \\ \hline 0 & H_{qq} \end{array}\right] J \begin{bmatrix} H_p \\ H_q \end{bmatrix} = (-H_{qq}H_{pp}H_q, H_{pp}H_{qq}H_p) \tag{90}$$

$$f_3 = -\frac{1}{4}\left(H_{qqq}(H_p, H_p) + \frac{1}{3}H_{qq}H_{pp}H_q, 0\right)$$

$$+ \frac{1}{6}\left(J\nabla^3 H(J\nabla H, J\nabla H) + J\nabla^2 H J \nabla^2 H J \nabla H\right) \tag{91}$$

$$= \left(\frac{11}{12}H_{qq}H_{pp}H_q - \frac{7}{12}H_{qqq}(H_p, H_p), -\frac{5}{6}H_{pp}H_{qq}H_p\right) \text{wrong need to revise this}$$

4.2.3 Modified equations for the Numerical flow of Projection methods

$$\rho(y) = y + Dg^T\mu \qquad , g : \mathbb{R}^{2d} \to \mathbb{R}^m \quad g = 0 \quad \text{defines a manifold} \tag{92}$$

Above μ is an appropriate m-vector, it's components are of the form $\frac{\beta_0 - \beta(y)}{\nabla\beta(y)^2}\nabla\beta(y)$, where β is a first integral and β_0 is the constant value that defines an invariant level set wrt to β.

We wish to study the behaviour of the projection methods we have analytically, in order to do so, we find equations for the modified numerical flow and doubly modify the modified equations.

Given the naive projection method (92), which we use in conjunction with a numerical flow (93)

$$\phi_h(y) = y + hf(y) + h^2 d_2(y) + h^3 d_3(y) + O(h^4) \tag{93}$$

Our new flow is $\hat{\phi}_h := \rho \circ \phi_h$. To simplify notation for the time being we assume $m = 1$ and there is only one first integral, that we project onto a $2d - 1$ dimensional invariant level surface defined by $\mathfrak{b} := \{y : \beta(y) = \beta_0\}$.

$$\hat{\phi}_h(y) = \phi_h(y) + \frac{\beta_0 - \beta(\phi_h(y))}{\nabla\beta(\phi_h(y))^2}\nabla\beta(\phi_h(y)) \tag{94}$$

expanding we find

$$\frac{\beta(\phi_h(y))}{\nabla\beta(\phi_h(y))^2}\nabla\beta(\phi_h(y)) = \frac{\beta(y + hf + h^2 d_2 + h^3 d_3 + o(h^4))}{\nabla\beta(y + hf + h^2 d_2 + O(h^3))^2}\nabla\beta(y + hf + h^2 d_2 + O(h^3)) \tag{95}$$

we expand each term in taylor series. Reminder : since β is a first integral and f is along the conserved manifold, we have that $\nabla\beta(y)^T f(y) = 0$ or in shorthand $\nabla\beta^T f = 0$ (In the following equations we omit the arguments y).

$$\begin{aligned}
\beta(\phi_h(y)) = {}& \beta(y) + \cancel{h\nabla\beta^T f} + \frac{h^2}{2}\left[D^2\beta(f,f) + 2\nabla\beta^T d_2\right] \\
& + \frac{h^3}{3!}\left[D^3\beta(f,f,f) + 6D^2\beta(d_2,f) + 6\nabla\beta^T d_3\right] + O(h^4)
\end{aligned} \tag{96}$$

$$\nabla\beta(\phi_h(y)) = \nabla\beta(y) + hD^2\beta f + \frac{h^2}{2}\left[D^3\beta(f,f) + 2D^2\beta d_2\right] + O(h^3) \tag{97}$$

squaring (97) we obtain the denominator (98)

$$|\nabla\beta|^2 \circ \phi_h(y) = |\nabla\beta|^2 + h\nabla\beta^T\left(D^2\beta f\right) + h^2\left(\nabla\beta^T\left(D^3\beta(f,f) + 2D^2\beta d_2\right) + \left(D^2\beta f\right)^2\right) + O(h^3) \tag{98}$$

we define $\alpha_1 := D^2\beta f$ and $\alpha_2 := \frac{1}{2}\left(D^3\beta(f,f) + 2D^2\beta d_2\right)$ and equation (98) simplifies to (99)

