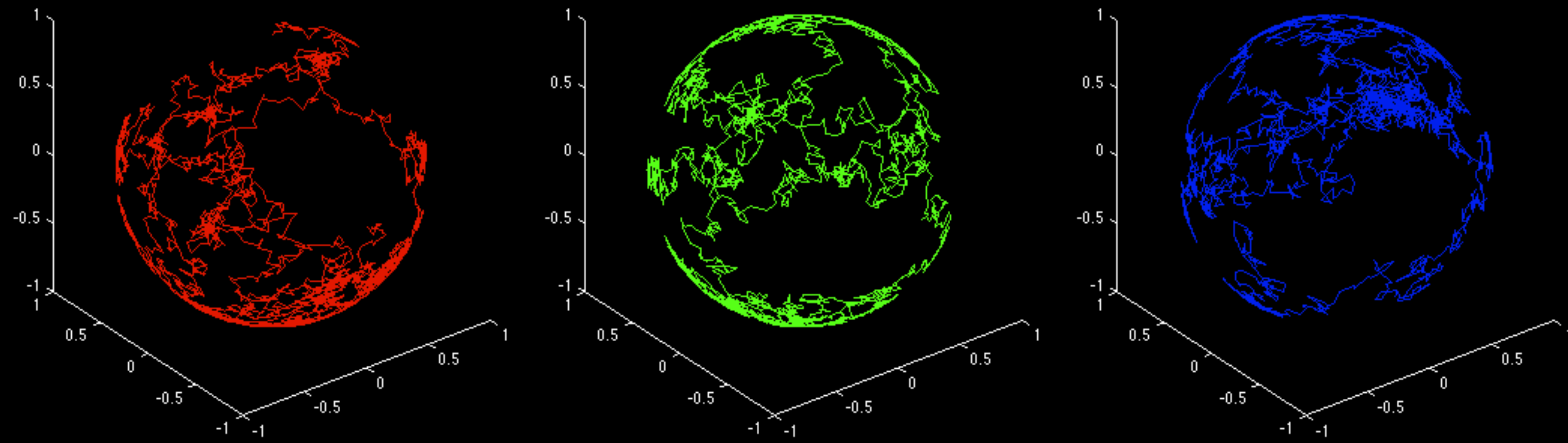
Geometric numerical integrators



OGS
Office of Graduate Studies

Books & Bagels interdisciplinary talk, June 2013

Sam Kennerly   Drexel class of 2013   PhD Physics

GSA
Graduate Student Association

This presentation was made possible by a Drexel Office of Graduate Studies Dissertation Fellowship.

Ordinary differential equations

- Low-jargon version: We want to predict some number $x(t)$ which depends on some other number *t*. Let $\dot{x}(t)$ denote the *t* derivative of $x(t)$. This is the "rate of change" of *x* as *t* changes. Suppose we know that $\dot{x}(t)$ obeys an **ordinary differential equation** (ODE) of the form:

$$\dot{x}(t) = f(x,t)$$

- Suppose we know $x(t_0)$ for some t_0. This is an **initial value problem.** A **numerical integrator** is a program for solving these problems.
- The number we want to predict is the **dependent variable** *x.* I like to call the **independent variable** *t* "time," but it can be any real number. *Ordinary* means *t* derivatives only; no other derivatives allowed!
- ODEs can include multiple variables $x(t), y(t), z(t), \ldots$ and/or higher-order derivatives like $\ddot{x}(t)$, which is the rate of change of $\dot{x}(t)$. **Reduction of order** is a trick for writing any ODE as a first-order vector ODE:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x},t)$$

Generator equations

- I use the name **generator equation** for any ODE of the form:

  $$\dot{\mathbf{x}}(t) = \hat{G}(\mathbf{x}, t) \cdot \mathbf{x}(t)$$

  x(t) is a column vector whose components are dependent variables, $G(t)$ is a matrix, and the dot means matrix multiplication.

- Any ODE can be rewritten in generator-equation form.

