Rigorous Bounds for the Errors of High-Order Transfer Maps

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Transfer Map Method

- The transfer map $\mathcal{M}$ is the flow of the system ODE.

$$\vec{z}_f = \mathcal{M}(\vec{z}_i, \vec{\delta}),$$

  where $\vec{z}_i$ and $\vec{z}_f$ are the initial and the final condition, $\vec{\delta}$ is system parameters.

Transfer Map Method and Differential Algebras

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  where $\vec{z}_i$ and $\vec{z}_f$ are the initial and the final condition, $\vec{\delta}$ is system parameters.

- For a repetitive system, only one cell transfer map has to be computed. Thus, it is much faster than ray tracing codes (i.e. tracing each individual particle through the system).
- The Differential Algebraic method allows a very efficient computation of high order Taylor transfer maps.
- The Normal Form method can be used for analysis of nonlinear behavior.

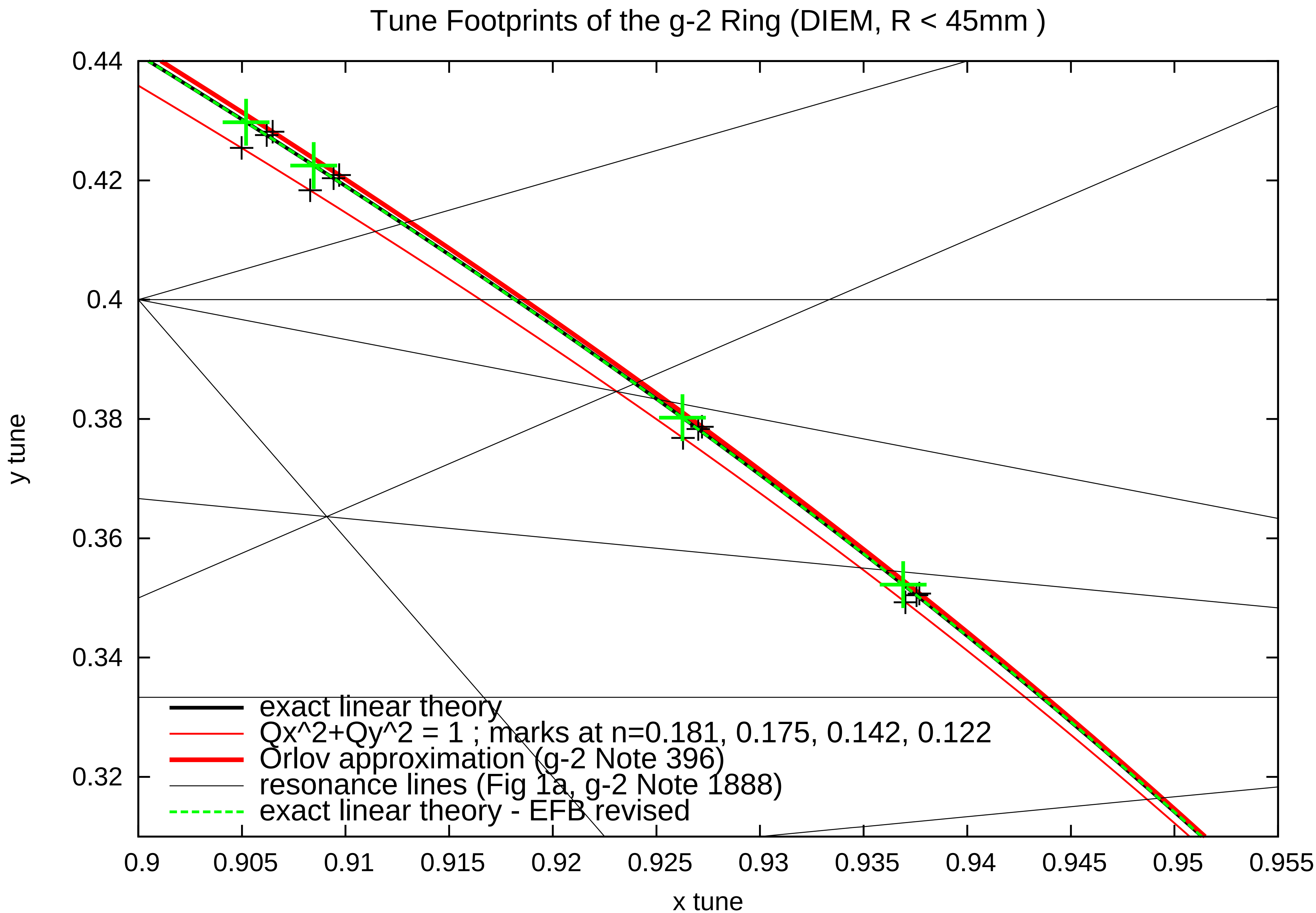
Differential Algebras (DA)

- it works to arbitrary order, and can keep system parameters in maps.
- very transparent algorithms; effort independent of computation order.

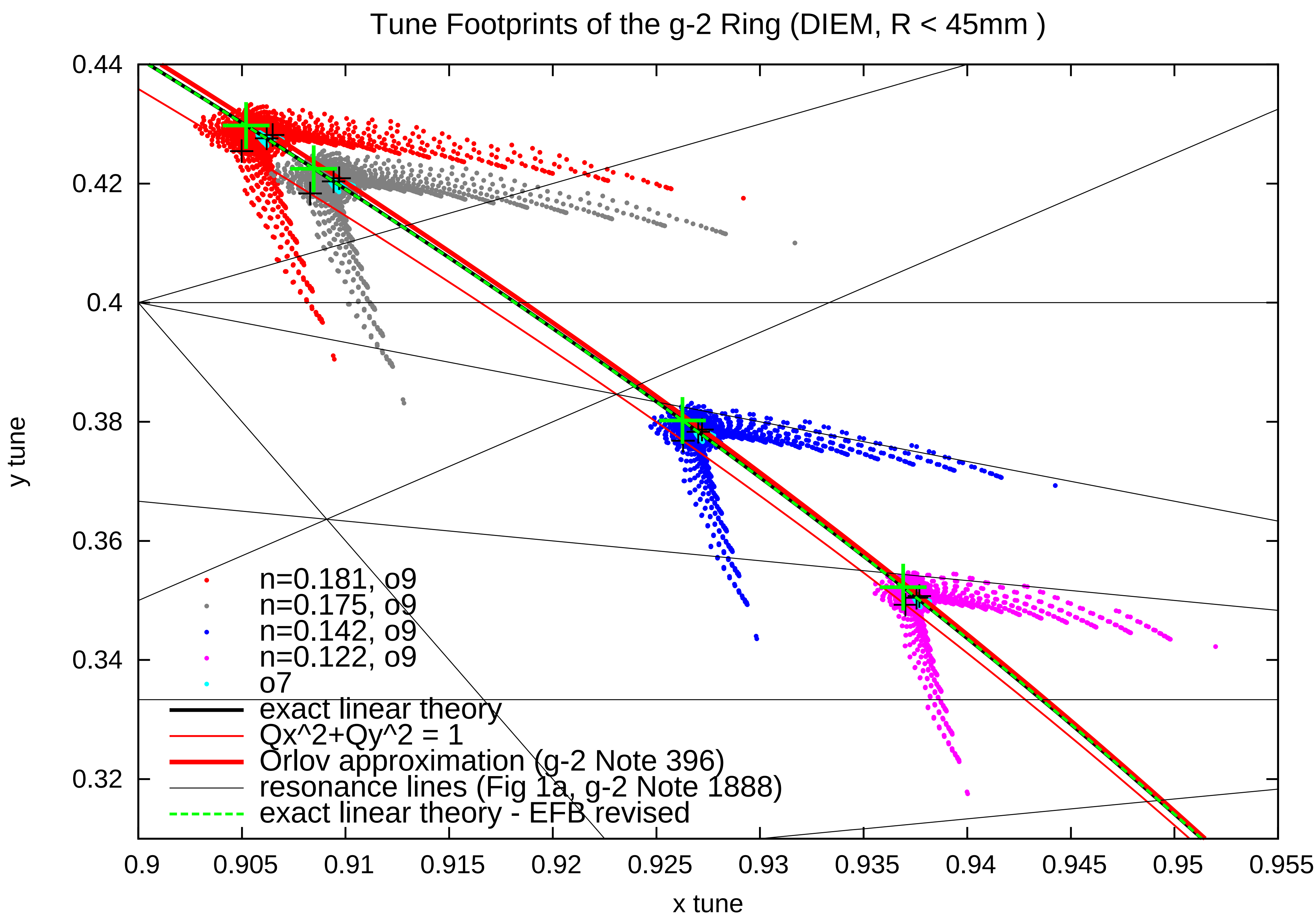
The code **COSY Infinity** has many tools and algorithms necessary.

High-Order Contributions

- Typically decreases as the order gets higher
- But, sometimes it is not the case



Tune Footprints of the g-2 Ring (DIEM, R < 45mm)
0.44
0.42
0.4
0.38
0.36
0.34
0.32
y tune
0.9
0.905
0.91
0.915
0.92
0.925
0.93
0.935
0.94
0.945
0.95
0.955
x tune
exact linear theory
Qx^2+Qy^2 = 1 ; marks at n=0.181, 0.175, 0.142, 0.122
Orlov approximation (g-2 Note 396)
resonance lines (Fig 1a, g-2 Note 1888)
exact linear theory - EFB revised



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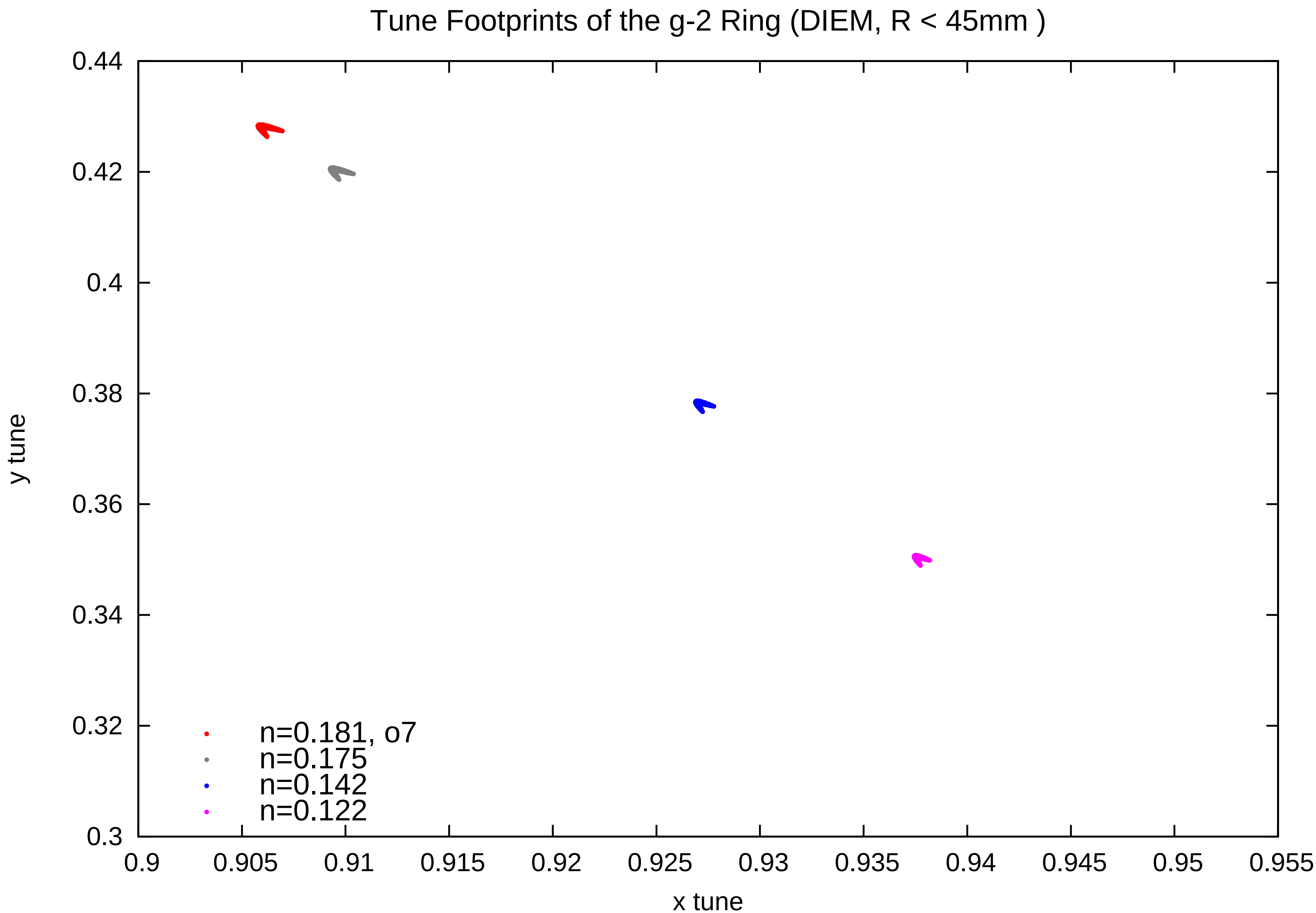

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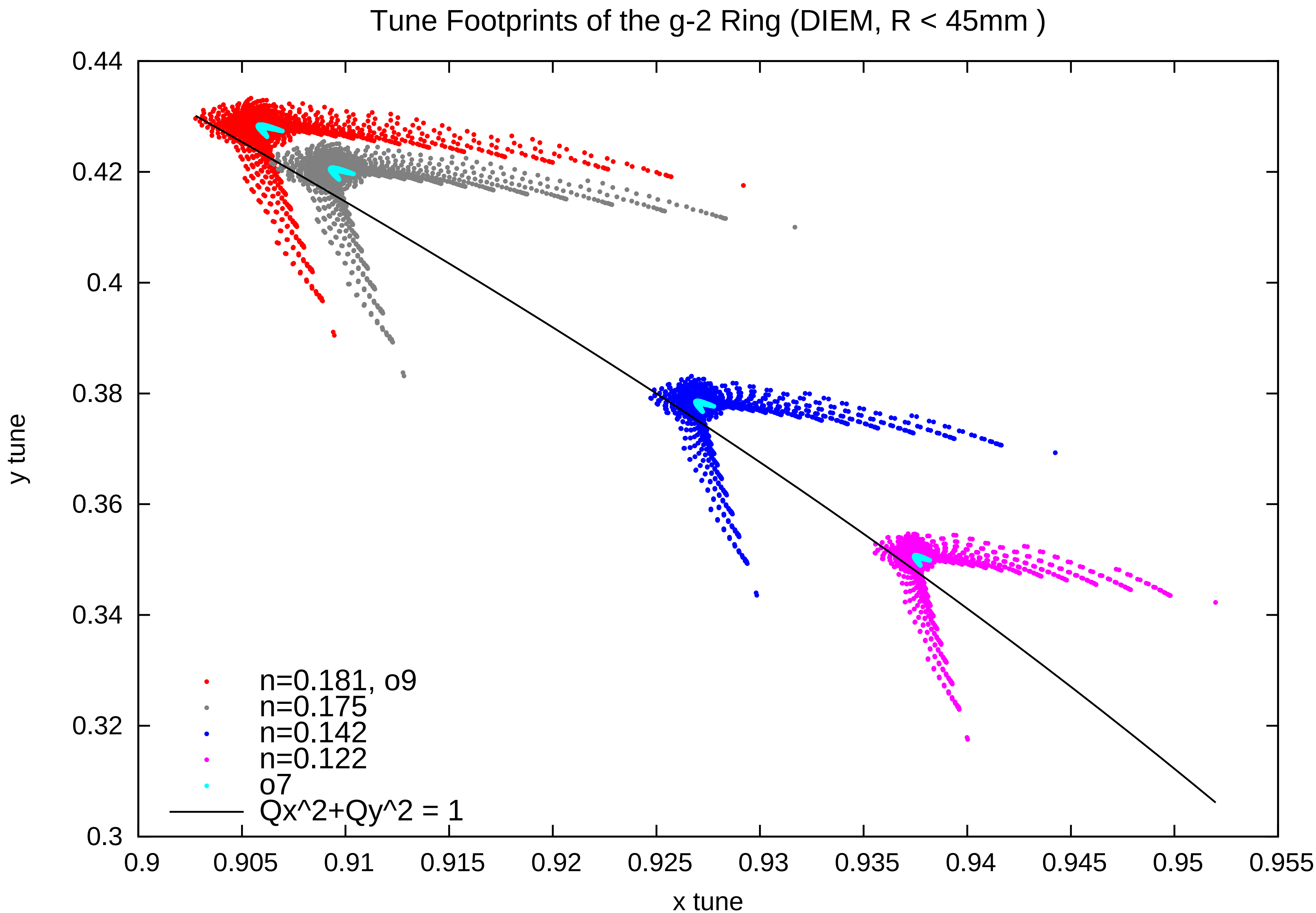
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High-Order Contributions

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- For example, the Muon g-2 Ring has large 9^{th} order contributions

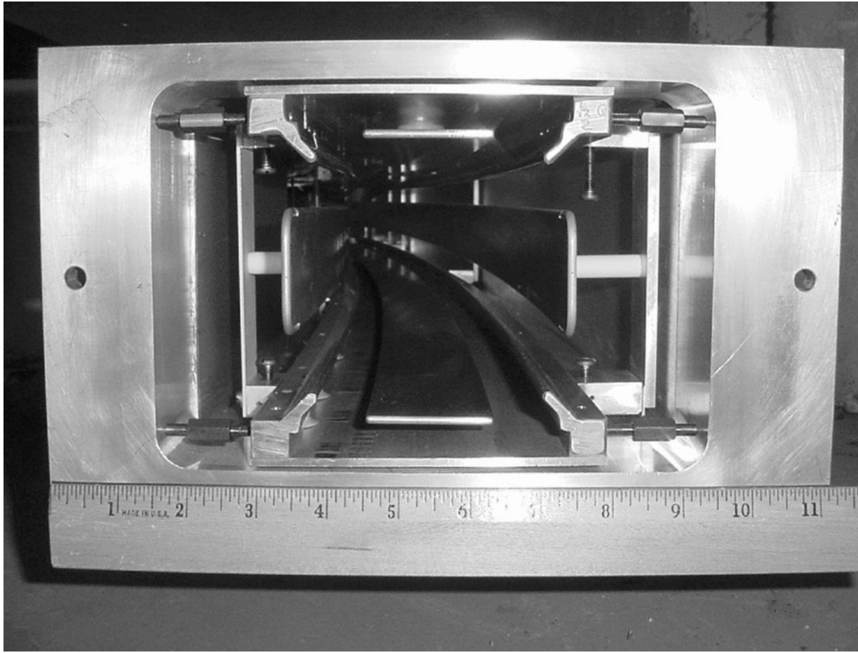

Fig. 6. A photograph taken from the end of a vacuum chamber housing the quadrupole plates; the ring center is on the left. The distance between quadrupole plates at equal potential is 10 cm. The bottom left and the top right rails are where the cable NMR trolley rides when measuring the magnetic field. The other two rails were used to keep the symmetry in the quadrupole region. The ruler units are in inches.