$$|\nabla\beta|^2 \circ \phi_h(y) = |\nabla\beta|^2\left(1 - 2h\frac{\nabla\beta^T\alpha_1}{|\nabla\beta|^2} + h^2\frac{2\nabla\beta^T\alpha_2 + |\alpha_1|^2}{|\nabla\beta|^2}\right) + O(h^3) \tag{99}$$

using the identity $\frac{1}{1+x} = 1 - x + x^2 - x^3 + x^4 - \ldots$ we obtain an expression

$$\frac{1}{|\nabla\beta \circ \phi_h(y)|^2} = \frac{1}{|\nabla\beta|^2}\left(1 - 2h\frac{\nabla\beta^T\alpha_1}{|\nabla\beta|^2} + h^2\left[\frac{4\left(\nabla\beta^T\alpha_1\right)^2}{|\nabla\beta|^4} - \frac{2\nabla\beta^T\alpha_2 + \alpha_1^2}{|\nabla\beta|^2}\right]\right) + O(h^3) \tag{100}$$

combining (96) and (100) we obtain the coefficients λ_2 and λ_3 as in (101) and (102) in terms of $f = J^{-1}\nabla H$, using these we derive an $O(h^3)$ expression for the pertubation (103)

$$\lambda_2 := \frac{\nabla^2\beta\left(J^{-1}\nabla H, J^{-1}\nabla H\right)}{2|\nabla\beta|^2} + \frac{\nabla\beta^T d_2}{|\nabla\beta|^2} \tag{101}$$

$$\begin{aligned}
\lambda_3 := {}& \frac{D^3\beta\left(J^{-1}\nabla H, J^{-1}\nabla H, J^{-1}\nabla H\right)}{6|\nabla\beta|^2} + \frac{D^2\beta\left(J^{-1}\nabla\beta, d_2\right)}{|\nabla\beta|^2} + \frac{\nabla\beta^T d_3}{|\nabla\beta|^2} \\
& - \frac{\nabla\beta^T\left(D^2\beta J^{-1}\nabla H\right)}{|\nabla\beta|^2} \cdot \frac{D^2\beta\left(J^{-1}\nabla H, J^{-1}\nabla H\right) + 2\nabla\beta^T d_2}{|\nabla\beta|^2}
\end{aligned} \tag{102}$$

Therefore

$$\frac{\beta(y) - \beta(\phi_h(y))}{\nabla\beta^T\nabla\beta(\phi_h(y))}\nabla\beta(\phi_h(y)) = -h^2\lambda_2\nabla\beta(y) - h^3\left(\lambda_3\nabla\beta(y) + \lambda_2 D^2\beta J^{-1}\nabla H(y)\right) + O(h^4) \qquad (103)$$

Thus the numerical flow (94) expanded becomes

$$\hat{\phi}_h(y) = y + hf(y) + h^2\left(d_2(y) - \lambda_2\nabla\beta\right) + h^3\left(d_3(y) - \lambda_3\nabla\beta - \lambda_2\nabla^2\beta J^{-1}\nabla H\right) + O(h^4) \qquad (104)$$

we can also define modified terms of the numerical flow

$$\begin{aligned}
\hat{d}_2 &:= d_2 - \lambda_2\nabla\beta \\
\hat{d}_3 &:= d_3 - \lambda_3\nabla\beta - \lambda_2\nabla^2\beta J^{-1}\nabla H
\end{aligned} \qquad (105)$$

and so the terms of the modified equation also change

$$\hat{f}_2(y) = \hat{d}_2(y) - \frac{1}{2}f^{(1)}f(y) = d_2 - \lambda_2\nabla\beta - \frac{1}{2}f^{(1)}f \qquad (106)$$

$$\dot{\widetilde{y}} = g(\widetilde{y}) = f(\widetilde{y}) + h\left(d_2(\widetilde{y}) - \lambda_2\nabla\beta(\widetilde{y}) - \frac{1}{2}f^{(1)}f(\widetilde{y})\right) + O(h^2) \qquad (107)$$

When we project onto multiple manifolds, for the naive projection method this means, we will assume that the other projection methods' qualitative behaviour is the same as for the naive method (which is easiest to analyze), having obtained evidence for this in the Kepler integration experiments (there are a tonne of pngs you can look at on the github repo in `./figures/`). For multiple projections for the naive projection method it suffices to make the following substitution

$$\lambda_2\nabla\beta \longleftrightarrow \sum_i \lambda_{2,i}\nabla\beta_i$$

given that we projection onto a set of first integrals $\{\beta_i\}$. The substitution is similarly linear for higher order terms.

