Fourth International Workshop on Taylor Methods

Boca Raton, Florida
December 16-19, 2006

http://bt.pa.msu.edu/TM/BocaRaton2006/

Topics:
High-Order Methods
Verification & Taylor Models
Automatic Differentiation
Differential Algebraic Tools

and their use for:
ODE and PDE Solvers
Global Optimization
Constraint Satisfaction
Dynamical Systems
Beam Physics

Support: Department of Energy
Michigan State University

Recent Advances in Taylor Model-based ODE Integration

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Outline

1. The Reference Trajectory
2. The Flow Operator
3. Defect-Based Verification
4. Step Size Control
5. Example: The Double Pendulum
6. Example / Outlook: Manifolds of the Henon Map

The Reference Trajectory

First Step: Obtain Taylor expansion in time of solution of ODE of center point c, i.e. obtain

$$c(t) = c_0 + c_1 \cdot (t - t_0) + c_2 \cdot (t - t_0)^2 + ... + c_n \cdot (t - t_0)^n$$

Very well known from day one how to do this with automatic differentiation. Rather convenient way: can be done by n iterations of the Picard Operator

$$c(t) = c_0 + \int_0^t f(r(t'), t) dt'$$

in one-dimensional Taylor arithmetic. Each iteration raises the order by one; so in each iteration i, only need to do Taylor arithmetic in order i. In either way, this step is **cheap** since it involves only **one-dimensional** operations.

The Nonlinear Flow

Second Step: The goal is to obtain Taylor expansion in time to order n **and** initial conditions to order k. Note:

1. This is usually the most **expensive** step. In the original Taylor model-based algorithm, it is done by n **iterations** of the Picard Operator in multi-dimensional Taylor arithmetic, where c_0 is now a polynomial in initial conditions.
2. The case $k = 1$ has been known for a long time. Traditionally solved by setting up **ODEs for sensitivities** and solving these as before.
3. The case of higher k goes back to Beam Physics (M. Berz, Particle Accelerators 1988)
4. Newest Taylor model arithmetic naturally supports different expansions orders k for initial conditions and n for time.

Goal: Obtain flow with one **single evaluation** of right hand side.

The Nonlinear Relative ODE

We now develop a better way for second step.
First: introduce new "perturbation" variables $\tilde{r}$ such that

$$r(t) = c(t) + A \cdot \tilde{r}(t).$$

The matrix A provides **preconditioning**. ODE for $\tilde{r}(t)$:

$$\tilde{r}' = A^{-1}\left[f(c(t) + A \cdot \tilde{r}(t)) - c'(t)\right]$$

Second: evaluate ODE for $\tilde{r}'$ in Taylor arithmetic. Obtain a Taylor expansion of the ODE, i.e.

$$\tilde{r}' = P(\tilde{r}, t)$$

up to order n in time and k in $\tilde{r}$. **Very important** for later use: the polynomial P will have no constant part, i.e.

$$P(0, t) = 0.$$

Reminder: The Lie Derivative

Let
$$r' = f(r,t)$$
be a dynamical system. Let g be a variable in state space, and let us study $g(r(t))$, i.e. along a solution of the ODE. We have
$$\frac{d}{dt}g(t) = f \cdot \nabla g + \frac{\partial g}{\partial t}$$
Introducing the **Lie Derivative** $L_f = f \cdot \nabla + \partial/\partial t$, we have
$$\frac{d^n}{dt^n}g = L_f^n g \text{ and } g(t) \approx \sum_{i=0}^{n} \frac{(t-t_0)^i}{i!} \, L_f^i g\Big/_{t=t_0}$$

Differential Algebras on Taylor Polynomial Spaces

Consider space ${}_nD_v$ of Taylor polynomials in v variables and order n with truncation multiplication. Formally: introduce **equivalence relation** on space of smooth functions

$$f =_n g$$

if all derivatives from 0 to n agree at 0. **Class** of f is denoted $[f]$. This induces addition, multiplication and scalar multiplication on classes. The resulting structure forms an algebra.

An algebra is a **Differential Algebra** if there is an operation ∂, called a derivation, that satisfies

$$\partial(s \cdot a + t \cdot b) = s \cdot \partial a + t \cdot \partial b \text{ and}$$
$$\partial(a \cdot b) = a \cdot (\partial b) + (\partial a) \cdot b$$

for any vectors a and b and scalars s and t. **Unfortunately**, the **natural partial derivative** operations $[f] \to [\partial_i f]$ does **not** introduce a differential algebra, because of loss of highest order.

Differential Algebras on Taylor Polynomial Spaces

However, consider the modified operation

$$\partial_f \text{ with } \partial_f g = f \cdot \nabla g$$

If f is origin preserving, i.e. $f(0) = 0$, then ∂_f is a derivation on the space ${}_nD_v$. Why?

- Each derivative operation in the gradient ∇g looses the highest order;
- but since $f(0) = 0$, the missing order in ∇g **does not matter** since it does not contribute to the product $f \cdot \nabla g$.

Polynomial Flow from Lie Derivative

Remember the ODE for $\tilde{r}'$:

$$\tilde{r}' = P(\tilde{r}, t)$$

up to order n in time and k in $\tilde{r}$. And remember $P(0, t) = 0$. Thus we can obtain the n-th order expansion of the flow as

$$\tilde{r}(t) = \sum_{i=0}^{n} \frac{(t - t_0)^i}{i!} \cdot \left(P \cdot \nabla + \frac{\partial}{\partial t} \right)^i \tilde{r}_0 \Bigg/_{t=t_0}$$

- The fact that $P(0, t) = 0$ restores the derivatives lost in ∇
- The fact that $\partial / \partial t$ appears without origin-preserving factor limits the expansion to order n.

Performance of Lie Derivative Flow Methods

Apparently we have the following:

- Each term in the Lie derivative sum requires $v+1$ derivations (very cheap, just re-shuffling of coefficients)
- Each term requires v multiplications
- We need **one** evaluation of f in ${}_nD_v$ (to set up ODE)

Compare this with the conventional algorithm, which requires n evaluations of the function f of the right hand side. Thus, roughly, if the evaluation of f requires more than v multiplications, the new method is more efficient.

- Many practically appearing right hand sides f satisfy this.
- But on the other hand, if the function f does not satisfy this (for example for the linear case), then also P will be simple (in the linear case: P will be linear), and thus less operations appear

Error Analysis via Interval Defect

Third step of rigorous method: provide rigorous error estimate. We now try to introduce a set of variables $\tilde{e}$, the error variables, such that the flow rigorously satisfies

$$r(t) = c(t) + A \cdot \tilde{r}(t) + \tilde{e}.$$

ODE for $\tilde{e}(t)$:

$$\tilde{e}' = f(c(t) + A \cdot \tilde{r}(t) + \tilde{e}) - c'(t) - A \cdot \tilde{r}'(t)$$

Now again evaluating ODE for $\tilde{e}'$ in Taylor arithmetic. Obtain a Taylor expansion of the ODE:

$$\tilde{e}' = 0$$

up to order n in time and k in initial conditions(!)

