# Taylor Model-based Verified Integrators

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## The Lorenz Equations

The equations describe a simplified model of unpredictable turbulent flows in fluid dynamics.
Exhibits sensitive dependence on initial conditions and chaoticity.

$$\begin{aligned}\dot{x} &= \sigma(y - x)\\ \dot{y} &= x(\rho - z) - y\\ \dot{z} &= xy - \beta z\end{aligned}$$

The standard parameter values are

$$\sigma = 10, \beta = \frac{8}{3}, \rho = 28$$

and $\rho$ is often varied. The fixed points are

$$(0,0,0), \quad (\pm\sqrt{\beta(\rho - 1)}, \pm\sqrt{\beta(\rho - 1)}, \rho - 1).$$

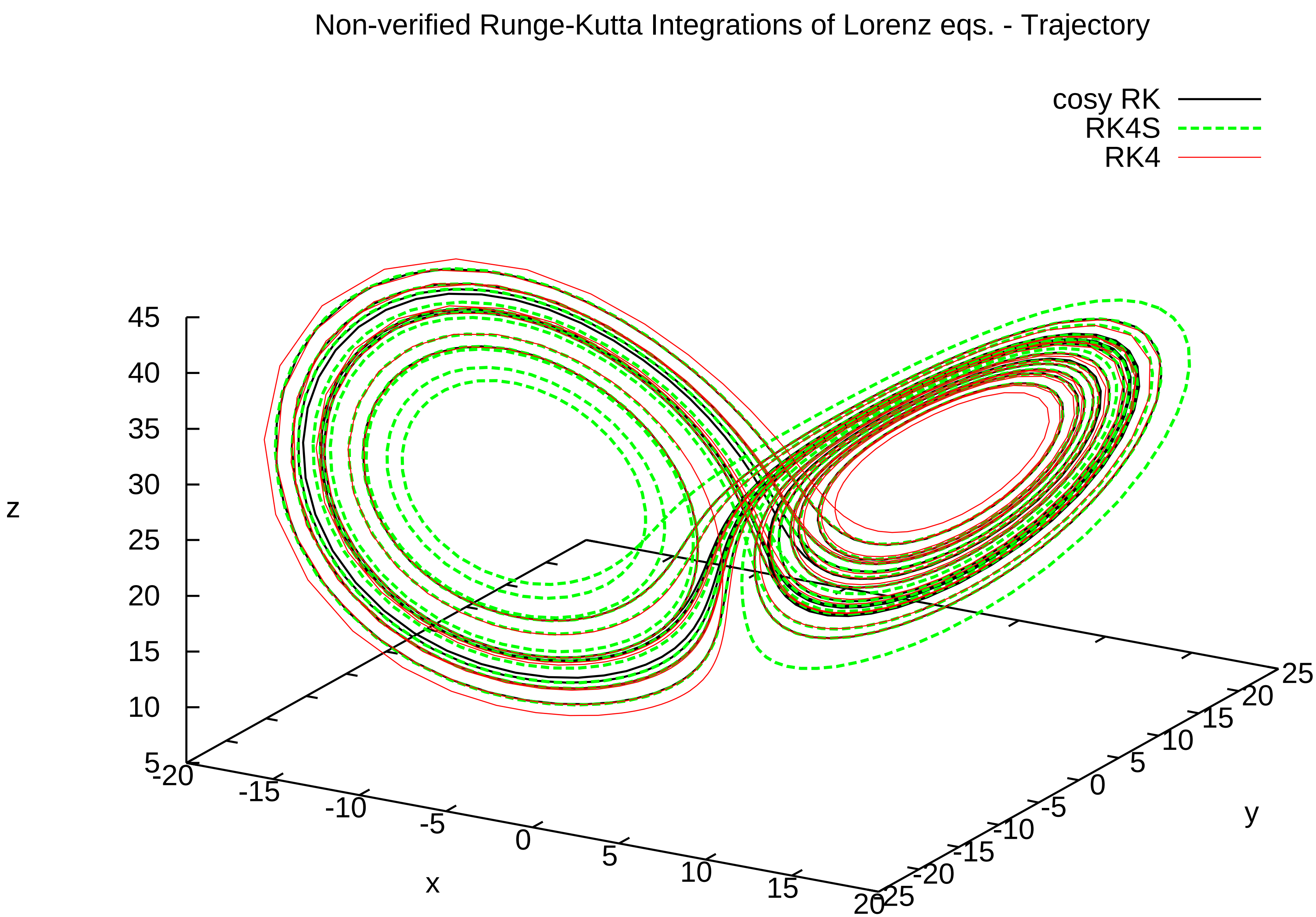
## Study Trajectories of the Lorenz System

Using conventional Runge Kutta integrators, study trajectories of an initial point

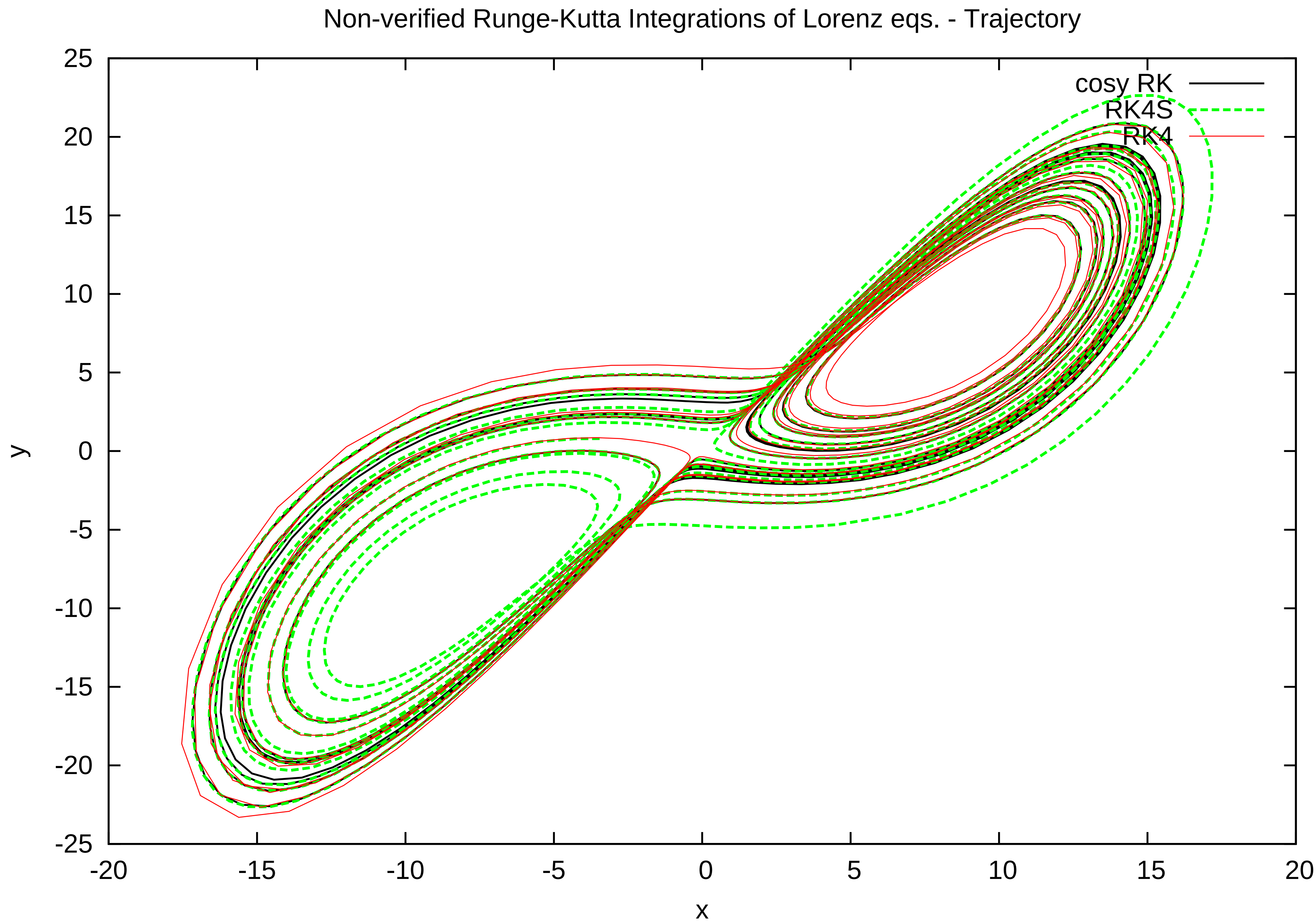
$$(x, y, z)|_0 = (15, 15, 36).$$

Integration from $t = 0$ to $t = T = 20$.

RK4: the 4th order RK
RK4S: 4th order RK with automatic step size control
COSY-RK8: 8th order RK implemented in COSY



Non-verified Runge-Kutta Integrations of Lorenz eqs. - Trajectory
cosy RK
RK4S
RK4
z
45
40
35
30
25
20
15
10
5
x
-20
-15
-10
-5
0
5
10
15
20
y
-25
-20
-15
-10
-5
0
5
10
15
20
25


Non-verified Runge-Kutta Integrations of Lorenz eqs. - Trajectory
cosy RK
RK4S
RK4
y
x
25
20
15
10
5
0
-5
-10
-15
-20
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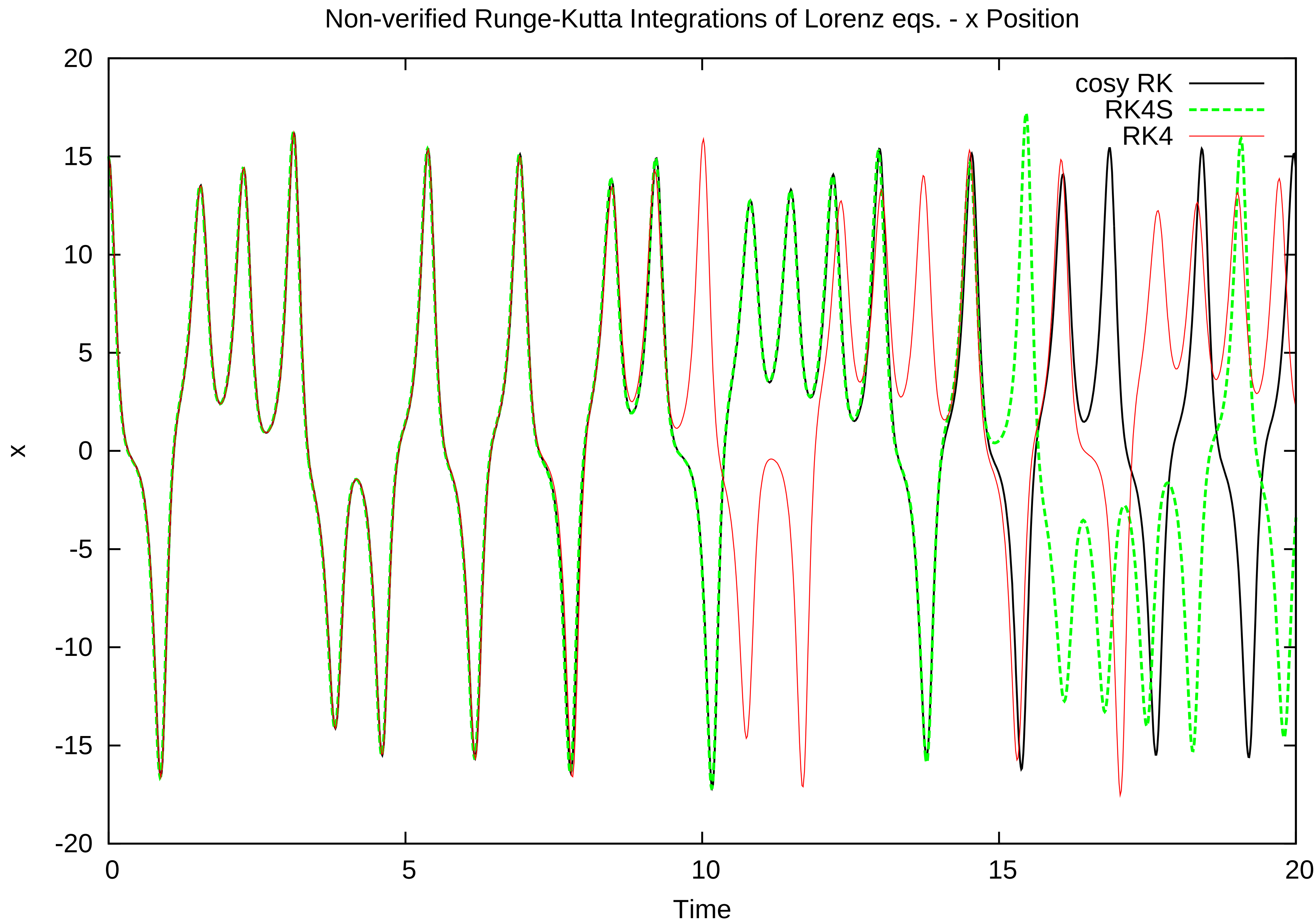
-10
-5
0
5
10
15
20



Non-verified Runge-Kutta Integrations of Lorenz eqs. - x Position
cosy RK
RK4S
RK4
x
Time
20
15
10
5
0
-5
-10
-15
-20
0
5
10
15
20

## Study Trajectories of the Lorenz System

Using conventional Runge Kutta integrators, study trajectories of an initial point

$$(x, y, z)|_0 = (15, 15, 36).$$

Integration from $t = 0$ to $t = T = 20$.

| | $x(T)$ | $y(T)$ | $z(T)$ | single step error | CPU |
|---|---|---|---|---|---|
| RK4 | 2.205 | 1.030 | 22.282 | | 0.689 |
| RK4S | -3.388 | 0.796 | 27.582 | 1.27e-2 | 0.904 |
| COSY-RK8 | 14.309 | 9.591 | 39.039 | 1.21e-7 | 1 |

RK4S: 4th order RK with automatic step size control
COSY-RK8: 8th order RK implemented in COSY

## Study Trajectories of the Lorenz System

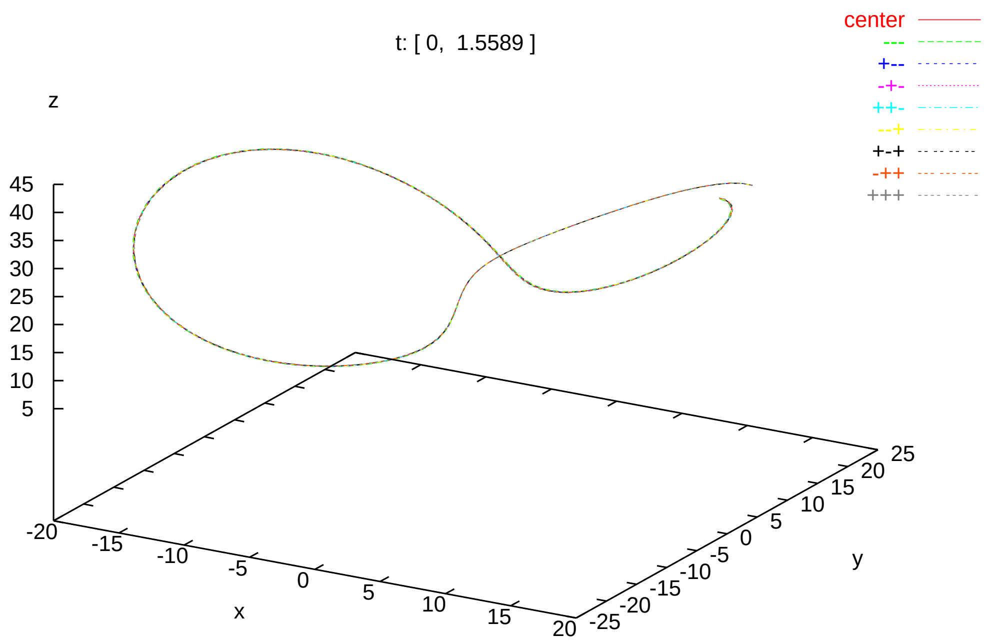
Using COSY-RK8, study trajectories of initial points

