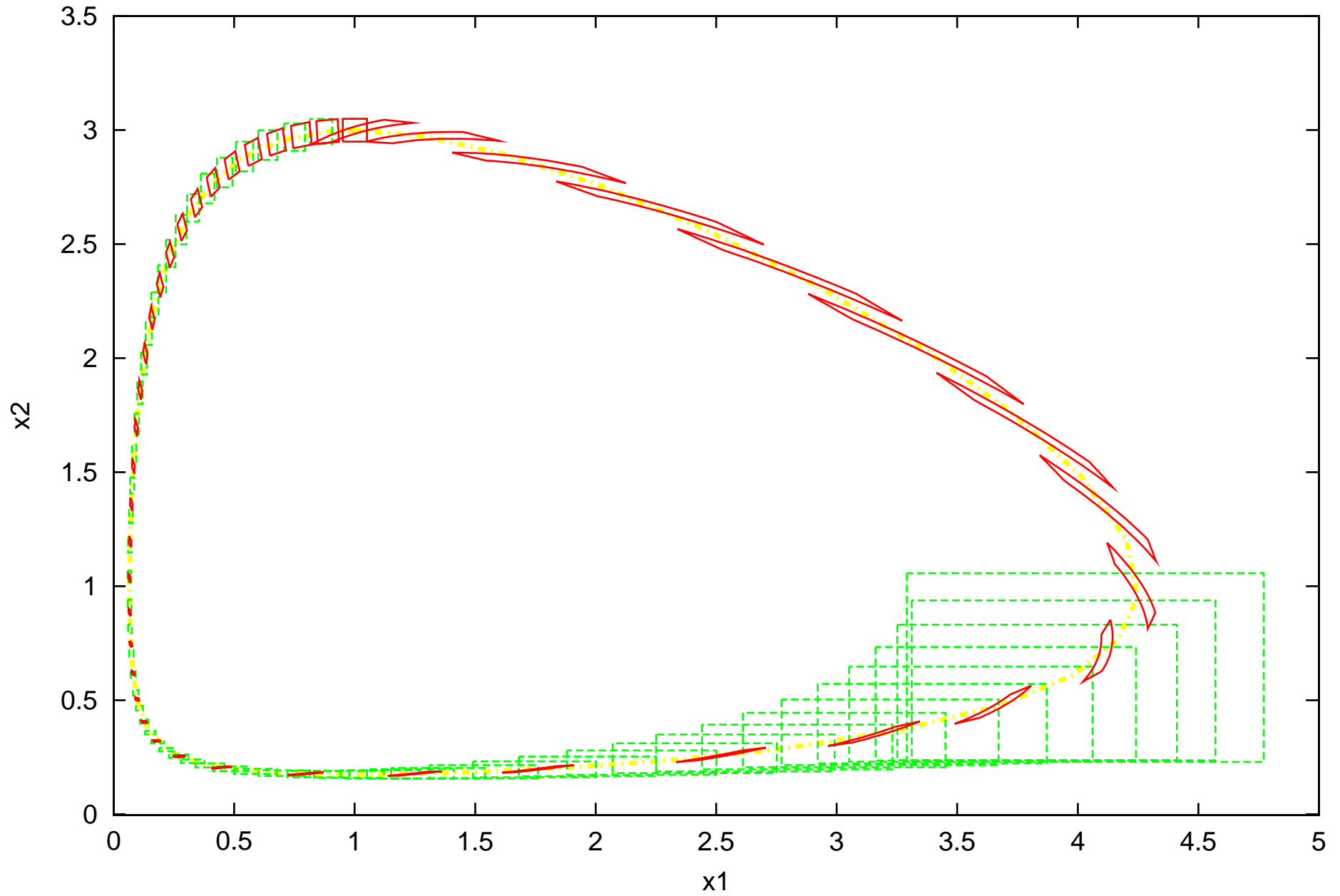


Recent Advances in the Validated Integration of ODEs

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Integration of the Volterra eq. COSY-VI and AWA



Definitions - Taylor Models and Operations

We begin with a review of the definitions of the basic operations.

Definition (Taylor Model) Let $f : D \subset R^v \rightarrow R$ be a function that is $(n + 1)$ times continuously partially differentiable on an open set containing the domain v -dimensional domain D . Let x_0 be a point in D and P the n -th order Taylor polynomial of f around x_0 . Let I be an interval such that

$$f(x) \in P(x - x_0) + I \text{ for all } x \in D.$$

Then we call the pair (P, I) an n -th order Taylor model of f around x_0 on D .

Definition (Addition and Multiplication) Let $T_{1,2} = (P_{1,2}, I_{1,2})$ be n -th order Taylor models around x_0 over the domain D . We define

$$T_1 + T_2 = (P_1 + P_2, I_1 + I_2)$$

$$T_1 \cdot T_2 = (P_{1,2}, I_{1,2})$$

where $P_{1,2}$ is the part of the polynomial $P_1 \cdot P_2$ up to order n and

$$I_{1,2} = B(P_e) + B(P_1) \cdot I_2 + B(P_2) \cdot I_1 + I_1 \cdot I_2$$

where P_e is the part of the polynomial $P_1 \cdot P_2$ of orders $(n + 1)$ to $2n$, and $B(P)$ denotes a bound of P on the domain D . We demand that $B(P)$ is at least as sharp as direct interval evaluation of $P(x - x_0)$ on D .

The Operator ∂^{-1} on Taylor Models

Let (P_n, I_n) be an n -th order Taylor model of f . From this we can obtain a Taylor model for the indefinite integral $\partial_i^{-1} f = \int f dx'_i$ with respect to variable x_i .

Taylor polynomial part: $\int_0^{x_i} P_{n-1} dx'_i,$

Remainder Bound: $(B(P_n - P_{n-1}) + I_n) \cdot B(x_i)$, where $B(P)$ is a polynomial bound.

So define the operator ∂_i^{-1} on space of Taylor models as

$$\begin{aligned} & \partial_i^{-1}(P_n, I_n) \\ &= \left(\int_0^{x_i} P_{n-1} dx'_i, (B(P_n - P_{n-1}) + I_n) \cdot B(x_i) \right) \end{aligned}$$

TM Scaling Theorem

Theorem (Scaling Theorem) Let $f, g \in C^{n+1}(D)$ and $(P_{f,h}, I_{f,h})$ and $(P_{g,h}, I_{g,h})$ be n -th order Taylor models for f and g around x_h on $x_h + [-h, h]^v \subset D$. Let the remainder bounds $I_{f,h}$ and $I_{g,h}$ satisfy $I_{f,h} = O(h^{n+1})$ and $I_{g,h} = O(h^{n+1})$. Then the Taylor models $(P_{f+g}, I_{f+g,h})$ and $(P_{f \cdot g}, I_{f \cdot g,h})$ for the sum and products of f and g obtained via addition and multiplication of Taylor models satisfy

$$I_{f+g,h} = O(h^{n+1}), \text{ and } I_{f \cdot g,h} = O(h^{n+1}).$$

Furthermore, let s be any of the intrinsic functions defined above, then the Taylor model $(P_{s(f)}, I_{s(f),h})$ for $s(f)$ obtained by the above definition satisfies

$$I_{s(f),h} = O(h^{n+1}).$$

We say the Taylor model arithmetic has the $(n+1)$ -st order scaling property.

Proof. The proof for the binary operations follows directly from the definition of the remainder bounds for the binaries. Similarly, the proof for the intrinsics follows because all intrinsics are composed of binary operations as well as an additional interval, the width of which scales at least with the $(n+1)$ -st power of a bound B of a function that scales at least linearly with h .

Important TM Algorithms

- **Range Bounding** (Evaluate f as TM, bound polynomial, add remainder bound)
- **Quadrature** (Evaluate f as TM, integrate polynomial and remainder bound)
- **Implicit Equations** (Obtain TMs for implicit solutions of TM equations)
- **Superconvergent Interval Newton Method** (Application of Implicit Equations)
- **ODEs** (Obtain TMs describing dependence of final coordinates on initial coordinates)
- **Implicit ODEs and DAEs**
- **Complex Arithmetic** (Describe complex ranges as two-dimensional TMs)

Implementation of TM Arithmetic

Validated Implementation of TM Arithmetic exists. The following points are important

- Strict requirements for **underlying FP arithmetic**
- Taylor models require cutoff threshold (**garbage collection**)
- Coefficients remain FP, not intervals
- Package quite **extensively tested** by Corliss et al.

For practical considerations, the following is important:

- Need **sparsity** support
- Need efficient coefficient **addressing** scheme
- About 50,000 lines of code
- **Language Independent** Platform, coexistence in F77, C, F90, C++

Multiplication - Weighting

Sometimes important: Carry different variables x_i to different orders w_i .

Can be achieved by simply "seeding" original variables as

$$P(x) = (x_1^{w_1}, x_2^{w_2}, \dots, x_v^{w_v}).$$

Then in all subsequent operations, only multiples of w_i appear as powers of x_i . Optimal reduction of speed by sparsity.

Order n	Variables v	Weighting w	Order n_i	Cosy Coefs	AWA Coefs
17	3	9	1	41	144
17	5	9	1	57	216
17	10	9	1	97	396
17	20	9	1	177	756
17	3	5	3	135	144
17	5	5	3	308	216
17	10	5	3	1248	396
17	20	5	3	6578	756
13	5	3	4	504	168
13	10	3	4	3094	308
15	5	3	5	882	192
15	10	3	5	7098	352

TABLE 1. Number of floating point numbers necessary to store all appearing partial derivatives in COSY to order n_i in initial conditions, and in the first order code AWA

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

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

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

The Volterra Equation

Describe dynamics of two conflicting populations

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

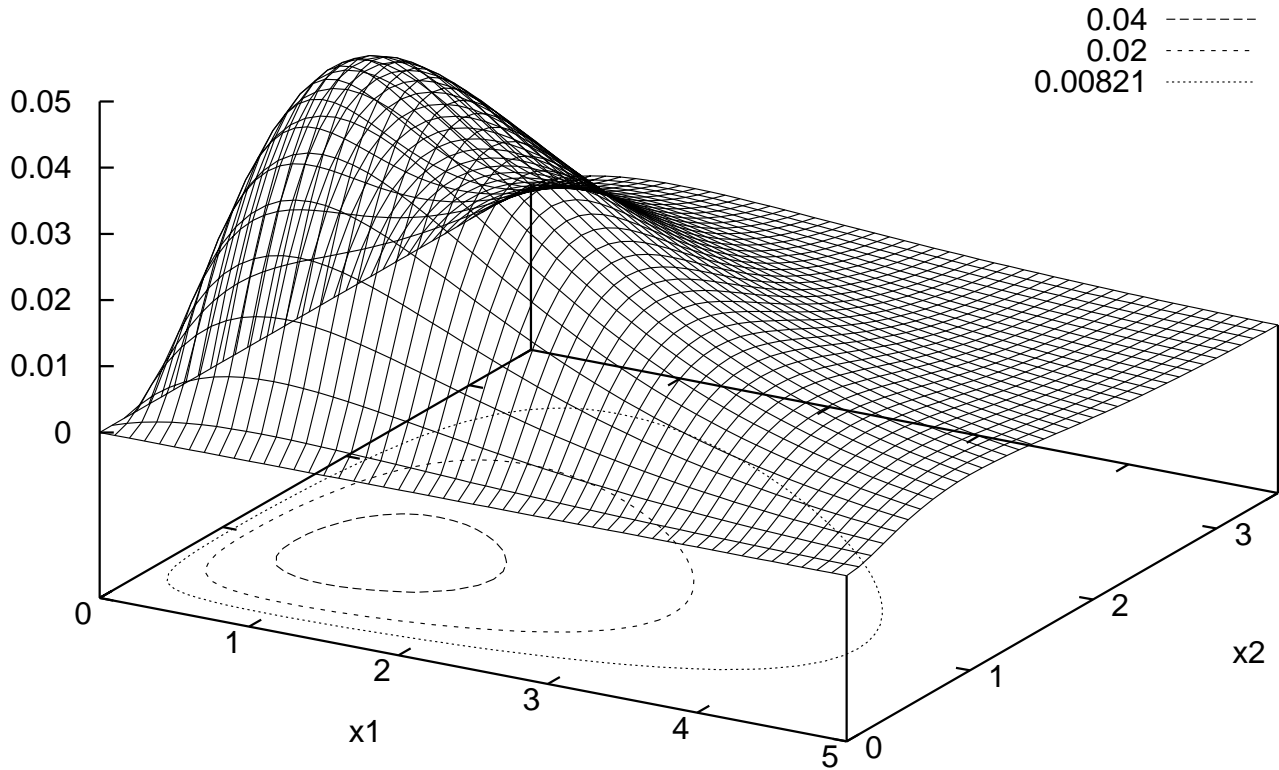
Interested in initial condition

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

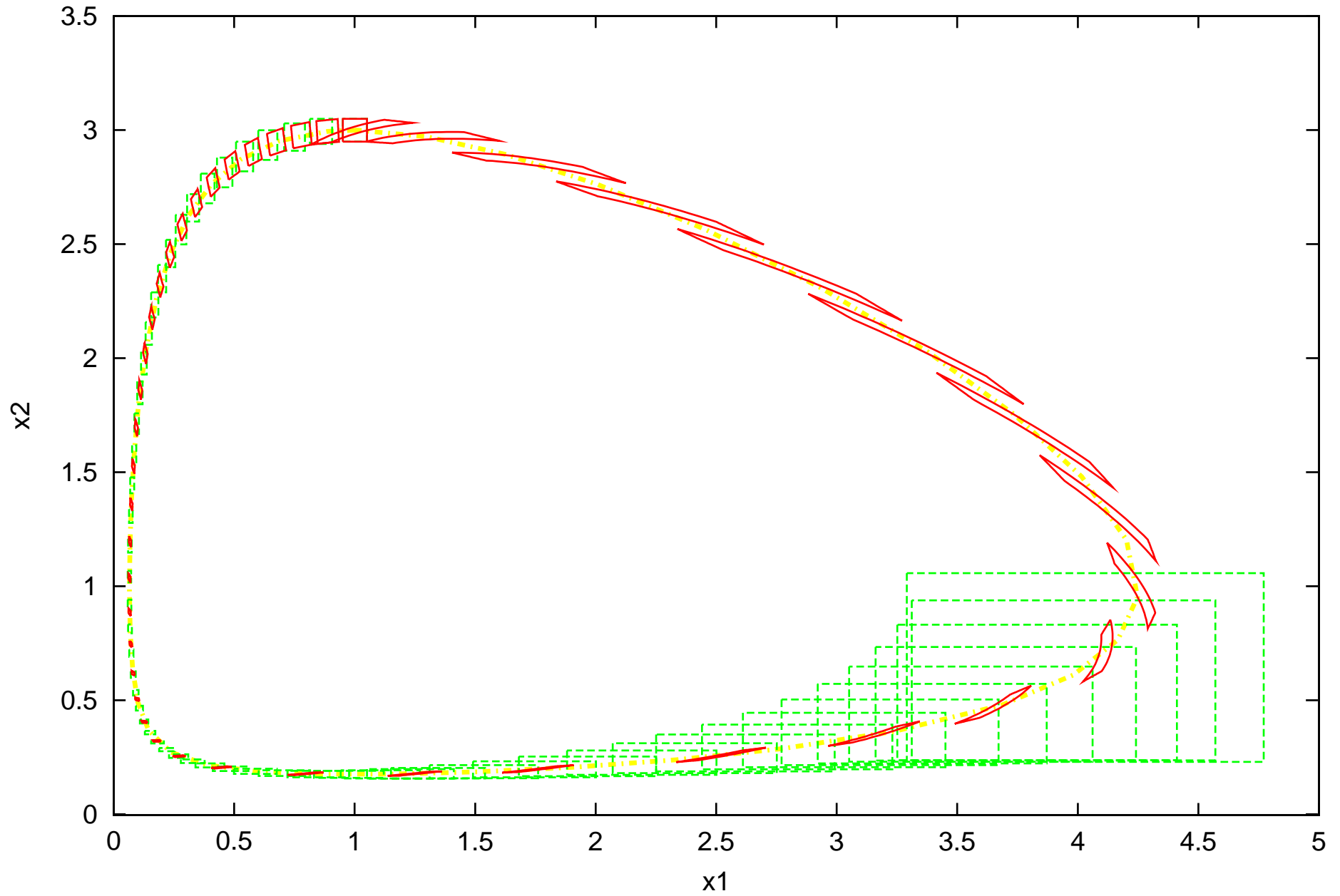
Satisfies constraint condition

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

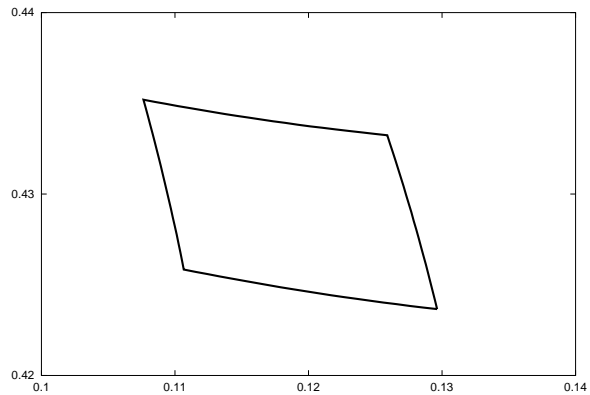
$f(x_1, x_2)$



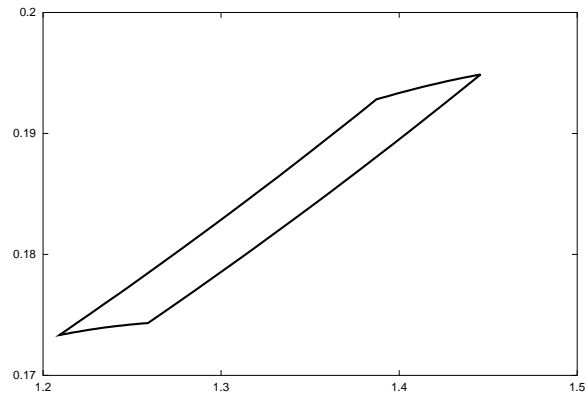
Integration of the Volterra eq. COSY-VI and AWA



