Time Parallel Time Integration

Part I

Multiple Shooting Type Methods

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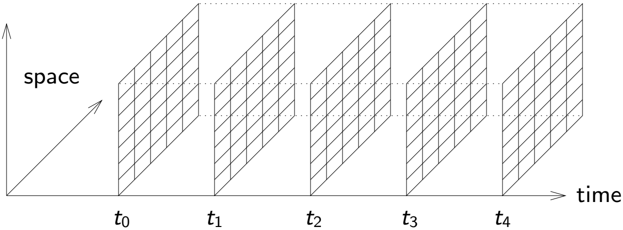
Solving Evolution Problems in Parallel ?

Heat equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + f$, $u(x, y, t_0) = u_0(x, y)$



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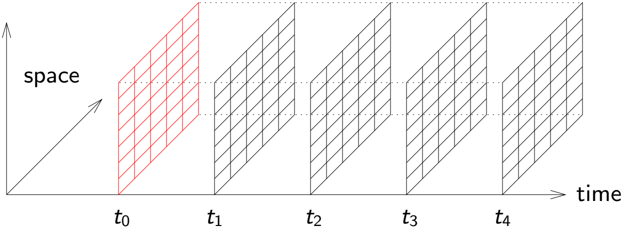

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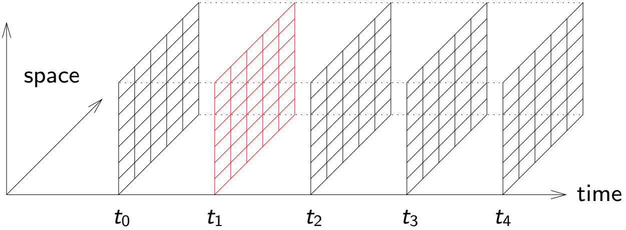

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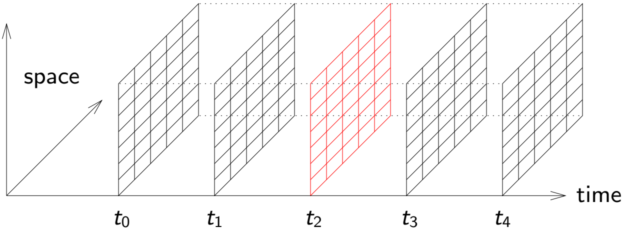

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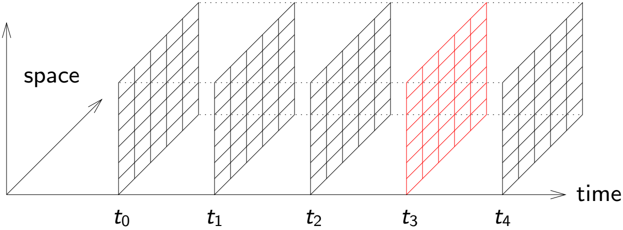

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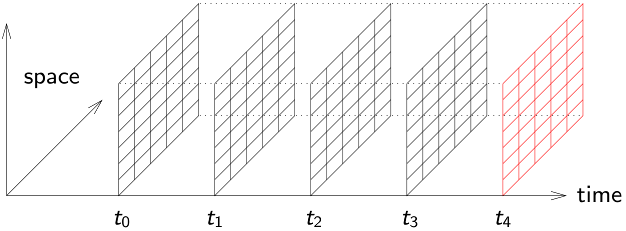

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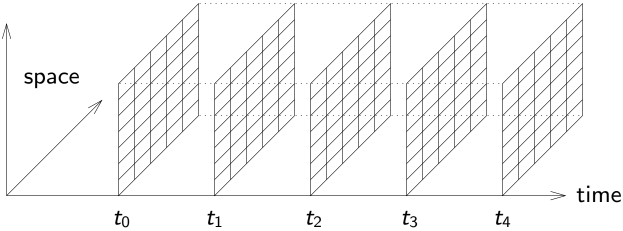

Simpler: $\frac{du}{dt} = f(u)$, $u(t_0) = u_0$, discretized by Forward Euler

$$u_{n+1} = u_n + \Delta t f(u_n).$$

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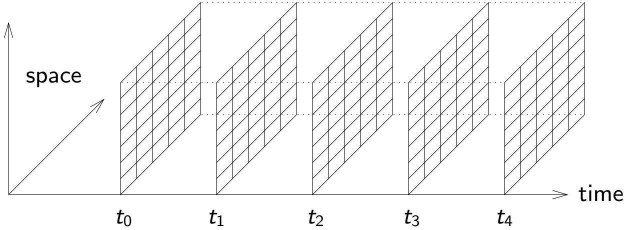

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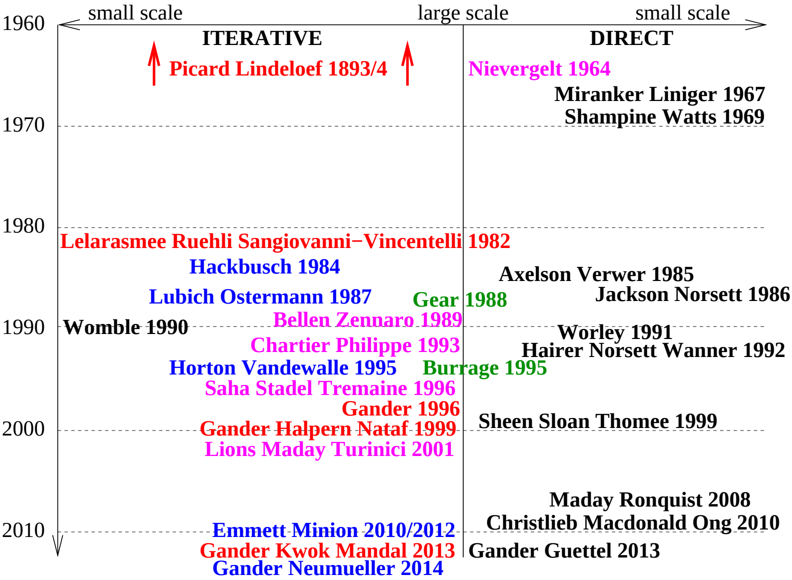
$$u_{n+1} = u_n + \Delta t f(u_n).$$

Triangular solve in the linear case $u' = au + f(t)$:

$$\begin{pmatrix} 1 & & & \\ -1 - a\Delta t & 1 & & \\ & -1 - a\Delta t & 1 & \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} \Delta t f(t_0) + (1 + a\Delta t) u_0 \\ \Delta t f(t_1) \\ \Delta t f(t_2) \\ \vdots \end{pmatrix}$$

