Solving PDEs with PGI CUDA Fortran
Part 4: Initial value problems for ordinary differential equations

Outline

ODEs and initial conditions. Explicit and implicit Euler methods. Runge-Kutta methods. Multistep Adams' predictor-corrector and Gear's BDF methods. Example: Lorenz attractor.

Ordinary differential equations and initial conditions

1 ordinary differential equation for 1 unknown function y(x) of 1 variable x

$$dy(x)/dx \equiv y'(x) = f(x, y(x))$$

For a unique solution, the initial condition is required

$$y(x_0) = y_0$$

A set of M ordinary differential equations for M unknown functions $y_m(x)$ of 1 variable x

$$dy_m(x)/dx = f_m(x, y_1(x), \ldots, y_M(x)), \quad m = 1, \ldots, M$$

$$dY(x)/dx \equiv Y'(x) = F(x, Y(x))$$

for vector Y of unknown functions y_m and vector F of right-hand-side functions f_m

For a unique solution, M initial conditions are required

$$y_m(x_0) = y_{m0} \quad \text{or} \quad Y(x_0) = Y_0$$

These are initial value problems (IVPs) for ordinary differential equations (ODEs).

Higher-order ODEs can be rewritten into a set of 1st-order ODEs (see, e.g., Numerical Recipes).

Ordinary differential equations and initial conditions

Discretization

x-grid and stepsize $x_n, \quad h_n = x_{n+1} - x_n, \quad n = 0, 1, \ldots$

numerical solution $y_n \approx y(x_n)$

Numerical methods below are, for simplicity, formulated for 1 ODE
and the constant stepsize h.
However, they all also work for y replaced by Y and h replaced by h_n.

Explicit Euler method

the left-hand 1st-order finite-difference scheme for the 1st derivative

$$y'(x_n) \approx (y(x_{n+1}) - y(x_n))/h$$

after substitution into the ODE, we get the approximate explicit Euler method

$$y_{n+1} = y_n + hf(x_n, y_n)$$

it is an explicit formula as all terms on the right-hand side are known

accuracy: 1st-order method (corresponds to the truncated Taylor expansion with the 0th and 1st term only)

Explicit Euler method

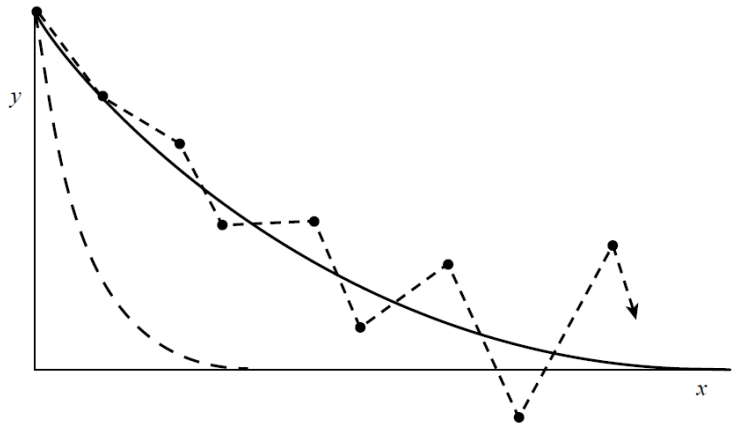
stability: consider a linear problem with constant coefficients

$$y'(x) = -cy, \quad y(0) = 1, \quad c > 0$$ (solution: $y(x) = e^{-cx}$)

Euler method: $y_{n+1} = y_n + h(-cy_n) = (1 - ch)y_n$

but for $h > 2/c : |y_{n+1}| > |y_n|$, or $|y_n| \to \infty$

thus, there is a stepsize limit due to stability



Pros: a simple explicit formula
Cons: low accuracy => higher-order explicit methods
low stability => implicit methods