4.2.4 Calculations of projection terms.

We calculate λ_2 (101) for the energy manifold (108)

$$\lambda_2 = \nabla^2 H\left(J\nabla H, J\nabla H\right) = \left(H_q^T H_{pp}H_q \ , \ H_p^T H_{qq}H_p\right) \qquad (108)$$

The gradient and Hessian of the angular momentum we calculated for the two body problem in two dimensions (23),(24), it is similar the n body problem in three dimensions. We calculate the hessian of the x, y, z componants of angular momentum $L_3 = p_1 x_2 - p_2 x_1$

$$\lambda_2 = \nabla^2 L_z\left(J\nabla H, J\nabla H\right) = \qquad (109)$$

5 Chaos, the Lyapunov spectrum and do the projection methods give rise to an attractor?

In this section we search for an attractor in the modified (with projection terms) Kepler and n-body equations. My suspicions where first aroused by the stabilizing of some solutions in the Kepler problem when running some numerical experiments, the orbits with low eccentricity seemed to converge onto circular orbits (figure 2), this is what prompted the search for an attractor. Liouville's theorem states that phase space volume is conserved in Hamiltonian systems, this result also follows from symplecticity and conservation of the symplectic two form; it follows from Liouville's theorem that symplectic systems do not have attractors In fact, the chaotic ones are often ergodic on their conserved manifolds (LAST LINE: EITHER GET RID OF THIS GLIB STATEMENT OR MAKE IT RIGOROUS).
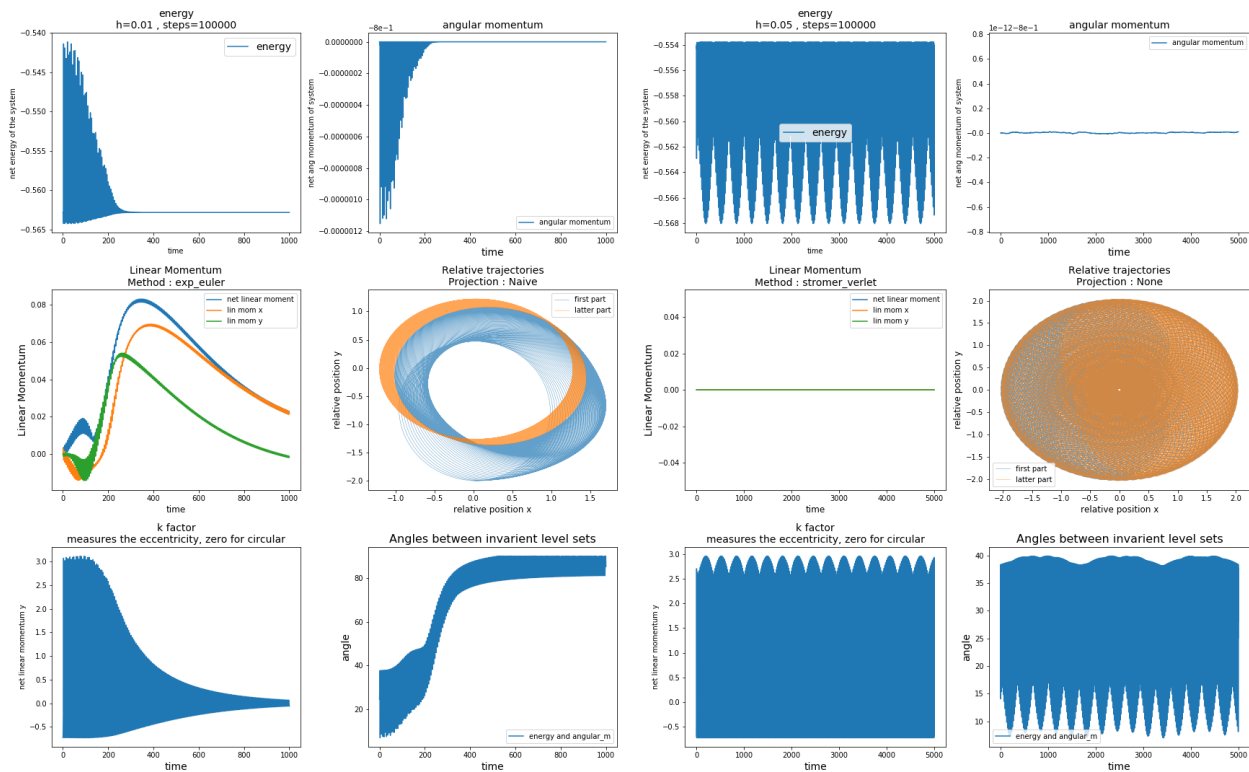

Figure 2: Numerical Experiments with Kepler System. Left: projection method. Right: Strömer Verlet symplectic integrator.