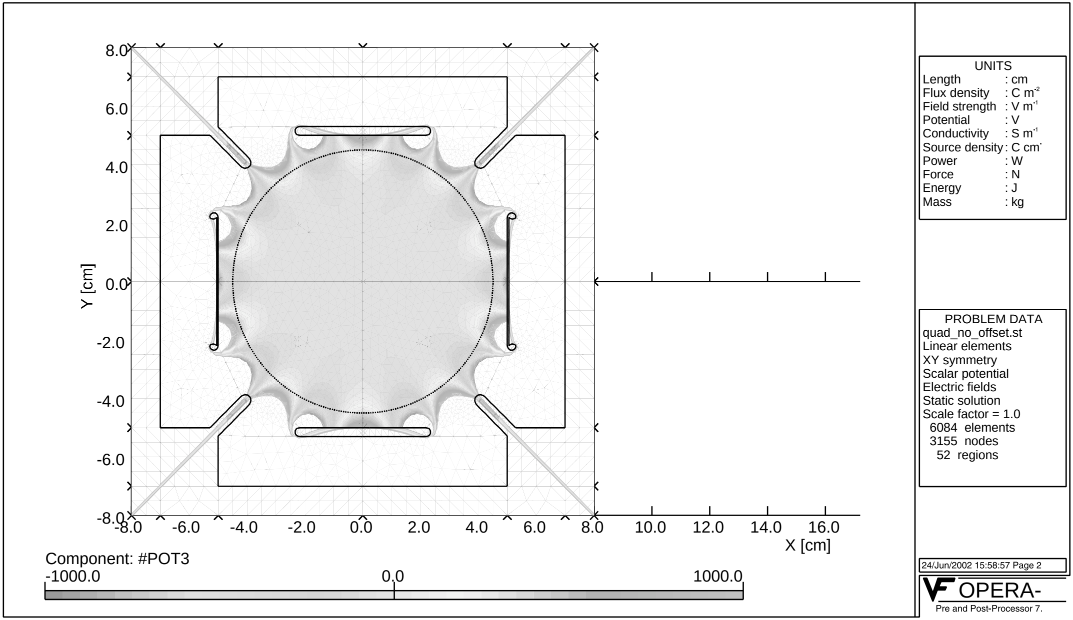

Fig. 18. The plotted parameter #POT3 is the regular potential (plotted in Fig. 17) minus the quadrupole potential and is defined as #POT3 $= \mathrm{POT} - (\mathrm{POT}_{2\,\mathrm{cm}}/2^2)*(x^2 - y^2)$. The dominance of the 20 pole, $b_{10}/b_2 = 1.9\%$ on the circle with $r = 4.5$ cm, is clearly visible.

High-Order Contributions

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  - due to the 20th pole components in the Electrostatic Quads

Related Talks

- Nonlinear Beam Dynamics, DA (Differential Algebras), COSY INFINITY
  Sat 05/10, **9:30am**, Main Auditorium, **Martin Berz**
  "Nonlinear beam dynamics tools for
  field treatment, symplectic tracking and spin in COSY INFINITY"
- Muon g-2 Experiment, Beam Dynamics, Simulations
  - The Storage Ring
  Fri 04/10, **9:00am**, Main Auditorium, **Eremey Valetov**
  "Beam Dynamics of the Muon g-2 Experiment"
  - The Beam Delivery System
  Thu 03/10, **4:50pm**, Main Auditorium, **Eremey Valetov**
  "New Muon Campus Simulations for
  the Muon g-2 Experiment at Fermilab"

High-Order Contributions

- Typically decreases as the order gets higher
- But, sometimes it is not the case
- For example, the Muon g-2 Ring has large 9th order contributions
  - due to the 20th pole components in the Electrostatic Quads
- How to catch known/unknown effects from the higher-order contributions
  - Use rigorous computation methods
    * Interval Methods?
    * DA related methods?

Interval Arithmetic

A method to perform guaranteed calculations on computer by presenting all numbers by intervals.

$$[a,b]+[c,d]=[a+c,b+d]$$
$$[a,b]-[c,d]=[a-d,b-c]$$
$$[a,b]\cdot[c,d]=[\min(ac,ad,bc,bd),\max(ac,ad,bc,bd)]$$
$$[a,b]/[c,d]=[\min(a/c,a/d,b/c,b/d),\max(a/c,a/d,b/c,b/d)]$$

Not a group because $[a,b]-[c,d]\neq[0,0]$ unless $a=b, c=d$.
In particular,

$$[a,b]-[a,b]=[a-b,b-a]$$
$$[a,b]/[a,b]=[\min(1,a/b,b/a),\max(1,a/b,b/a)]$$

Thus, operations lead to over estimation, which can become large with time to blow up.

Verified ODE Integrations

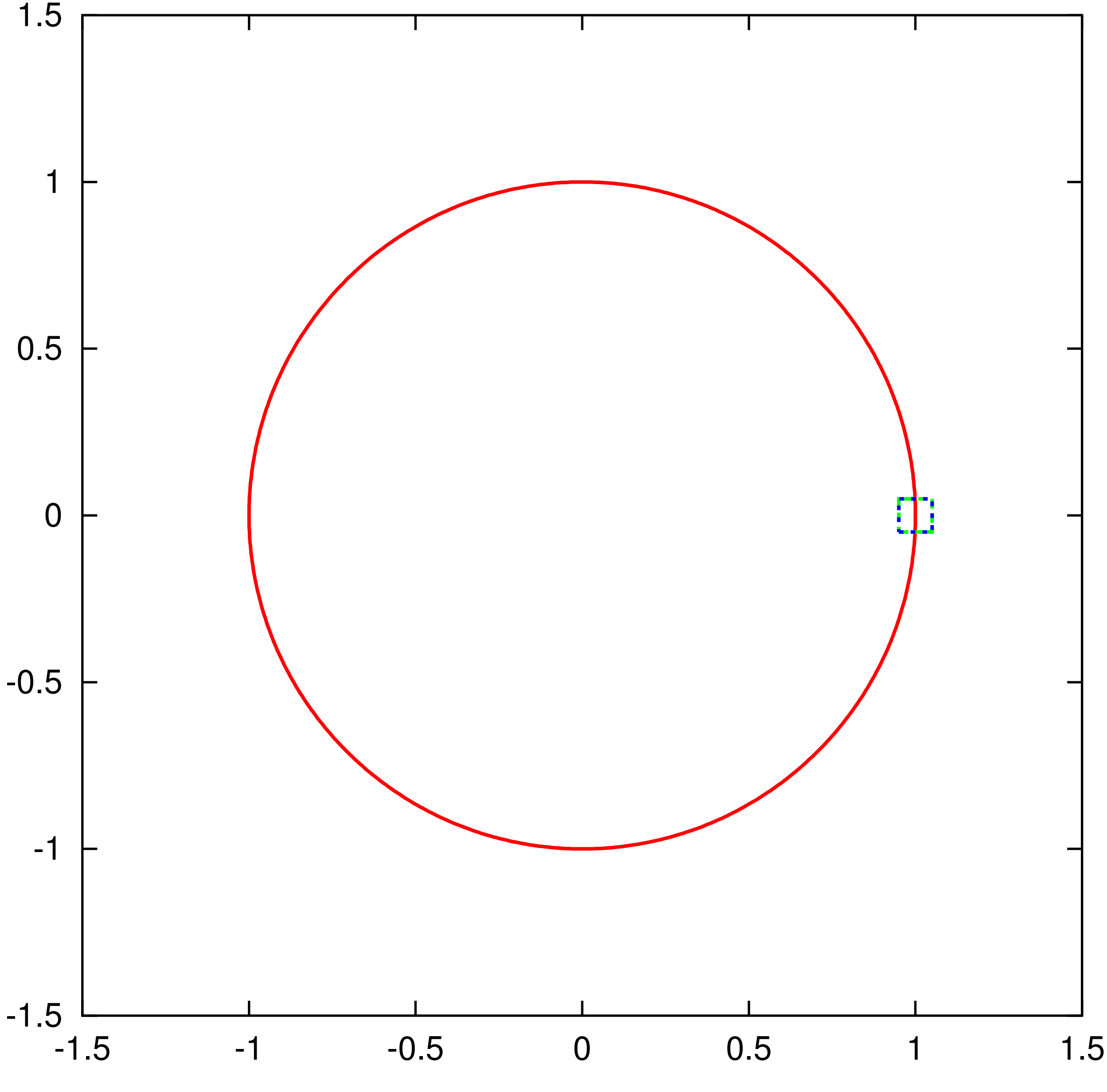
Using the interval method, typical issues in general are

- overestimation
- the dependency problem
- the dimensionality curse

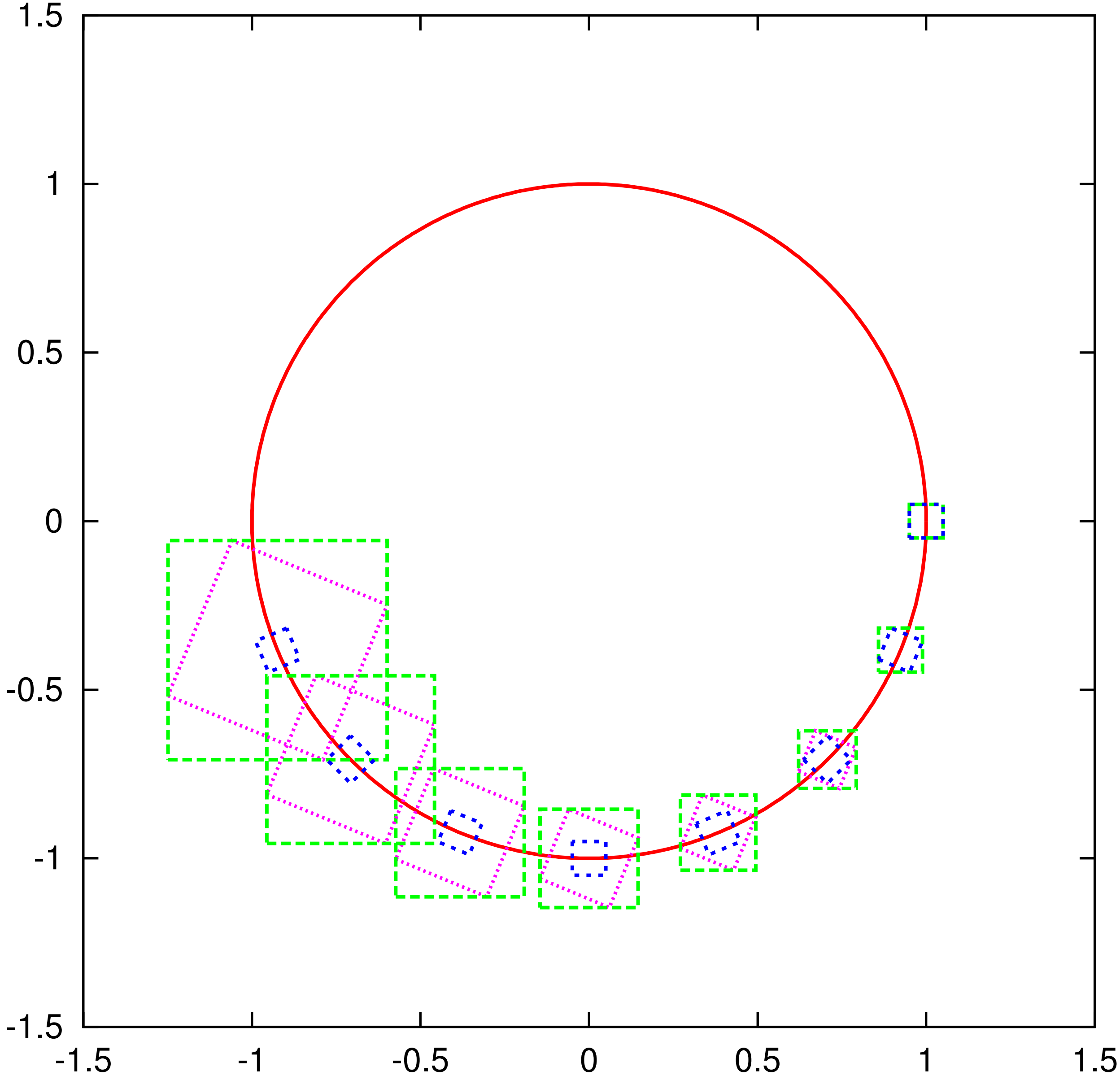
When geometric transformations of sets are involved,
such as ODE integrations, there arises an additional issue

- the wrapping effect

To transport a large phase space volume with validation,



Over Estimation has to be controlled.



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How to handle the wrapping effect in

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

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

Taylor models

For $f : D \subset R^v \to R$ that is $(n+1)$ times continuously partially differentiable,

$P(x - x_0)$: the n-th order Taylor polynomial of f around $x_0 \in D$

e: a small remainder bounding set of the deviation of P from f

$$f(x) - P(x - x_0) \in e, \quad \forall x \in D \quad \text{where} \quad x_0 \in D.$$

We call the combination of P and e as a Taylor model.

$$T = (P, e) = P + e.$$

T depends on the order n, the domain D, and the expansion point x_0.

Taylor Model Arithmetic

Define Taylor model addition, multiplication for $T_1 = (P_1, e_1)$, $T_2 = (P_2, e_2)$ with the same conditions $\{n, D, x_0\}$.

$$\begin{aligned} T_1 + T_2 &= (P_1 + P_2, e_1 + e_2), \\ T_1 \cdot T_2 &= (P_{1\cdot 2}, e_{1\cdot 2}). \end{aligned}$$

$P_{1\cdot 2}$: the part of the polynomial $P_1 \cdot P_2$ up to the order n.
$e_{1\cdot 2} = B(P_{>n}) + B(P_1) \cdot e_2 + B(P_2) \cdot e_1 + e_1 \cdot e_2$.
$P_{>n}$: the higher order part from $(n+1)$ to $2n$.
$B(P)$: an enclosure bound of P over D.
Operations on sets e_i follow set theoretical operations and outward rounding.

Taylor Model Arithmetic – and Intrinsic Functions

Define Taylor model addition, multiplication for $T_1 = (P_1, e_1)$, $T_2 = (P_2, e_2)$ with the same conditions $\{n, D, x_0\}$.

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Intrinsic functions for Taylor models can be defined by performing various manipulations using these. The particularly nice is ∂_i^{-1}, antiderivation, being a Taylor model intrinsic function; because obtaining the integral with respect to variable x_i of P is straightforward, so is an integral of a Taylor model.

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.

Taylor Models for the Flow

Goal: Determine a Taylor model, consisting of a Taylor Polynomial and an interval bound for the remainder, for the flow of the differential equation

$$\frac{d}{dt}\vec{r}(t) = \vec{F}(\vec{r}(t), t)$$

where $\vec{F}$ is sufficiently differentiable. The Remainder Bound should be fully rigorous for all initial conditions $\vec{r}_0$ and times t that satisfy

$$\vec{r}_0 \in [\vec{r}_{01}, \vec{r}_{02}] = \vec{B}$$
$$t \in [t_0, t_1].$$

In particular, $\vec{r}_0$ itself may be a Taylor model, as long as its range is known to lie in $\vec{B}$.

The Use of Schauder's Theorem

Re-write differential equation as integral equation

$$\vec{r}(t) = \vec{r}_0 + \int_{t_0}^{t} \vec{F}(\vec{r}(t'), t')\, dt'.$$

Now introduce the operator

$$A : \vec{C}^0[t_0, t_1] \to \vec{C}^0[t_0, t_1]$$

on space of continuous functions via

$$A\left(\vec{f}\right)(t) = \vec{r}_0 + \int_{t_0}^{t} \vec{F}\left(\vec{f}(t'), t'\right) dt'.$$

Then the solution of ODE is transformed to a fixed-point problem on space of continuous functions

$$\vec{r} = A(\vec{r}).$$

Theorem (Schauder): *Let A be a continuous operator on the Banach Space X. Let $M \subset X$ be compact and convex, and let $A(M) \subset M$. Then A has a fixed point in M, i.e. there is an $\vec{r} \in M$ such that $A(\vec{r}) = \vec{r}$.*

The Polynomial of the Self-Including Set

Attempt sets M^* of the form

$$M^* = M_{\vec{P}^* + \vec{I}^*} \text{ where}$$
$$\vec{P}^* = \mathcal{M}_n(\vec{r}_0, t),$$

the n-th order Taylor expansion of the flow of the ODE. It is to be expected that $\vec{I}^*$ can be chosen smaller and smaller as order n of $\vec{P}^*$ increases.