Implicit Euler method

the right-hand 1st-order finite-difference scheme for the 1st derivative

$$y'(x_{n+1}) \approx (y(x_{n+1}) - y(x_n))/h$$

after substitution into the ODE, we get the implicit Euler method

$$y_{n+1} = y_n + hf(x_{n+1}, y_{n+1})$$

it is an implicit formula as there are references to unknown y_{n+1} on the right-hand side

again, it is only 1-st order accurate

Implicit Euler method

stability: as above, consider the problem

$$y'(x) = -cy, \quad y(0) = 1, \quad c > 0$$ (solution: $y(x) = e^{-cx}$)

the implicit formula: $y_{n+1} = y_n + h(-cy_{n+1}) = y_n/(1 + ch)$

thus, implicit Euler method is stable for any (positive) h, it has an infinite region of absolute stability

Semi-implicit Euler method for $Y' = F(Y)$

solving implicit Euler method by linearization of F(Y)
(similarly as in the Newton method for root finding)

$$Y_{n+1} = Y_n + hF(Y_{n+1}) \approx Y_n + h\left[F(Y_n) + (\partial F/\partial Y)_{Y_n} \cdot (Y_{n+1} - Y_n)\right]$$

$$Y_{n+1} = Y_n + h[I - h(\partial F/\partial Y)]^{-1} \cdot F(Y_n)$$

i.e., in each step, MxM (Jacobian) matrix assembly and inversion is required

Runge-Kutta methods

– more accurate, higher-order methods for integrating ODEs

– approximate the Taylor expansion by averaging the appropriately chosen dy/dx along y(x) between x_n and x_{n+1}

– RK1: the explicit Euler method, the simplest RK method

$$y_{n+1} = y_n + hk_1$$
$$k_1 = f(x_n, y_n)$$

for f(x) independent of y, it is equivalent to the rectangle quadrature rule

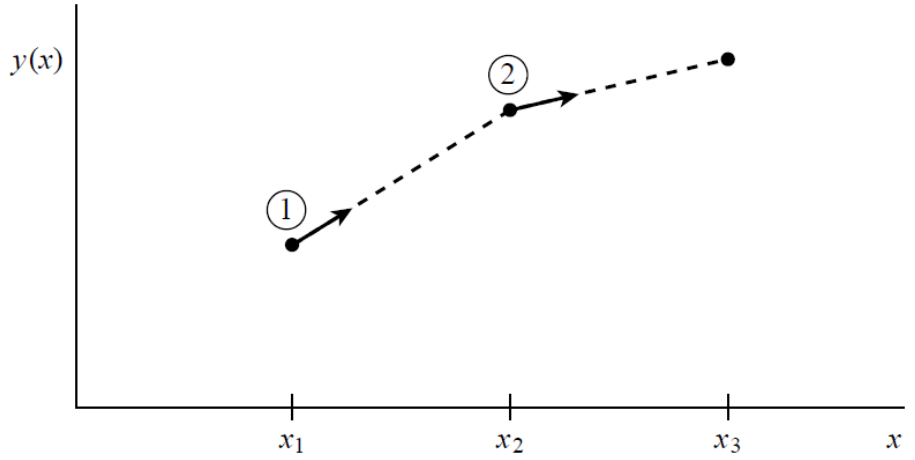
– RK2: the 2nd-order RK method (midpoint method)

$$y_{n+1} = y_n + hk_2$$
$$k_1 = f(x_n, y_n), \quad k_2 = f(x_n + h/2, y_n + hk_1/2)$$

