Geometric Integration and the Parareal Algorithm

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The Lotka-Volterra Equations

Lotka Volterra System of differential equations with predator y and prey x[1]

$$\begin{array}{rcrcrcrl} \dot{x} & = & x & - & xy & = & -xy\frac{\partial H}{\partial y}; & x(0)=\hat{x}, \\ \dot{y} & = & -y & + & xy & = & xy\frac{\partial H}{\partial x}; & y(0)=\hat{y}. \end{array}$$

with the function $H(x,y) = x + y - \ln x - \ln y$. The exact solution is thus a cycle, and is known in closed form.[2]

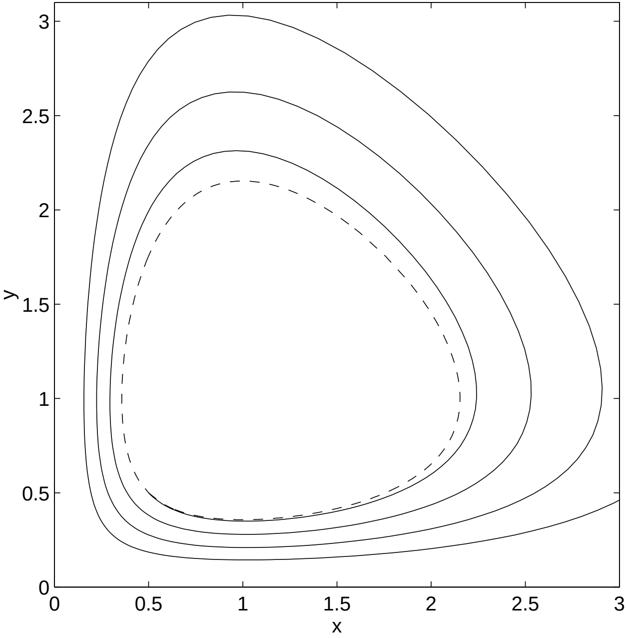
Discretization by Forward Euler:

$$\begin{array}{rcrcrcl} \frac{x_{n+1}-x_n}{\Delta t} & = & x_n & - & x_n y_n & ; & x_0 = \hat{x}, \\ \frac{y_{n+1}-y_n}{\Delta t} & = & -y_n & + & x_n y_n & ; & y_0 = \hat{y}. \end{array}$$

[1] Alfred J. Lotka, Elements of Physical Biology (1925), and Vito Volterra, Variazioni e fluttuazioni del numero d'individui in specie animali conviventi (1927)

[2] A. Steiner and M. Arrigoni, "Die Lösung gewisser Räuber-Beute-Systeme", Studia Biophysica vol. 123 (1988) No. 2.

Forward Euler Solution (exact solution dashed)



A Geometric Method for Lotka Volterra

Using a small modification[3]

$$\begin{aligned}
\frac{x_{n+1} - x_n}{\Delta t} &= \quad x_n \quad - \quad x_n y_n \quad ; \quad x_0 = \hat{x}, \\
\frac{y_{n+1} - y_n}{\Delta t} &= -y_n \quad + \quad x_{n+1} y_n \quad ; \quad y_0 = \hat{y},
\end{aligned}$$

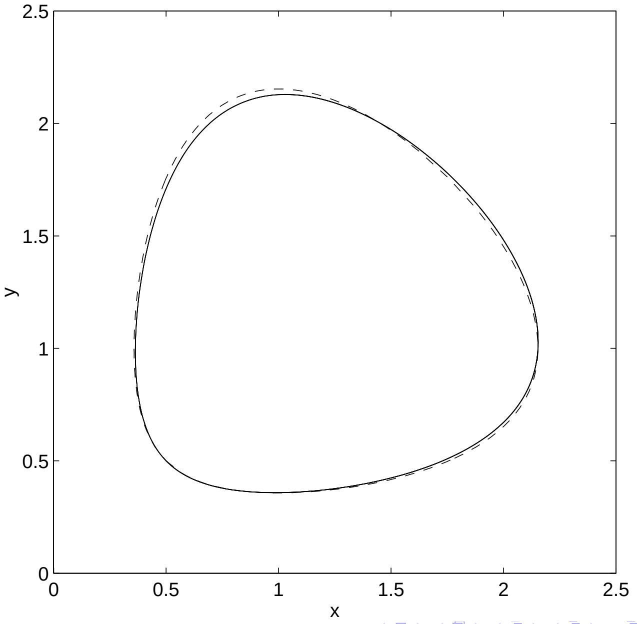
leads to a physically correct so called *Poisson Integrator*.