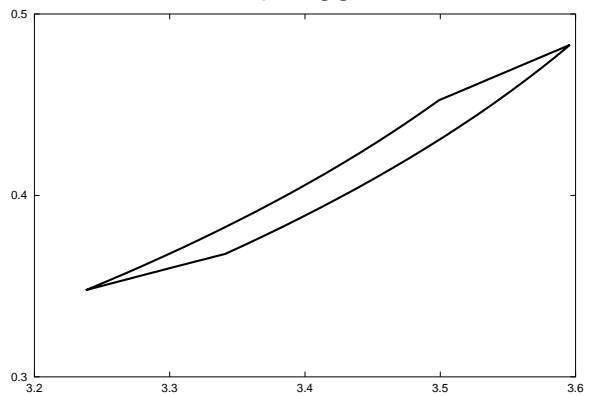
t=2.33



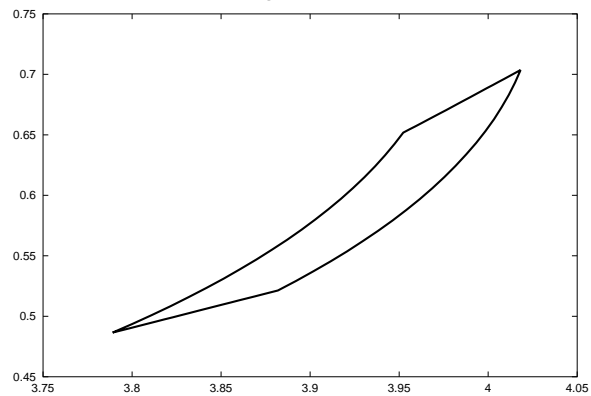
t=3.94



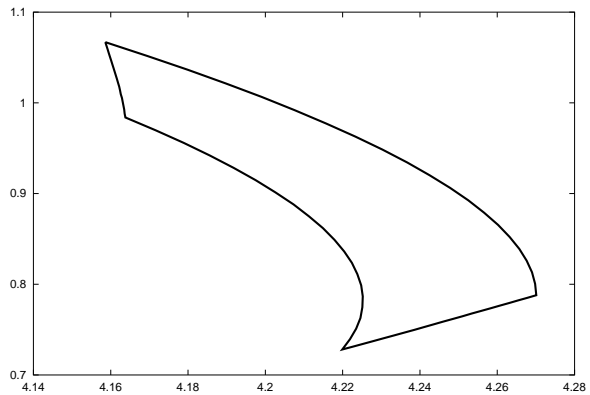
t=4.58



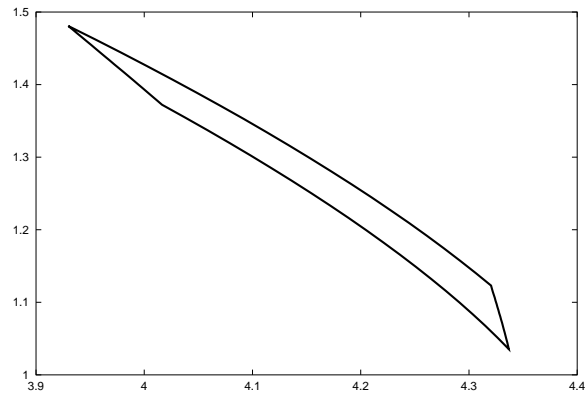
t=4.71



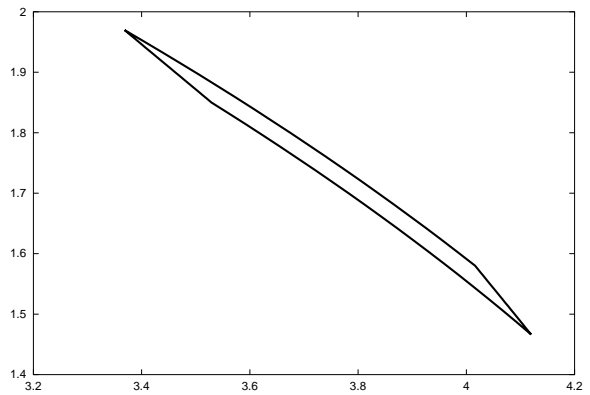
t=4.85



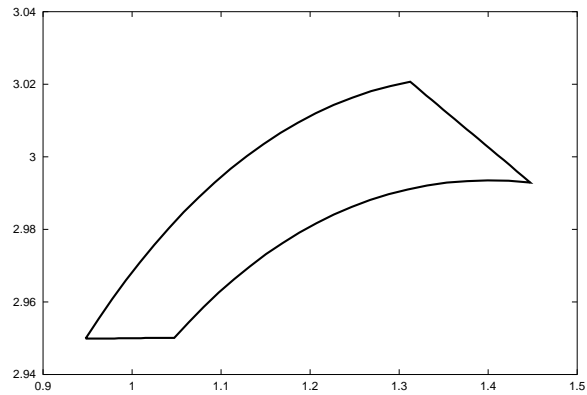
t=4.95

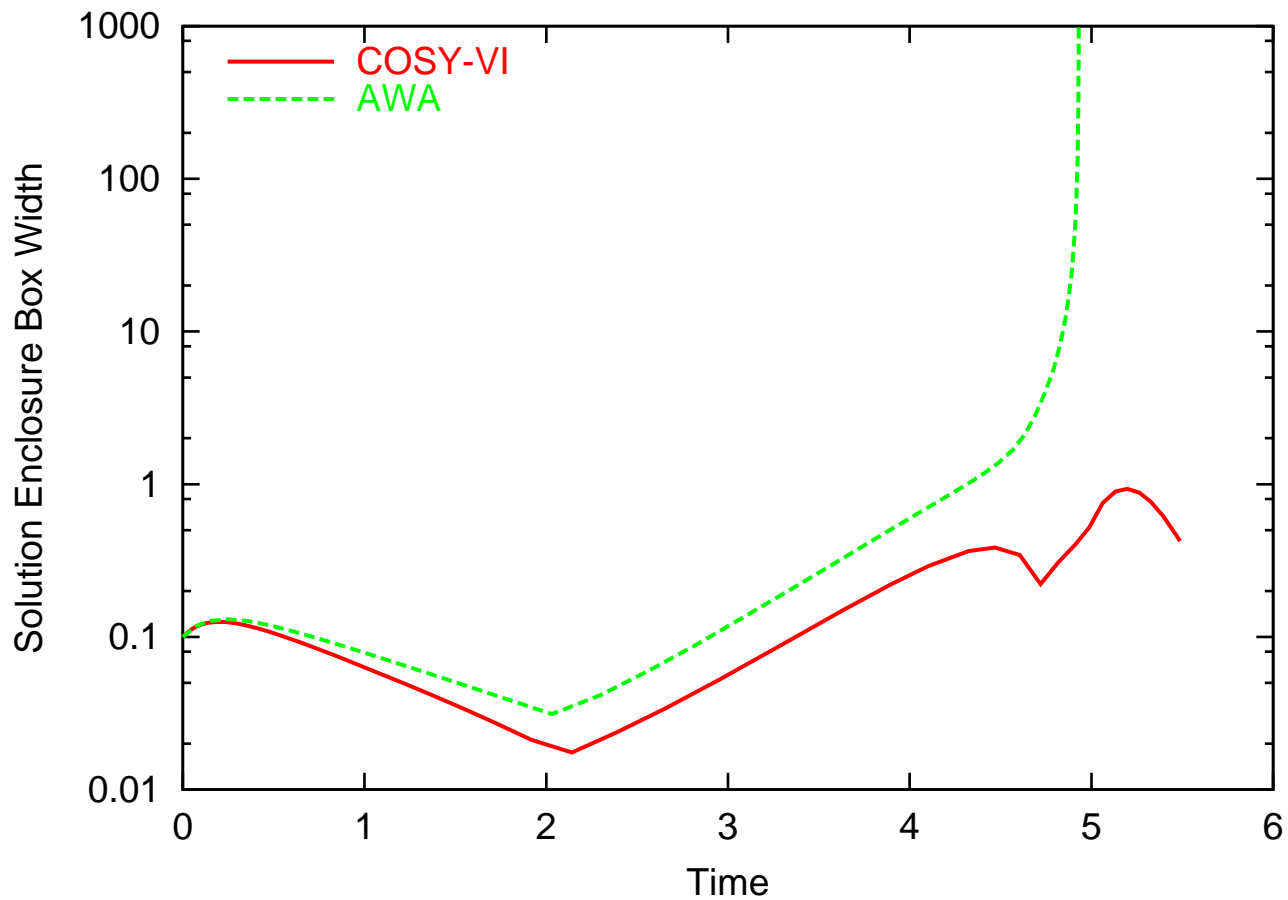


t=5.06

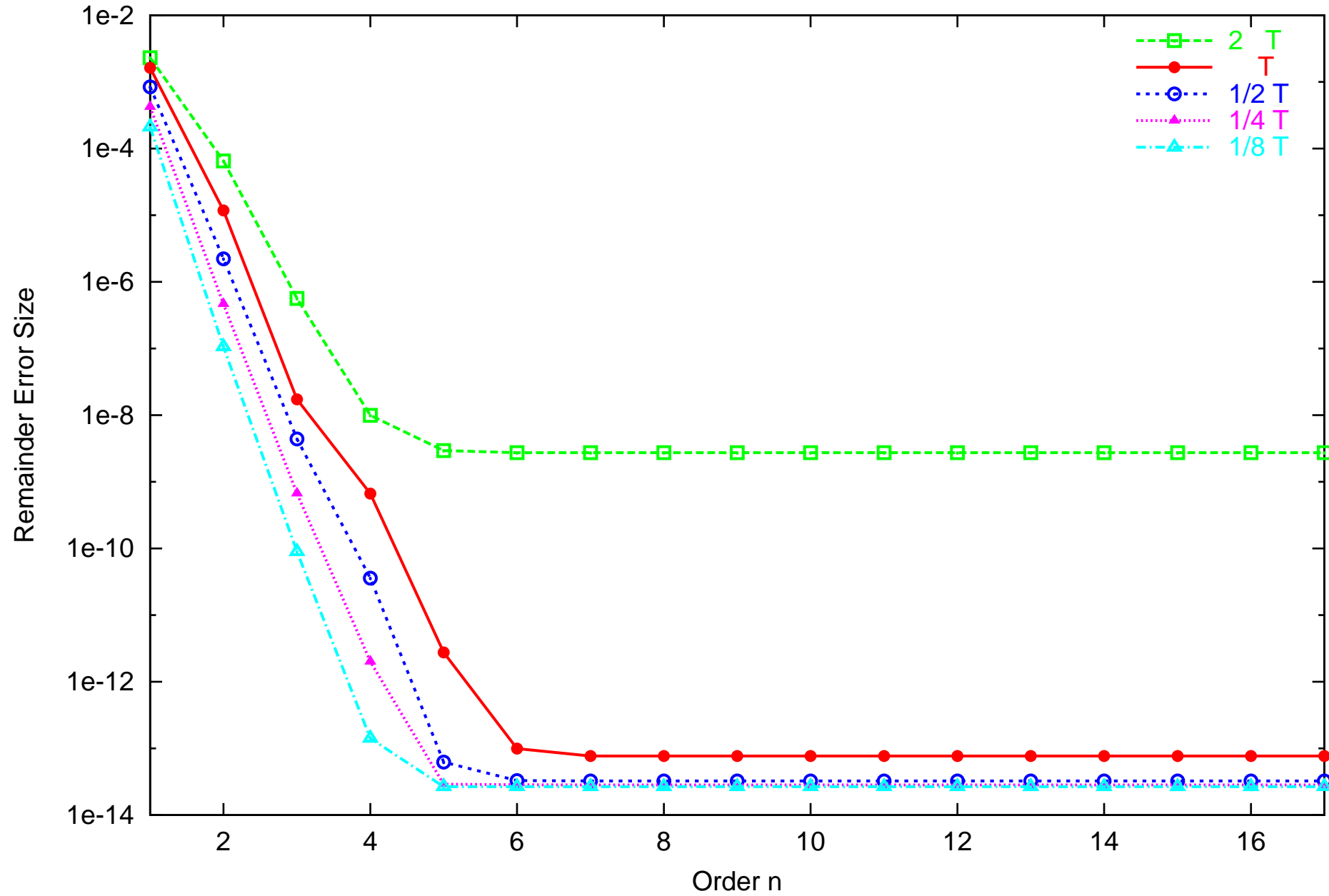


t=5.45

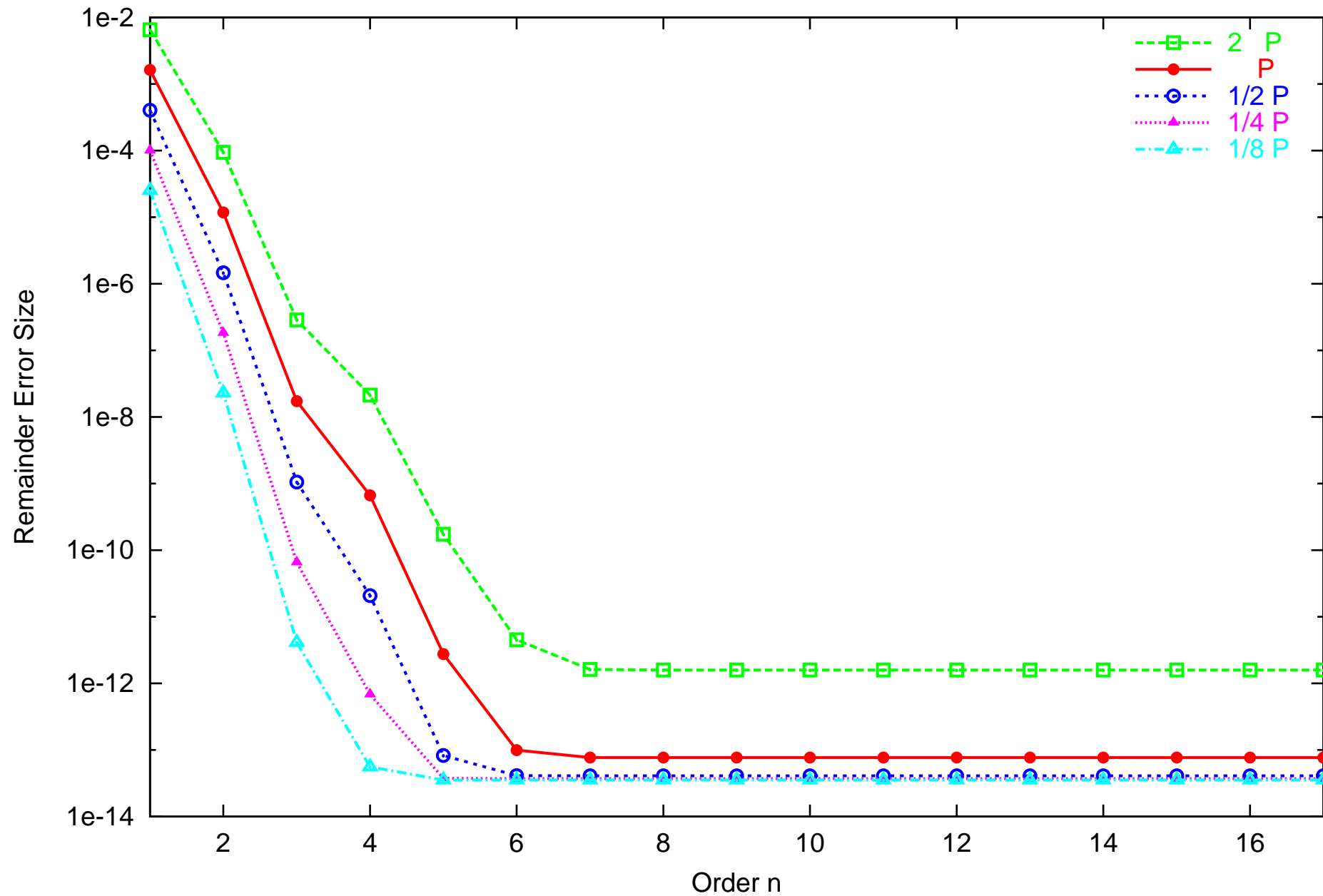


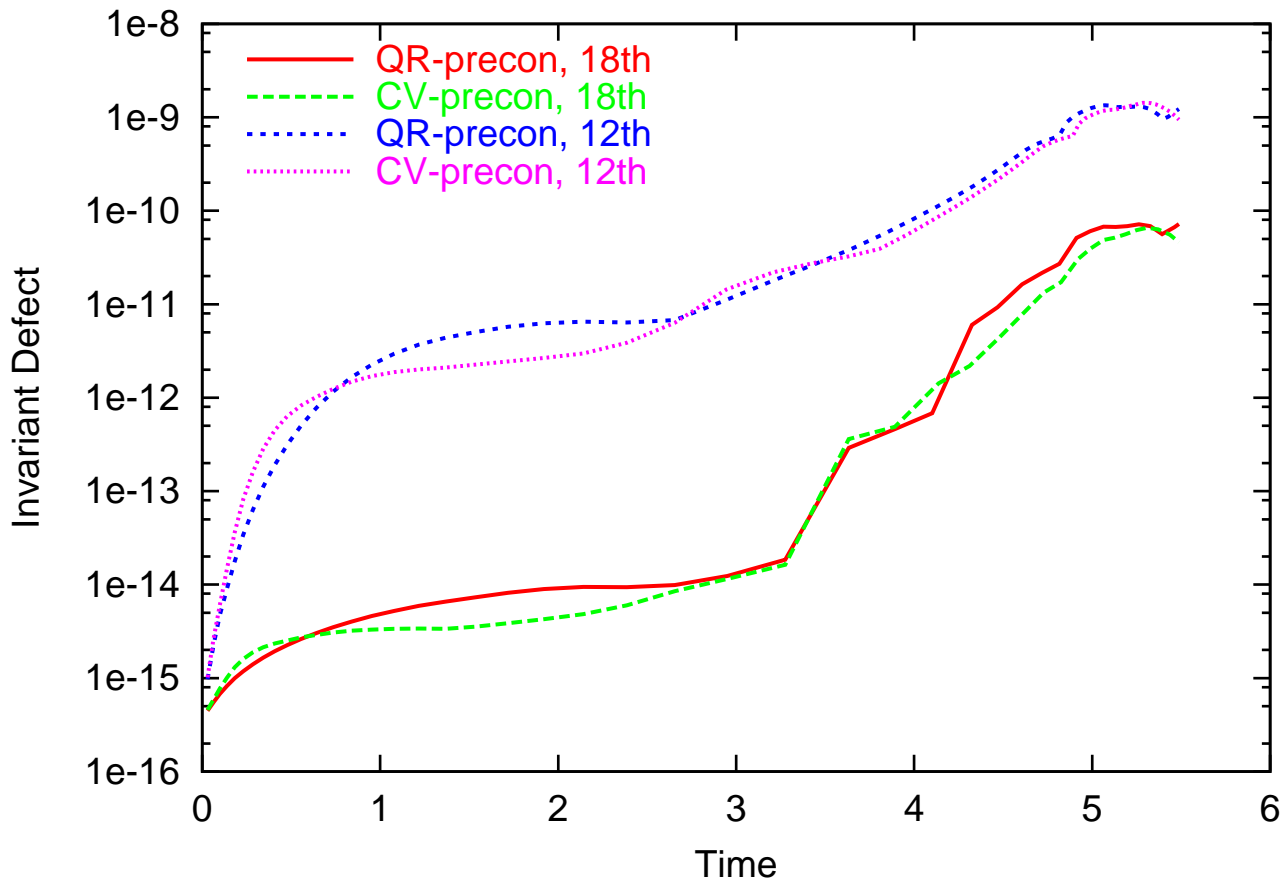


Volterra 18th, IC: P1, Result: $P_n + \{B(P_{n+1} \text{ to } P_{18}) + IR\}$, same P



Volterra 18th, IC: P1, Result: $P_n + \{B(P_{n+1} \text{ to } P_{18}) + IR\}$, same T





Shrink Wrapping I

A method to remove the remainder bound of a Taylor model by increasing the polynomial part.