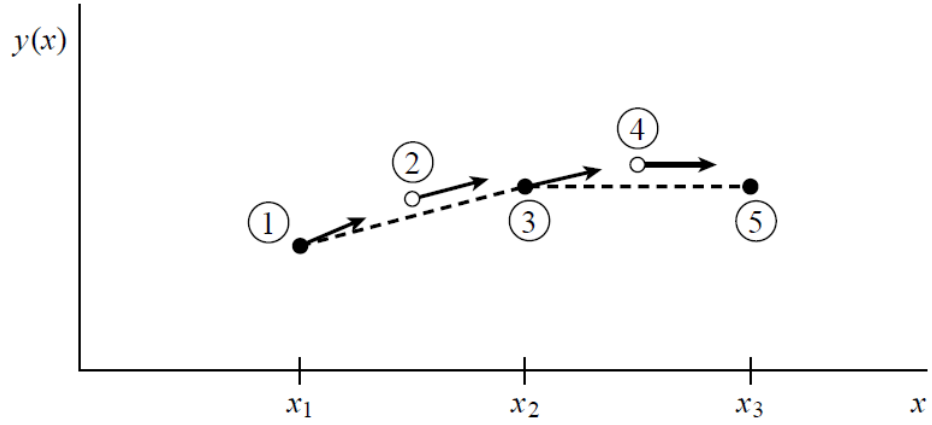
for f(x) independent of y, it is equivalent to the trapezoidal quadrature rule

Runge-Kutta methods

RK1:
one f(x,y) evaluation
per step



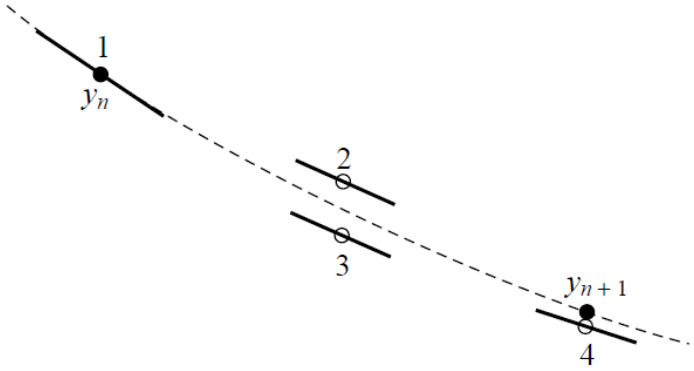
RK2:
two f(x,y) evaluations
per step



Runge-Kutta methods

– RK4: the most popular, 4th-order RK method

$$
\begin{aligned}
y_{n+1} &= y_n + h(k_1 + 2k_2 + 2k_3 + k_4)/6 \\
k_1 &= f(x_n, y_n) \\
k_2 &= f(x_n + h/2, y_n + hk_1/2) \\
k_3 &= f(x_n + h/2, y_n + hk_2/2) \\
k_4 &= f(x_n + h, y_n + hk_3)
\end{aligned}
$$



for f(x) independent of y, it is equivalent to the Simpson's quadrature rule

– a general p-step (explicit) RK method

$$
\begin{aligned}
y_{n+1} &= y_n + h\sum_{i=1}^{p} c_i k_i \\
k_1 &= f(x_n, y_n) \\
k_i &= f(x_n + \alpha_i h, y_n + h\sum_{j=1}^{i-1} \beta_{ij} k_j), \quad i = 2, \ldots, p
\end{aligned}
$$

Runge-Kutta methods

– stepsize control (different h in each step): guess a step size,
or make a few runs with step doubling,
or use RK methods with adaptive stepsize control
(e.g., Numerical Recipes, Chapter 16.2)

– pros: higher accuracy, better stability (not as much as in implicit variants)
than explicit Euler

– implicit RK methods available (more stable than the explicit methods,
but not infinitely stable)

Multistep methods

A general linear multistep method

$$y_{n+1} = \sum_{i=1}^{p} a_i y_{n+1-i} + h \sum_{i=0}^{p} b_i f_{n+1-i}$$

with a_p or b_p nonzero

The methods are explicit and p-step for $b_0=0$

and implicit and (p+1)-step otherwise.

