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Perspectives on geometric numerical integration

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ABSTRACT

Geometric numerical integration concerns the development, analysis, and use of algorithms for the numerical solution of differential equations that preserve a geometric or qualitative property of the exact solutions, such as an integral or symmetry, or preservation of a differential invariant such as symplecticity or phase space volume. The leapfrog method and the midpoint rule exemplify two major directions of development in the subject. It is an instance of the more general problem of structure-preserving model reduction: which features of reality should be preserved when building a model? We review some recent developments in geometric numerical integration, including the structure of Butcher series, symplectic integrators on non-Euclidean phase spaces, and symplectic integrators for boundary value problems.

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Introduction

A diagram from Book I, Theorem I of Newton's *Principia* is shown in Figure 1. It proves that a body moving under a central force sweeps out equal areas in equal times, or, in modern terms, the conservation of angular momentum for motion in a central force field. Since 1918 this property has been understood as an example of Noether's theorem, a cornerstone result in geometric mechanics. Newton has *discretised* the smooth motion of the planet into a repeated sequence of two steps ('For suppose the time to be divided into equal parts'). In the first step (AB), the planet moves in a straight line. In the second step, the planet does not move, but its velocity vector is changed under the influence of the central force from Bc to BC . The triangles SAB and SBC have the same area. He then lets the step size tend to zero ('Now let the number of those triangles be augmented ... *ad infinitum*'), arriving at the desired result for the continuous system.

To a modern reader, coming to this for the first time, there is a lot in this. First, Newton proves the result without using calculus, even though he had invented and used calculus in the previous decades. There is a long-running debate as to why Newton presented his results in geometric language (Guicciardini 1998). Second, he achieves an exact result, which holds for all future time of the motion, for all possible central force systems. Third, his method looks strikingly similar to the modern process of discretizing a differential equation in order to approximate its solution on a computer, especially in situations where an exact solution cannot be obtained using calculus. Not just similar—it is *exactly*

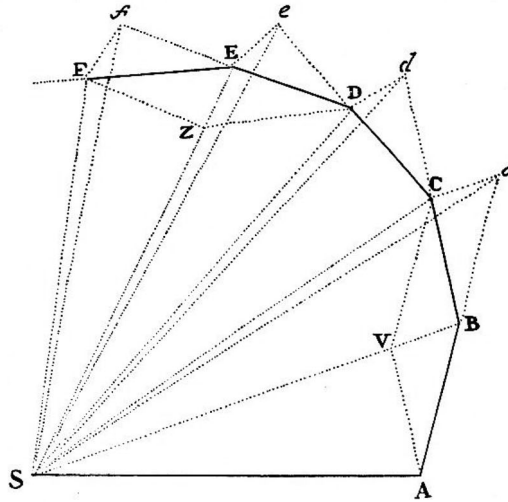
SECTION II

The determination of centripetal forces.

PROPOSITION I. THEOREM I

The areas which revolving bodies describe by radii drawn to an immovable centre of force do lie in the same immovable planes, and are proportional to the times in which they are described.

For suppose the time to be divided into equal parts, and in the first part of that time let the body by its innate force describe the right line AB. In the second part of that time, the same would (by Law 1), if not hindered,



proceed directly to c , along the line Bc equal to AB ; so that by the radii AS , BS , cS , drawn to the centre, the equal areas ASB , BSc , would be described. But when the body is arrived at B , suppose that a centripetal force acts at once with a great impulse, and, turning aside the body from the right line Bc , compels it afterwards to continue its motion along the right line BC .

Figure 1. Newton's proof of conservation of angular momentum for motion in a central force field.

the same as what is now known, from its alternation of position and velocity updates, as the leapfrog method, introduced in modern times by Verlet (1967) as a method for simulating the motion of large numbers of molecules. What could not have been anticipated by Verlet is that, fifty years later, it remains one of the most widely used and fundamental algorithms in computational physics and chemistry. Fourth, while Newton knows that the discrete motion ABC is only an approximation that wanders away from the true motion ('their ultimate perimeter ADF will be a curve line'), the discrete motion satisfies the equal area property *exactly*, for all time, and not merely approximately.