Of course this is not the real ODE: we are missing the remainder errors. However, evaluating the ODE for $\tilde{e}'$ in **Taylor Model** arithmetic, we obtain a (very small) interval term R, the Taylor model remainder, such that

$$\tilde{e}' \in R$$

Error Analysis via Defect - Implementation

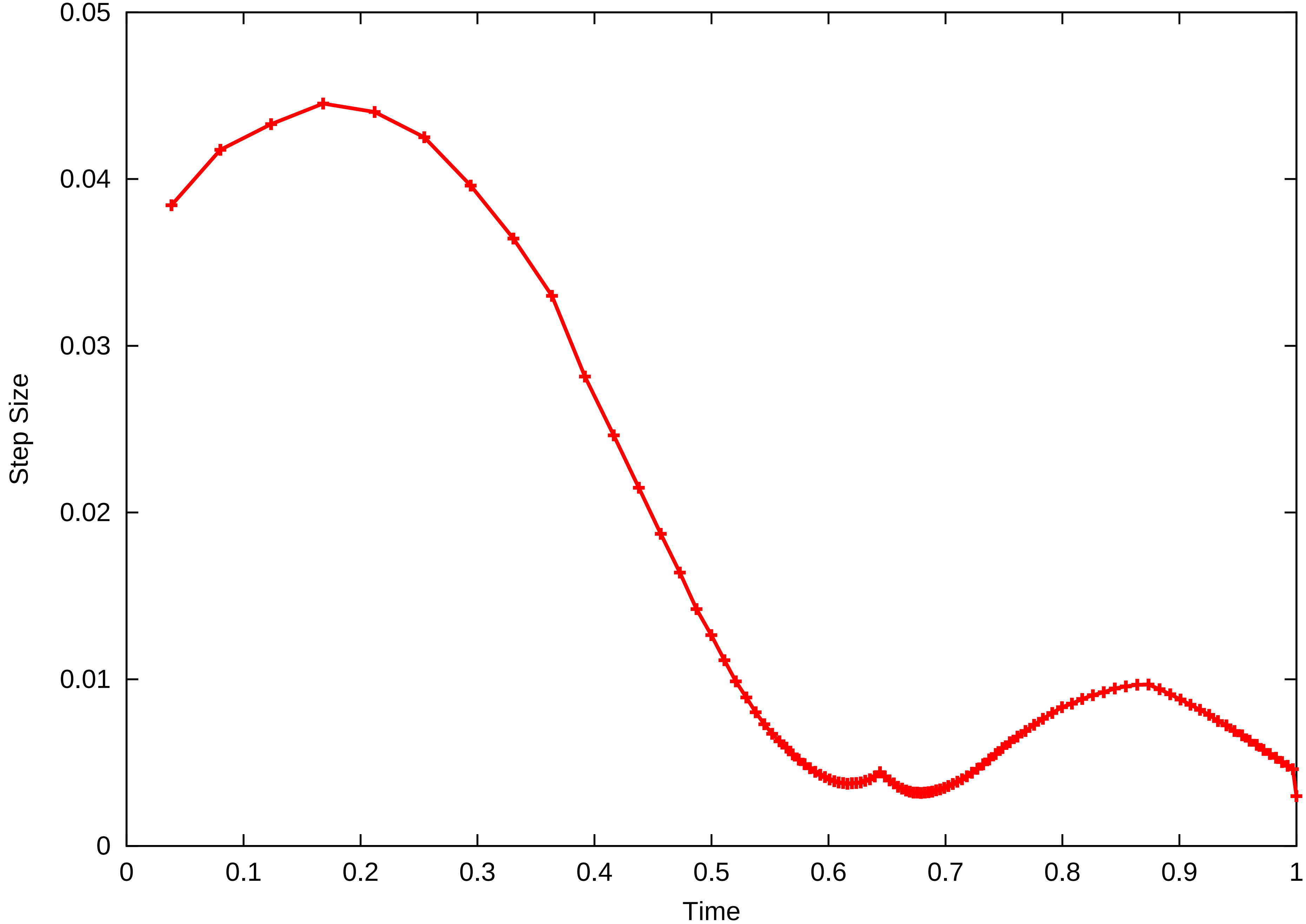
For practical implementation, the following aspects are critical:

1. Make sure $\tilde{r}'(t)$ numerically fits with $\tilde{r}(t)$. Solution: obtain approximate value of $\tilde{r}'(t)$, and then obtain a Taylor model for $\int \tilde{r}'(t)$ to represent $\tilde{r}$. Can be done
2. Defect ODE can be solved with very simple Euler-type integrator.
3. Simplest possible case: treat $\tilde{e}$ as intervals. Leads to a cone-type flow enclosure.
4. Next more sophisticated case: treat $\tilde{e}$ as additional variables (to very low order). Leads to linear inhomogeneous ODE.

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 $\Delta t_3 = c \cdot \Delta t_2$



Step Size
0.05
0.04
0.03
0.02
0.01
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time

Dynamic Domain Decomposition

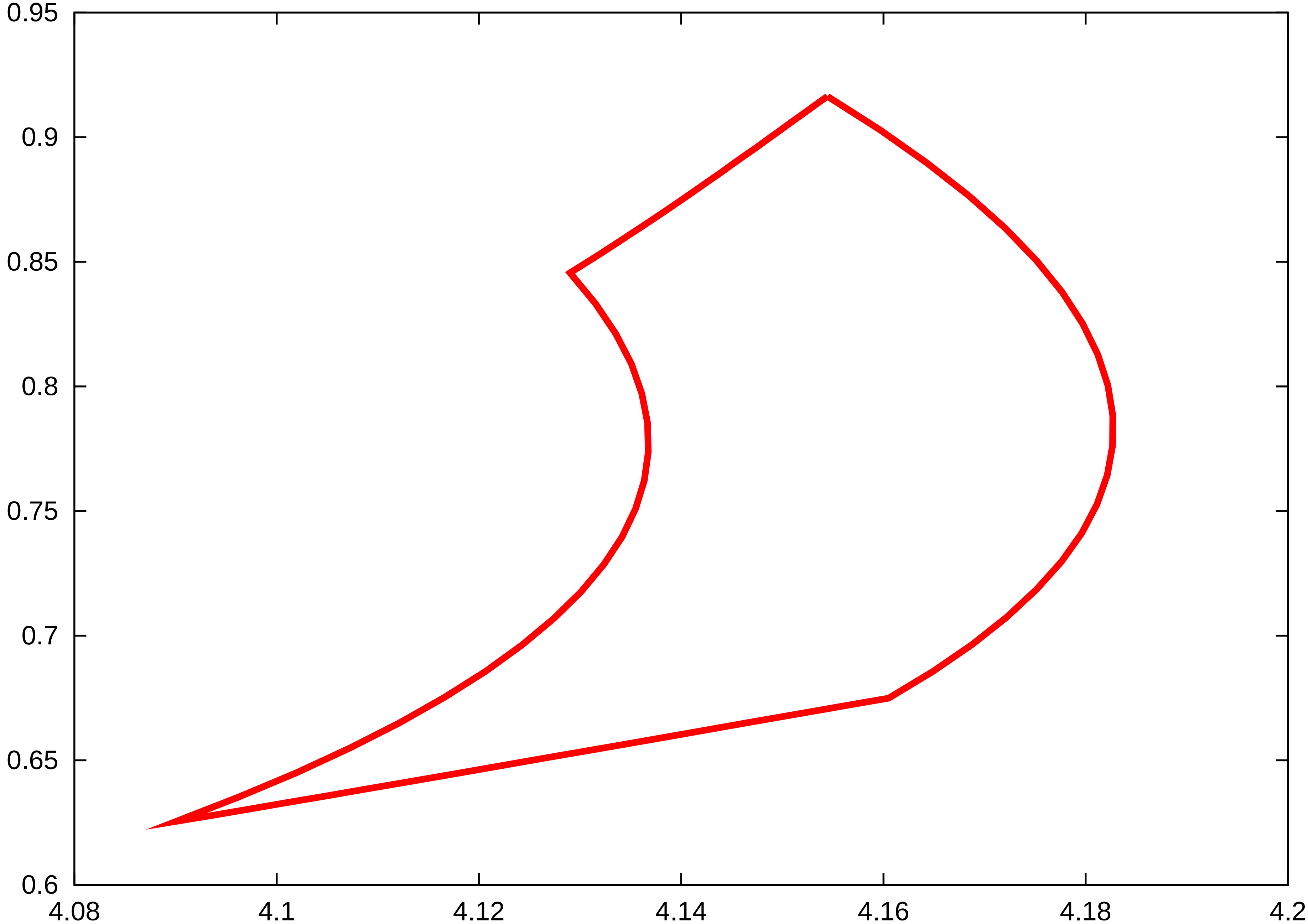
For extended domains (i.e. not only point solutions), this is **natural equivalent** to step size control. Similarity to what's done in global optimization.