$$(x, y, z)|_0 = (15, 15, 36)$$

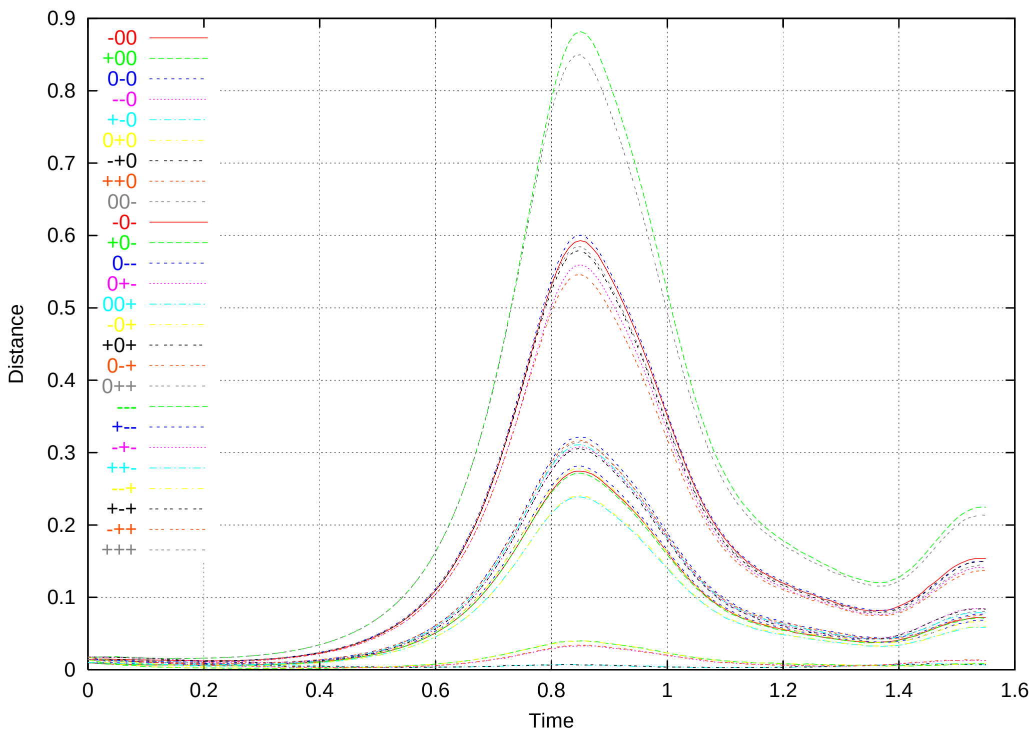
and

$$(x, y, z)|_0 = (15, 15, 36) + (\pm 0.01, \pm 0.01, \pm 0.01)$$

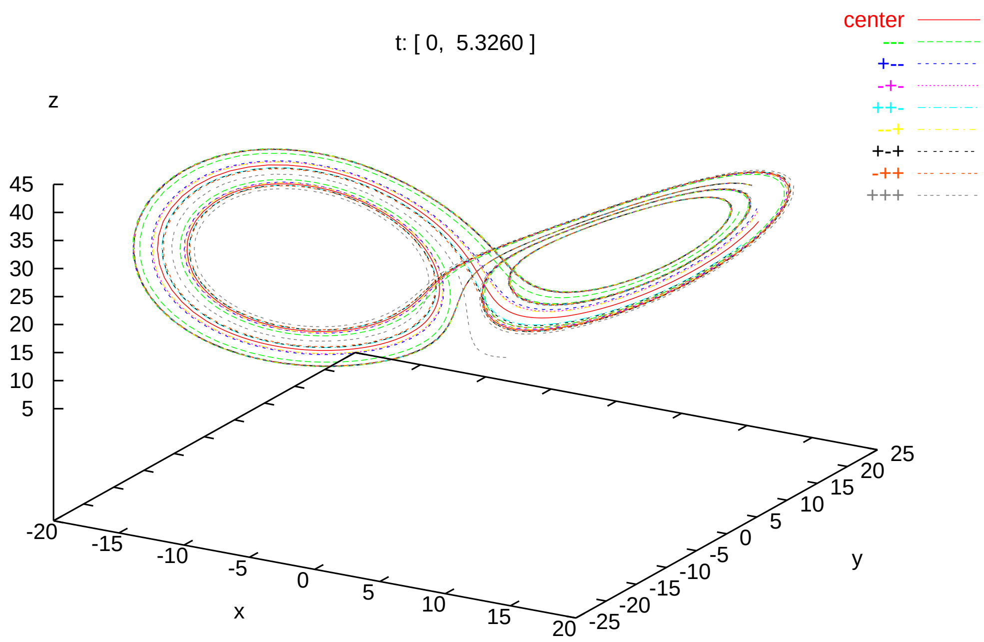
$t \in [0, 1.56]$



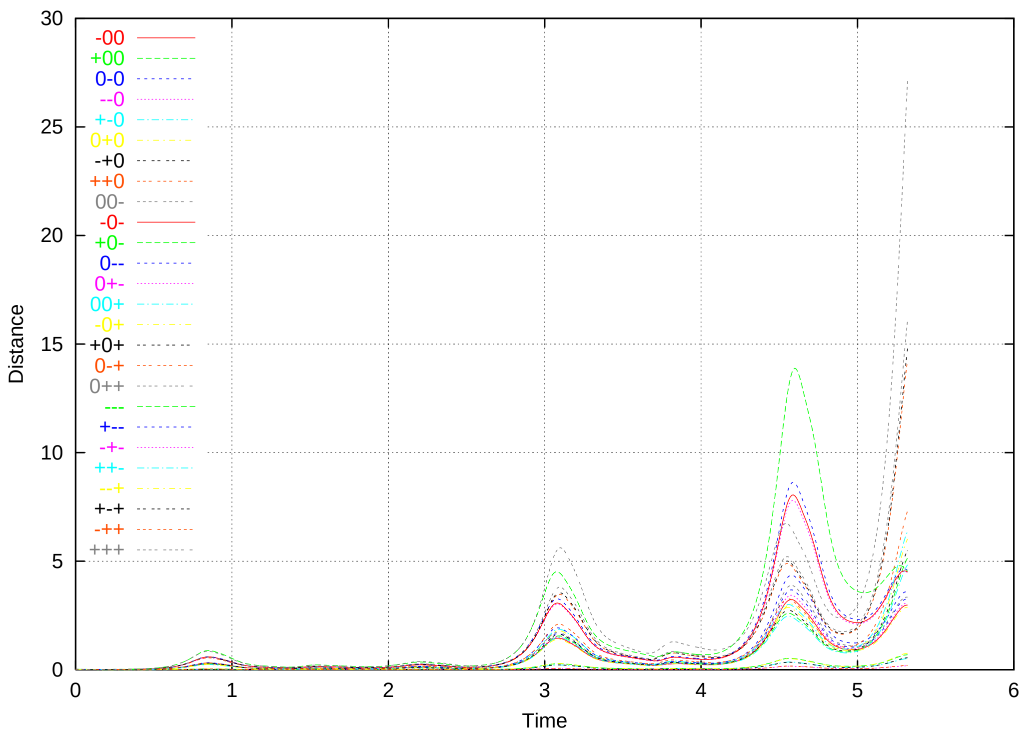

Distance to the Center Trajectory



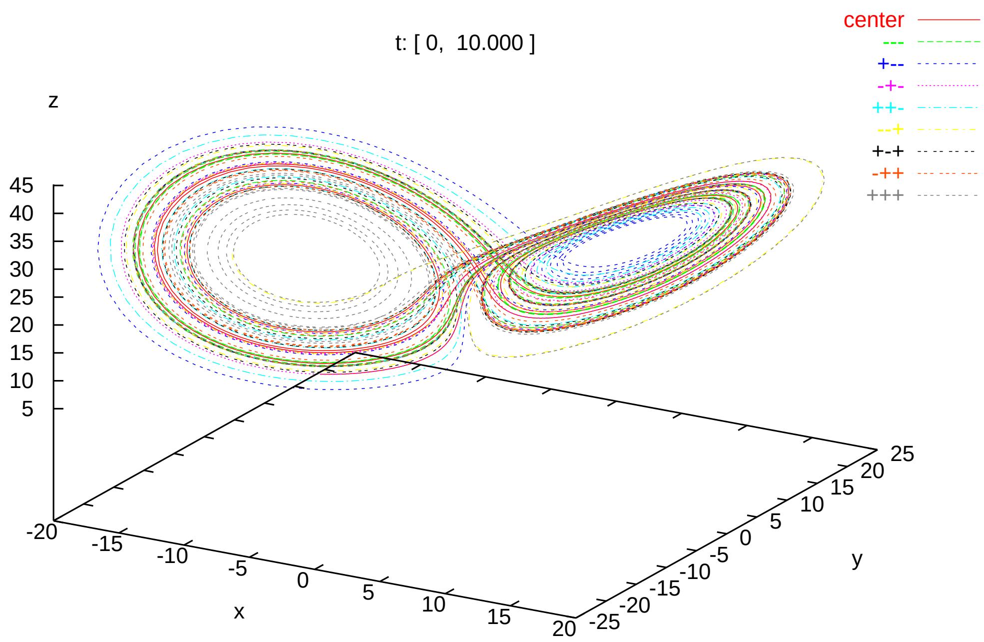
$t \in [0, 5.326]$



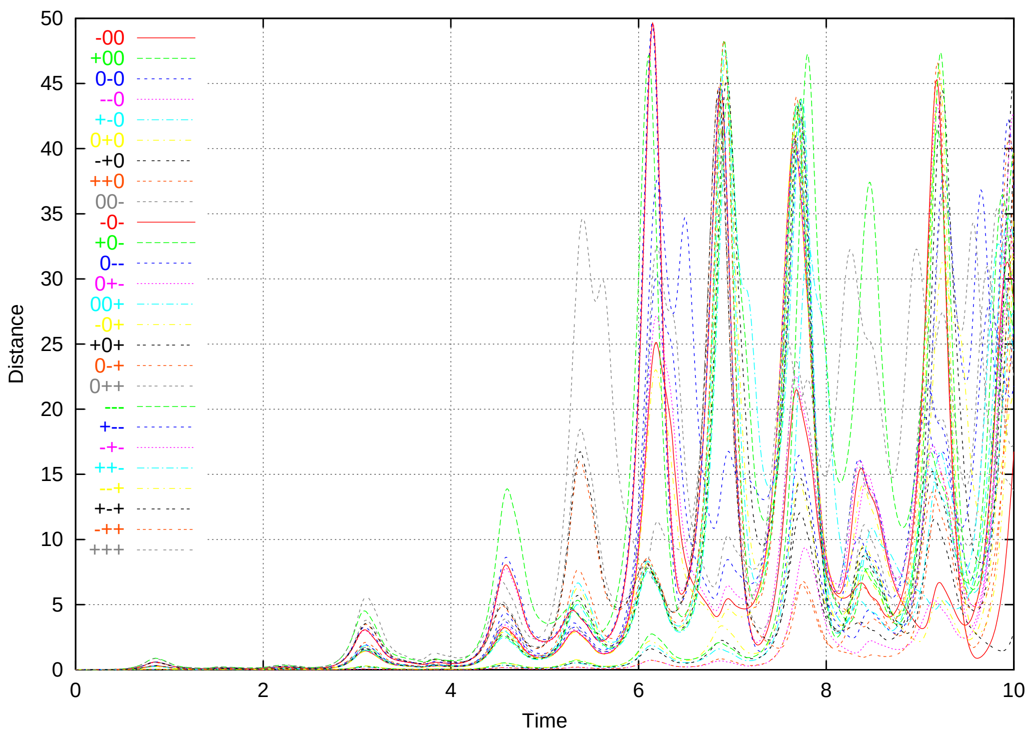

Distance to the Center Trajectory



$t \in [0, 10]$




Distance to the Center Trajectory



## Rigorous Integrations of the Lorenz System

As a test case, transport an area of initial condition

$$(x, y, z)|_0 = (15, 15, 36) + (\pm 0.01, \pm 0.01, \pm 0.01)$$

using rigorous ODE integrators.

AWA: An interval based ODE integrator by R. Lohner

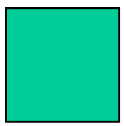
COSY-VI: Taylor model based ODE integrator in COSY

– Computed in 2001, using COSY-VI version 1

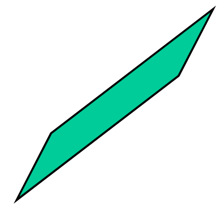
# Taylor Model based Integrator COSY-VI version 1 (1997–)

- High order expansion not only in time $t$ but also in transversal variables $\vec{x}$.
- One time step integration via Picard iterations based on the Shauder fixed point theorem.
- Shrink wrapping algorithm, a simplified version

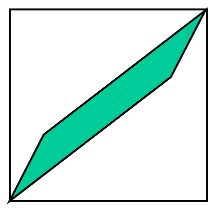
# The Wrapping Effect in Linear ODEs



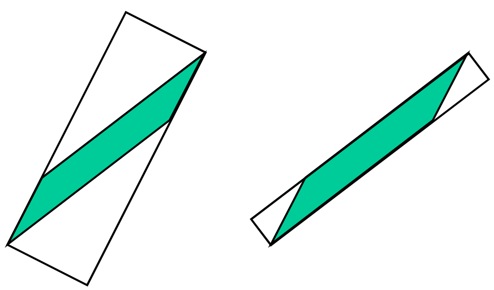
Initial Condition Interval Box



Solution Set

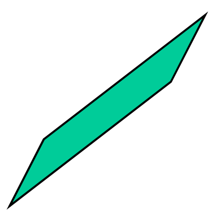


Solution Set in the Optimal Interval Box



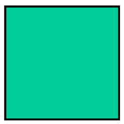
Solution Set in Rotated Rectangles

( Here, the Right One is Optimal. )

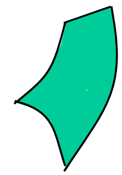


Solution Set by Taylor Models

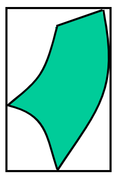
# The Wrapping Effect in Nonlinear ODEs



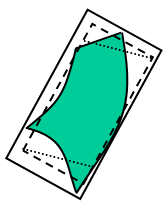
Initial Condition Interval Box



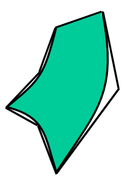
Solution Set



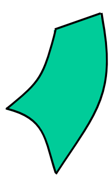
Solution Set in the Optimal Interval Box



Solution Set in an Optimal Rotated Rectangle



Solution Set in an Optimal Eight-Corner Polygon



Solution Set by Taylor Models

# The Henon Map

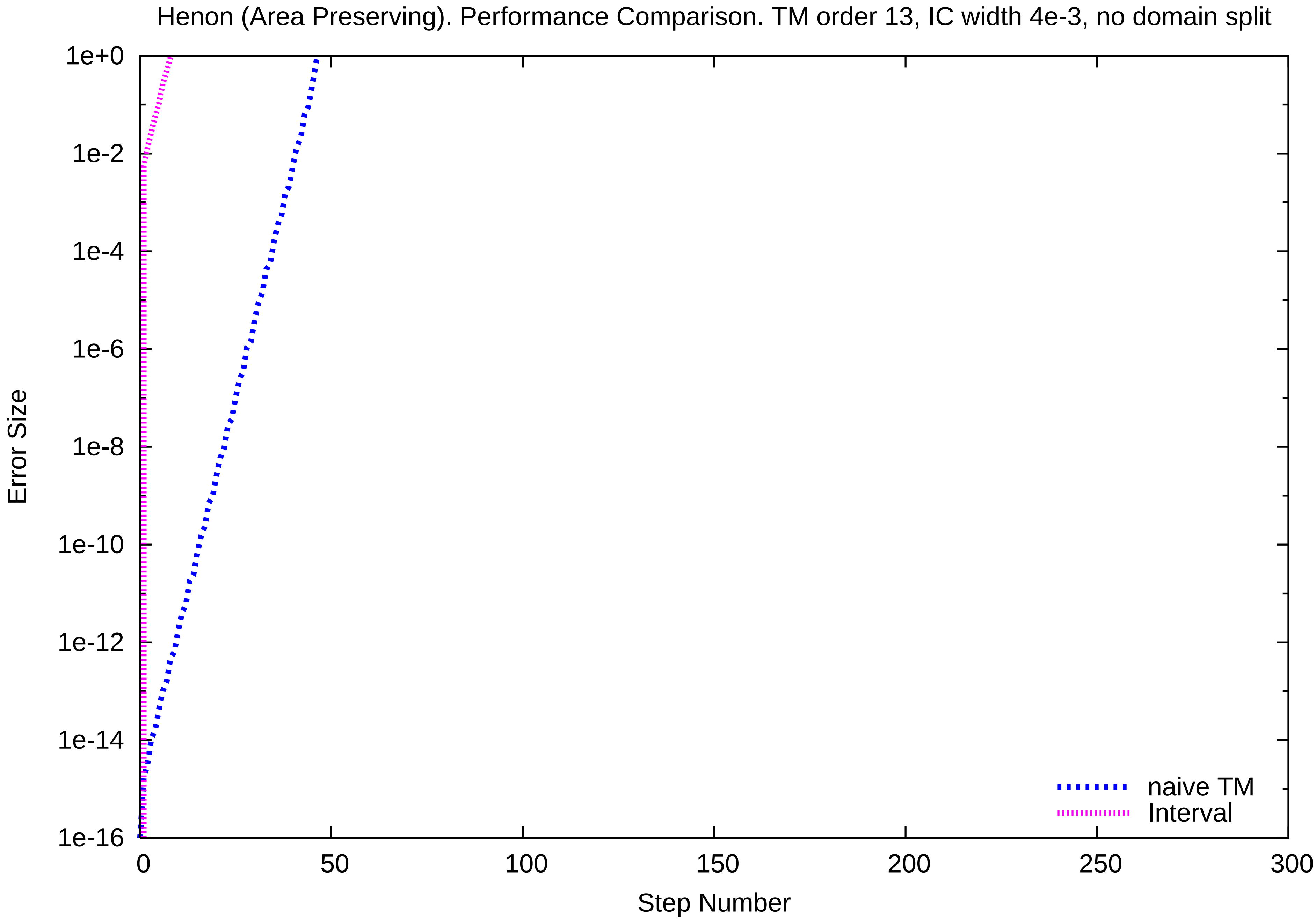
Henon Map: frequently used elementary example that exhibits many of the well-known effects of nonlinear dynamics, including chaos, periodic fixed points, islands and symplectic motion. The dynamics is two-dimensional, and given by

$$x_{n+1} = 1 - \alpha x_n^2 + y_n$$
$$y_{n+1} = \beta x_n.$$

It can easily be seen that the motion is area preserving for $|\beta| = 1$.We consider

$$\alpha = 2.4 \text{ and } \beta = -1,$$

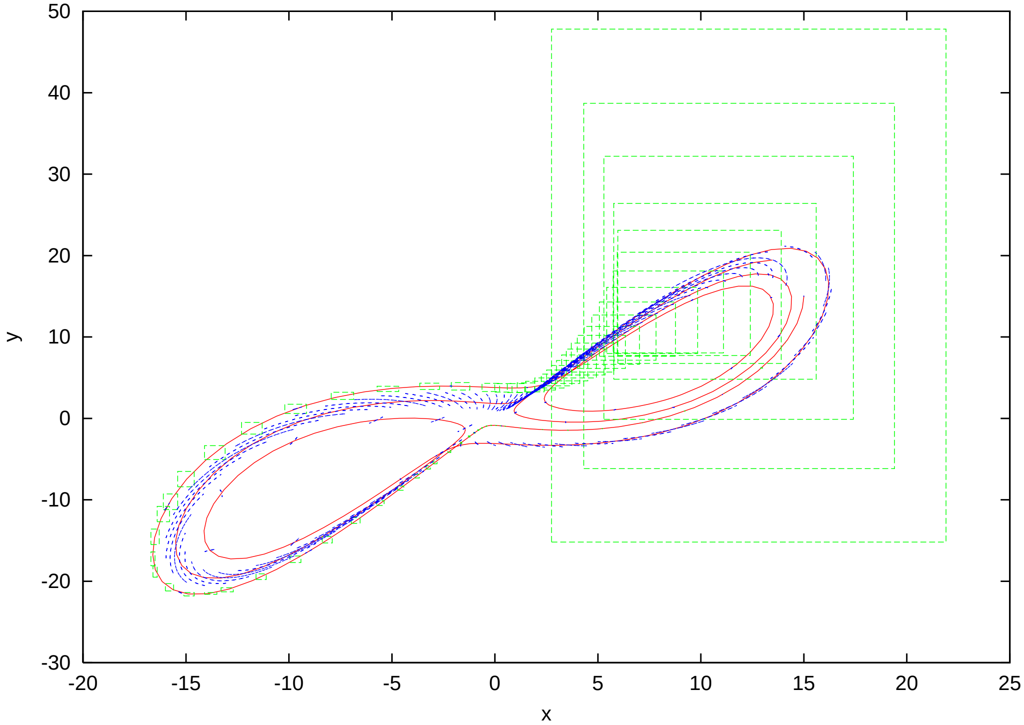
and concentrate on initial boxes of the from $(x_0, y_0) \in (0.4, -0.4) + [-d, d]^2$.