Multistep methods

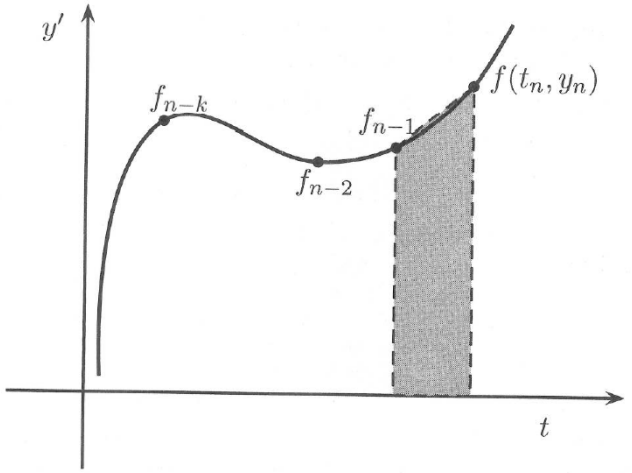
Adams' family of multistep methods

– based on polynomial approximation of f(x,y(x)) between x_{n+1-p} and x_n
(x_{n+1} for implicit methods)
and analytical integration of the approximating polynomial between x_n and x_{n+1}

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} N_p(x)\,dx = y_n + h\sum_{i=0}^{p} b_i f_{n+1-i}$$

– the order (i.e., the coincidence with the truncated Taylor expansion) is p for explicit and p+1 for implicit methods

– the explicit p=1 method is the explicit Euler,
the implicit p=0 method is the implicit Euler



Multistep methods

Coefficients a_i and b_i of Adams' methods

explicit (Adams-Bashforth) methods

all p:	a_1 = 1, other a_i = 0					
	i:	0	1	2	3	4
p=0:	b_i	–				
p=1:	b_i	0	1			
p=2:	$2b_i$	0	3	–1		
p=3:	$12b_i$	0	23	–16	5	
p=4:	$24b_i$	0	55	–59	37	–9

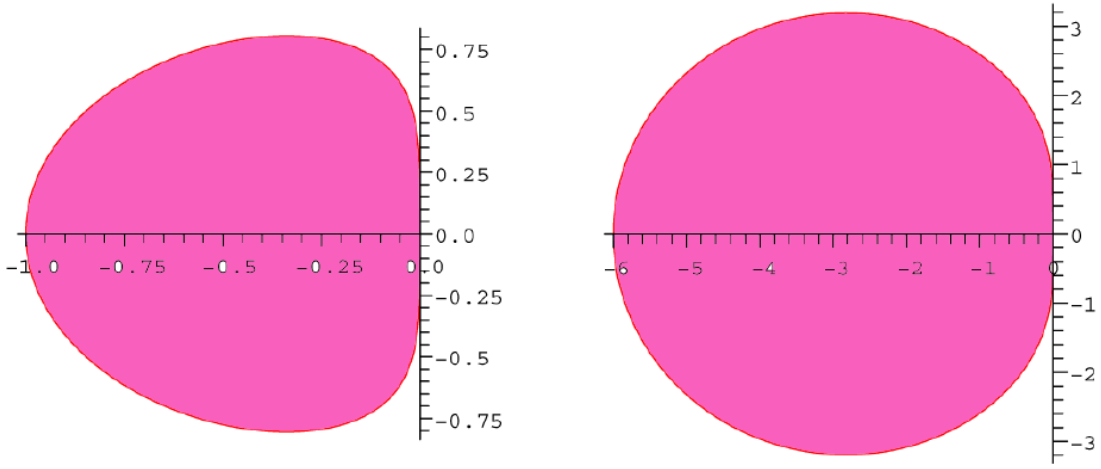
e.g., explicit p=2: $y_{n+1} = y_n + h(3f_n - f_{n-1})/2$

implicit (Adams-Moulton) methods

all p:	a_1 = 1, other a_i = 0					
	i:	0	1	2	3	4
p=0:	b_i	1				
p=1:	$2b_i$	1	1			
p=2:	$12b_i$	5	8	–1		
p=3:	$24b_i$	9	19	–5	1	
p=4:	$720b_i$	251	646	–264	106	–19

implicit p=1: $y_{n+1} = y_n + h(f_{n+1} + f_n)/2$

Regions of absolute stability
of explicit and implicit
2nd-order Adams methods



Multistep methods

The predictor-corrector algorithm: conventional application of Adams' methods

step P (predictor): applies an explicit Adams' formula of a given order,
ynew = y_{n+1}[explicit](x_{n+1})
step E (evaluation): updates f_{n+1} = f(x_{n+1},ynew)
step C (corrector): applies an implicit Adams' formula of the same order,
ynew = y_{n+1}[implicit](x_{n+1})
steps E and C can be repeated: variants PEC, PECE, $P(EC)^2E$
i.e., a predictor extrapolates f into x_{n+1},
a corrector makes use of this value for polynomial interpolation

