Rigorous Reachability Analysis and Domain Decomposition of Taylor Models

Martin Berz and Kyoko Makino

Department of Physics and Astronomy
Michigan State University

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Verified ODE Integrations

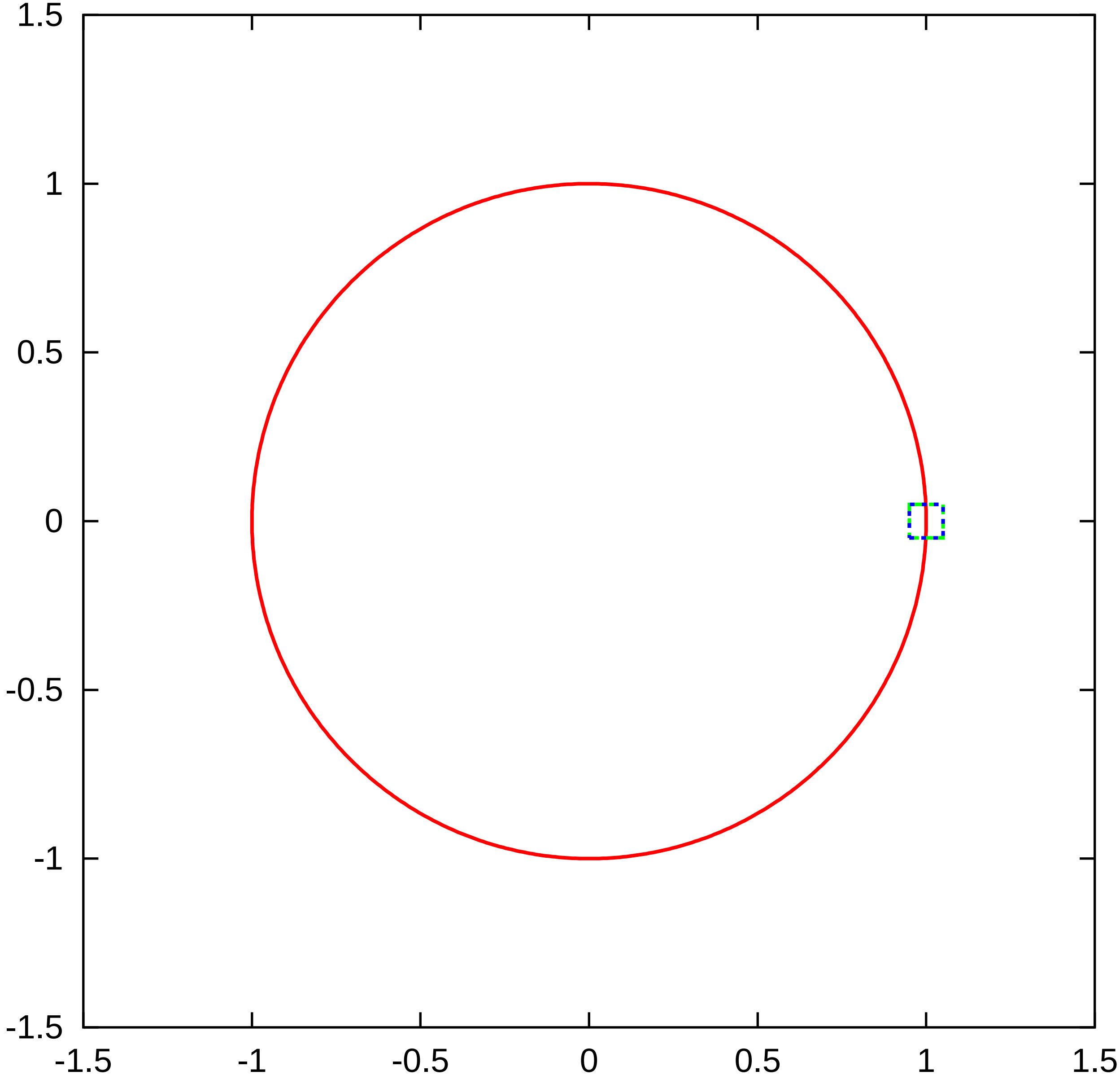
Using the interval method, typical issues in general are

- overestimation
- the dependency problem
- the dimensionality curse

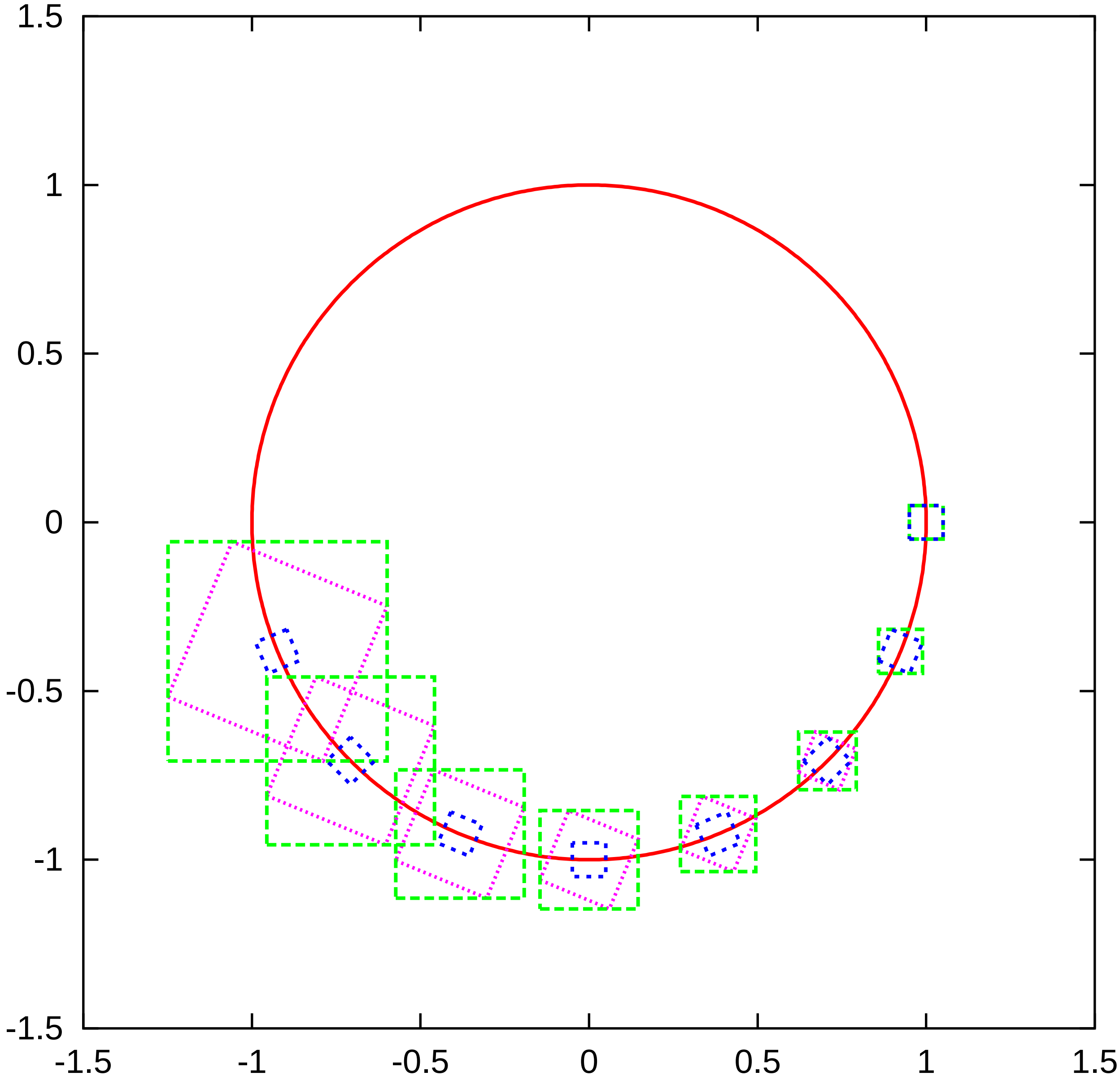
When geometric transformations of sets are involved,
such as ODE integrations, there arises an additional issue

- the wrapping effect

To transport a large phase space volume with validation,



Over Estimation has to be controlled.



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Using the interval method, typical issues in general are

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- the dependency problem
- the dimensionality curse

When geometric transformations of sets are involved, such as ODE integrations, there arises an additional issue

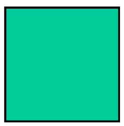
- the wrapping effect

How to handle the wrapping effect in

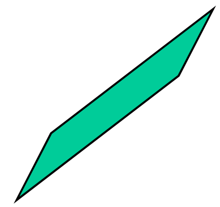
- the interval method
- the Taylor model method; $T = (P, e) = P + e$ where

$$f(x) - P(x - x_0) \in e, \quad \forall x \in D,\ x_0 \in D$$

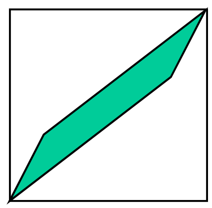
The Wrapping Effect in Linear ODEs



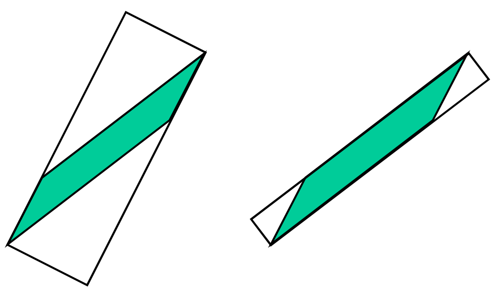
Initial Condition Interval Box



Solution Set

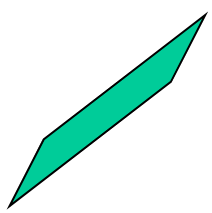


Solution Set in the Optimal Interval Box



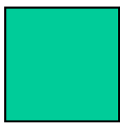
Solution Set in Rotated Rectangles

(Here, the Right One is Optimal.)

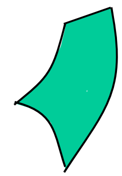


Solution Set by Taylor Models

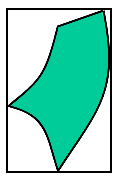
The Wrapping Effect in Nonlinear ODEs



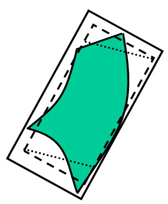
Initial Condition Interval Box



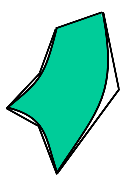
Solution Set



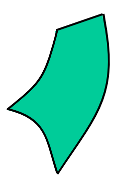
Solution Set in the Optimal Interval Box



Solution Set in an Optimal Rotated Rectangle



Solution Set in an Optimal Eight-Corner Polygon



Solution Set by Taylor Models

ODE Integration with Taylor Models

Idea: retain full **dependence on initial conditions** as Taylor model (Non-verified version: big breakthrough in particle optics and beam physics, 1984 - allows to calculate "aberrations" to any order, from earlier order three)

1. Different from other validated methods, the approach is **single step** - no need for a separate coarse enclosure and subsequent verification step
2. Error due to **time stepping** is $O(n_t + 1)$
3. Error due to **initial variables** is $O(n_v + 1)$, **not** $O(2)$ as in other methods
4. By choosing n_t and n_v appropriately, the error due to finite domain and time stepping can be made **arbitrarily small.**
5. Overall, **never** leave the TM represenation until possibly the very end. Doing so may remove higher order dependence.

Refer to the references in the proceedings paper.

The Volterra Equation

Describe dynamics of two conflicting populations

$$\frac{dx_1}{dt} = 2x_1(1 - x_2), \quad \frac{dx_2}{dt} = -x_2(1 - x_1)$$

Interested in initial condition

$$x_{01} \in 1 + [-0.05, 0.05], \quad x_{02} \in 3 + [-0.05, 0.05] \quad \text{at } t = 0.$$

Satisfies constraint condition

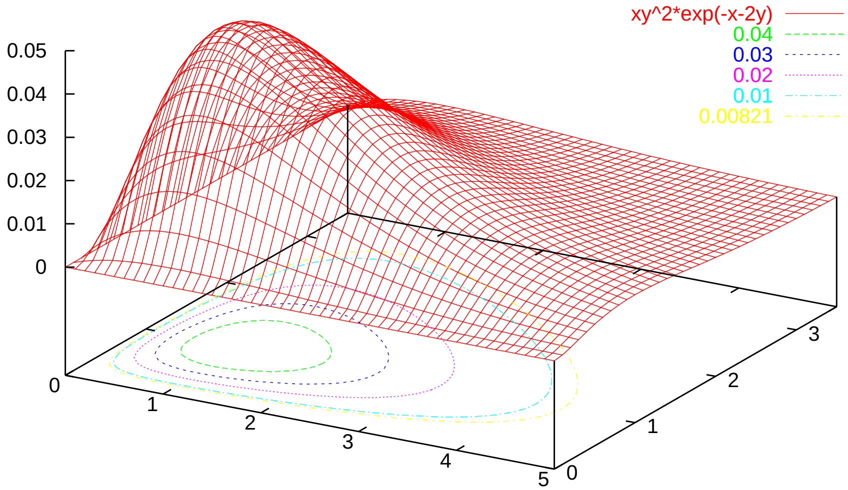
$$C(x_1, x_2) = x_1 x_2^2 e^{-x_1 - 2x_2} = \text{Constant}$$

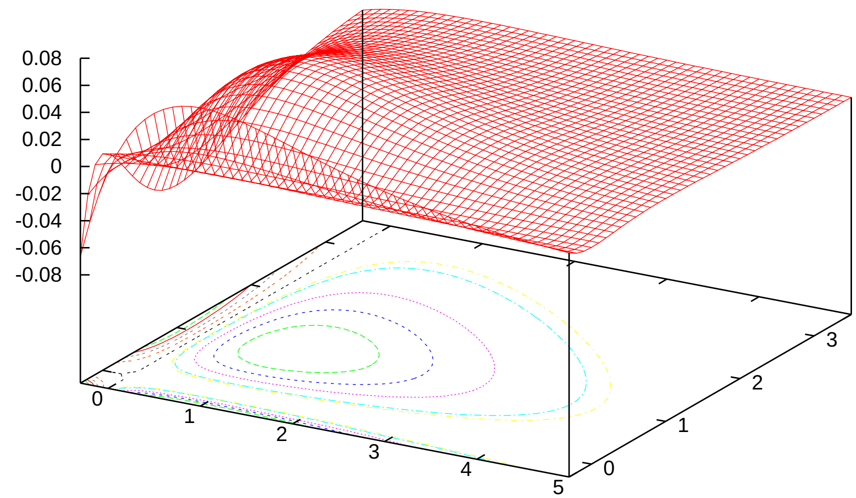
Trajectories of the Volterra Equations

The solutions have to satisfy the constraint

$$C(x_1, x_2) = x_1 x_2^2 e^{-x_1 - 2x_2} = \text{constant},$$

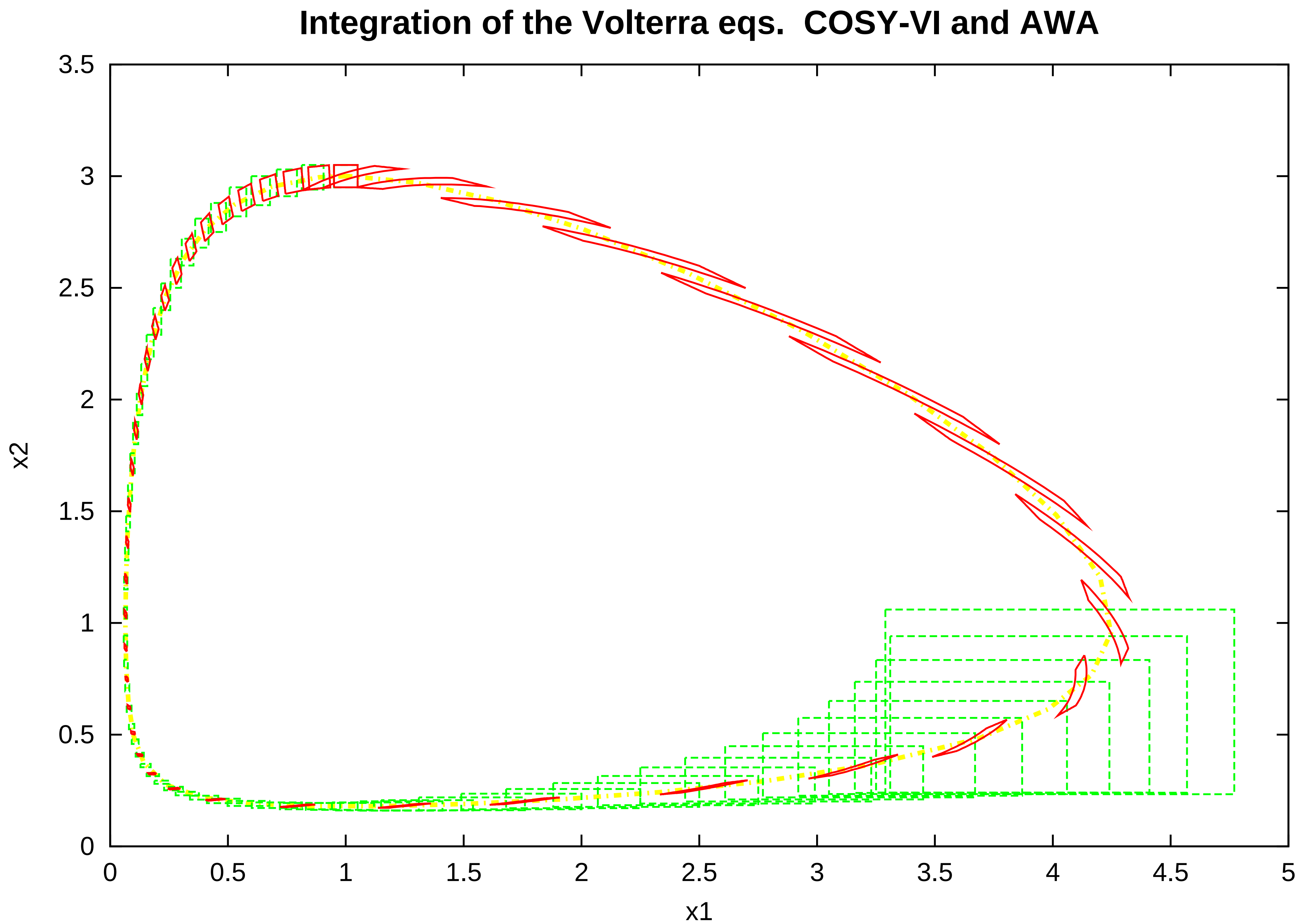
so the trajectories follow the contour lines of $C(x_1, x_2)$.