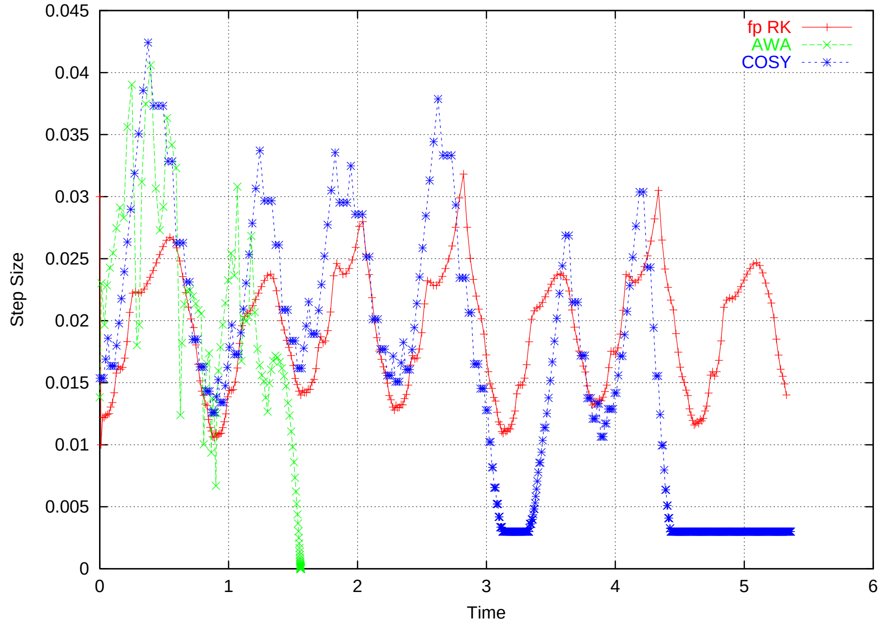
Henon (Area Preserving). Performance Comparison. TM order 13, IC width 4e-3, no domain split
Error Size
1e+0
1e-2
1e-4
1e-6
1e-8
1e-10
1e-12
1e-14
1e-16
0
50
100
150
200
250
300
Step Number
naive TM
Interval

$$x_0 = 15 \pm 0.01, \; y_0 = 15 \pm 0.01, \; z_0 = 36 \pm 0.01$$

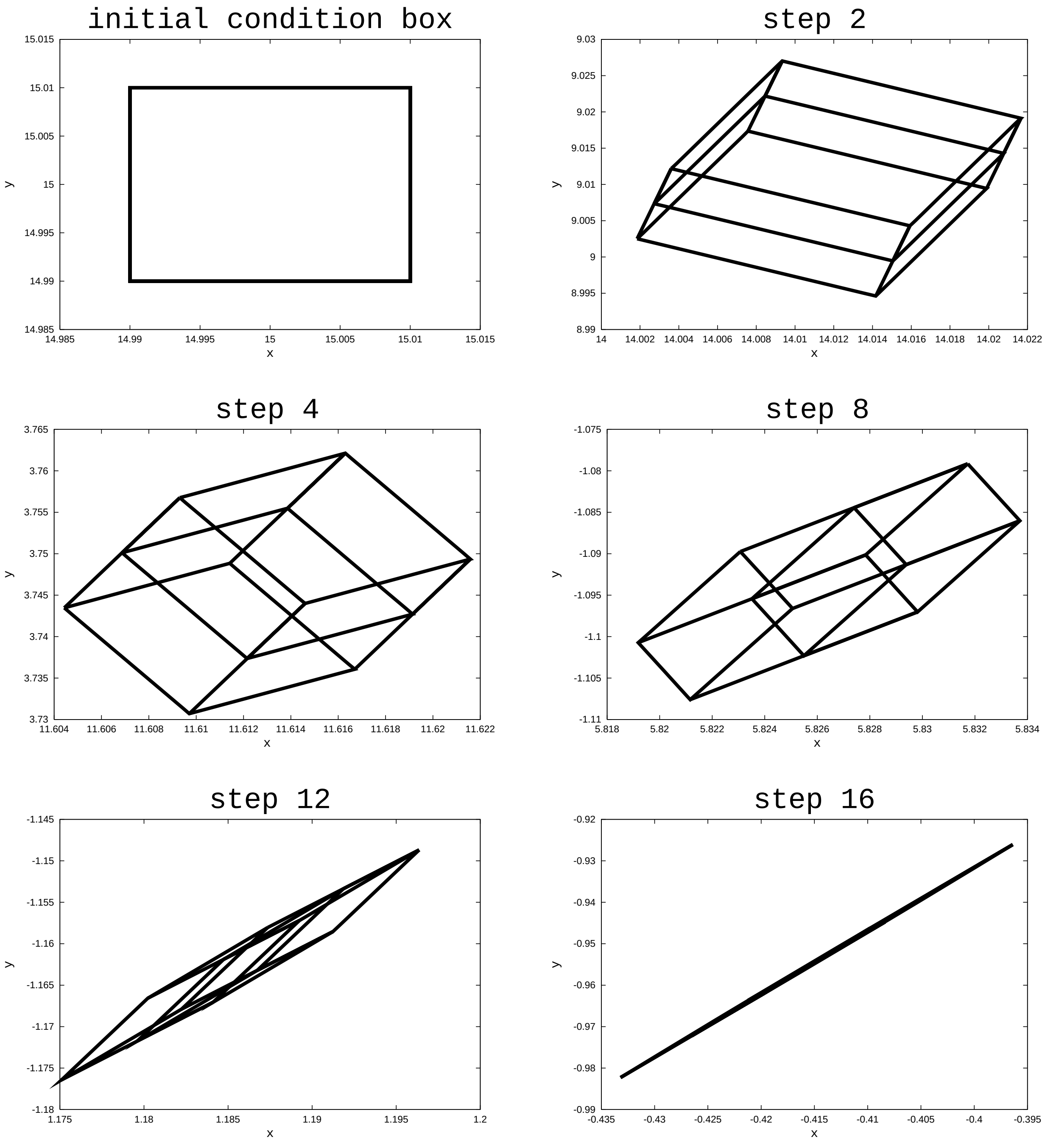
Solution Ranges by COSY and AWA (18th Order)




Step Size

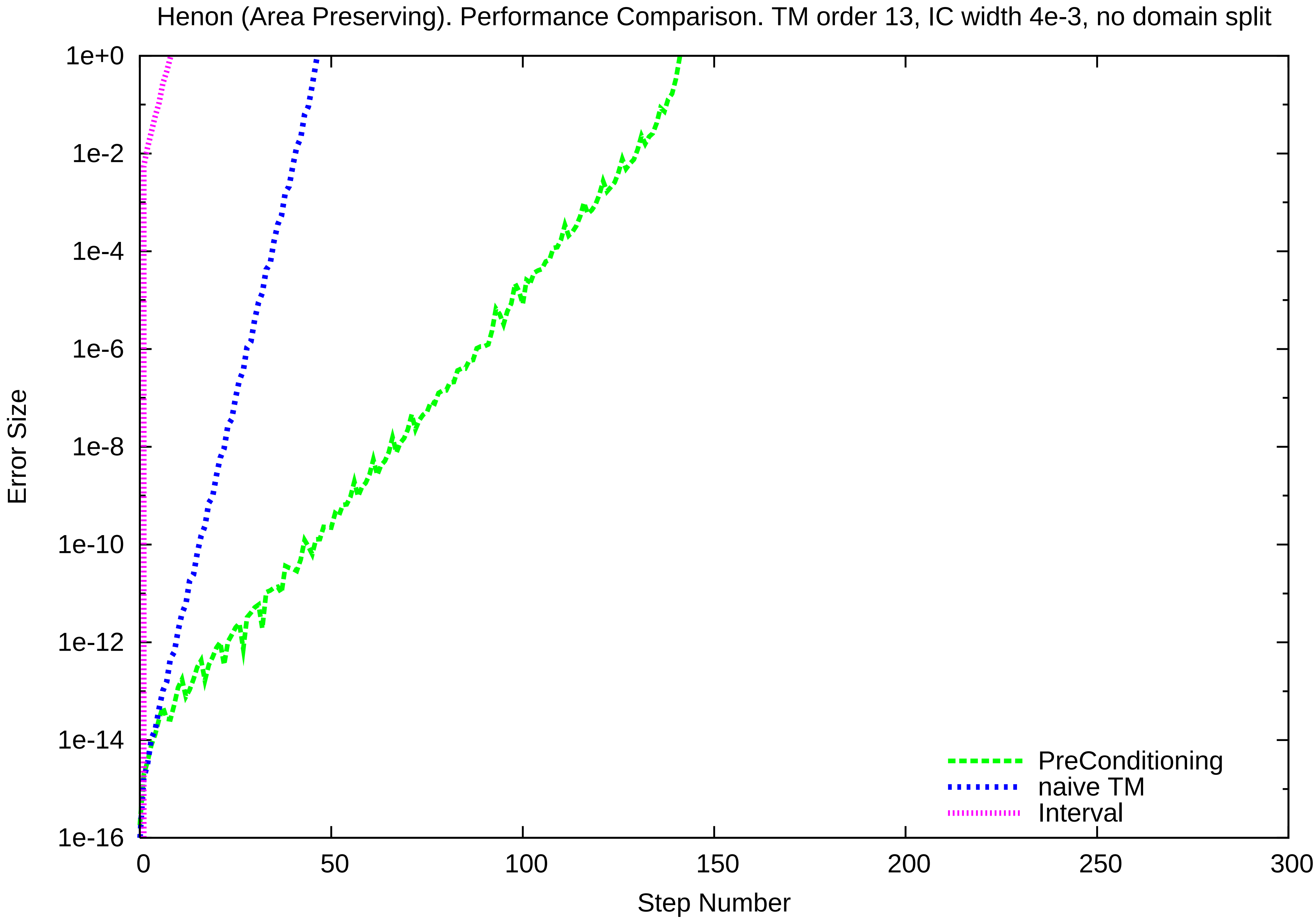


# Flow Enclosures of the Lorenz System



# Taylor Model based Integrator COSY-VI version 2 (2002-)

- Shrink wrapping algorithm including blunting to control ill-conditioned cases.
- Pre-conditioning algorithms based on the Curvilinear, QR decomposition, and blunting pre-conditioners.
- Capability of weighted order computation, allowing to suppress the expansion order in transversal variables $\vec{x}$.



Henon (Area Preserving). Performance Comparison. TM order 13, IC width 4e-3, no domain split
1e+0
1e-2
1e-4
1e-6
1e-8
1e-10
1e-12
1e-14
1e-16
Error Size
0
50
100
150
200
250
300
Step Number
PreConditioning
naive TM
Interval

# Taylor Model based Integrator COSY-VI version 3 (2007-)

- More economical one time step integration using the reference trajectory and the Lie derivative based flow operator on the deviation equations.
- Non aborting mechanism when prohibited arithmetic happens such as $1/f$ for $0 \in f$.
- Improvement of step size control.
- Error parametrization of Taylor models.
- Dynamic domain decomposition.

## Error Parametrization of Taylor models

**Motivation:** Is it possible to absorb the remainder error bound intervals of Taylor models into the polynomial parts using additional parameters?

Phrase the question as the following problem:

1. Have Taylor models with 0 remainder error interval, which depend on the independent variables $\vec{x}$ and the parameters $\vec{\alpha}$.

$$\vec{T}_0 = \vec{P}_0(\vec{x}, \vec{\alpha}) + \overrightarrow{[0,0]}.$$

2. Perform Taylor model arithmetic on $\vec{T}_0$, namely $\vec{F}(\vec{T}_0)$

$$\vec{F}(\vec{T}_0) = \vec{P}(\vec{x}, \vec{\alpha}) + \vec{I}_F, \text{ where } \vec{I}_F \neq \overrightarrow{[0,0]}.$$

3. Try to absorb $\vec{I}_F$ into the polynomial part that depends on $\vec{\alpha}$

$$\vec{P}(\vec{x}, \vec{\alpha}) + \vec{I}_F \subseteq \vec{P}'(\vec{x}, \vec{\alpha}) + \overrightarrow{[0,0]}. \qquad \text{(A)}$$

## Error Absorption

We limit the explicitly $\vec{\alpha}$-dependent part $\vec{P}_\alpha(\vec{x},\vec{\alpha})$ to be only **linearly** dependent on $\vec{\alpha}$, and express $\vec{I}_F$ by the matrix form.

$$\vec{P}_\alpha(\vec{x},\vec{\alpha}) + \vec{I}_F \subseteq \left(\widehat{M} + \widehat{\bar{M}}(\vec{x})\right) \cdot \vec{\alpha} + \left(\widehat{I}_F + \widehat{\bar{I}}_F(\vec{x})\right) \cdot \vec{\beta}.$$

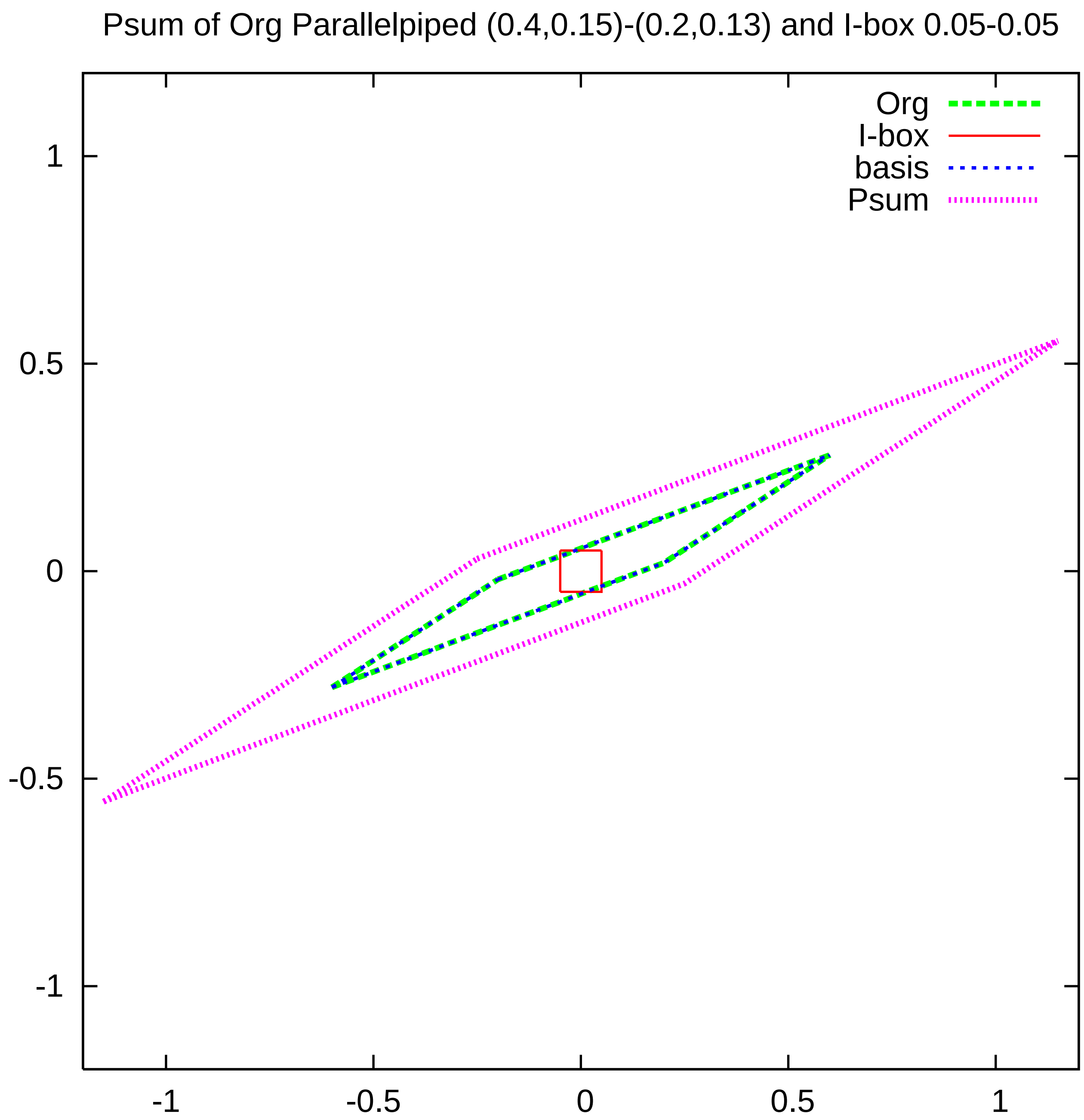
where $(\widehat{I}_F)_{ii} = |I_{Fi}|$ , $\widehat{\bar{I}}_F(\vec{x}) = 0$. The problem is now to find a **set sum of two parallelepipeds**. Choose a favoured collection of $v$ column vectors $\widehat{L} + \widehat{\bar{L}}(\vec{x})$ using the **Psum algorithm.**