– initialization of multistep methods by their lower-order relatives or by RK methods

– the predictor-corrector algorithm is essentially explicit,
its stability is therefore worse than that of the corrector

– adaptive stepsize control is laborious

Multistep methods

Backward differentiation formulas (BDFs, Gear's method)

– based on polynomial approximation of y(x) between x_{n+1-p} and x_{n+1} and analytical differentiation of the approximating polynomial at x_{n+1}

$$y_{n+1} = \sum_{i=1}^{p} a_i y_{n+1-i} + h b_0 f_{n+1}$$

– implicit p-step methods of the order p; for p=1: implicit Euler method

– BDFs combined with the Newton method are known to have excellent stability (for $p \leq 6$)

– inevitable for stiff problems with two or more very different scales of the variable x on which the unknowns y are changing (stability conditions require to accommodate to the fastest scale, i.e., with small stepsize, while the process under study usually develops on the slowest scale,
i.e., too many small steps would be necessary with explicit methods)

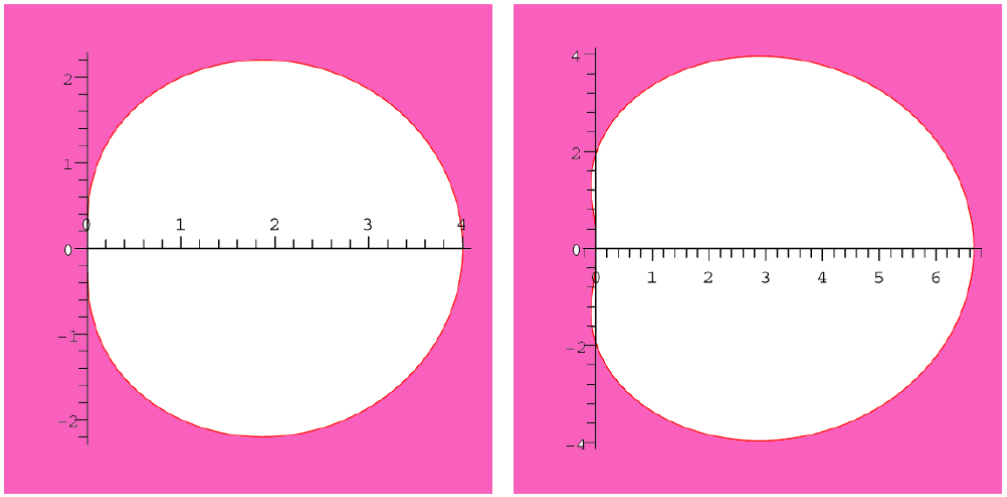
Multistep methods

Coefficients a_i and b_i of Gear's methods

	i:	1	2	3	4	5	6	i:	0	> 0
p=1:	a_i	1						b_i	1	0
p=2:	$3a_i$	4	–1					$3b_i$	2	0
p=3:	$11a_i$	18	–9	2				$11b_i$	6	0
p=4:	$25a_i$	48	–36	16	–3			$25b_i$	12	0
p=5:	$137a_i$	300	–300	200	–75	12		$137b_i$	60	0
p=6:	$147a_i$	360	–450	400	–225	72	–10	$147b_i$	60	0

e.g., p=2: $y_{n+1} = (4y_n - y_{n-1})/3 + 2f_{n+1}/3$

Regions of absolute stability
of 2nd- and 3rd-order
BDF methods (regions in color)



On the crossroads

Euler methods
are extremely simple but inaccurate, too; the implicit variant is necessary when stability matters, i.e., when larger stepsize is required than a stability condition allows.