Geometric Numerical Integration, Hairer, Lubich, Wanner, Springer Verlag, 2002:

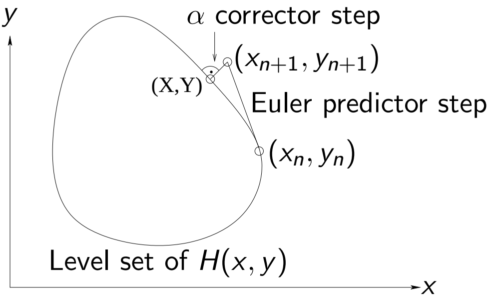
"The subject of this book is numerical methods that preserve geometric properties of the flow of a differential equation: symplectic integrators for Hamiltonian systems, symmetric integrators for reversible systems, methods preserving first integrals and numerical methods on manifolds, including Lie group methods and integrators for constrained mechanical systems, and methods for problems with highly oscillatory solutions."

[3] A Non Spiraling Integrator for the Lotka Volterra Equation, G., Il Volterriano No. 4, pp. 21–28, Liceo Cantonale e Biblioteca Cantonale di Mendrisio, 1994.

Poisson Integrator for Lotka Volterra



Preservation of the Hamiltonian



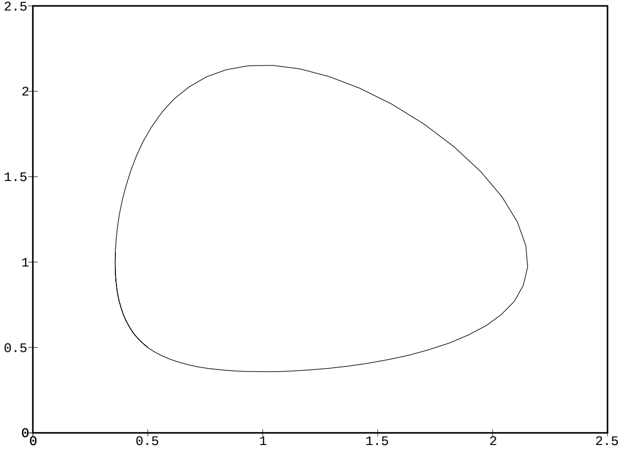
$$
\begin{aligned}
X &= x_{n+1} + \alpha \frac{\partial H}{\partial x}(X,Y) \\
Y &= y_{n+1} + \alpha \frac{\partial H}{\partial y}(X,Y)
\end{aligned}
$$

For the new approximation (X, Y), determine α such that

$$H(X(x_{n+1}, y_{n+1}, \Delta t, \alpha), Y(x_{n+1}, y_{n+1}, \Delta t, \alpha)) = H(x_n, y_n).$$

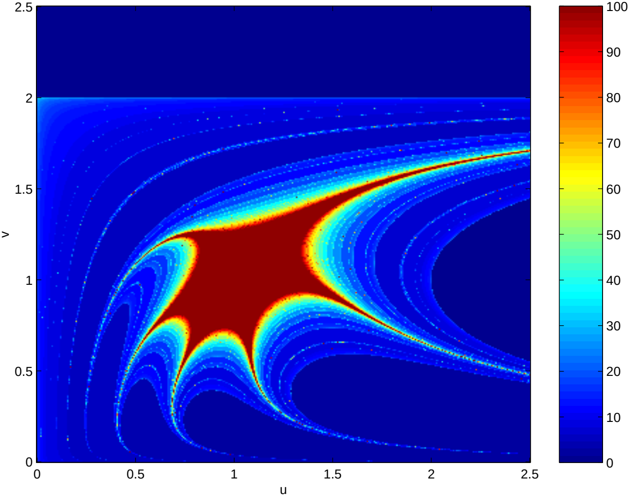
(could also evaluate gradient at x_{n+1}, y_{n+1})

Hamiltonian Preserving Integrator



However: Tupper (2005): A test problem for molecular dynamics integration: "The computed covariance function is clearly not converging to C as $n \to \infty$"

Positivity as a Geometric Property



On the Positivity of Poisson Integrators for the Lotka-Volterra Equations, M. Beck and M.J. Gander, BIT Numerical Mathematics, Vol. 55, No. 2, pp. 319–340, 2015.