This requires knowledge of nth order flow $\mathcal{M}_n(\vec{r}_0, t)$, including time dependence. It can be obtained by iterating in polynomial arithmetic, or Taylor models without treatment of a remainder. To this end, one chooses an initial function $\mathcal{M}_n^{(0)}(\vec{r}, t) = \mathcal{I}$, where $\mathcal{I}$ is the identity function, and then iteratively determines

$$\mathcal{M}_n^{(k+1)} =_n A(\mathcal{M}_n^{(k)}).$$

This process converges to the exact result $\mathcal{M}_n$ in exactly n steps.

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

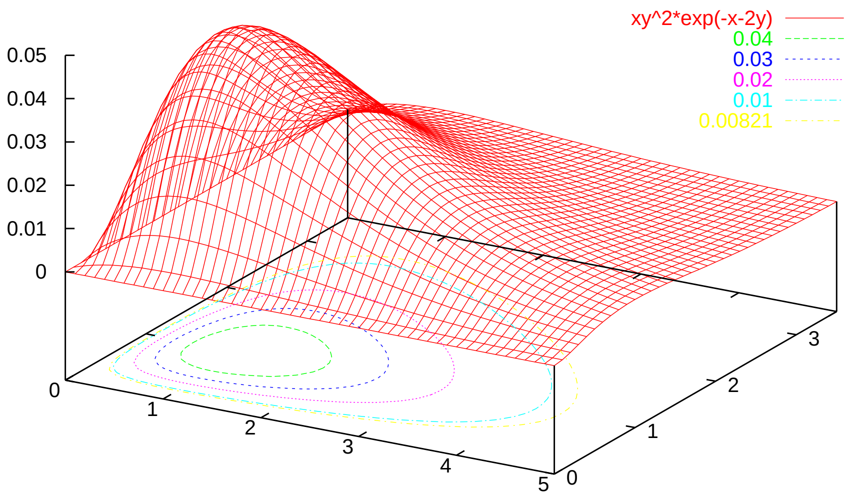
$$C(x_1, x_2) = x_1 x_2^2 e^{-x_1 - 2x_2} = \text{Constant}$$

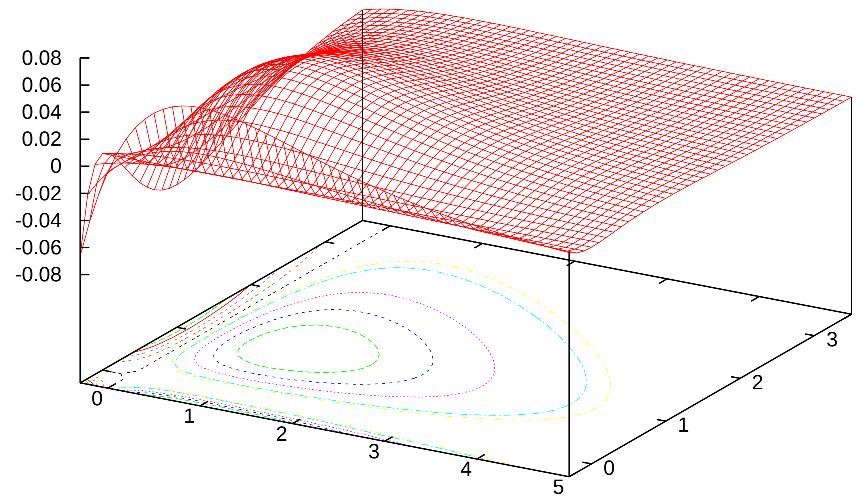
Trajectories of the Volterra Equations

The solutions have to satisfy the constraint

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

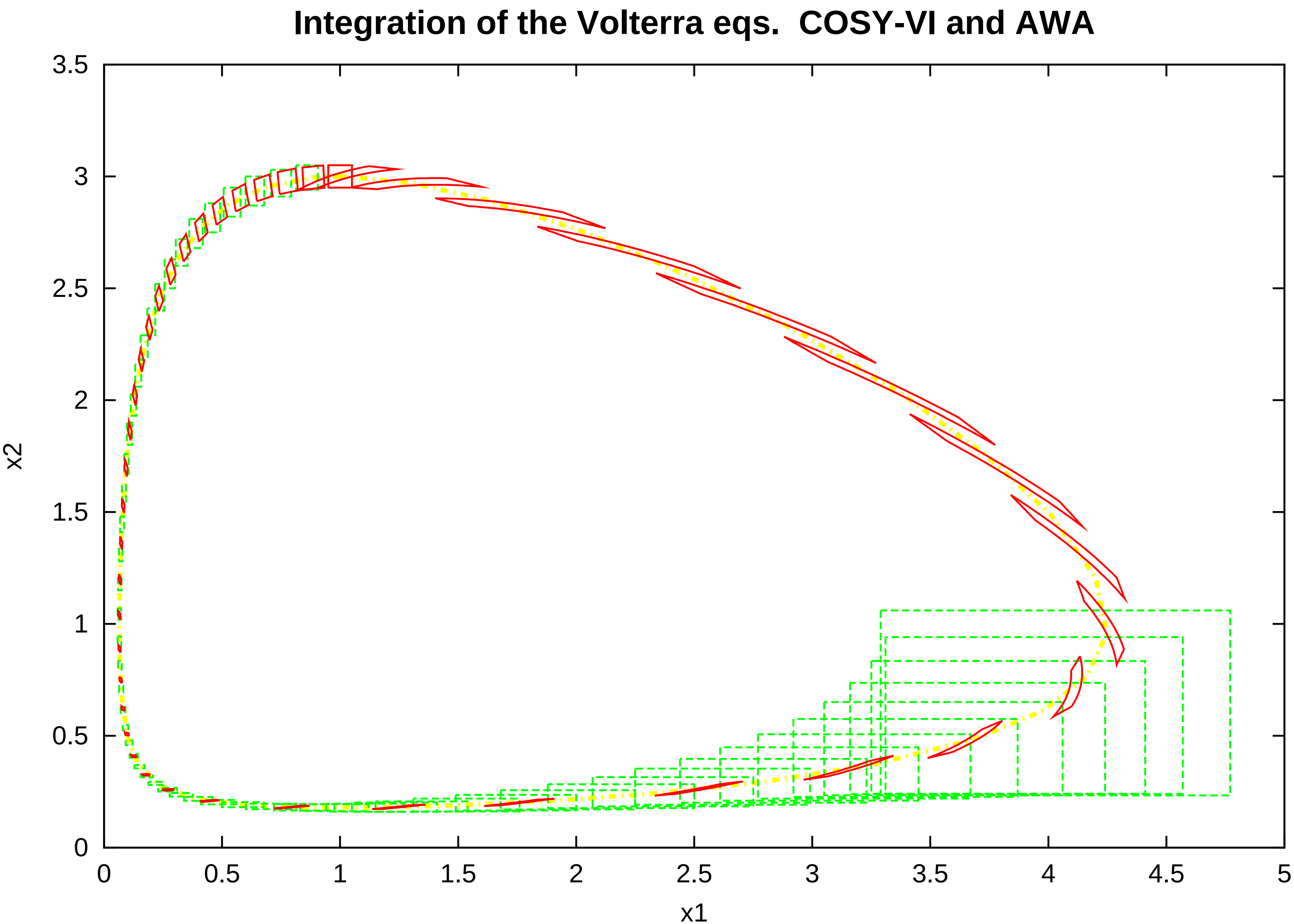
so the trajectories follow the contour lines of $C(x_1, x_2)$.





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

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
x1
3.5
3
2.5
2
1.5
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0
0.5
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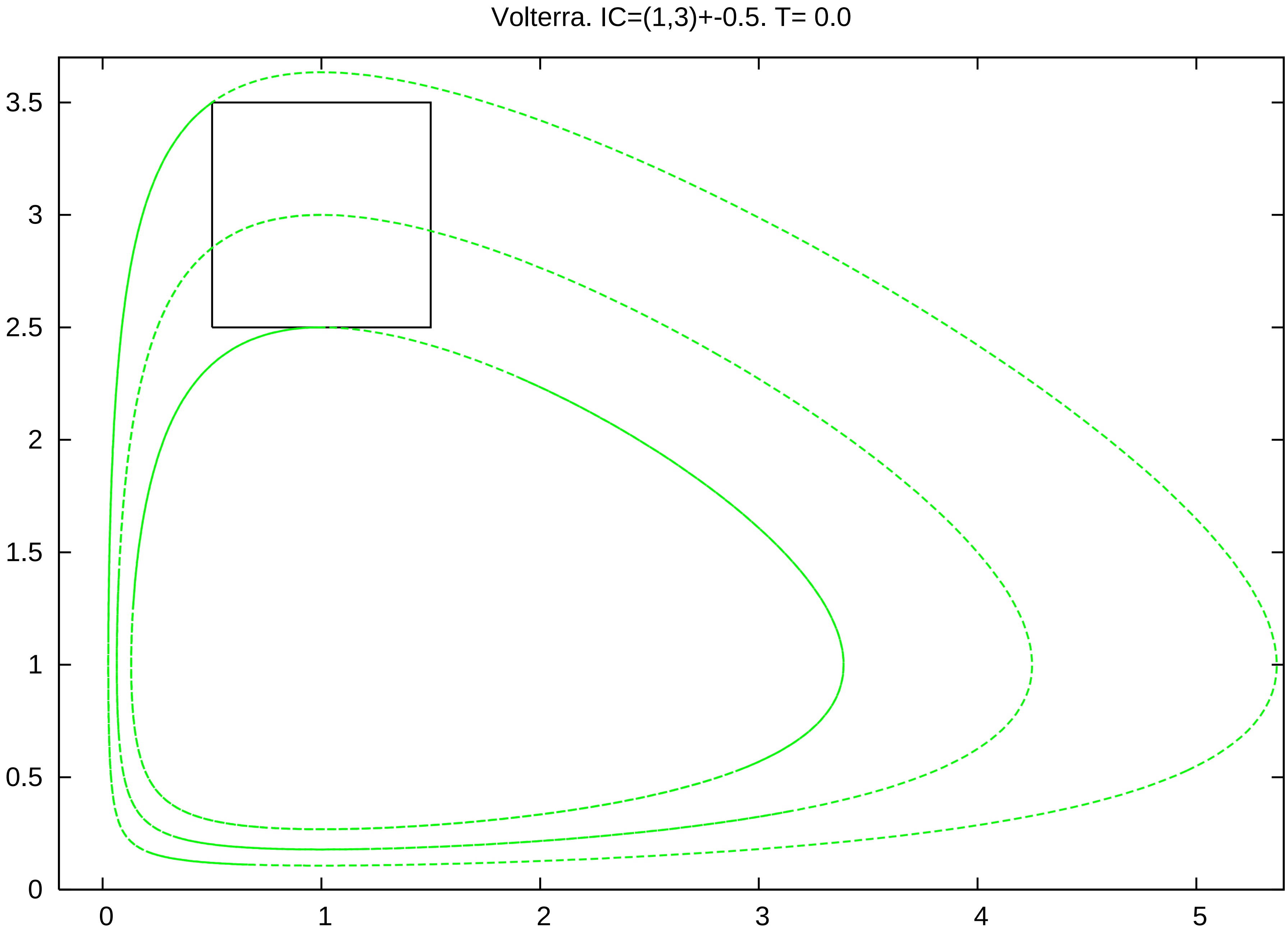
3.5
4
4.5
5



Volterra. IC=(1,3)+-0.5. T= 0.0
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5

Step Size Control

Step size control to maintain approximate error ε in each step. Based on a suite of tests:

1. Utilize the **Reference Orbit.** Extrapolate the size of coefficients for estimate of remainder error, scale so that it reaches and get Δt_1. Goes back to Moore in 1960s. This is one of conveniences when using Taylor integrators.
2. Utilize the **Flow.** Compute flow time step with Δt_1.Extrapolate the contributions of each order of flow for estimate of remainder error to get update Δt_2.
3. Utilize a **Correction factor** c to account for overestimation in TM arithmetic as $c = \sqrt[n+1]{|R|/\varepsilon}$. Largely a measure of complexity of ODE. Dynamically update the correction factor.
4. Perform verification attempt for $\Delta t_3 = c \cdot \Delta t_2$

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:

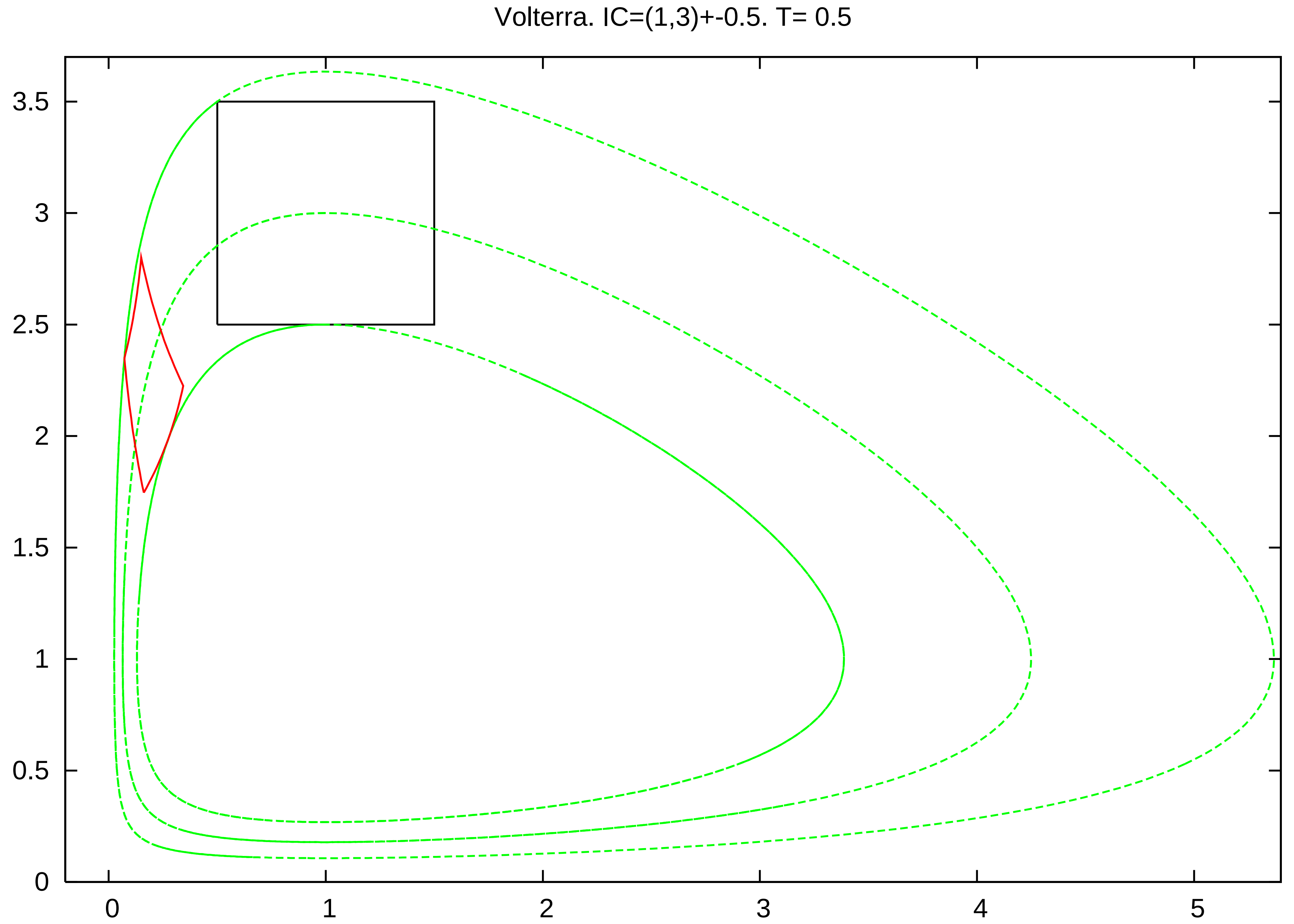
- Utilize "First-in-last-out" stack; minimizes stack length. Special adjustments for stack management in a parallel environment, including load balancing.
- Outlook: also dynamic order control for dependence on initial conditions