After the k th step of the integration, the region occupied by the final variables is given by

$$A \subseteq \vec{I}_0 + \bigcup_{\vec{x}_0 \in \vec{B}} \mathcal{M}_0(\vec{x}_0),$$

where \vec{x}_0 are the initial variables, \vec{B} is the original box of initial conditions, \mathcal{M}_0 is the polynomial part of the Taylor model, and \vec{I}_0 is the remainder bound interval. \mathcal{M}_0 is scaled such that the original box \vec{B} is unity, i.e. $\vec{B} = [-1, 1]^v$. \vec{I}_0 accounts for the local approximation error of the expansion in time carried out in the k th step as well as floating point errors and potentially other accumulated errors from previous steps; it is usually very small. Try to “absorb” the small remainder interval into a set very similar to the first part via

$$A \subset A^* \subseteq \vec{I}_0^* + \bigcup_{\vec{x}_0 \in \vec{B}} \mathcal{M}_0^*(\vec{x}_0),$$

where \mathcal{M}_0^* is a slightly modified polynomial, and \vec{I}_0^* is significantly reduced

Shrink Wrapping

Theorem (Shrink Wrapping) Let $\mathcal{M} = \mathcal{I} + \mathcal{S}(\vec{x})$, where \mathcal{I} is the identity. Let $\vec{I} = d \cdot [-1, 1]^v$, and

$$A \subseteq \vec{I} \boxplus \bigcup_{\vec{x} \in \vec{B}} \mathcal{M}(\vec{x})$$

be the set sum of the interval $\vec{I} = [-d, d]^v$ and the range of \mathcal{M} over the original domain box \vec{B} . So A is the range enclosure of the flow of the ODE over the interval \vec{B} provided by the Taylor model. Let q be the shrink wrap factor of \mathcal{M} ; then we have

$$A \subset \bigcup_{\vec{x} \in \vec{B}} (q\mathcal{M})(\vec{x}),$$

and hence multiplying \mathcal{M} with the number q allows to set the remainder bound to zero.

Shrink Wrapping

We define q , the so-called shrink wrap factor, as

$$q = 1 + d \cdot \frac{1}{(1 - (v - 1)t) \cdot (1 - s)}.$$

The bounds s and t for the polynomials \mathcal{S}_i and $\partial\mathcal{S}_i/\partial x_j$ can be computed by interval evaluation. The factor q will prove to be a factor by which the Taylor polynomial $\mathcal{I} + \mathcal{S}$ has to be multiplied in order to absorb the remainder bound interval.

Remark (Typical values for q) To put the various numbers in perspective, in the case of the verified integration of the Asteroid 1997 XF11, we typically have $d = 10^{-7}$, $s = 10^{-4}$, $t = 10^{-4}$, and thus $q \approx 1 + 10^{-7}$. It is interesting to note that the values for s and t are determined by the non-linearity in the problem at hand, while in the absence of “noise” terms in the ODEs described by intervals, the value of d is determined mostly by the accuracy of the arithmetic. Rough estimates of the expected performance in quadruple precision arithmetic indicate that with an accompanying decrease in step size, if desired d can be decreased below 10^{-12} , resulting in $q \approx 1 + 10^{-12}$.

Long-Term Behavior - Validated Case

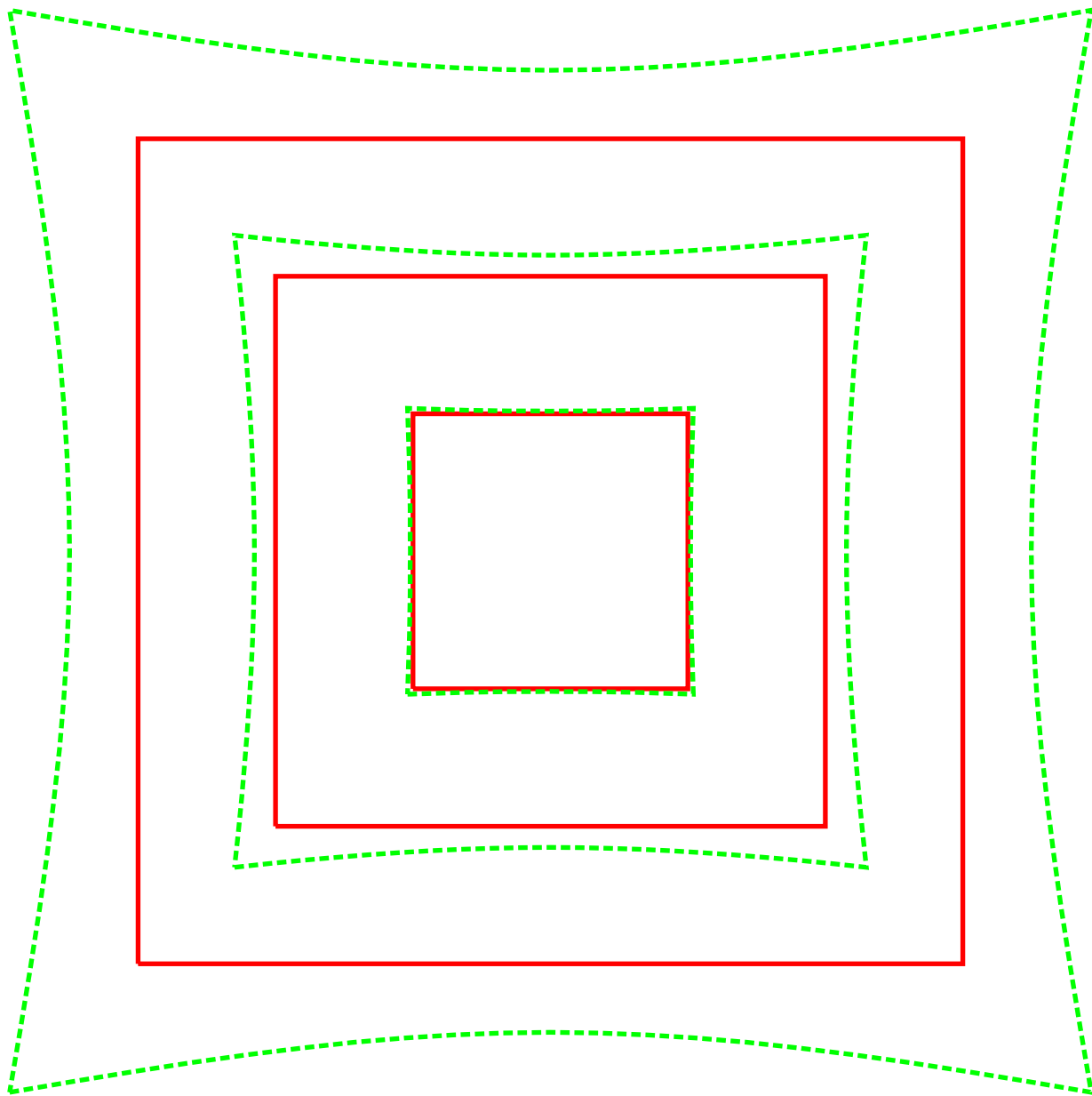
Consider very simple two-state dynamical system:

$$x_{n+1} = x_n \cdot \sqrt{1 + x_n^2 + y_n^2} \text{ and } y_{n+1} = y_n \cdot \sqrt{1 + x_n^2 + y_n^2}$$

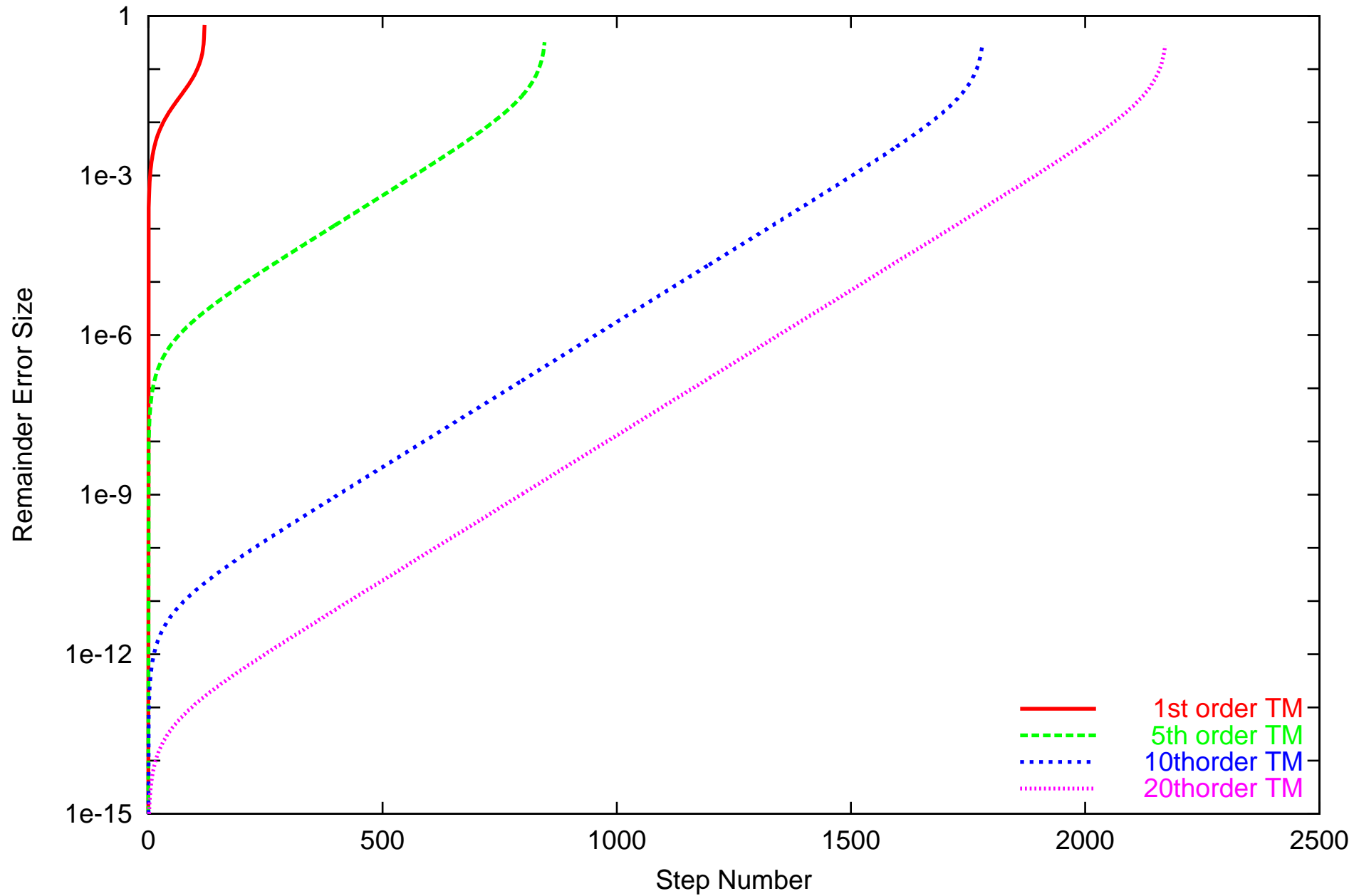
$$x_{n+2} = x_{n+1} \cdot \sqrt{\frac{2}{1 + \sqrt{1 + 4(x_{n+1}^2 + y_{n+1}^2)}}} \text{ and}$$

$$y_{n+2} = y_{n+1} \cdot \sqrt{\frac{2}{1 + \sqrt{1 + 4(x_{n+1}^2 + y_{n+1}^2)}}}.$$

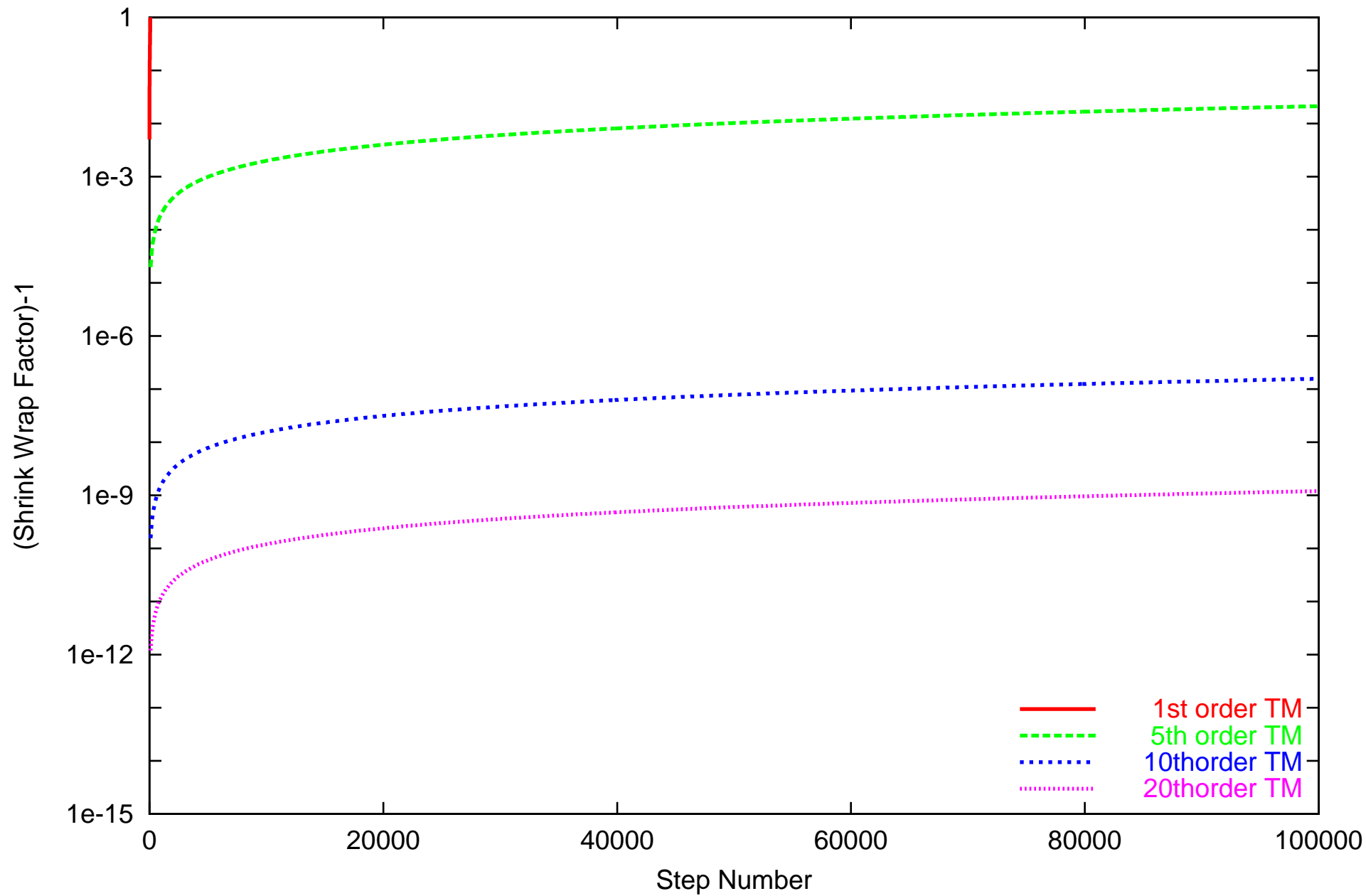
Simple arithmetic shows that, also here we have $(x_{n+2}, y_{n+2}) = (x_n, y_n)$.



Stretch by $\sqrt{1+x^2+y^2}$ and unstretch back, $DX=0.05$, $(0,0)$, noSW



Stretch by $\sqrt{1+x^2+y^2}$ and unstretch back, $DX=0.05$, $(0,0)$, SW



Shrink Wrapping II

Let us consider the practical limitations of the method; apparently the measures of the nonlinearities s and t must not become too large

Remark (Limitations of shrink wrapping) Apparently the shrink wrap method discussed above has the following limitations

Remark 1 *1. The measures of nonlinearities s and t must not become too large*

2. The application of the inverse of the linear part should not lead to large increases in the size of remainder bounds.

Apparently the first requirement limits the domain size that can be covered by the Taylor model, and it will thus happen only in extreme cases. Furthermore, in practice the case of s and t becoming large is connected to also having accumulated a large remainder bound, since the remainder bounds are calculated from the bounds of the various orders of s . In the light of this, not much additional harm is done by removing the offending s into the remainder bound and create a linearized Taylor model.

Definition (Blunting of an Ill-Conditioned Matrix)

Let \hat{A} be a regular matrix that is potentially ill-conditioned and $\vec{q} = (q_1, \dots, q_n)$ a vector with $q_i > 0$. Arrange the column vectors \vec{a}_i of \hat{A} by size.

Let \vec{e}_i be the familiar orthonormal vectors obtained through the Gram-Schmidt procedure, i.e.

$$\vec{e}_i = \frac{\vec{a}_i - \sum_{k=1}^{i-1} \vec{e}_k (\vec{a}_i \cdot \vec{e}_k)}{\left| \vec{a}_i - \sum_{k=1}^{i-1} \vec{e}_k (\vec{a}_i \cdot \vec{e}_k) \right|}.$$

We form vectors \vec{b}_i via

$$\vec{b}_i = \vec{a}_i + q_i \vec{e}_i$$

and assemble them columnwise into the matrix \hat{B} . We call \hat{B} the \vec{q} -blunted matrix belonging to \hat{A}

Intuitively, the effect of blunting is that each vector \vec{b}_i is being "pulled away" from the space spanned by the previous vectors $\vec{b}_1, \dots, \vec{b}_{i-1}$, and more strongly so if q_i becomes bigger and bigger. In fact, we have the following result: .

Preconditioning the Flow

Idea: write the Taylor model of the solution as a composition of two Taylor models $(P_l + I_l)$ and $(P_r + I_r)$, and then choose $P_l + I_l$ in such a way that in each step, the operations appearing on I_r are minimized. At the same time, I_l will be chosen as small as possible. Can be viewed as a coordinate transformation.

In the factorization, we impose that $(P_r + I_r)$ is normalized such that each of its components has a range in $[-1, 1]$, and even near the boundaries.

Definition (Preconditioning the Flow) Let $(P + I)$ be a Taylor model. We say that $(P_l + I_l), (P_r + I_r)$ is a factorization of $(P + I)$ if $B(P_r + I_r) \in [-1, 1]$ and

$$(P + I) \in (P_l + I_l) \circ (P_r + I_r) \text{ for all } x \in \mathcal{D}$$

where \mathcal{D} is the domain of the Taylor model $(P_r + I_r)$.