In this section we look for evidence of an attractor, analytically in the modified equations and numerically in experiments.

An **Attractor** is DEFINE ATTRACTOR (I think it's just a submanifold embedded in the phase space which attracts things, it has a basin of attraction)

The **basin of attraction** of an attractor DEFINE BASIN OF ATTRACTOR (PROBABLY EXACTLY WHAT I THINK IT IS)

5.1 Lyapunov Exponents

DEFINITON OF LYAPUNOV EXPONENTS

THEOREM, IN HAMILTONIAN SYSTEMS, THE LYAPUNOV EXPONENTS ARE THE SAME EVERYWHERE

5.1.1 Gramm Schmidt decomposition : Algorithm for finding Lyapunov exponents 1

IMPLEMENT SPECTRUM FINDER OF LYAPUNOV EXPONENTS, FIND THE SPECTRUM FOR SOME SYMPLECTIC METHOD, THE BIGGEST ONE SHOULD BE POSITIVE AND THEIR SUM SHOULD ADD TO ZERO.

5.2 Calculating Lyapunov exponents for symplectic integrators.

We expect the Lyapunov spectrum to be independent of initial conditions.

5.3 Implementation of modified equations for the Kepler problem.

We implement the modified equations, expanded to second order, and integrate them with a small step size to see if they behave similarly to the integrators with larger step-sizes. A welcome side-effect of implementing these is that the code provides us with strong evidence that the results from the previous section, 'Backwards Error Analysis' are correct.

5.3.1 Implementing the modified equation integrator for the Explicit Euler method (no projection)

The modified equation is

$$g(\widetilde{y}) = f(\widetilde{y}) - \frac{1}{2}f^{(1)}f(y) + O(h^2) = J^{-1}\nabla H - \frac{1}{2}J^{-1}\nabla^2 H J^{-1}\nabla H$$

we integrate with 100* smaller step-sizes.

5.3.2 Implementing the modified equation integrator for the Strömer Verlet method

We implement the 'Projected Strömer Verlet' modified equation with $h = 0.1$ and integrate it using the explicit Euler method but with a much smaller step-size. For ease of reference the 'Projected Strömer Verlet' method is written below (**??**).

5.3.3 Implementing exaggerated modified equations

We then multiply the $O(h^2)$ projection terms by a constant to make them more pronounced, to see if this would give me an attractor. (this ended up being very messy and didn't give me results I'd hoped it would)

6 Conclusions

6.1 Mathematical Conclusions

Did some theoretical and applied mathematics: studied ordinary differential equations paying attention to symmetries (important in physics), hamiltonian systems & symplectic manifolds.

What did I learn about numerical integrators (history + people, how the methods evolved, why they evolved, for what where they used in the early days)?

What did I learn about symplectic geometry (as an old field, as a theory that comes from mathematical physics and that was a generalization from Hamiltonians, how it's worded today in terms of exterior calculus skew-symmetric two-forms, about the emerging field of geometric information theory)?

What did you read about that was out of your depths (renormalization of manifolds, ...)?

6.2   Critical analysis of learning and process

One of the aims of this project was to learn how to do research independently. I can't make up my mind whether the problem stems from disorganization, or some deeper lack of connection with the subject matter which prevents flow; or perhaps it is just a normal part of the learning process to struggle and feel somewhat inadequate at times.

I read a lot of random articles that were only vaguely relevant to what I was working on, many things I read I also didn't understand. Don't know if this is a good or bad thing.