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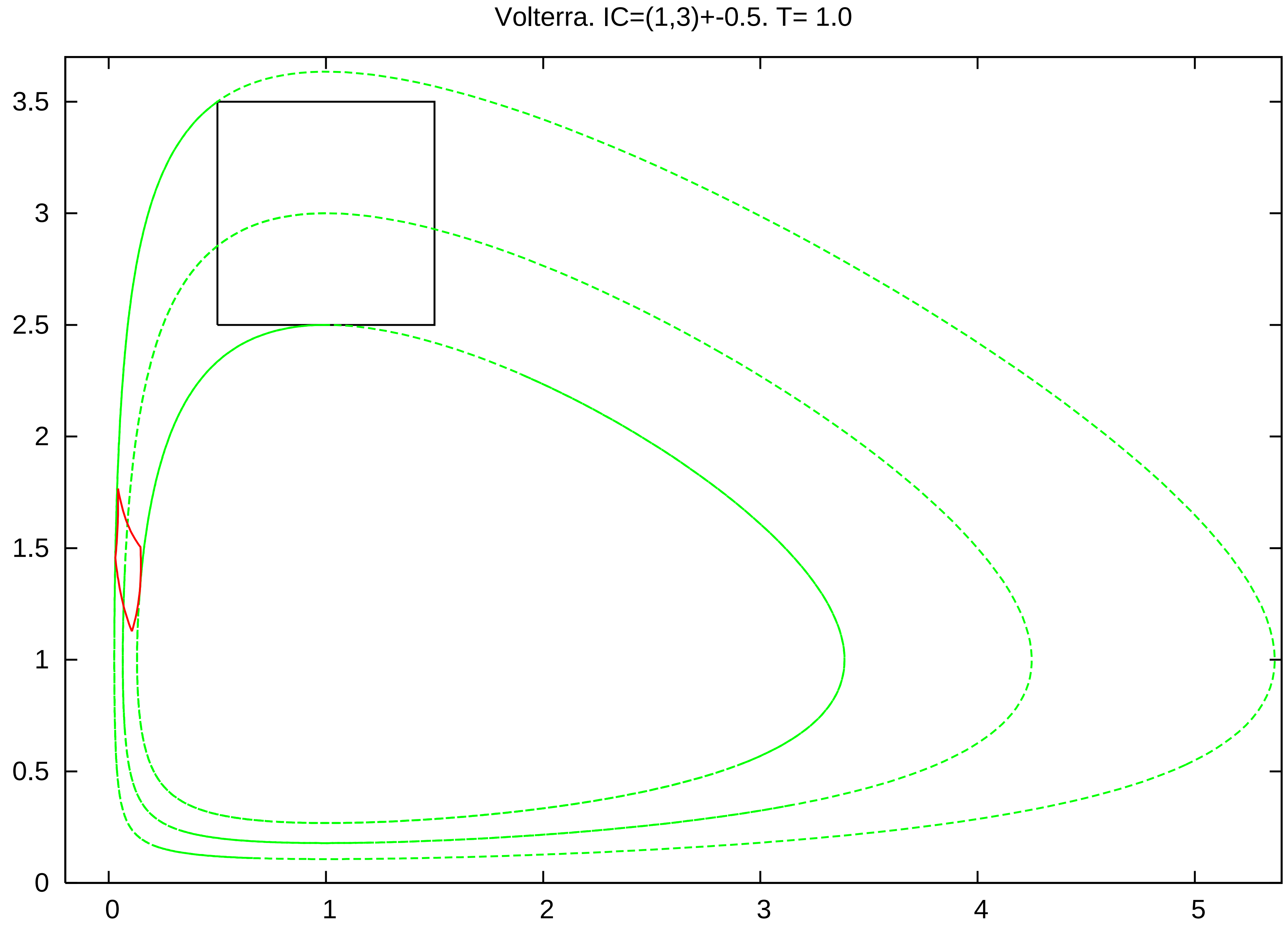
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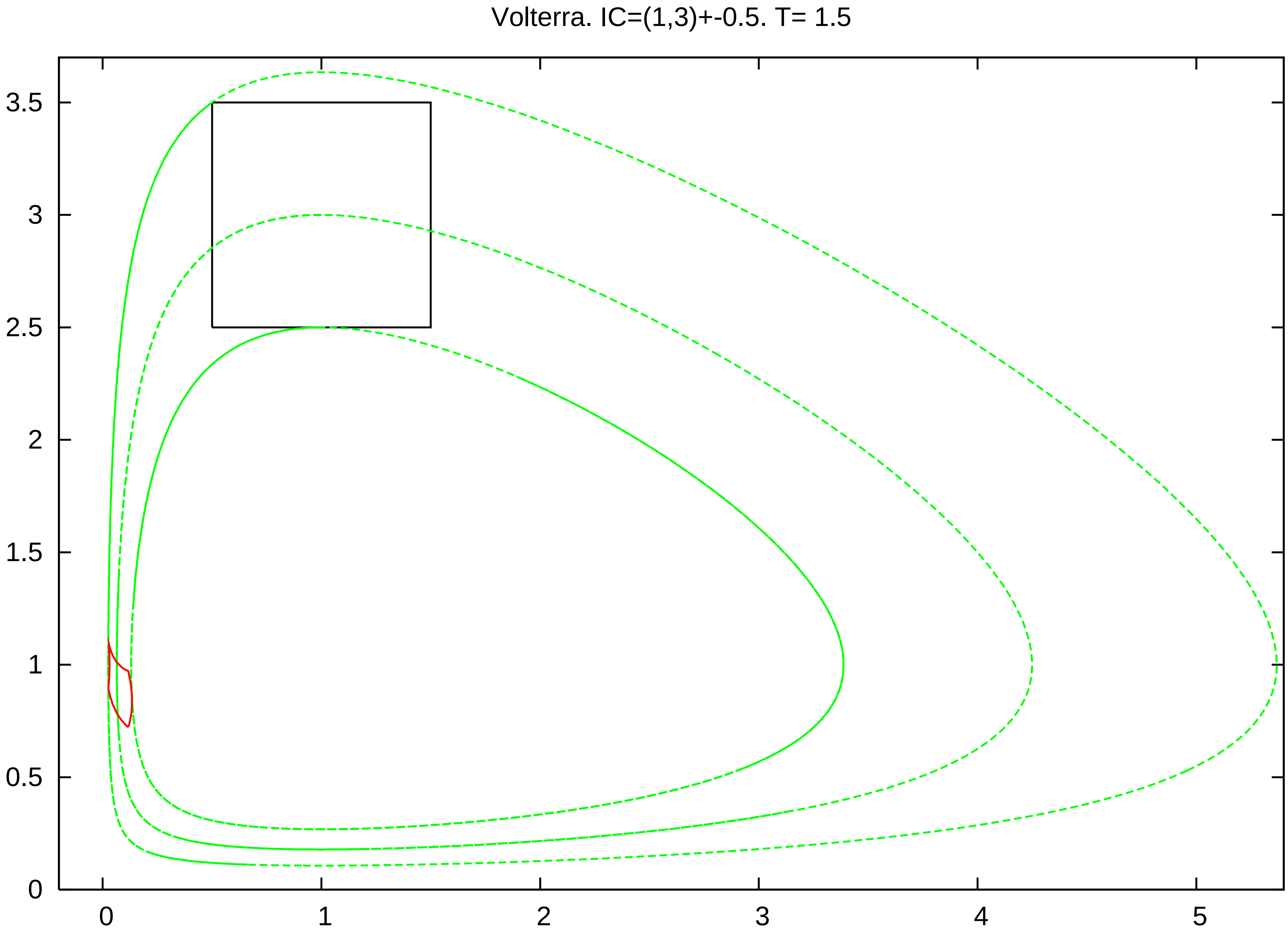
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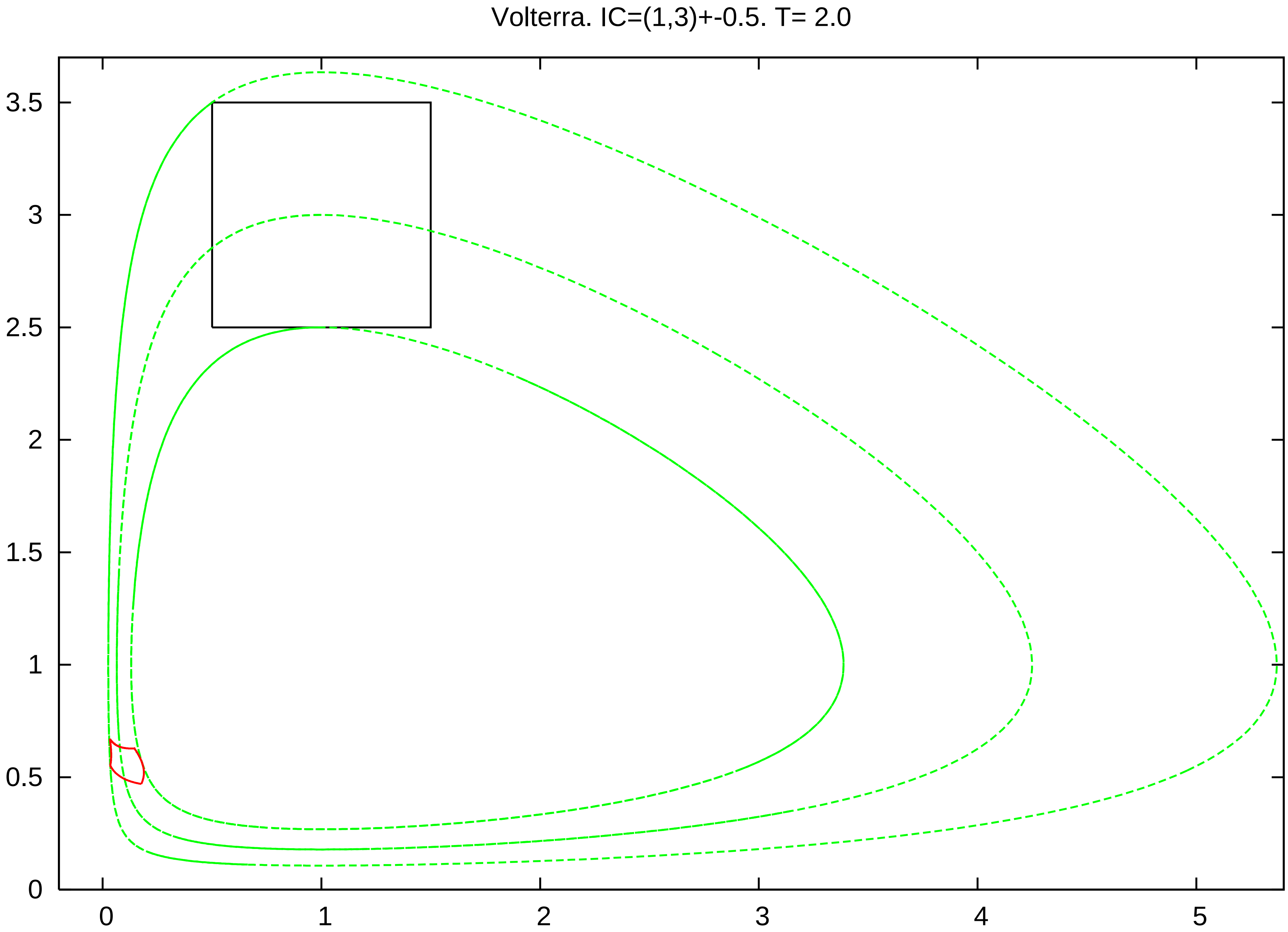

