Are Discrete Models More Accurate?

N ewton's second law describes the motion of the center of mass of most objects that we encounter in everyday life, including the complex motion of a spoon when we eat, the acceleration of a car, and even the trajectories of planets and stars. Only if objects move extremely fast, do we need to replace Newton's second law with Einstein's theory of relativity, and only if objects are extremely small, do we need to use the laws of quantum mechanics.

Newton's second law states that the net force F on an object equals the product of its mass m and its acceleration a: $F = m \times a$. Unfortunately, the acceleration of the center of mass of an object is hard to measure. It is the rate of change of the velocity, where the velocity of the center of mass is its change in position per unit of time. Most of the time, we cannot determine the acceleration or the velocity directly but measure the location of the surface of the object at fixed time intervals. We use this data to estimate the position of the center of mass and then compute its acceleration. This is a complicated procedure.

It is equally complicated to solve Newton's second law on a computer numerically, because it is a second-order differential equation. Typically, the net force depends on the position of the object $F = F(x)$ and the acceleration is the second time derivative of the position $a = \frac{d^2x}{dt^2}$. There are a few simple systems, such as mass–spring systems, where Newton's second law has an analytical solution, but in all real life situations, one needs a sophisticated procedure, such as a fourth to fifth order Runge-Kutta method to integrate Newton's second law. Predicting the motion of a planetary system with two or more planets requires a super computer.

In the following, we study the motion of an object by starting at the molecular level and then moving up to the macroscopic level. Using this method, Newton's law in differential form is overly complicated. In contrast, Newton's law as a difference equation can easily be solved on a computer and experimentally verified. Its predictions are closer to experimental observations.

Every macroscopic object consists of many molecules. To determine the center of mass motion, we first consider the motion of the molecules relative to each other: vibrational modes. There are roughly the same numbers of vibrational modes as there are molecules. We sort the vibrational modes according to their frequency and time average their impact on the center of mass motion, one-by-one, starting with the mode with the highest frequency [1, 2]. To illustrate this procedure, we assume that all vibrational modes have been time averaged, except

ALFRED HÜBLER AND AUSTIN GERIG

Alfred Hübler is the director of the Center for Complex Systems Research at the University of Illinois at Urbana-Champaign, Urbana, Illinois (hubler.alfred@gmail.com or http://server17.how-why.com/blog/)

Austin Gerig is an Associate Member of the Quantitative Finance Research Centre at the School of Finance and Economics of the University of Technology, Sydney, Australia (austin.gerig@uts.edu.au or http://datasearch.uts.edu.au/business/staff/finance/details.cfm?StaffId=7748)

FIGURE 1
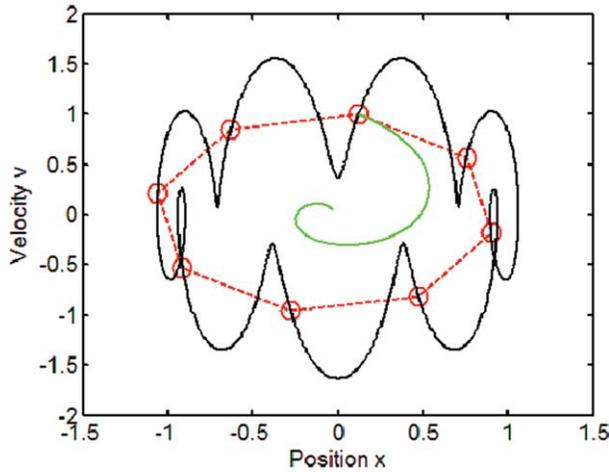
A phase space representation of the original dynamics (black), the dynamics of the averaged differential equation (green), and the dynamics of the mapping function (red circles). The dashed line connects the states predicted by the mapping function. The mapping function makes accurate predictions, whereas the differential equation provides only a rough approximation of the original dynamics.

but not zero, then without any further approximations, we write Eq. (2) as a mapping function:

$$x_{n+1} - x_n = T \, \bar{f}(x_n) \qquad (4)$$

where $x_n = x(n \cdot T)$, $n = 0, 1, \ldots$ This mapping function describes the motion of the center of mass of soft and rigid objects, whereas Eq. (3) applies only for rigid objects. The mapping function is generally more accurate because its derivation requires only one approximation, whereas the equation of motion in differential form requires a second approximation.

As an example, consider a linear oscillator with a high-frequency vibration: $\frac{d^2x}{dt^2} + x = F \sin(\omega t)$, where $\omega = \frac{2\pi}{T} \gg 1$. We use averaging to find a low-dimensional model of the slow center of mass motion.[1] Figure 1 shows the dynamics of this system, the dynamics of the averaged differential equation, and the dynamics of the mapping function.