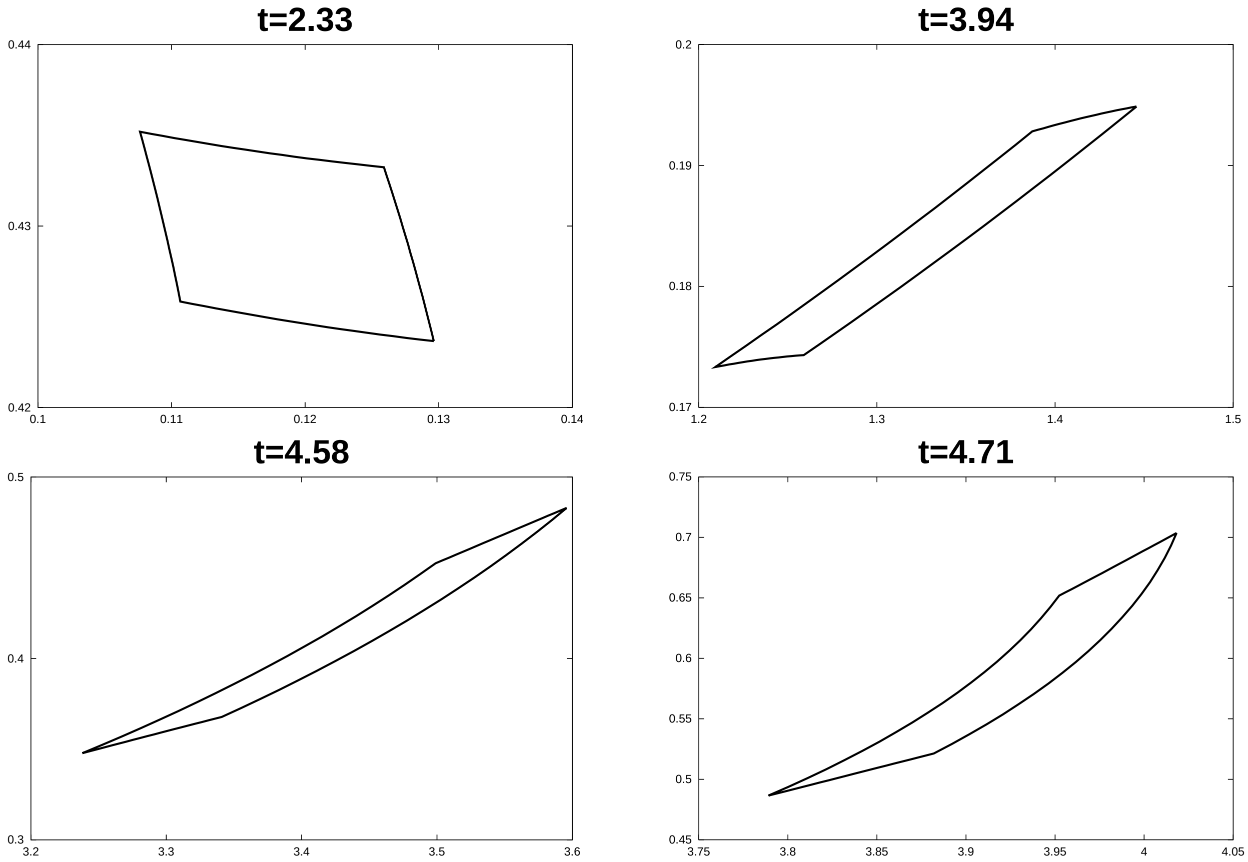


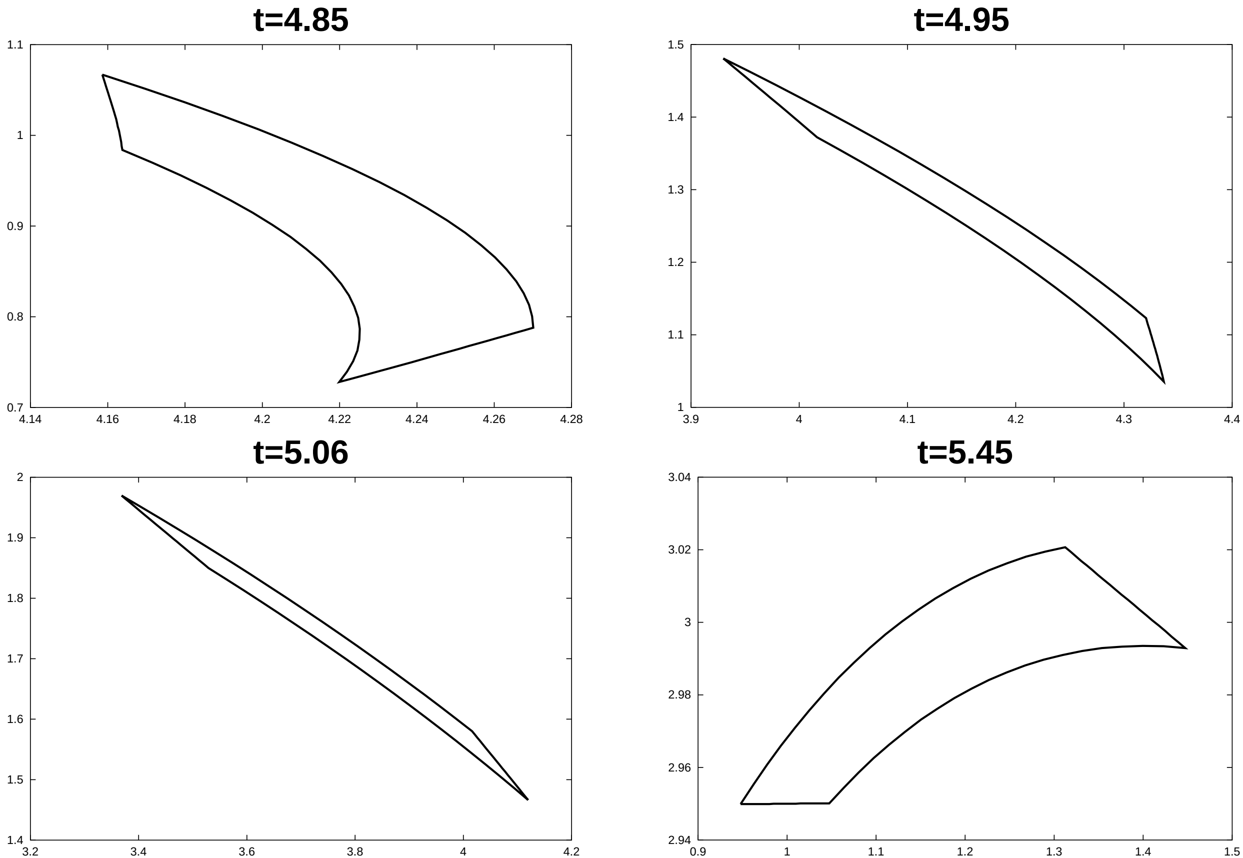


$0 \le x_1 \le 5, \quad 0 \le x_2 \le 3.5.$ $\qquad -0.3 \le x_1 \le 5, \quad -0.3 \le x_2 \le 3.5.$

In the positive quadrant (Left), the trajectories form closed orbits. However, it's not the case in the other quadrants (Right).


Integration of the Volterra eqs. COSY-VI and AWA
x2
3.5
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
x1


t=2.33
0.44
0.43
0.42
0.1
0.11
0.12
0.13
0.14
t=3.94
0.2
0.19
0.18
0.17
1.2
1.3
1.4
1.5
t=4.58
0.5
0.4
0.3
3.2
3.3
3.4
3.5
3.6
t=4.71
0.75
0.7
0.65
0.6
0.55
0.5
0.45
3.75
3.8
3.85
3.9
3.95
4
4.05


t=4.85
1.1
1
0.9
0.8
0.7
4.14
4.16
4.18
4.2
4.22
4.24
4.26
4.28
t=4.95
1.5
1.4
1.3
1.2
1.1
1
3.9
4
4.1
4.2
4.3
4.4
t=5.06
2
1.9
1.8
1.7
1.6
1.5
1.4
3.2
3.4
3.6
3.8
4
4.2
t=5.45
3.04
3.02
3
2.98
2.96
2.94
0.9
1
1.1
1.2
1.3
1.4
1.5

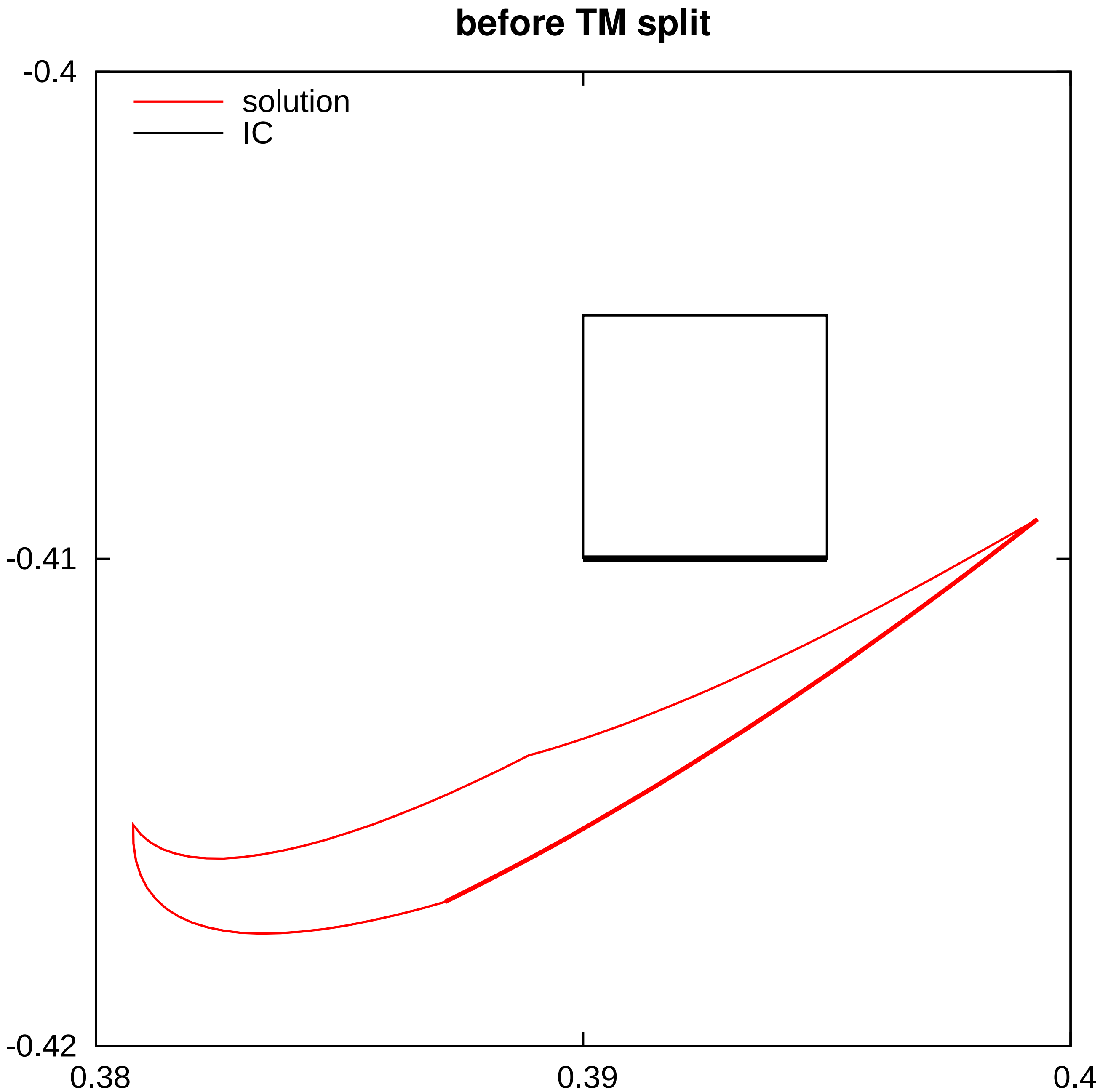
Dynamic Domain Decomposition

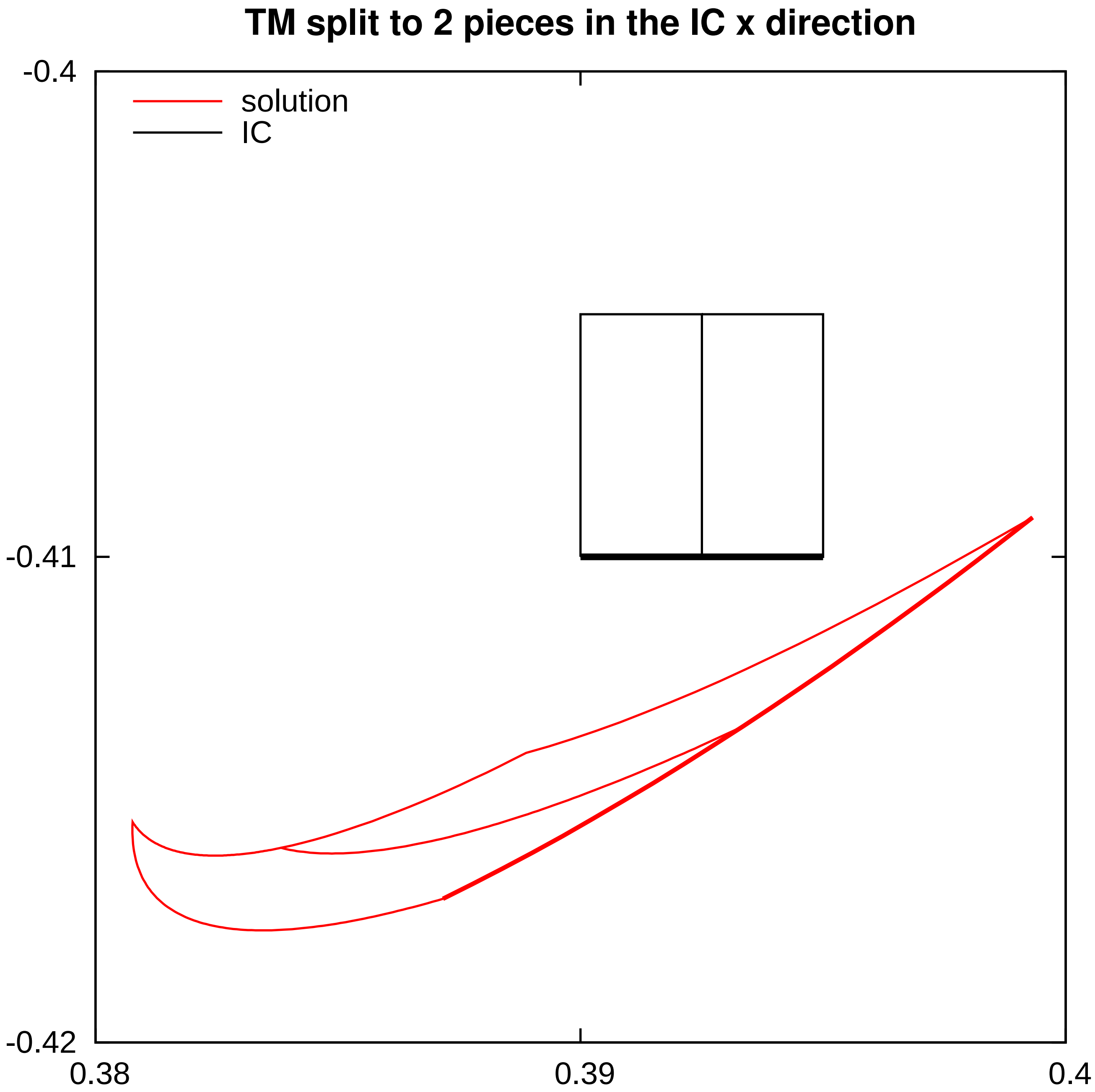
For extended domains, this is **natural equivalent** to step size control. Similarity to what's done in global optimization.

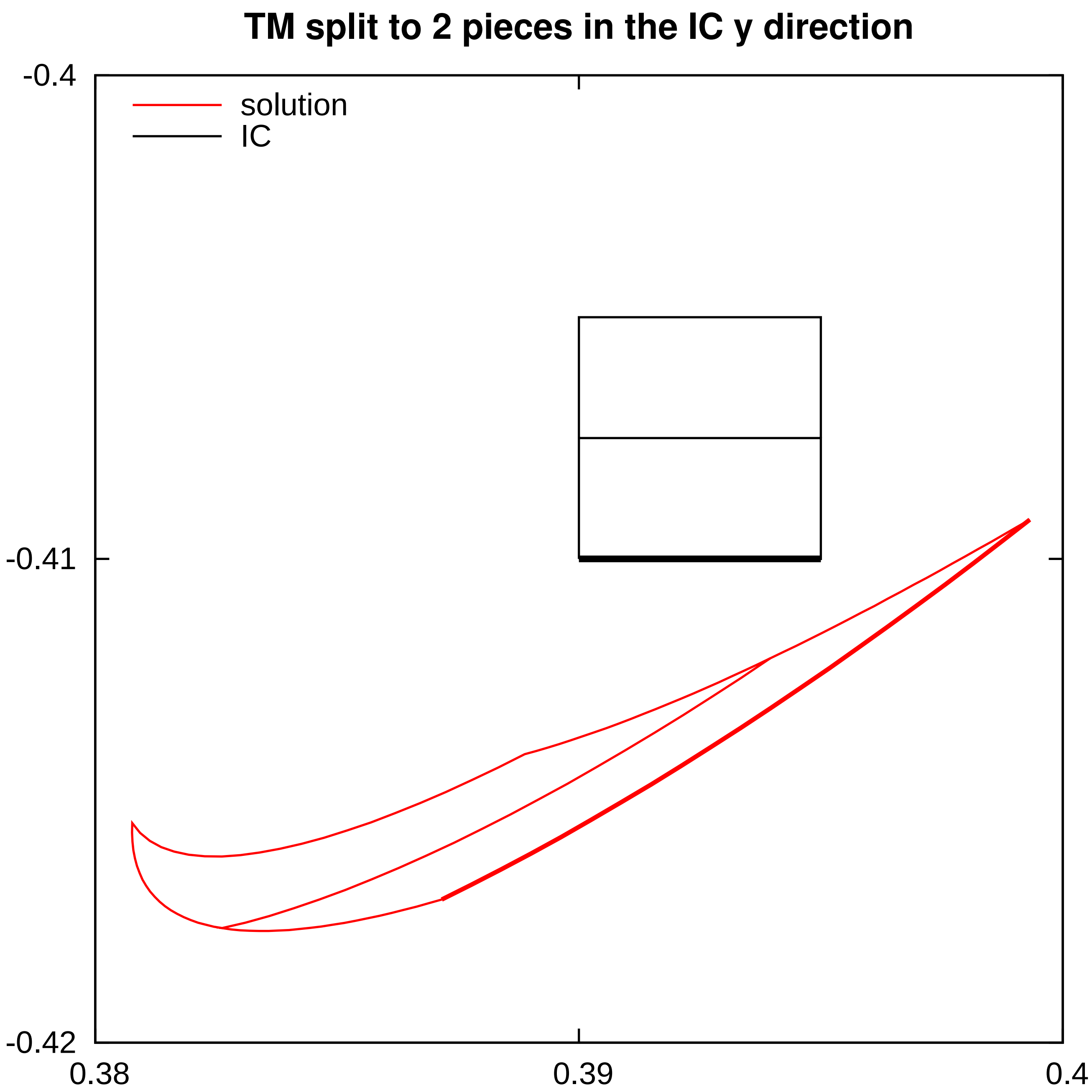
1. Evaluate ODE for $\Delta t = 0$ for current flow.
2. If resulting remainder bound R greater than ε, split the domain along variable leading to longest axis.
3. Absorb R in the TM polynomial part using the error parametrization method. If it fails, split the domain along variable leading to largest 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


before TM split
solution
IC
-0.4
-0.41
-0.42
0.38
0.39
0.4


TM split to 2 pieces in the IC x direction
solution
IC
-0.4
-0.41
-0.42
0.38
0.39
0.4


TM split to 2 pieces in the IC y direction
solution
IC
-0.4
-0.41
-0.42
0.38
0.39
0.4

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The solutions have to satisfy the constraint

$$C(x_1, x_2) = x_1 x_2^2 e^{-x_1 - 2x_2} = \text{constant},$$

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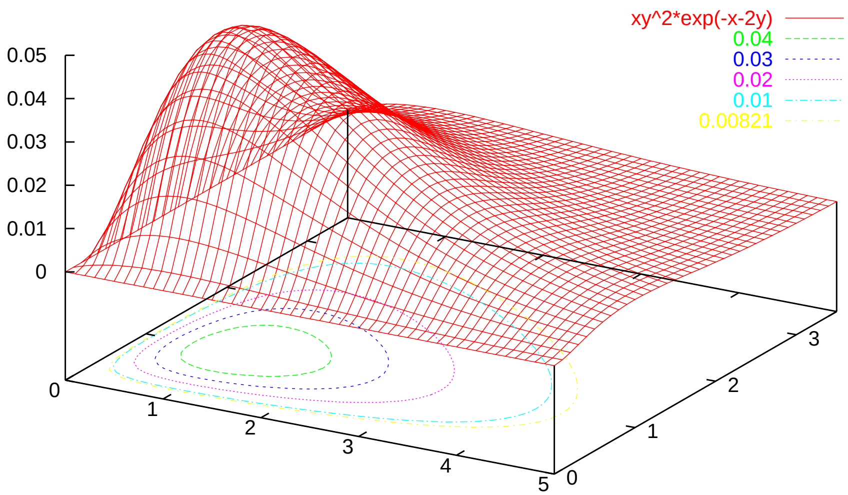

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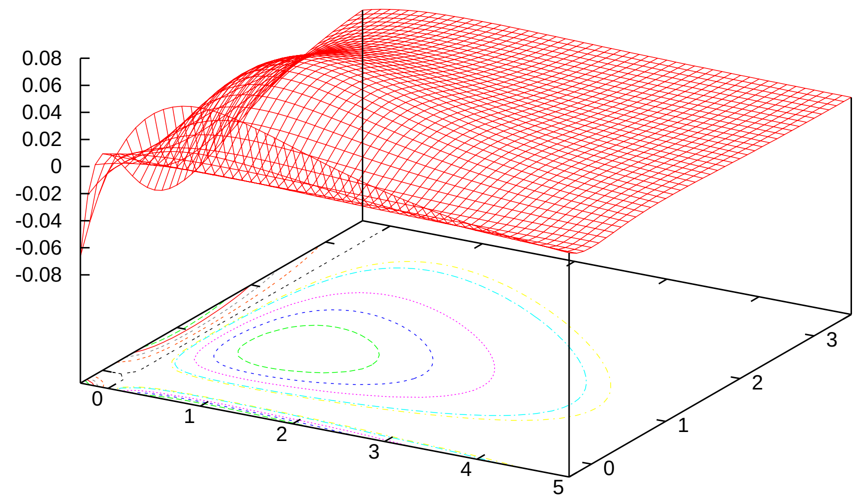