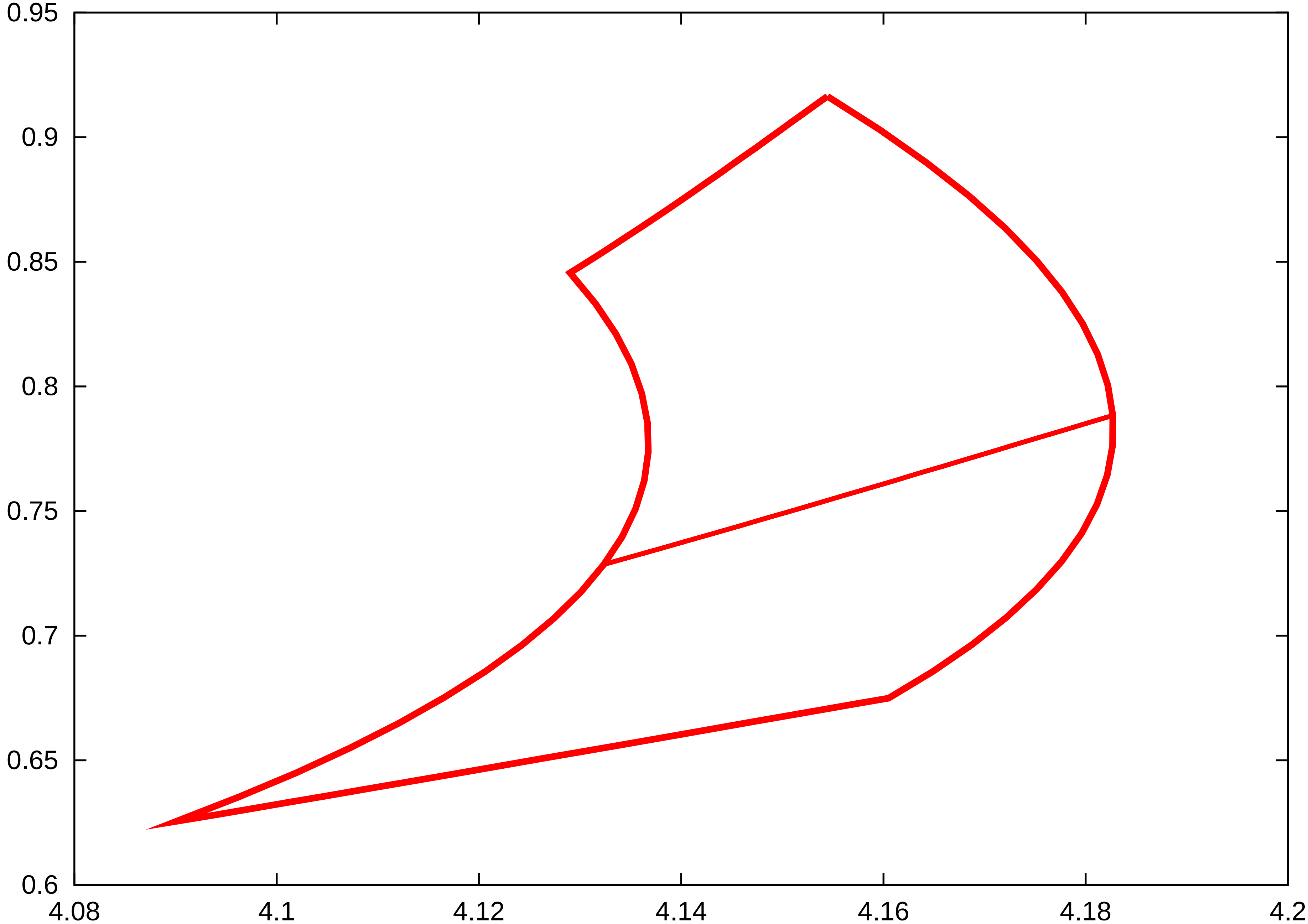
1. Evaluate ODE for $\Delta t = 0$ for current flow.
2. If remainder resulting remainder bound R greater than say $\varepsilon/10$, split domain along variable leading to longest axis.
3. Put one half of the box on stack for future work.

Things to consider:

- Since TM provides inner and outer estimate, R is very convenient measure for actual overstimation
- Utilize "First-in-last-out" stack; minimizes stack length. Special adjustments for stack management in a parallel environment, including load balancing.