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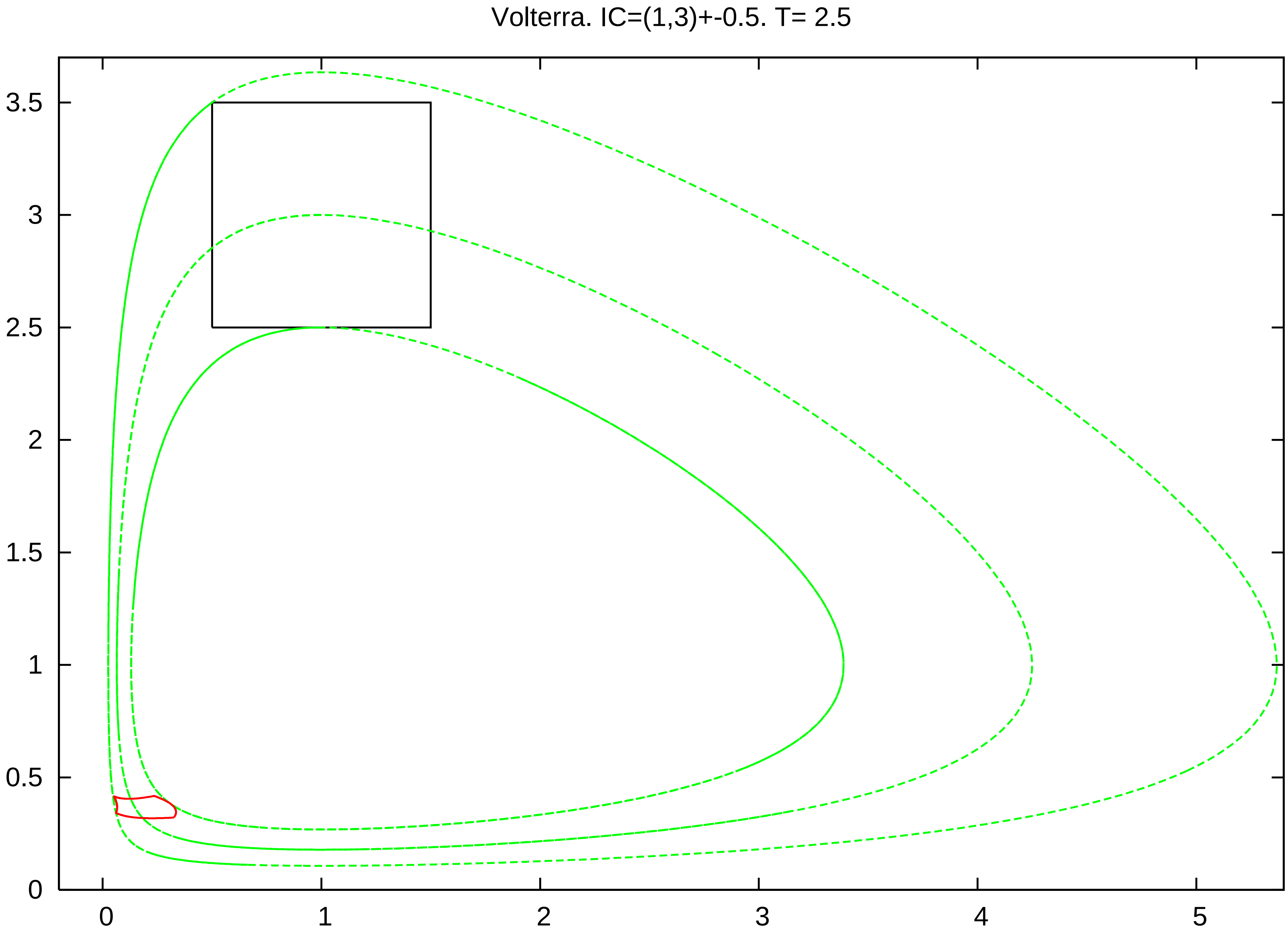
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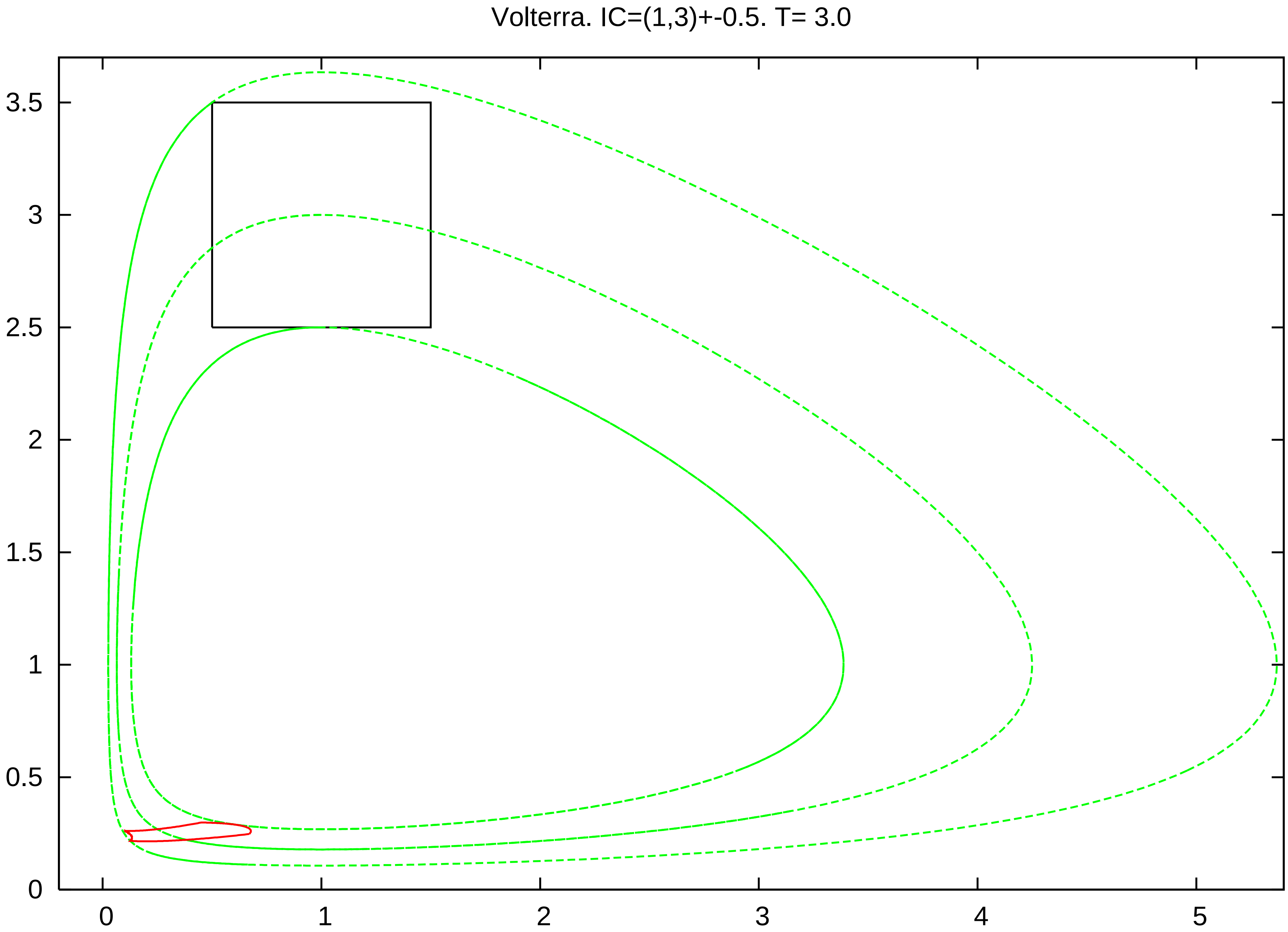
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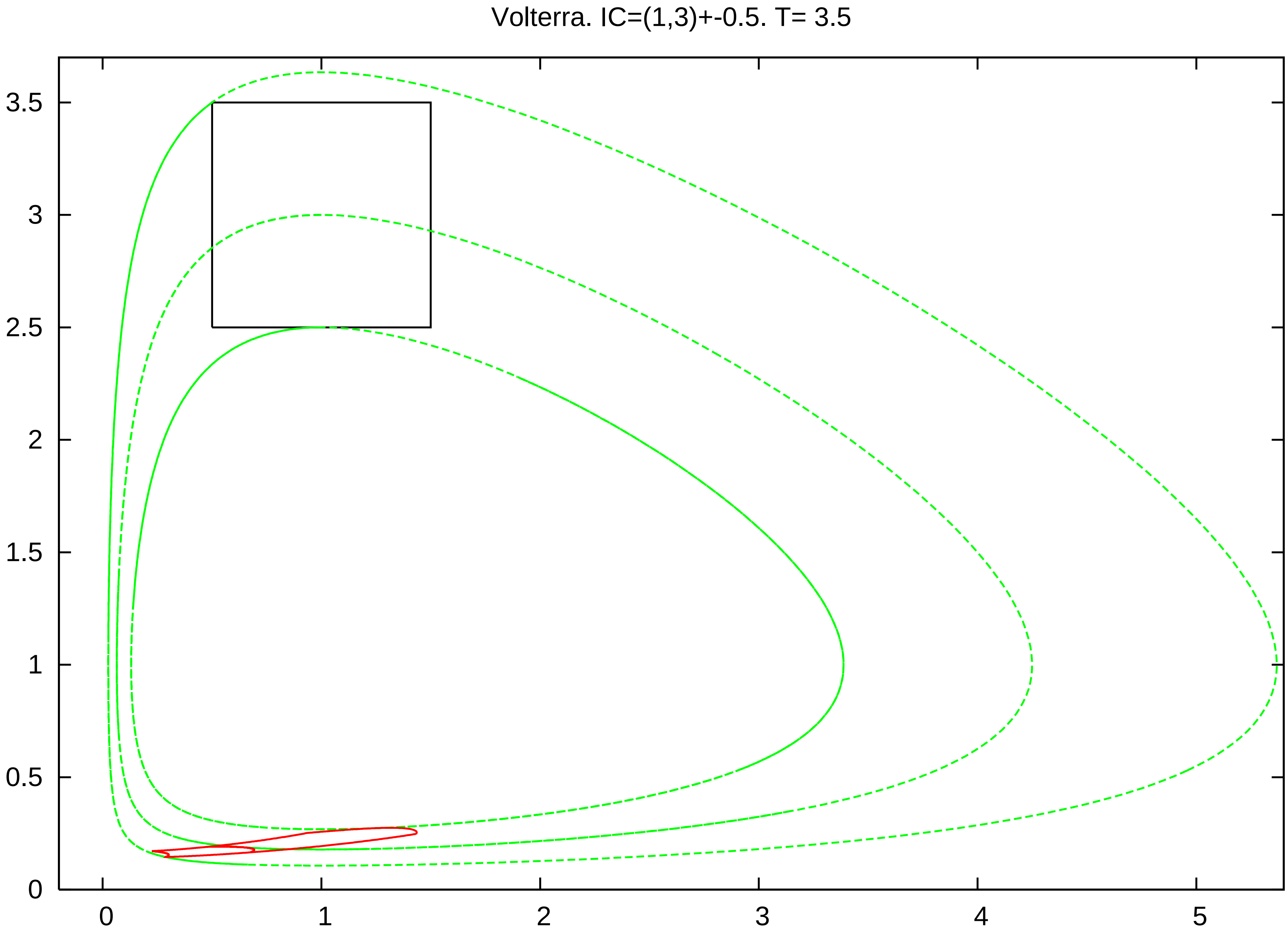
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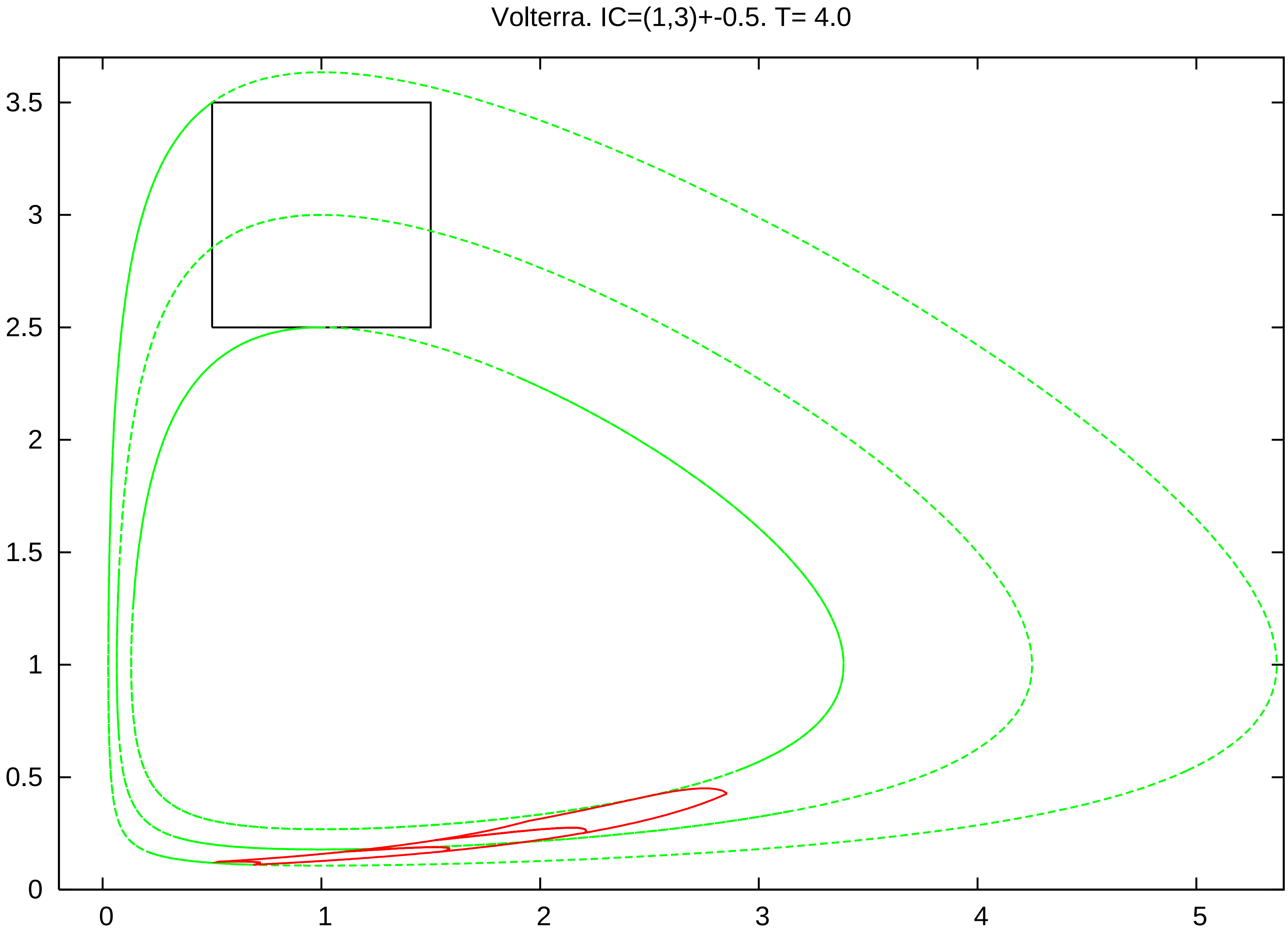
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0.5
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3.5
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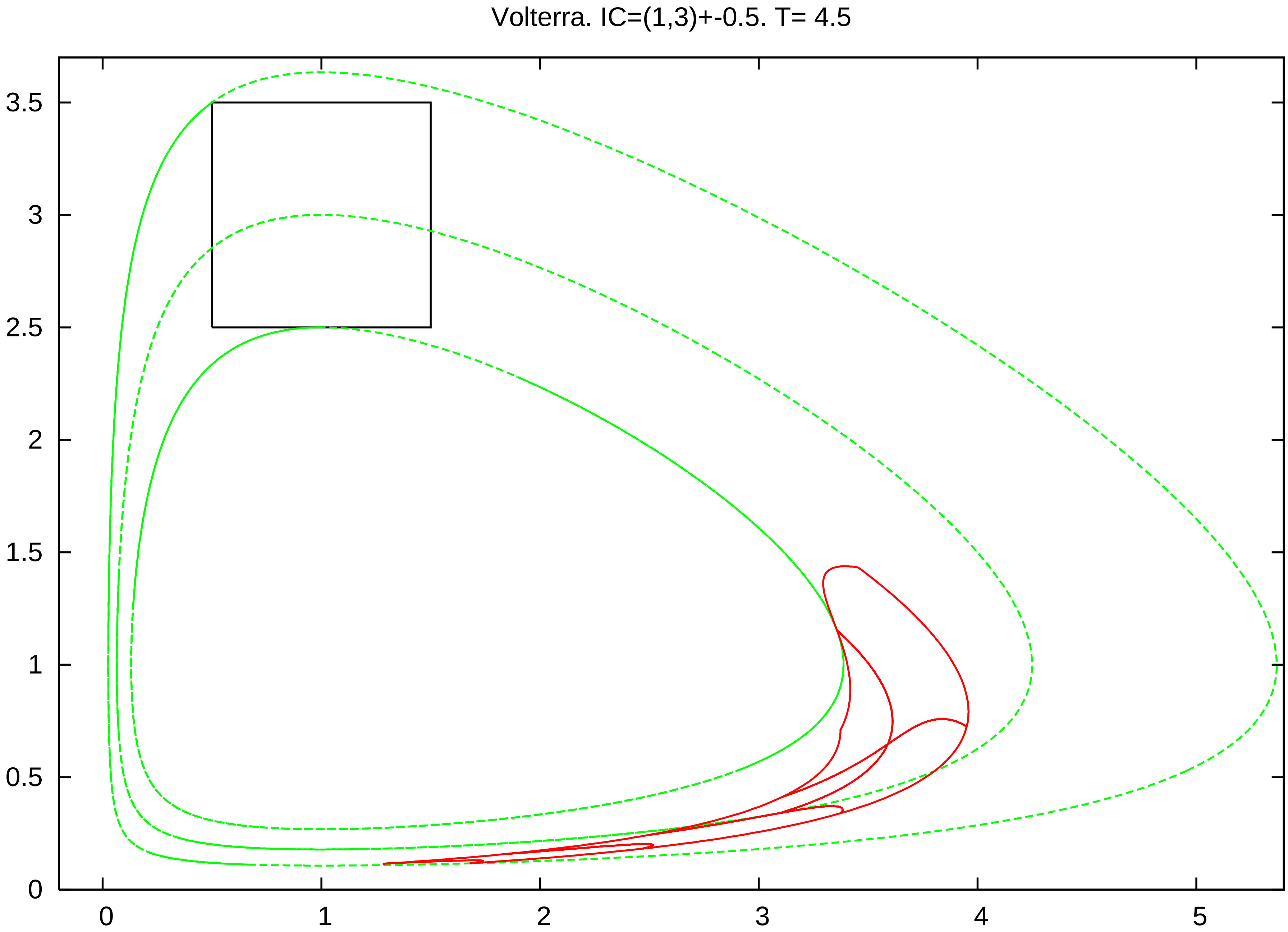
Volterra. IC=(1,3)+-0.5. T= 4.5
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3.5
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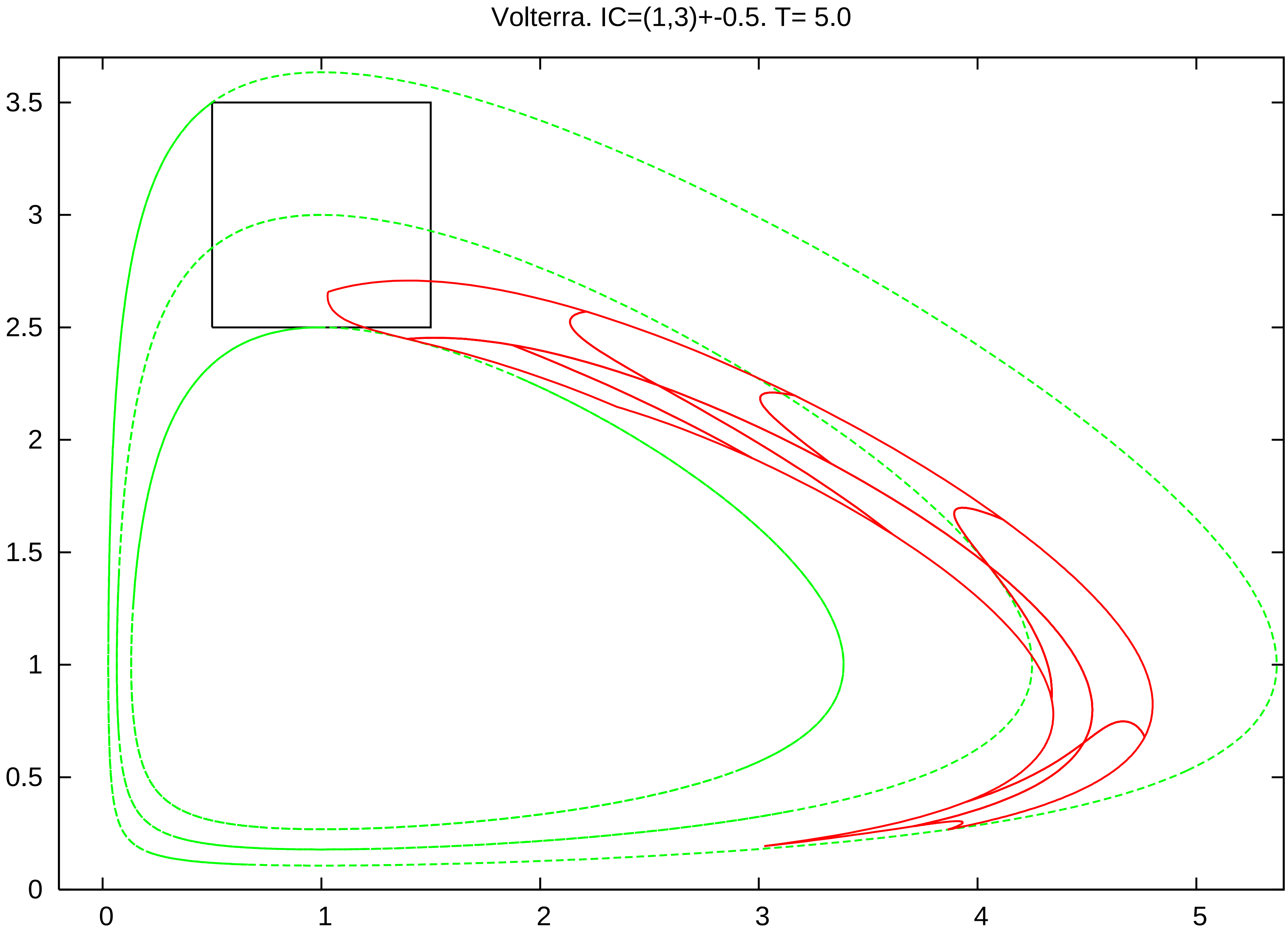