Time Parallel Methods Over the Course of Time



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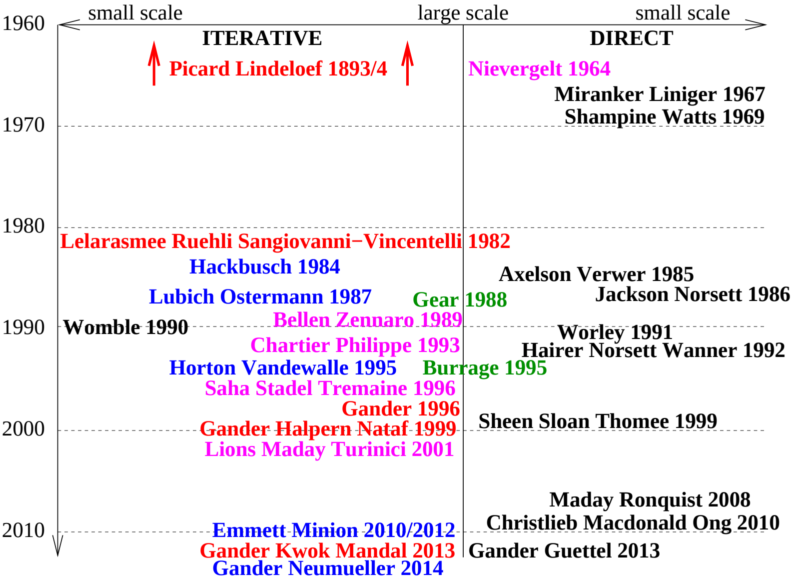
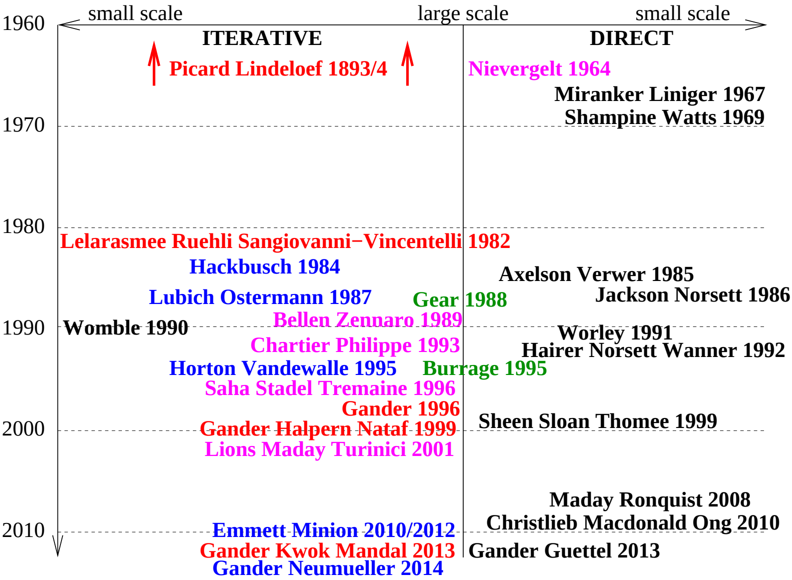


50 Years of time parallel time integration (G, 2015)

Multiple Shooting Type Methods

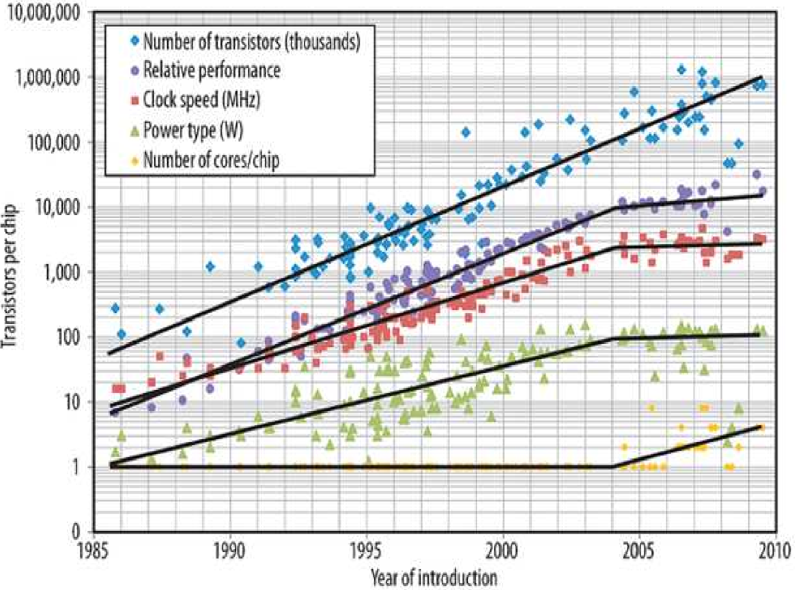


Jörg Nievergelt 1964

Parallel Methods for Integrating Ordinary Differential Equations. Comm. of the ACM, Vol 7(12), 1964.

> *"For the last 20 years, one has tried to speed up numerical computation mainly by providing ever faster computers.* **Today, as it appears that one is getting closer to the maximal speed of electronic components**, *emphasis is put on allowing operations to be performed in parallel. In the near future, much of numerical analysis will have to be recast in a more 'parallel' form."*

“Today” of Nievergelt precisely 40 years later



Jörg Nievergelt 1964

Parallel Methods for Integrating Ordinary Differential Equations. Comm. of the ACM, Vol 7(12), 1964.

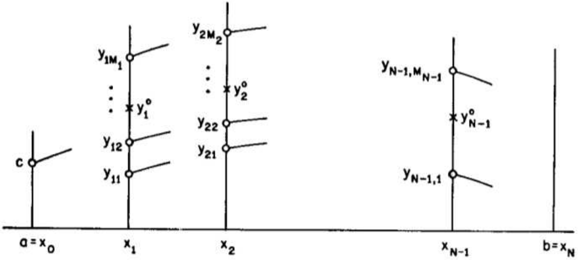
Model problem treated:

$$y' = f(y), \quad y(x_0) = y_0$$

> *"As an example, a method is proposed for 'parallelizing' the numerical integration of an ordinary differential equation, which process, by all standard methods, is entirely serial"*

Nievergelt's Method from 1964

The idea is to divide the integration interval [a, b] into N equal subintervals $[x_{i-1}, x_i]$, $x_0 = a$, $x_N = b$, $i = 1, 2, \cdots, N$, to make a rough prediction y_i^0 of the solution $y(x_i)$, to select a certain number M_i of values y_{ij}, $j = 1, 2, \cdots, M_i$ in the vicinity of y_i^0, $i = 1, 2, \cdots, N$, and then to integrate *simultaneously* with an accurate integration method $\mathfrak{M}$ all the initial value problems



. The connection between the branches is now brought about by interpolating the end value of the unique branch in $[x_0, x_1]$

Alfredo Bellen and Marino Zennaro 1989

Parallel algorithms for initial-value problems for difference and differential equations. J. Comp. and Appl. Math. Vol 25, 1989.

> *"In addition to the two types of parallelism mentioned above, we wish to isolate a third which is analogous to what Gear has more recently called parallelism* across the time*. Here it is more appropriately called parallelism across the steps. In fact, the algorithm we propose is a realization of this kind of parallelism. Without discussing it in detail here, we want to point out that* **the idea is indeed that of multiple shooting** *and parallelism is introduced at the cost of redundancy of computation."*

Bellen and Zennaro's Method from 1989

Consider the difference equation

$$y_{n+1} = F_{n+1}(y_n), \quad y_0 \text{ known.}$$

With $\mathbf{y} := (y_0, y_1, \ldots, y_n, \ldots)$ this represents a fixed point problem of the form

$$\mathbf{y} = \mathbf{\Phi}(\mathbf{y}),$$

where $\mathbf{\Phi}(\mathbf{y}) = (y_0, F_1(y_0), F_2(y_1), \ldots, F_n(y_{n-1}), \ldots)$.

Steffensen's method applied to the fixed point problem gives

$$\mathbf{y}^{k+1} = \mathbf{\Phi}(\mathbf{y}^k) + \Delta\mathbf{\Phi}(\mathbf{y}^k)(\mathbf{y}^{k+1} - \mathbf{y}^k)$$

where $\Delta\mathbf{\Phi}$ is an approximation to the differential $D\mathbf{\Phi}$, and Bellen and Zennaro chose $y_n^0 = y_0$.

Properties of the Algorithm

Steffensen's method for $f(x) = 0$:

$$\begin{aligned} x_{k+1} &= x_k - g(x_k)^{-1} f(x_k) \\ g(x_k) &:= \frac{f(x_k + f(x_k)) - f(x_k)}{f(x_k)}. \end{aligned}$$

Bellen and Zennaro's Results:

1. each iteration gives one more exact value, so convergence is guaranteed
2. convergence is locally quadratic
3. corrections can be computed in parallel
4. numerically estimated speedups of 29-53 with for 400 steps

Philippe Chartier and Bernard Philippe 1993

A Parallel Shooting Technique for Solving Dissipative ODE's. Computing, Vol 51, 1993.