The composition of the Taylor models is here to be understood as insertion of the Taylor model $P_r + I_r$ into the polynomial P_l via Taylor model addition and multiplication and subsequent addition of the remainder bound I_l . For the study of the solutions of ODEs, the following result is important

Preconditioning the Flow II

Proposition Let $(P_{l,n} + I_{l,n}) \circ (P_{r,n} + I_{r,n})$ be a factored Taylor model that encloses the flow of the ODE at time t_n . Let $(P_{l,n+1}^*, I_{l,n+1}^*)$ be the result of integrating $(P_{l,n} + I_{l,n})$ from t_n to t_{n+1} . Then solution is in

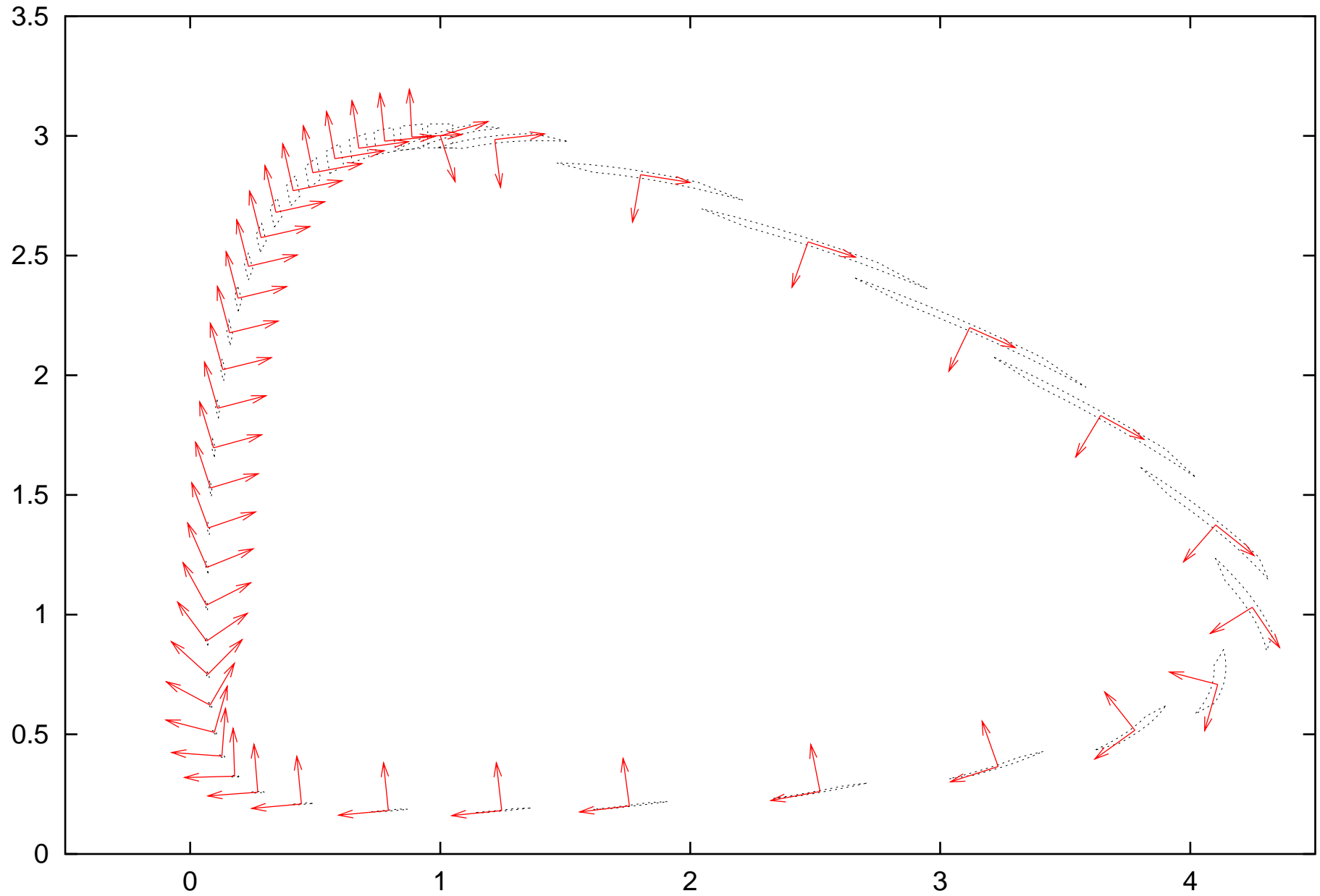
$$(P_{l,n+1}^*, I_{l,n+1}^*) \circ (P_{r,n} + I_{r,n})$$

Definition (Curvilinear Preconditioning) Let $x^{(m)} = f(x, x', \dots, x^{(m-1)}, t)$ be an m -th order ODE in n variables. Let $x_r(t)$ be a solution of the ODE and $x_r'(t), \dots, x_r^{(k)}(t)$ its first k time derivatives. Let $\vec{e}_1, \dots, \vec{e}_l$ be the l unit vectors not in the span of $x_r'(t), \dots, x_r^{(k)}(t)$, sorted by distance from the span. Then we call the Gram-Schmidt orthonormalization of the set $(x_r'(t), \dots, x_r^{(k)}(t), \vec{e}_1, \dots, \vec{e}_l)$ the curvilinear basis of depth k .

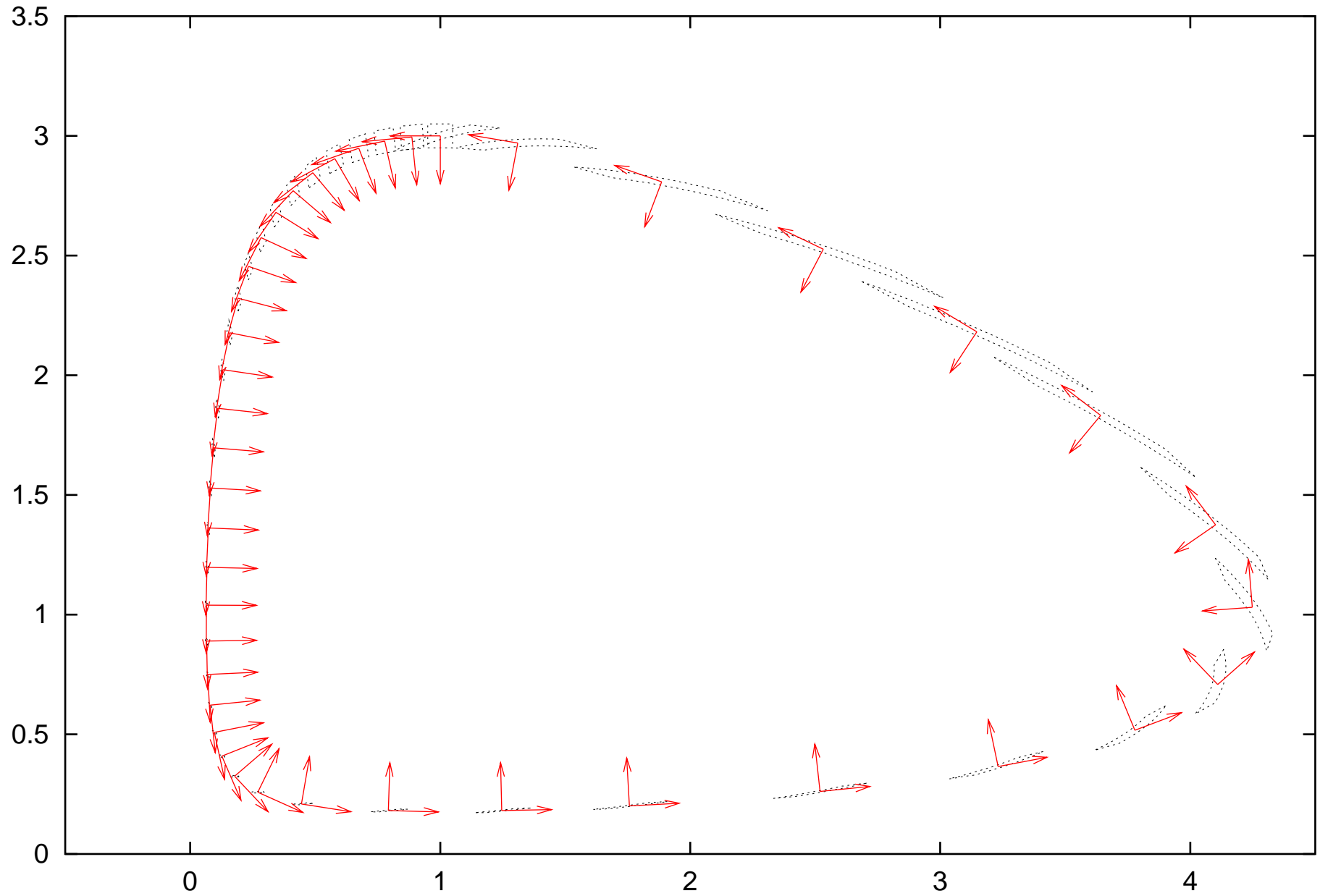
Curvilinear coordinates have long history. Study of solar system, Beam Physics,

Example (Curvilinear Solar System and Particle Accelerators) In this case, $n = 3$, and one usually chooses $k = 2$. The first basis vector points in the direction of motion of the reference orbit. The second vector is perpendicular to it and points approximately to the sun or the center of the accelerator. The third vector is chosen perpendicular to the plane of the previous two.

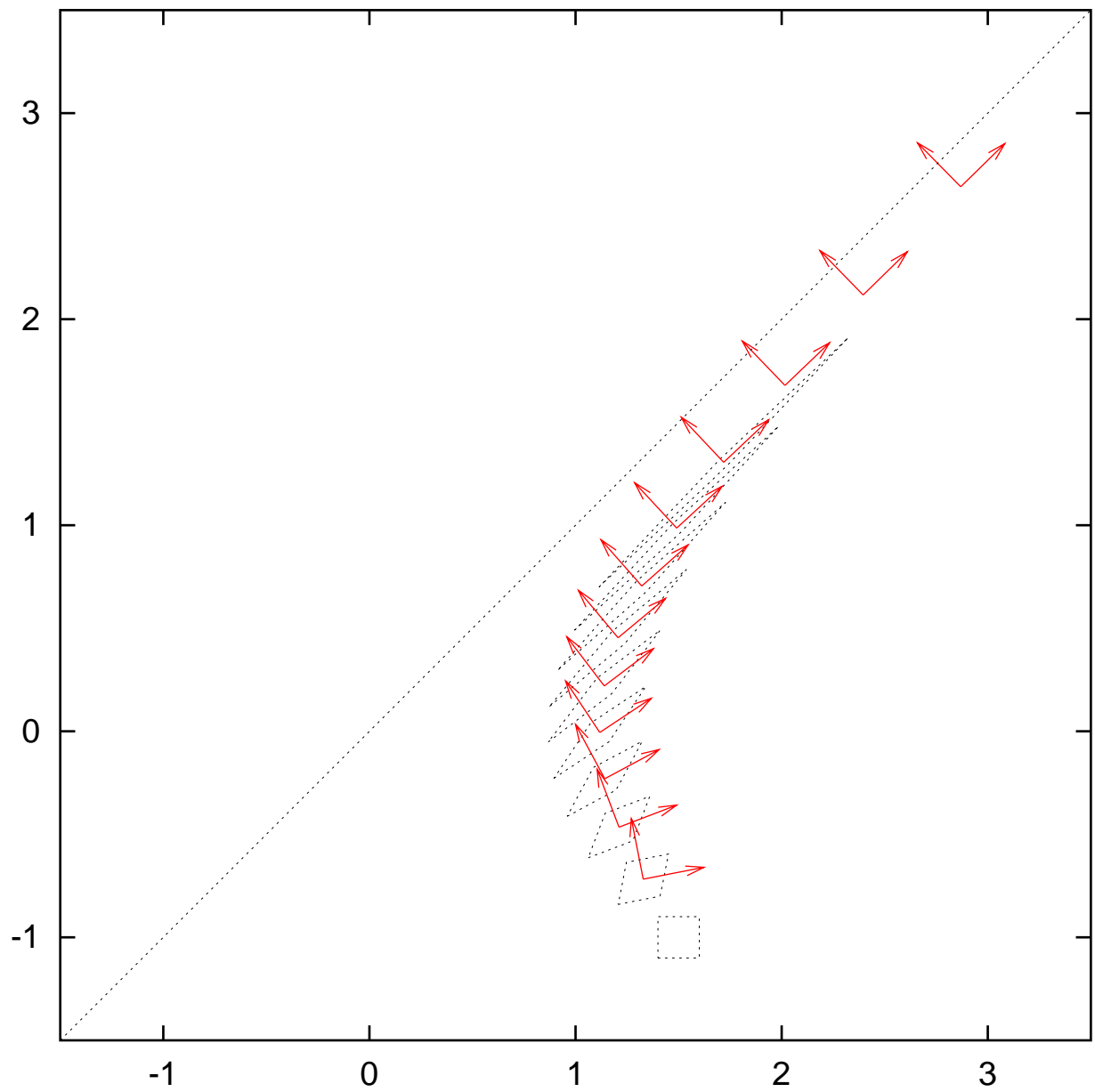
Volterra - QR based preconditioning



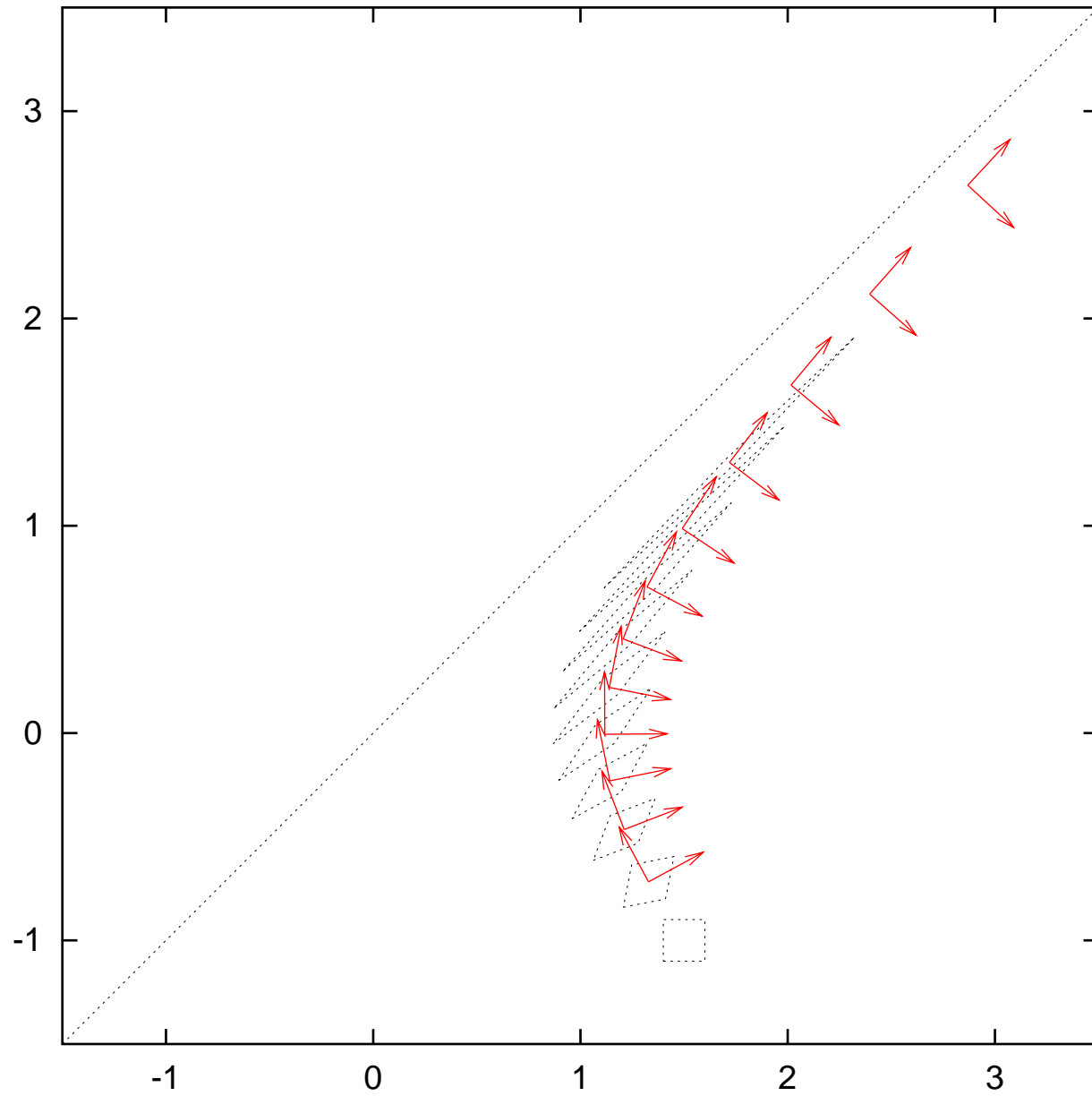
Volterra - Curvilinear preconditioning



needle IC(1.5,-1) - QR based preconditioning



needle IC(1.5,-1) - Curvilinear preconditioning



Random Matrices - Discrete

Select 1000 twodimensional random matrices with coefficients in $[-1, 1]$. Sort according to eigenvalues into seven sub-cases.

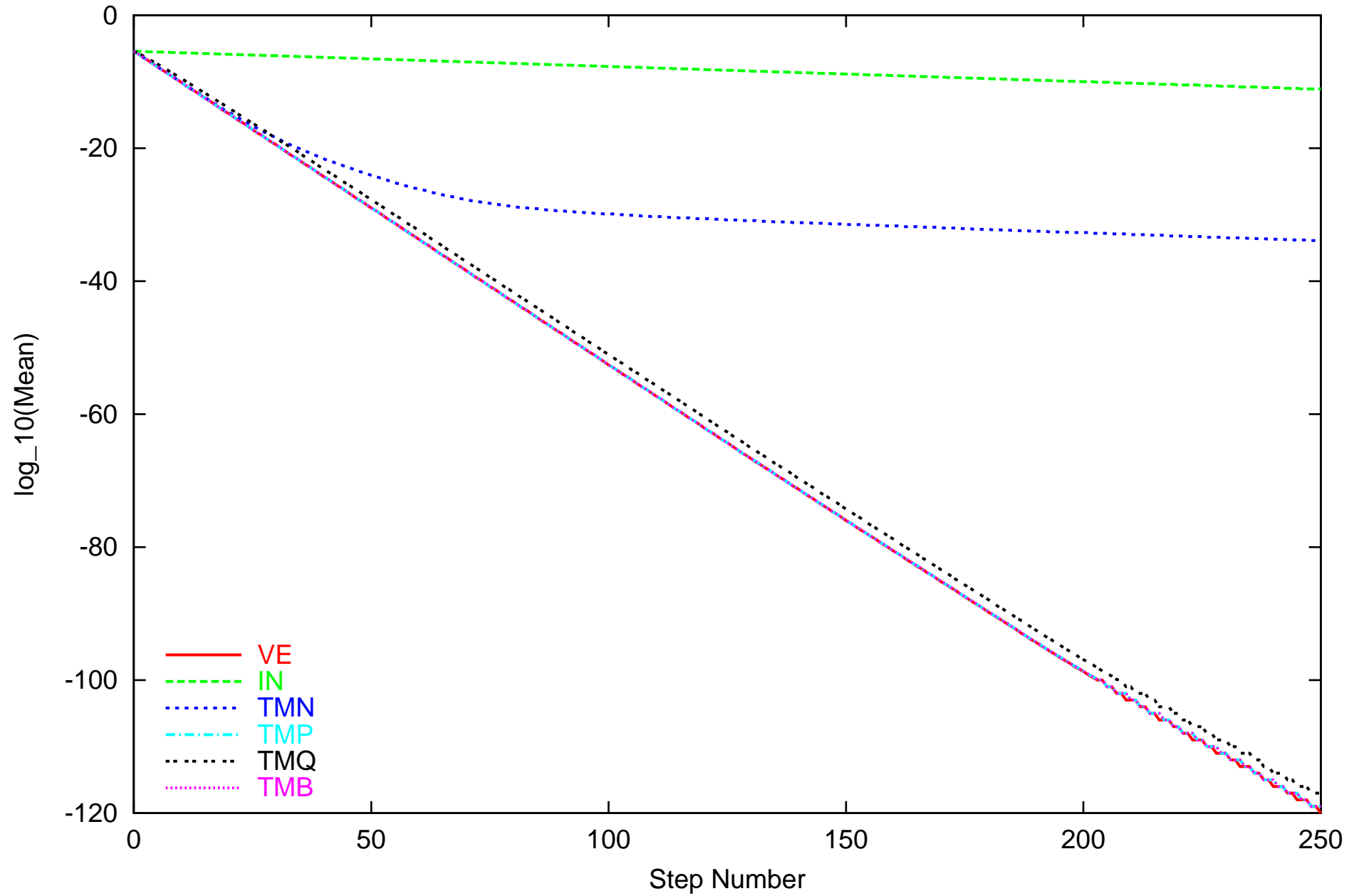
Perform iteration in the following ways:

- Naive Interval
- Naive Taylormodel
- Parallelepiped-preconditioned Taylormodel
- **QR**-preconditioned \square Taylormodel
- Blunted preconditioned TM, various blunting factors
- Set of four floating point corner points for volume estimation

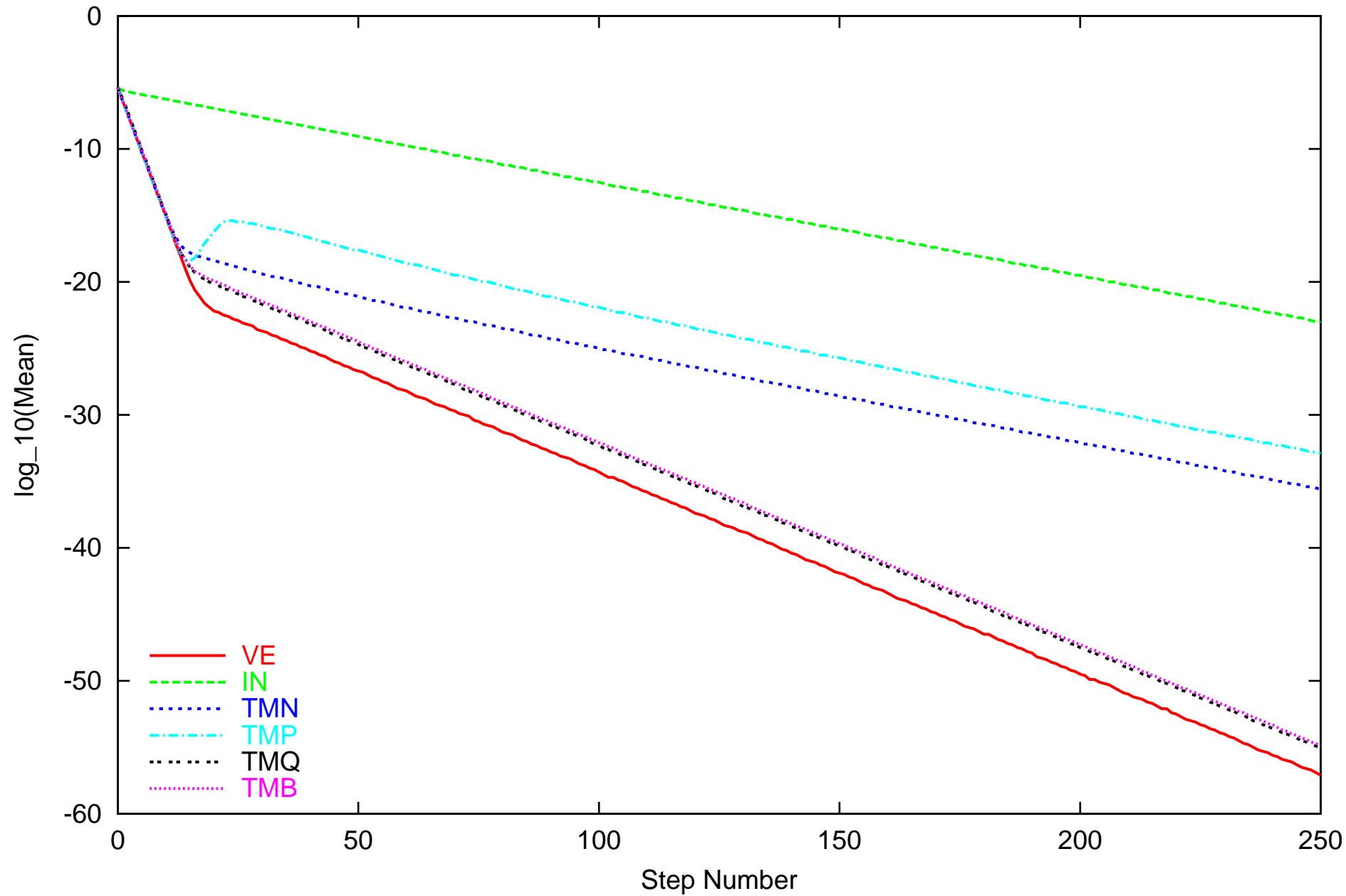
Perform the following tasks:

- Iterations through matrix
- Sets of iterations through matrix and its inverse

325 Conjugate EVs Random Matrices



80 Real EVs (5 =< ratio < 10) Random Matrices



Random Matrices - Discrete

Select 1000 twodimensional random matrices with coefficients in $[-1, 1]$. Sort according to eigenvalues into seven sub-cases.

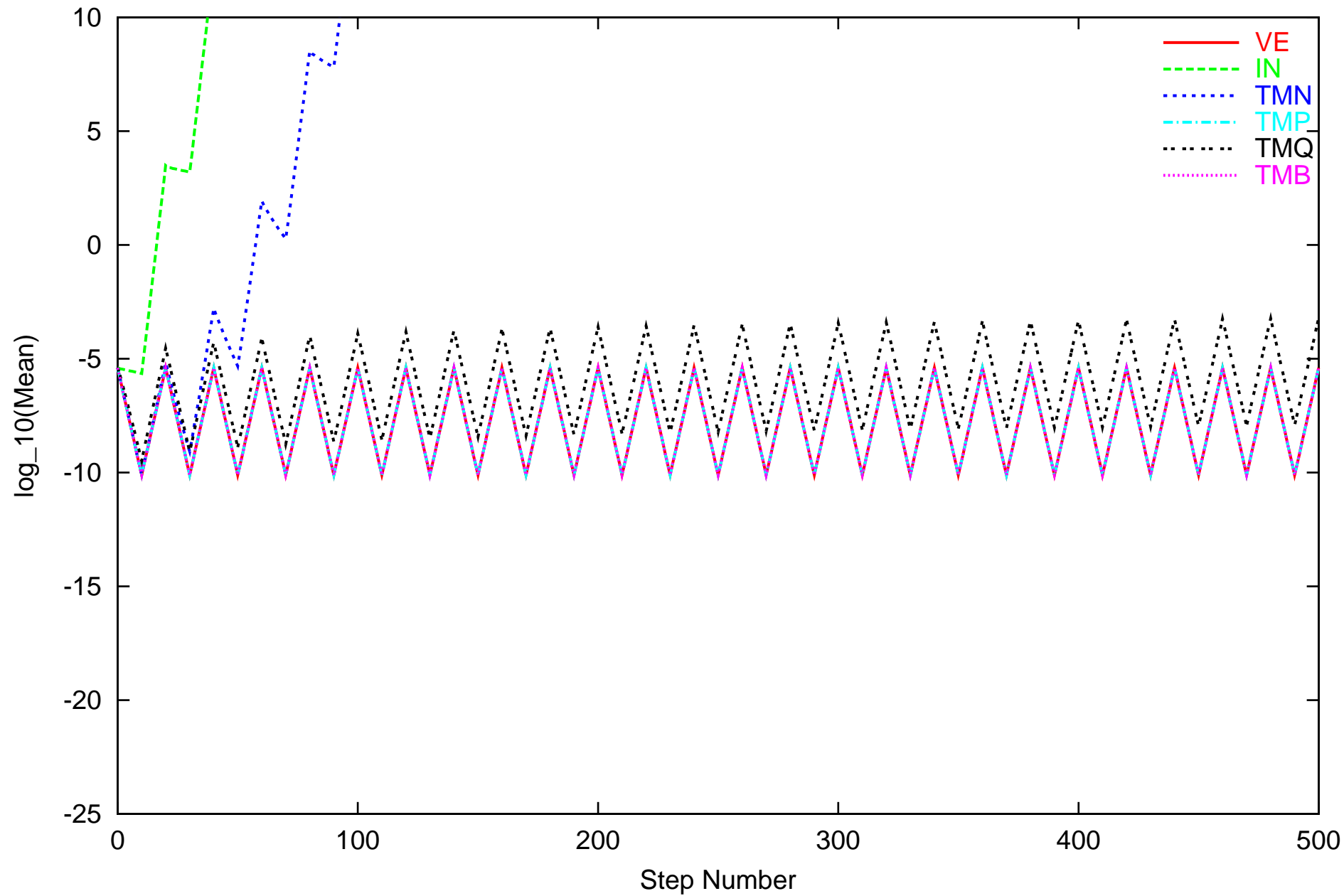
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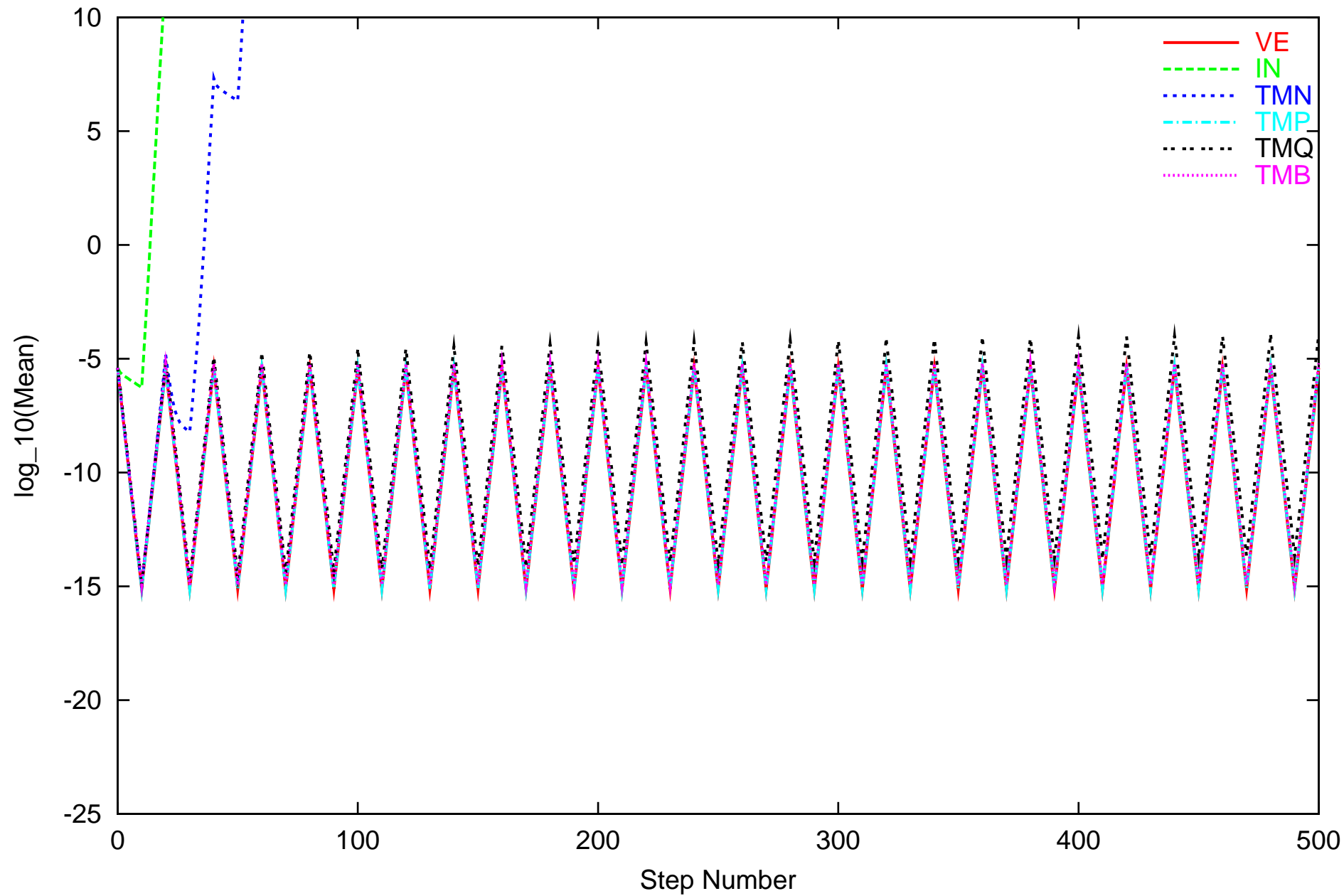
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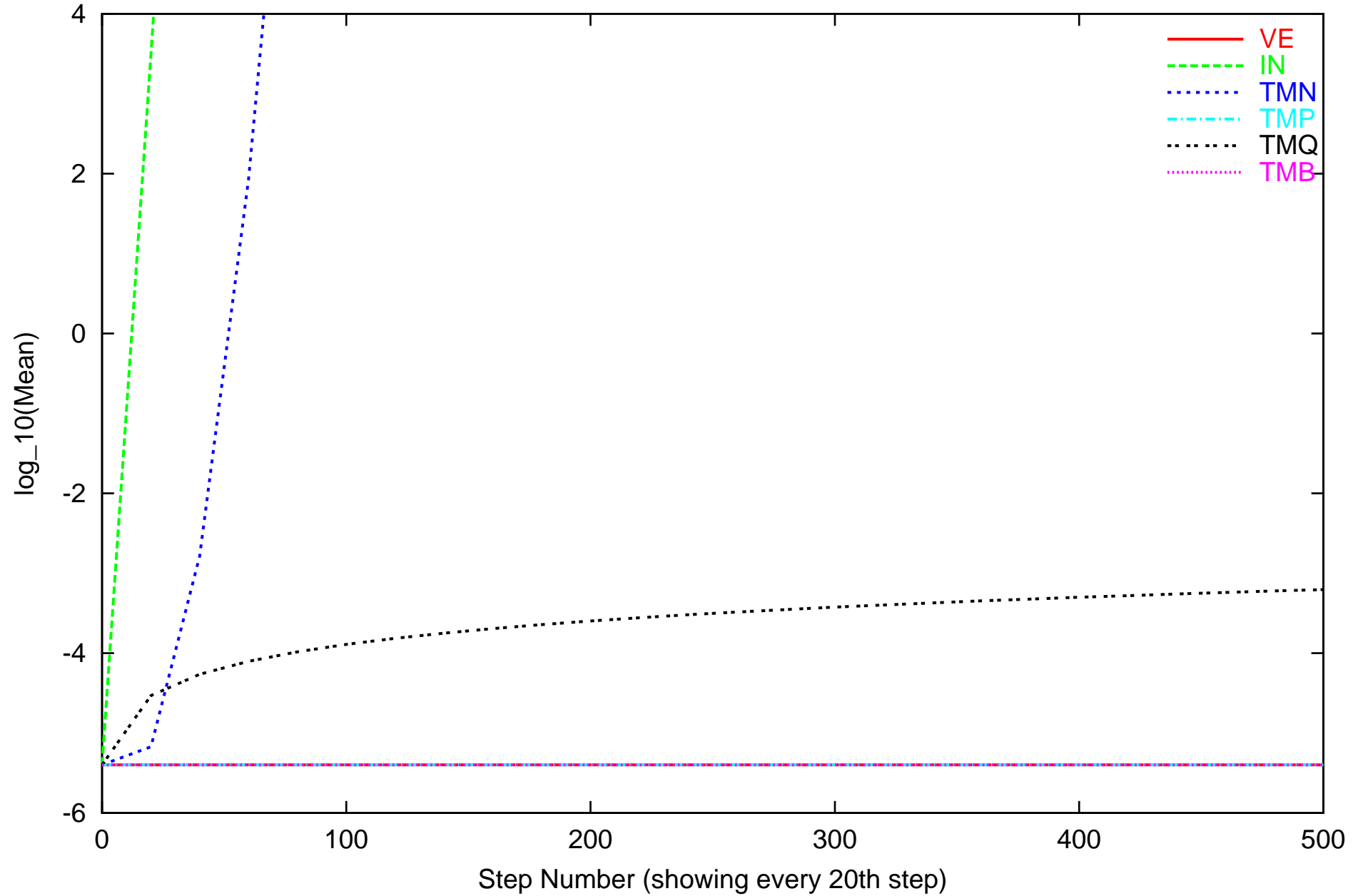
325 Conjugate EVs Random Matrices



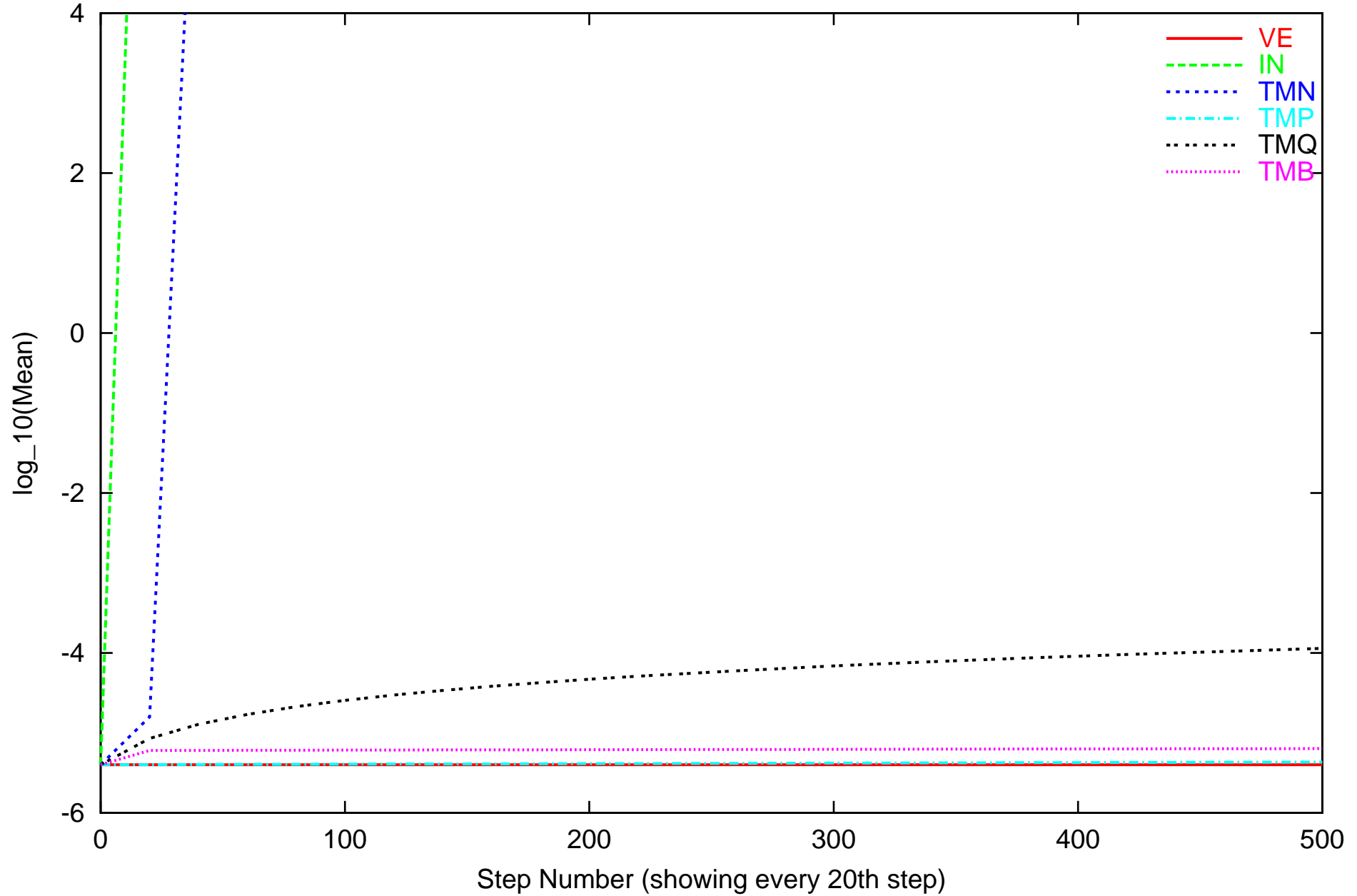
80 Real EVs ($5 \leq \text{ratio} < 10$) Random Matrices