- When using QR preconditioning, make sure longest side stays longest. (Not a problem for CV preconditioning)
- 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
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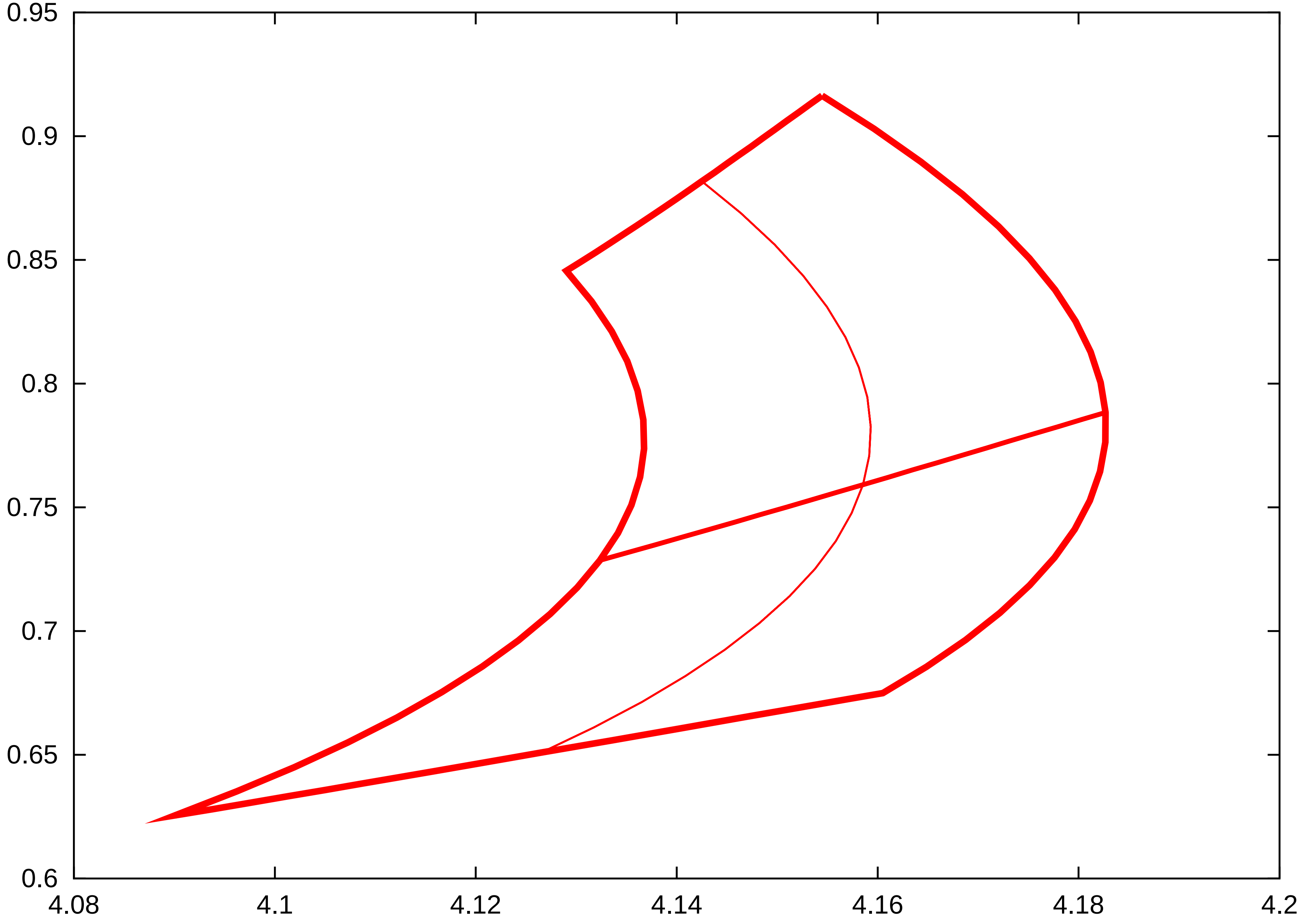
0.6
4.08
4.1
4.12
4.14
4.16
4.18
4.2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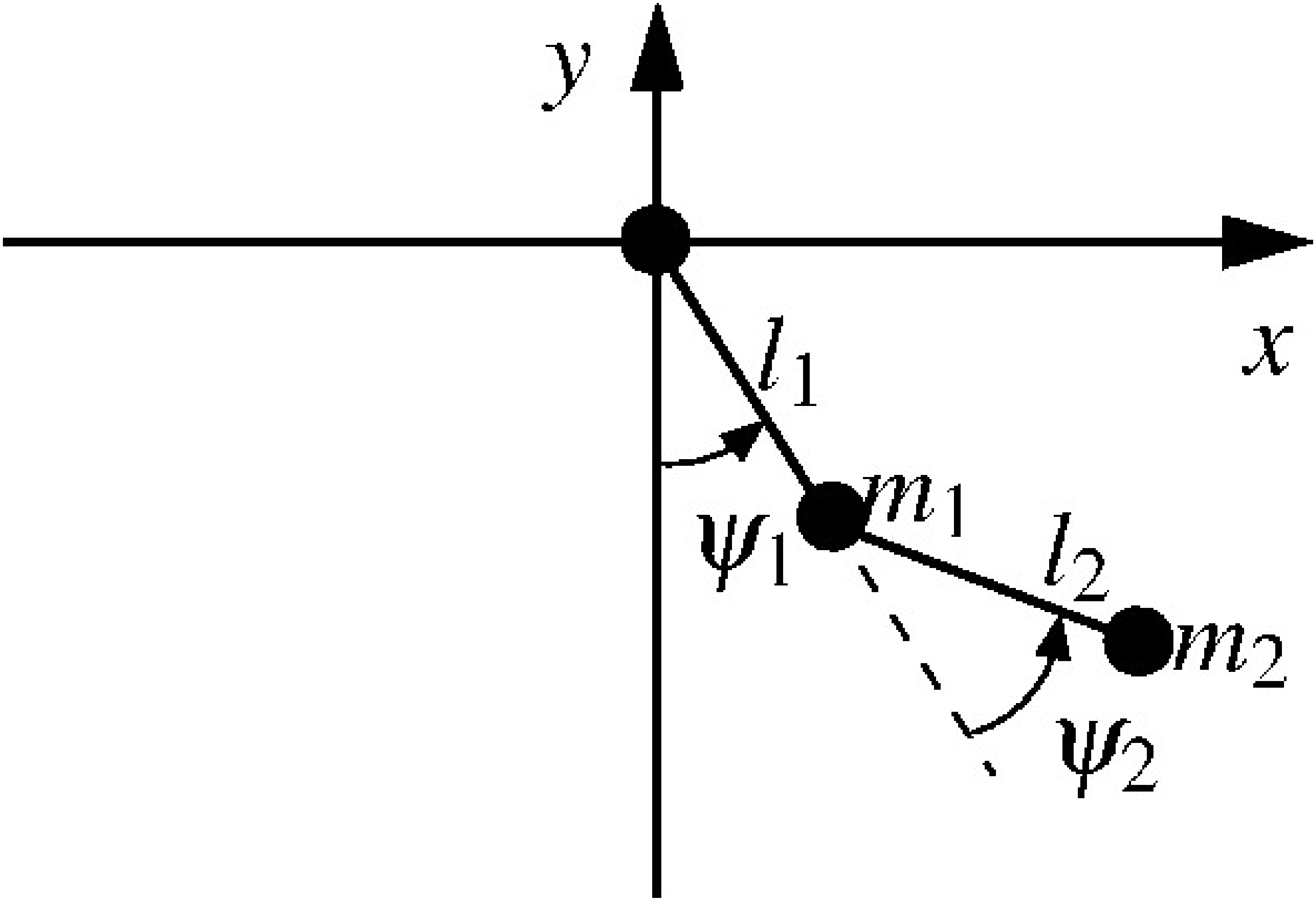


y
x
l1
m1
ψ1
l2
m2
ψ2

The Double Pendulum - a Chaotic System

$$\frac{d^2}{dt^2}\psi_1 = \frac{l_1 m_2 \left[l_2(\dot\psi_1 + \dot\psi_2)^2 + l_1 \dot\psi_1^2 \cos\psi_2\right]}{l_1^2\left[m_1 + m_2 \sin^2\psi_2\right]} \sin\psi_2 + g \cdot \frac{-l_1(m_1+m_2)\sin\psi_1 + l_1 m_2 \cos\psi_2 \sin(\psi_1+\psi_2)}{l_1^2\left[m_1 + m_2\sin^2\psi_2\right]}$$

$$\begin{aligned}\frac{d^2}{dt^2}\psi_2 = &-\frac{(l_1(m_1+m_2) + l_2 m_2 \cos\psi_2) l_1 \dot\psi_1^2}{l_1 l_2 (m_1 + m_2\sin^2\psi_2)}\sin\psi_2 \\ &- \frac{l_2 m_2 (l_2 + l_1\cos\psi_2)(\dot\psi_1+\dot\psi_2)^2}{l_1 l_2(m_1+m_2\sin^2\psi_2)}\sin\psi_2 \\ &+ g\cdot\frac{(m_1+m_2)(l_2+l_1\cos\psi_2)\sin\psi_1}{l_1 l_2(m_1+m_2\sin^2\psi_2)} \\ &- g\cdot\frac{(l_1(m_1+m_2)+l_2 m_2\cos\psi_2)\sin(\psi_1+\psi_2)}{l_1 l_2(m_1+m_2\sin^2\psi_2)}\end{aligned}$$

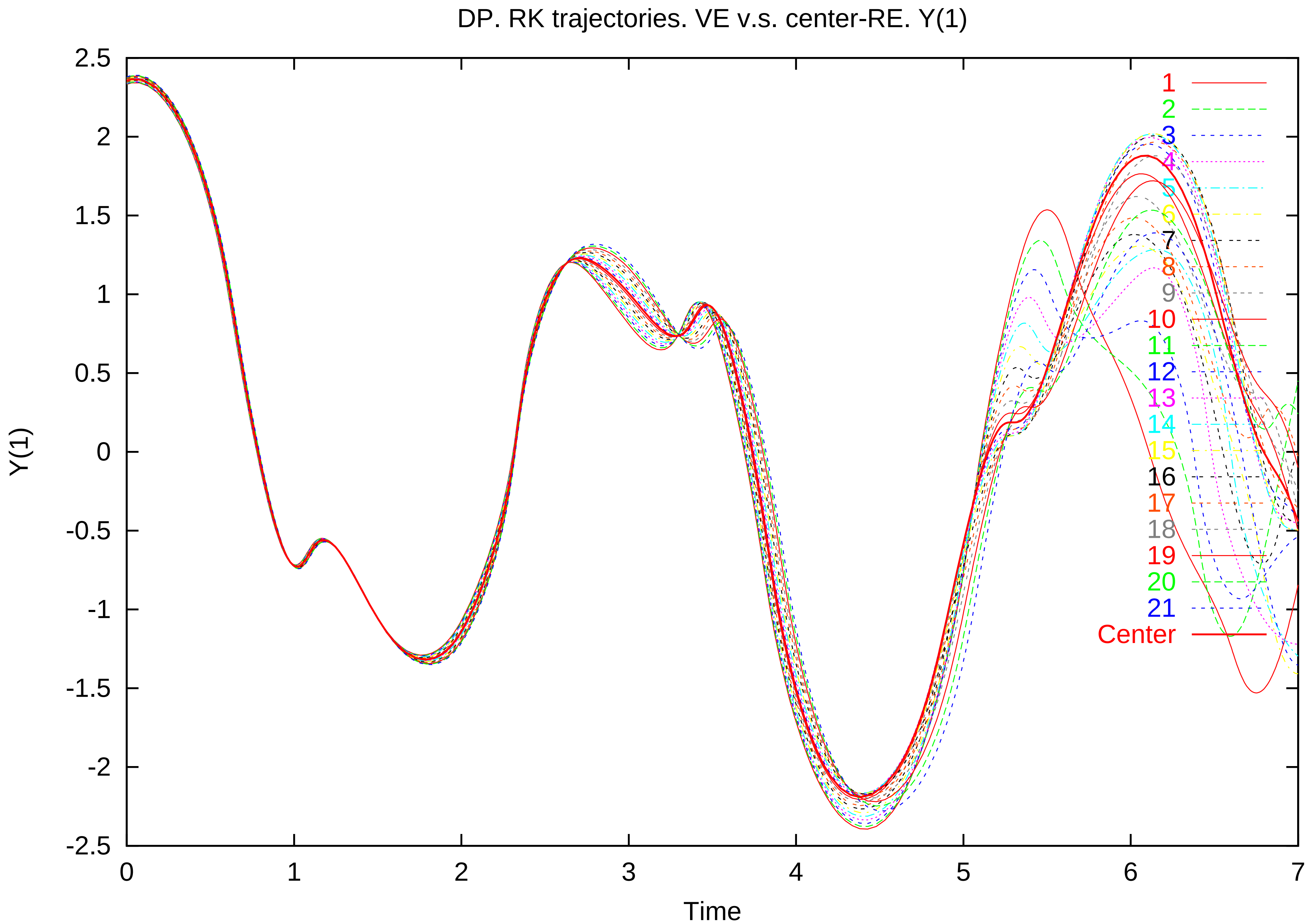
The Double Pendulum - Initial Conditions