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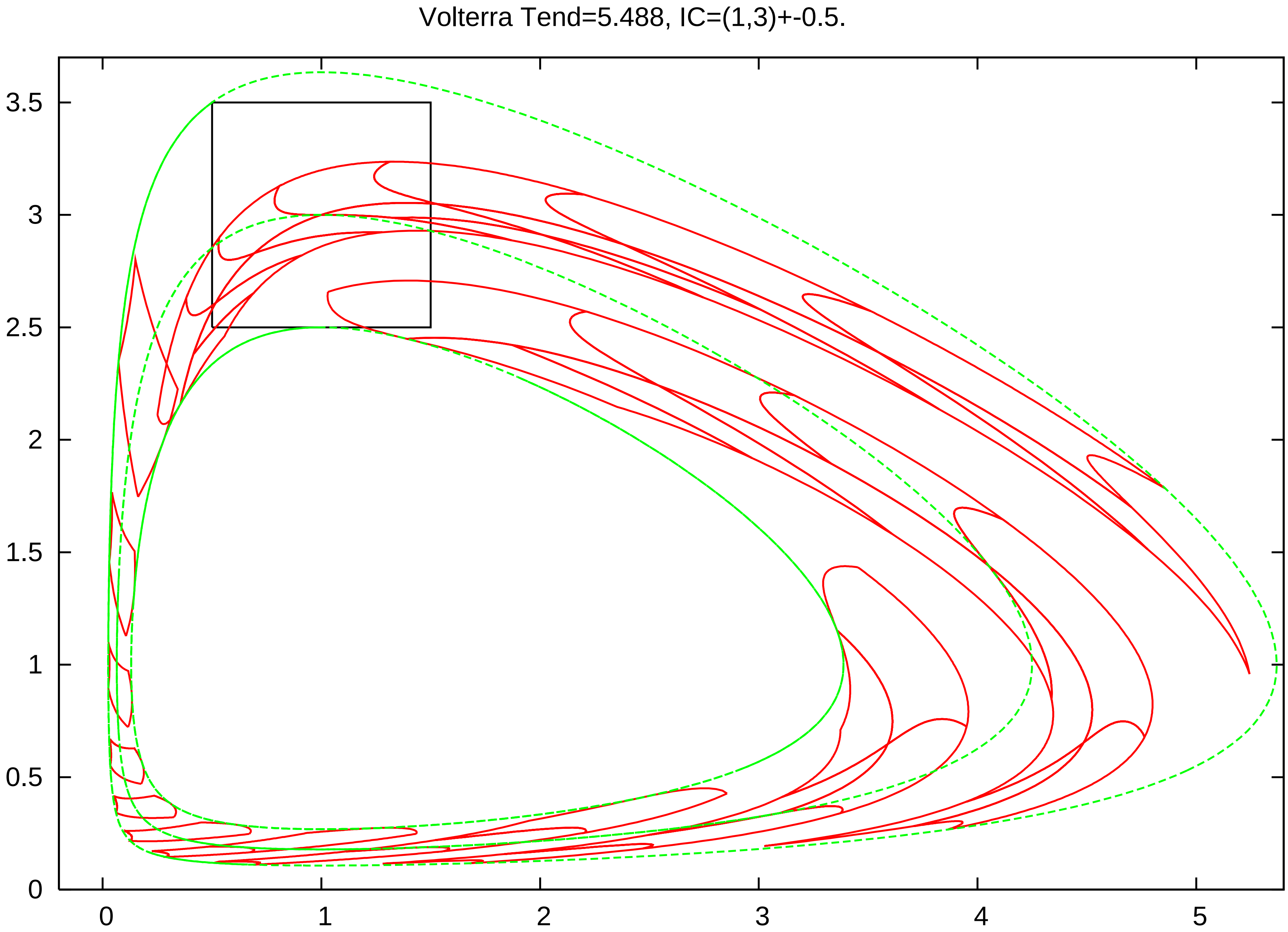
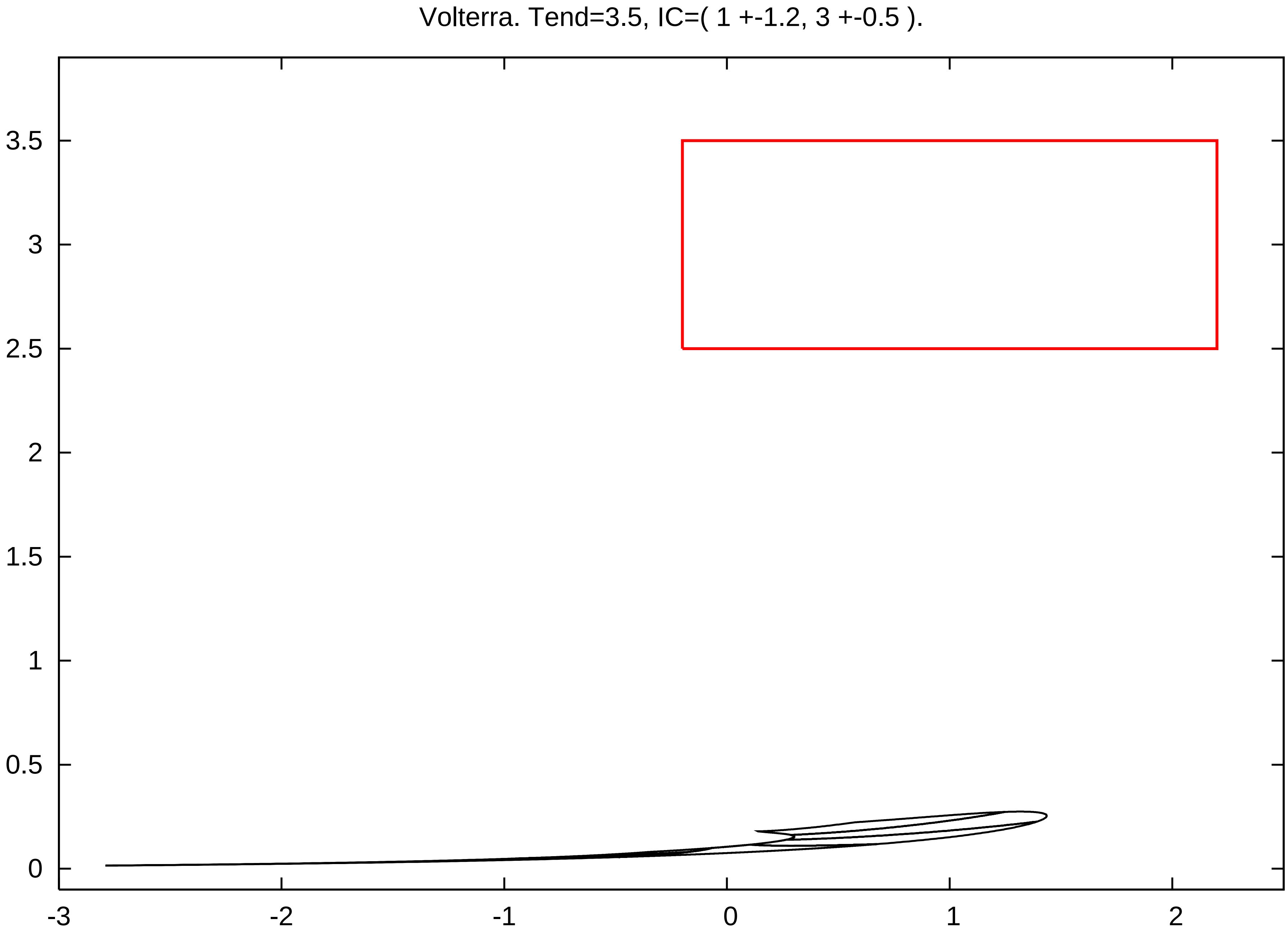
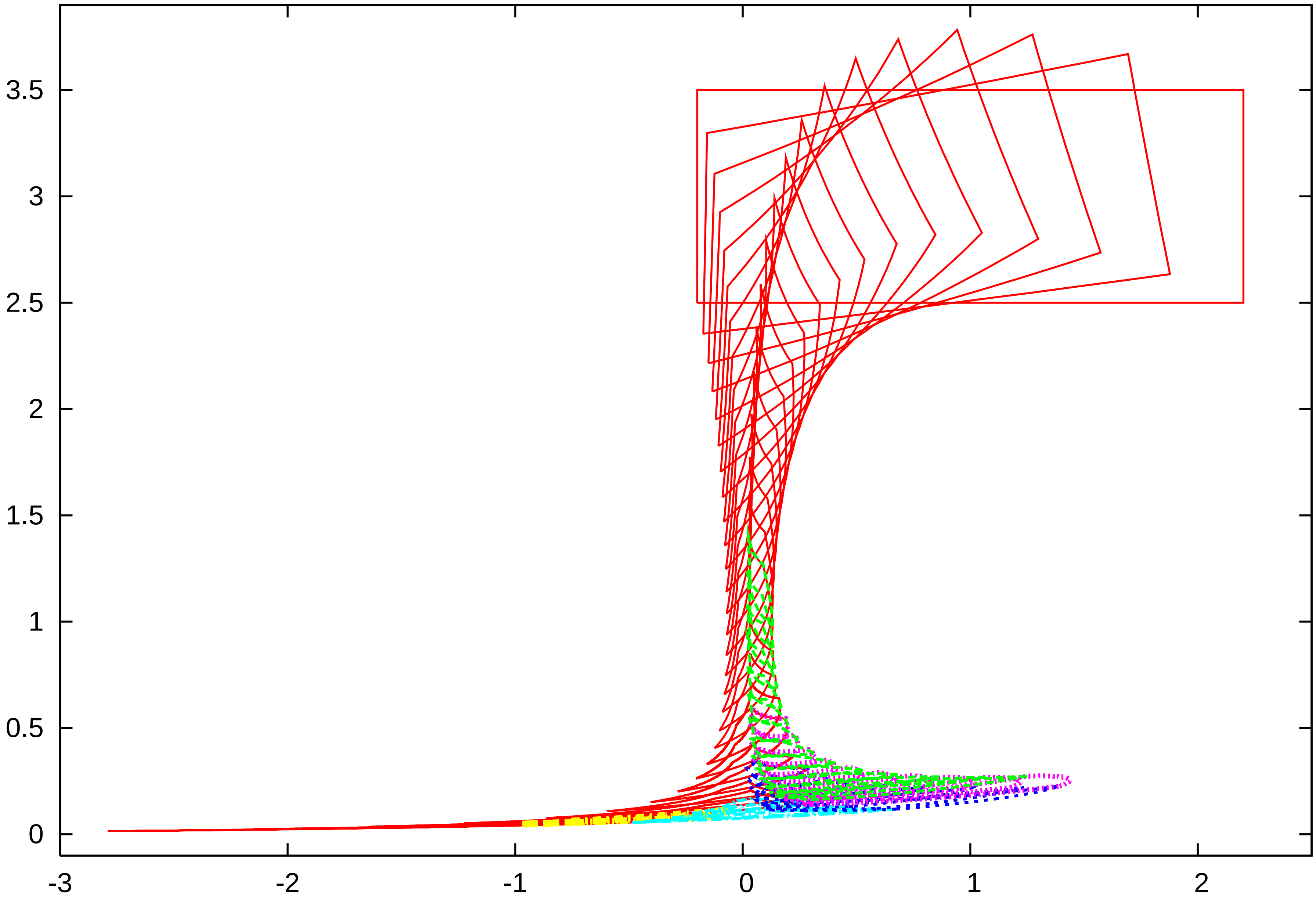
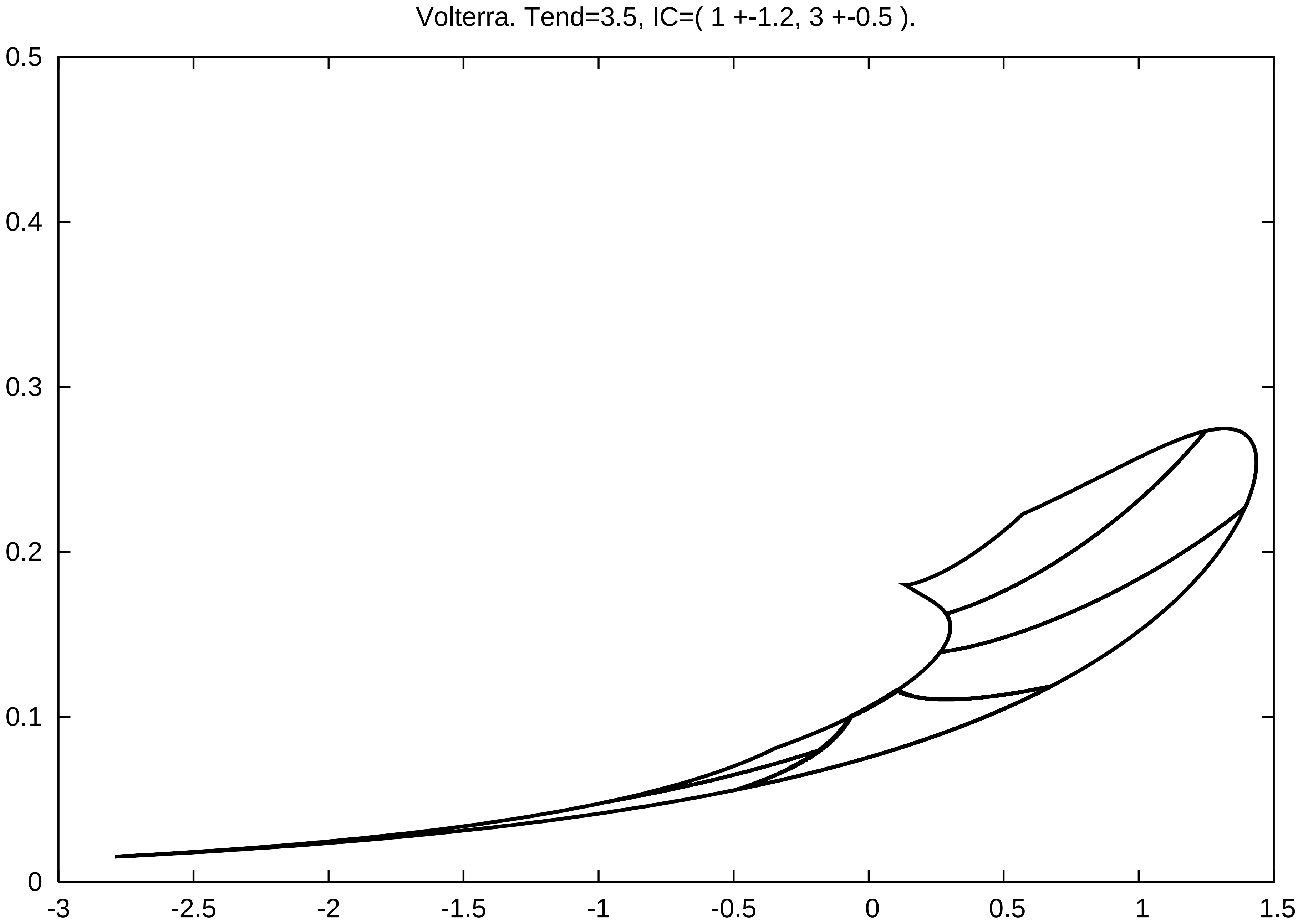

Volterra Tend=5.488, IC=(1,3)+-0.5.
0
0.5
1
1.5
2
2.5
3
3.5
0
1
2
3
4
5



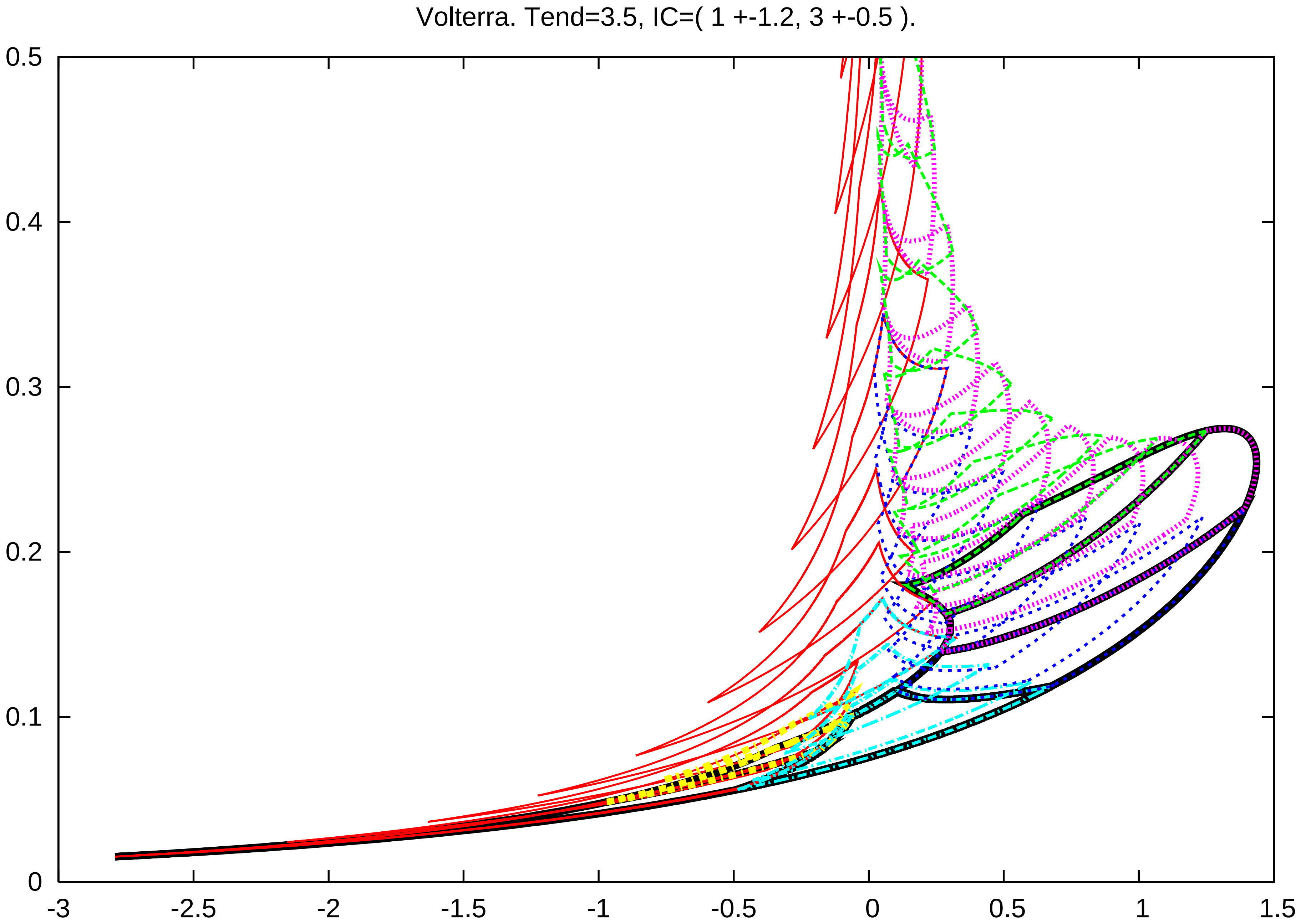
Volterra. Tend=3.5, IC=(1 +-1.2, 3 +-0.5).
3.5
3
2.5
2
1.5
1
0.5
0
-3
-2
-1
0
1
2

Volterra. Tend=3.5, IC=(1 +-1.2, 3 +-0.5).





Volterra. Tend=3.5, IC=(1 +-1.2, 3 +-0.5).
0.5
0.4
0.3
0.2
0.1
0
-3
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5


Volterra. Tend=3.5, IC=(1 +-1.2, 3 +-0.5).
0.5
0.4
0.3
0.2
0.1
0
-3
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5

Rigorous Reachability Analysis

- Obtain a rigorous flow of a large area of interest by integrating the ODEs using Taylor models for the time step of interest
- During the verified integration process, conduct domain decompositions dynamically as needed

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

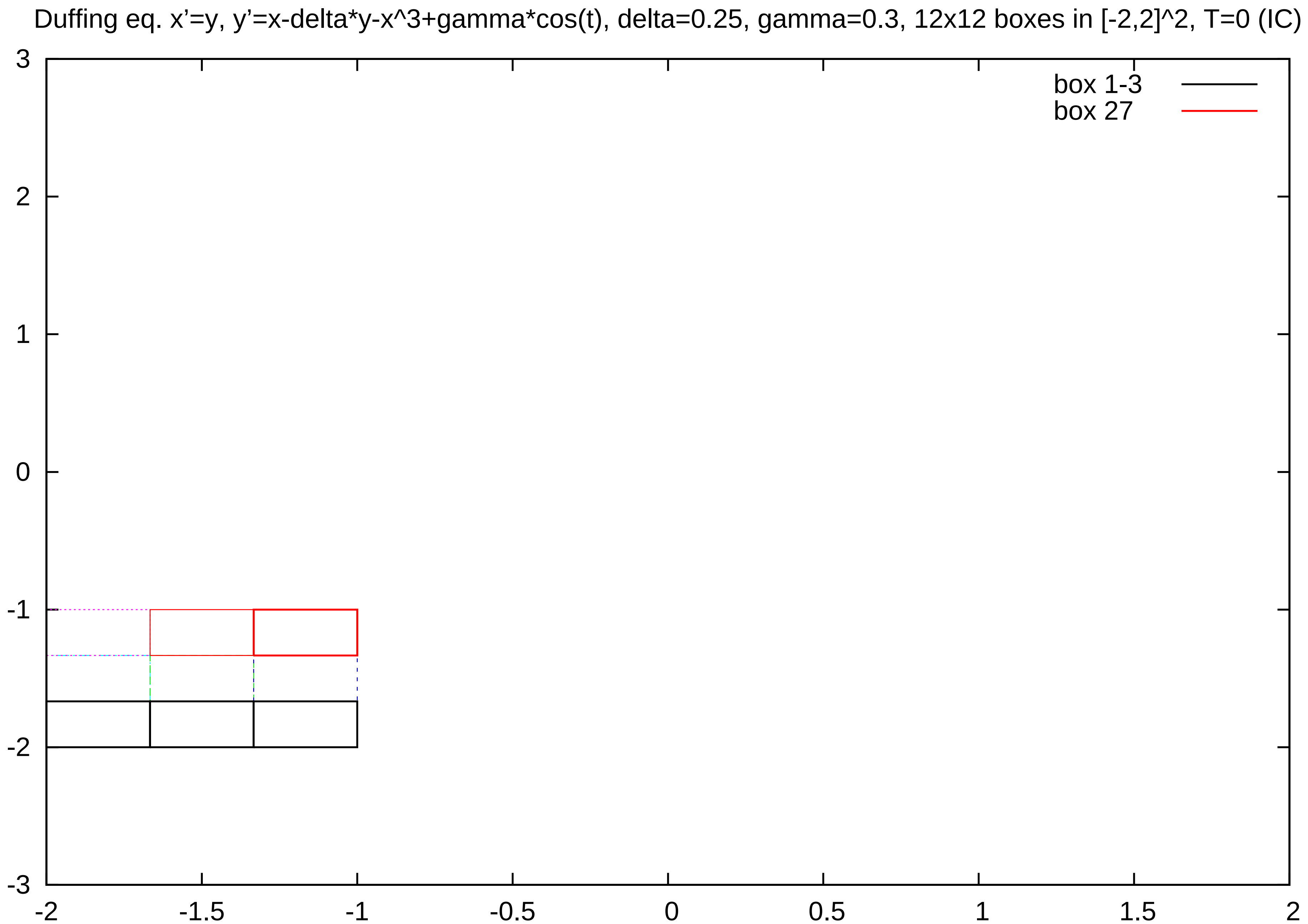
$$\begin{aligned}\dot{x} &= y\\ \dot{y} &= x - \delta y - x^3 + \gamma\cos(t)\end{aligned}$$