325 Conjugate EVs Random Matrices



80 Real EVs ($5 \leq \text{ratio} < 10$) Random Matrices



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

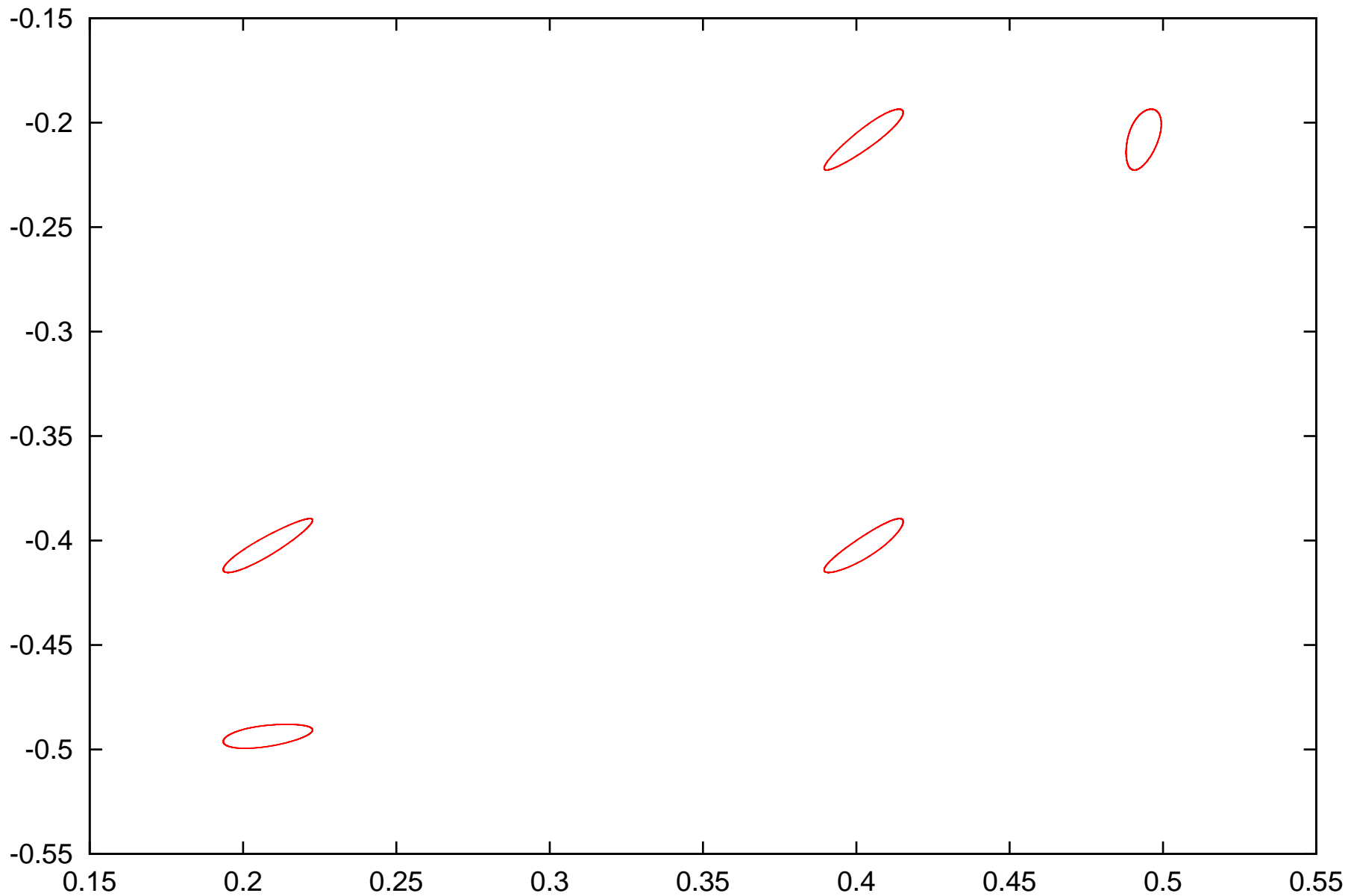
$$\begin{aligned}x_{n+1} &= 1 - \alpha x_n^2 + y_n \\ y_{n+1} &= \beta x_n.\end{aligned}$$

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

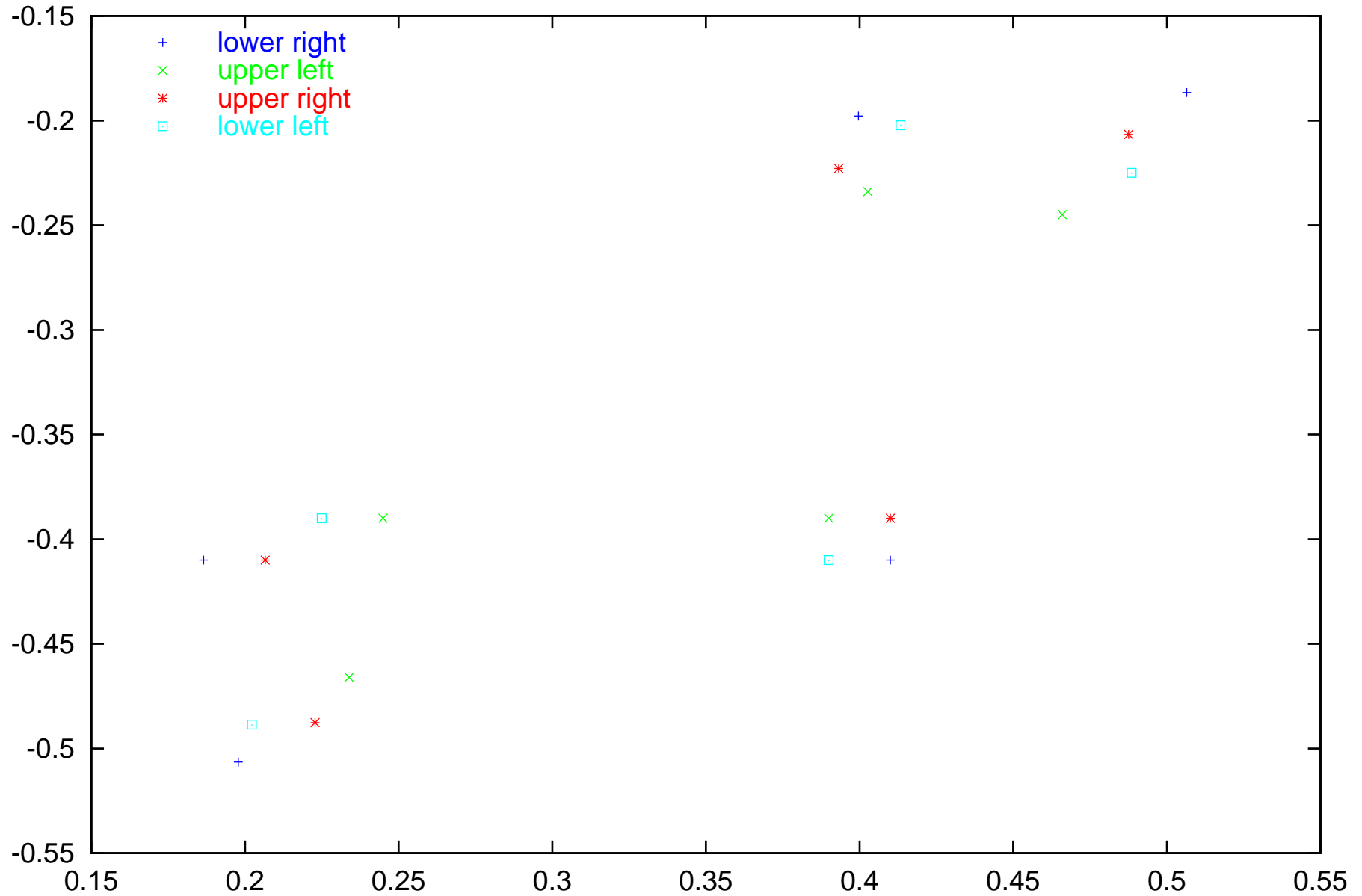
$$\alpha = 2.4 \text{ and } \beta = -1,$$

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

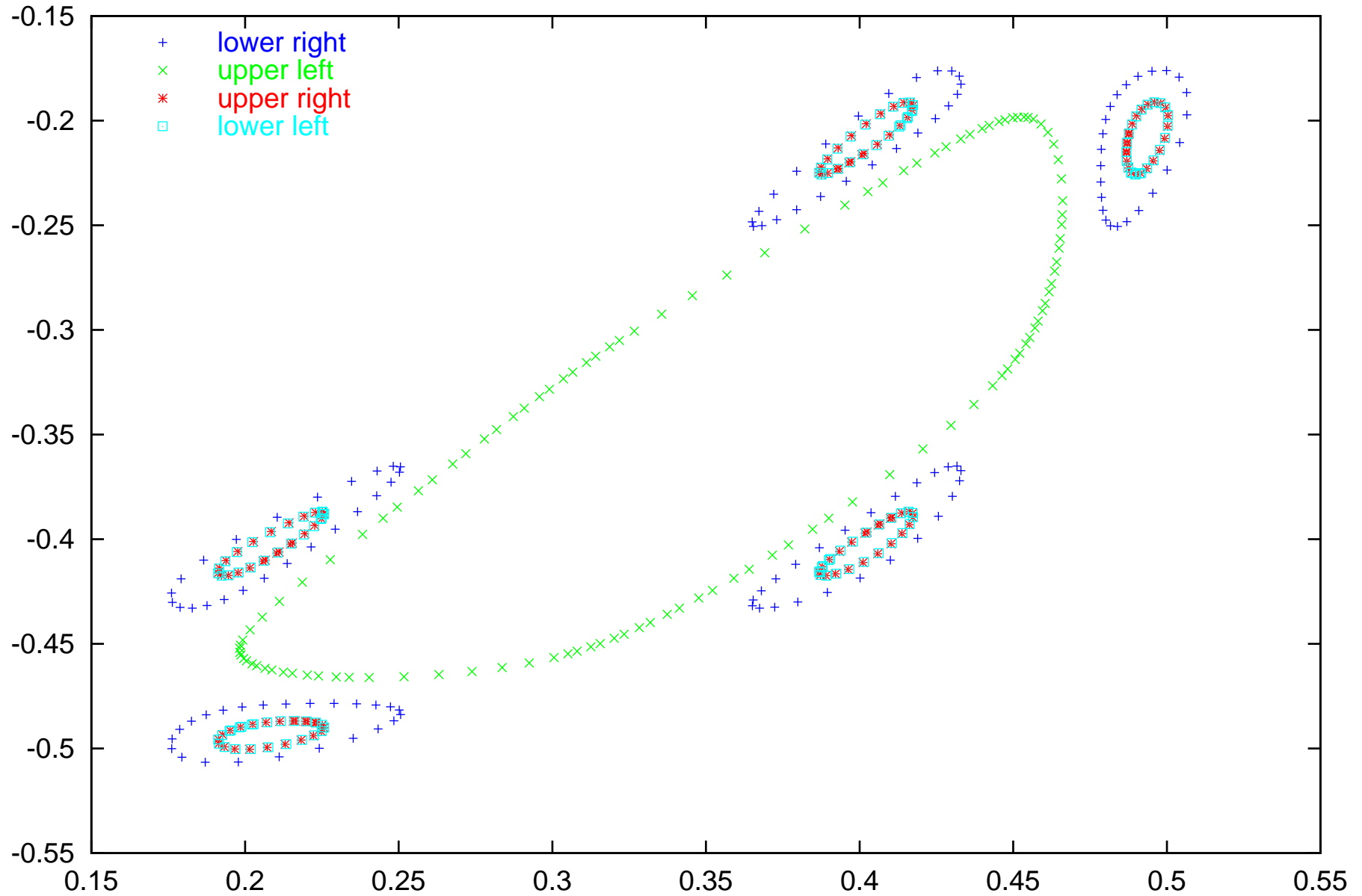
Henon system, $x_n = 1 - 2.4x^2 + y$, $y_n = -x$, the positions at each step



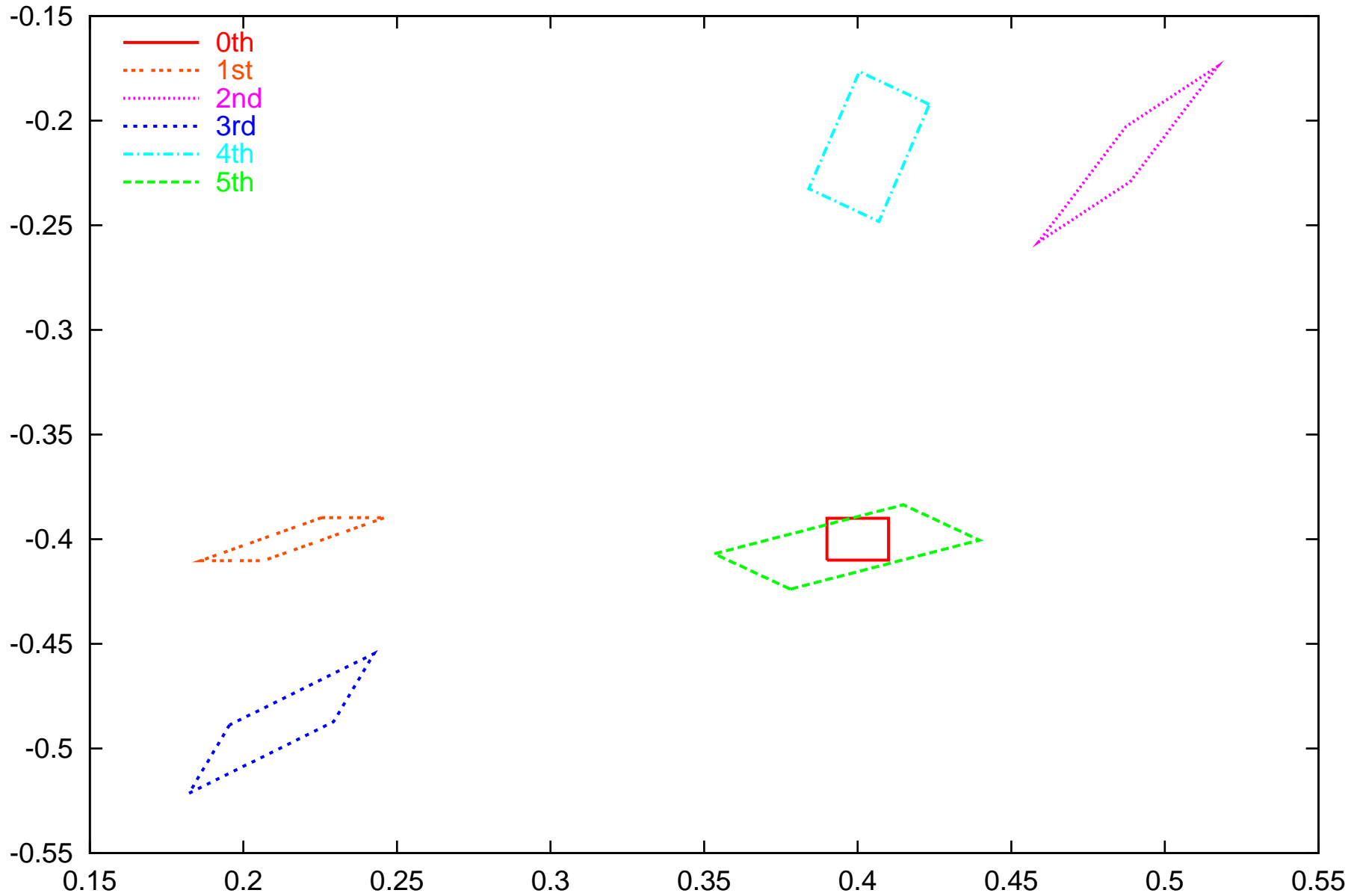
Henon system, $x_n = 1 - 2.4x^2 + y$, $y_n = -x$, corner points (± 0.01) the first 5 steps



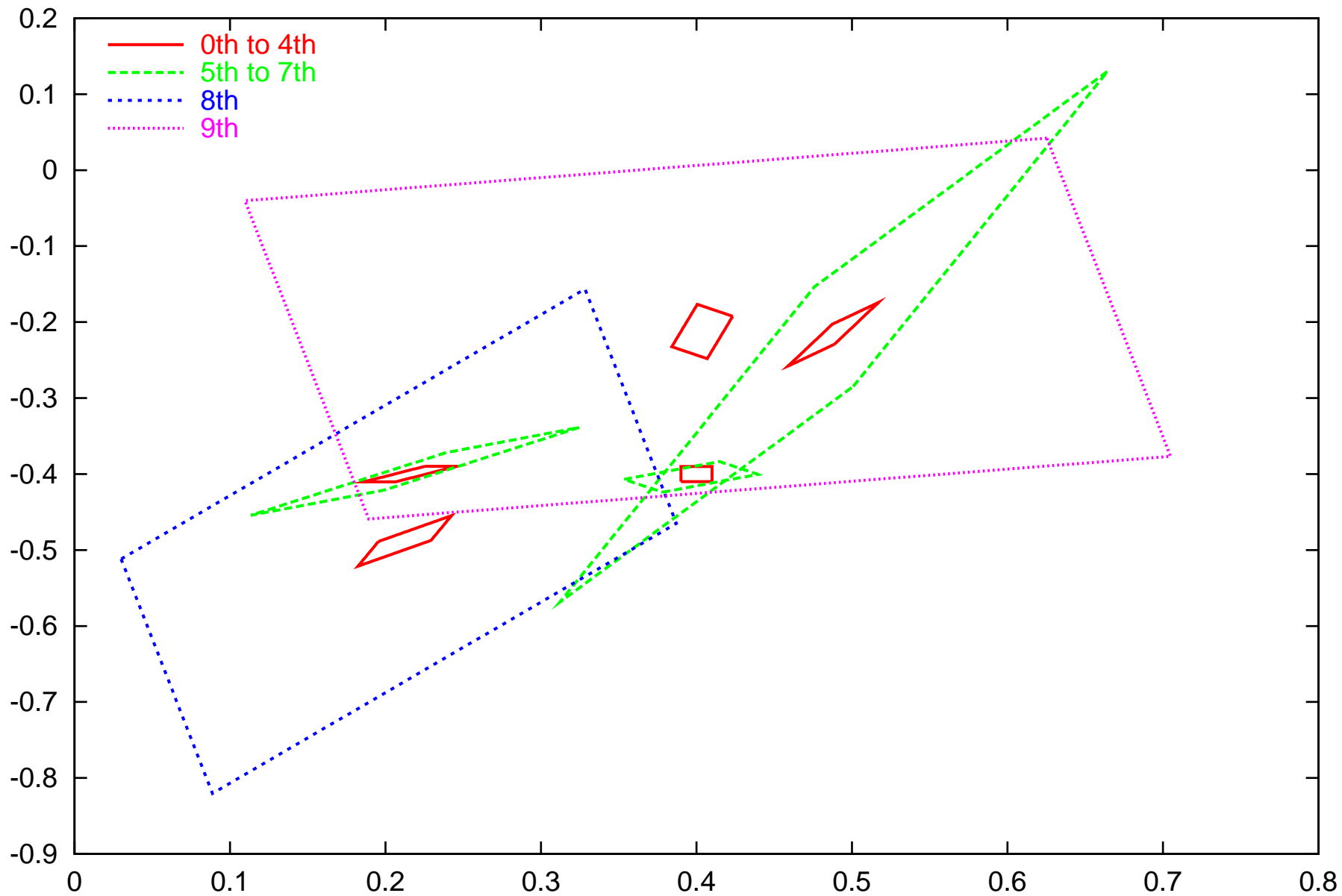
Henon system, $x_n = 1 - 2.4x^2 + y$, $y_n = -x$, corner points (± 0.01) the first 120 steps