> *"In this paper, we study different modifications of a class of parallel algorithms, initially designed by A. bellen and M. Zennaro for difference equations and called 'across the steps' methods by their authors, for the purpose of solving initial value problems in ordinary differential equations (ODE's) on a massively parallel computer."*

> *"It is indeed generally admitted that the integration of a system of ordinary differential equations in a step-by-step process is inherently sequential."*

"In diesem Artikel studieren wir verschieden Versionen einer Klasse paralleler Algorithmen, die ursprünglich von A. Bellen und M. Zennaro für Differenzengleichungen konzipiert und von ihnen 'across the steps' Methode genannt worden ist."

Multiple Shooting for Initial Value Problems

To solve the initial value problem

$$u' = f(u), \quad u(0) = u^0, \qquad x \in [0,1]$$

by **multiple shooting**, one splits the time interval into subintervals $[0,\frac{1}{3}]$, $[\frac{1}{3},\frac{2}{3}]$, $[\frac{2}{3},1]$, and then solves on each subinterval

$$\begin{array}{rcl} u_0' &=& f(u_0), \\ u_0(0) &=& U_0, \end{array} \qquad \begin{array}{rcl} u_1' &=& f(u_1), \\ u_1(\frac{1}{3}) &=& U_1, \end{array} \qquad \begin{array}{rcl} u_2' &=& f(u_2), \\ u_2(\frac{2}{3}) &=& U_2, \end{array}$$

together with the matching conditions

$$U_0 = u^0, \quad U_1 = u_0(\frac{1}{3}, U_0), \quad U_2 = u_1(\frac{2}{3}, U_1)$$

$$\Longleftrightarrow \quad F(\mathbf{U}) = \begin{pmatrix} U_0 - u^0 \\ U_1 - u_0(\frac{1}{3}, U_0) \\ U_2 - u_1(\frac{2}{3}, U_1) \end{pmatrix} = 0, \; \mathbf{U} = (U_0, U_1, U_2)^T.$$

Using Newton's Method

$$F(\mathbf{U}) = \begin{pmatrix} U_0 - u^0 \\ U_1 - u_0(\frac{1}{3}, U_0) \\ U_2 - u_1(\frac{2}{3}, U_1) \end{pmatrix} = 0$$

$$\begin{pmatrix} U_0^{k+1} \\ U_1^{k+1} \\ U_2^{k+1} \end{pmatrix} = \begin{pmatrix} U_0^{k} \\ U_1^{k} \\ U_2^{k} \end{pmatrix} - \begin{bmatrix} 1 & & \\ -\frac{\partial u_0}{\partial U_0}(\frac{1}{3}, U_0^k) & 1 & \\ & -\frac{\partial u_1}{\partial U_1}(\frac{2}{3}, U_1^k) & 1 \end{bmatrix}^{-1} \begin{pmatrix} U_0^k - u^0 \\ U_1^k - u_1(\frac{1}{3}, U_0^k) \\ U_2^k - u_1(\frac{2}{3}, U_1^k) \end{pmatrix}$$

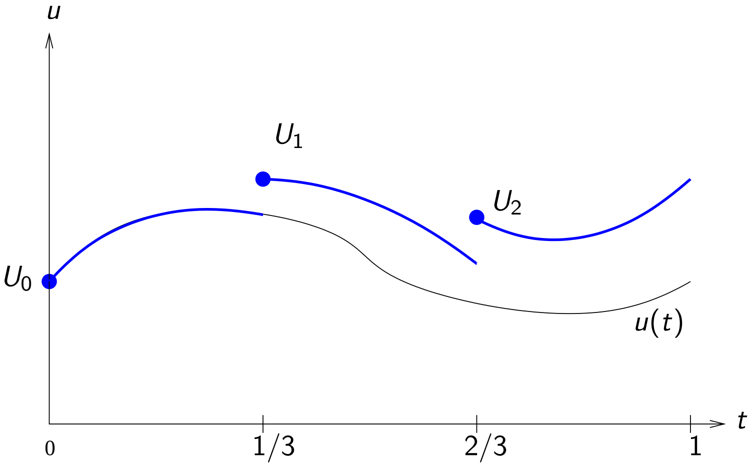
Multiplying through by the matrix, we find the recurrence

$$\begin{aligned} U_0^{k+1} &= u^0, \\ U_1^{k+1} &= u_0(\tfrac{1}{3}, U_0^k) + \tfrac{\partial u_0}{\partial U_0}(\tfrac{1}{3}, U_0^k)(U_0^{k+1} - U_0^k), \\ U_2^{k+1} &= u_1(\tfrac{2}{3}, U_1^k) + \tfrac{\partial u_1}{\partial U_1}(\tfrac{2}{3}, U_1^k)(U_1^{k+1} - U_1^k). \end{aligned}$$

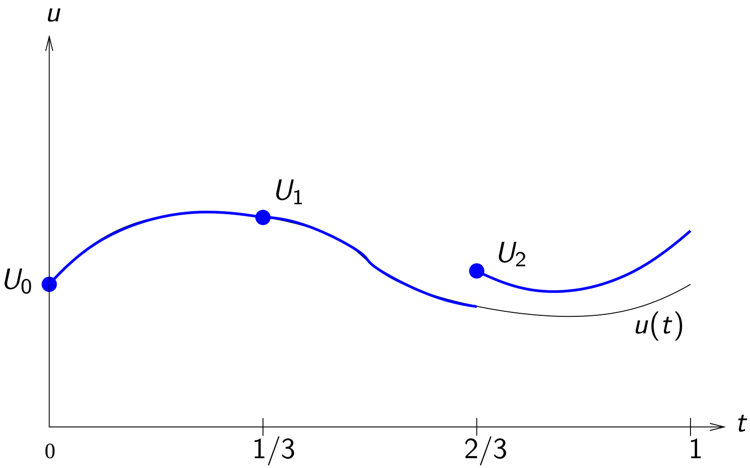
General case with N intervals:

$$U_{n+1}^{k+1} = u_n(t_{n+1}, U_n^k) + \frac{\partial u_n}{\partial U_n}(t_{n+1}, U_n^k)(U_n^{k+1} - U_n^k).$$

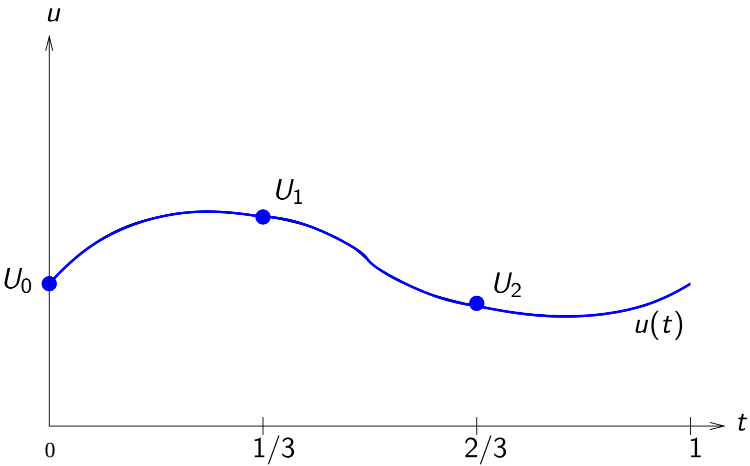
Example: first iteration



Example: second iteration



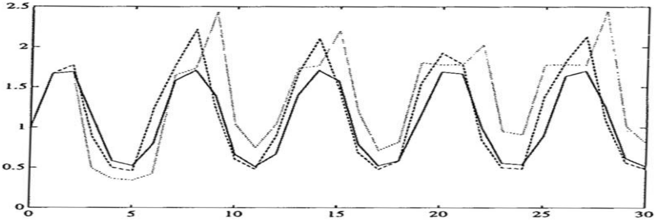
Example: third iteration



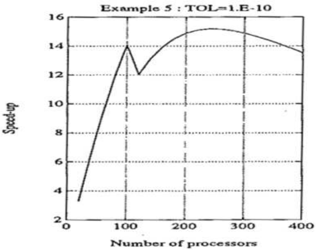
Results of Chartier and Philippe

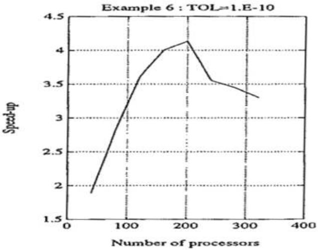
- The algorithm converges locally quadratically
- Global convergence is proved for dissipative systems