The Parareal Algorithm

J-L. Lions, Y. Maday, G. Turinici (2001): A "Parareal" in Time Discretization of PDEs

The parareal algorithm for the model problem

$$u' = f(u)$$

is defined using two propagation operators:

1. $G(t_2, t_1, u_1)$ is a rough approximation to $u(t_2)$ with initial condition $u(t_1) = u_1$,
2. $F(t_2, t_1, u_1)$ is a more accurate approximation of the solution $u(t_2)$ with initial condition $u(t_1) = u_1$.

Starting with a coarse approximation U_n^0 at the time points $t_1, t_2, \ldots, t_N$, parareal performs for $k = 0, 1, \ldots$ the correction iteration

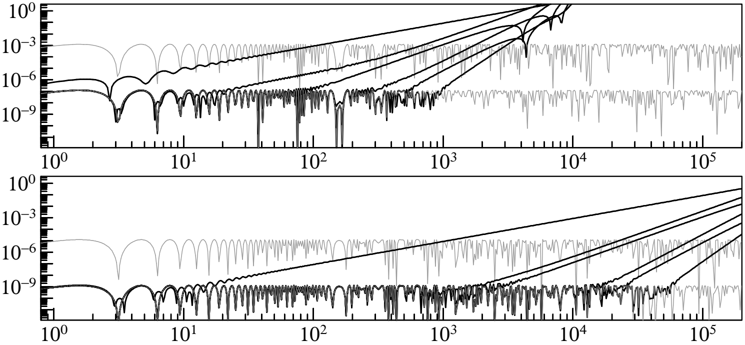
$$U_{n+1}^{k+1} = G(t_{n+1}, t_n, U_n^{k+1}) + F(t_{n+1}, t_n, U_n^k) - G(t_{n+1}, t_n, U_n^k).$$

Geometric Parareal Algorithms ?

- **Bal and Wu (DD17, 2008):** Symplectic Parareal. Non-iterative: "the two-step IPC scheme can be arbitrarily accurate"
- **Audouze, Massot, Volz (2009):** Symplectic multi-time step parareal algorithms applied to molecular dynamics. "We also prove the symplecticity of this method, which is an expected behavior of the molecular dynamics integrators"
- **Jiménez-Pérez, Laskar (2011):** A time-parallel algorithm for almost integrable Hamiltonian systems. "In this paper we propose a refinement of the SST97 algorithm to accelerate the solution and to preserve the accuracy of the sequential integrator"
- **Dai, Le Bris, Legoll, Maday (2013):** Symmetric parareal algorithms for Hamiltonian systems. "Using a symmetrization procedure and/or a projection step, we introduce here several variants of the original plain parareal in time algorithm"

Harmonic Oscillator

$$H(p,q) = \frac{1}{2}(p^2 + q^2), \quad q(0) = 1, p(0) = 0$$



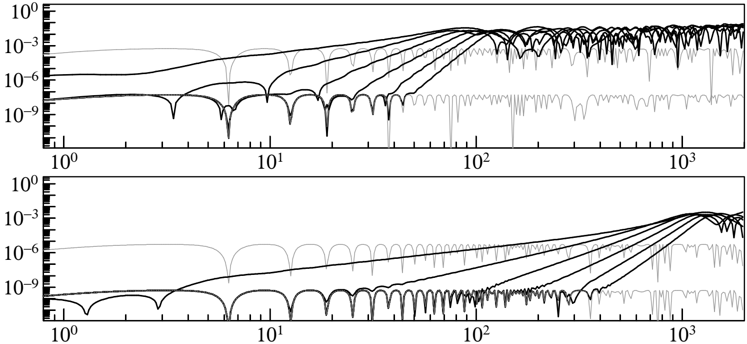
Störmer-Verlet for $\Delta T = 0.1$ and $\Delta T = 0.01$:

Theorem (G, Hairer 2014)

For the harmonic oscillator with G of order ε, convergence can be achieved on a time window of length $O(\varepsilon^{-1})$.