Volterra. IC=(1,3)+-0.5. T= 5.0
0
0.5
1
1.5
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2.5
3
3.5
0
1
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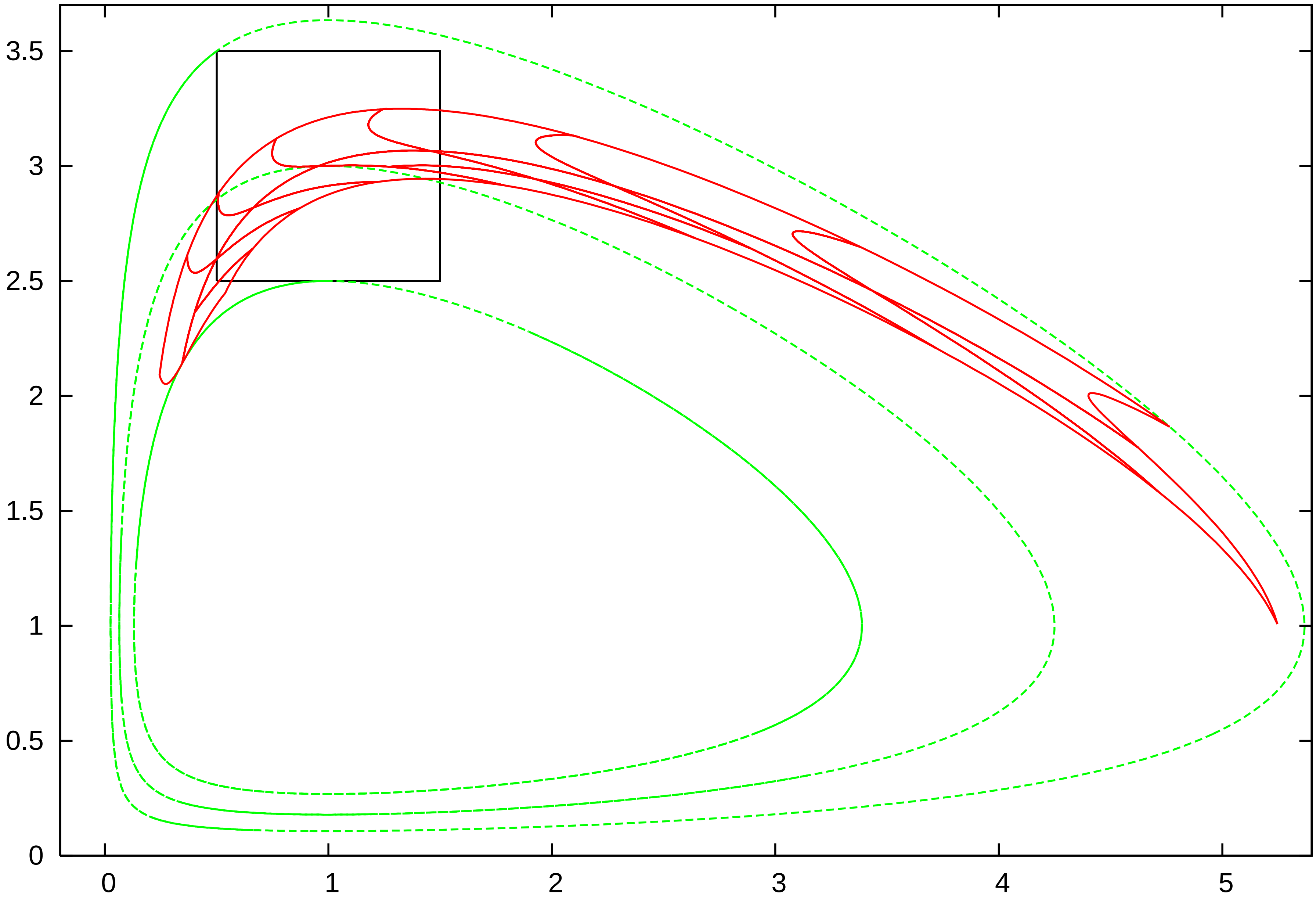
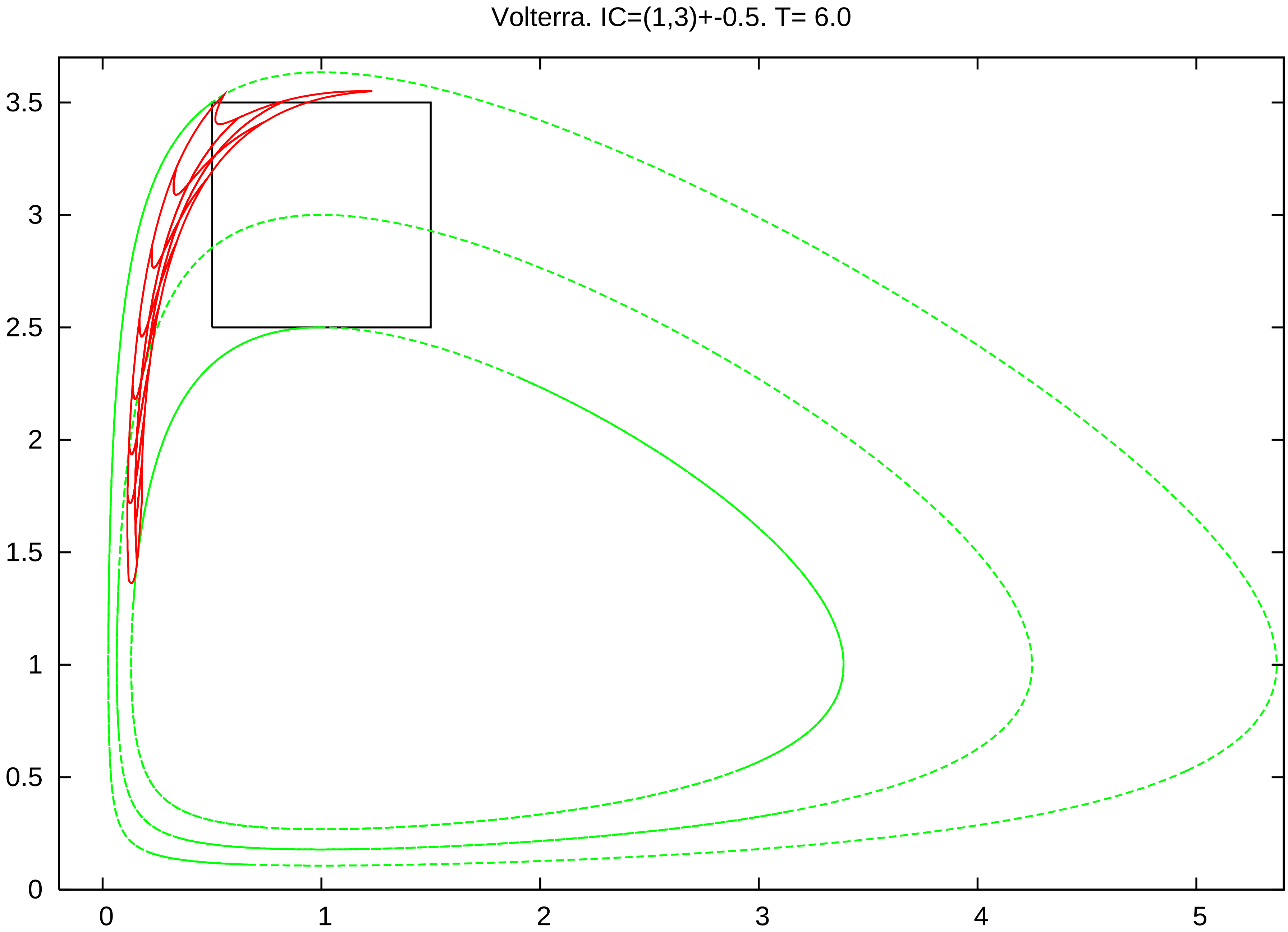
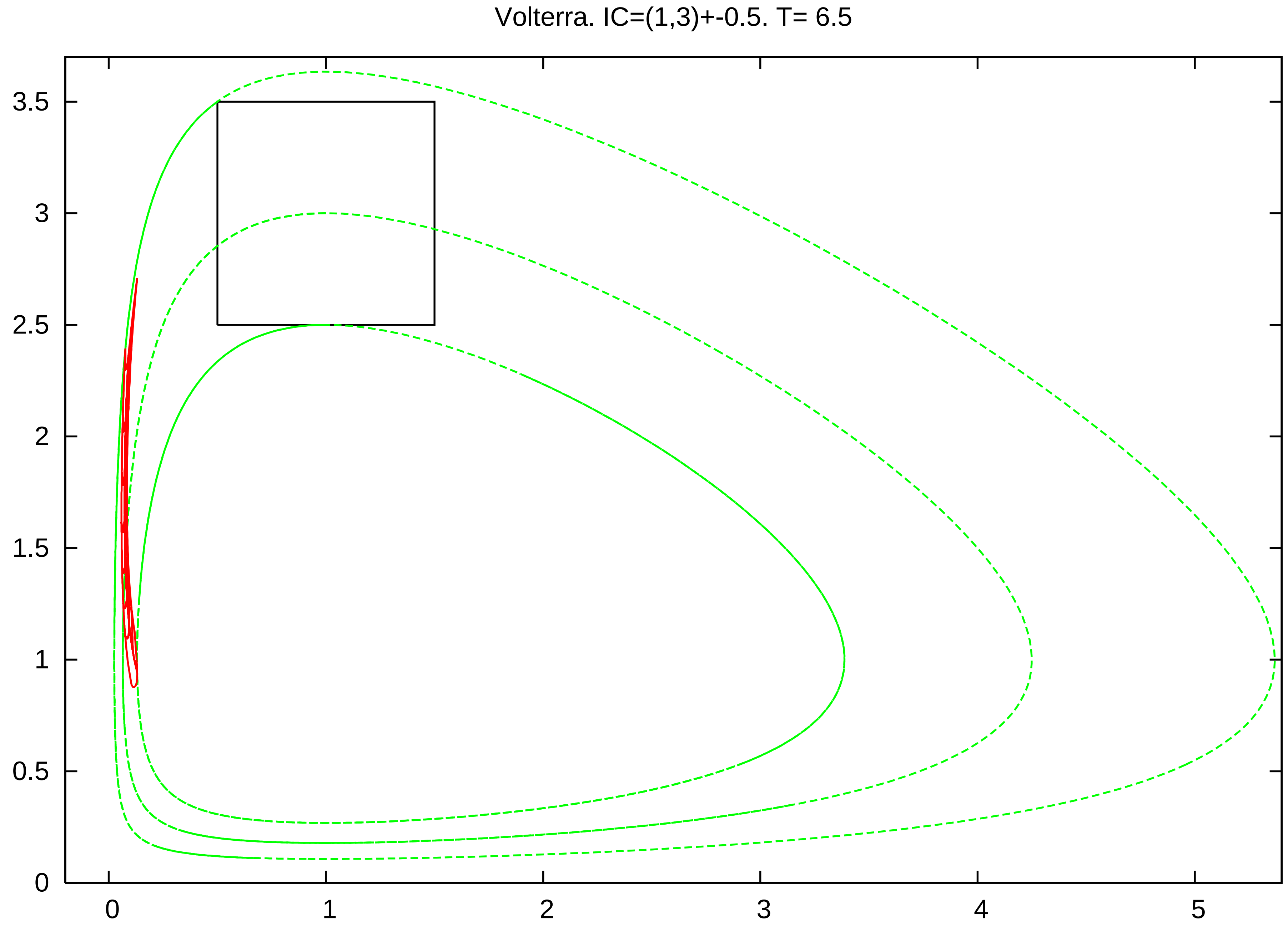
5