Non-dissipative example $y' = \cos x \sin y^2$, $y(0) = 1$



Speedup for a dissipative scalar ODE and a system of 3 ODEs





Prasenjit Saha, Joachim Stadel, Scott Tremaine

A parallel integration method for solar system dynamics. The Astronomical Journal, Vol 114(1), 1997.

> *"We describe how long-term solar system orbit integration could be implemented on a parallel computer. The interesting feature of our algorithm is that each processor is assigned not to a planet or a pair of planets, but to a time-interval. Thus, the 1st week, 2nd week, . . . , 1000th week of an orbit are computed concurrently. The problem of matching the input to the $(n+1)$-st processor with the output of the n-th processor can be solved efficiently by an iterative procedure. Our work is related to the so-called* ***waveform relaxation methods****. . . ".*

The Idea of Saha, Stadel and Tremaine

Consider the system of ordinary differential equations

$$\dot{y} = f(y), \quad y(0) = y_0,$$

or equivalently the set of quadratures

$$y(t) = y(0) + \int_0^t f(y(s))ds.$$

Approximating the quadrature by sums gives

$$y_n = y_0 + h \sum_{m=0}^{n-1} f(\frac{1}{2}(y_m + y_{m-1})), \quad n = 1, \ldots, N.$$

This is again a fixed point equation of the form

$$\mathbf{y} = F(\mathbf{y}),$$

which can be solved by an iterative process.

Algorithm of Saha, Stadel and Tremaine

Algorithm for a Hamiltonian problem with a small perturbation

$$\dot{p} = -H_q,\ \dot{q} = H_p, \quad H(p,q,t) = H^0(p) + \epsilon H^1(p,q,t).$$

Denoting $y := (p,q)$, $f(y) := (-H_q(y), H_p(y))$, they derive Newton's method for the associated fixed point problem (as Chartier Philippe)

$$Y_{n+1}^{k+1} = y_n^\epsilon(t_{n+1}, Y_n^k) + \frac{\partial y_n^\epsilon}{\partial Y_n}(t_{n+1}, Y_n^k)(Y_n^{k+1} - Y_n^k)$$

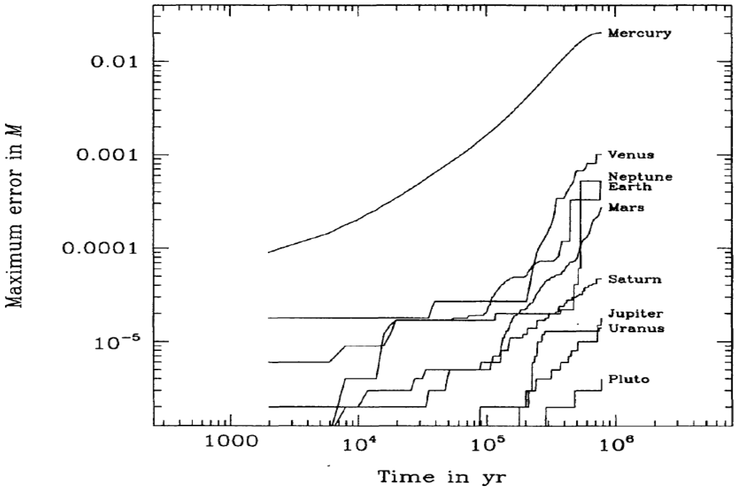
but now propose to approximate the derivative by a cheap difference for the unperturbed Hamiltonian

$$Y_{n+1}^{k+1} = y_n^\epsilon(t_{n+1}, Y_n^k) + y_n^0(t_{n+1}, Y_n^{k+1}) - y_n^0(t_{n+1}, Y_n^k).$$

They argue that each iteration now improves the error by a factor ϵ, instead of quadratically.

Results for our solar system

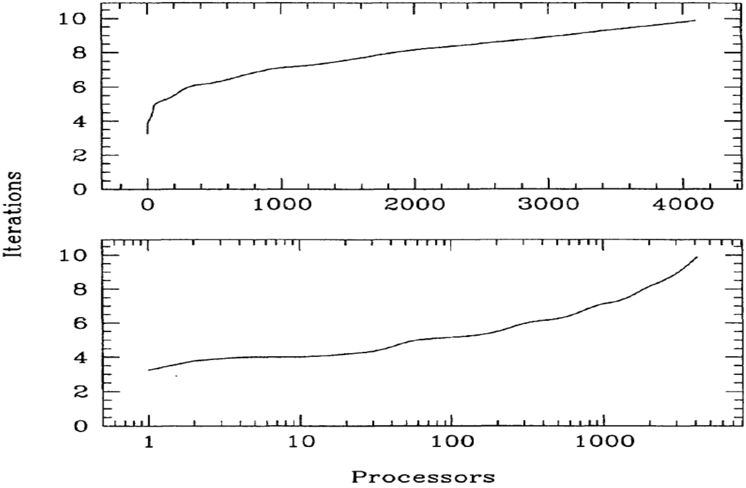
Using for H^0 Kepler's law, and ϵH^1 planetary perturbations



Maximum error in mean anomaly M versus time, $h = 7\frac{1}{32}$ days, compared to results from the literature

Possible Speedup

Iterations needed to converge to relative error $1e-15$



Top linear scaling, and bottom logarithmic scaling

Lions, Maday, Turinici 2001

Résolution d'EDP par un schéma en temps "pararéel".
C. R. Acad. Sci. Paris.

> *"Elle a pour principale motivation les problèmes en temps réel, d'où la terminologie proposée de pararéel."*

$$\dot{y} = -ay, \quad \text{on } [0, T], \quad y(0) = y_0.$$

First use Backward Euler on grid T_n with step ΔT

$$Y_{n+1}^1 - Y_n^1 + a\Delta T Y_{n+1}^1 = 0, \quad Y_0^1 = y_0.$$

Then compute on each interval $[T_n, T_{n+1}]$ exactly

$$\dot{y}_n^1 = -ay_n^1, \quad y_n^1(T_n) = Y_n^1.$$

Iteration for $k = 1, 2, \ldots$:

1. Compute jumps $S_n^k := y_{n-1}^k(T_n) - Y_n^k$
2. Propagate jumps $\delta_{n+1}^k - \delta_n^k + a\Delta T \delta_{n+1}^k = S_n^k$, $\delta_0^k = 0$
3. Set $Y_n^{k+1} := y_{n-1}^k(T_n) + \delta_n^k$ and solve in parallel

$$\dot{y}_n^{k+1} = -ay_n^{k+1}, \quad \text{on } [T_n, T_{n+1}], \quad y_n^{k+1}(T_n) = Y_n^{k+1}.$$