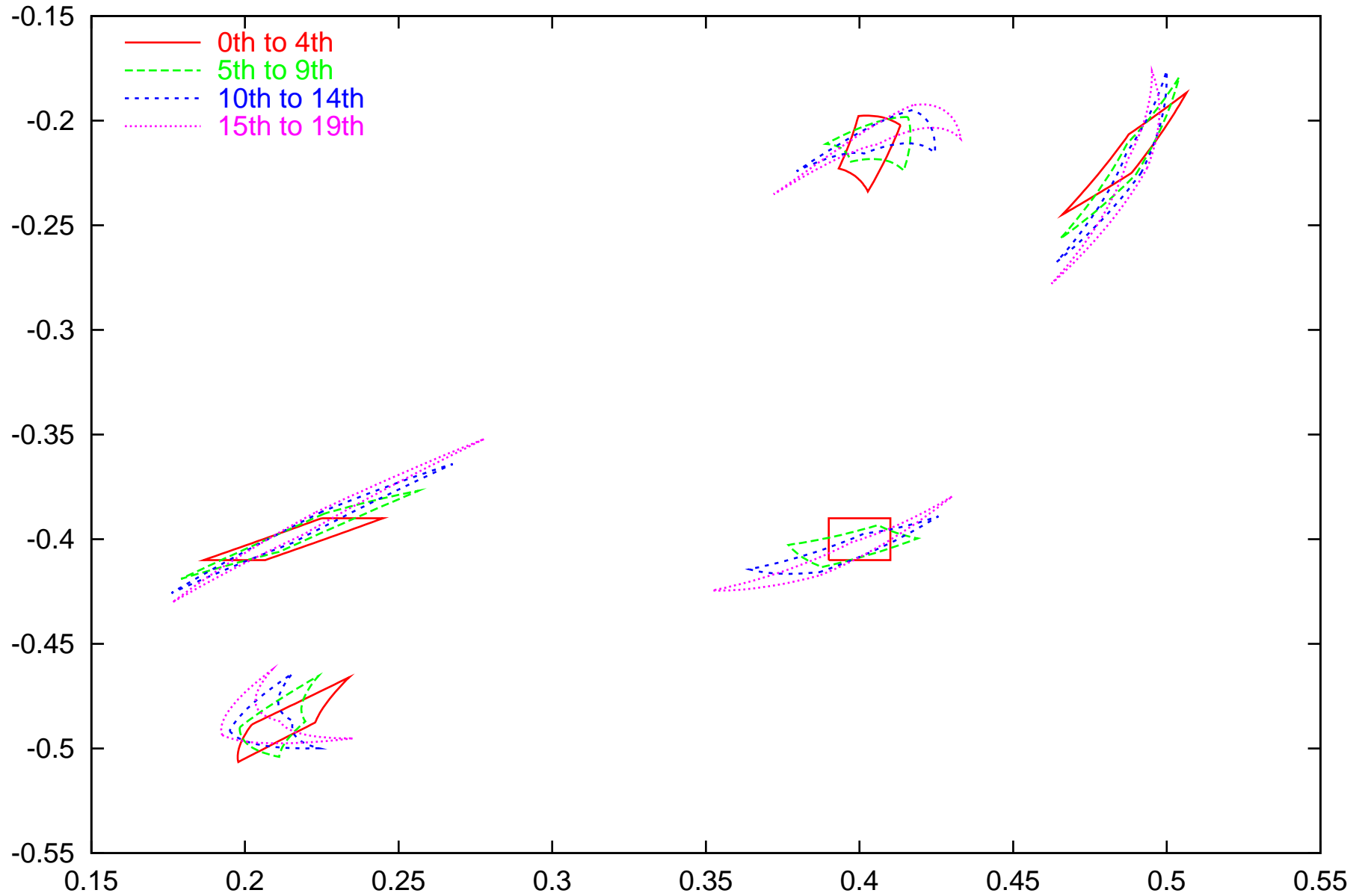
Henon system, $x_n = 1 - 2.4x^2 + y$, $y_n = -x$, NO=1, SW



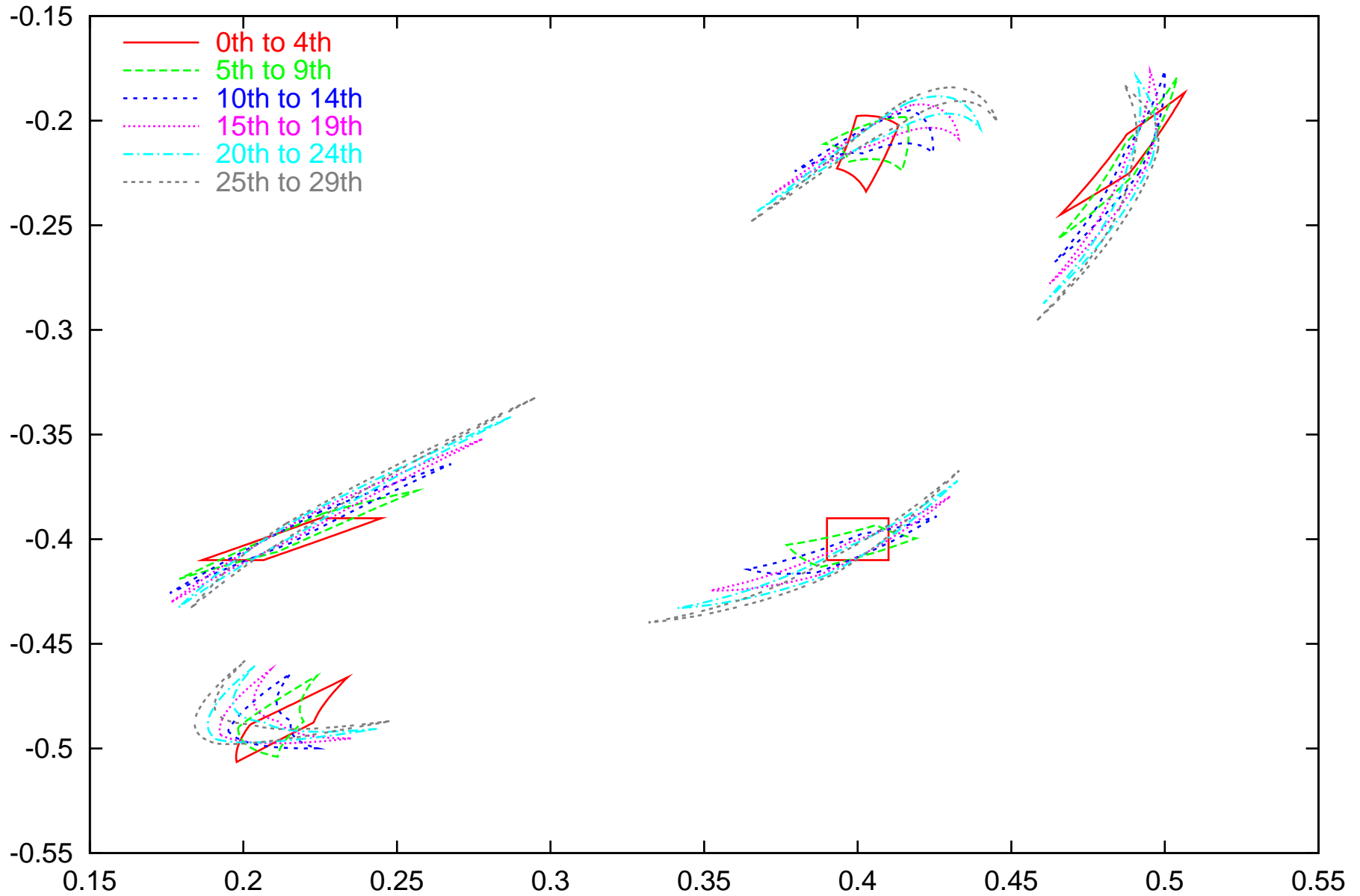
Henon system, $x_n = 1 - 2.4x^2 + y$, $y_n = -x$, NO=1, SW

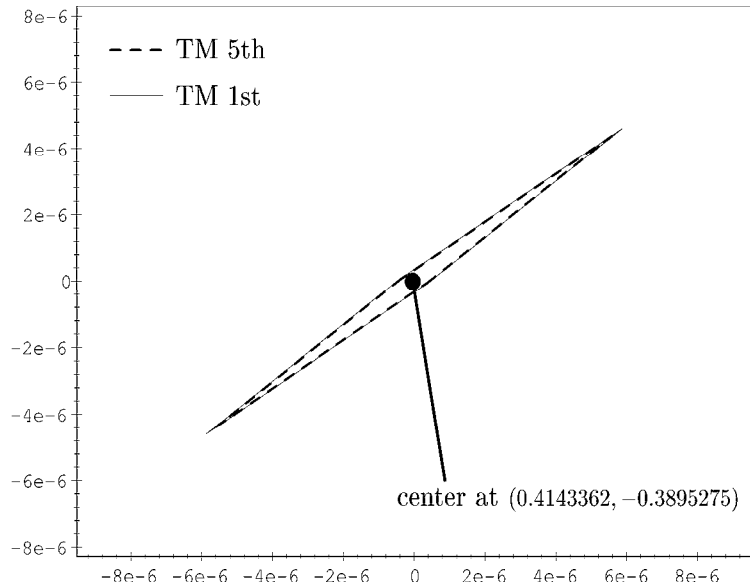
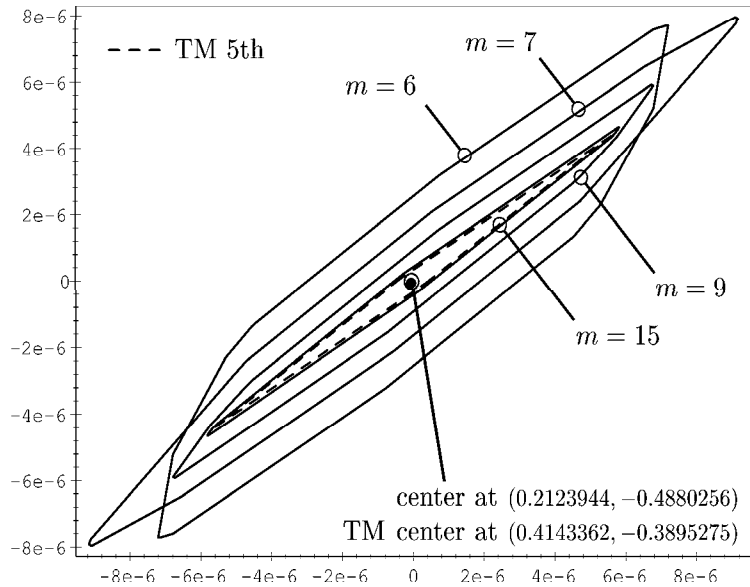


Henon system, $x_n = 1 - 2.4x_n^2 + y_n$, $y_n = -x_n$, NO=20, SW

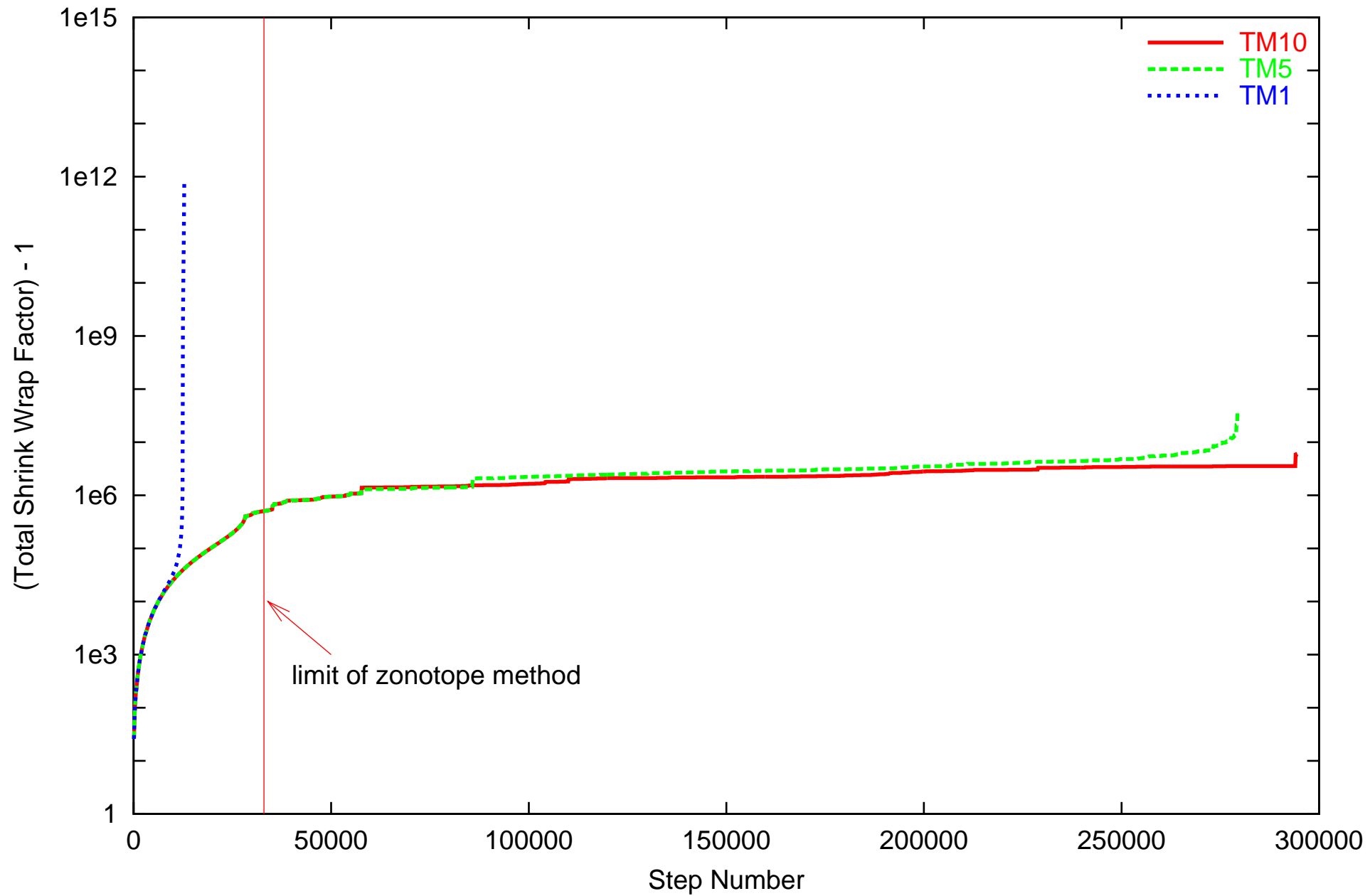


Henon system, $x_n = 1 - 2.4x_n^2 + y_n$, $y_n = -x_n$, NO=20, SW





Henon system, $x_n = 1 - 2.4x^2 + y$, $y_n = -x$, $DX = 1e-14$, $(0.4, -0.4)$, SW



A Muon Cooling Ring

Example from Beam Physics: Simple model of muon cooling ring, using curvilinear preconditioning.

Simultaneous damping via matter, and azimuthal accelerations. Equations of motion:

$$\begin{aligned}\dot{x} &= p_x \\ \dot{y} &= p_y \\ \dot{p}_x &= p_y - \frac{\alpha}{\sqrt{p_x^2 + p_y^2}} \cdot p_x + \frac{\alpha}{\sqrt{x^2 + y^2}} \cdot y \\ \dot{p}_y &= -p_x - \frac{\alpha}{\sqrt{p_x^2 + p_y^2}} \cdot p_y - \frac{\alpha}{\sqrt{x^2 + y^2}} \cdot x\end{aligned}$$

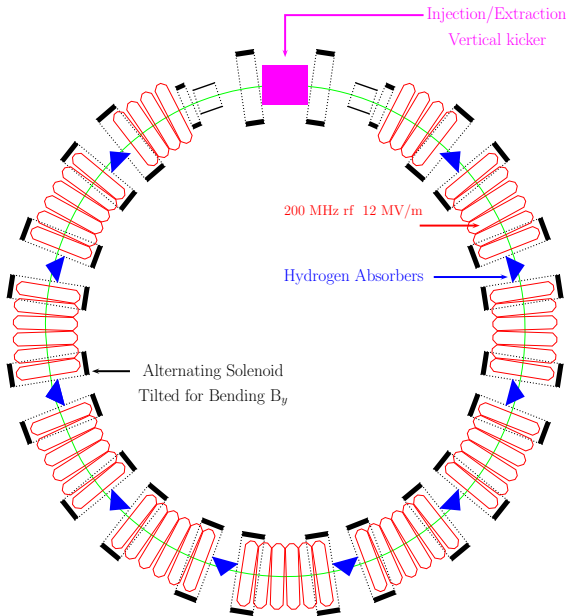
Has invariant solution

$$(x, y, p_x, p_y)_I(t) = (\cos t, -\sin t, -\sin t, -\cos t),$$

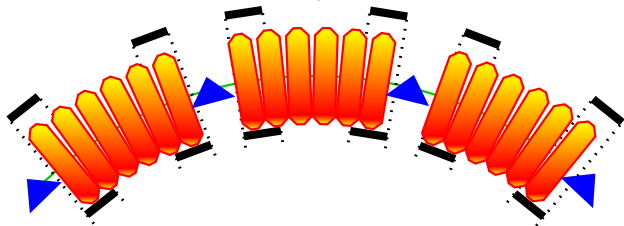
ODE asymptotically approach circular motion of the form

$$(x, y, p_x, p_y)_a(t) = (\cos(t - \phi), -\sin(t - \phi), -\sin(t - \phi), -\cos(t - \phi)),$$

where ϕ is a characteristic angle for each particle.



a)

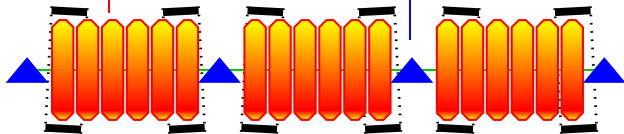


b)