There where periods when I felt inspired and spent hours reading or coding at a time, and there were periods when I felt uninspired and either did something else or forced myself to do research despite myself. I'm struggling to find a good balance between straining myself and doing too little work; when you feel lethargic is it the case that you should force yourself to work until you are more inspired or should will that just demotivate you? And when you *are* motiviated should you keep working until you don't? - this strikes me as counter-productive because ideally you want to finnish well with a good idea of what you want to do next, rather than keep going until you trail off. The question of finding inspiration and flow has been plaguing me for a while but I don't seem to have made much headway answering it - am I asking the wrong question?

different take on same theme as above paragraph: I'm disappointed that I didn't end up getting completely absolved by the project, I think my approach to learning is definitely improving (becomming more effective) and there where times when all I could think about was the project and what I was currently doing, but this feeling didn't permeate everything. What I mean to say is that the project was enjoyable but not something I would loose sleep over, or wake up in the middle of the night with a revelation about, as was the case in high-school sometimes I lay awake for hours thinking about math, and on a few occasions it woke me up up at 3am and I would just start writing math for the next couple hours; this level of inspiration is something I'm trying to master and tame so as to be able to make more of it and get it on demand, I haven't got there yet - my aim is to try achieve this before end of undergrad.

Future work. It seems I opened some doors which lead down various avenues of exploration: I want to learn more about Lie groups & algebras (this is what I'm currently reading about), hamiltonian systems, the poisson braket, numerical schemes ++; then I also want to capitalize on my code to make more simulations of realistic n-body problems such as earth / sun / moon system, or a real solar system, or satalites and display the Lyapunov of different integrators for these types of problem with different integrators. I also want to read more articles about integration methods to know more about the context into which my project fits so that I can write something reasonable if I make an article for arxiv or to send to journals.

6.3 Skills acquired

Got better at reading literature. More coding is never a bad thing, I actually had quite a bit of fun coding.

6.4 Future work

7 Articles to refrence that I have not added to bibtex yet

COMMENTED ARTICLE HERE

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A Peter E. Hydon, Symmetry Methods for Differential Equations - A Beginner's Guide

B Geometric Numerical Integrations - Structure Preserving Algorithms for Ordinary Differential Equations.

C Papers

D Appendix B - Log

D.1 Friday 8 May 2020

D.1.1 Goals

- skim 'Numerical integration structure preserving...' book

- understand what a symplectic manifold is abstractly and wrt hamiltonian systems

- read a little about symplectic transformations

- re-read ex undergrad paper on numerical integration

- read Omar's paper once though (just skim)

- skim 'symmetry methods...' book once more and finish in-depth reading of chapter 2

D.1.2 Log

Went on a Wikipedia spree : KAM, Pertubation theory, Numerical Integration, Hamiltonian mechanics, Fiber bundle, Jet bundle, Spray, Riemannian geometry, Symplectic vector space, Symplectic matrix, Symplectic - learned some meta-things perhaps slightly meta / intangible but nevertheless I think useful knowledge.

D.2 Weekly Goals - week of 2020.05.11

Read in depth symmetry methods for differential equations, answering all the questions.
Skim-read one chapter of the numerical methods for integration every day.
At the end of each day do a review session where you go over what you learned.
Do this at the end of the week too, this one you document.

D.3 Monday 11 May 2020

Read mainly the symmetry book today.

D.4 Thursday 11 May 2020

Goal for week : implement the runga-kunga methods from [3] and see what you can find on the projection methods discussed with Gantumur during the meeting.