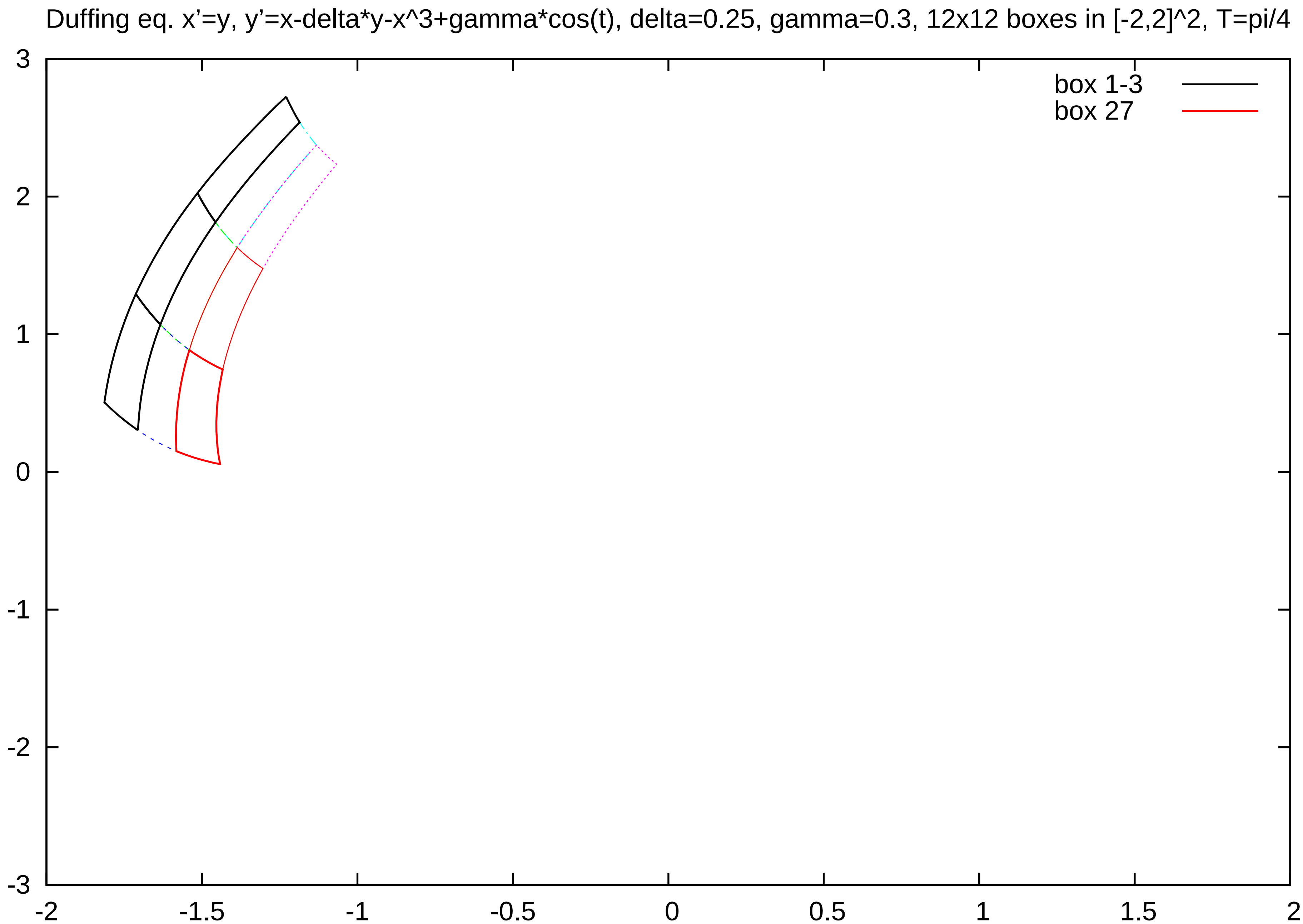
with

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

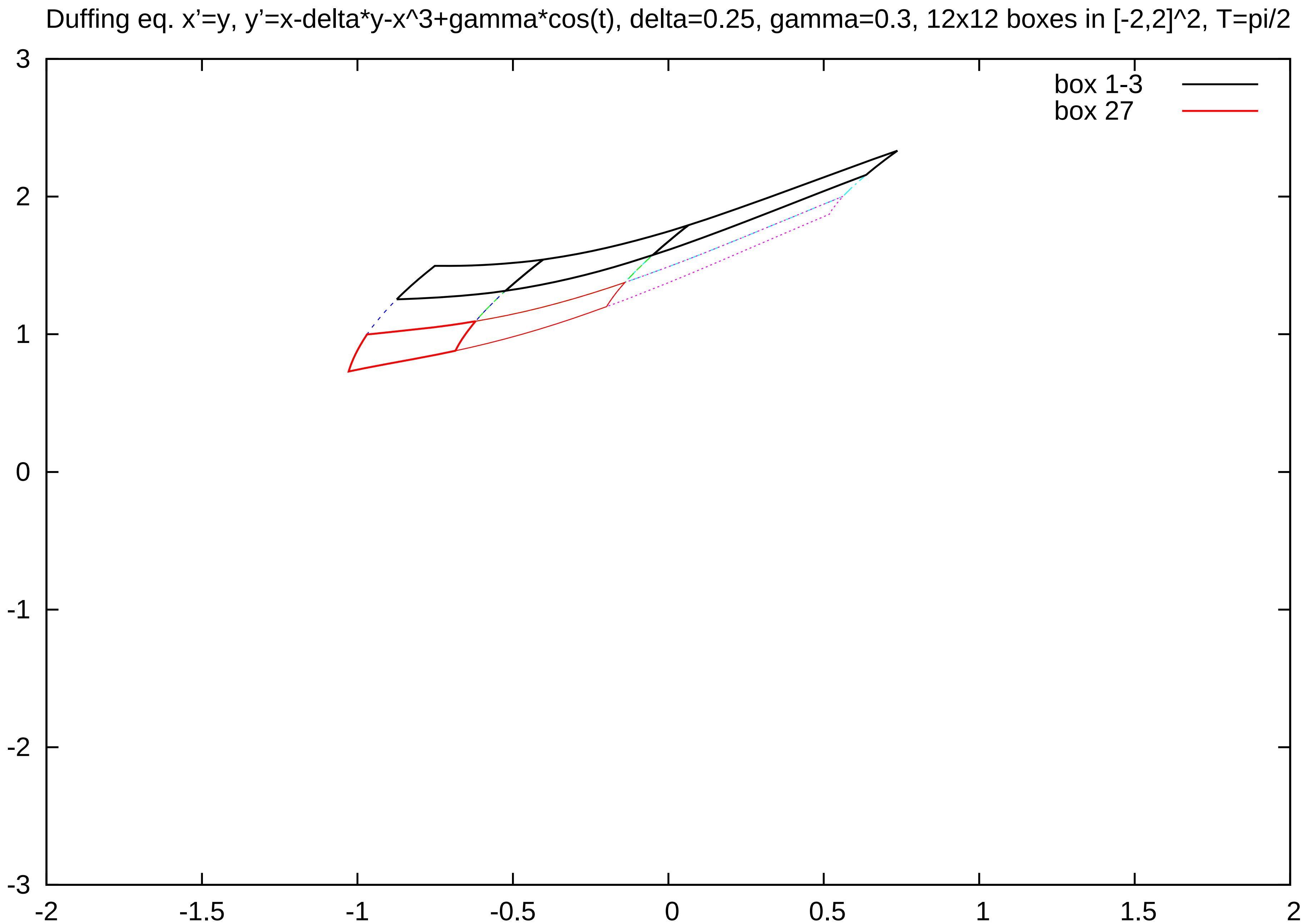
for

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

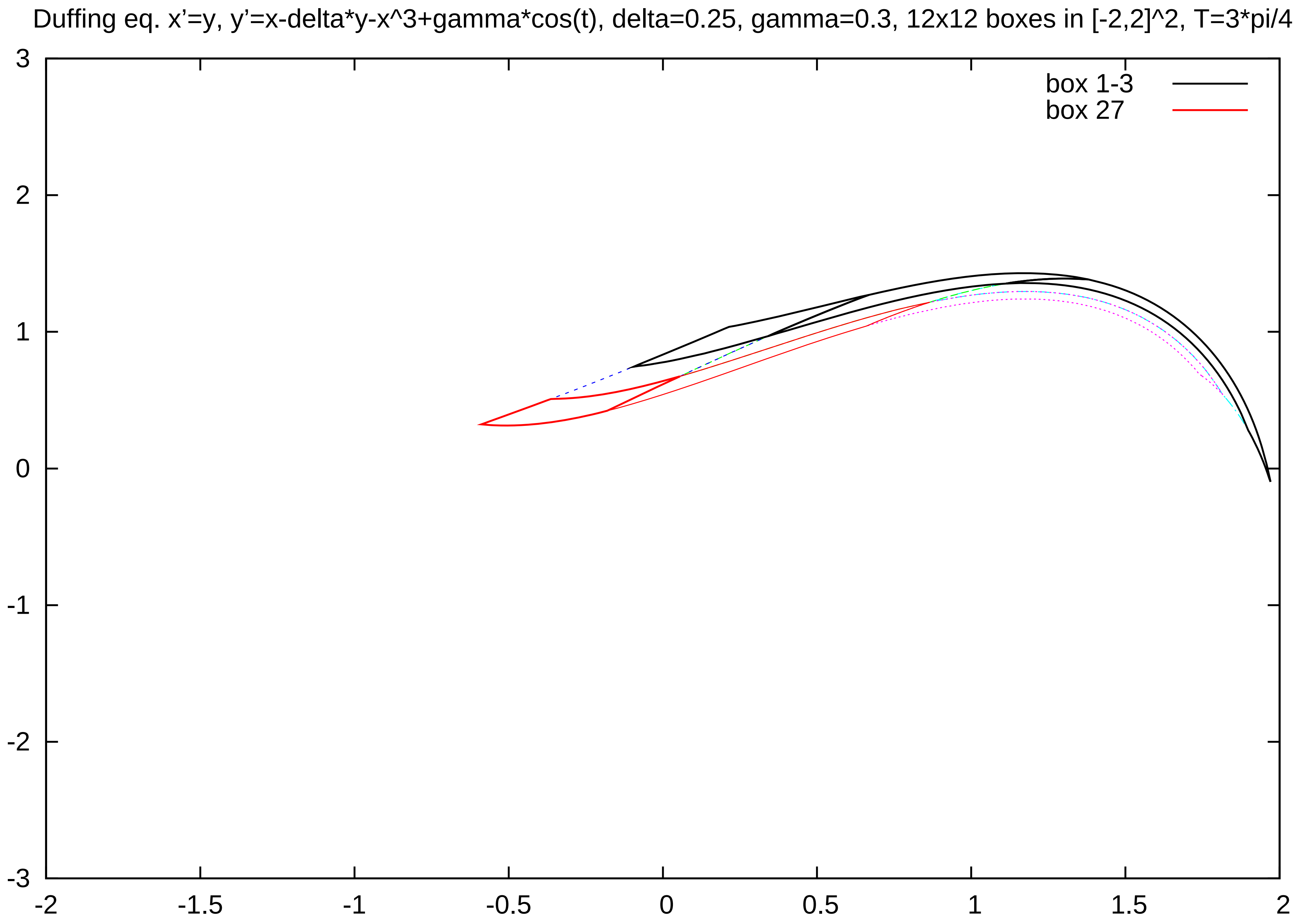

Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=0 (IC)
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

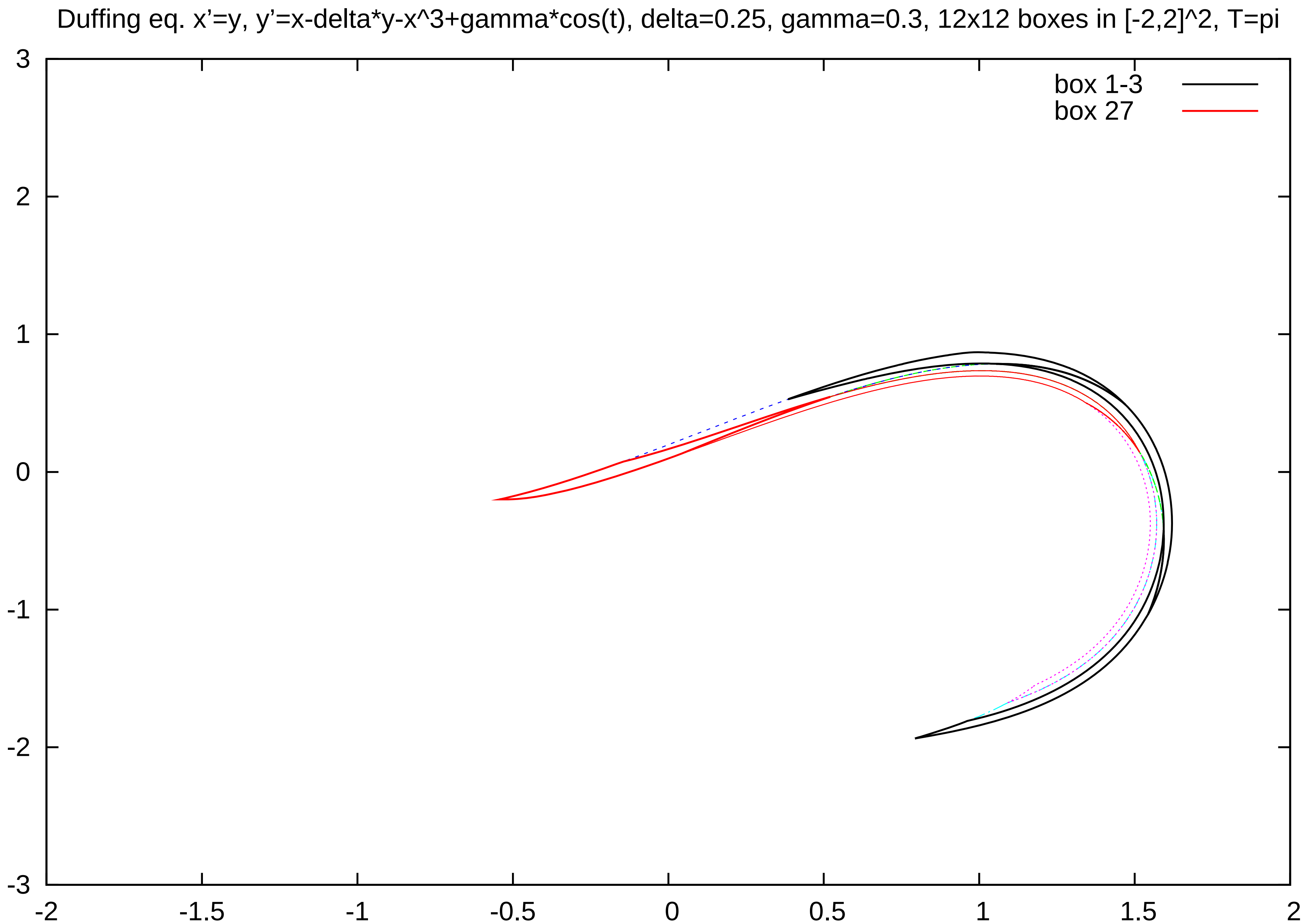


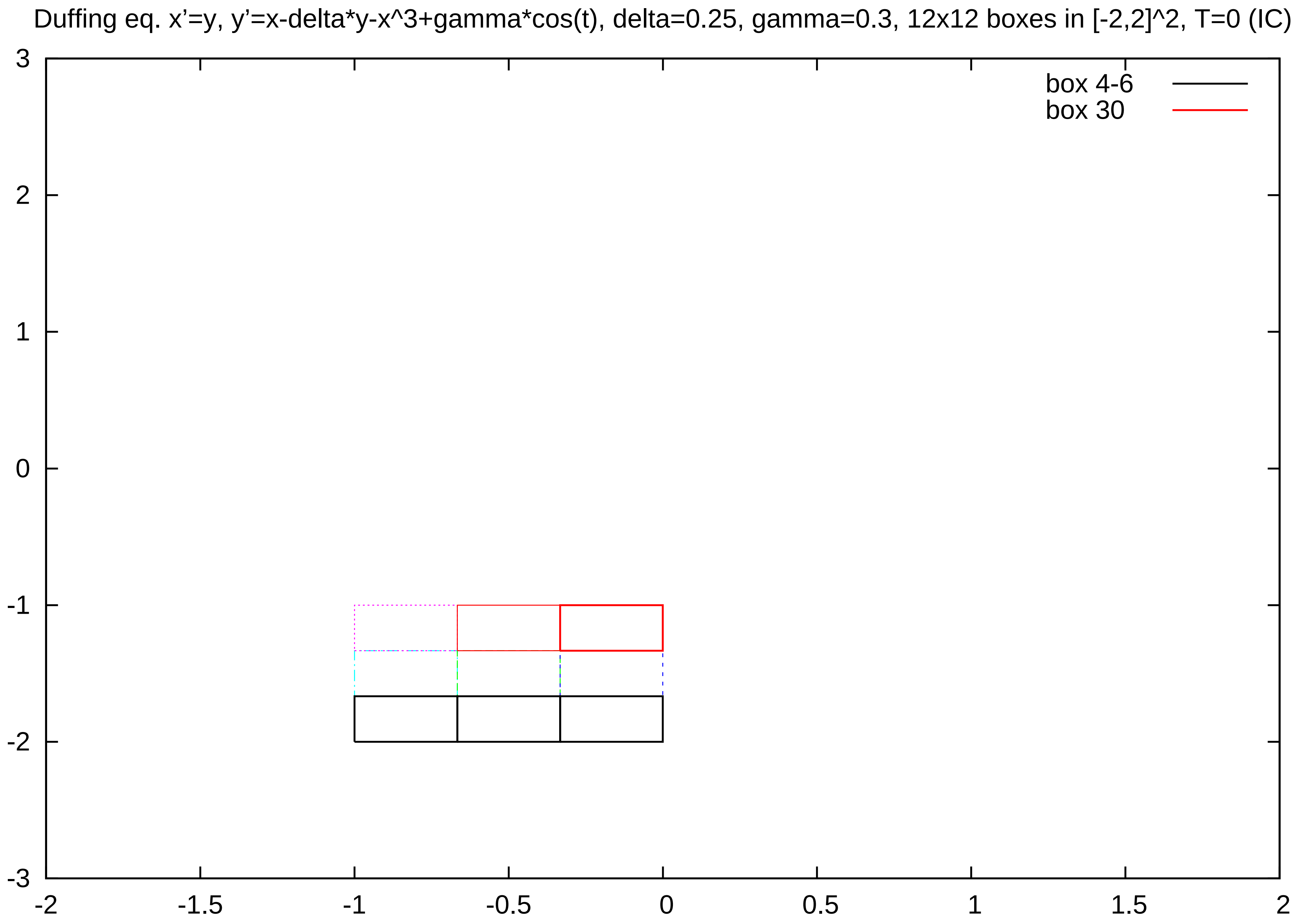
Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=pi/4
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2



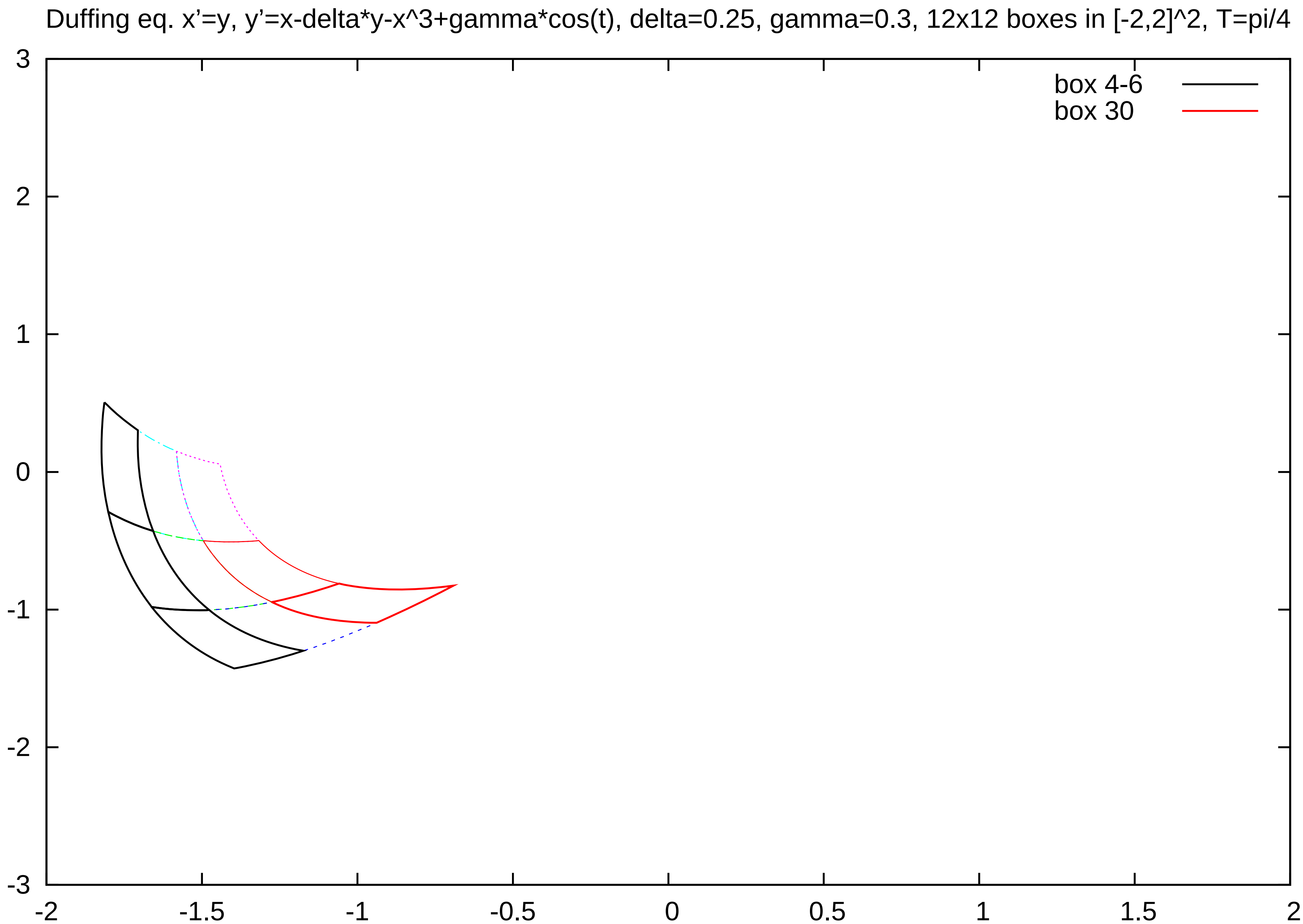
Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=pi/2
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2