Symplecticity

This possibility of a computational method preserving some aspect of the true solution exactly, without any error even over long times, is the foundation of geometric numerical integration. Newton's diagram shows that the leapfrog method preserves angular momentum. However, it also preserves another property of Newton's equations, namely

symplecticity. The word symplectic is from the Greek *symplegma*, or intertwined together, and refers to the special way that the position and velocity components are linked in the equations of motion. They are dual to each other in a way that is not obvious to our immediate experience, where they seem to have separate natures.

After a long gestation beginning in the eighteenth century, the symplectic property was strongly exploited by Poincaré in the 1890s in his studies of celestial mechanics. This was made possible by his clear understanding of the concept of phase space (which itself has a long and tangled history Nolte 2010). If the positions of a system of particles are $q_1, \dots, q_n$, and their momenta are $p_1, \dots, p_n$, then the system's phase space is $\mathbb{R}^{2n}$ with coordinates $(q_1, \dots, q_n, p_1, \dots, p_n)$, which is conveniently collected into a vector z . Moreover, instead of considering the path taken by a single trajectory $z(t)$, he considered the evolution of a whole ensemble of nearby initial conditions (Poincaré 1893, §233):

Consider the fluid molecules which initially form a certain figure F_0 ; when these molecules are displaced, their ensemble forms a new figure which will be deformed in a continuous manner, and at the instant t the envisaged ensemble of molecules will form a new figure F ...