- Group theorists call G an *infinitesimal generator*. If G is constant, then the exact solution is "generated" by a matrix exponential:

  $$\mathbf{x}(t) = \exp\left[(t - t_0)\hat{G}\right] \cdot \mathbf{x}(t_0)$$

  If G is not constant, then things can get complicated. If G does not depend on **x**(t), then the ODE is **linear**. Otherwise it is **nonlinear**.

- If G is a nice, smooth function of **x** and t, then it is approximately constant over small timesteps. This was Sophus Lie's big idea which led to modern theories of *Lie groups* and *Lie algebras*.

Symmetry and conservation laws

- In many applications, $\mathbf{x}(t)$ obeys some conservation law. Examples:

  Classical mechanics: Energy and momentum are conserved.

  Quantum mechanics: Wavefunctions remain normalized.

  Engineering / Control Theory: Parameters are constrained to a surface.

  Chemistry / Ecology / Economics: Lotka-Volterra V is constant.

- Roughly speaking, **Noether's theorem** says: any system with a *continuous symmetry group* has a corresponding conservation law.

- Many numerical integrators (Euler, Runge-Kutta, Adams) ignore symmetry groups and violate conservation laws. **Geometric integrators** are designed to preserve symmetries and respect conservation laws.

- Examples: *Symplectic integrators* are used for orbital mechanics, particle physics, and molecular dynamics. *Magnus expansion* is used for nuclear magnetic resonance calculations in physics, chemistry, and medicine. It is also very good at solving finite-dimensional Schrödinger equations.

The exponential midpoint method

- The **Euler method** is a simple (and unstable) integrator:

$$\mathbf{x}(t + \mathrm{h}) \;\approx\; \mathbf{x}(t) + \mathrm{h}\hat{G}(\mathbf{x}(t), t) \cdot \mathbf{x}(t)$$

- The **exponential Euler method** is a simple geometric integrator which calculates a matrix exponential on each timestep:

$$\mathbf{x}(t + \mathrm{h}) \;\approx\; \exp\left[\mathrm{h}\hat{G}(\mathbf{x}(t), t)\right] \cdot \mathbf{x}(t)$$

- The **exponential midpoint method** (ExpMid) uses the exponential Euler method to “look a half-step into the future” on each timestep:

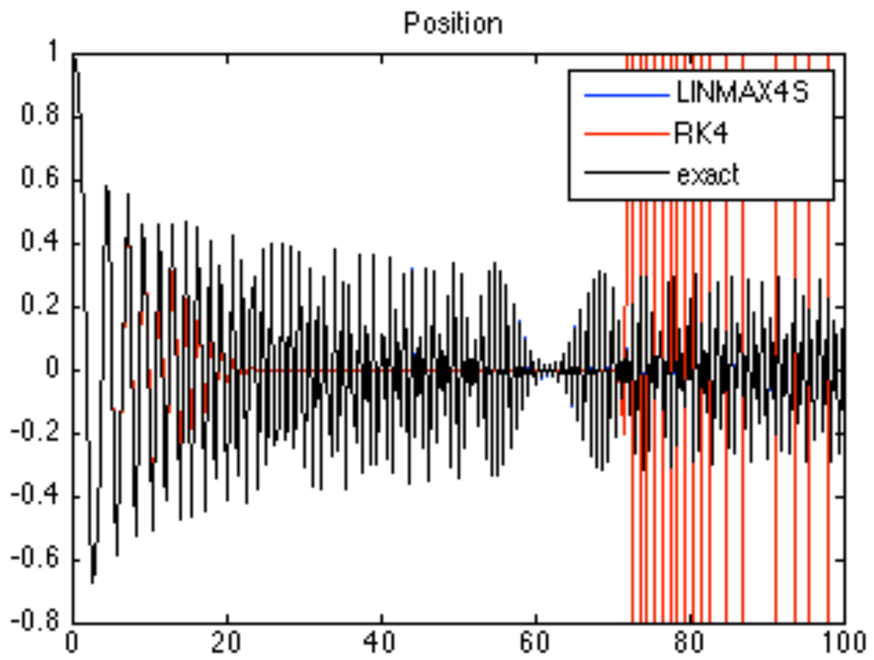
$$\mathbf{x}^\sharp \equiv \exp\left[\tfrac{1}{2}\mathrm{h}\hat{G}\big(\mathbf{x}(t), t\big)\right] \cdot \mathbf{x}(t) \qquad t^\sharp \equiv t + \tfrac{1}{2}\mathrm{h}$$