In agreement with recent work of Rauh et al. (SCAN2006), we consider the parameter values $(l_1, l_2, m_1, m_2, g) = (1, 1, 1, 1, 9.81)$.

$$\psi_1(t=0) \in \frac{3\pi}{4} + \frac{1}{100}\frac{3\pi}{4}[-1,+1]$$
$$\psi_2(t=0) = -1.726533538$$
$$\dot{\psi}_1(t=0) = 0.4138843714$$
$$\dot{\psi}_2(t=0) = 0.6724072960$$

These initial conditions are in the **chaotic regime**. Illustration of motion (for similar, but not identical initial conditions):

`http://www.vis.uni-stuttgart.de/~kraus/`
`LiveGraphics3D/examples/parametrized/pendulum.html`



DP. RK trajectories. VE v.s. center-RE. Y(1)
Y(1)
Time
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
0
1
2
3
4
5
6
7
1
2
3
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19
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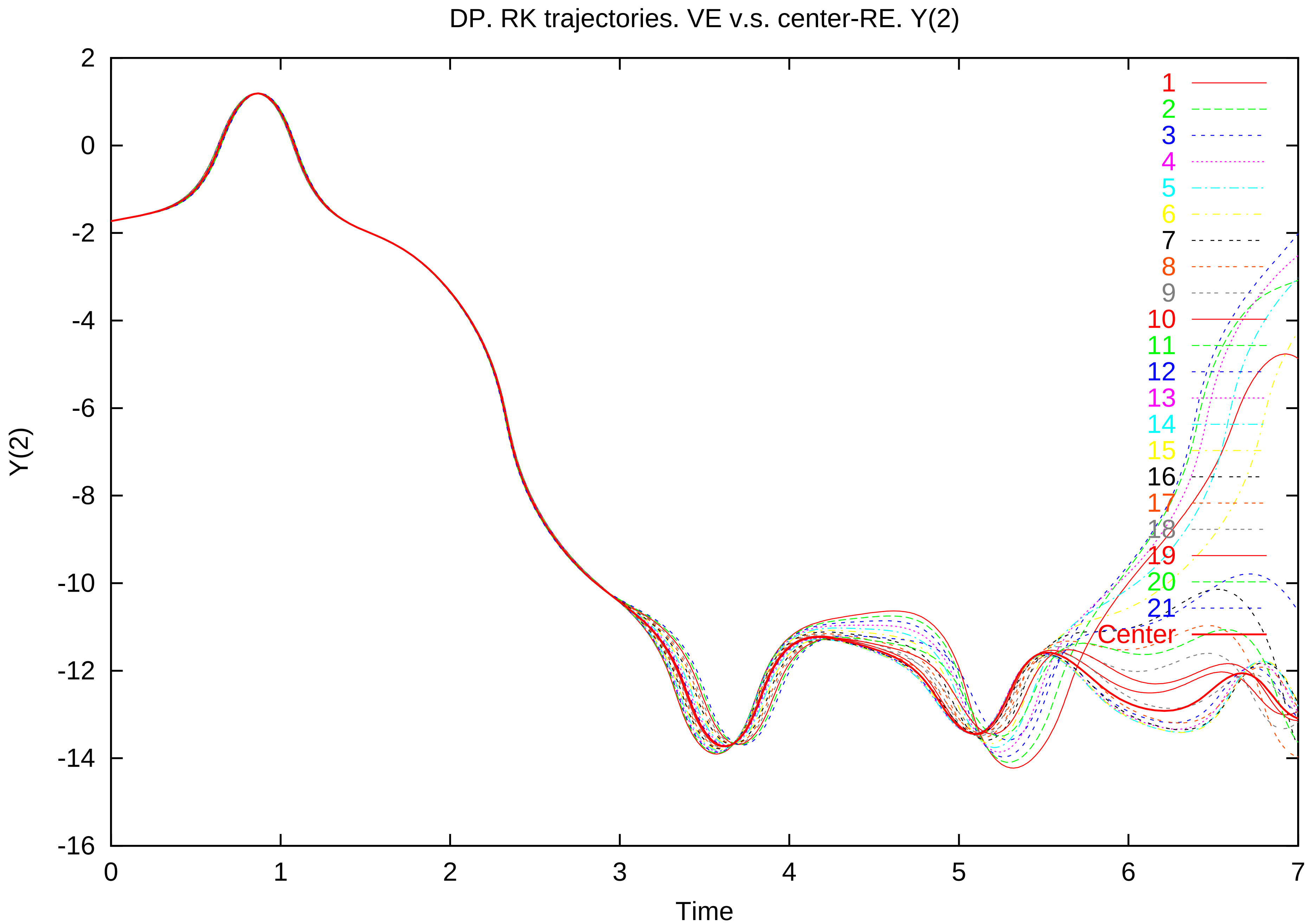
21
Center