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

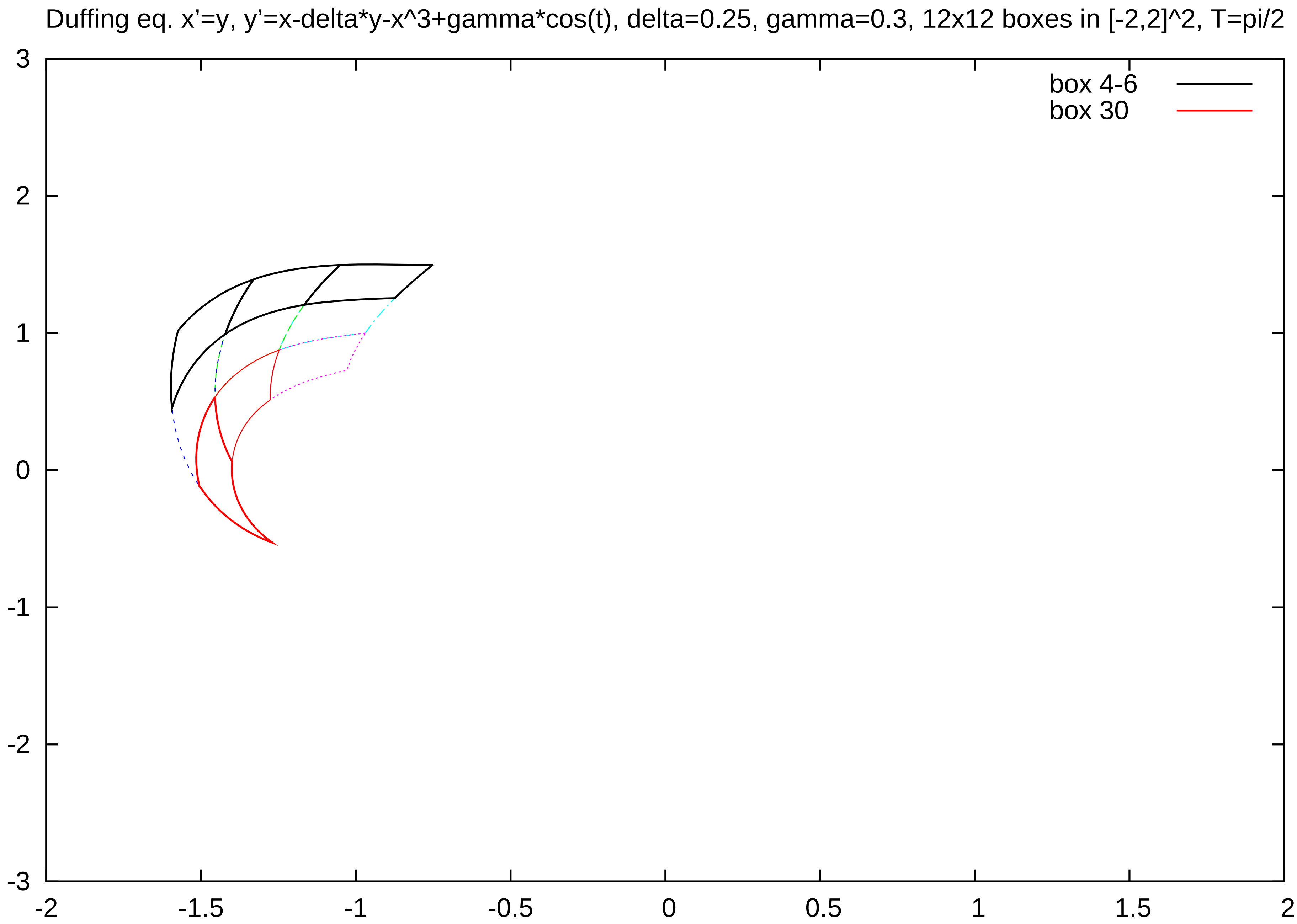

Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=pi
box 1-3
box 27
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

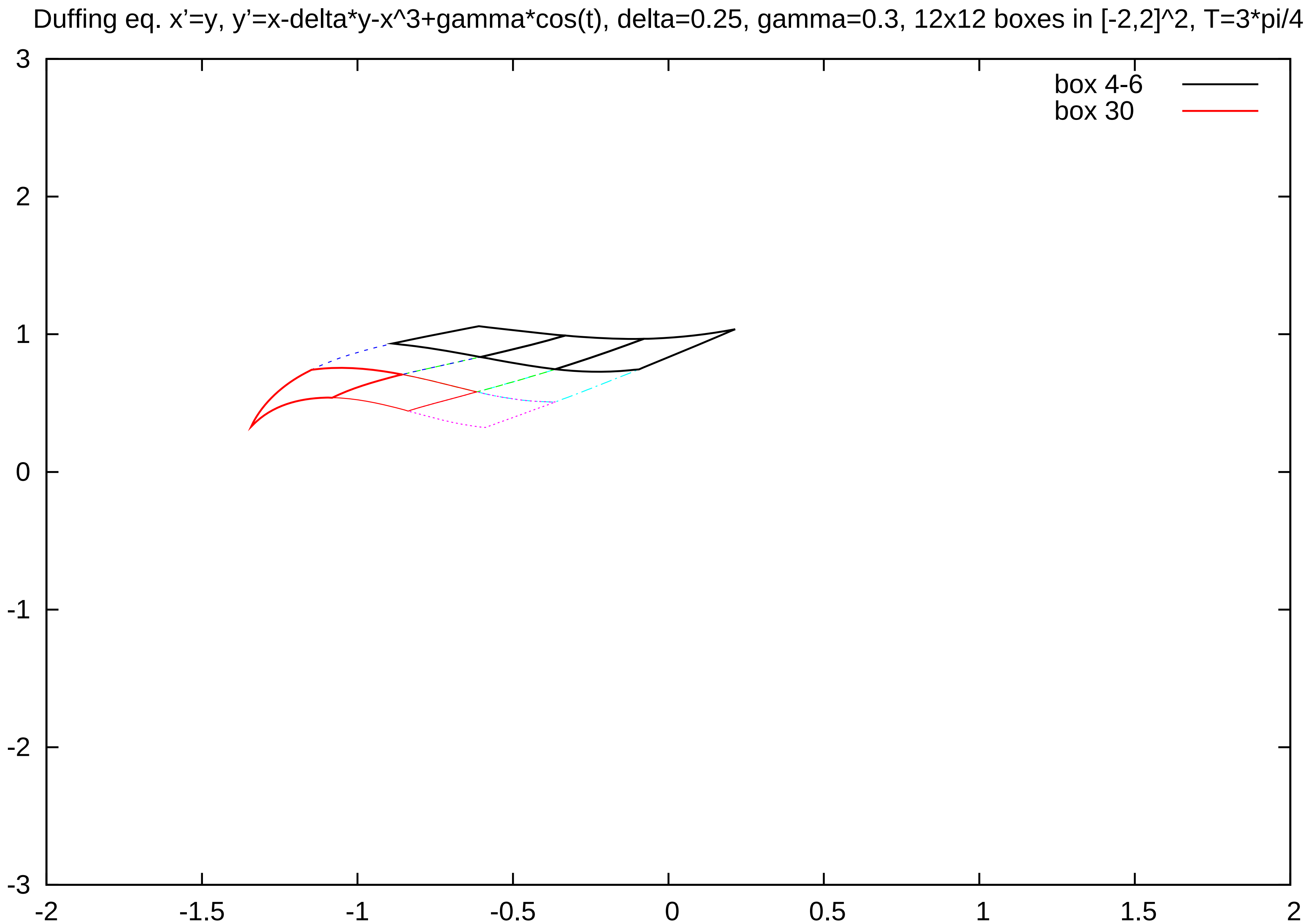


Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=0 (IC)
box 4-6
box 30
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

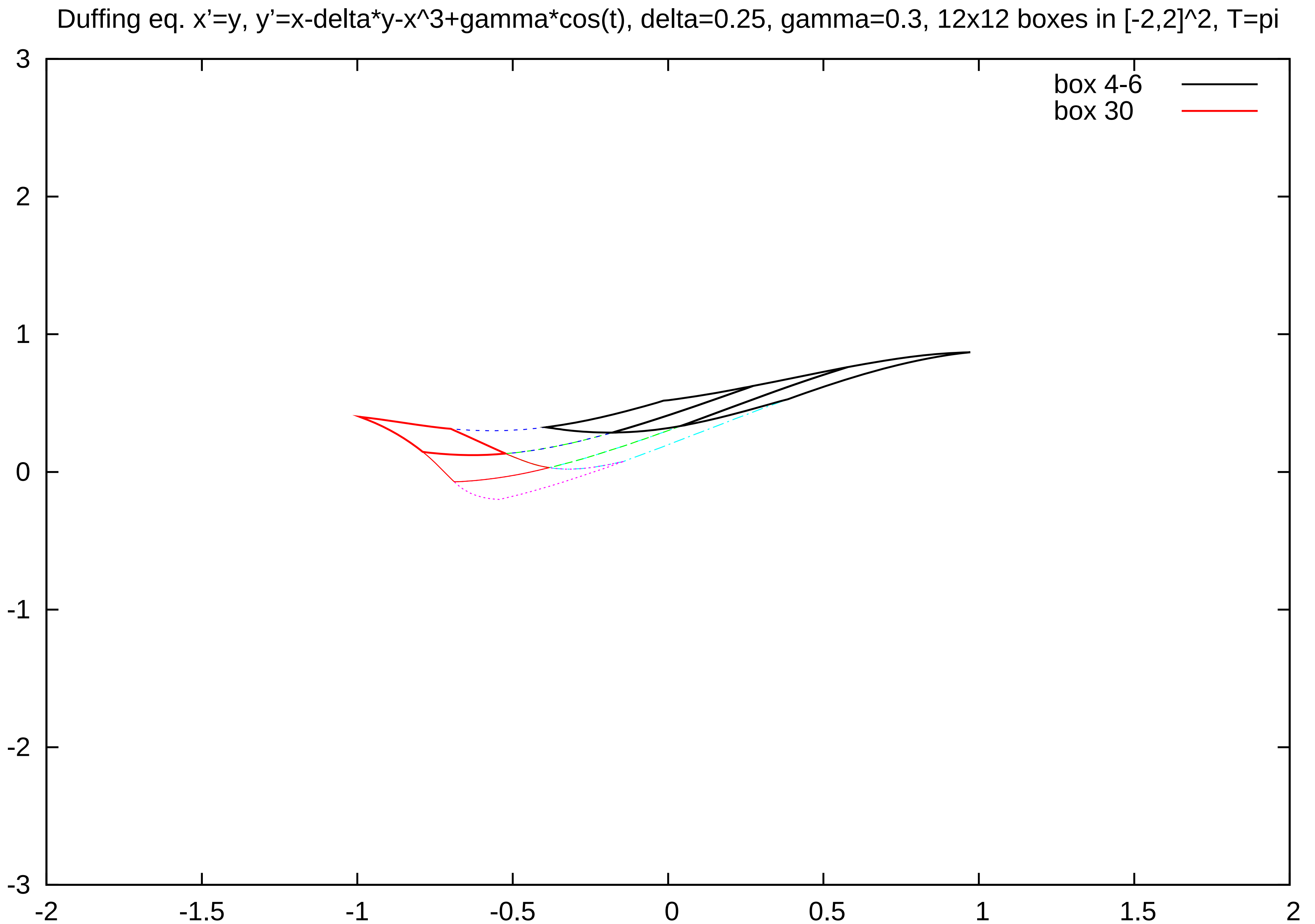


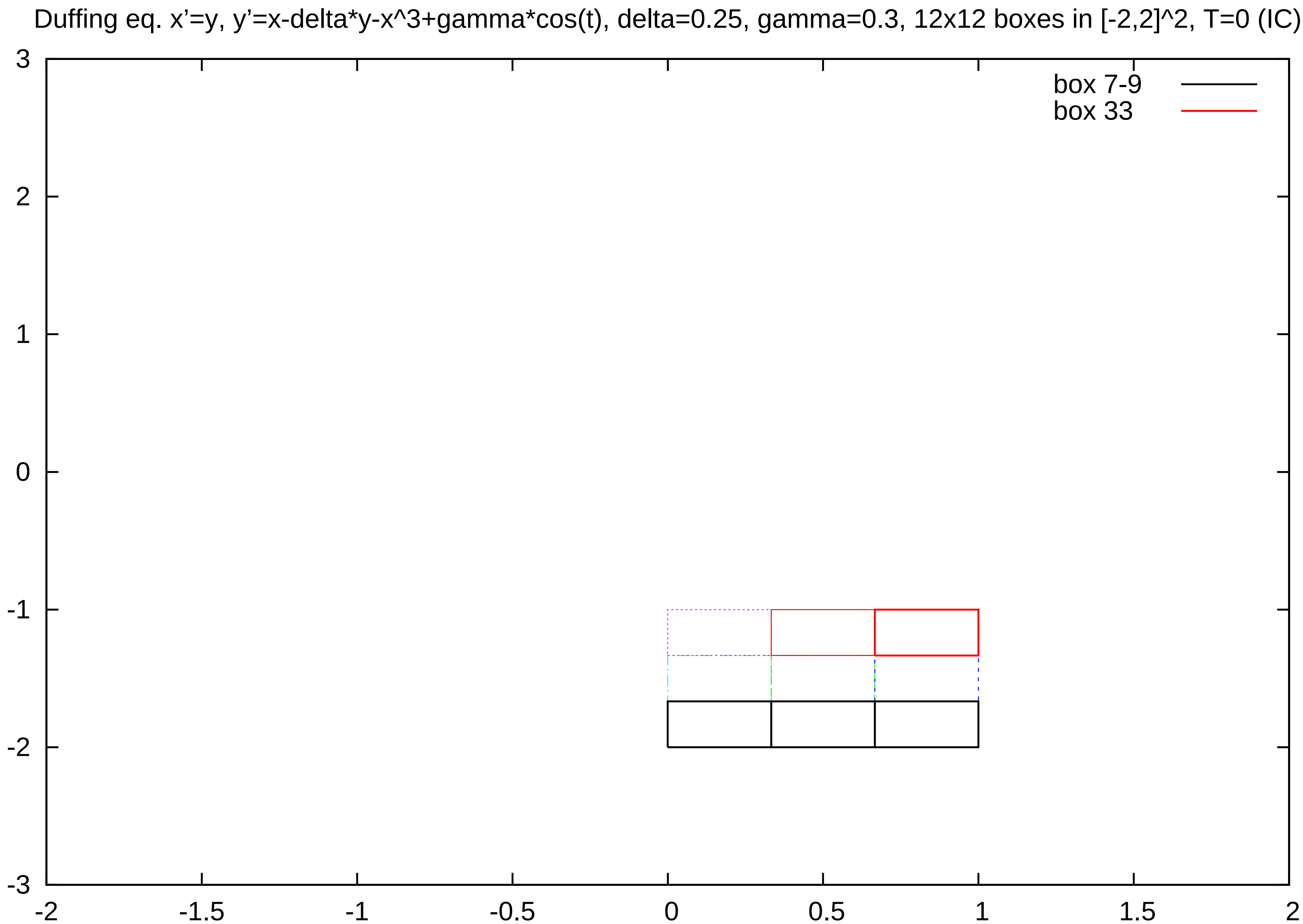
Duffing eq. x'=y, y'=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=pi/4
box 4-6
box 30
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2


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/2
box 4-6
box 30
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

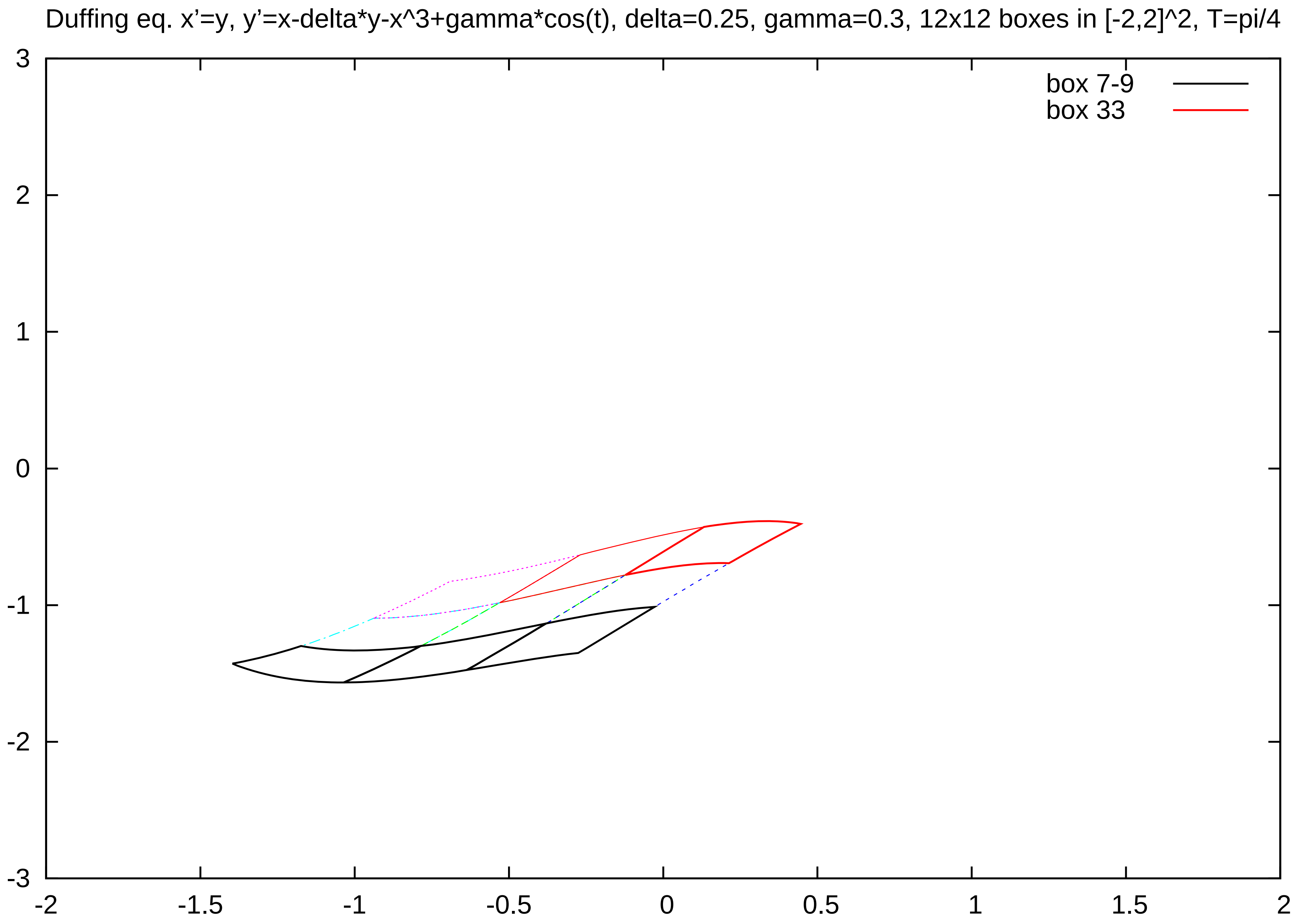


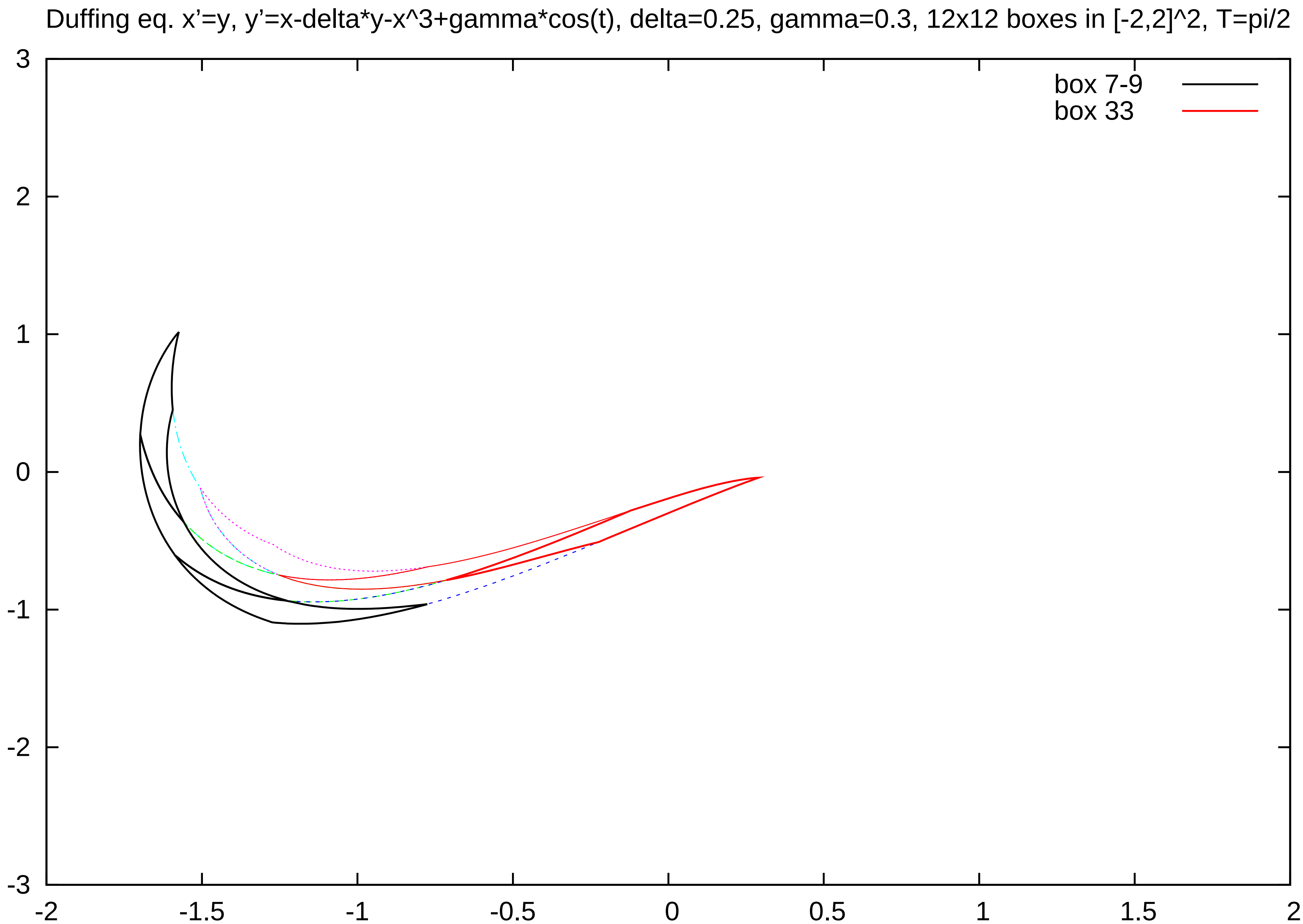
Duffing eq. x’=y, y’=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=3*pi/4
box 4-6
box 30
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2