"C'est alors un exercice que de montrer la:"

Proposition: The parareal scheme is order k, i.e. there exists c_k s.t.

$$|Y_n^k - y(T_n)| + \max_{t\in[T_n,T_{n+1}]} |y_n^k(t) - y(t)| \leq c_k \Delta T^k.$$

Parareal Algorithm in Modern Notation for $u' = f(u)$

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

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

G, Vandevalle 2007: Parareal is multiple shooting with the Jacobian approximated by differences on a coarser grid

Precise Convergence Estimate for Parareal

Theorem (G, Hairer 2007)

Let $F(t_{n+1}, t_n, U_n^k)$ denote the exact solution at t_{n+1} and $G(t_{n+1}, t_n, U_n^k)$ be a one step method with local truncation error bounded by $C_1 \Delta T^{p+1}$. If

$$|G(t + \Delta T, t, x) - G(t + \Delta T, t, y)| \leq (1 + C_2 \Delta T)|x - y|,$$

then

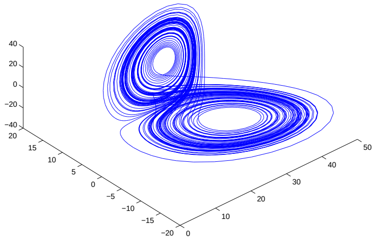
$$\max_{1\leq n\leq N} |u(t_n) - U_n^k| \leq \frac{C_1 \Delta T^{k(p+1)}}{k!}(1 + C_2 \Delta T)^{N-1-k} \prod_{j=1}^{k}(N-j) \max_{1\leq n\leq N} |u(t_n) - U_n^0|$$
$$\leq \frac{(C_1 T)^k}{k!} e^{C_2(T-(k+1)\Delta T)} \Delta T^{pk} \max_{1\leq n\leq N} |u(t_n) - U_n^0|.$$

G and Hairer: Nonlinear Convergence Analysis for the Parareal Algorithm, Domain Decomposition Methods in Science and Engineering XVII, Springer-Verlag, 2007.

Results for the Lorenz Equations

Suggested by Jean-Pierre Eckmann (2004)

$$\begin{aligned}\dot{x} &= -\sigma x + \sigma y\\ \dot{y} &= -xz + rx - y\\ \dot{z} &= xy - bz\end{aligned}$$

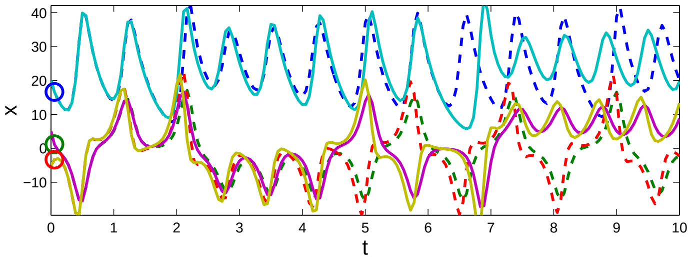


Parameters: $\sigma = 10$, $r = 28$ and $b = \frac{8}{3} \Longrightarrow$ chaotic regime.

Initial conditions: $(x, y, z)(0) = (20, 5, -5)$

Simulation time: $t \in [0, T = 10]$

Discretization: Fourth order Runge Kutta, $\Delta T = \frac{T}{180}$,
$\Delta t = \frac{T}{1800}$.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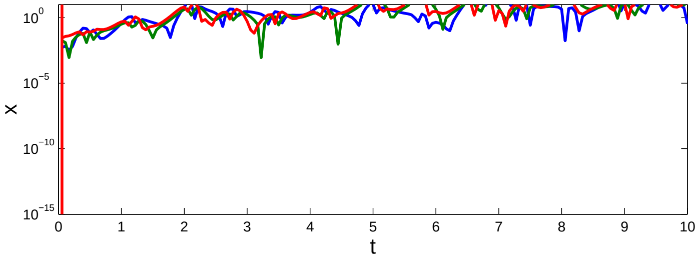
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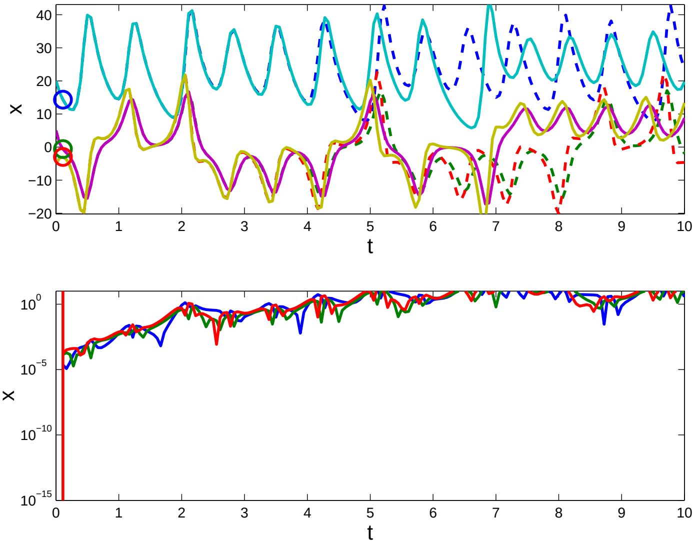
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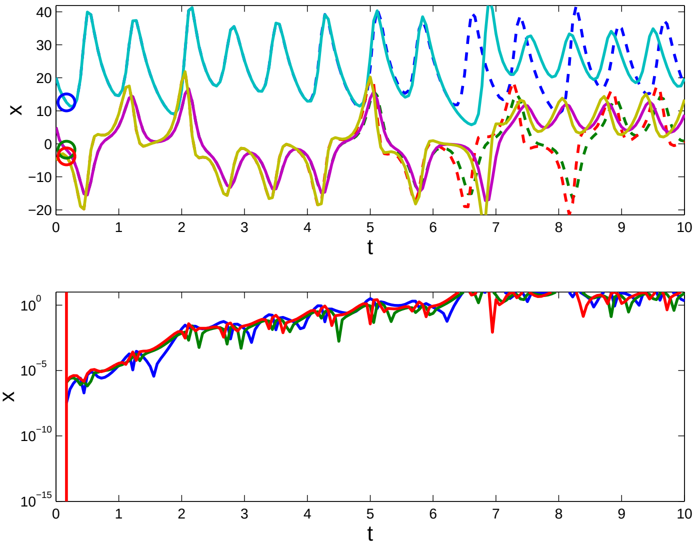
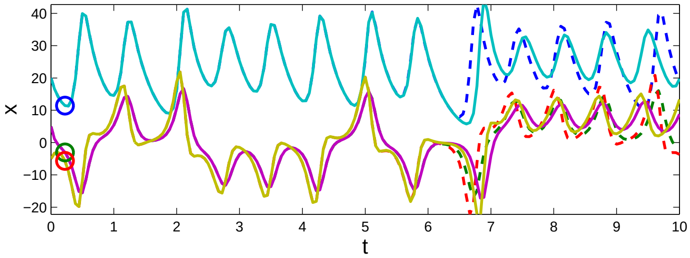
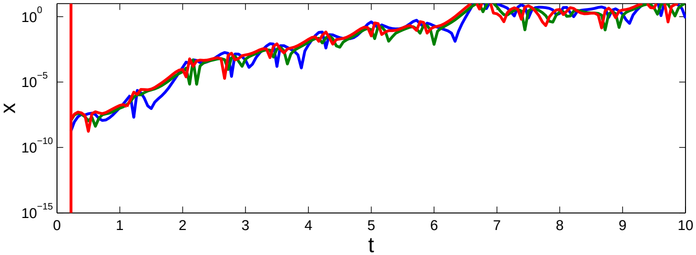
t