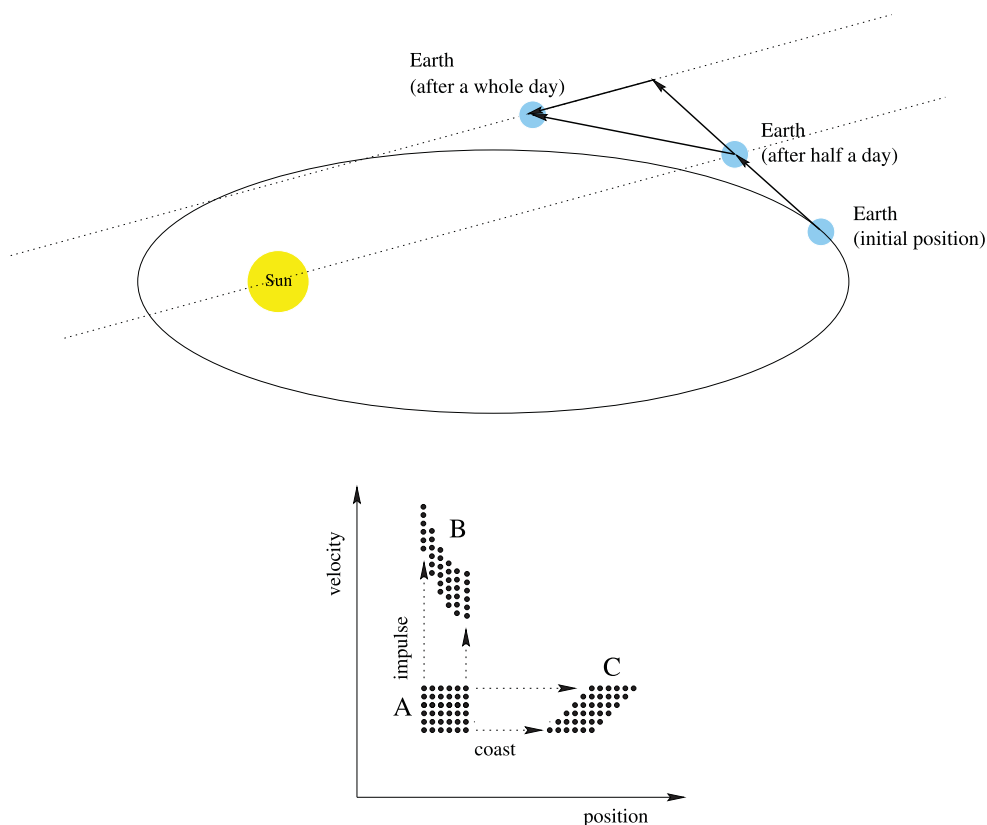


Figure 2. The leapfrog method illustrated in real space (top) and in phase space (bottom), illustrating its property of preservation of phase space area, an instance of symplecticity. Point A shows an ensemble of 25 virtual Earths close to the actual Earth; C shows how they would spread out in phase space during the initial ‘coast’ step; B shows how they would spread out during the ‘impulse’ step. The area occupied by the ensembles B and C is the same as that occupied by A.

This is what is now called the flow map.

The symplectic property of the leapfrog method is illustrated in Figure 2. Consider an ensemble of particles, initially at A. They will slowly spread out. During the ‘coast’ step, the faster bodies in the ensemble coast a little bit further, to C, but the whole ensemble continues to occupy the same area. Similarly, when the force acts ‘at once with a great impulse’ (Newton), the velocities of the bodies closer to the sun receive a greater impulse, but the whole ensemble still occupies the same area, at B. The area is preserved regardless of the shape of the ensemble. It is preserved for all time, and this is the symplectic conservation law. Just as Newton did, letting the steps ‘be diminished *in infinitum*’ shows that the continuous motion also obeys the same conservation law.

With one position and one momentum variable, as in Figure 2, symplecticity is just planar area and is easy to visualise given the idea of phase space. For larger systems, symplecticity is the sum of the areas projected to each (q_i, p_i) plane, and its impact is subtle and far-reaching, giving rising to the modern, highly active fields of symplectic geometry and topology.

Switching to calculus, consider systems obeying Hamilton’s equations of motion

$$\begin{aligned}\dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i}\end{aligned}\tag{1}$$

for $i = 1, \dots, n$, where $H(q, p)$ is the Hamiltonian, the total energy of the system. The Equations (1) may be written in matrix form as or

$$J\dot{z} = \nabla H(z), \quad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}.\tag{2}$$

Systems in which $H(q, p) = \sum_{i=1}^n p_i^2/(2m_i) + V(q)$ lead to $m\ddot{q}_i = -\nabla V(q)$, or Newton’s second law.

The relative motion of nearby trajectories $z(t)$ and $z(t) + \varepsilon u(t)$ can be studied by differentiating with respect to ε , giving the variational equation

$$J\dot{u} = H''(z)u$$

where $H''(z)$ is the symmetric matrix of second partial derivatives of H . The symplectic form ω is then the bilinear function of two first variations u and v given by $\omega(u, v) := u^T J v$. The property that the flow of (2) is symplectic is then verified by

$$\frac{d}{dt} \omega(u, v) = u^T J \dot{v} + \dot{u}^T J v = u^T (J \dot{v}) - (J \dot{u})^T v = u^T (H''(z)v) - (H''(z)u)^T v = 0.$$

Following an explosion of interest in the 1990s, it is now known that symplectic integrators, like the leapfrog method, can provide excellent results for Hamiltonian systems, even over very long times and when the dynamics exhibits chaos (Sanz-Serna and Calvo 1994; Hairer et al. 2006; McLachlan and Quispel 2006). Any features that are robust and generic for Hamiltonian systems are preserved. They are fast and simple, and can be used reliably both when the time steps are small (when quantitative accuracy is required) or large (when qualitative preservation of phase space structures is sufficient).