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 4-6
box 30
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=0 (IC)
box 7-9
box 33
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
box 7-9
box 33
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/2
box 7-9
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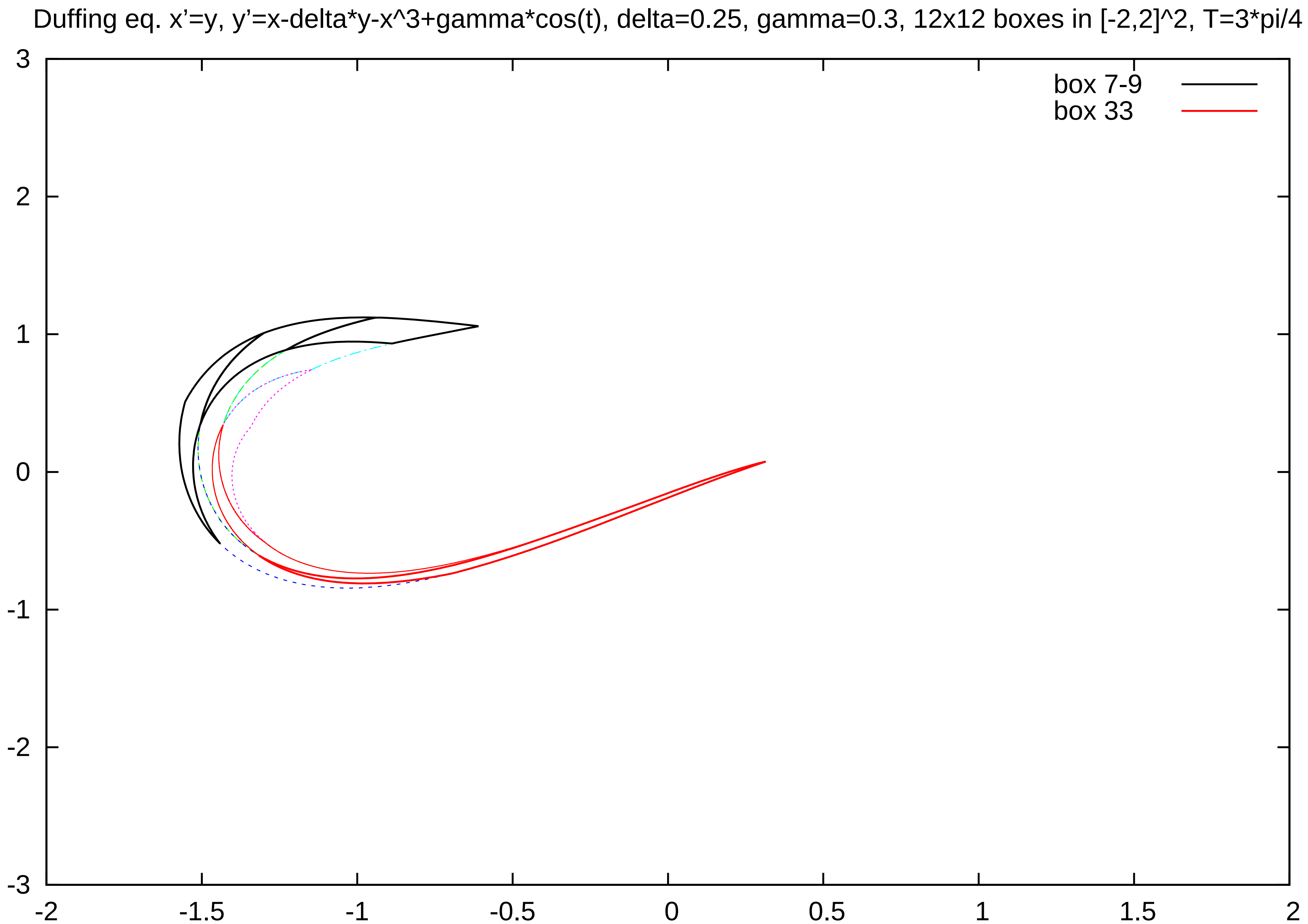
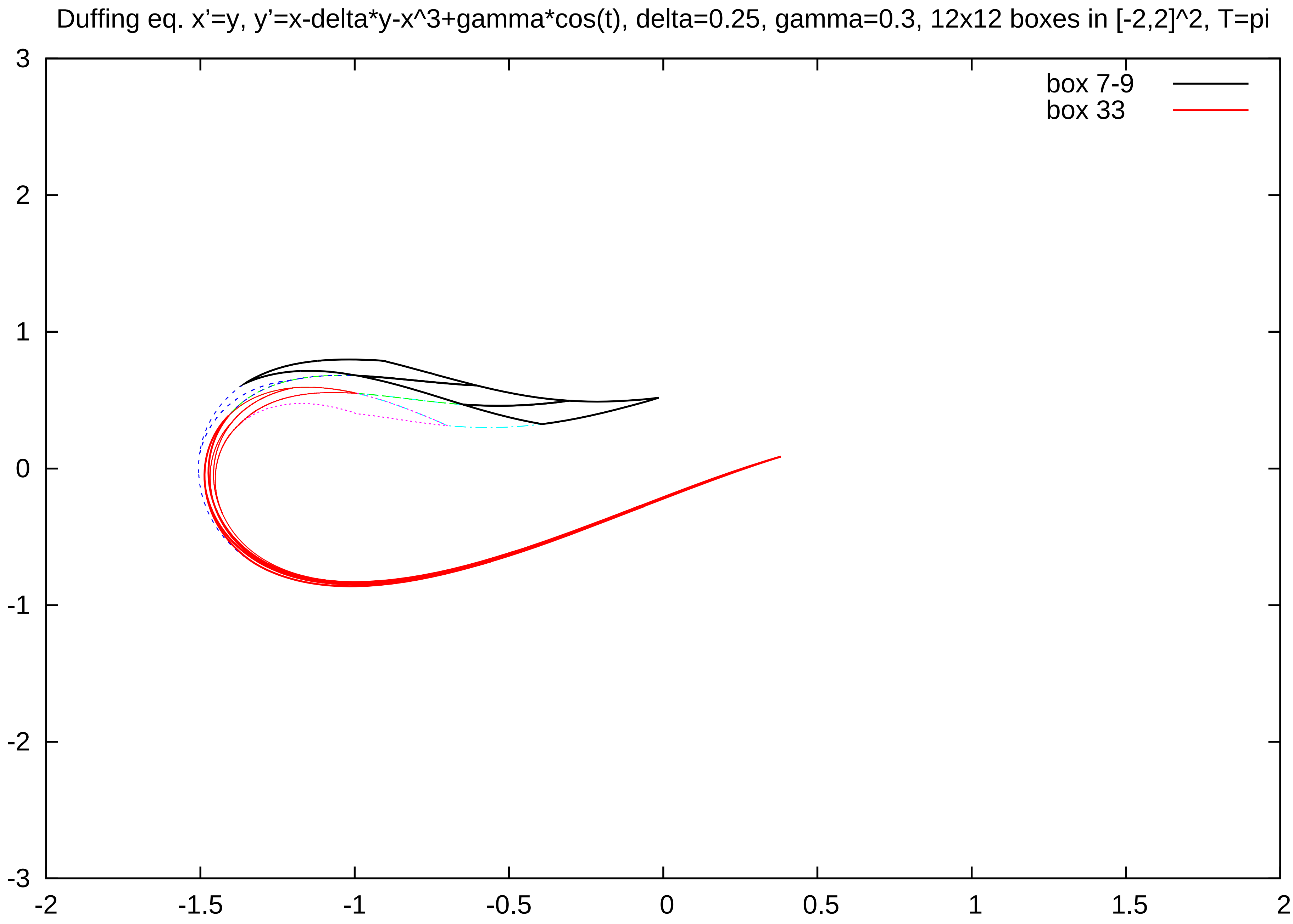
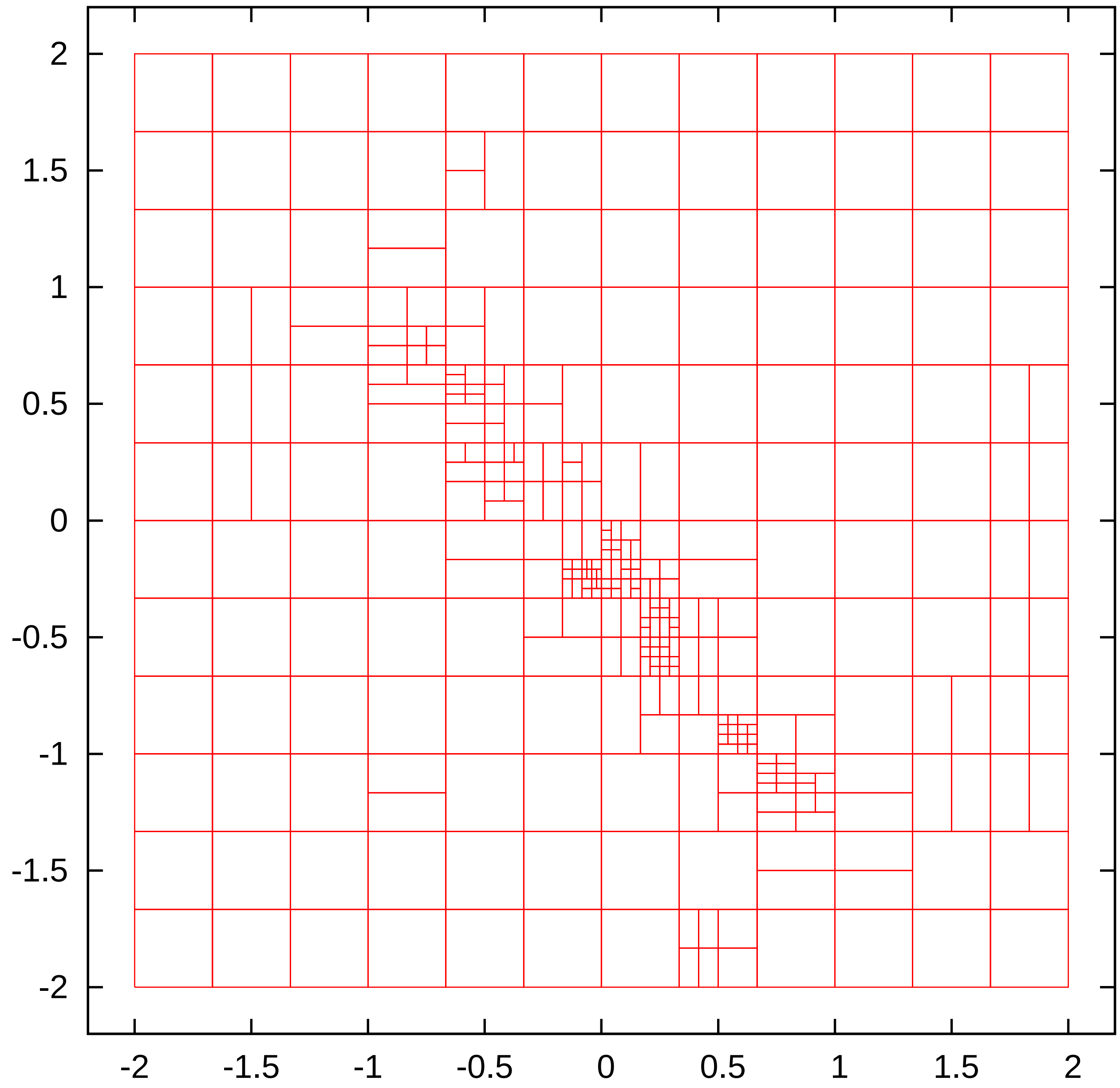
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

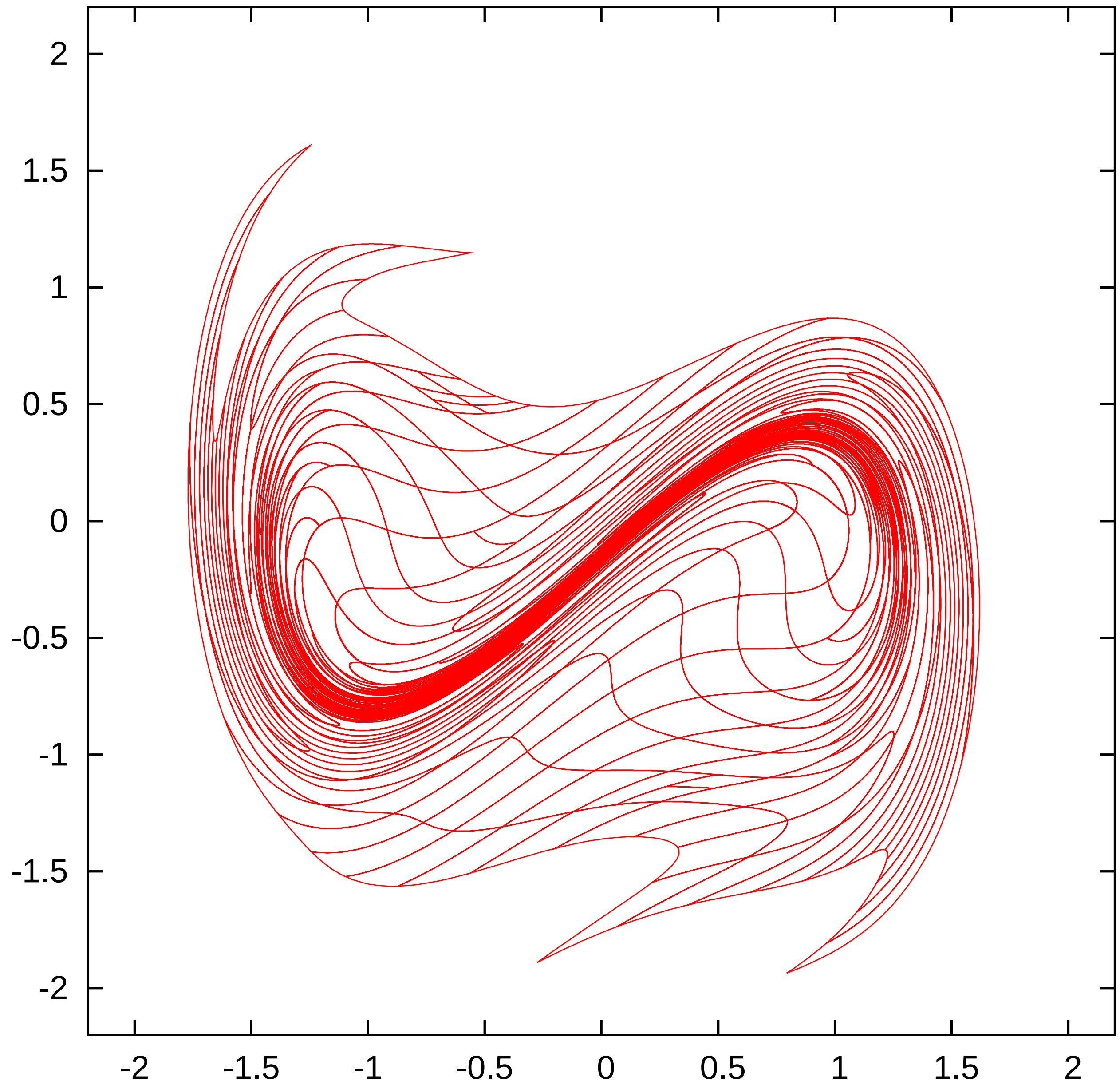

Duffing eq. x’=y, y’=x-delta*y-x^3+gamma*cos(t), delta=0.25, gamma=0.3, 12x12 boxes in [-2,2]^2, T=3*pi/4
box 7-9
box 33
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2


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 7-9
box 33
3
2
1
0
-1
-2
-3
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

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



Duffing. Time 0 to pi. 12x12 ICs. VIRDA=0.50. 343 Objs



Allows graph theoretical treatment (Morse decomposition, Conley index etc)

CPU Time:

~ 20 min (1E-5 accuracy)

~ 100 min (1E-10 accuracy)

Graph-Based Methods

Problem: Many problems of dynamical systems are statements about behavior at infinity. Examples: attracting regions, limit cycles, etc. How can these be studied using finite integration?