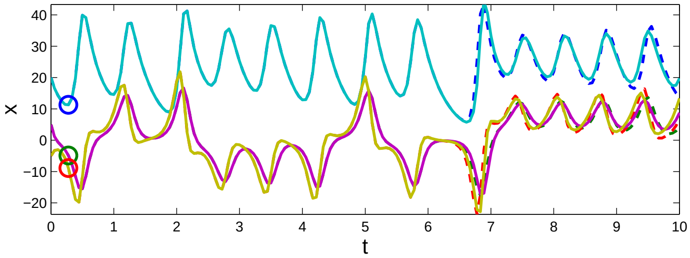

x
t
40
30
20
10
0
−10
−20
0
1
2
3
4
5
6
7
8
9
10
x
t
10^{0}
10^{-5}
10^{-10}
10^{-15}



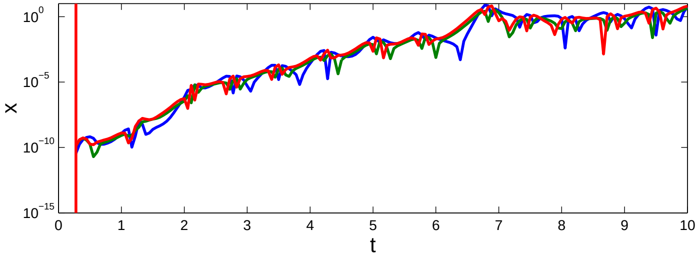
40
30
20
10
0
−10
−20
x
0
1
2
3
4
5
6
7
8
9
10
t



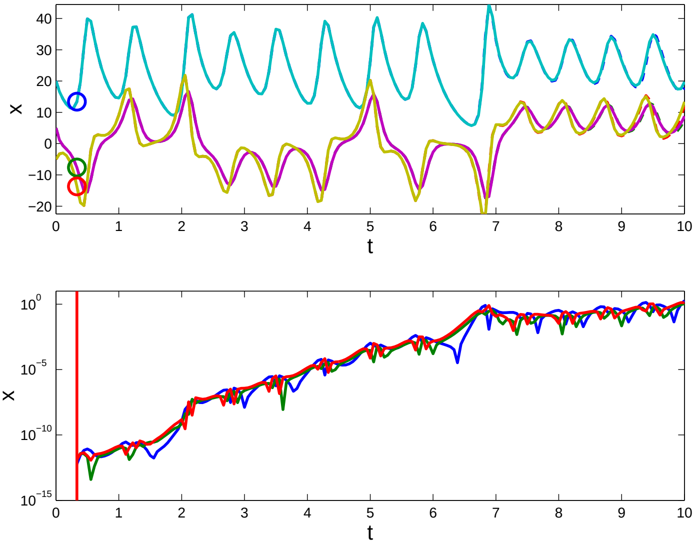
10^{0}
10^{-5}
10^{-10}
10^{-15}
x
0
1
2
3
4
5
6
7
8
9
10
t

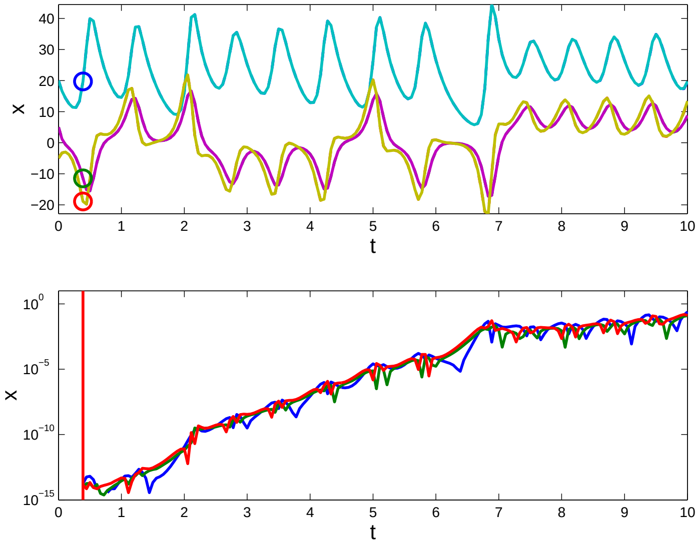


40
30
20
10
0
−10
−20
x
0
1
2
3
4
5
6
7
8
9
10
t

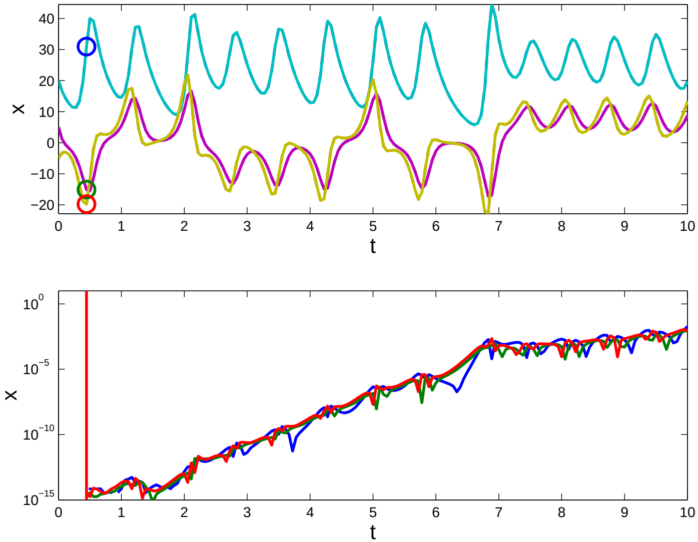


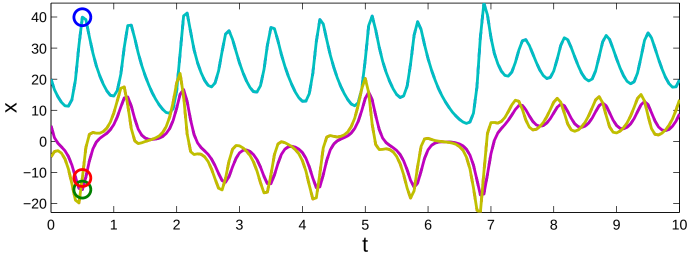
10^{0}
10^{-5}
10^{-10}
10^{-15}
x
0
1
2
3
4
5
6
7
8
9
10
t

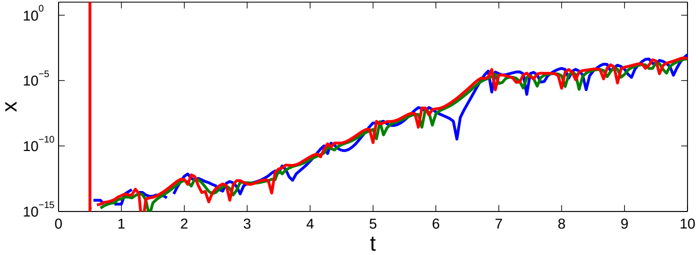

40
30
20
10
0
−10
−20
x
0 1 2 3 4 5 6 7 8 9 10
t
10^{0}
10^{-5}
10^{-10}
10^{-15}
x
0 1 2 3 4 5 6 7 8 9 10
t