The motion of the solar system provides a striking example, of interest from the time of Plato (*Timaeus* 46c)

... the god invented and gave us vision in order that we might observe the circuits of intelligence in the heavens ... that, by learning to know them and acquiring the power to compute them rightly according to nature, we might reproduce the perfectly unerring revolutions of the god and reduce to settled order the wandering motions in ourselves.

through Jefferson (1819)

I am indebted to you for Mr. Bowditch's very learned mathematical papers ... One of these impairs the confidence I had reposed in La Place's demonstration that the excentricities of the planets of our system could oscillate only within narrow limits, and therefore could authorise no inference that the system must, by its own laws, come one day to an end.

to Poincaré, whose study mentioned above led him to the discovery of chaotic dynamics, to today: on time scales up to 2 Myr, simulations of the solar system have given accurate values for solar insolation, one of the key forcings for the ice ages (Edvardsson et al. 2002); on time scales up to 40 Myr, they have led to a substantial recalibration of the geological epochs, and allowed the dating of some geological samples to an accuracy of 40 kyr (Laskar et al. 2004); and on time scales of a few Gyr they have allowed the study of chaos in and evolution of the solar system—and indeed of extrasolar systems (Barnes and Raymond 2004).

What kinds of dynamical systems are there?

Success here has been due both to the importance of symplecticity and to the structure of the particular system at hand. What other properties can dynamical systems have that influence their behaviour? Some examples are conserved quantities (like energy and momentum); symmetries; time reversibility; and volume preservation (as in incompressible fluids). These properties influence the characteristic dynamics, bifurcations, and invariant sets of the systems. Thus we are asking for a natural classification of dynamical systems, ideally according to some algebraic structure. This approach is something that is a characteristic of mathematics as a whole that is distinct from other disciplines. Once an interesting example of something is known, it is natural to ask for all possible examples. This may turn out to be easy (there are just seven types of symmetry in frieze patterns Knight 1984) or extremely difficult (prime numbers are the building blocks of the integers, but understanding all their properties is difficult), but it is always important. Attempts to classify dynamical systems were made early on by Lie and by Cartan (1909), but have not led to a satisfactory general theory. Nevertheless, the known examples are important because, as most differential equations cannot be solved exactly, it is helpful to know at least the typical or characteristic features of each class.

Often, in modelling situations, even the equations of motion are not known precisely. In this case knowing general features like symmetries and dimensions is vital, as is knowing whether any phenomena that are discovered are robust under changes to the model. From this point of view, geometric numerical integration is a special case of the fundamental scientific challenge of *structure preserving model reduction*, passing from a more exact description of nature to a less exact one, in order to understand it better. In such approximations, it is important to understand what can be retained and what should be retained.

While this problem pervades science, and is always difficult to handle, in one respect dynamical systems and statistics face a worse situation than do most parts of science:

they are trying to predict the future. As Silver (2012) remarked (paraphrasing the serenity prayer):

Prediction is difficult for us for the same reason that it is so important: it is where objective and subjective reality intersect. Distinguishing the signal from the noise requires both scientific knowledge and self-knowledge: the serenity to accept the things we cannot predict, the courage to predict the things we can, and the wisdom to know the difference.

Returning to earth, let us suppose that a dynamical model has been constructed of some situation—meteorology, say, or the interaction of molecules—and that the details of the model are assumed to be accurate and knowable in as much precision as desired, and that the model is well-posed and does in fact reflect reality. This leaves the mathematical problem of drawing conclusions from the model, which almost always requires further simplifications. Even here there are limitations. It is not always easy to discover the important structures in an equation, or to know how they affect its solutions. Furthermore, it is now known that some important properties *cannot* be preserved by numerical methods. For example, no method can preserve both energy and symplecticity. No method can preserve phase space volume and arbitrary linear symmetries. There is also a large grey area in which no method with the desired properties is known to exist, but nor is such a method known to be impossible (McLachlan and Quispel 2006).

The sequel reviews three topics in geometric numerical integration. They range from the abstract (the algebraic structure of numerical integration methods in general), to the geometric (the construction of symplectic integrators on spheres), to the important yet poorly understood (partial differential equations).