Runge-Kutta explicit methods
are simple and fast enough both to code and to run, as each step requires just evaluation of an explicit formula, and for many problems, they are accurate enough. However, they are explicit and stepsize is limited.

Predictor-corrector
implementation, including stepsize adaptivity, is rather an artwork, but it was done and can be reused from available packages. Still, stability is limited.

Backward differentiation formulas,
as a multistep method, share many features with predictor-corrector methods, however, for their excellent stability, they are inevitable for stiff problems.

An example: Lorenz attractor

– a problem of the 2D convection in the atmosphere, mathematically simplified as much as possible
– a fully deterministic system with chaotic behavior

– a simplified problem: 3 ODEs for temporal evolution of 3 variables (coefficients of eigenvalue expansions of the stream function and temperature anomalies) in the 3D (phase) space

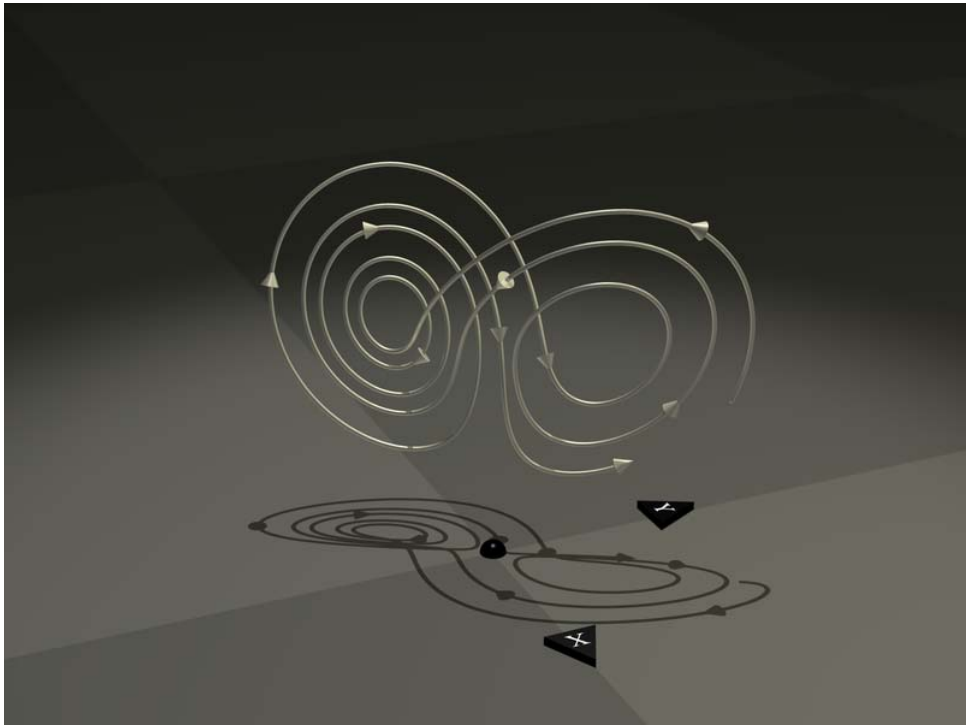
$$\begin{aligned} dA/d\tau &= P(B-A) \\ dB/d\tau &= rA - B - AC \\ dC/d\tau &= -bC + AB \end{aligned}$$