---

[1] *We transform the second-order equation to a first-order equation: $\frac{dx}{dt} = v$ and $\frac{dv}{dt} = -x + F \sin(\omega t)$, where v is the velocity. Both equations are averaged to eliminate the fast variable: $\frac{1}{T}\int_t^{t+T} \frac{dx}{dt} dt' = \frac{1}{T}\int_t^{t+T} v \, dt'$ and $\frac{1}{T}\int_t^{t+T} \frac{dv}{dt} dt' = \frac{1}{T}\int_t^{t+T} -x + F \sin(\omega t) dt'$. Evaluating the integrals gives for Eq. (2): $\frac{X(t+T)-X(t)}{T} = X(t)\frac{\cos(T)-1}{T} + V(t)\frac{\sin(T)}{T}$, $\frac{V(t+T)-V(t)}{T} = X(t)\frac{-\sin(T)}{T} + V(t)\frac{\cos(T)-1}{T}$, where $t = n\,T + \Delta n = 0, 1, 2, \ldots$, $x(t) = X(t) + B\sin(\omega t)$, and $v(t) = V(t) + B\omega \sin(\omega t)$. The averaged differential equation is: $\frac{dX}{dt} = X(t)\frac{\cos(T)-1}{T} + V(t)\frac{\sin(T)}{T}$, $\frac{dV}{dt} = +X(t)\frac{-\sin(T)}{T} V(t)\frac{\cos(T)-1}{T}$, and the mapping function is $X_{n+1} = X_n\frac{\cos(T)}{T} + V_n\frac{\sin(T)}{T}$, $V_{n+1} = X_n\frac{-\sin(T)}{T} + V_n\frac{\cos(T)}{T}$. Figure 1 shows the analytic solutions of the original equation, the dynamics of the mapping function, and a simulation where the averaged differential equation is integrated with Euler's method with time step $t = \frac{T}{100}$. The parameters are $A = 1$, $\omega = 8$, $F = 5$, and $\Delta = .2, T = \frac{2\pi}{\omega}, B = \frac{F}{1-\omega^2}$.*

---

one. In this case, the equation of motion of the center of mass x might read: $dx/dt = f(x,y)$, where t is time, y is a vibration such as $y = y_0 \sin\left(\frac{2\pi}{T} t\right)$, with a short period of oscillation, $T \ll 1$, and a small amplitude $y_0 < f$.

Next, we time average both sides of the differential equation $\frac{1}{T}\int_t^{t+T} \frac{dx}{dt} dt' = \frac{1}{T}\int_t^{t+T} f(x,y) dt'$ and obtain the difference equation:

$$\frac{x(t+T) - x(t)}{T} = \frac{1}{T}\int_t^{t+T} f(x(t'), y(t')) dt' \qquad (1)$$

This equation is exact. To evaluate the remaining integral, we assume that $x(t')$ changes only slightly and approximate its change by a constant, such as $x(t') \approx x(t)$, or a Taylor expansion, such

as $x(t') \approx x(t) + f(x(t), y(t')) \cdot t' + \ldots$ (Approximation I), and evaluate the integral. Then, Eq. (1) reads:

$$\frac{x(t+T) - x(t)}{T} = \bar{f}(x(t)) \qquad (2)$$

Now there are two ways to proceed:
i. We assume that the object is rigid and therefore the period of oscillation is effectively zero, i.e., $T \approx 0$, then the difference can be approximated by a differential $\frac{x(t+T)-x(t)}{T} \approx \lim_{T \to 0}\left(\frac{x(t+T)-x(t)}{T}\right) = \frac{dx}{dt}$ (Approximation II). With this second approximation, Eq. (2) turns into a differential equation for x:

$$\frac{dx}{dt} = \bar{f}(x) \qquad (3)$$

Such an approach is used to derive Newton's second law in differential form.
ii. If the object is not rigid, i.e., the period of the fast oscillation is small

The original dynamics is not damped but the dynamics of the averaged differential equation is damped. The dynamics of the mapping function matches the original dynamics exactly.

Most of the laws of Physics, including the laws of thermodynamics, electrodynamics, quantum mechanics, those that govern fluid flow, and those that describe the averaged motion of many particle systems, can be formulated as mapping functions. Mapping functions are easy to work with, can be iterated quickly and efficiently with computers, produce time series that are naturally compatible with discrete experimental data, and, as shown above, can be more accurate than differential equations.

It is conceivable that in the future, many of the laws of Physics will be formulated as difference equations instead of differential equations. This paradigm shift would have a large impact on Physics education. Currently, Physics is taught in upper level high school classes because calculus is a prerequisite. If the fundamental concepts are formulated as algebraic difference equations, they can be taught at the middle school level and reach a much larger fraction of the student population. In other disciplines such as finance and economics, the situation is similar. Formulating fundamental concepts with the tools of discrete mathematics may help to explain them to a larger fraction of the population.

In summary, the dynamics of macroscopic variables, such as the center of mass of an object, can be modeled by equations of motion in differential form if the separation of time scales of the slowest modes is very large. If the separation of time scales is not that large, mapping functions, such as Newton's second law written as a difference equation, provide the most accurate models for macroscopic variables. In both cases, averaging provides low-dimensional equations of motion for macroscopic variables, no matter if the underlying high-dimensional model is time discrete or time continuous.

There is a third class of systems, however, where the modes cannot be sorted by time and amplitude because their time scales are variable, or because the amplitude of the higher frequency modes is not smaller, or because there is strong coupling between all modes across scales. In this case, there is most likely no accurate low-dimensional model. For these systems, the underlying high-dimensional model has irreducible complexity: averaging does not provide accurate low-dimensional models. If the system has billions of parts, such as the molecules in a flickering flame, it is practically impossible to simulate and predict its dynamics, including the dynamics of the center of mass.

REFERENCES
1. Lichtenberg, A.J.; Lieberman, M.A. Regular and Chaotic Dynamics, 1st ed.; Applied Mathematical Sciences, Vol. 38; Springer-Verlag: New York, NY, 1983.
2. Guckenheimer, J.; Holmes, P. Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields. Applied Mathematical Science No. 42; Springer-Verlag: New York, Heidelberg, Berlin, 1983.