The midpoint rule, and Butcher series

Although Poincaré used analytical and topological methods, rather than numerical methods, he did introduce one transformation that is now recognised as a fundamental example of a symplectic integrator. For a differential equation $\dot{z} = f(z)$, this is the midpoint rule with time step h ,

$$\frac{z_1 - z_0}{h} = f\left(\frac{z_0 + z_1}{2}\right). \quad (3)$$

Poincaré proved (Poincaré 1893, §319) that the transformation $z_0 \mapsto z_1$ is symplectic. In the notation of (2), we have

$$J(z_1 - z_0) = h\nabla H(\bar{z}), \quad \bar{z} = \frac{z_0 + z_1}{2}$$

with first variation

$$J(u_1 - u_0) = \frac{1}{2}hH''(\bar{z})(u_0 + u_1).$$

Therefore,

$$(u_0 + u_1)^T J(v_1 - v_0) = \frac{1}{2}h(u_0 + u_1)^T H''(\bar{z})(v_0 + v_1).$$

The right hand side is symmetric in u and v , so the left hand side is too. Therefore

$$0 = (u_0 + u_1)^T J(v_1 - v_0) - (v_0 + v_1)^T J(u_1 - u_0) = 2u_1^T Jv_1 - 2u_0^T Jv_0.$$

That is, the symplectic form $\omega(u, v) = u^T Jv$ is preserved, namely $\omega(u_1, v_1) = \omega(u_0, v_0)$.

Poincaré used this transformation to study periodic orbits. In this application, symplecticity was essential. However, when used as an integrator, the midpoint rule, in addition to symplecticity, has some other important properties that the leapfrog method does not have. It also preserves any quadratic conserved quantities, and any linear symmetries, exactly and automatically. (This is all the more remarkable because the method is provided only with the differential equation, and not with its conserved quantities.)

This feature is related to an underlying symmetry of the midpoint rule. Namely, it is invariant under all affine changes of variable in z , those of the form $\tilde{z} = Az + b$, including translations, rotations, and changes of scale and units. It's also an example of the widely used class of *Runge-Kutta methods*. Beginning in 1963, the New Zealand mathematician John Butcher revolutionised the study of numerical differential equations in a remarkable series of papers concerning what are now called Butcher series or B-series in his honour (Butcher 1963). Associated with the differential equation $\dot{z} = f(z)$, $z \in \mathbb{R}^n$, these are series of the form

$$c_0 z + c_1 h f + c_2 h^2 f'(f) + c_3 h^3 f'(f'(f)) + c_4 h^3 f''(f, f) + \dots,$$

where the vector field f and its derivatives $f', f'', \dots$ are evaluated at z and $c_0, c_1, \dots$ are constants. All Runge-Kutta methods can be expanded in B-series, some of which (like the midpoint rule) are symplectic, and others of which are energy preserving, when f is Hamiltonian. In recent years a rich additional structure of B-series, induced by these properties, has been discovered (McLachlan et al. 2017). Over time, many other families of numerical methods have also been found to possess B-series, prompting the question of exactly which methods have one. What property—ideally, what simple geometric property—characterises methods that have a B-series?

This problem was solved in McLachlan et al. (2016). A method has a B-series if, and only if, it respects all affine maps between spaces of any dimension. Namely, if $\dot{z} = f(z)$ and $\dot{y} = g(y)$ are differential equations related by $y = Az + b$, then a numerical method has a B-series if and only if it yields related maps when applied to these two equations; informally, if and only if the results do not depend on the choice of coordinates.