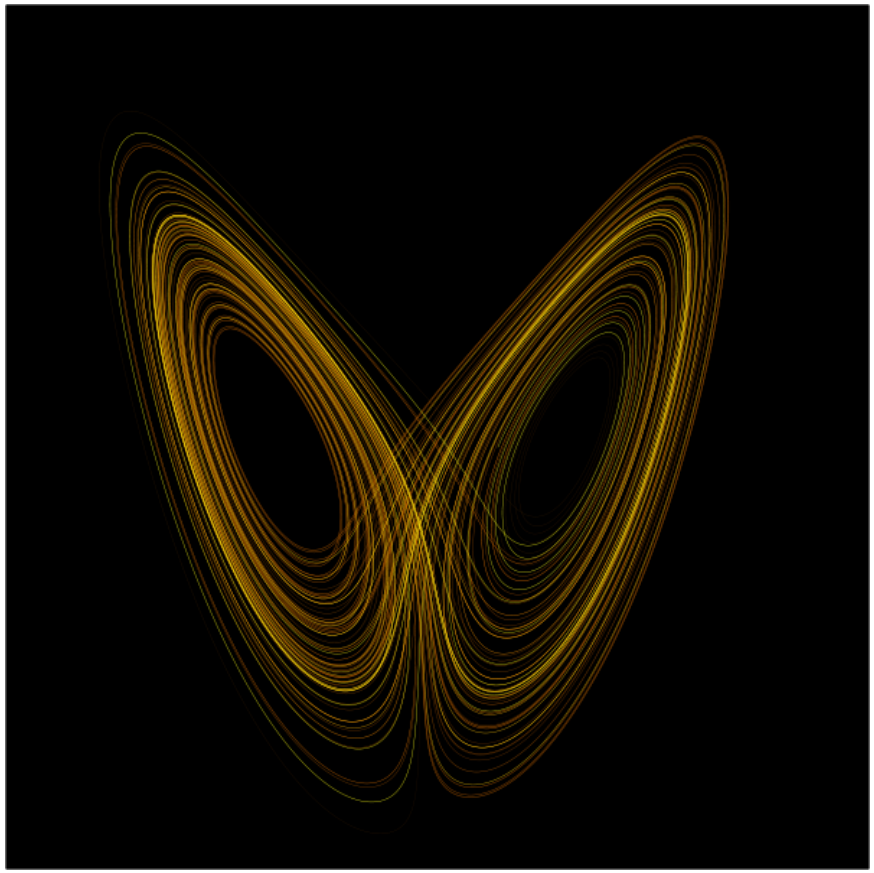
where A is a stream-function coefficient, B and C coefficients of temperature anomalies, P the Prandtl number, r=Ra/Ra_{CR} with Ra the Rayleigh number, $b = 4/(1+(2/\lambda)^2)$ corresponds to the size of a convection roll and τ is nondimensionalized time

– parameters used by Lorenz (1963): P=10, r=28 and b=8/3, a sufficient time interval: 0..20

Lorenz attractor

– temporal solutions roll around two fixed points (the strange attractors) along a lemniscate-shaped trajectory (like ∞)
– physically: the boundary layer of a convection cell grows, at some point it becomes unstable, convection resumes, either as a clockwise or counterclockwise roll: chaotic behavior in a deterministic system
– popular vizualization: A-B-C phase portraits





Lorenz attractor

Source codes
CPU: an arbitrary A-B-C point undergoes NT Runge-Kutta time steps, they are recorded and plotted
CPU: NX x NY x NZ points, spread within a 3D cube, undergo NT time steps, each independent of others, only final positions of all points are recorded and plotted
GPU: the previous case with one kernel
GPU: the previous case, now with a smaller kernel called repeatedly
Goals: a massively parallel compute-bound kernel, SP/DP execution times, avoiding kernel execution timeout, stability limits of explicit schemes

Links and references

Numerical methods

Ascher U. M. and Petzold L. R., Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations, SIAM, 1998

Press W. H. et al., Numerical Recipes in Fortran 77: The Art of Scientific Computing, Second Edition, Cambridge, 1992
Chapter 16.1: Runge-Kutta method
Chapter 16.2: Adaptive stepsize control for Runge-Kutta
Chapter 16.6: Stiff sets of equations
http://www.nr.com, PDFs available at http://www.nrbook.com/a/bookfpdf.php

Lorenz attractor

Schubert G. et al., Mantle Convection in the Earth and Planets, Cambridge, 2001, p. 332–337
http://ebookee.org/Mantle-Convection-in-the-Earth-and-Planets_661884.html