DP. RK trajectories. VE v.s. center-RE. Y(2)
Y(2)
Time
2
0
-2
-4
-6
-8
-10
-12
-14
-16
0
1
2
3
4
5
6
7
1
2
3
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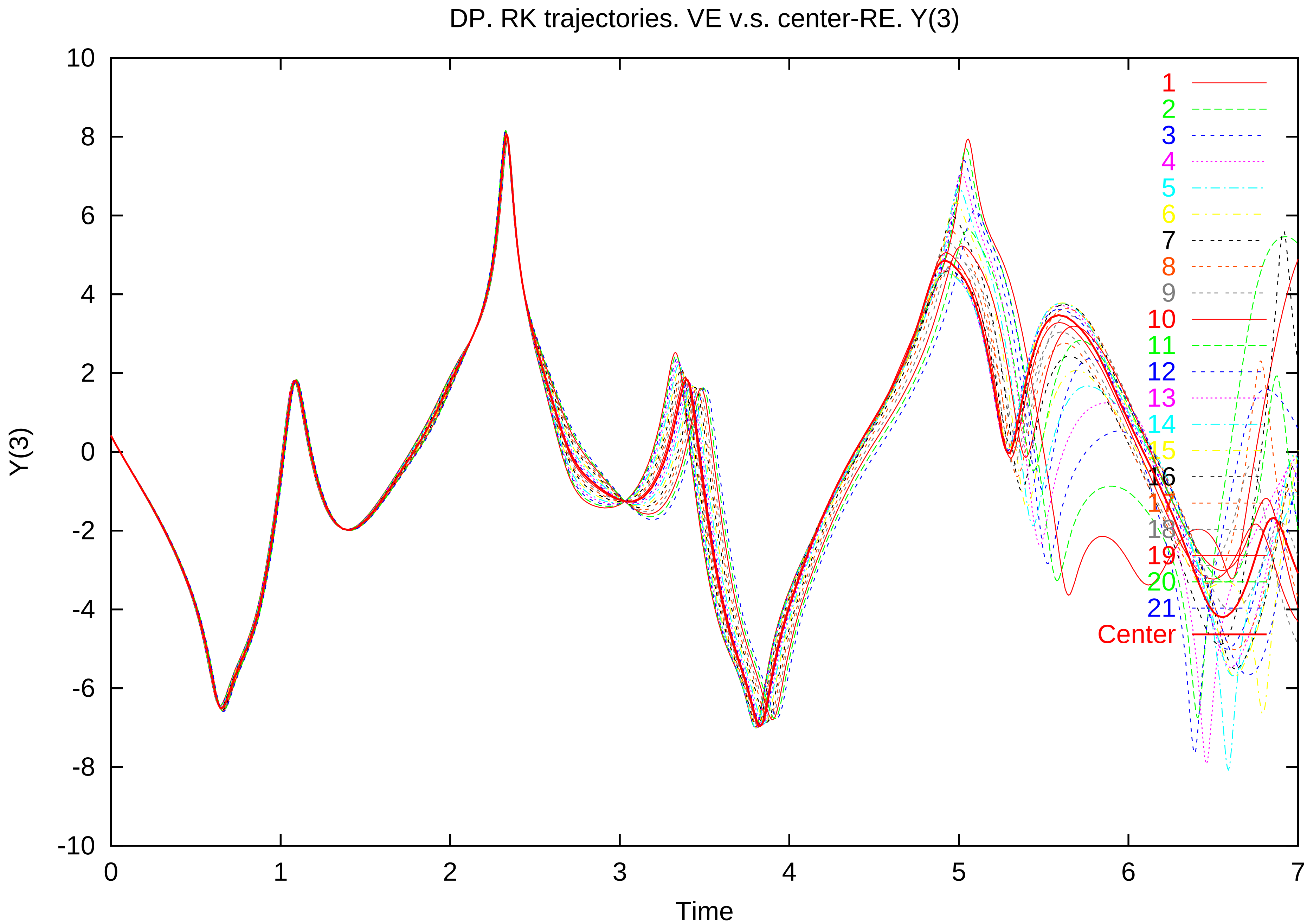
21
Center



DP. RK trajectories. VE v.s. center-RE. Y(3)
Y(3)
Time
10
8
6
4
2
0
-2
-4
-6
-8
-10
0
1
2
3
4
5
6
7
1
2
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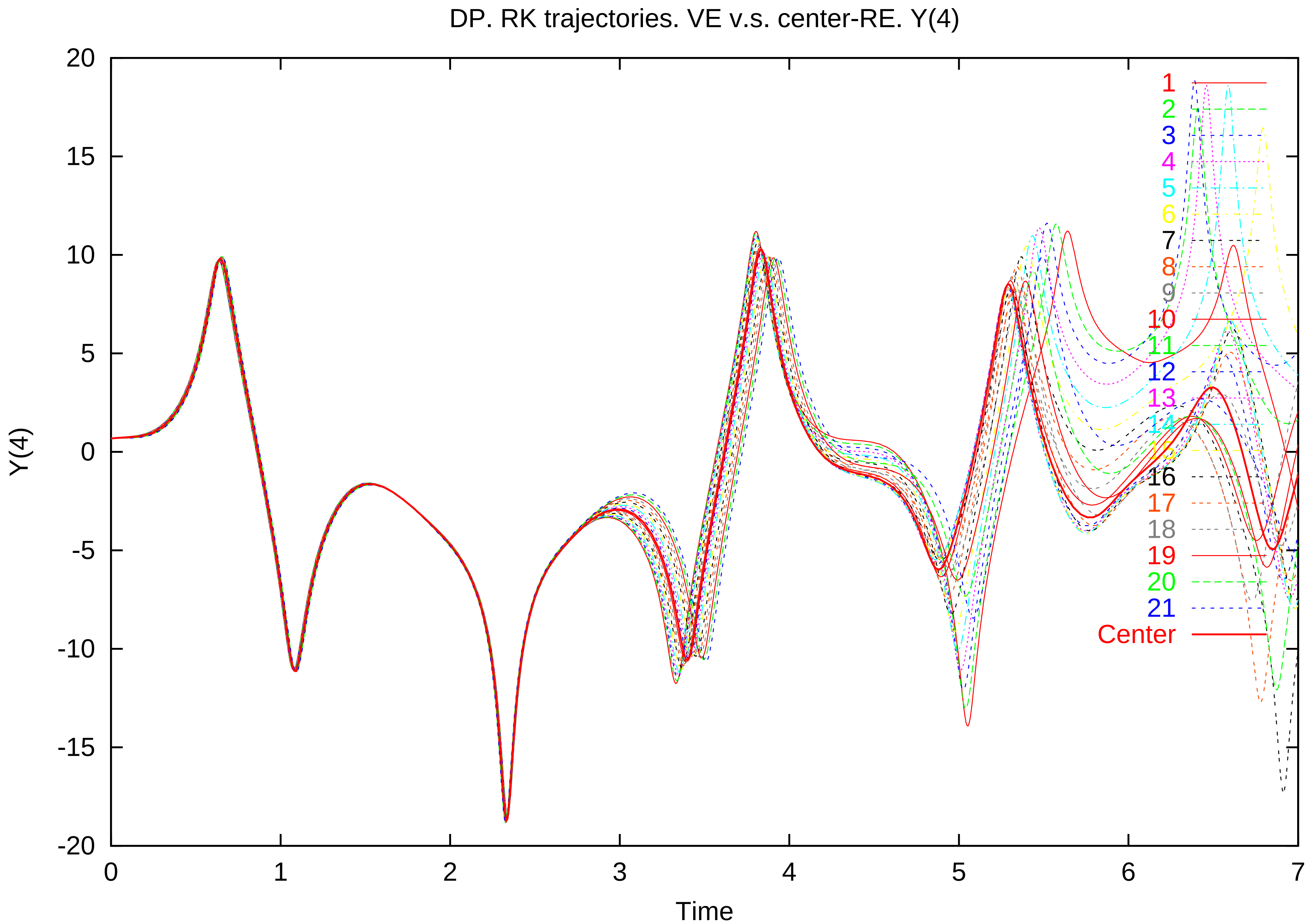
Center