Kepler Problem (Completely Integrable)

$$H(p,q) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$



Simulations for $\Delta T = 0.1$ and $\Delta T = 0.01$:

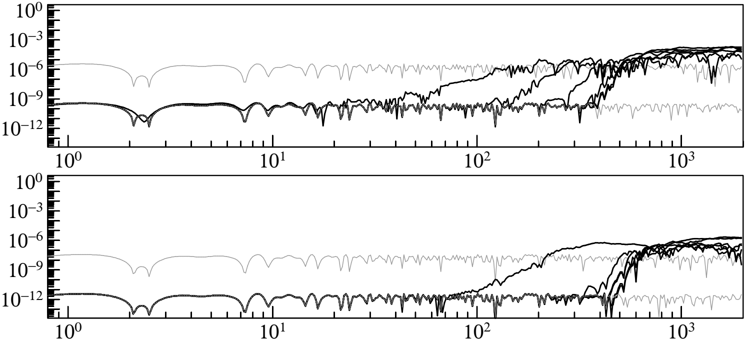
Theorem (G, Hairer 2014)

For integrable systems with G of order ε, convergence can be achieved on a time window of length $O(\varepsilon^{-1/2})$.

Hénon-Heiles Equation (Chaotic)

$$H(p,q) = \frac{1}{2}(p_1^2 + p_2^2) + U(q_1, q_2)$$

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



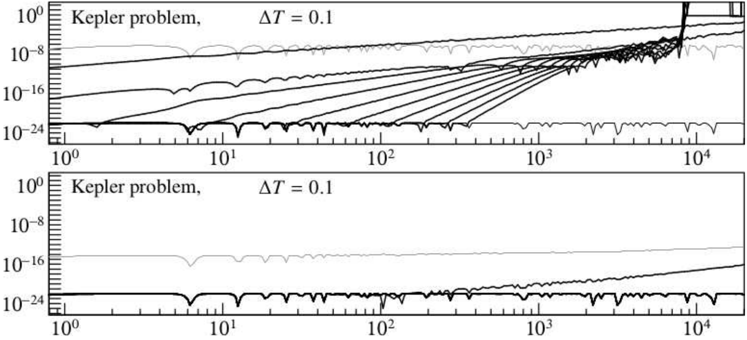
Simulations for $\Delta T = 0.01$ and $\Delta T = 0.001$:

Theorem (G, Hairer 2014)

For general systems with G of order ε, convergence can be achieved only on a time window of length $O(1)$.

Derivative Parareal Algorithm

One step back in the derivation of parareal to avoid cancellation: $G(U_n^{k+1}) - G(U_n^k) \approx G'(U_n^k)(U_n^k - U_n^{k-1})$.



- Fine integrator quadruple precision implementation of Gauss-Runge-Kutta method of order 12
- Coarse integrator 21 steps of Störmer-Verlet (top) and Gauss-Runge-Kutta of order 8 (below), both double precision

Conclusions

- The parareal algorithm can not preserve symplectic properties of $\varphi^F_{\Delta T}$ and $\varphi^G_{\Delta T}$
- Nevertheless the parareal algorithm can benefit from the symplectic structure in certain cases (e.g. completely integrable systems)
- It is really the coarse integrator that is key for performance

Analysis for parareal algorithms applied to Hamiltonian differential equations, M.J. Gander and E. Hairer, Journal of Computational and Applied Mathematics, 259, pp. 1–13, 2014.

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- There are however many other time parallel methods:

50 Years of Time Parallel Time Integration, G., to appear in 'Multiple Shooting and Time Domain Decomposition', T. Carraro, M. Geiger, S. Körkel, R. Rannacher, editors, Springer Verlag, 2015.