Answer: Discretize space into disjoint sub-regions R_i, study flow for fixed Δt. Consider the directed graph described by the following incidence matrix:

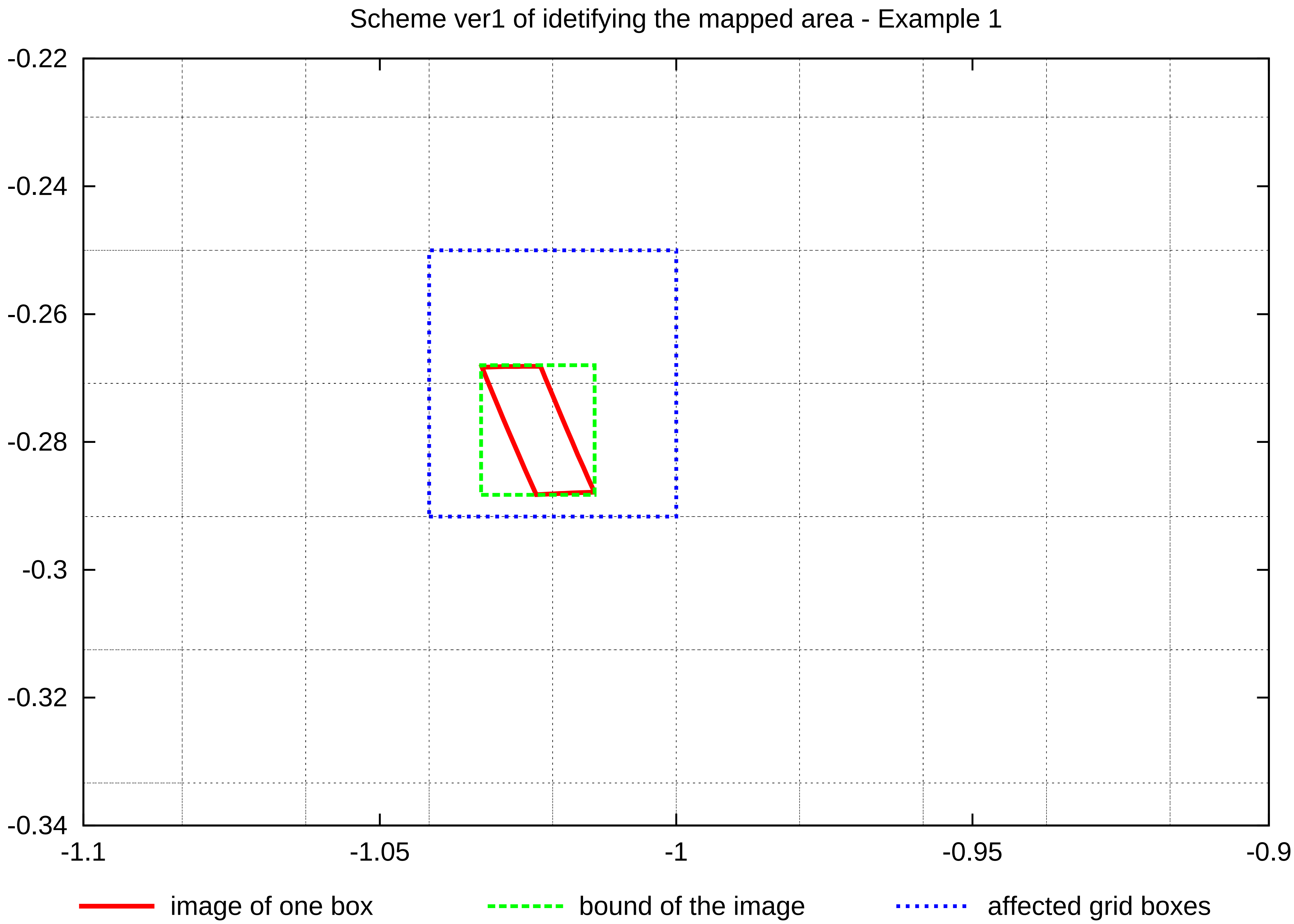
$$\hat{A}_{ij} = \begin{cases} 0 & \text{if } M(R_i) \text{ is certain not to reach } R_j \\ 1 & \text{else} \end{cases}$$

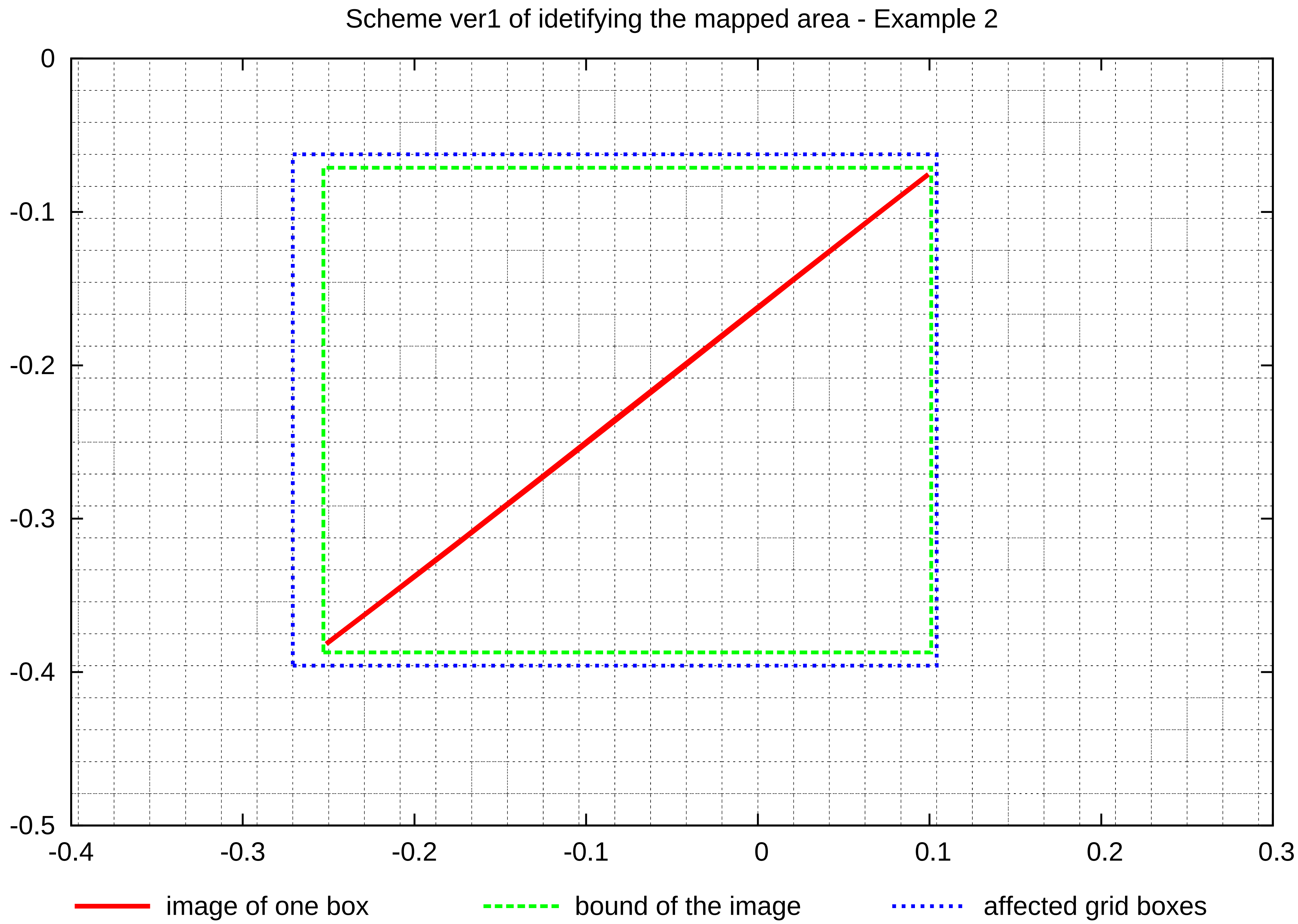
Studying the graph allows to rigorously identify basins of attraction, invariant sets, isolating neighborhoods, etc.

Problem: The quality of the analysis directly depends on the fineness of the mesh and the reduction of overestimation

Rigorous Reachability Analysis

- Obtain a rigorous flow of a large area of interest by integrating the ODEs using Taylor models for the time step of interest
- During the verified integration process, conduct domain decompositions dynamically as needed
- Discretize the space into disjoint sub-regions for studying graphs


Scheme ver1 of idetifying the mapped area - Example 1
-0.22
-0.24
-0.26
-0.28
-0.3
-0.32
-0.34
-1.1
-1.05
-1
-0.95
-0.9
image of one box
bound of the image
affected grid boxes

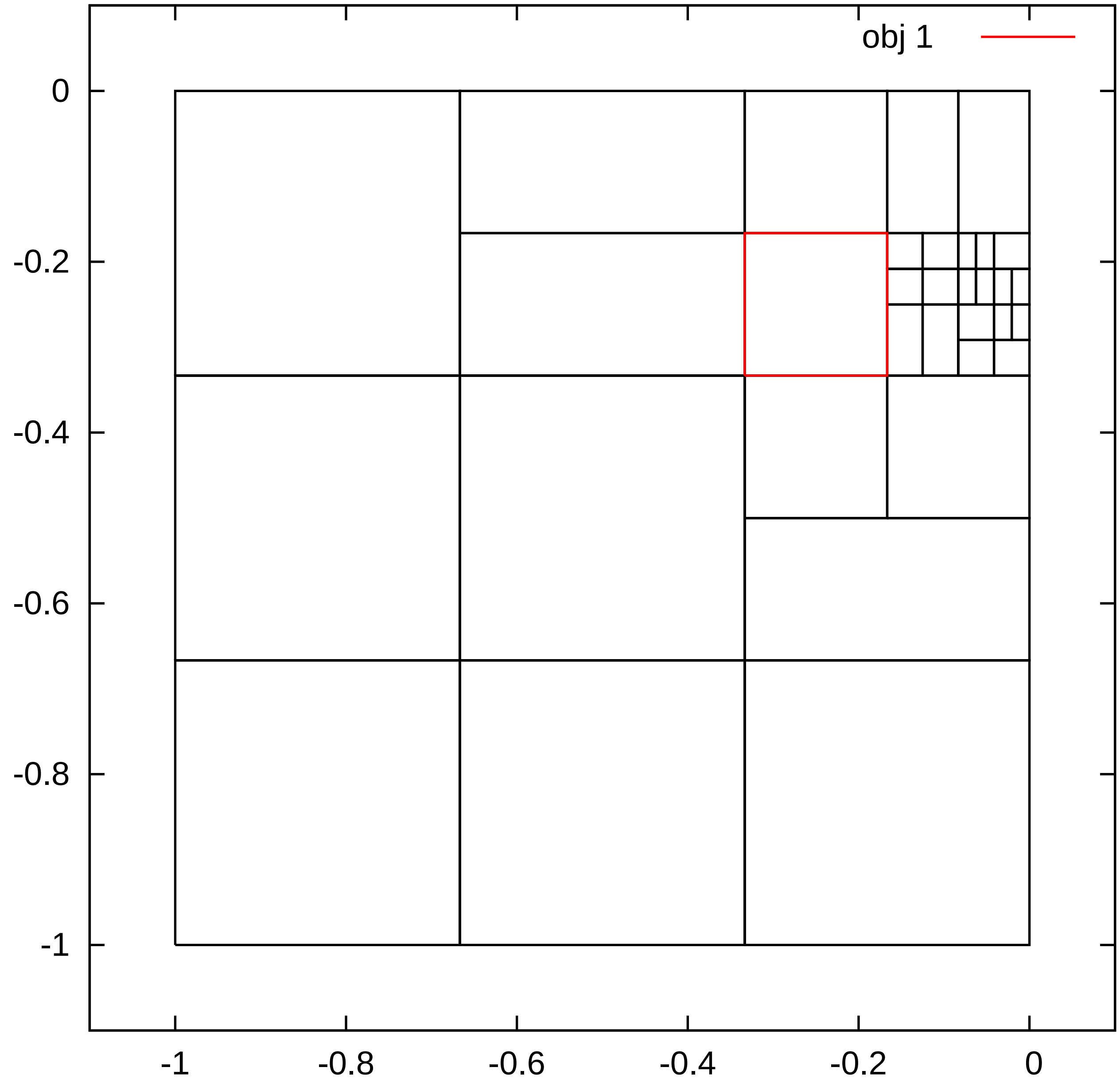


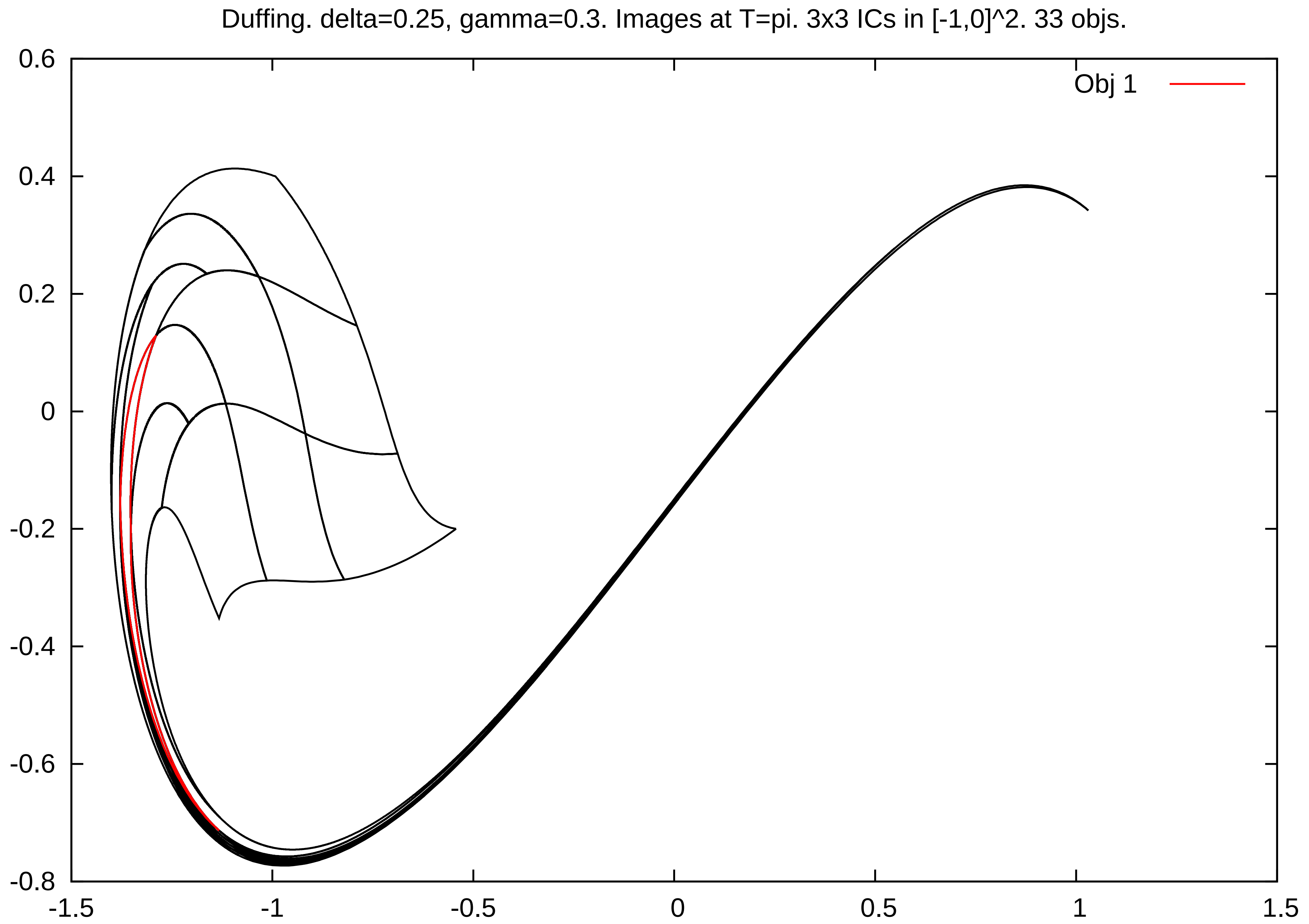
Scheme ver1 of idetifying the mapped area - Example 2
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
image of one box
bound of the image
affected grid boxes

Rigorous Reachability Analysis

- Obtain a rigorous flow of a large area of interest by integrating the ODEs using Taylor models for the time step of interest
- During the verified integration process, conduct domain decompositions dynamically as needed
- Discretize the space into disjoint sub-regions for studying graphs
  - In Taylor models, it's possible to discretize the resulting flow in a similar manner as of dynamic domain decompositions.

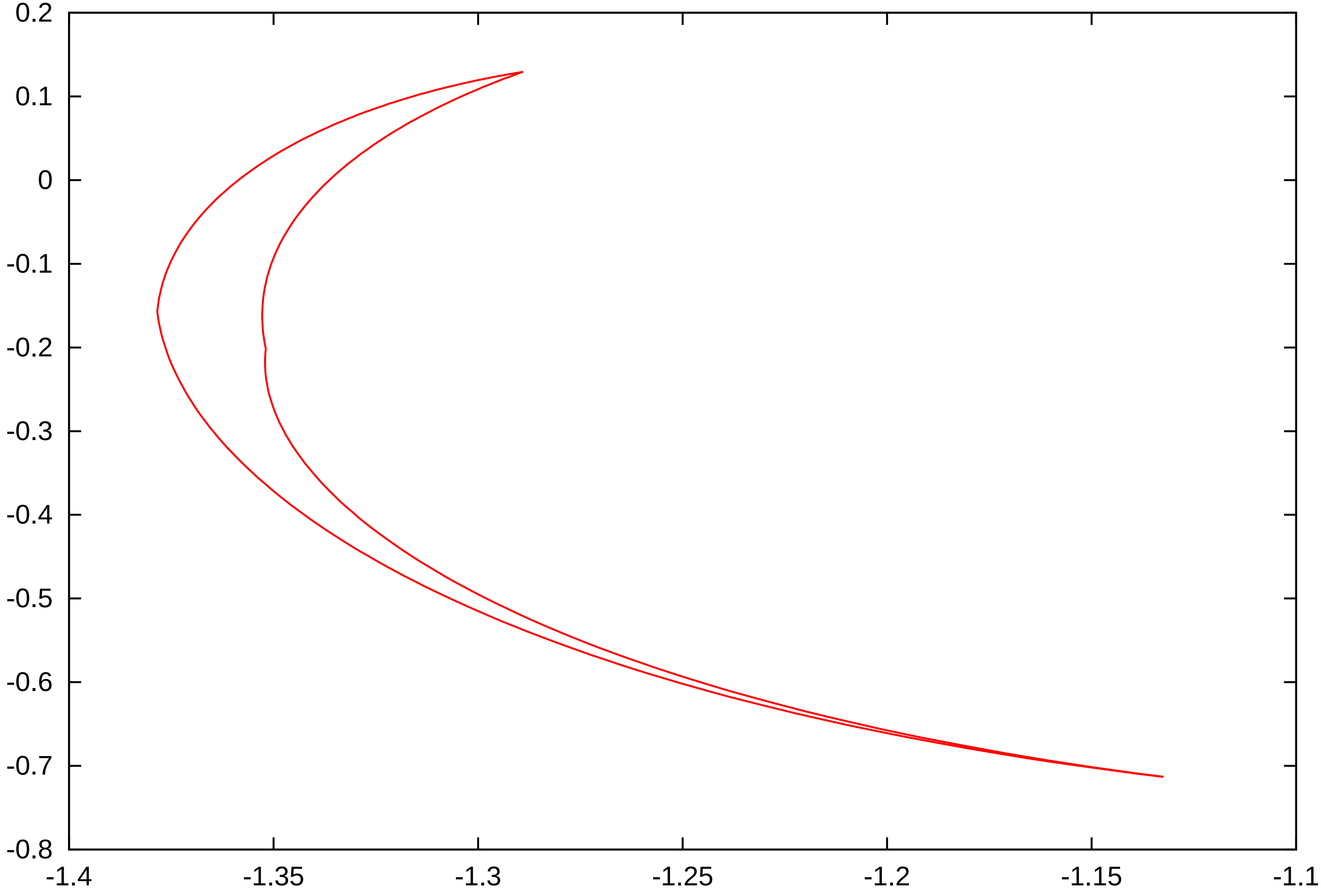
Duffing. delta=0.25, gamma=0.3. IC split map. 3x3 ICs in [-1,0]^2. T 0 to pi. 33 objs.