E   Appendix C

E.1   Random Attractors

Here are twelve of my favourite random attractors generated using code form Paul Bourke's website, thank you Paul Bourke. The way the algorithm works is it randomly generates a 5th order (non linear) ODE in two variables, then solves for the trajectories of several randomly generated points. Most of the time the orbits tend to infinity, sometimes there is an integer dimensional (Hausdorff dimension) attractor, but sometimes these equations give rise to a strange attractors (3 , 4).
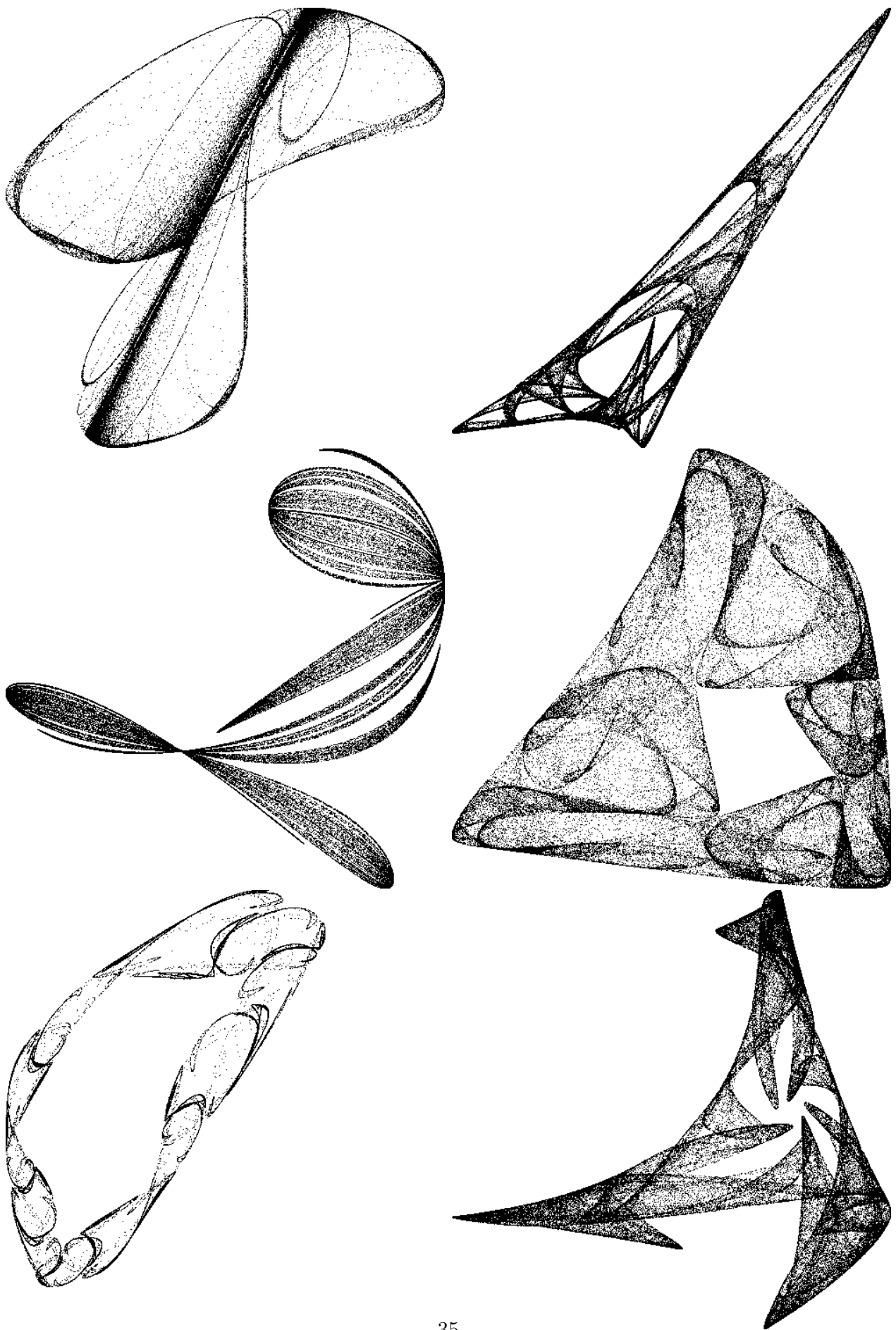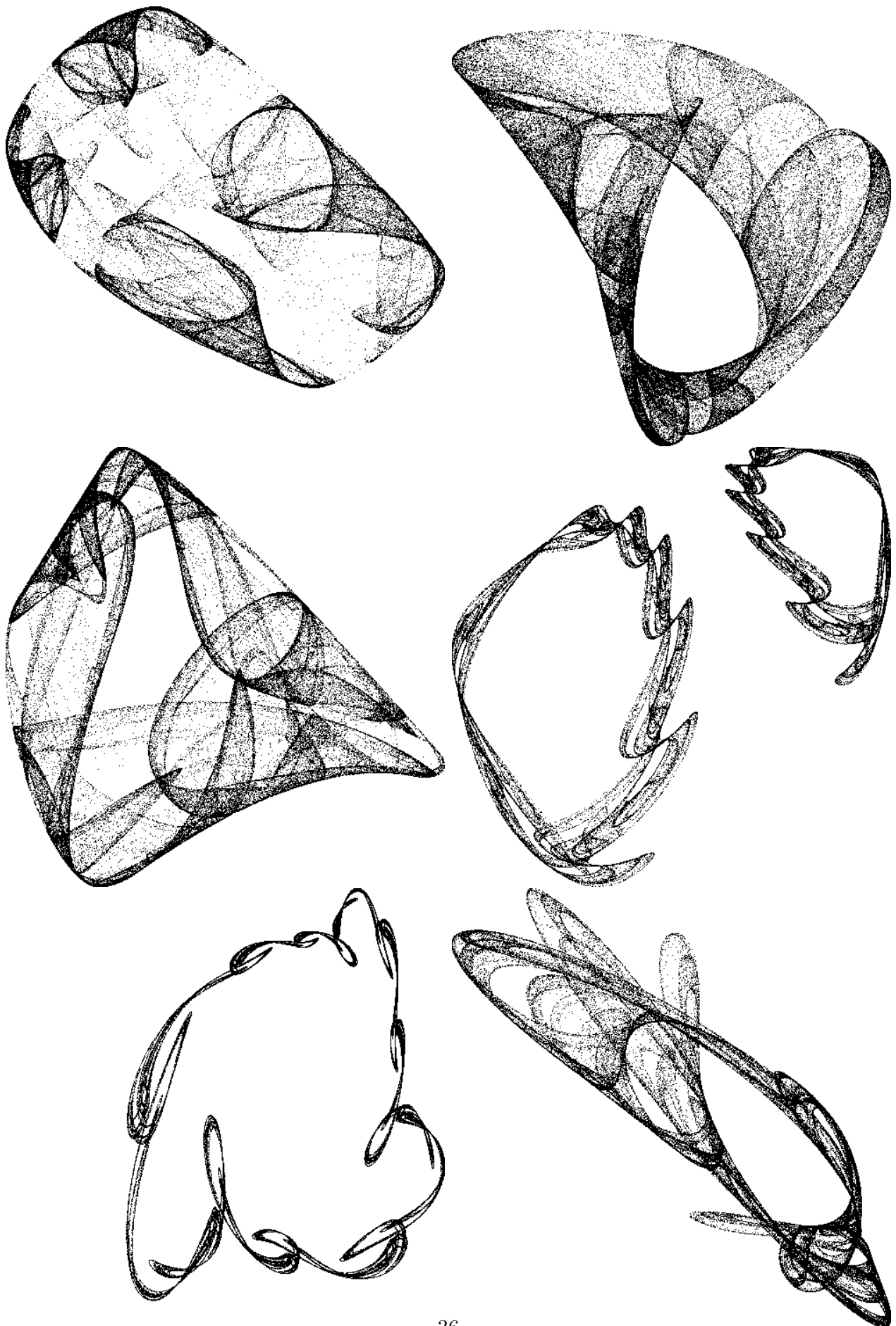
Figure 3: Random Chaotic Attractors