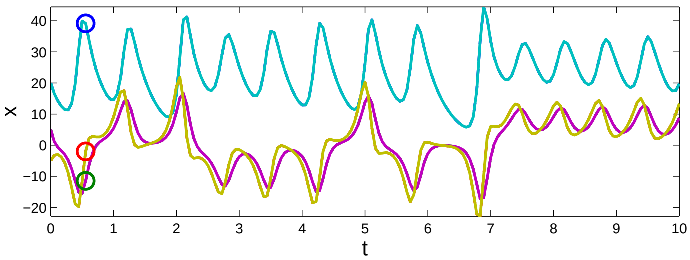


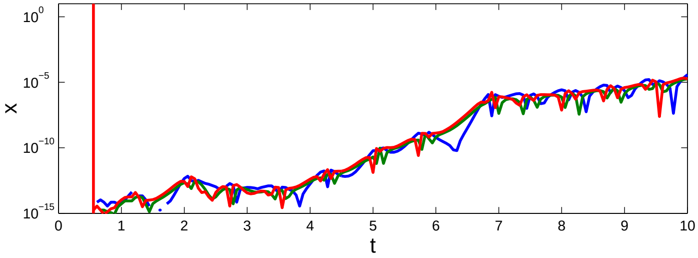
40
30
20
10
0
−10
−20
x
0 1 2 3 4 5 6 7 8 9 10
t
10^{0}
10^{-5}
10^{-10}
10^{-15}
x
0 1 2 3 4 5 6 7 8 9 10
t

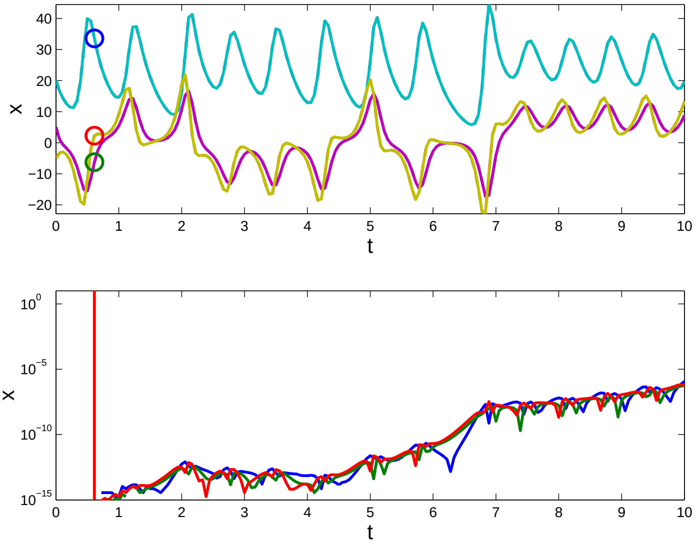

x
t
0
1
2
3
4
5
6
7
8
9
10
40
30
20
10
0
−10
−20
10^{0}
10^{-5}
10^{-10}
10^{-15}


x
t
0
1
2
3
4
5
6
7
8
9
10
40
30
20
10
0
−10
−20

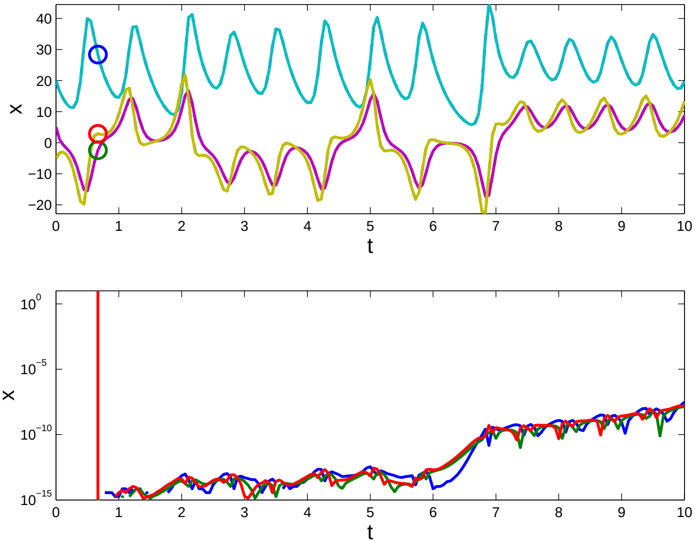

x
t
0
1
2
3
4
5
6
7
8
9
10
10^{0}
10^{-5}
10^{-10}
10^{-15}


40
30
20
10
0
−10
−20
x
0 1 2 3 4 5 6 7 8 9 10
t


10^{0}
10^{-5}
10^{-10}
10^{-15}
x
0 1 2 3 4 5 6 7 8 9 10
t

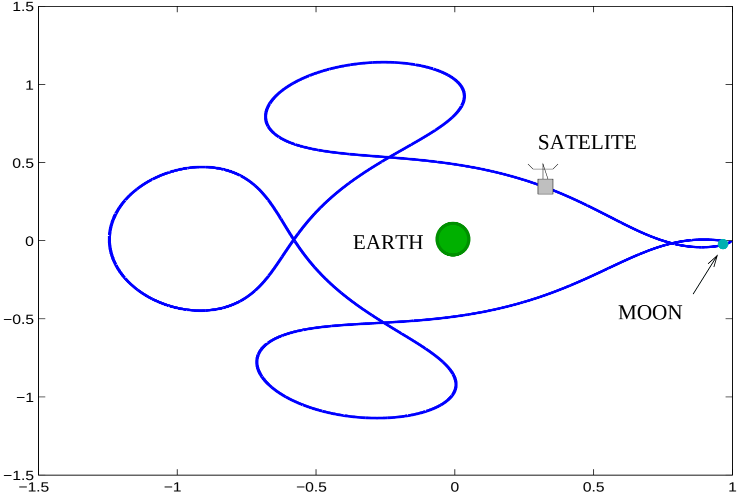


40
30
20
10
0
−10
−20
x
0
1
2
3
4
5
6
7
8
9
10
t
10^{0}
10^{-5}
10^{-10}
10^{-15}
x
t



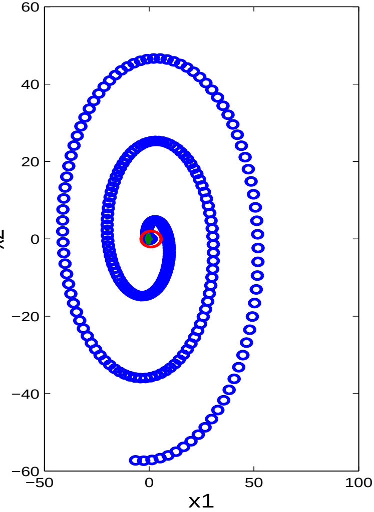
40
30
20
10
0
−10
−20
x
0
1
2
3
4
5
6
7
8
9
10
t
10^0
10^−5
10^−10
10^−15
x
t