DP. RK trajectories. VE v.s. center-RE. Y(4)
Y(4)
Time
20
15
10
5
0
-5
-10
-15
-20
0
1
2
3
4
5
6
7
1
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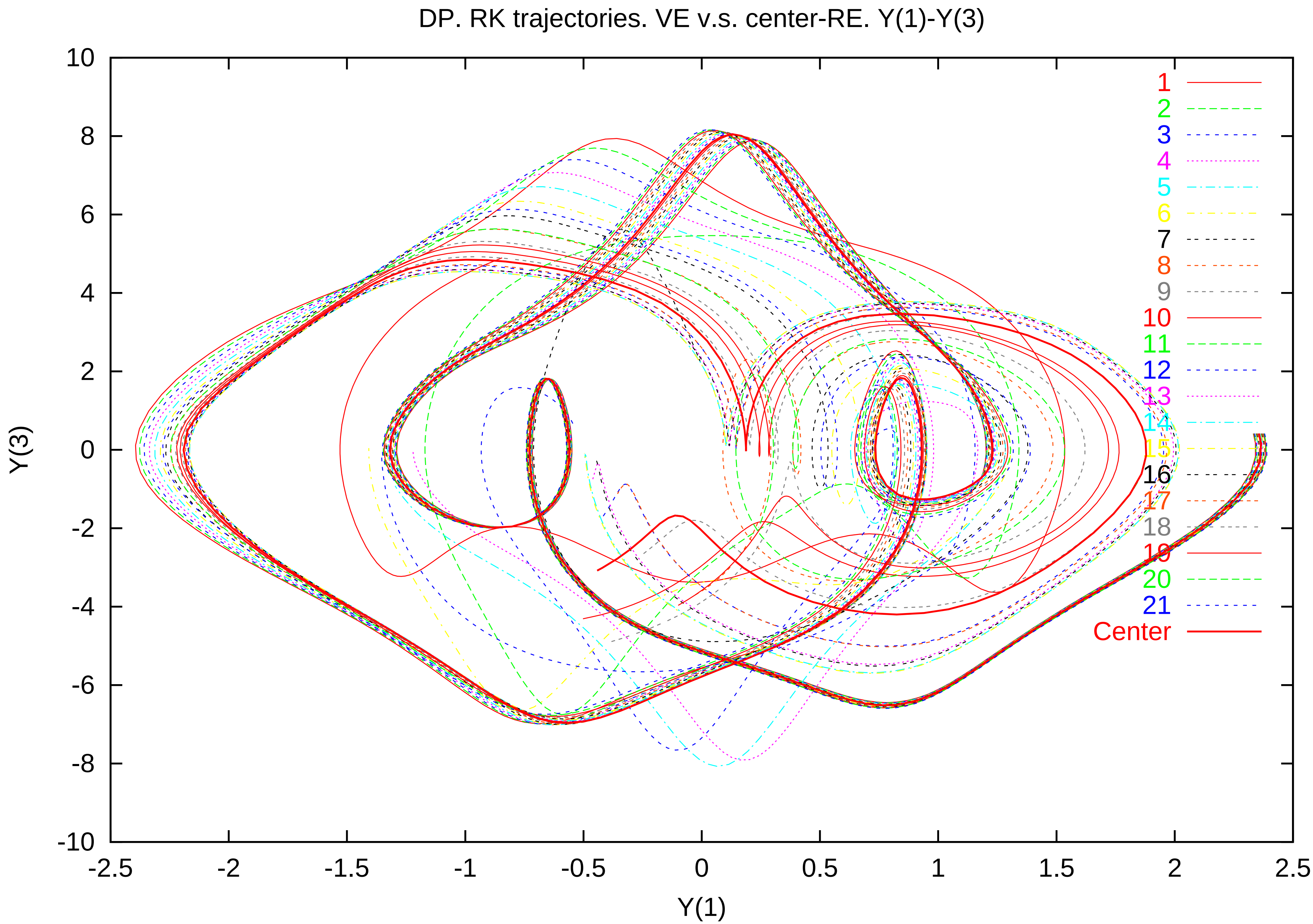
DP. RK trajectories. VE v.s. center-RE. Y(1)-Y(3)
Y(3)
Y(1)
10
8
6
4
2
0
-2
-4
-6
-8
-10
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
2.5
1
2
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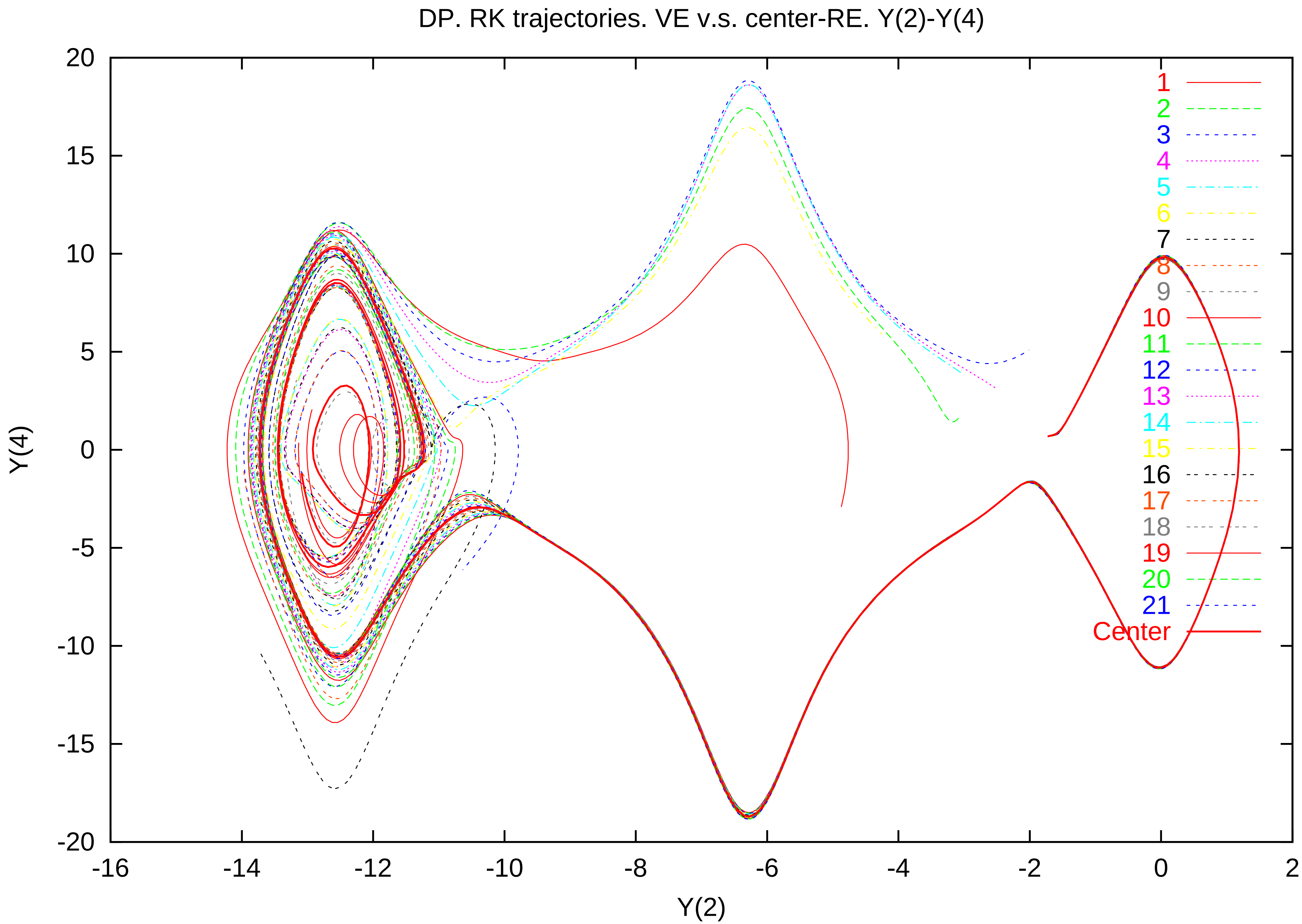
DP. RK trajectories. VE v.s. center-RE. Y(2)-Y(4)
Y(4)
Y(2)
20
15
10
5
0
-5
-10
-15
-20
-16
-14
-12
-10
-8
-6
-4
-2
0
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21
Center

The Double Pendulum - Code Performance

Integration was carried out from $t = 0$ until $t = 0.5$ sec.
VNODE (Ned Nedialkov), QR method
ValEncIA-IVP (Rauh and Auer), Domain decomposition by lots of intervals, forward/backward integration for pruning
COSY-VI Taylor models, no domain decomposition at $t = 1.0$.
(The data reported for VNODE and ValEncIA-IVP are quoted from Rauh et al., SCAN2006).

Time t	**CPU VNODE**	**CPU ValEncIA**	**CPU COSY**
0.5	15.4 sec	5880 / 94 sec *	0.51 sec
1.0	(breakdown $t < 0.6$)	(breakdown $t < 0.6$)	2.04 sec

* First number: Implementation using Matlab-Intlab,
second number: using C++ interval library

The Double Pendulum - Check of COSY-VI

The doule pendulum **preservers energy**. Evaluating energy in Taylor model arithmetic over the entire flow at any two points in the integration, and subtracting the results, must result in a **tight enclosure of zero**.