Figure 4: Random Chaotic Attractors

E.2 Henon-Heiles Attractor

"The Hénon-Heiles model was created for describing stellar motion, followed for a very long time, inside the gravitational potential $U_0(r, z)$ of a galaxy with cylindrical symmetry (Hénon & Heiles 1964). Extensive numerical experimentations should help to answer the question, if there exists, besides the known invariants H and L, a *third* invariant. Despite endless tentatives of analytical calculations during many decades, such a formula had not been found.

After a reduction of dimension, a Hamiltonian in two degrees of freedom of the form

$$H(p, q) = \frac{1}{2}\left(p_1^2 + p_2^2\right) + U(q) \tag{110}$$

is obtained and the question is, if such an equation has a *second* invariant. Here Hénon and Heiles put aside the astronomical origin of the problem and choose

$$U(q) = \frac{1}{2}\left(q_1^2 + q_2^2\right) + q_1^2 q_2 - \frac{1}{3}q_2^3$$

When U approaches $\frac{1}{6}$, the level curves of U tend to an equilateral triangle, whose verties are saddle points of U. The corresponding system has solutions with nontrivial properties. For given initial values with $H(p_0, q_0) < \frac{1}{6}$ and q_0 inside the triangle $U \le \frac{1}{6}$, the solution stays there and moves somehow like a mass point gliding on this surface (see figure 5).