The spherical midpoint rule

From this point of view, B-series methods such as the midpoint rule (3) can be considered as fairly fundamental objects in numerical analysis. They are defined on vector spaces independently of the choice of coordinates. A key development of modern geometric mechanics has been to study dynamical systems on general manifolds such as spheres, tori, and Lie groups, not only on vector spaces. These spaces do not even have global coordinates. A key example is the motion of a freely rotating rigid body such as a hammer (Figure 3). Its three rotational degrees of freedom cannot be described by a single

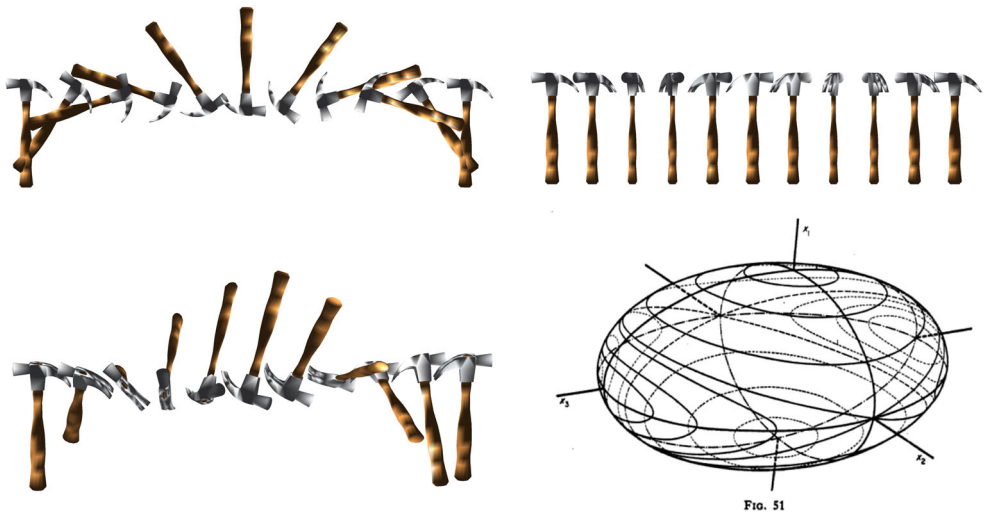


Figure 3. The motion of a free rigid body: the hammer rotates stably around its long and short axes (left), but not around its middle axis (top right). The dynamics of the angular momentum in the body frame takes place on the sphere of constant total angular momentum. As the kinetic energy, whose level sets are ellipsoids, is also conserved, the orbits are the intersection of spheres and ellipsoids, as drawn by Landau and Lifschitz (1960) and shown here (bottom right).

global coordinate chart. One way to represent its motion is as a *spin system* of the form

$$\dot{x} = f(x) := x \times \nabla H(x), \quad x \in \mathbb{R}^3. \quad (4)$$

Instead of the phase plane with coordinates (q, p) and symplectic form being planar area, we have the sphere $x_1^2 + x_2^2 + x_3^2 = 1$ with symplectic form being Euclidean area on the sphere. The standard midpoint rule (3) does not preserve area on the sphere. In McLachlan et al. (2014) a variant of the midpoint rule is described, called the *spherical midpoint rule*, that preserves the sphere and its area. Applied to (4), the spherical midpoint rule is

$$x_1 = x_0 + hf\left(\frac{\bar{x}}{\|\bar{x}\|}\right), \quad \bar{x} = \frac{x_0 + x_1}{2}. \quad (5)$$

An example is shown in Figure 4. Like Poincaré's midpoint rule, it is also invariant under symmetries of the phase space: affine for the standard midpoint rule, rotations of the sphere for the spherical midpoint rule. Both rules extend to larger, coupled systems. Although the spherical midpoint rule (5) is pleasingly simple, and also plausibly related to the original midpoint rule, so far it stands alone and no general method of constructing symplectic integrators on arbitrary symplectic manifolds is known.

Multisymplecticity and boundary value problems

The subject of numerical methods for differential equations can be broadly divided into methods for ordinary differential equations (ODEs, those with one independent variable, such as time) and partial differential equations (PDEs, those with more than one independent variable, such as space and time); it can also be divided into initial- and boundary-