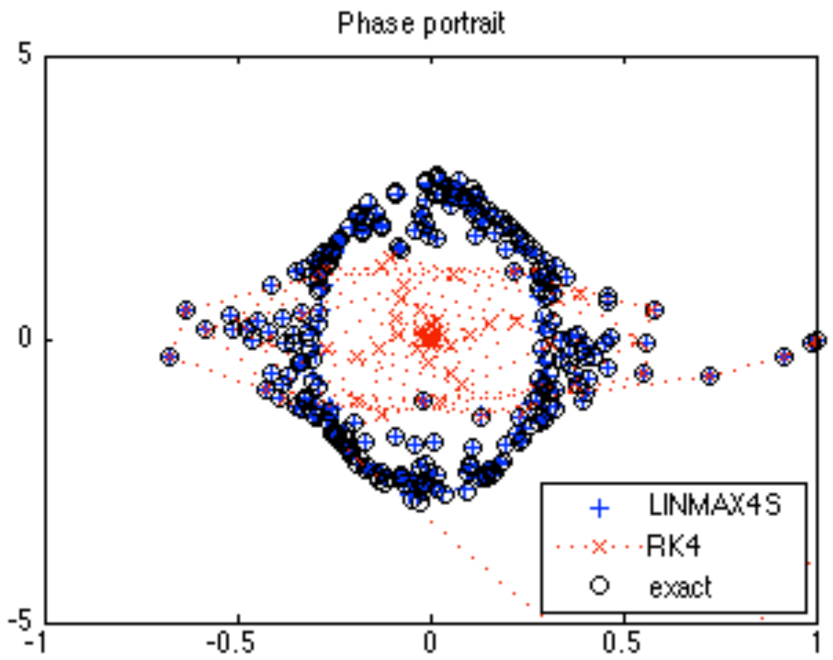
$$\mathbf{x}(t + \mathrm{h}) \approx \exp\left[\mathrm{h}\hat{G}\big(\mathbf{x}^\sharp, t^\sharp\big)\right] \cdot \mathbf{x}(t)$$

- ExpMid is only a *2nd-order* integrator, but it is general, easy to code, and very good at preserving Lie-group symmetries.

LINMAX and STRATOMAX

- LINMAX and STRATOMAX are open-source software packages I wrote for geometric numerical integration using MATLAB or Python / NumPy. I use them in my thesis, but they could have many other applications!





- LINMAX uses a 6th-order Magnus expansion to integrate linear ODEs. It is available at http://sites.google.com/site/samkennerly/programs .
- STRATOMAX is a Monte Carlo simulator which combines ExpMid with a *Castell-Gaines method* for stochastic differential equations (SDEs).

Recommended reading

Detailed explanations of geometric integrators for ODEs:

- S. Blanes, et al: “The Magnus expansion and some of its applications.” *Physics Reports* 470 p151-238 (2009)
- A. Iserles, et al: “Lie-group methods.” *Acta Numerica,* p215-365 (2000)

Methods using ODE integrators to solve SDEs:

- K. Burrage, et al: “Numerical methods for strong solutions of stochastic differential equations: an overview.” *Proc. R. Soc. Lond. A,* 460 (2004)
- F. Castell and J. Gaines: “The ordinary differential equation approach to asymptotically efficient schemes for solution of stochastic differential equations.” *Annales de l’I. H. P., section B* tome 32, no 2 (1996)

A textbook on scientific applications of Lie group theory:

- R. Gilmore: *Lie groups, physics, and geometry: an introduction for physicists, engineers, and chemists.* Cambridge University Press (2008)