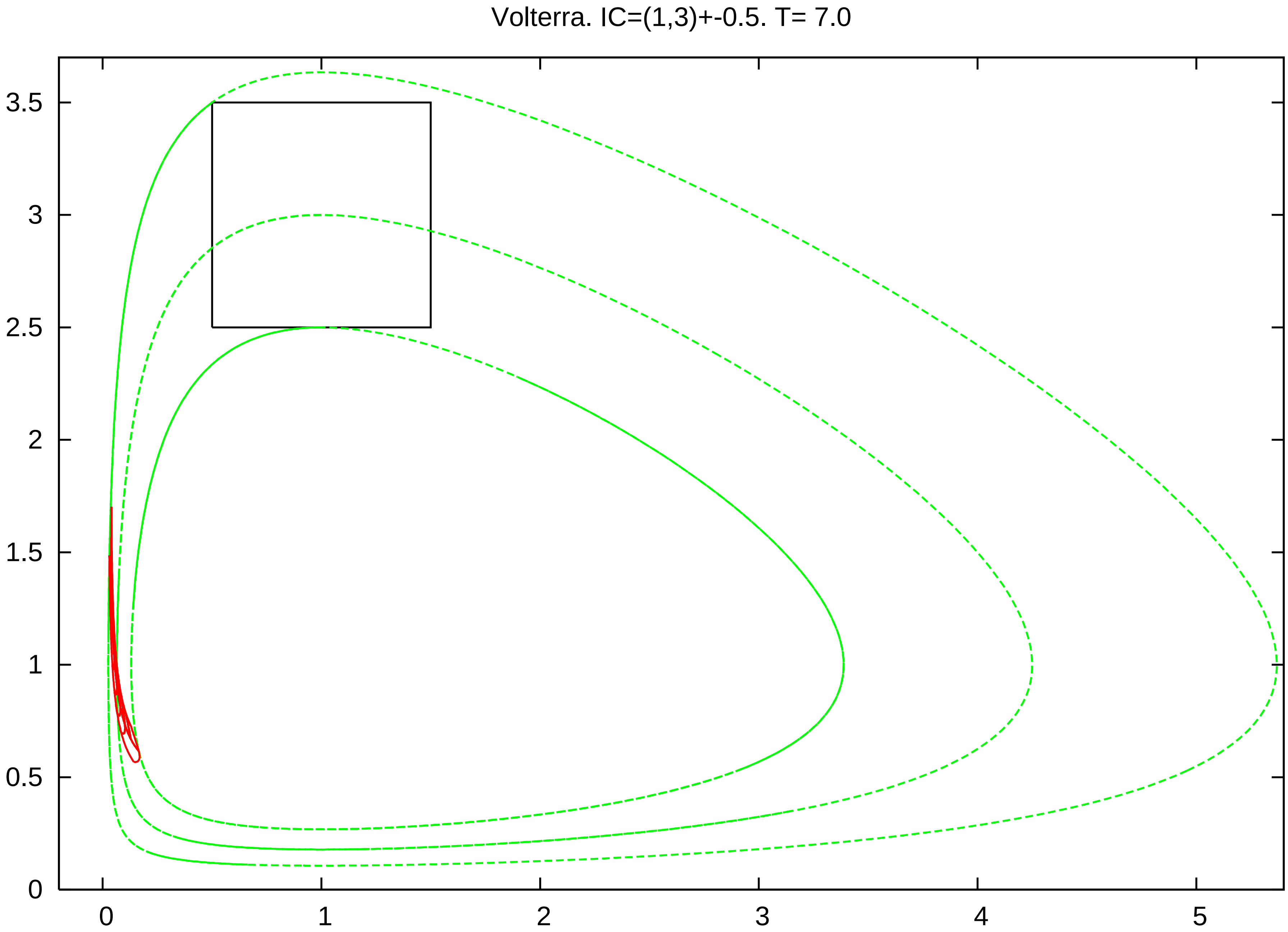
Volterra. IC=(1,3)+-0.5. T= 5.5



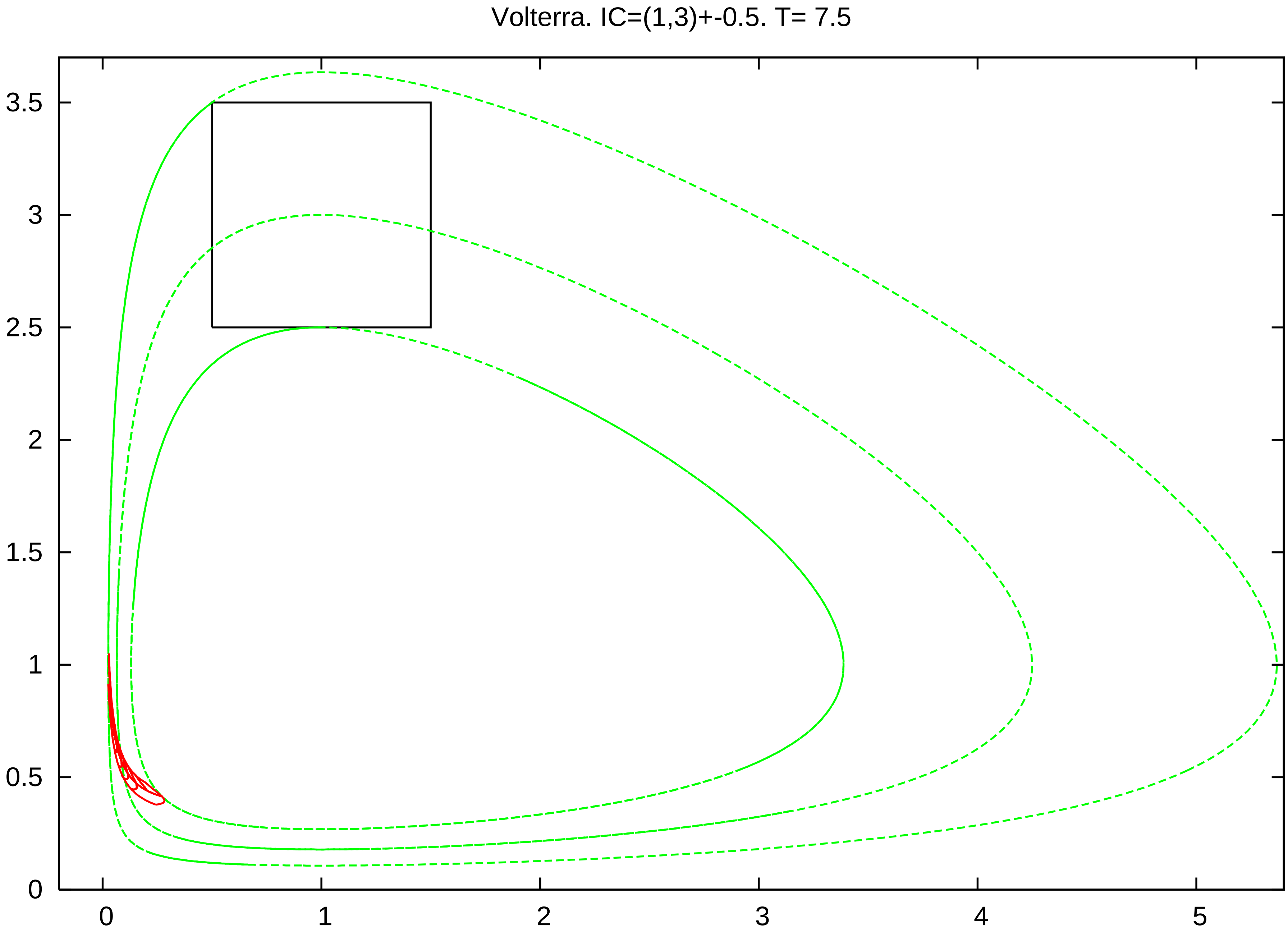


Volterra. IC=(1,3)+-0.5. T= 6.0
0
0.5
1
1.5
2
2.5
3
3.5
0
1
2
3
4
5

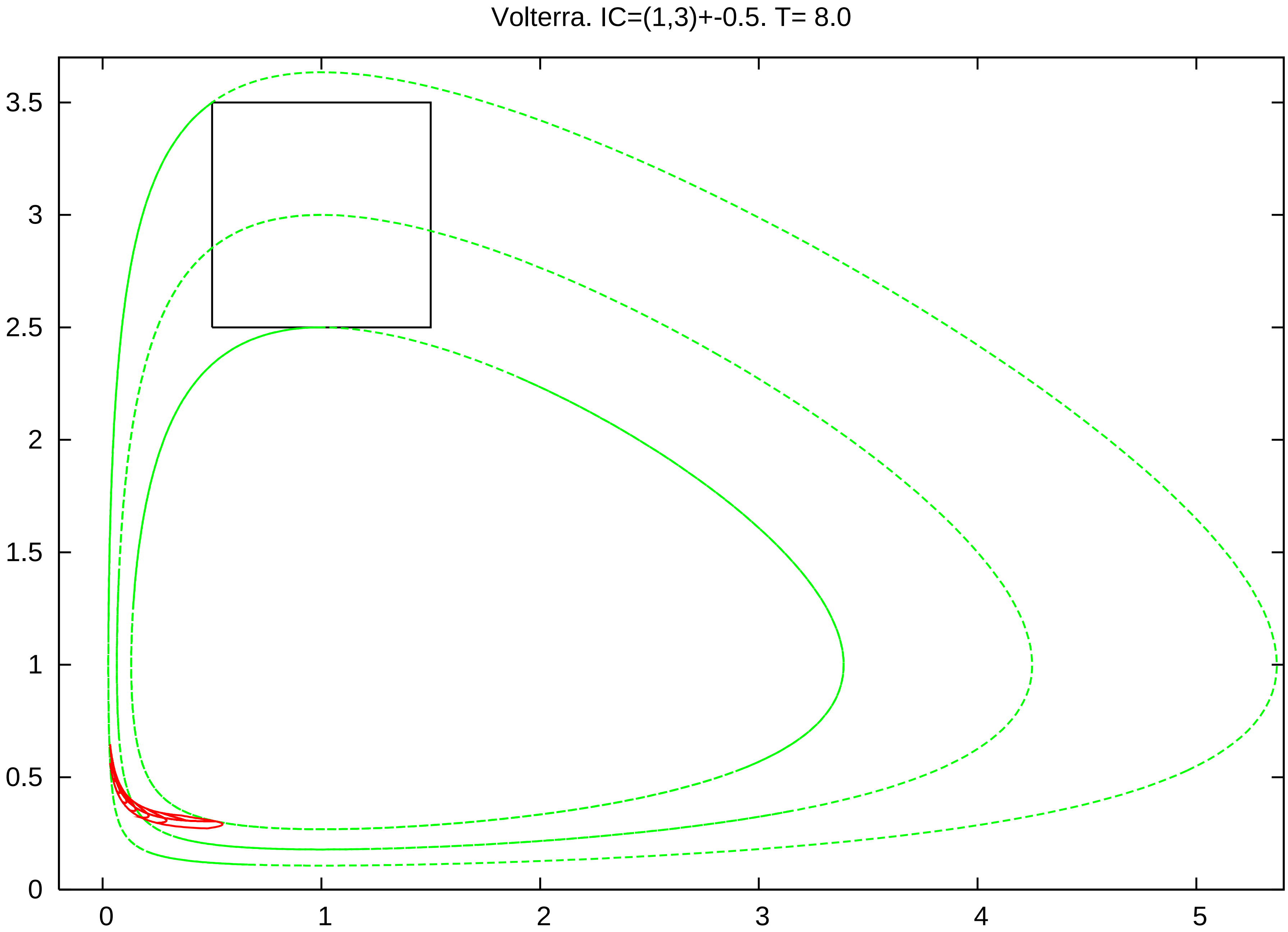

Volterra. IC=(1,3)+-0.5. T= 6.5
0
0.5
1
1.5
2
2.5
3
3.5
0
1
2
3
4
5



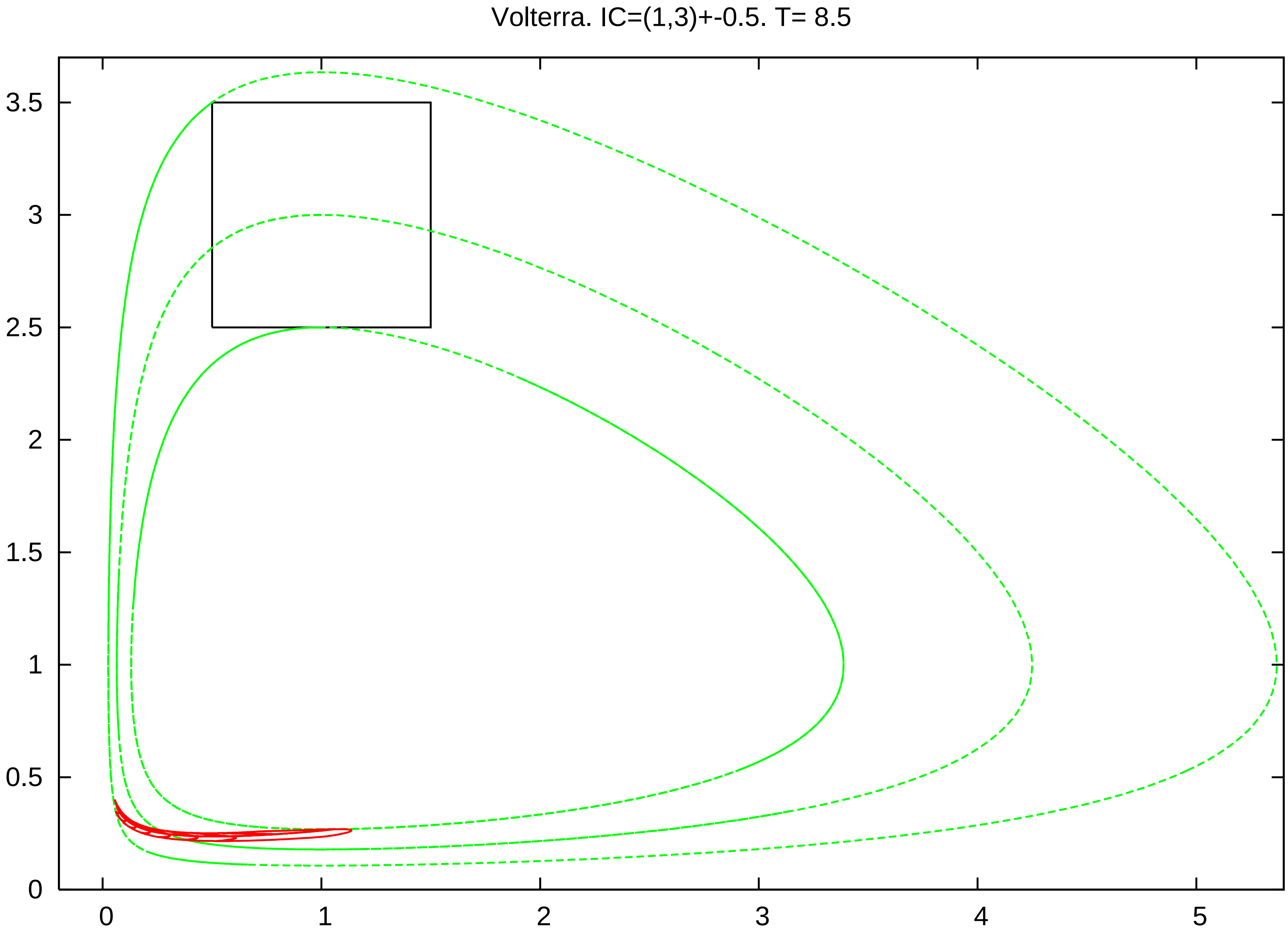
Volterra. IC=(1,3)+-0.5. T= 7.0
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5

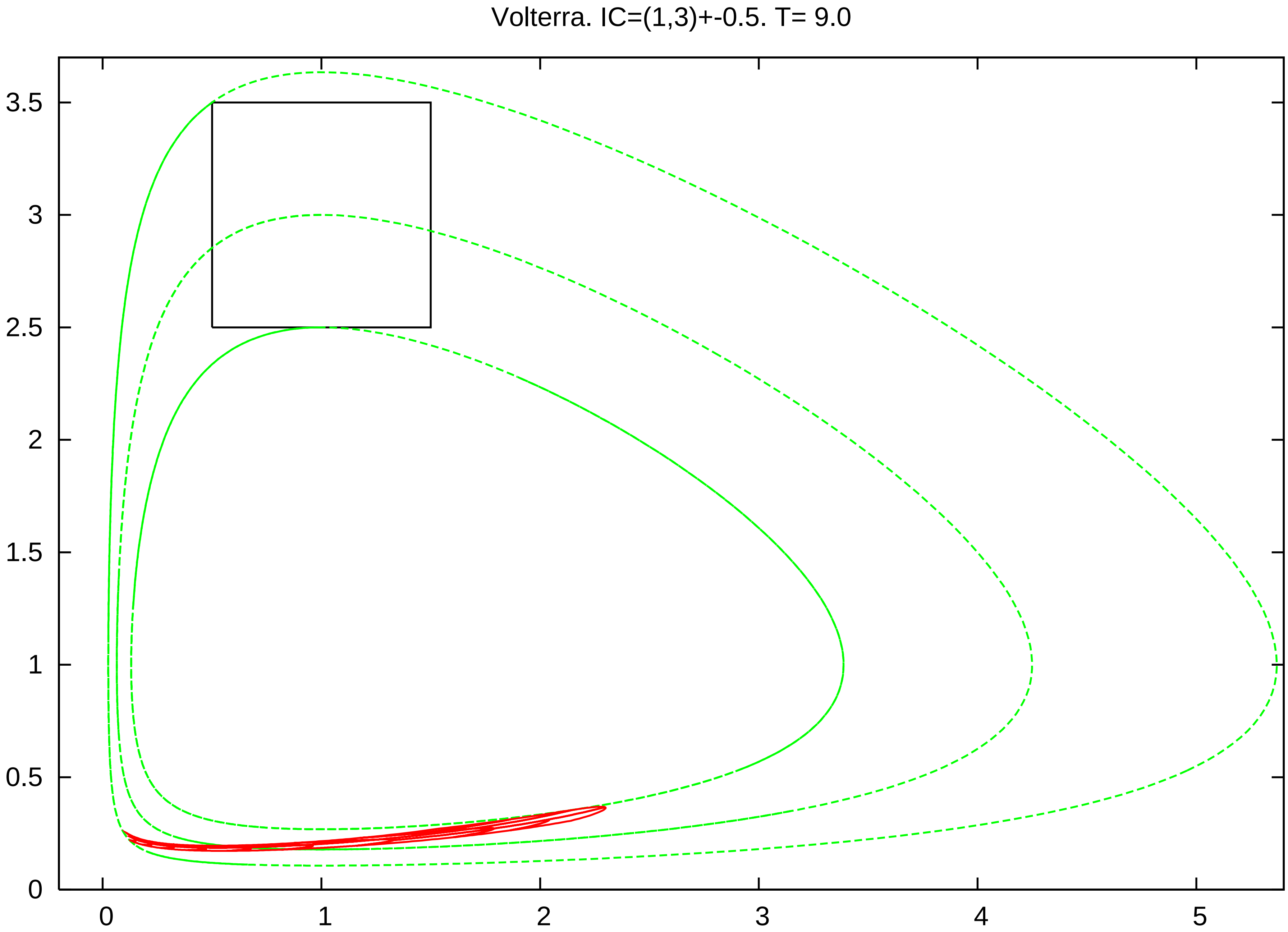


Volterra. IC=(1,3)+-0.5. T= 7.5
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5

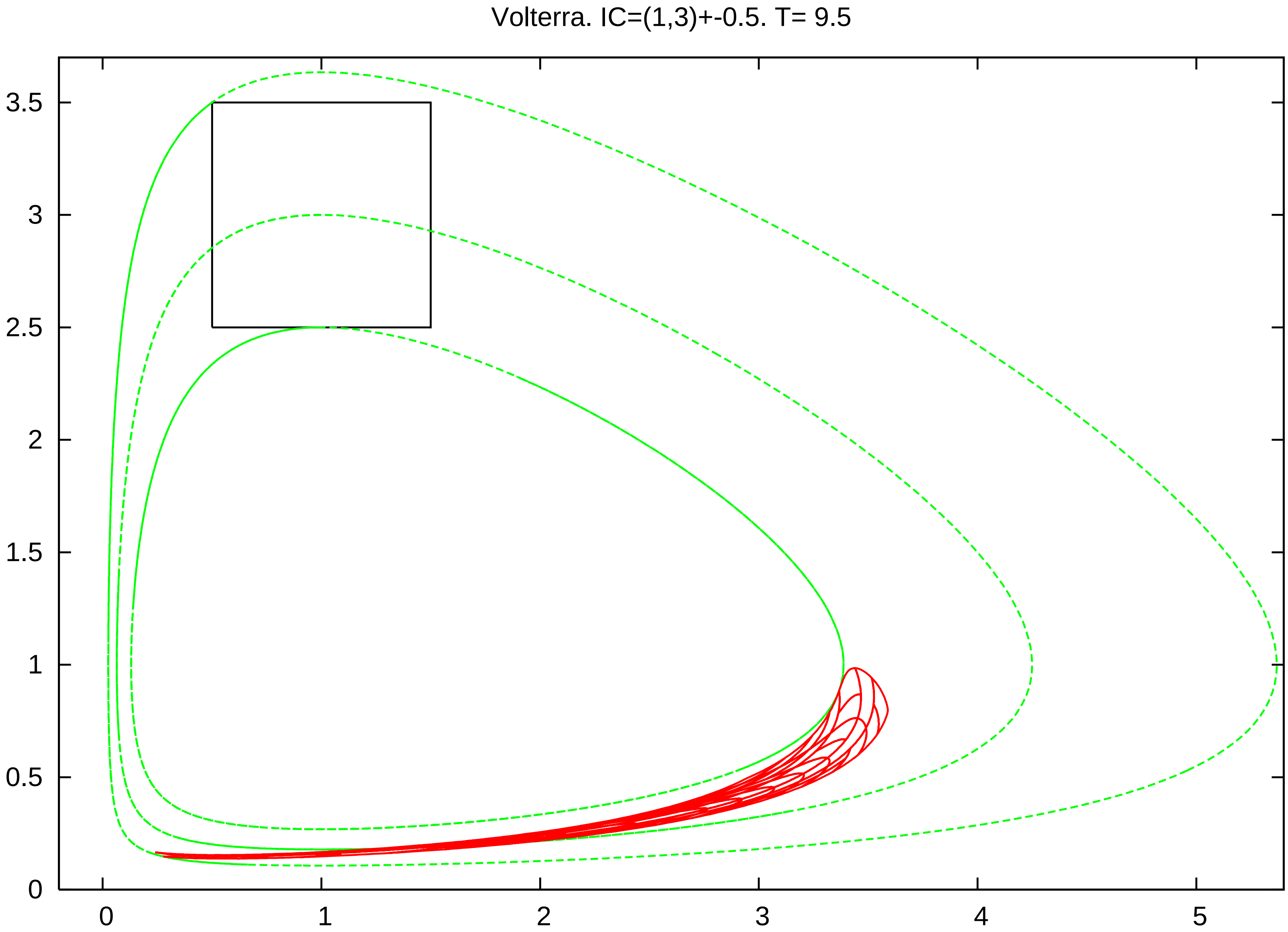


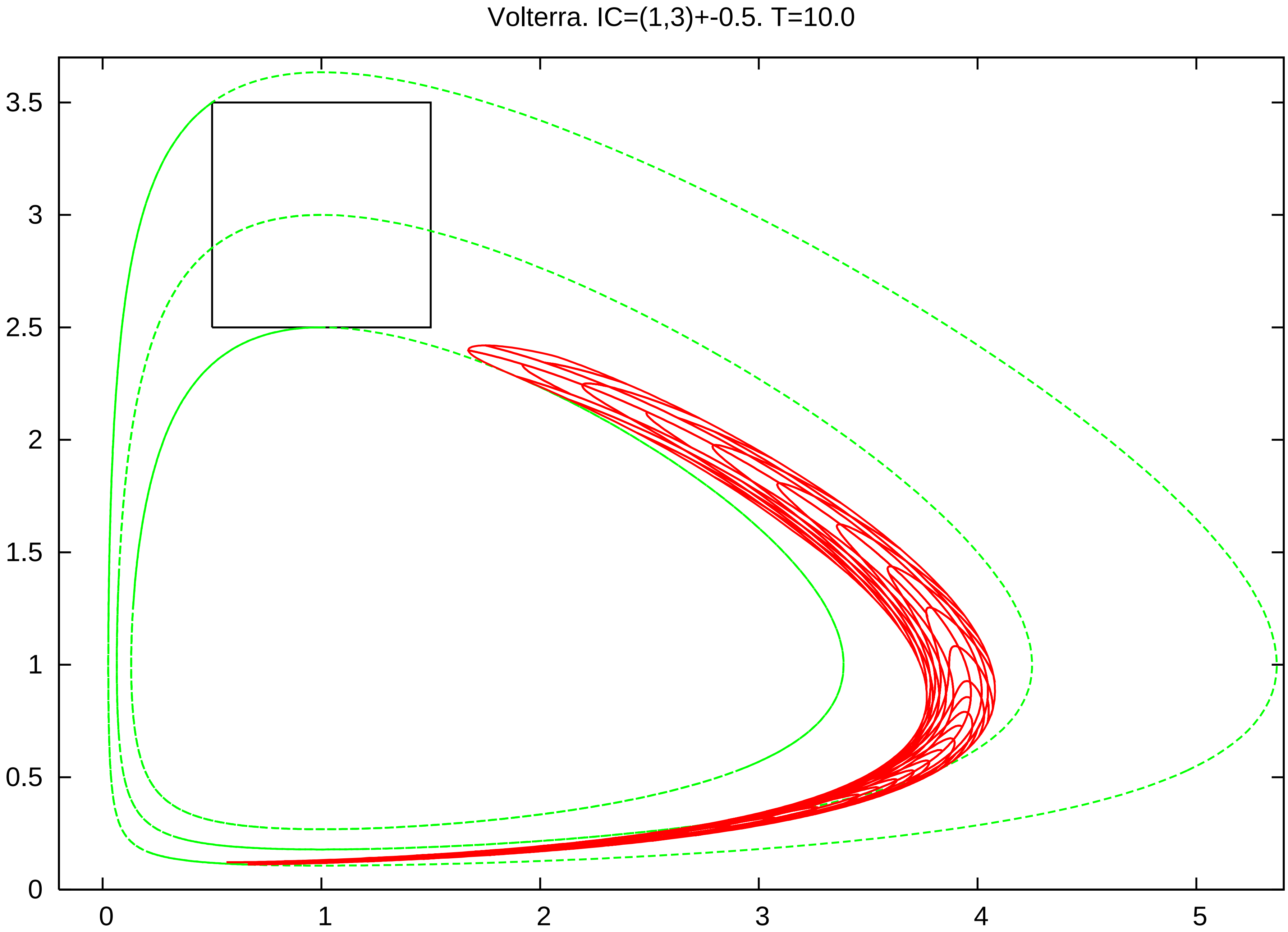
Volterra. IC=(1,3)+-0.5. T= 8.0
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5