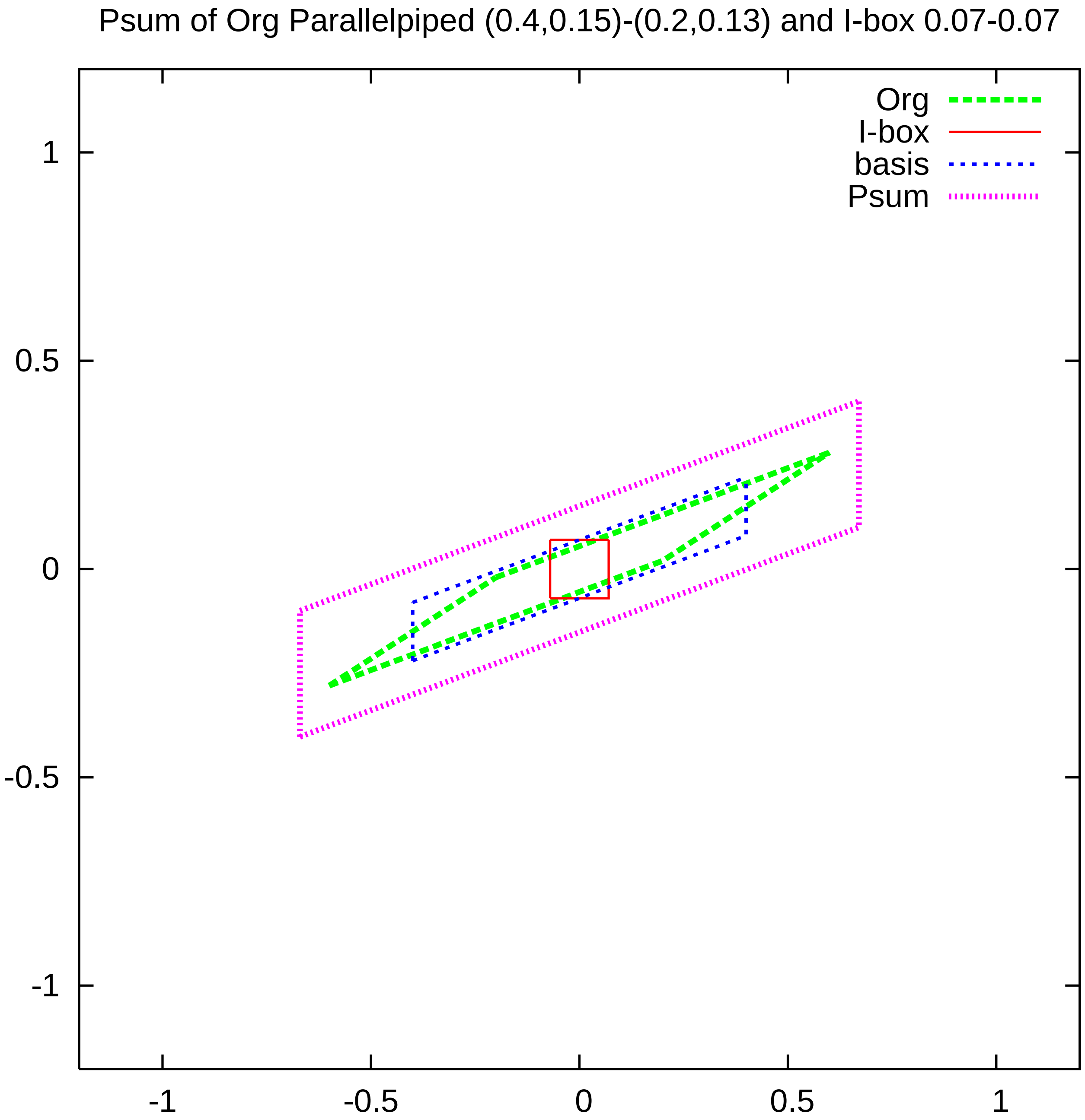
$$\begin{aligned}\vec{P}_\alpha(\vec{x},\vec{\alpha}) + \vec{I}_F &\subseteq \left(\widehat{L} + \widehat{\bar{L}}(\vec{x})\right) \cdot \vec{\alpha} + \left(\widehat{E} + \widehat{\bar{E}}(\vec{x})\right) \cdot \vec{\beta} \\ &\subseteq \widehat{L} \circ \left[\left(\widehat{I} + \widehat{L}^{-1} \circ \widehat{\bar{L}}(\vec{x})\right) \cdot \vec{\alpha} + \widehat{B} \cdot \vec{\beta}\right]\end{aligned}$$

where $\widehat{B}$ is diagonal, $(\widehat{B})_{ii} = |\text{bound}((\widehat{L}^{-1} \circ (\widehat{E} + \widehat{\bar{E}}(\vec{x})) \cdot \vec{\beta})_i)|$.

**If** the **diagonal terms** of $\left(\widehat{I} + \widehat{L}^{-1} \circ \widehat{\bar{L}}(\vec{x})\right)$ are **positive**,

$$\vec{P}_\alpha(\vec{x},\vec{\alpha}) + \vec{I}_F \subseteq \left(\widehat{L} + \widehat{\bar{L}}(\vec{x}) + \widehat{L} \circ \widehat{B}\right) \cdot \vec{\alpha}.$$


Psum of Org Parallelpiped (0.4,0.15)-(0.2,0.13) and I-box 0.05-0.05
Org
I-box
basis
Psum
1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1


Psum of Org Parallelpiped (0.4,0.15)-(0.2,0.13) and I-box 0.07-0.07
Org
I-box
basis
Psum
1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1

# Cost of Additional Parameters

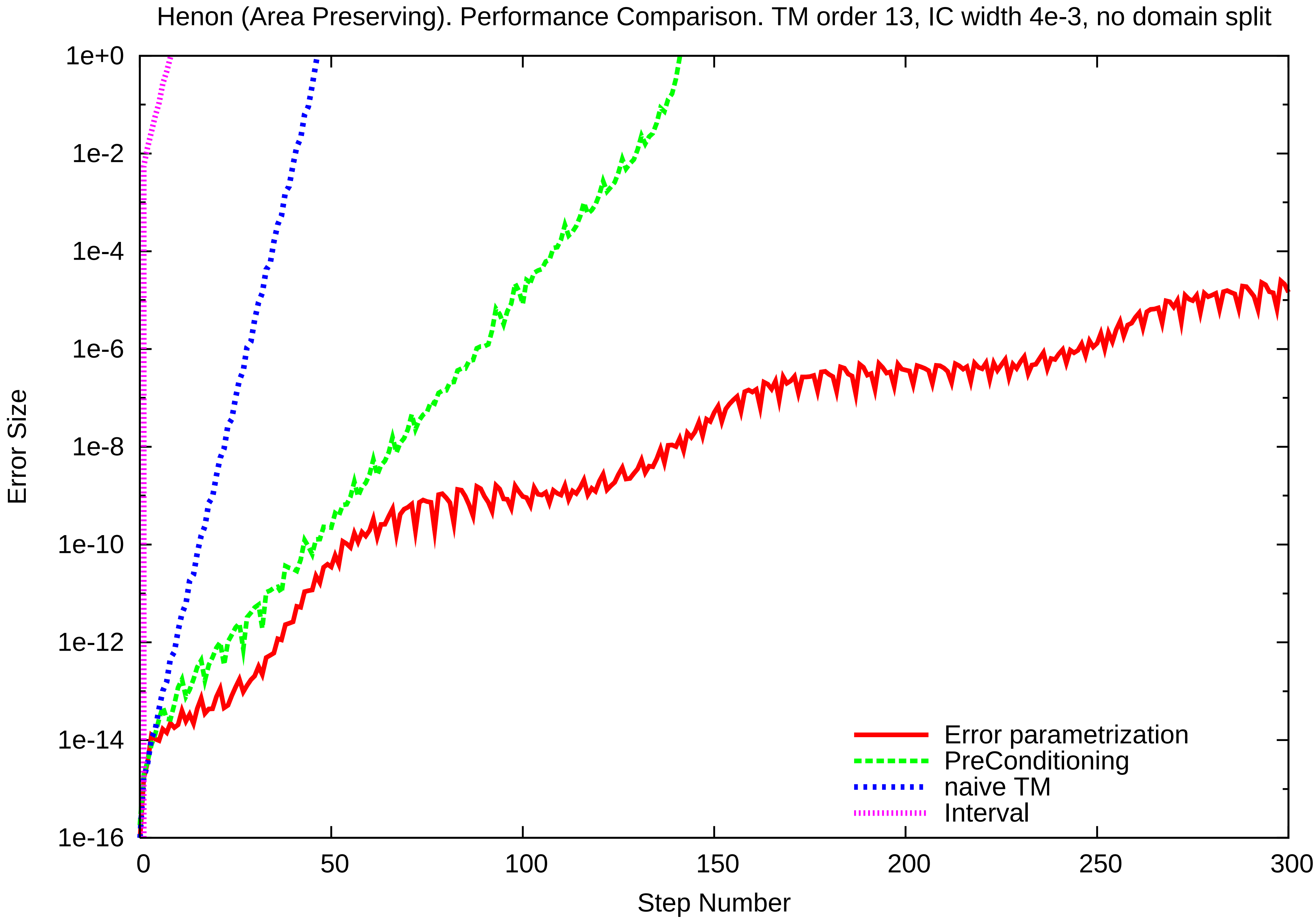
For a $v$ dimensional system, we need $v$ parameters $\vec{\alpha}$ to absorb Taylor model remainder error bound intervals. The dependence on $\vec{\alpha}$ is limited to **linear**. So, we use weighted DA. Choose an appropriate weight order $w$ for $\vec{\alpha}$.

- The dependence on $\vec{\alpha}$ has to be kept linear. Namely $2 \cdot w > n$, where $n$ is the computational order of Taylor models. Choose

$$w = \text{Int}\left(\frac{n}{2}\right) + 1.$$

Maximum size necessary for DA and TM for $v = 2$.

| $n$ | $v$ | DA | TM | $v$ | DA | TM | | $w$ | $v_w$ | DA | TM |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 13 | 2 | 105 | 140 | $2+2$ | 2380 | 2419 | | 7 | $2+2_w$ | 161 | 200 |
| 21 | 2 | 253 | 304 | $2+2$ | 12650 | 12705 | $\Rightarrow$ | 11 | $2+2_w$ | 385 | 440 |
| 33 | 2 | 595 | 670 | $2+2$ | 66045 | 66124 | | 17 | $2+2_w$ | 901 | 980 |


Henon (Area Preserving). Performance Comparison. TM order 13, IC width 4e-3, no domain split
1e+0
1e-2
1e-4
1e-6
1e-8
1e-10
1e-12
1e-14
1e-16
Error Size
0
50
100
150
200
250
300
Step Number
Error parametrization
PreConditioning
naive TM
Interval

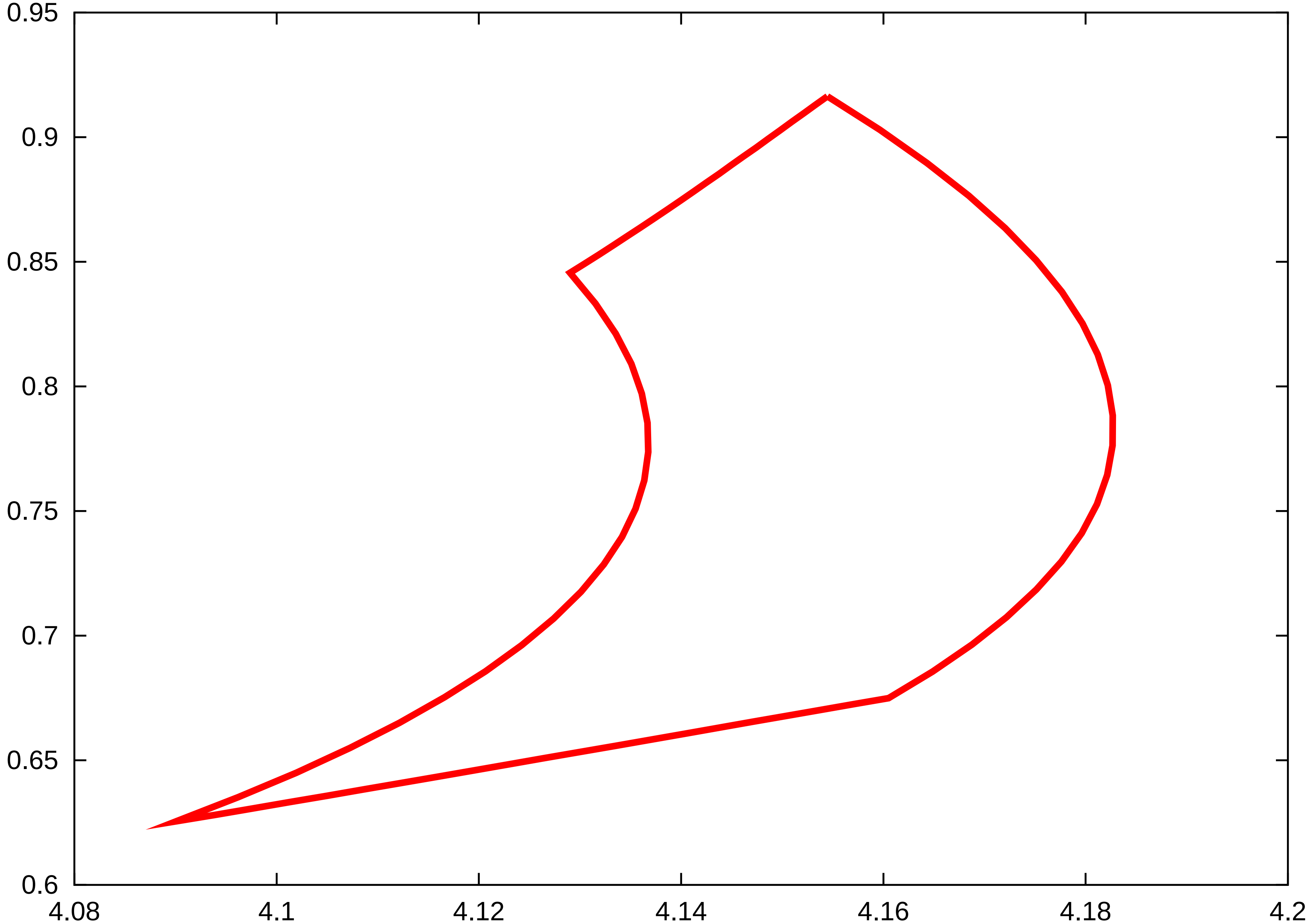
# Dynamic Domain Decomposition

For extended domains, this is **natural equivalent** to step size control. Similarity to what's done in global optimization.