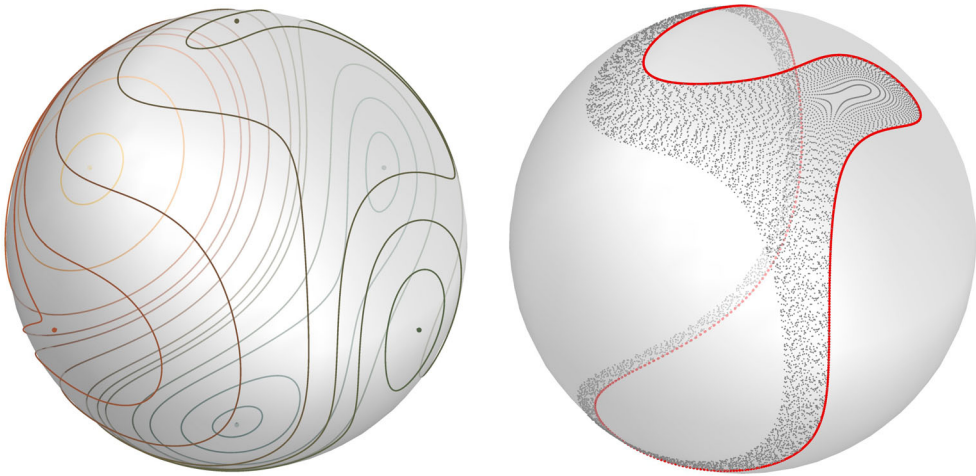


Figure 4. Left: Phase portrait of a Hamiltonian system on a curved phase space, a sphere. Right: An orbit computed using the classical midpoint rule shows a nonphysical drift (black); the orbit computed by the symplectic spherical midpoint rule (red) shows a correct periodic orbit with no drift.

value problems. The success of symplectic integrators largely rests on their performance for initial-value problem ODEs. What can be done for the other problem classes?

Not surprisingly, given its fundamental role in physics, investigation of these questions goes back a long way, at least to Weyl (1935). For a PDE such as the nonlinear wave equation

$$u_{tt} = u_{xx} + f(u), \quad (6)$$

perturbed solutions $u(x,t) + \varepsilon v(x,t)$ be studied using the variational equation

$$v_{tt} = v_{xx} + f''(u)v.$$

The differential forms ω and κ , where $\omega(v,w) = vw_t - wv_t$ and $\kappa(v,w) = vw_x - wv_x$ then obey the *multisymplectic* conservation law

$$\omega_t + \kappa_x = 0. \quad (7)$$

Just as in conservation of mass, a change in ω at any point (x,t) must be balanced by a flux κ .

Numerical methods can be developed that preserve discrete versions of (7). The simplest is the traditional 5-point scheme with time step Δt and space step Δx ,

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\Delta t)^2} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + f(u_i^n)$$

where $u_i^n \approx u(i\Delta x, n\Delta t)$. More sophisticated methods, including spectral and finite element methods, are also available (Bridges and Reich 2006). However, what is still not clear is the full influence of the conservation law (7) on the behaviour of solutions to the differential equation (6).

One point of view is provided by studying the simpler case of a boundary value problem. Consider the reaction–diffusion equation

$$u_t = u_{xx} + C e^u, \quad u(x,0) = u_0(x), \quad u(0,t) = u(1,t) = 0. \quad (8)$$

Here $u(x,t)$ is the temperature of a solid and $C > 0$ is a parameter that specifies the heat generated by an exothermic process. Steady-state solutions $u(x)$ obey the ODE boundary value problem

$$0 = u_{xx} + C e^u, \quad u(0) = u(1) = 0. \quad (9)$$

For $0 < C < C^* \approx 3.51$, this problem has two solutions; for $C > C^*$ it has none (see Figure 5). In the latter case, the original time-dependent problem (8) must result in an ignition, regardless of the original temperature distribution $u_0(x)$. The critical value C^* is called a bifurcation point. In this case it is the simplest of all types of bifurcation, a *fold*.

A crucial question in problems like this, therefore, is what kinds of bifurcations are possible? How common are they? Do they persist under small changes in the problem, or under discretization? How can they be detected?