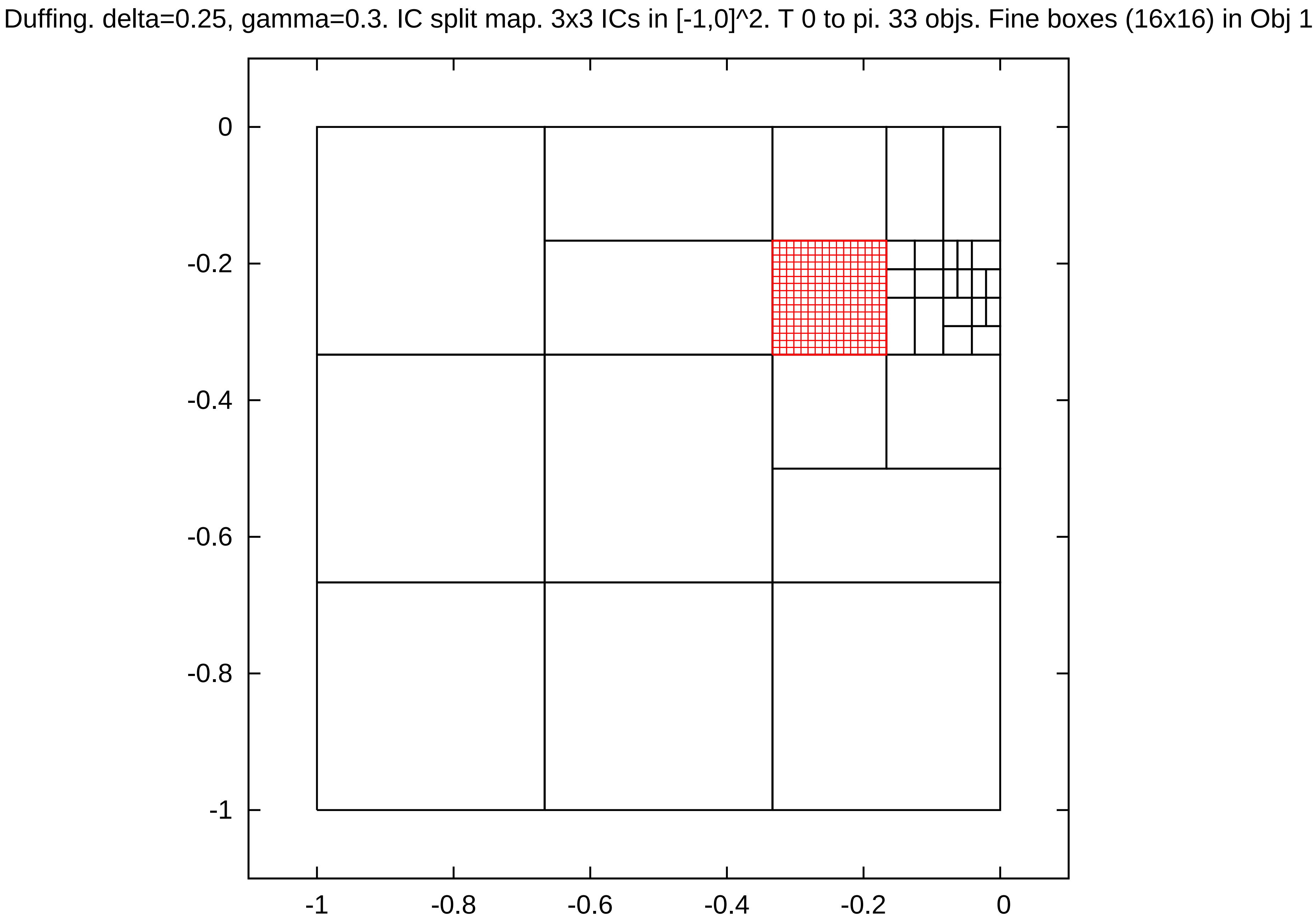


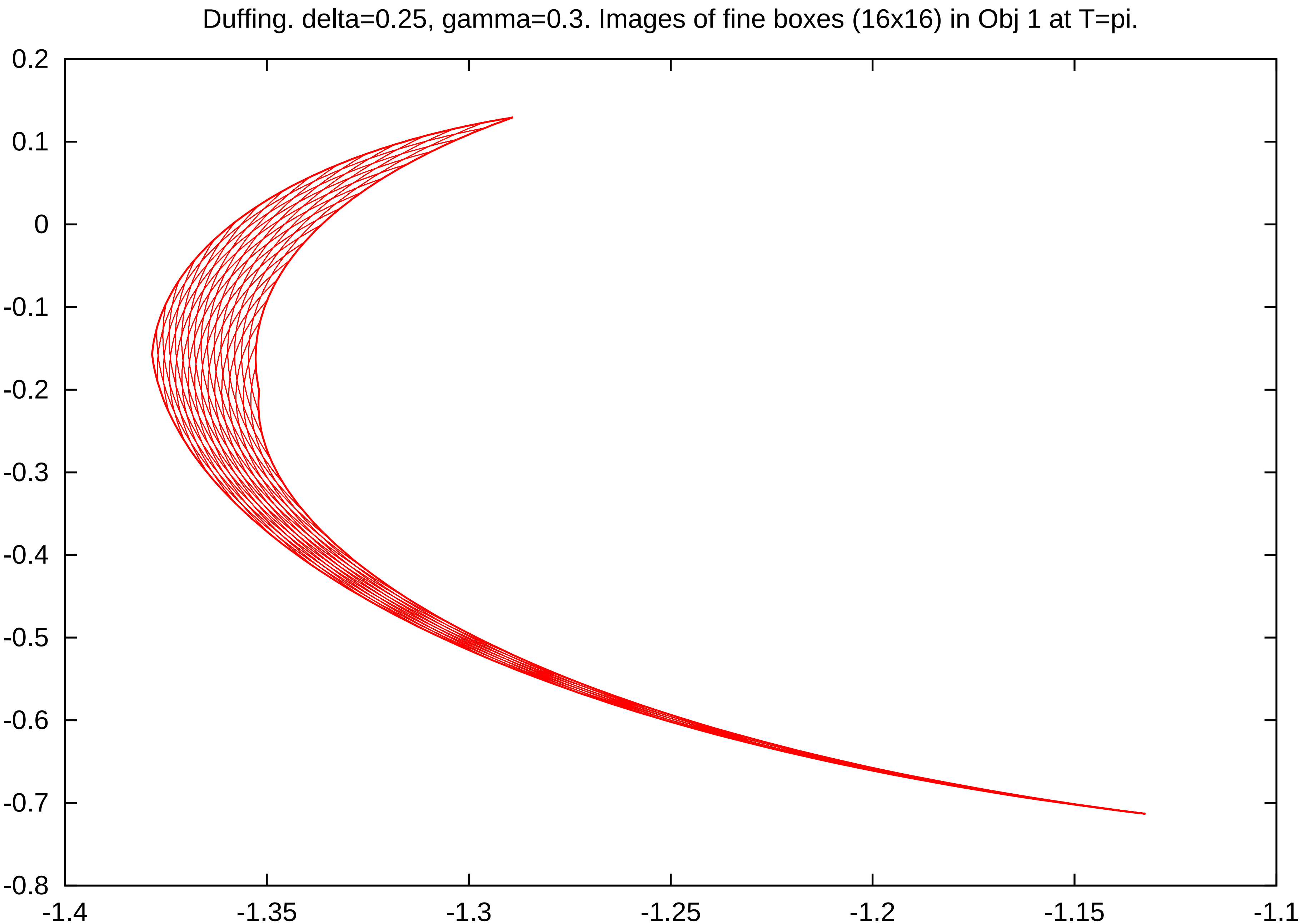


Duffing. delta=0.25, gamma=0.3. Images at T=pi. 3x3 ICs in [-1,0]^2. 33 objs.
Obj 1
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.5
-1
-0.5
0
0.5
1
1.5

Duffing. delta=0.25, gamma=0.3. Image of Obj 1 at T=pi.




Duffing. delta=0.25, gamma=0.3. IC split map. 3x3 ICs in [-1,0]^2. T 0 to pi. 33 objs. Fine boxes (16x16) in Obj 1
0
-0.2
-0.4
-0.6
-0.8
-1
-1
-0.8
-0.6
-0.4
-0.2
0


Duffing. delta=0.25, gamma=0.3. Images of fine boxes (16x16) in Obj 1 at T=pi.
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-0.8
-1.4
-1.35
-1.3
-1.25
-1.2
-1.15
-1.1

Rigorous Reachability Analysis

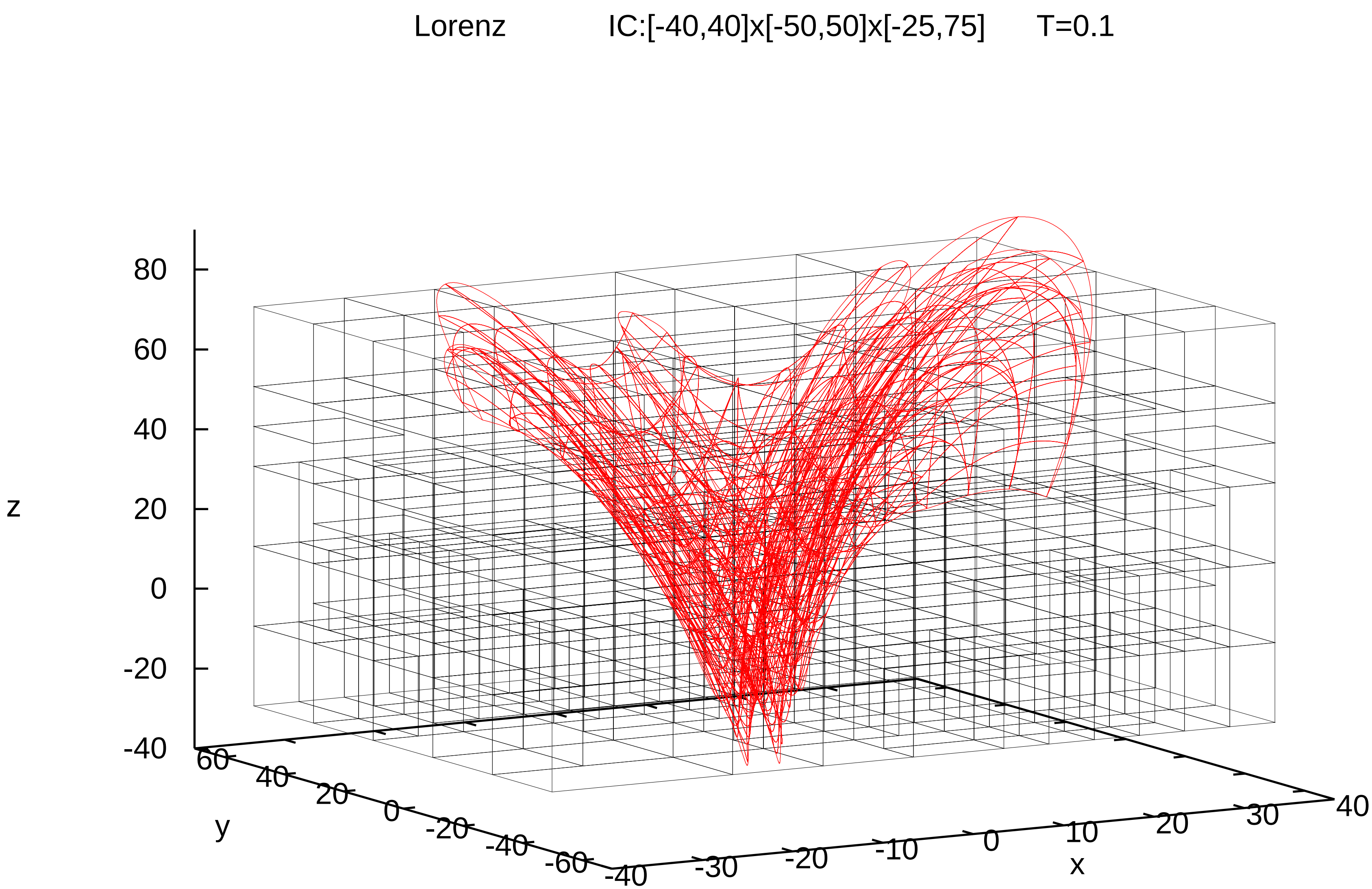
- Obtain a rigorous flow of a large area of interest by integrating the ODEs using Taylor models for the time step of interest
- During the verified integration process, conduct domain decompositions dynamically as needed
- Discretize the space into disjoint sub-regions for studying graphs
  - In Taylor models, it's possible to discretize the resulting flow in a similar manner as of dynamic domain decompositions.
  - The capability of dividing the Taylor model objects as needed – i.e., during the integration process, after obtaining the resulting flow – is a big advantage.
  - On the other hand, with the interval method, if further discretization is needed, it has to be done in the initial area of interest all over again.

Rigorous Integrations of the Lorenz System

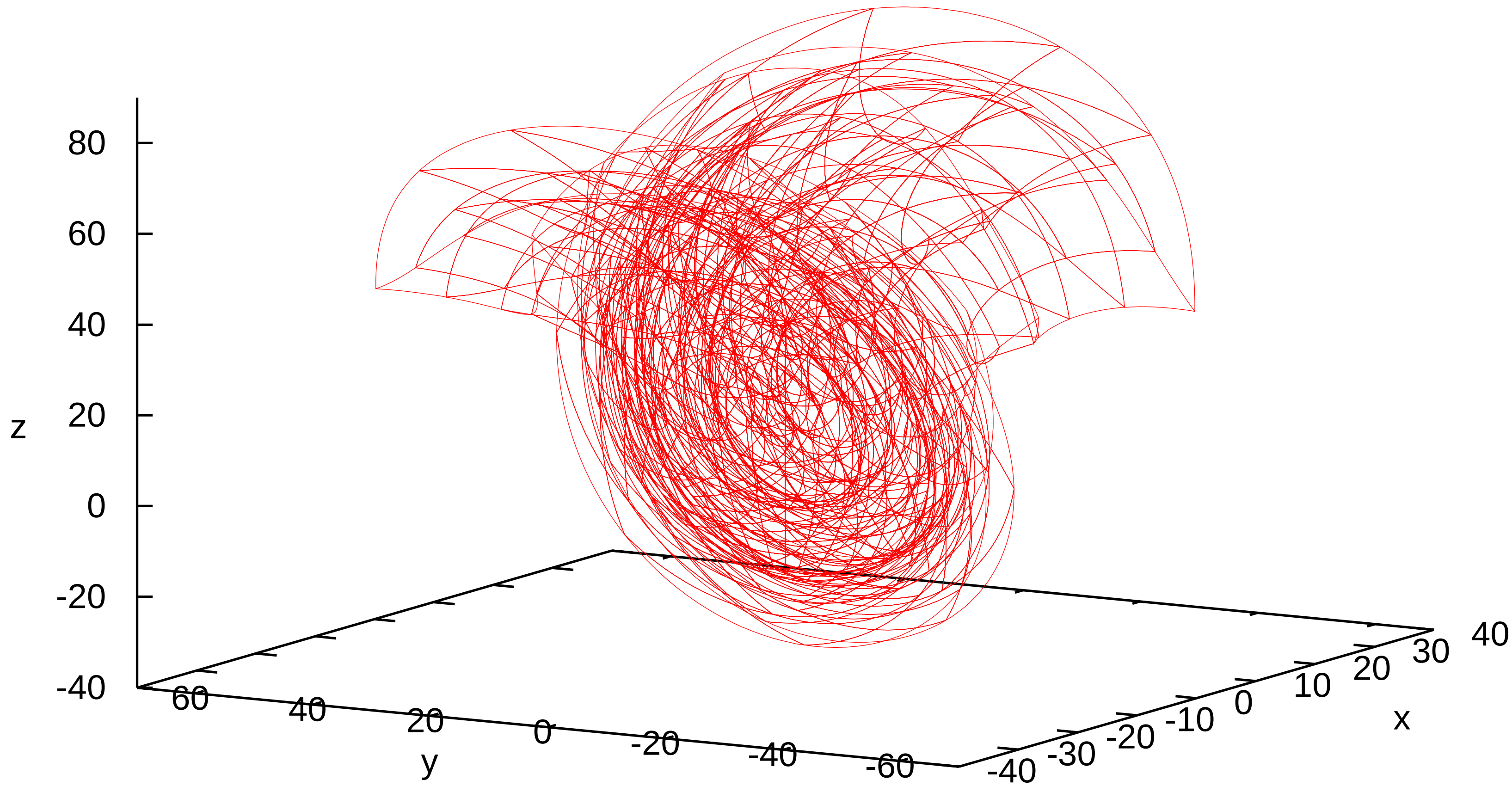
Rigorous flow integrations of large ranges of initial conditions have been computed using Taylor model based ODE integrators, particularly by COSY-VI version 3.

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

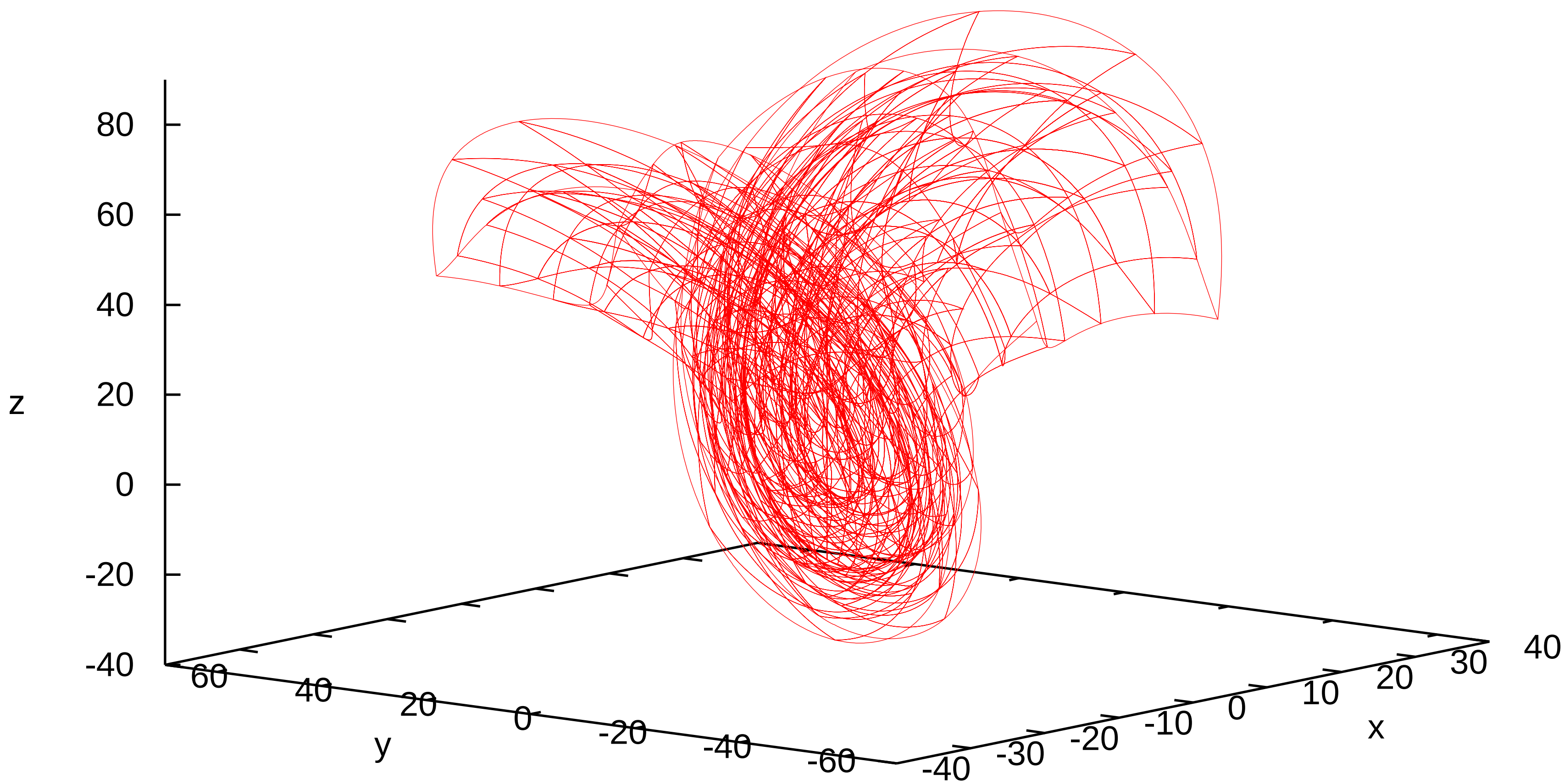
$$(x, y, z)|_0 = ([-40, 40], [-50, 50], [-25, 75])$$

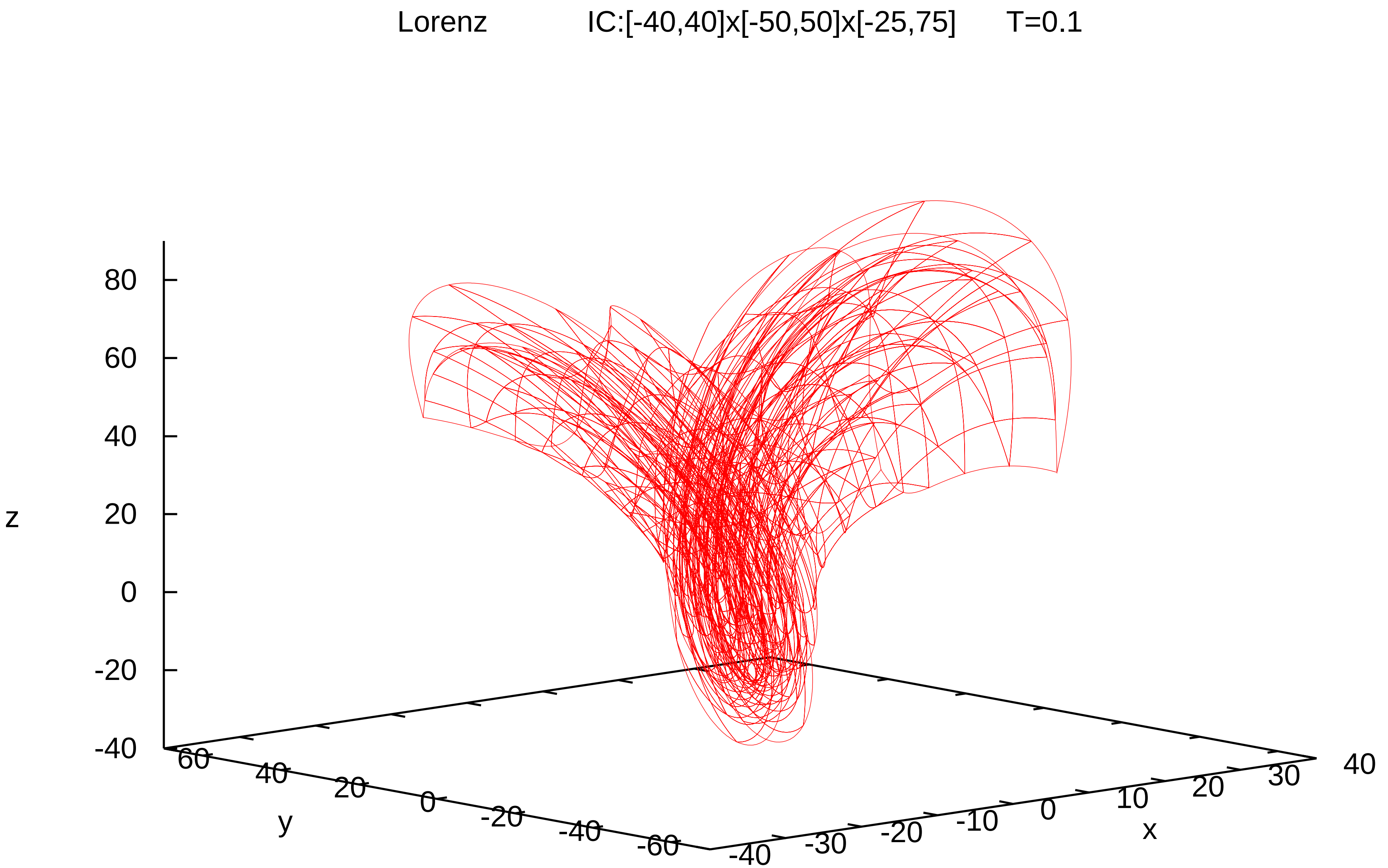

Lorenz IC:[-40,40]x[-50,50]x[-25,75] T=0.1
z
80
60
40
20
0
-20
-40
y
60
40
20
0
-20
-40
-60
x
-40
-30
-20
-10
0
10
20
30
40

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




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

Work in Progress

- Improvement of the Taylor model arithmetic package in COSY to allow arbitrarily high precision Taylor model computations
- Improvement of COSY-VI
  - Various schemes to conduct Poincare projections
  - Computations in parallel environment

Taylor Models 2017
Islamorada, Florida Keys
Dec 11-14

tm2017@taylormodel.org

tm2017.taylormodel.org

Photo: View from Meeting Room