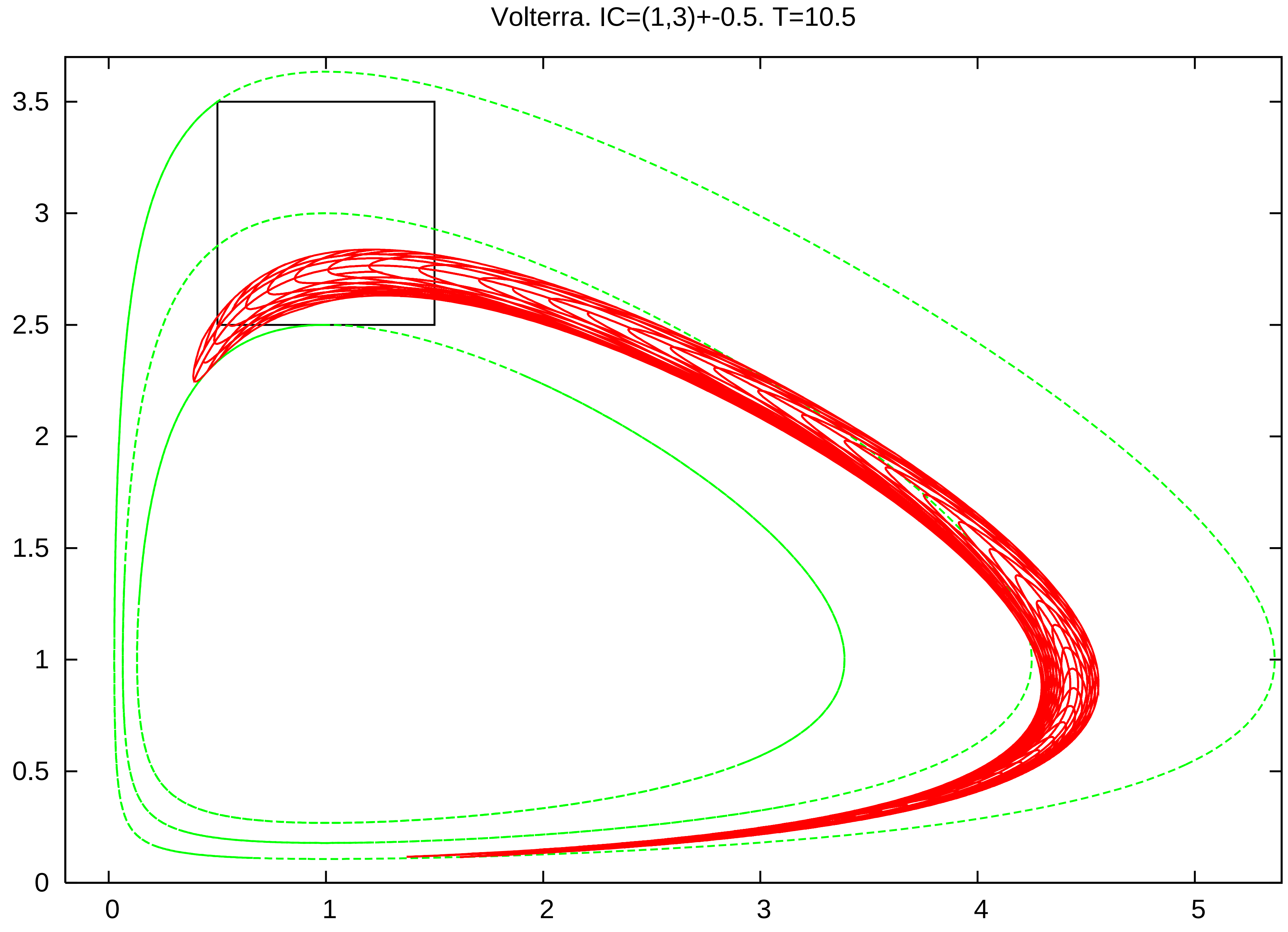

Volterra. IC=(1,3)+-0.5. T= 8.5
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5

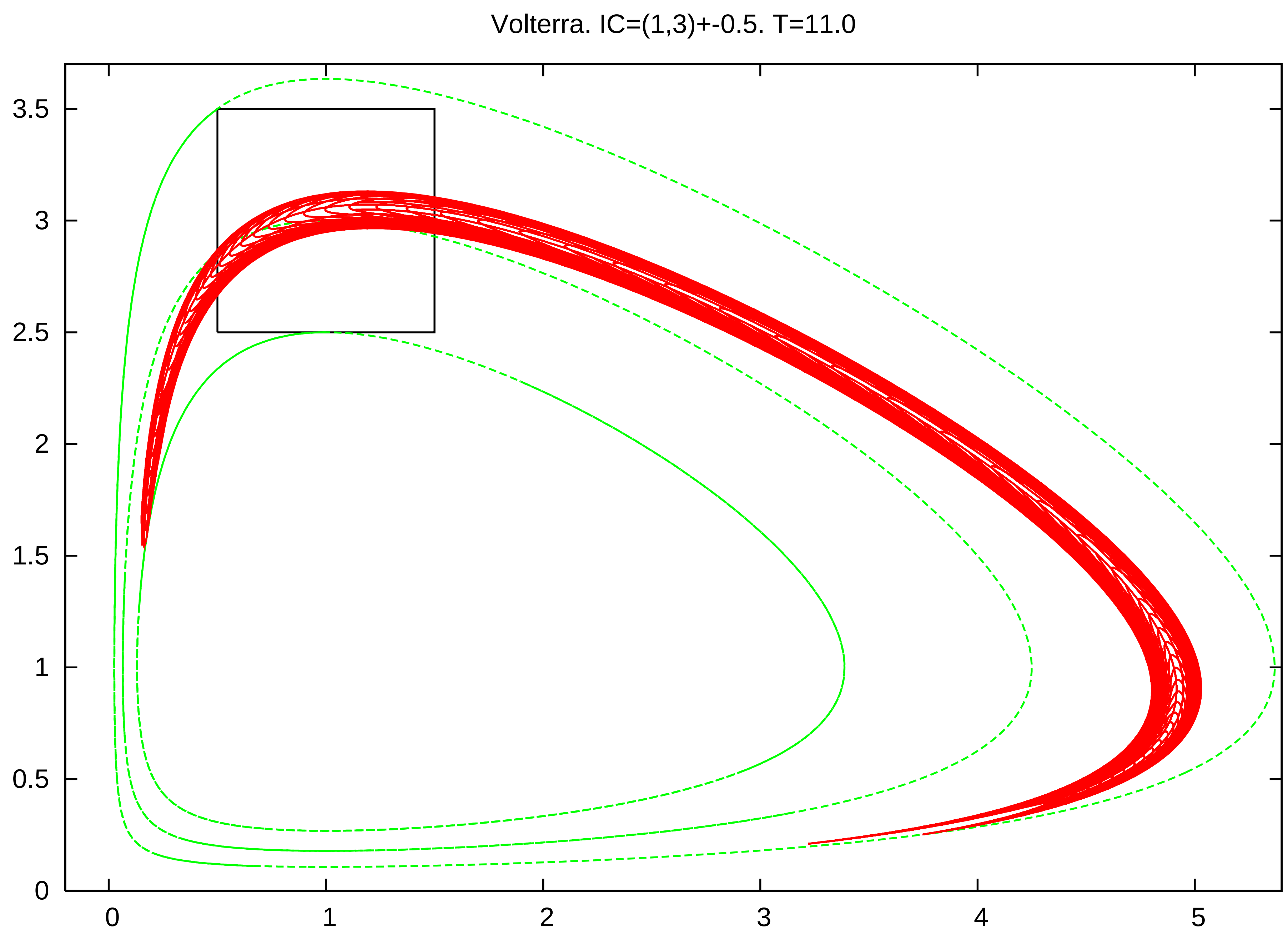


Volterra. IC=(1,3)+-0.5. T= 9.0
0
0.5
1
1.5
2
2.5
3
3.5
0
1
2
3
4
5


Volterra. IC=(1,3)+-0.5. T= 9.5
0
0.5
1
1.5
2
2.5
3
3.5
0
1
2
3
4
5


Volterra. IC=(1,3)+-0.5. T=10.0
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5


Volterra. IC=(1,3)+-0.5. T=10.5
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5


Volterra. IC=(1,3)+-0.5. T=11.0
0
0.5
1
1.5
2
2.5
3
3.5
0
1
2
3
4
5

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

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

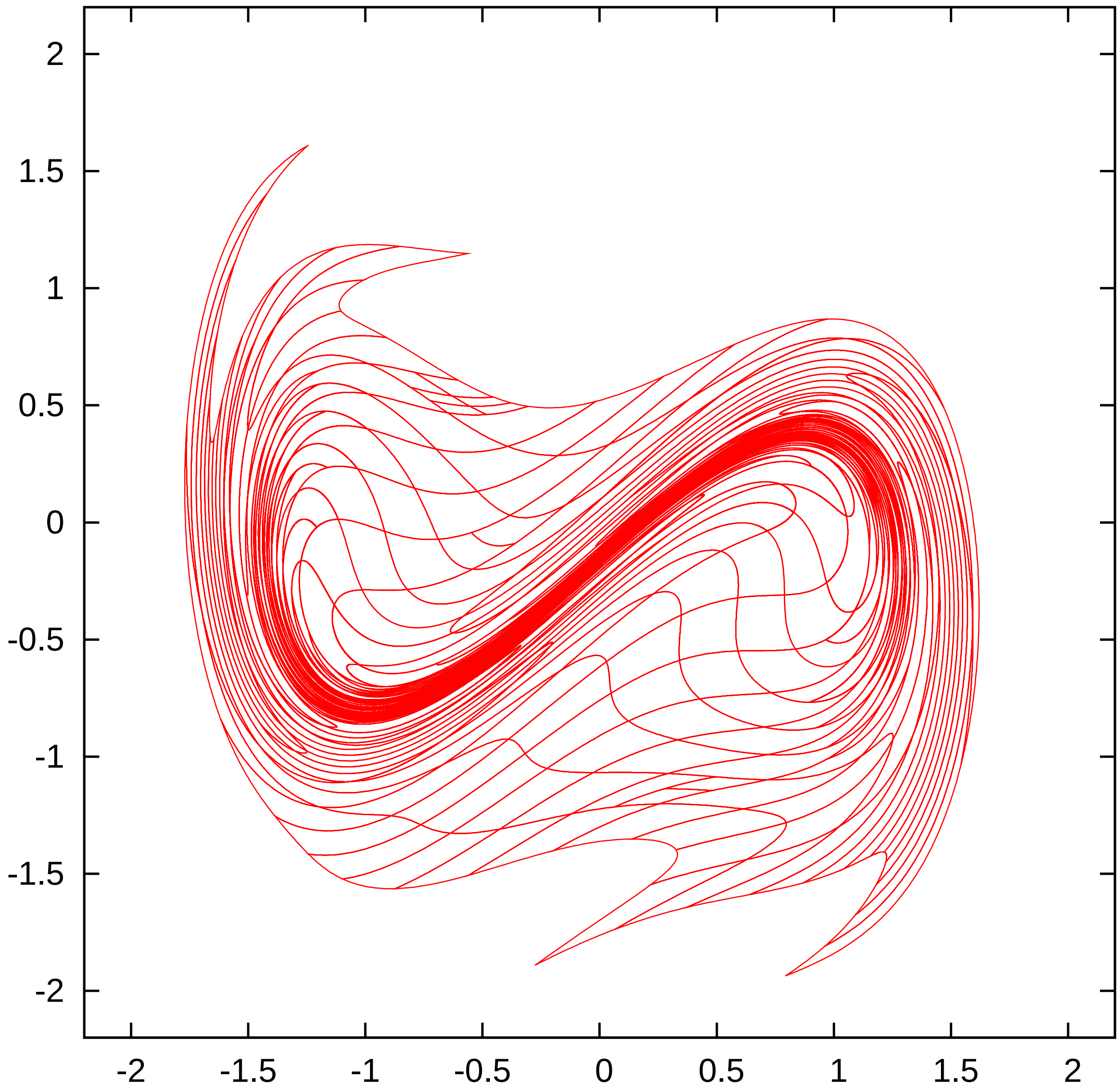
with

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

for

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

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



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

CPU Time:

~ 20 (1E-5 accuracy)

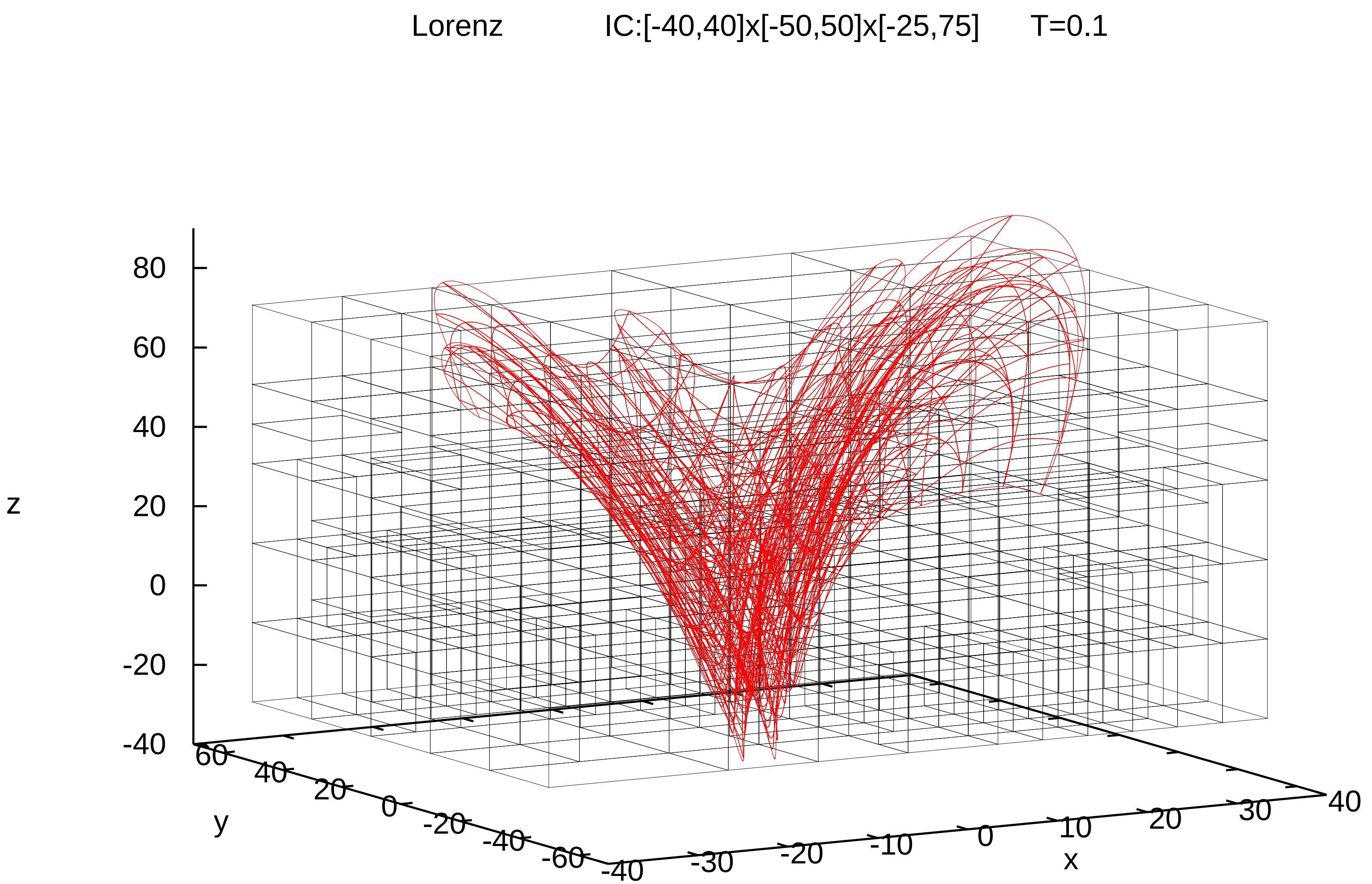
~ 100 (1E-10 accuracy)

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

Summary

- Transfer Map Method and Differential Algebras (DA)
- Rigorous Computation Methods
  - Interval Methods
  - Taylor Models (TM), and comparison
- Verified ODE Integrations
  - Things to care: overestimation, dependency, wrapping effect
  - Taylor Model based ODE Integrations
    - Mathematical backbones
    - Various enhancement methods
      - many methods possible with the DA/TM framework!
    - Examples: Volterra (contour trajectories)
Lorenz, Duffing (chaotic systems)
- Work in progress to improve the performances
  - Higher precision Taylor Model computations
  - Enhancements for the ODE integrations and more