In a recent study (McLachlan and Offen 2018), we have gone some way towards answering these questions in the framework of *catastrophe theory*, a branch of the theory of singularities of functions developed enormously during the 1960s and 1970s (Poston and Stewart 2014). Symplectic (and, for PDEs, multisymplectic) integrators can preserve these bifurcations; standard methods may not. Two more exotic bifurcations are shown in Figure 6.

So far, geometric numerical methods for PDEs have shown a high degree of success only for the simplest equations, such as (6). There is a long list of PDEs that are difficult to solve numerically, difficult to analyze, and also have a rich geometric structure, such as those in fluid mechanics, general relativity, optimal transport, curvature flow, and harmonic analysis. Often the solutions possess fine features and instabilities that preclude highly accurate solutions. Work in some of these areas such as fluid mechanics (Cotter and Thuburn 2014) and gravitational waves (Dietrich et al. 2015) is beginning that may form part of future operational methods. It is here that we can anticipate—or, at least, hope—that geometric numerical methods may continue to develop and to provide useful tools for understanding.

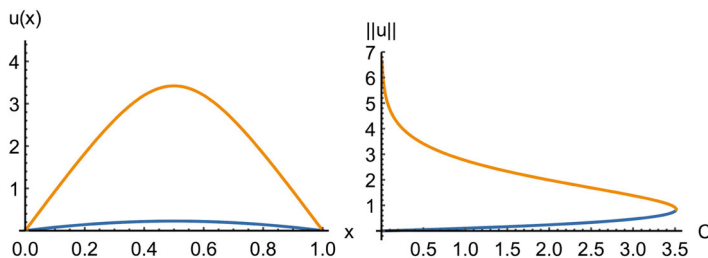


Figure 5. Bifurcation in the 2-point boundary value problem (9). For $C = 1.5 < C^*$ the problem has two solutions (shown at left); for $C > C^* \approx 3.51$ it has none. C^* is a fold bifurcation.

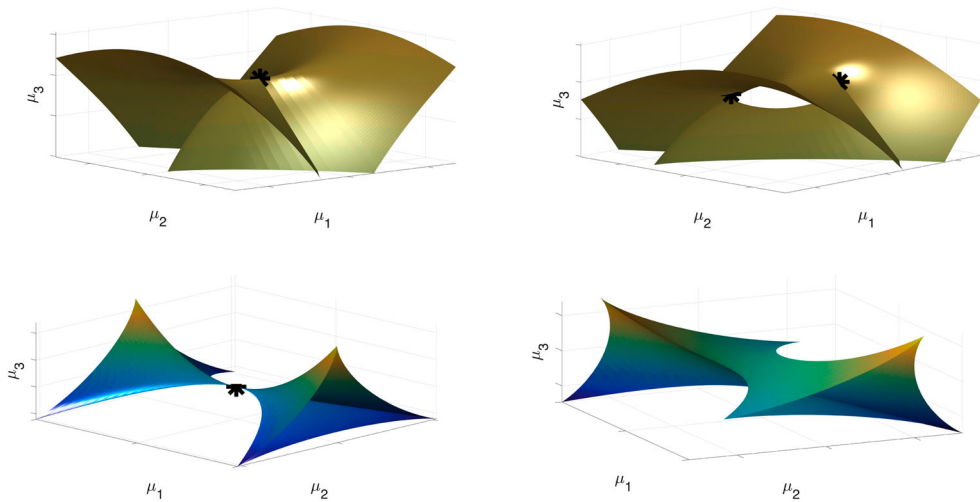


Figure 6. Schematic illustration of some codimension-3 bifurcations in Hamiltonian boundary value problems with parameters μ_1 , μ_2 , and μ_3 . Left: the bifurcation surfaces of the hyperbolic umbilic (top) and elliptic umbilic (bottom) bifurcations have a complicated but typical structure: any problem close to one of these will show a similar bifurcation. Right: A *non*-Hamiltonian problem close to one of these, or a discretization by a non-symplectic integrator, produces a qualitative change in the bifurcation diagram.

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