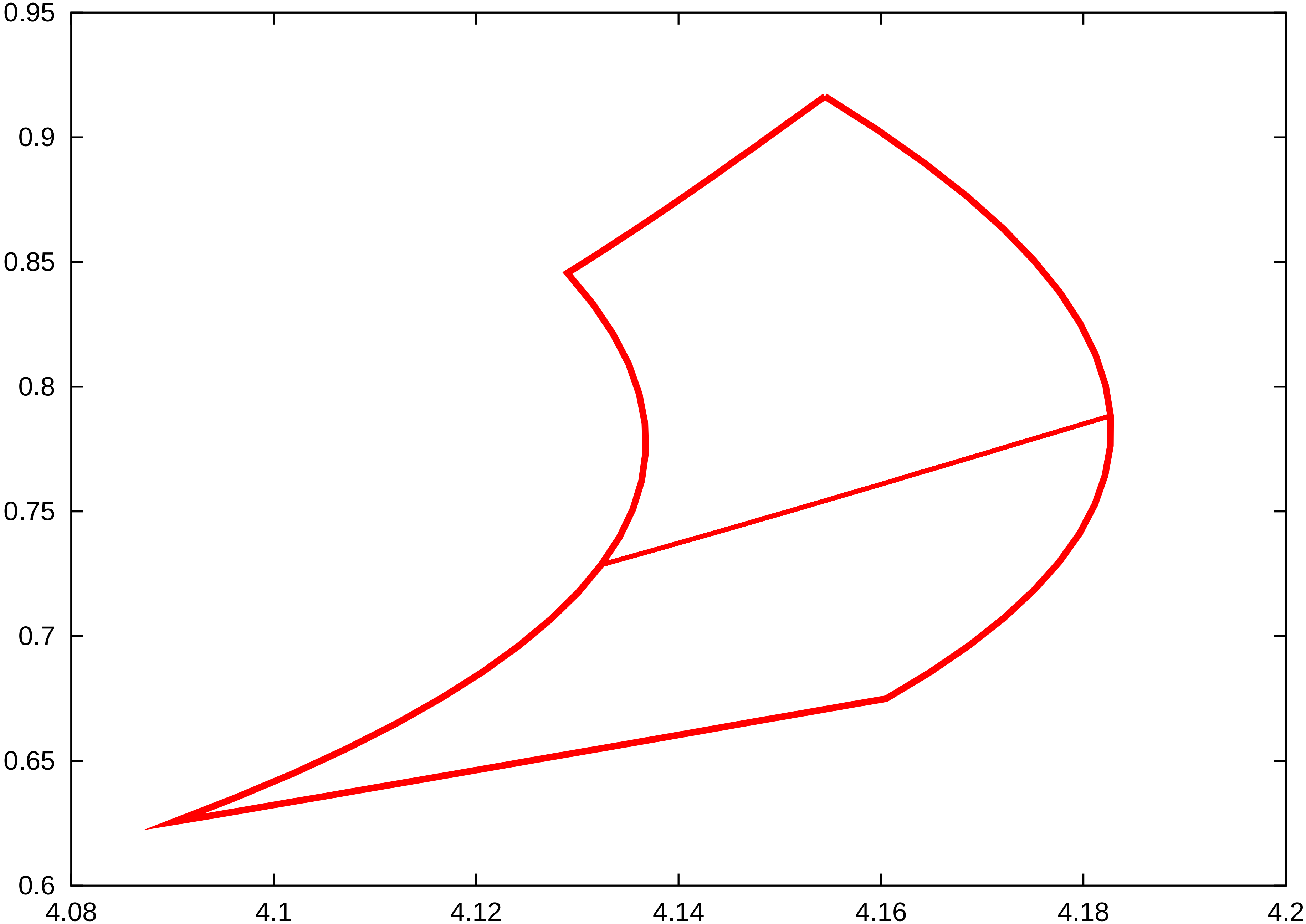
1. Evaluate ODE for $\Delta t = 0$ for current flow.
2. If resulting remainder bound $R$ greater than $\varepsilon$, split the domain along variable leading to longest axis.
3. Absorb $R$ in the TM polynomial part using the error parametrization method. If it fails, split the domain along variable leading to largest $x$ dependence of the error.
4. Put one half of the box on stack for future work.

Things to consider:

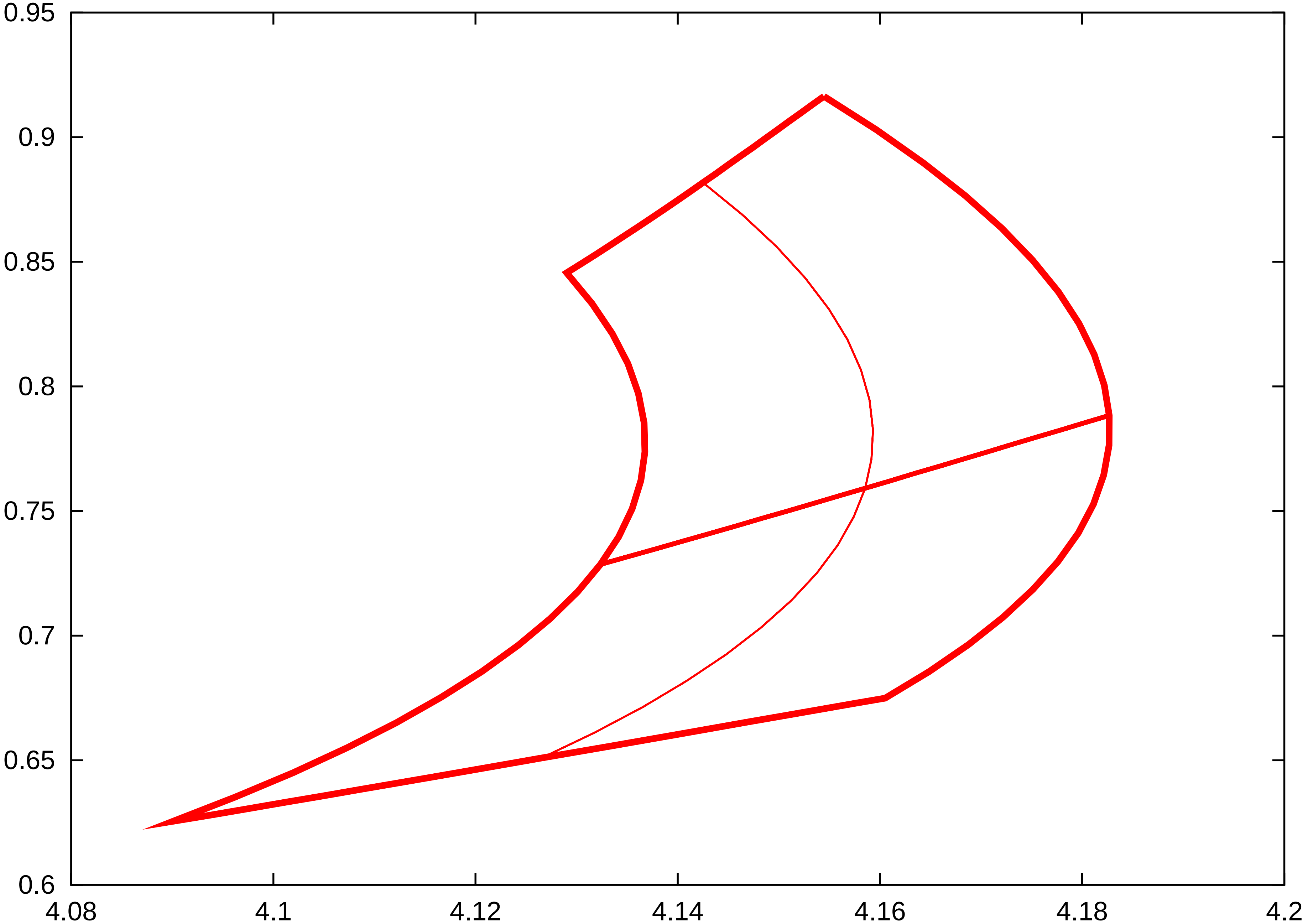
- Utilize "First-in-last-out" stack; minimizes stack length. Special adjustments for stack management in a parallel environment, including load balancing.
- Outlook: also dynamic order control for dependence on initial conditions



0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
4.08
4.1
4.12
4.14
4.16
4.18
4.2



0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
4.08
4.1
4.12
4.14
4.16
4.18
4.2


0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
4.08
4.1
4.12
4.14
4.16
4.18
4.2

## The Duffing Equation

The equation describes a damped and driven oscillator.
Exhibits sensitive dependence on initial conditions and chaoticity.

$$\ddot{x} + \delta\dot{x} + \alpha x + \beta x^3 = \gamma\cos(\omega t)$$

Example: Study

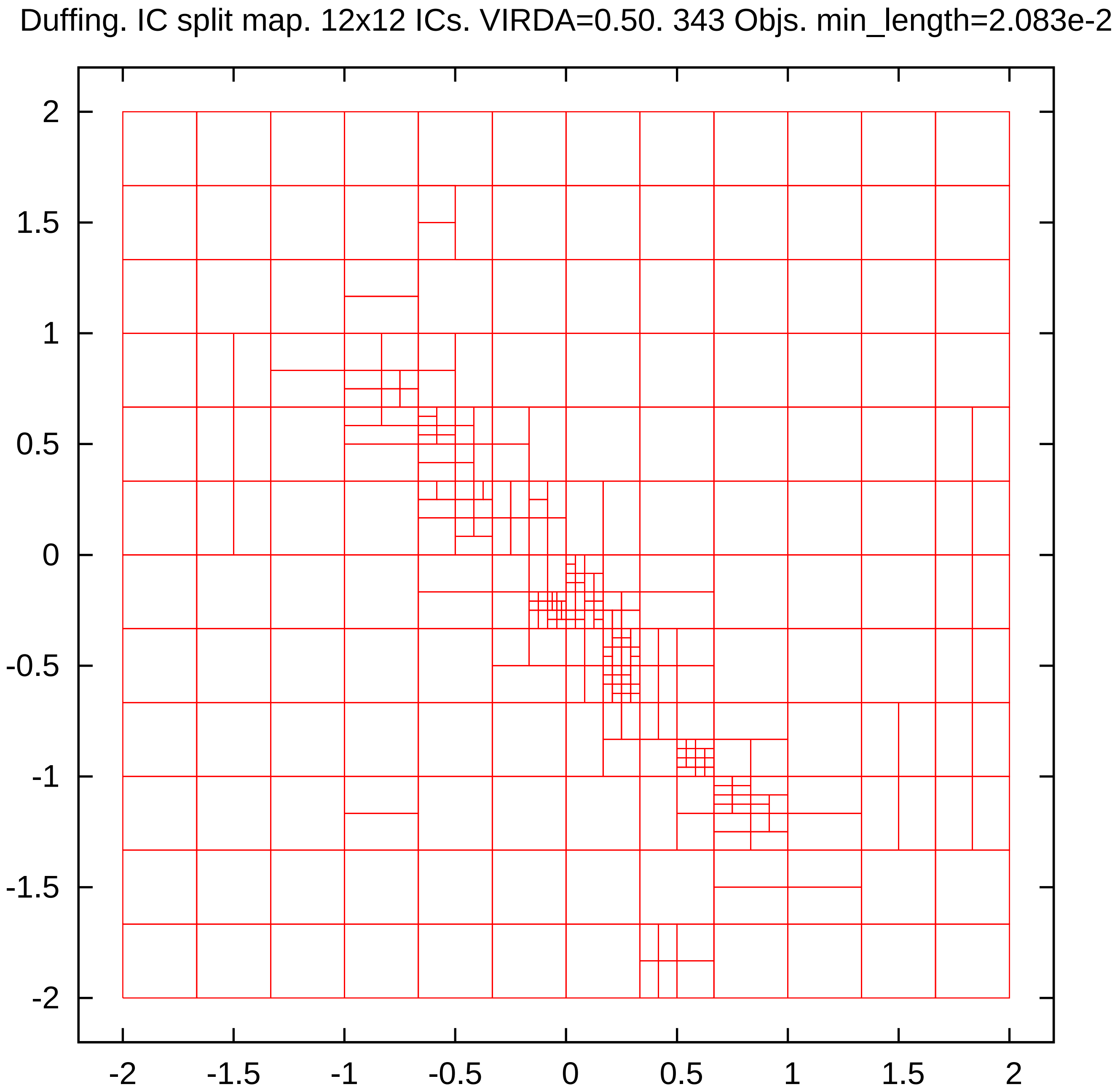
$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= x - \delta y - x^3 + \gamma\cos(t) \end{aligned}$$

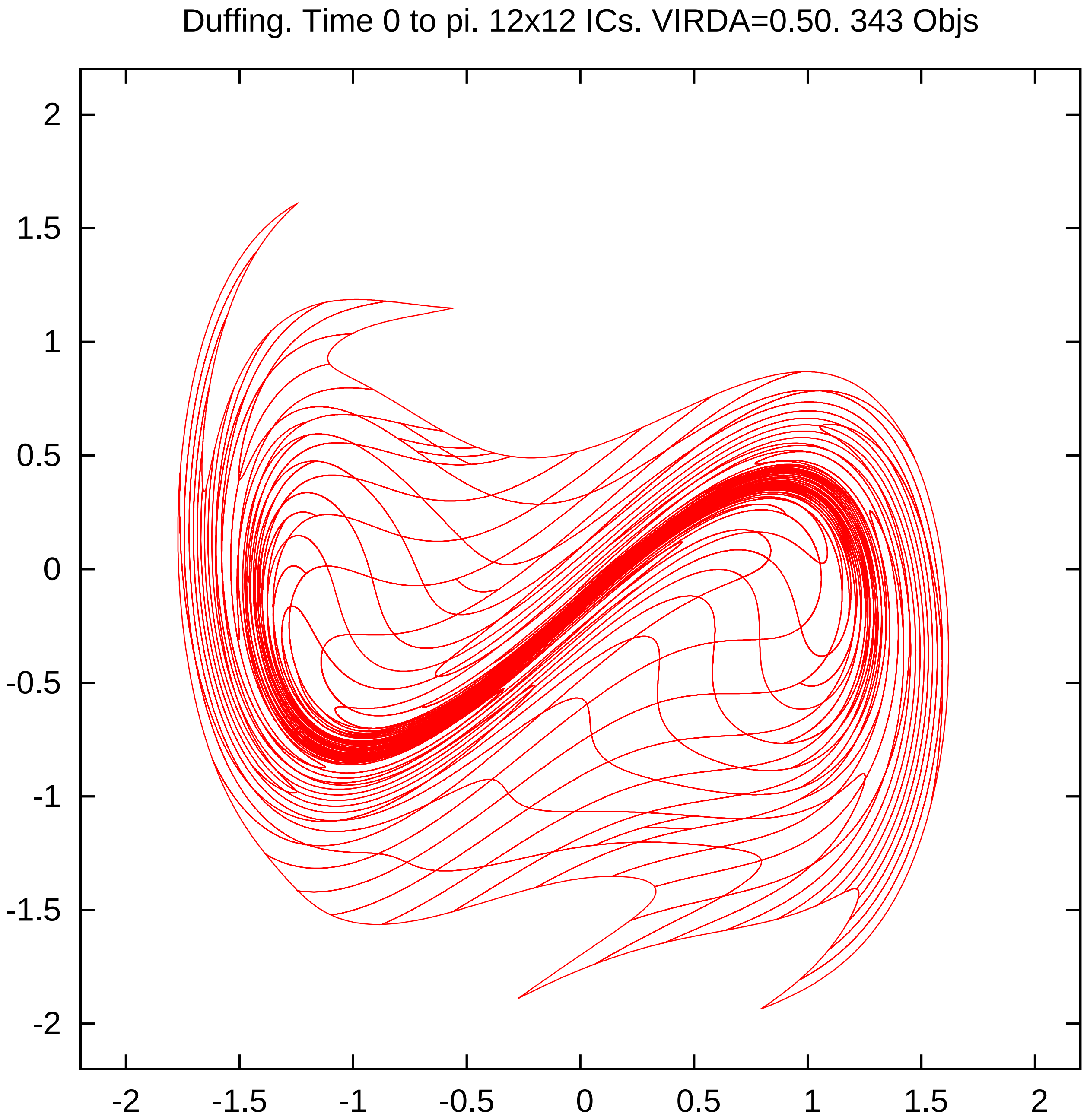
with

$$\delta = 0.25, \quad \gamma = 0.3,$$

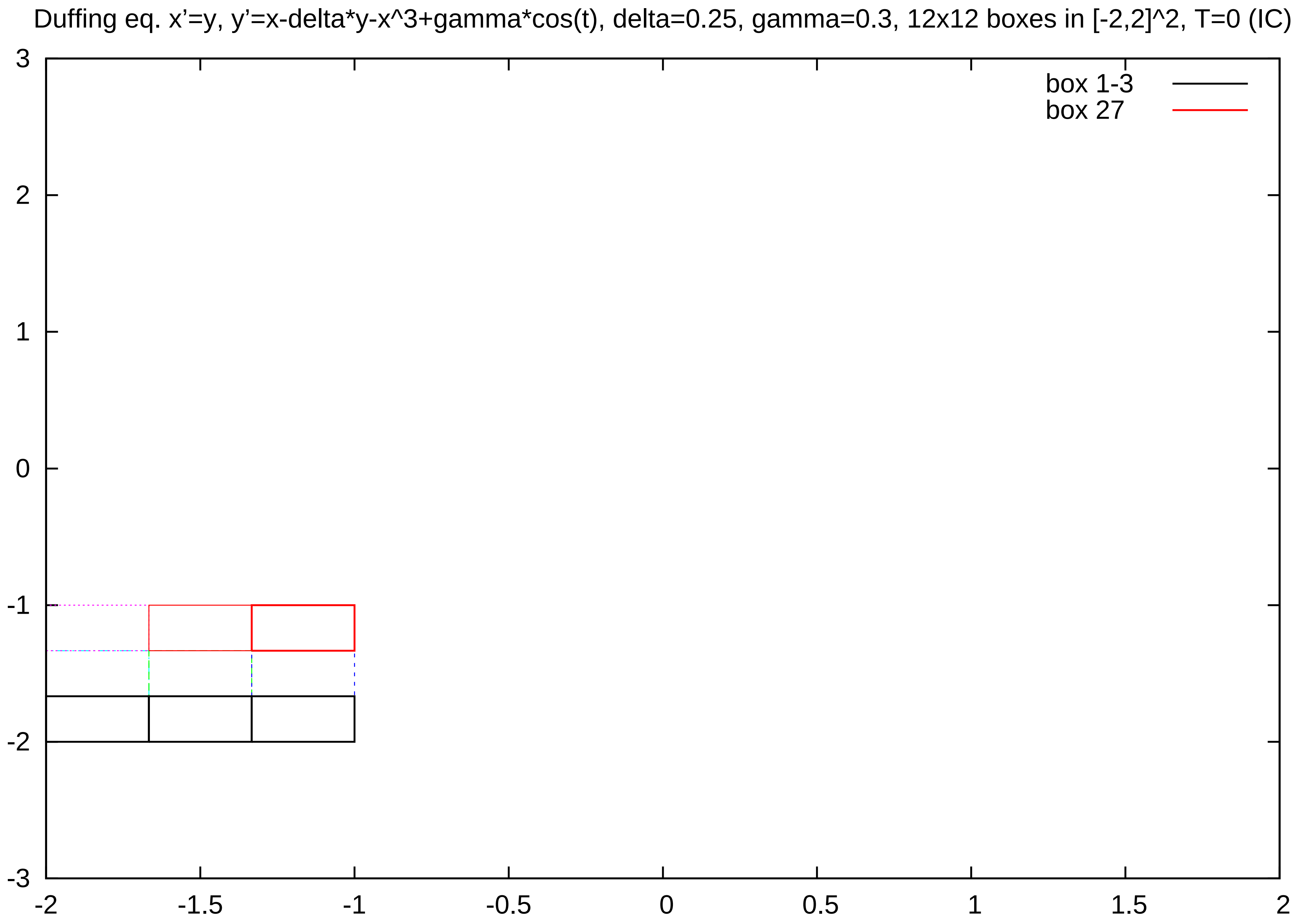
for

$$t \in [0, \pi], \quad (x, y)_{IC} \in [-2, 2] \times [-2, 2].$$


Duffing. IC split map. 12x12 ICs. VIRDA=0.50. 343 Objs. min_length=2.083e-2
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