Poincaré Cuts. We fix the energy H_0 and put $q_{10} = 0$. Then for any point $P_0 = (q_{20}, p_{20})$, we obtain p_{10} from (110) as $p_{10} = \sqrt{2H_0 - 2U_0 - p_{20}^2}$, where we choose the positive root. We then follow the solution until it hits again the surface $q_1 = 0$ in the positive direction $p_1 > 0$ and obtain a point $P_1 = (q_{21}, p_{21})$; in the same way we compute $P_2 = (q_{22}, p_{22})$, etc. For the same initial values and with $H_0 \in [\frac{1}{12}, \frac{1}{6}]$, the solution gives the Pointcaré cuts below (fig 5)" [4]
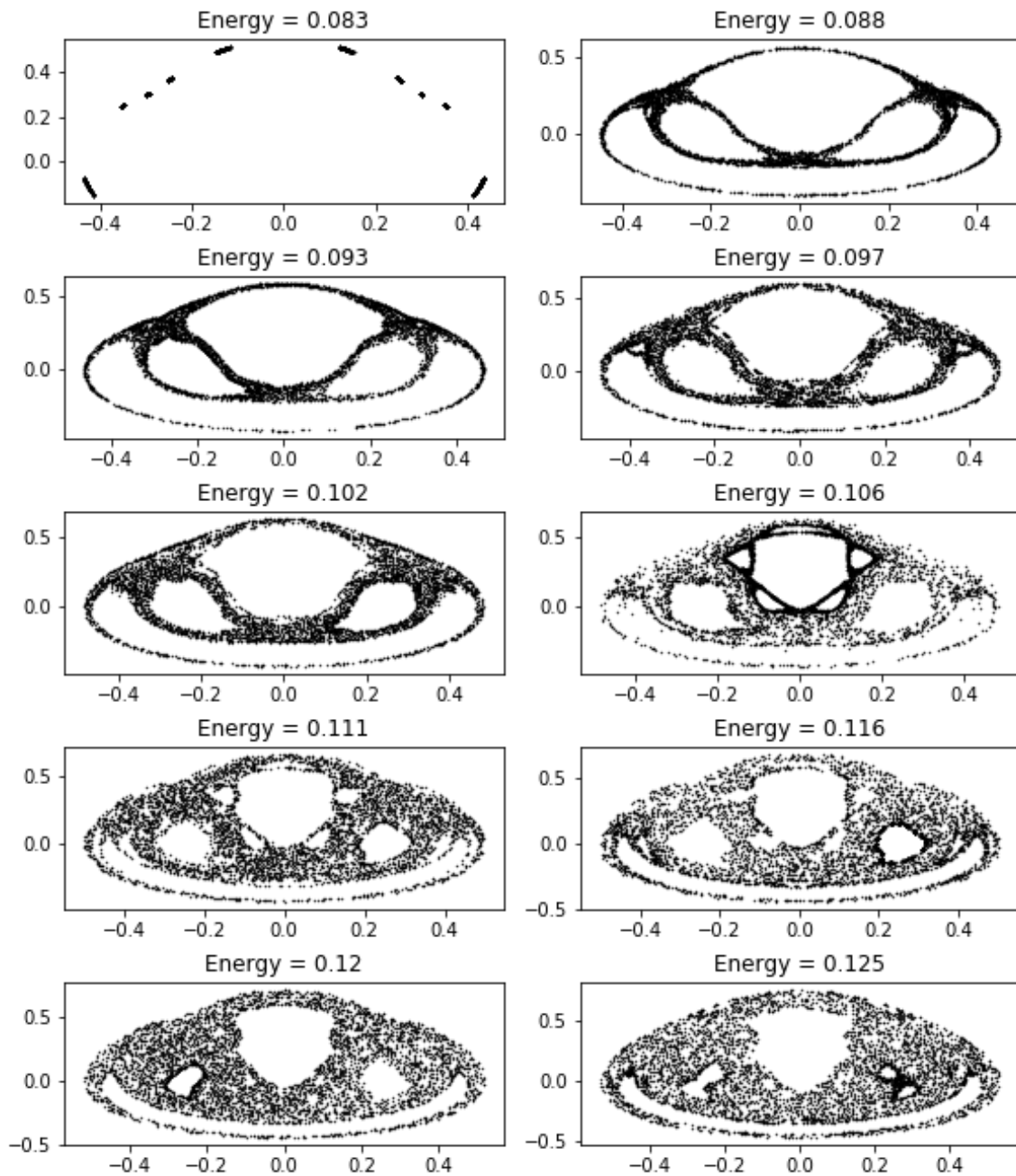
Figure 5: Hennon-Heiles System, Pointcaré Cuts

E.3 Other Stuff

Some symplectic integrators have cool graphical properties, here is a figure of the symplectic Strömer Verlet method applied to the kepler problem.