Numerical experiment: Arenstorf orbit

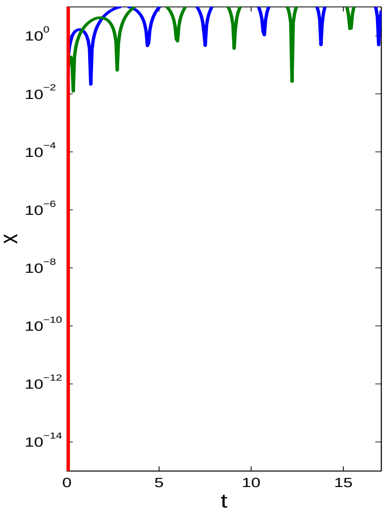


Lets try the parareal algorithm with 250 processors

Iteration 1

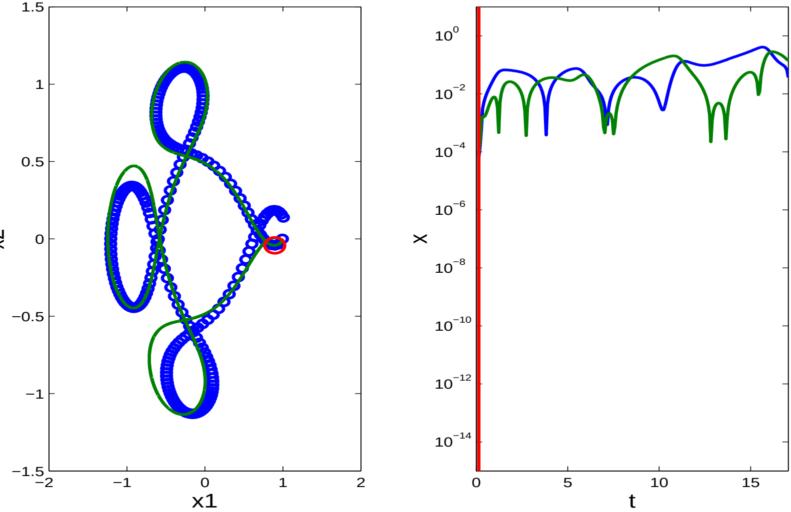


60
40
20
0
−20
−40
−60
−50
0
50
100
x1
x2

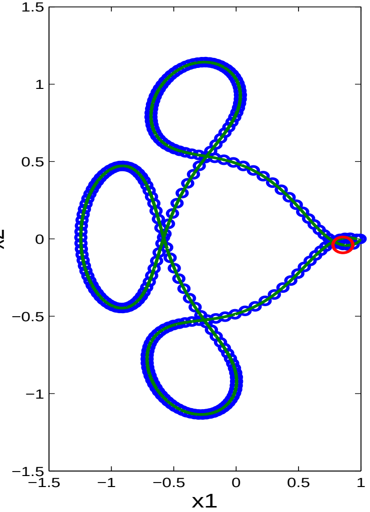


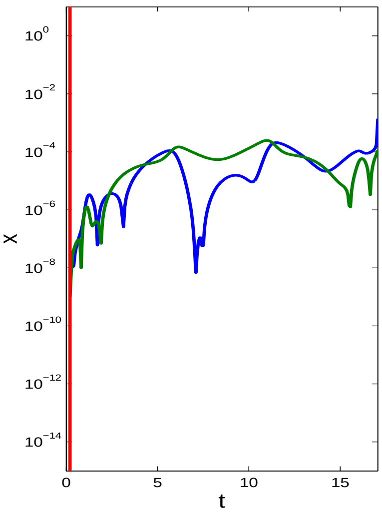
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
X
0
5
10
15
t

Iteration 2

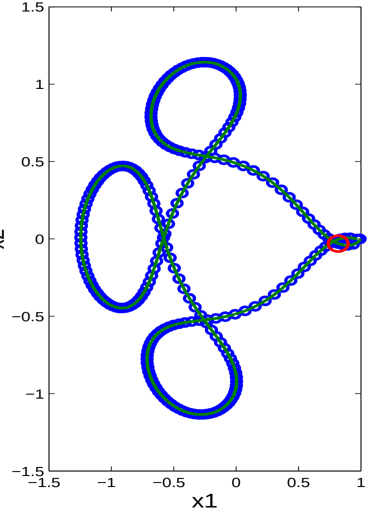

1.5
1
0.5
0
−0.5
−1
−1.5
−2
−1
0
1
2
x1
x2
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
0
5
10
15
t
X

Iteration 3

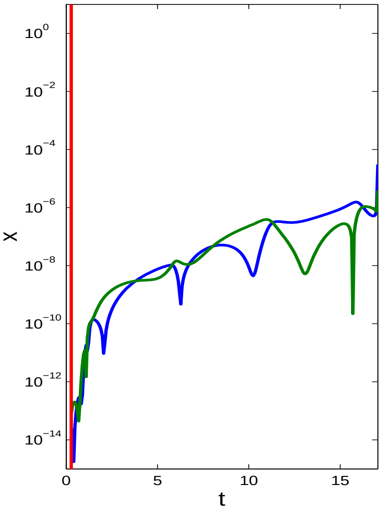

1.5
1
0.5
0
−0.5
−1
−1.5
−1.5
−1
−0.5
0
0.5
1
x1


10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
x
0
5
10
15
t

Iteration 4

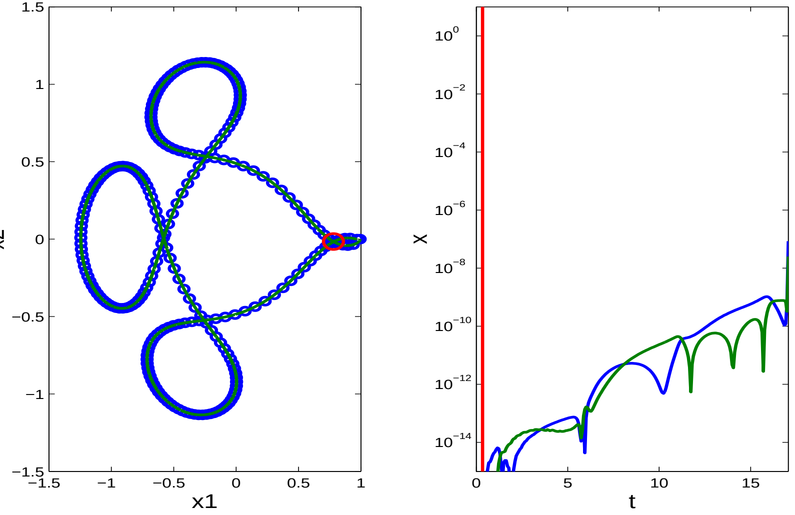


1.5
1
0.5
0
−0.5
−1
−1.5
x2
−1.5
−1
−0.5
0
0.5
1
x1

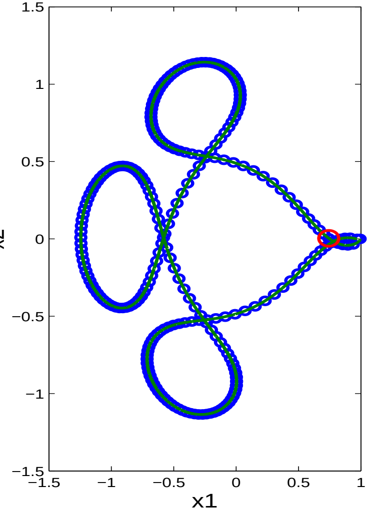


10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
x
0
5
10
15
t

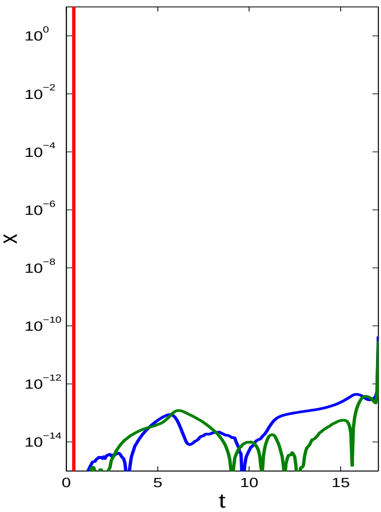
Iteration 5



Iteration 6



1.5
1
0.5
0
−0.5
−1
−1.5
−1.5
−1
−0.5
0
0.5
1
x1



10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
x
0
5
10
15
t

Conclusions Part I: Shooting Type Method

- The idea of parallelizing the solution of ODEs in the time direction goes back to Nievergelt (1964)
- Multiple shooting methods for initial value problems were investigated by Bellen and Zennaro (discrete case, 1989) and Chartier and Phillipe (continuous case, 1993)
- Approximating the Jacobian by a simpler model in multiple shooting for initial value problems was proposed by Saha, Stadel and Tremaine (1997)
- The parareal algorithm by Lions, Maday and Turinici (2001) uses an approximation of the Jacobian on a coarse grid

Preprints are available at www.unige.ch/∼gander