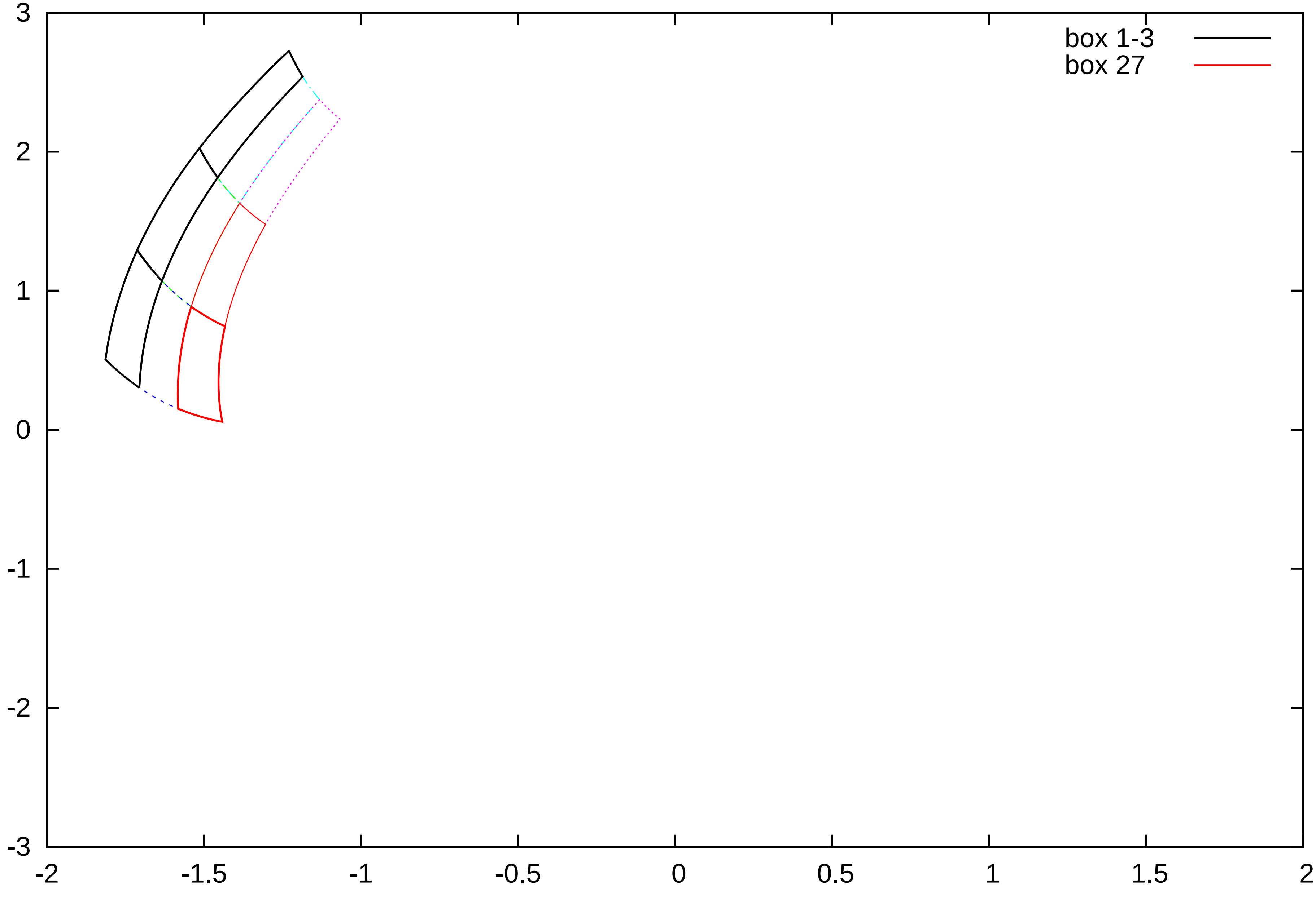


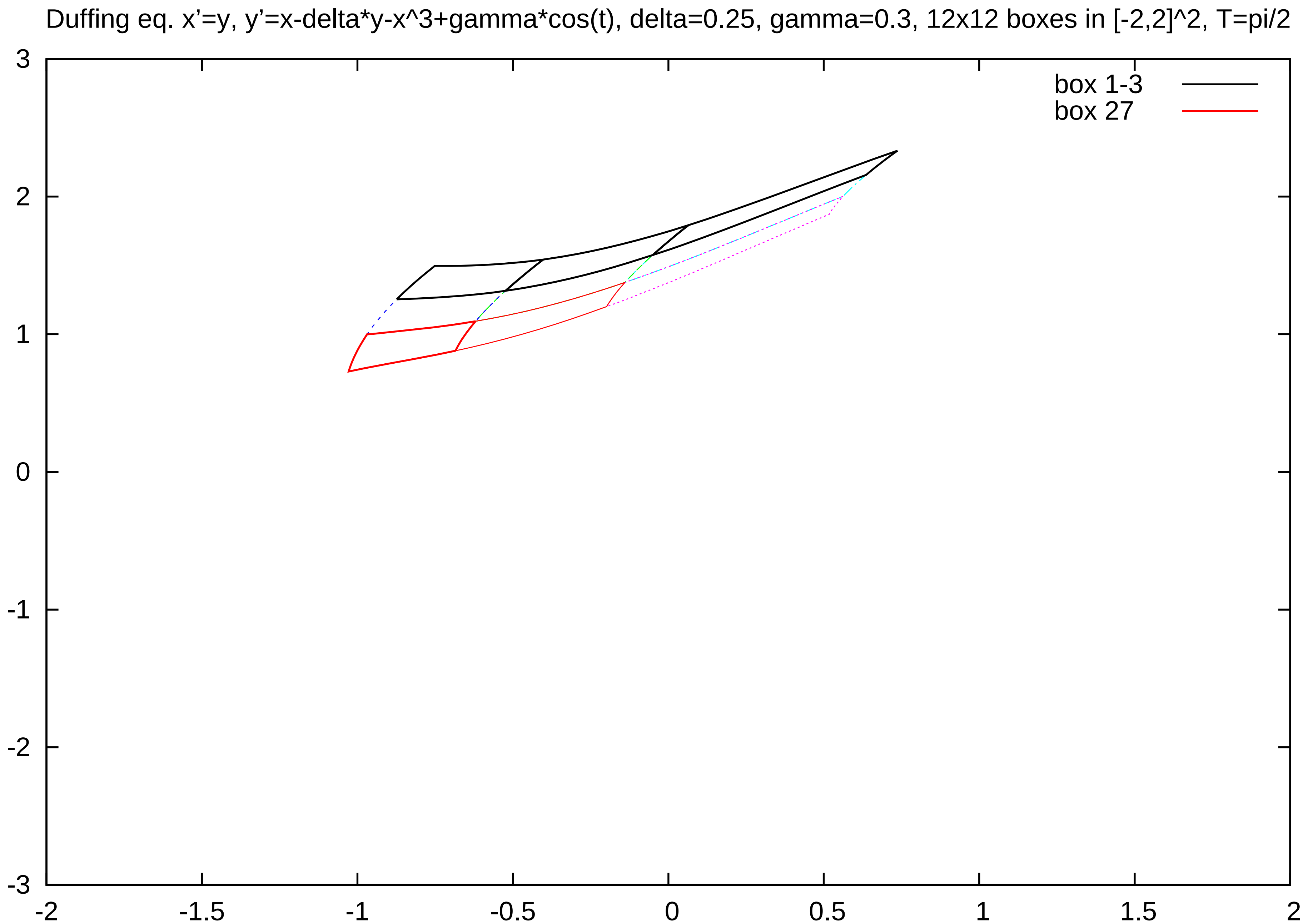
Duffing. Time 0 to pi. 12x12 ICs. VIRDA=0.50. 343 Objs
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2



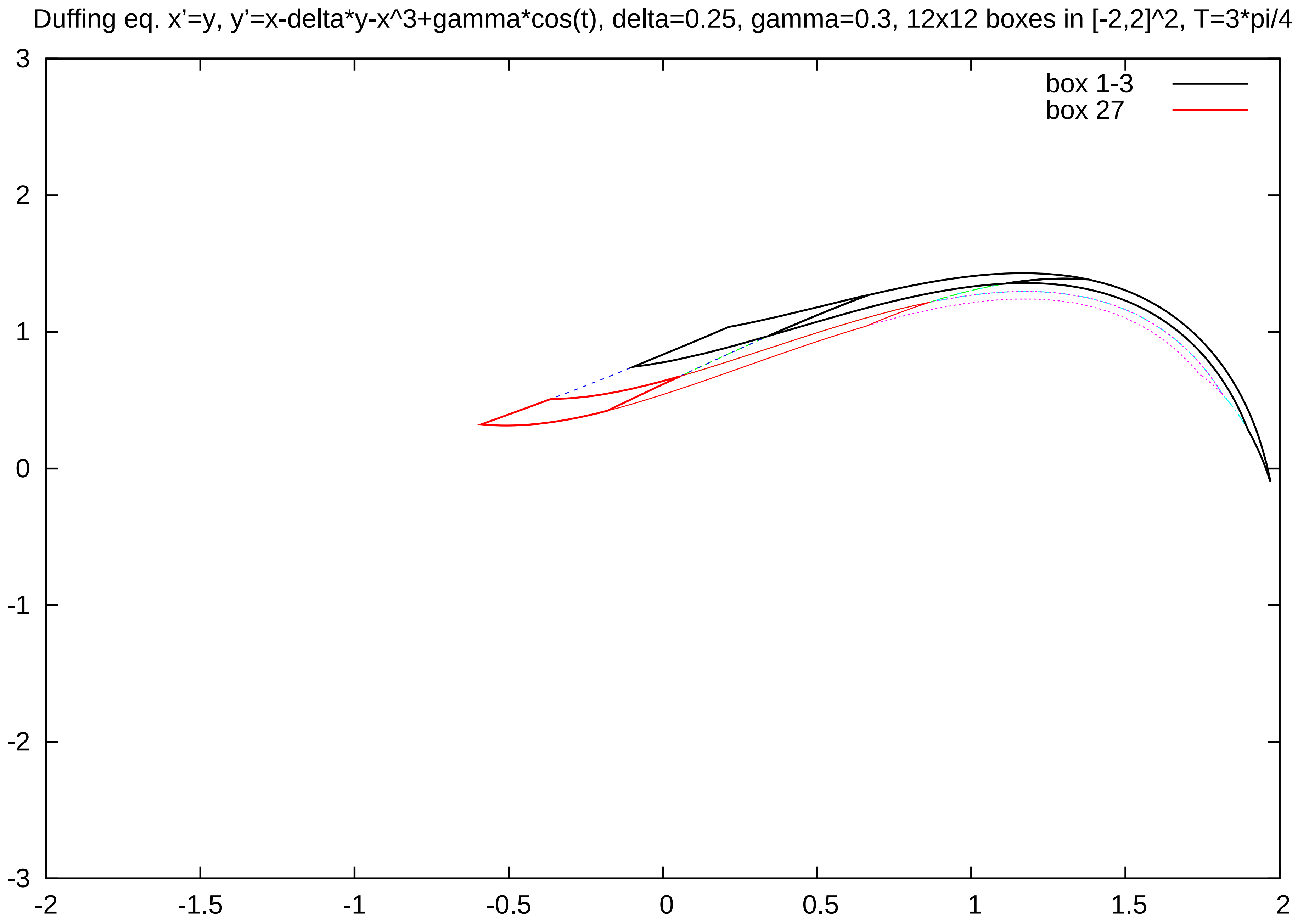
Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=0 (IC)
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=pi/4

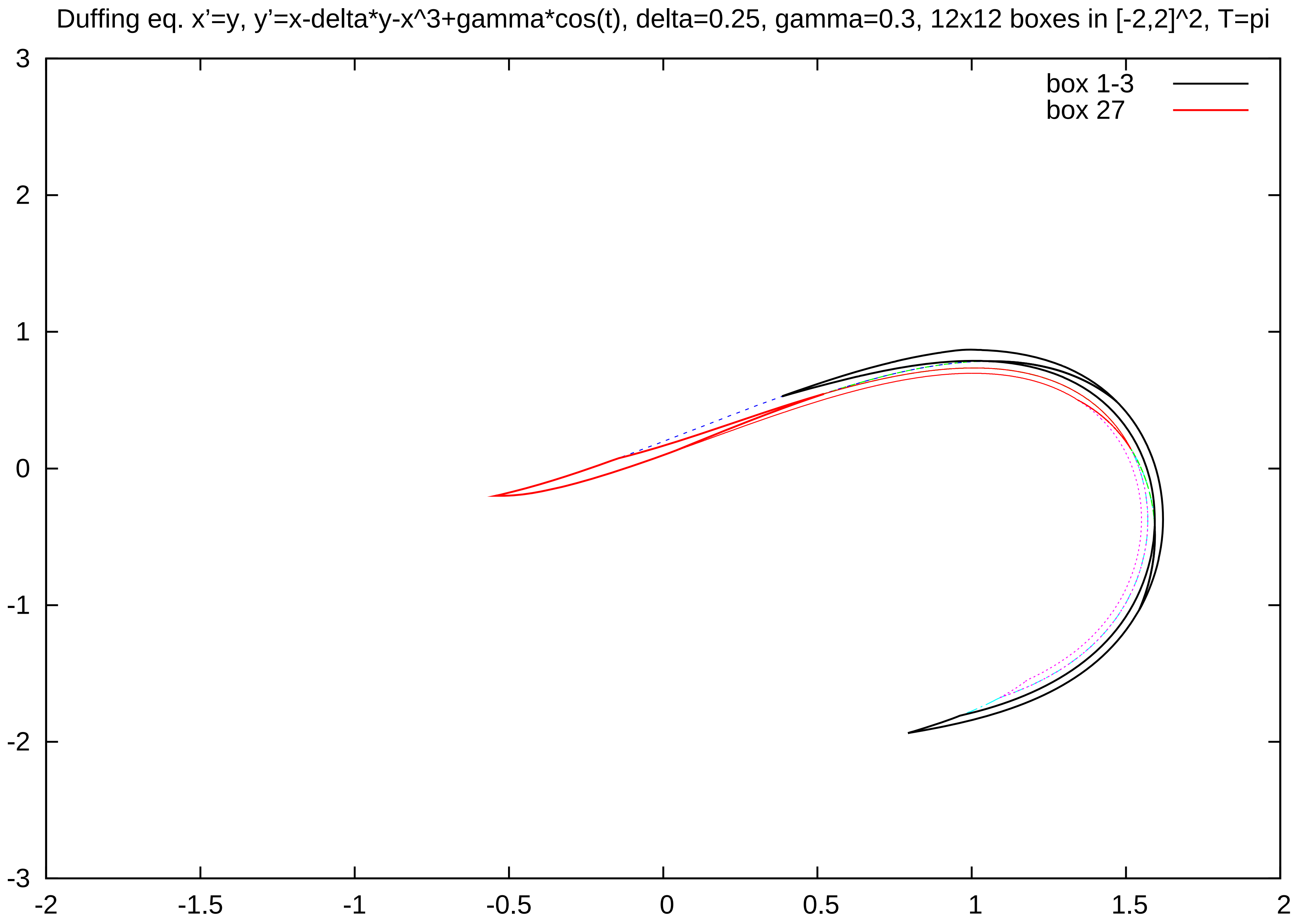




Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=pi/2
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2



Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=3*pi/4
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2



Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=pi
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

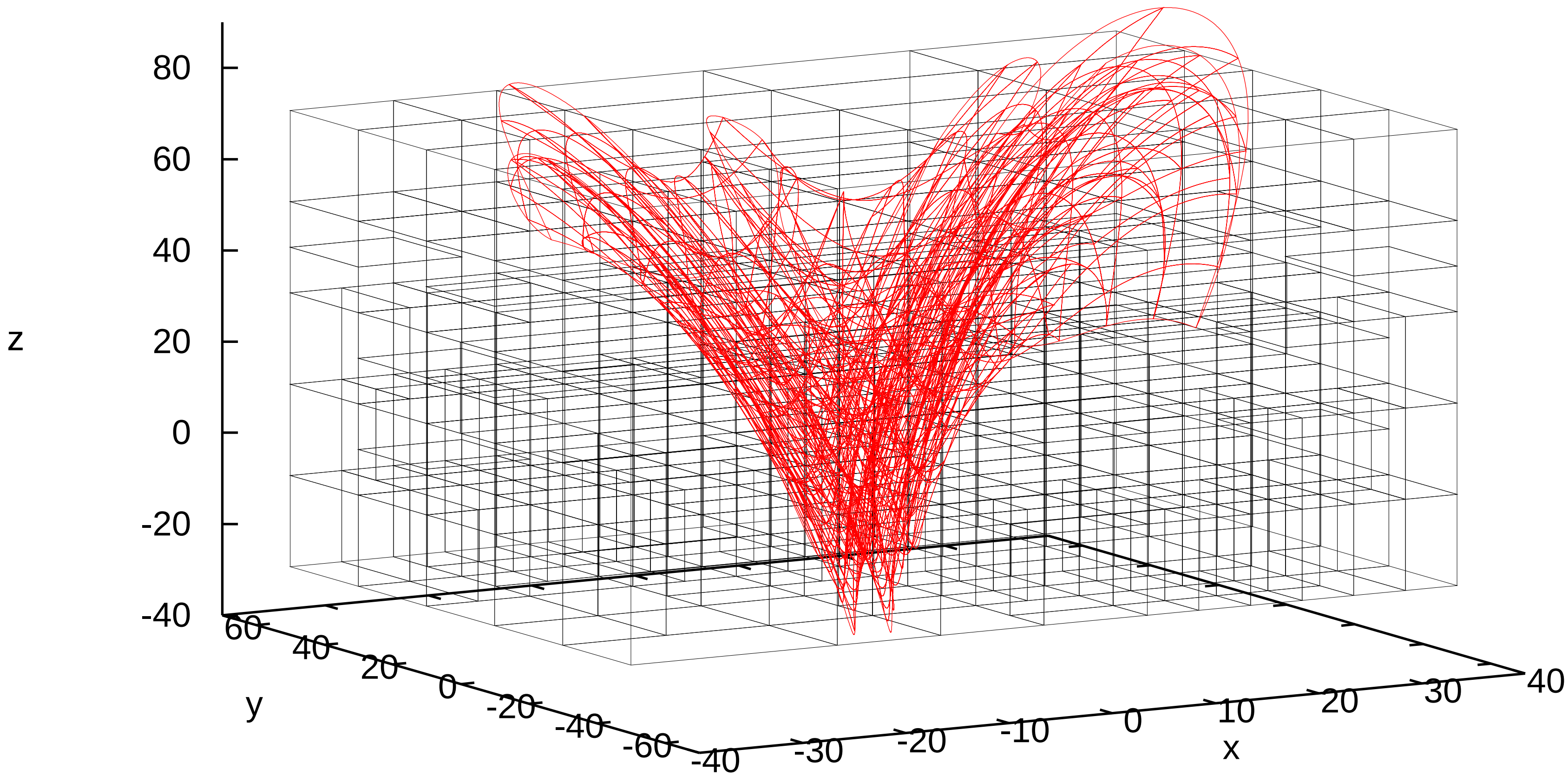
## Rigorous Integrations of the Lorenz System

Rigorous flow integrations of large ranges of initial conditions have been computed using Taylor model based ODE integrators, particularly by COSY-VI version 3.