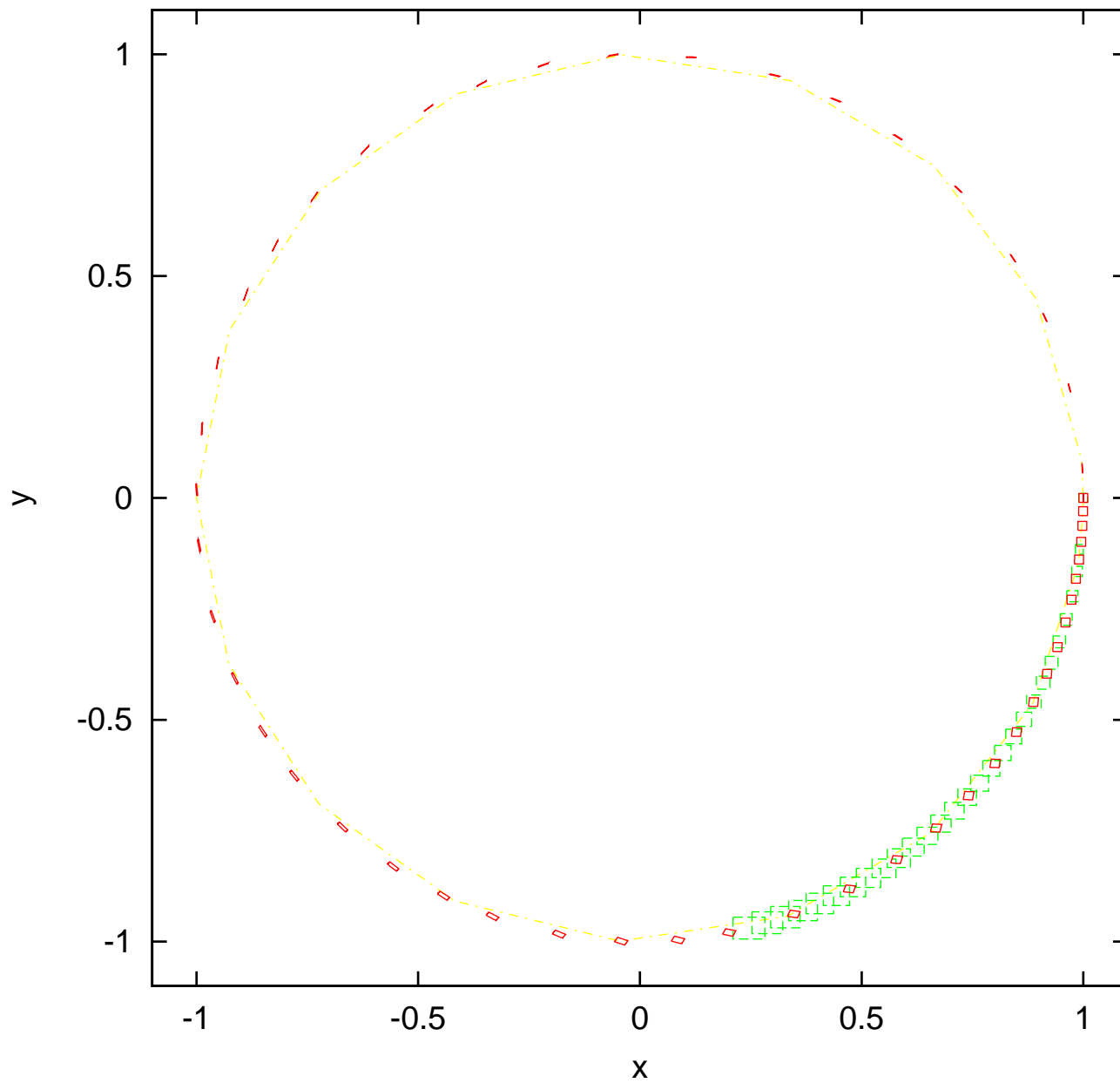
Tilted Solenoids

RF Cavities

H₂ Absorber



mucool, DX=0.01, preconditioned TM 12th, noSW



A Muon Cooling Ring - Results

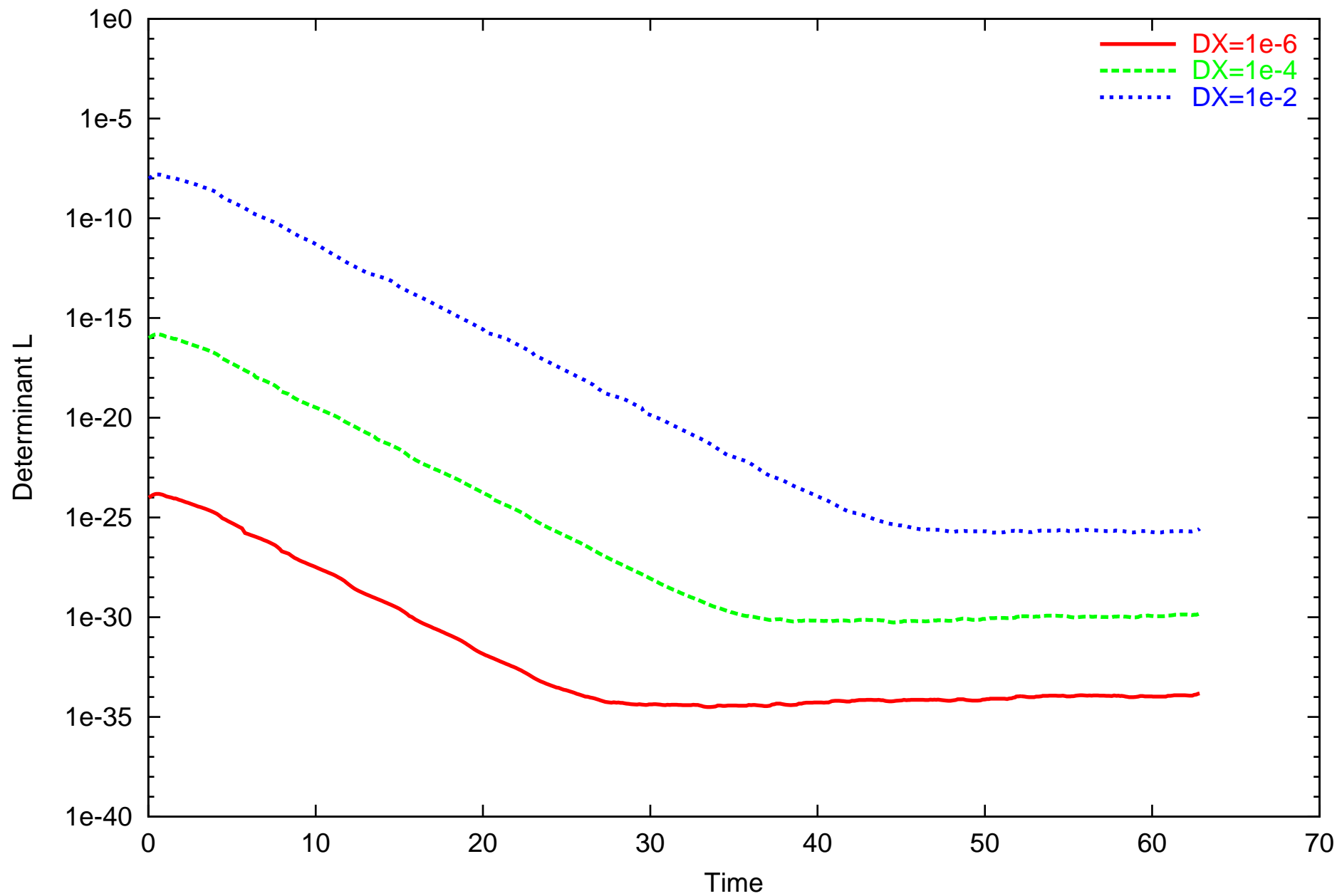
1. Need to treat a large box of $[-10^{-2}, 10^{-2}]^4$
2. Because of damping action towards the invariant limit cycle, the linear part of the motion is more and more ill-conditioned.

COSY easily integrates 10 cycles for $d = 10^{-2}$ with curvilinear preconditioning and QR preconditioning. AWA (method 4) behaves as follows:

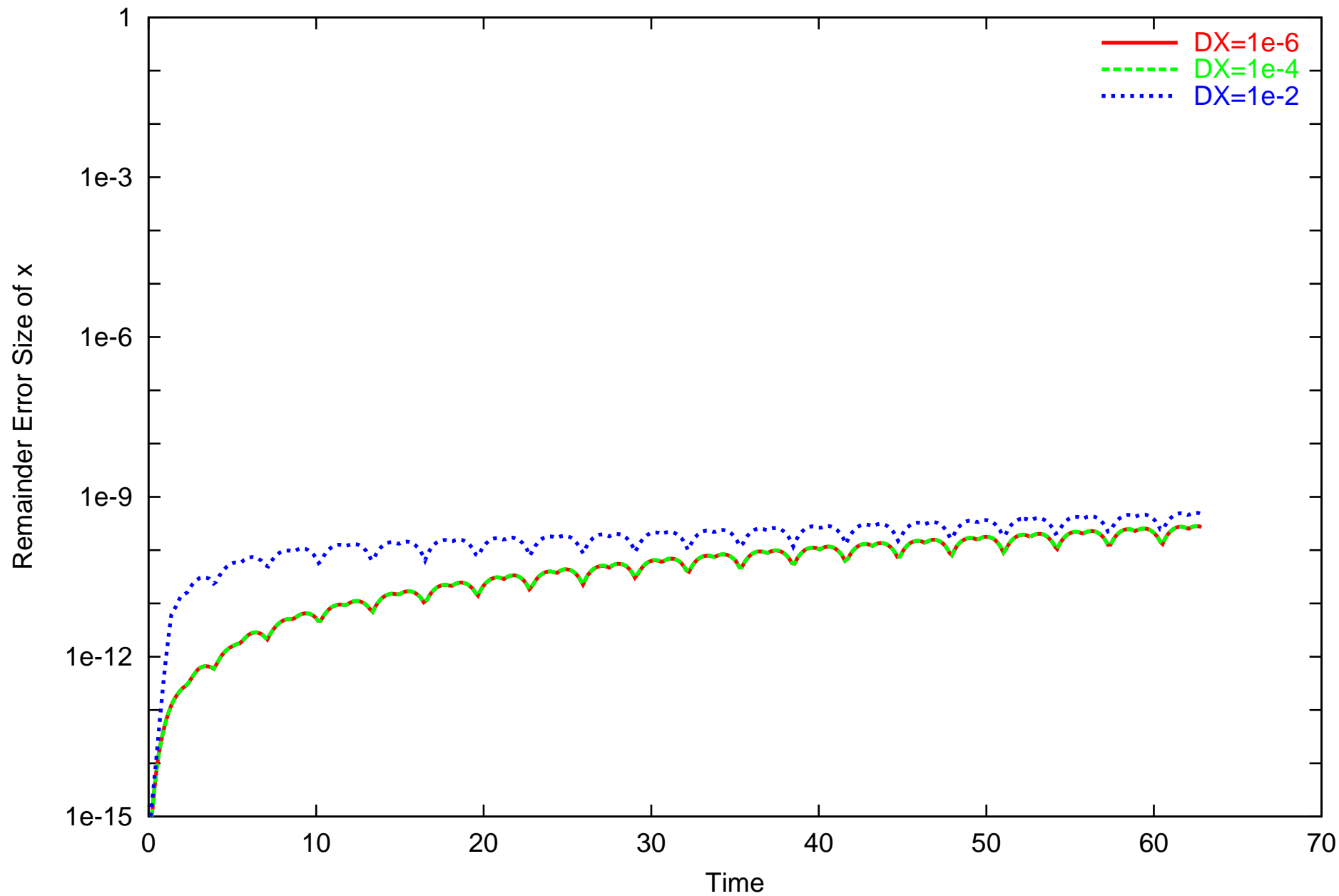
d	Cycles
10^{-2}	0.22
10^{-3}	1.25
10^{-4}	9.5

Thus, trying to simulate the system with AWA requires $> (10^2)^4 = 10^8$ subdivisions of the box that COSY can transport in one piece.

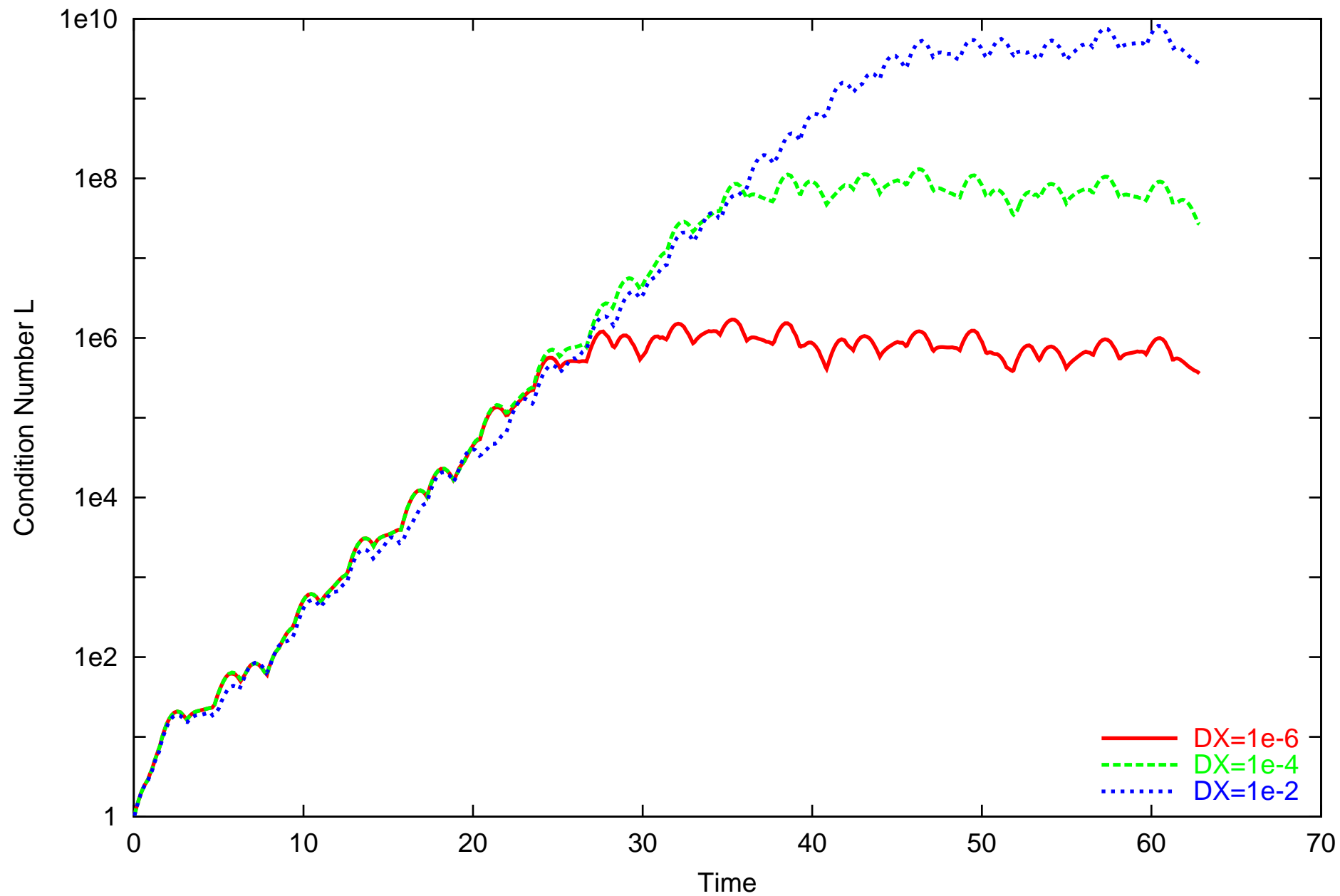
mucool ODE, (1,0,0,-1), Pre-conditioned TM 12th, noSW



mucool ODE, (1,0,0,-1), Pre-conditioned TM 12th, noSW

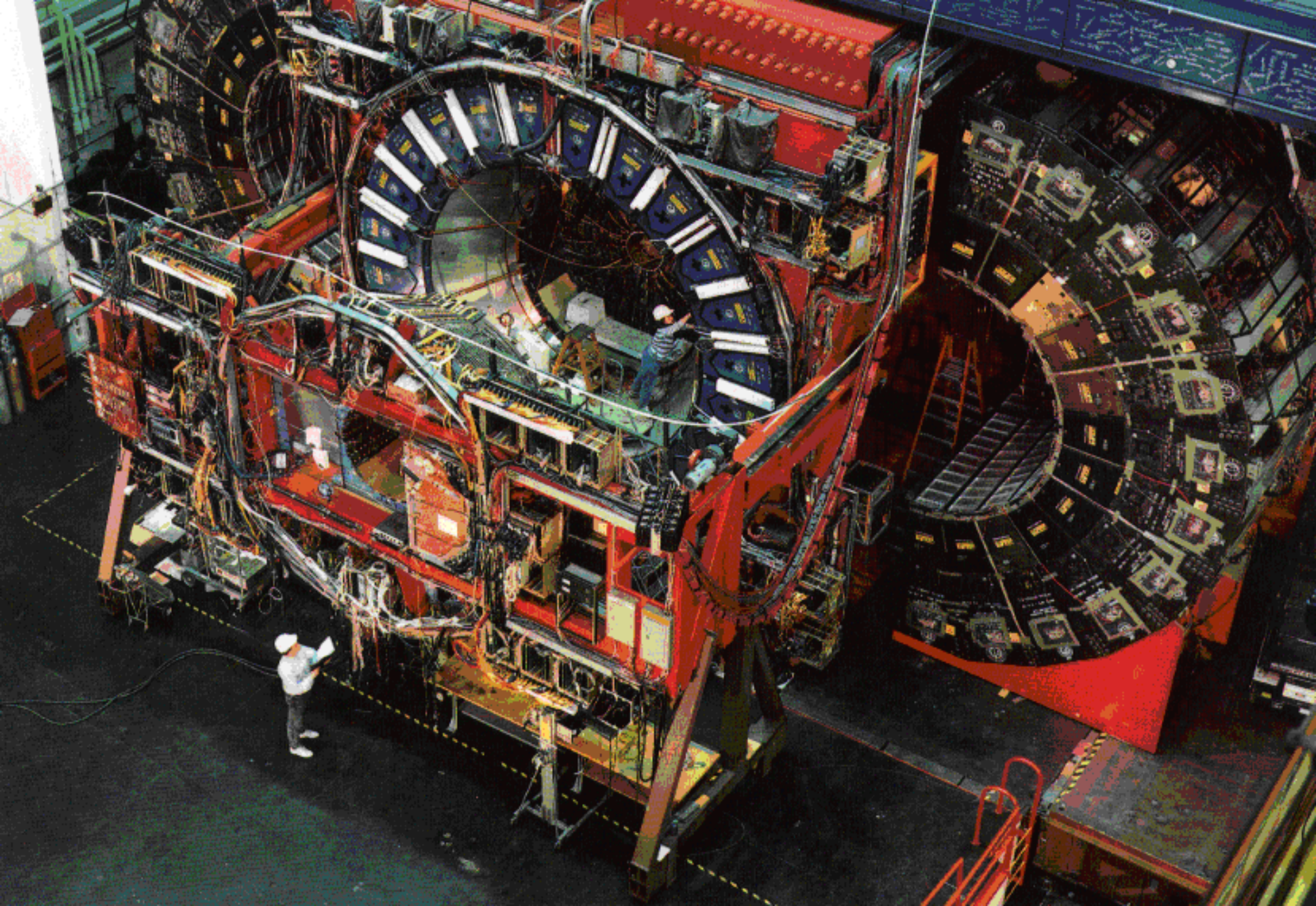


mucool ODE, (1,0,0,-1), Pre-conditioned TM 12th, noSW









Third International Workshop on Taylor Methods

Miami Beach, Florida
December 16-20, 2004

Topics:

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Automatic Differentiation
Validated Methods
Taylor Models

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