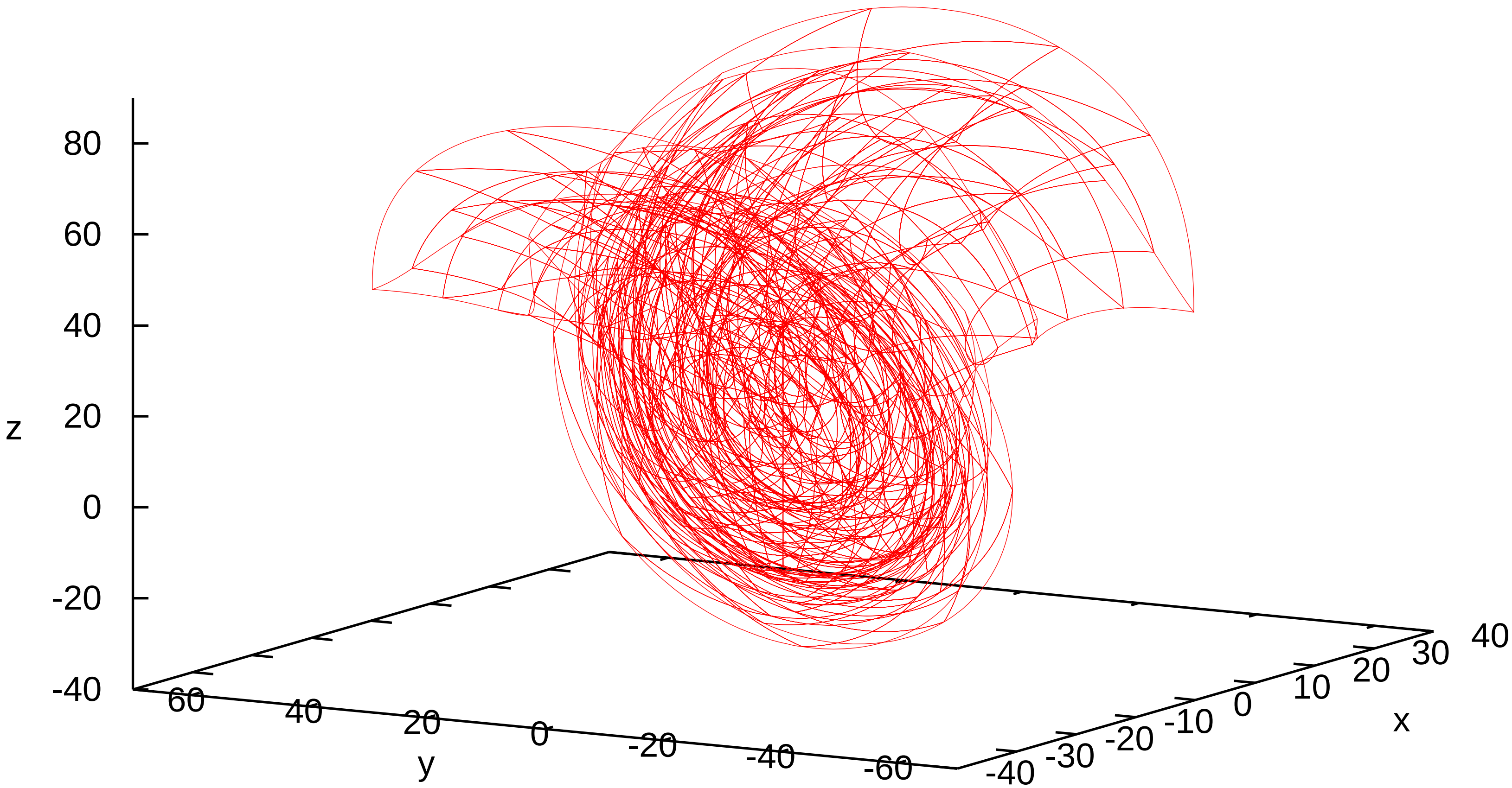
Example: Flow computations of the standard Lorenz equations for an area of initial condition

$$(x, y, z)|_0 = ([-40, 40], [-50, 50], [-25, 75])$$

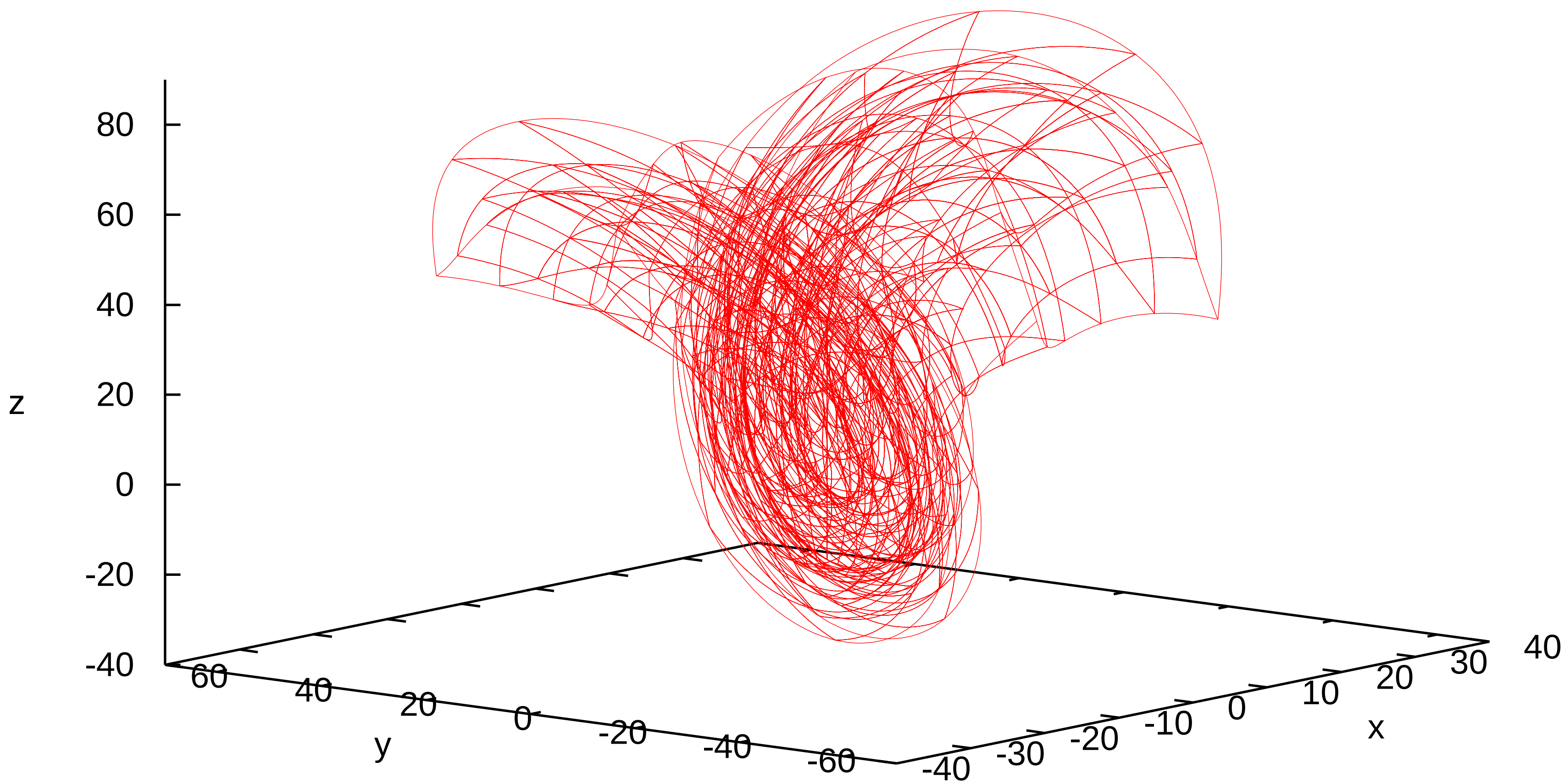
Lorenz IC:[-40,40]x[-50,50]x[-25,75] T=0.1

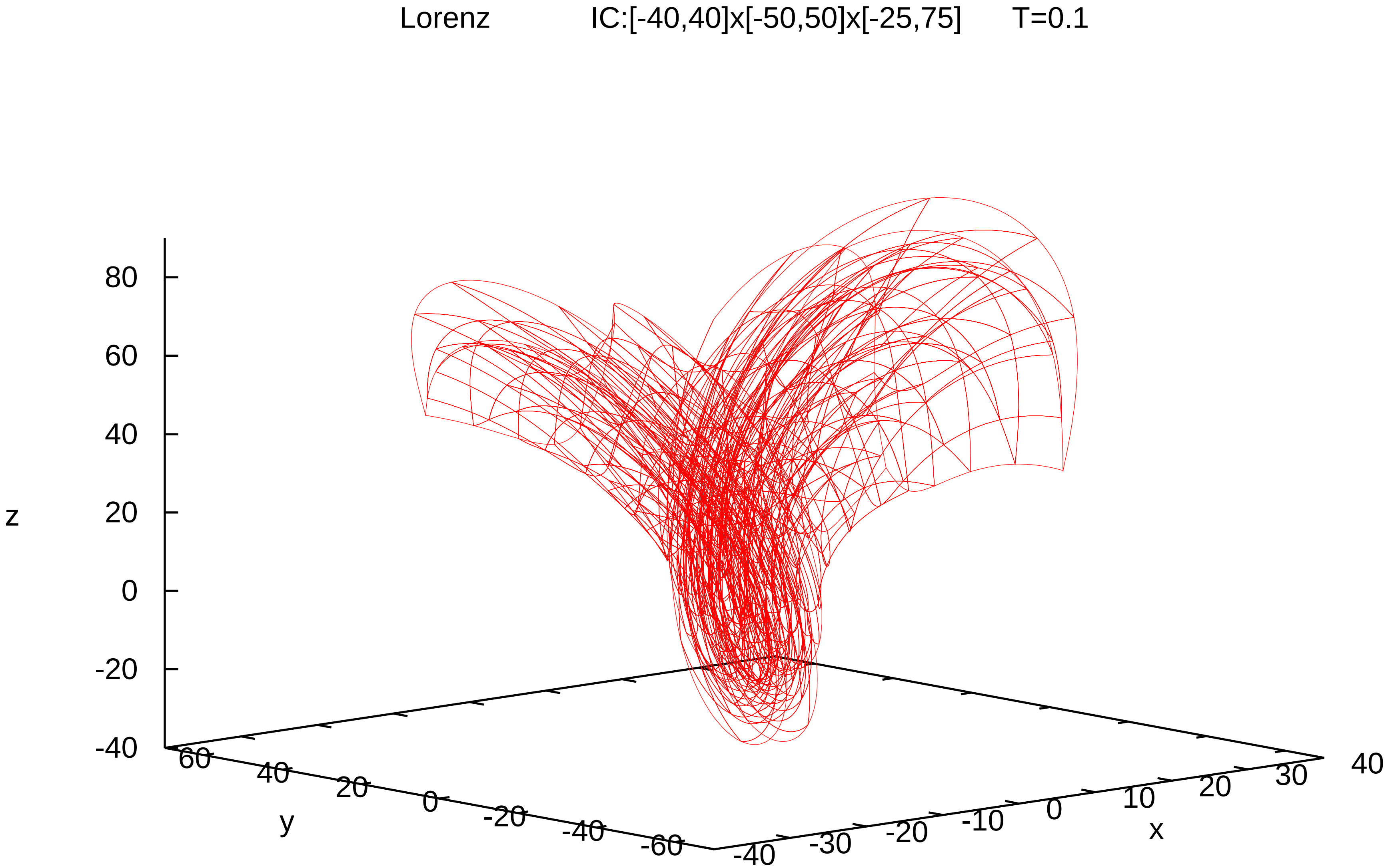


Lorenz IC:[-40,40]x[-50,50]x[-25,75] T=0.1



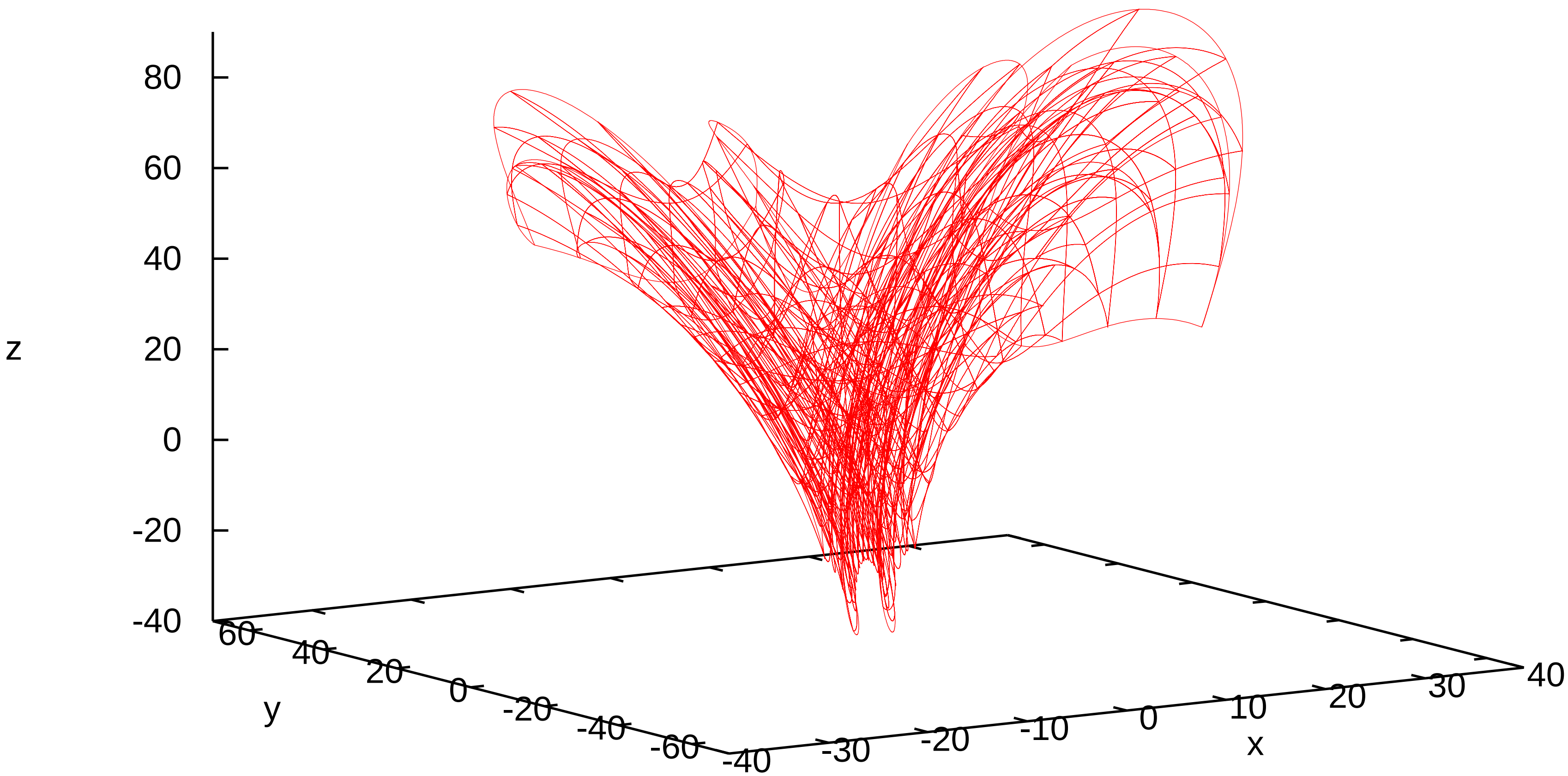
Lorenz IC:[-40,40]x[-50,50]x[-25,75] T=0.1



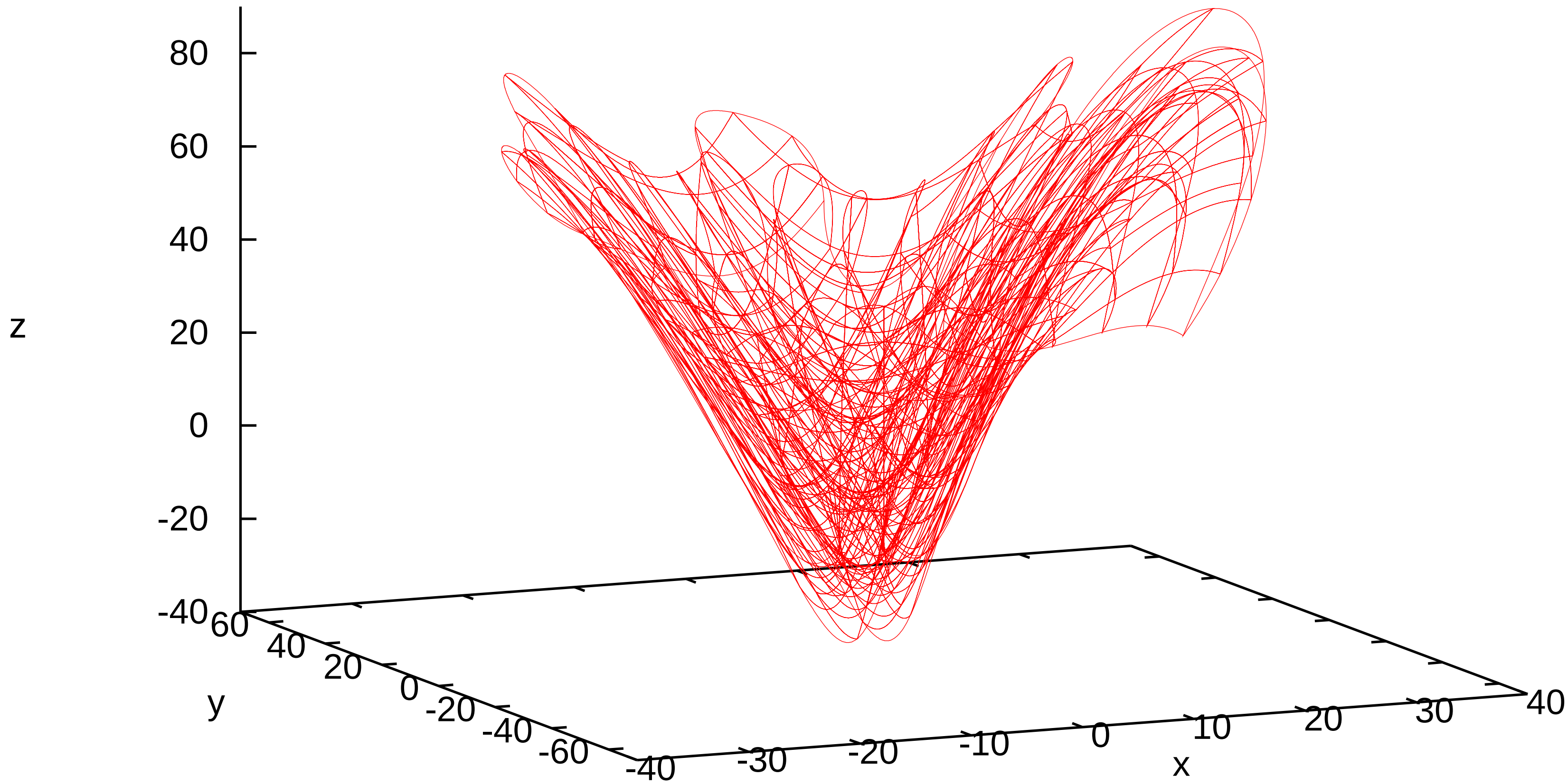


Lorenz IC:[-40,40]x[-50,50]x[-25,75] T=0.1
z
80
60
40
20
0
-20
-40
y
60
40
20
0
-20
-40
-60
x
-40
-30
-20
-10
0
10
20
30
40

Lorenz IC:[-40,40]x[-50,50]x[-25,75] T=0.1



Lorenz IC:[-40,40]x[-50,50]x[-25,75] T=0.1



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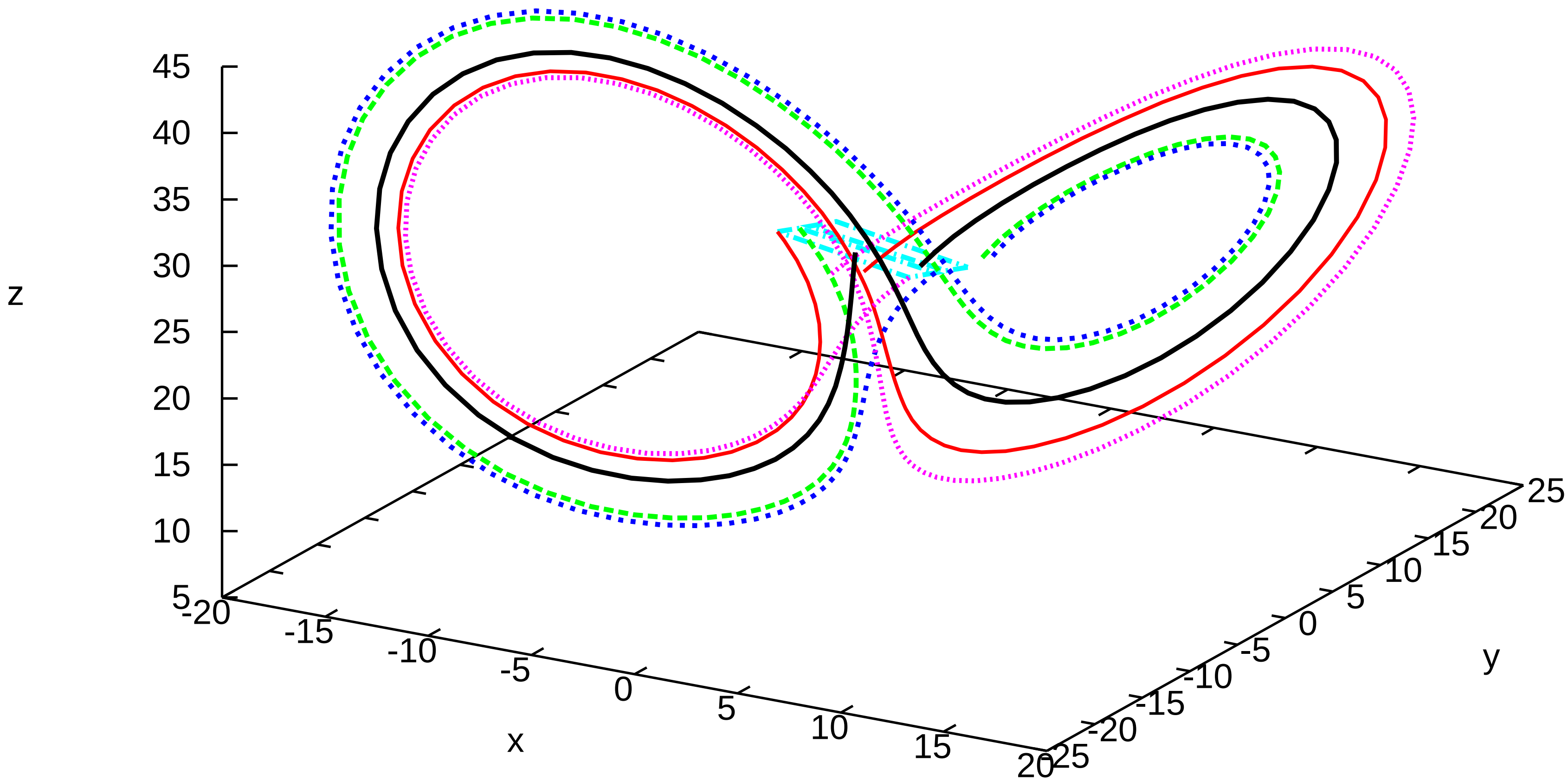
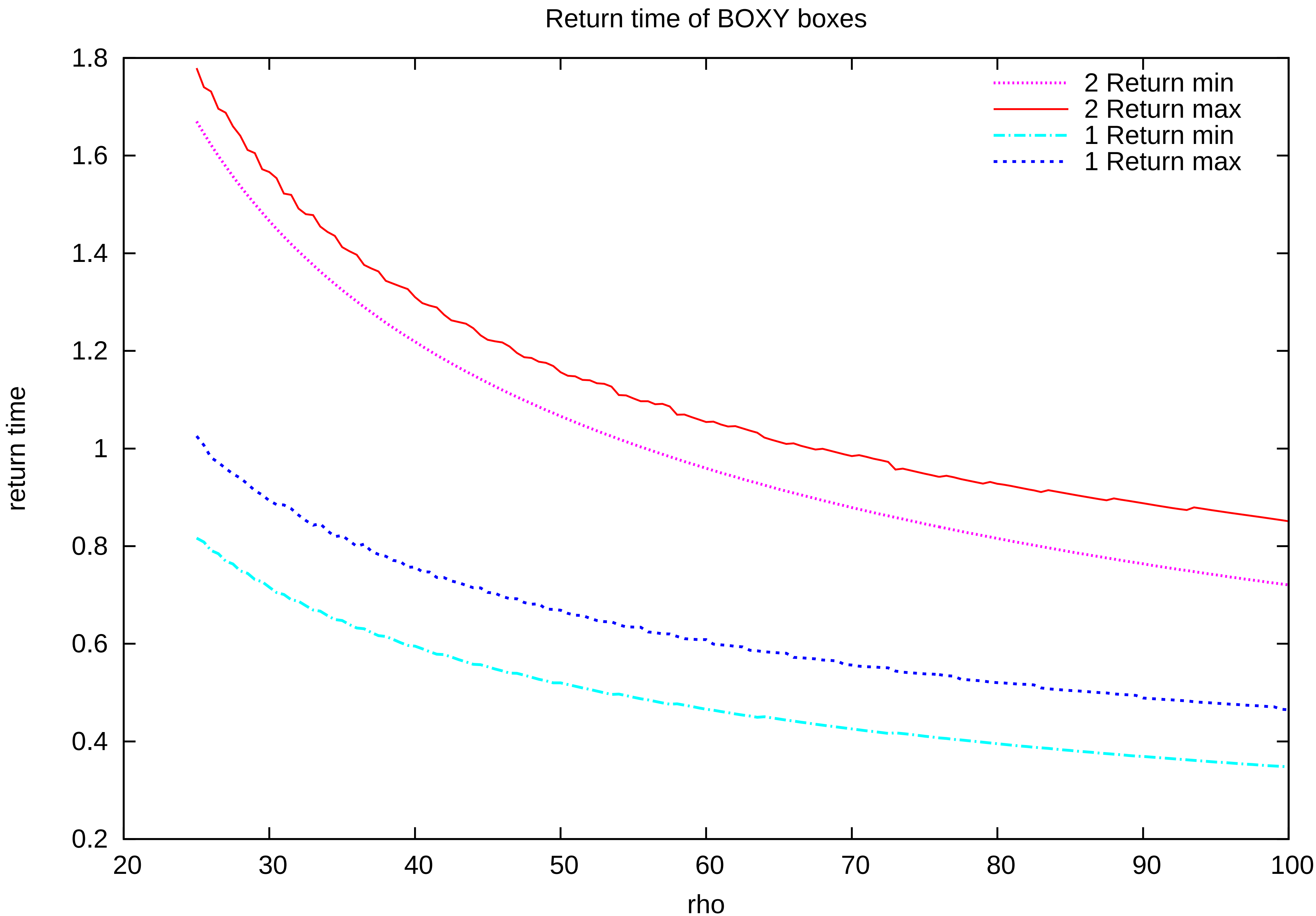
$$(x, y, z)|_0 = ([-40, 40], [-50, 50], [-25, 75])$$

Example: Rigorous mapping of the Lorenz system to study dynamics on Poincare surfaces. Particularly compute the second full return Poincare maps to the surface $z = \rho - 1$ with a wide range of $\rho$ dependence.

Lorenz, point integrations for the 2nd return to z=27 plane from the top

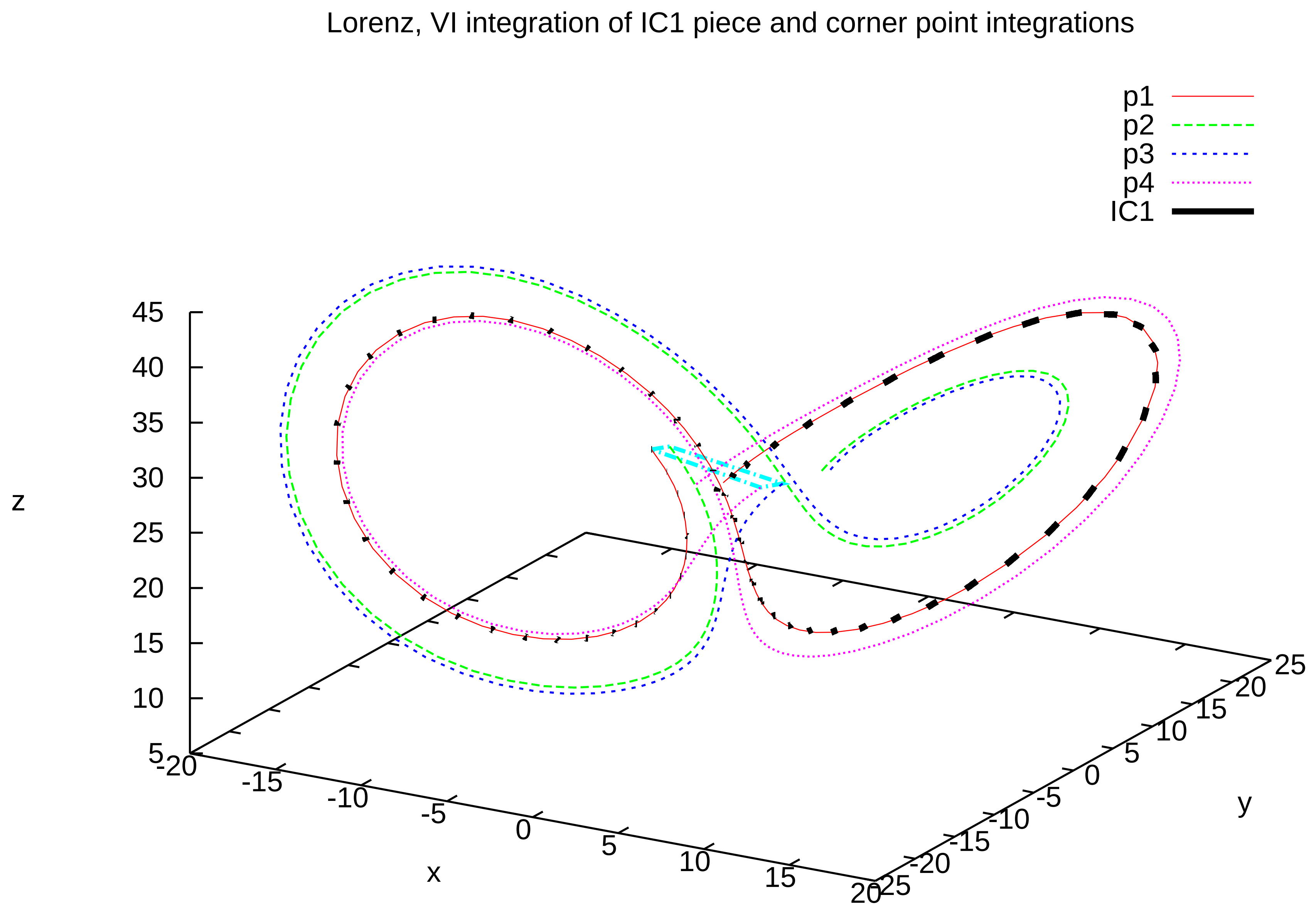



Return time of BOXY boxes
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
return time
20
30
40
50
60
70
80
90
100
rho
2 Return min
2 Return max
1 Return min
1 Return max

## Rigorous Flows and Poincare Projections

Rigorous flow computations using COSY-VI ver 3

- Integrate until an approximate return time $\tilde{t}_R$
- The last time step is arranged such that the initial Taylor models $T_i(r)$ of the time step is entirely before crossing the surface and the solution Taylor models $T_f(r)$ is entirely after crossing the surface.
- Using the explicit time dependent TM solution $T(r,t)$ of the last time step, generate the position dependent return time $t_R(r)$ as a Taylor model.
- $T(r, t_R(r))$ provides a projected solution up to the computation order; finally the small TM remainder is projected.


Lorenz, VI integration of IC1 piece and corner point integrations
p1
p2
p3
p4
IC1
z
45
40
35
30
25
20
15
10
5
x
-20
-15
-10
-5
0
5
10
15
20
y
-25
-20
-15
-10
-5
0
5
10
15
20
25

## Outlook

- Conduct Poincare projections more frequently, possibly at every time step.
- Improvement of the Taylor model arithmetic package in COSY to allow arbitrarily high precision Taylor model computations.
- Improvement of COSY-VI, associated to above and else.