Total Energy E is given as

$$E = m_1 \cdot g \cdot y_1 + m_2 \cdot g \cdot y_2 + \frac{1}{2} m_1 \left(\dot{x}_1^2 + \dot{y}_1^2 \right) + \frac{1}{2} m_2 \left(\dot{x}_2^2 + \dot{y}_2^2 \right).$$

Elementary arithmetic shows that

$$\begin{aligned}
&x_1 = l_1 \cdot \sin \psi_1,\ x_2 = x_1 + l_2 \cdot \sin(\psi_1 + \psi_2) \\
&y_1 = -l_1 \cdot \cos \psi_1,\ \ y_2 = y_1 - l_2 \cdot \cos(\psi_1 + \psi_1) \\
&\dot{x}_1 = \dot{\psi}_1 \cdot l_1 \cdot \cos \psi_1,\ \ \dot{x}_2 = \dot{x}_1 + (\dot{\psi}_1 + \dot{\psi}_2) \cdot l_2 \cdot \cos(\psi_1 + \psi_2) \\
&\dot{y}_1 = \dot{\psi}_1 \cdot l_1 \cdot \sin \psi_1,\ \ \dot{y}_2 = \dot{y}_1 + (\dot{\psi}_1 + \dot{\psi}_2) \cdot l_2 \cdot \sin(\psi_1 + \psi_2)
\end{aligned}$$

The Double Pendulum - Energy at t=0

```
I  COEFFICIENT              ORDER EXPONENTS
1   6.636304564436251         0    0 0  0 0  0
2  0.4629982784681443         1    1 0  0 0  0
3  -.1650152672869661E-02    2    2 0  0 0  0
4  -.4284009231437226E-04    3    3 0  0 0  0
5  0.7634228476230531E-07    4    4 0  0 0  0
6  0.1189166522762920E-08    5    5 0  0 0  0
7  -.1412752780648741E-11    6    6 0  0 0  0
8  -.1571866492860271E-13    7    7 0  0 0  0
R [-.1538109061161243E-012,0.1517608952722424E-012]
```

The Double Pendulum - Energy at t=0.5

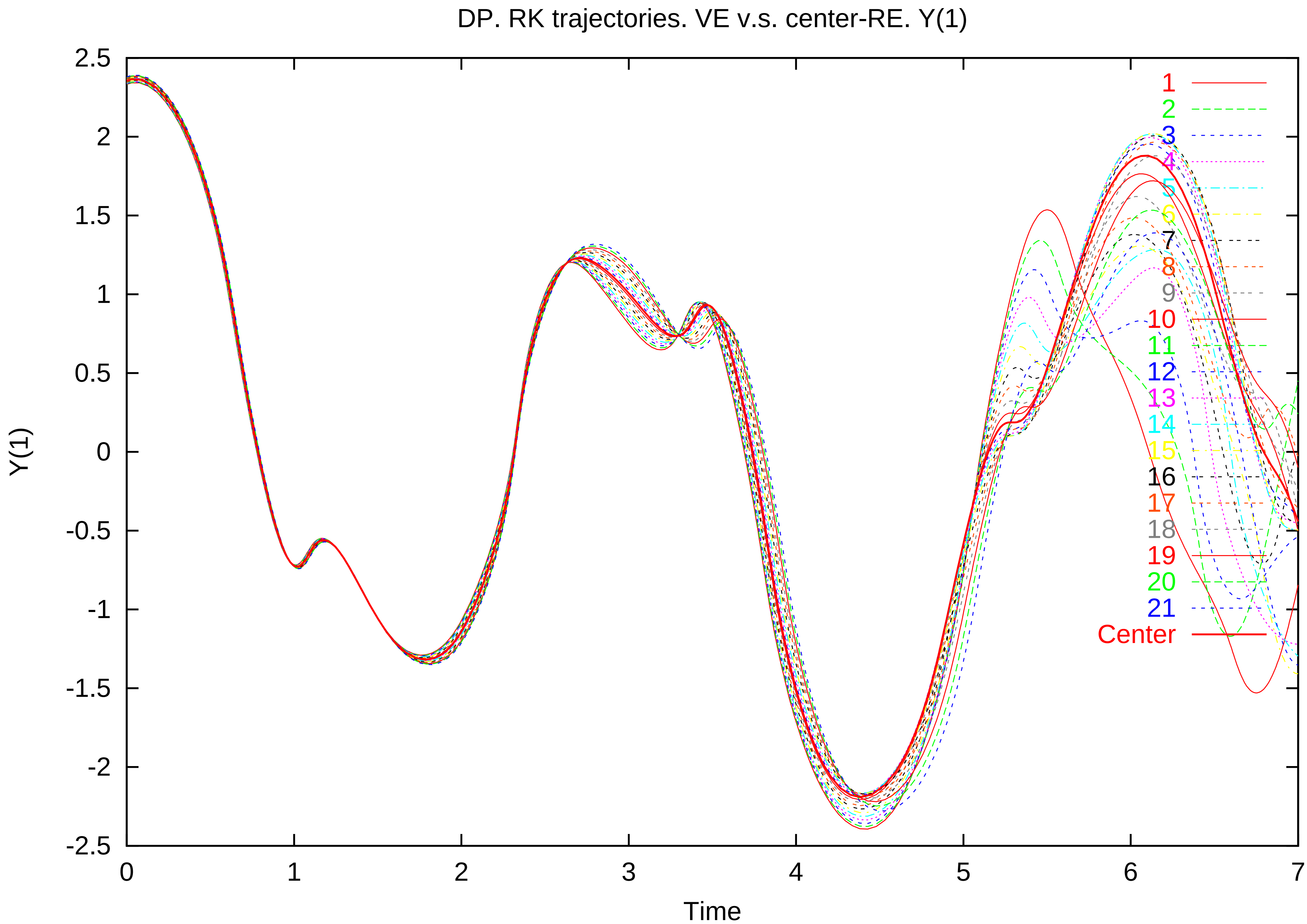
I	COEFFICIENT	ORDER	EXPONENTS				
1	6.636304564436253	0	0	0	0	0	0
2	0.4629982784681632	1	1	0	0	0	0
3	-.1650152672942219E-02	2	2	0	0	0	0
4	-.4284009217517837E-04	3	3	0	0	0	0
5	0.7634212049420934E-07	4	4	0	0	0	0
6	0.1189297979605227E-08	5	5	0	0	0	0
7	-.1487493064301731E-11	6	6	0	0	0	0
8	0.1498746352978318E-13	7	7	0	0	0	0
9	-.8978311500296960E-14	8	8	0	0	0	0
10	0.1732136627097570E-14	9	9	0	0	0	0
11	-.1410358744591400E-15	10	10	0	0	0	0
12	-.3488804283416099E-16	11	11	0	0	0	0
13	0.1647113913603616E-16	12	12	0	0	0	0

R [-.6845903858358710E-010,0.7016561210090576E-010]

The Double Pendulum - Energy Difference

I	COEFFICIENT	ORDER	EXPONENTS				
1	0.266453525910037E-14	0	0	0	0	0	0
2	0.188182802673964E-13	1	1	0	0	0	0
3	-.725584956701164E-13	2	2	0	0	0	0
4	0.139193893227990E-12	3	3	0	0	0	0
5	-.164268095972426E-12	4	4	0	0	0	0
6	0.131456842307669E-12	5	5	0	0	0	0
7	-.747402836529906E-13	6	6	0	0	0	0
8	0.307061284583859E-13	7	7	0	0	0	0
9	-.899231705828288E-14	8	8	0	0	0	0
10	0.173213662709757E-14	9	9	0	0	0	0
11	-.141035874459140E-15	10	10	0	0	0	0
12	-.348880428341609E-16	11	11	0	0	0	0
13	0.164711391360361E-16	12	12	0	0	0	0

R [-.686171064301878E-010,0.703257299583504E-010]


DP. RK trajectories. VE v.s. center-RE. Y(1)
Y(1)
Time
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
0
1
2
3
4
5
6
7
1
2
3
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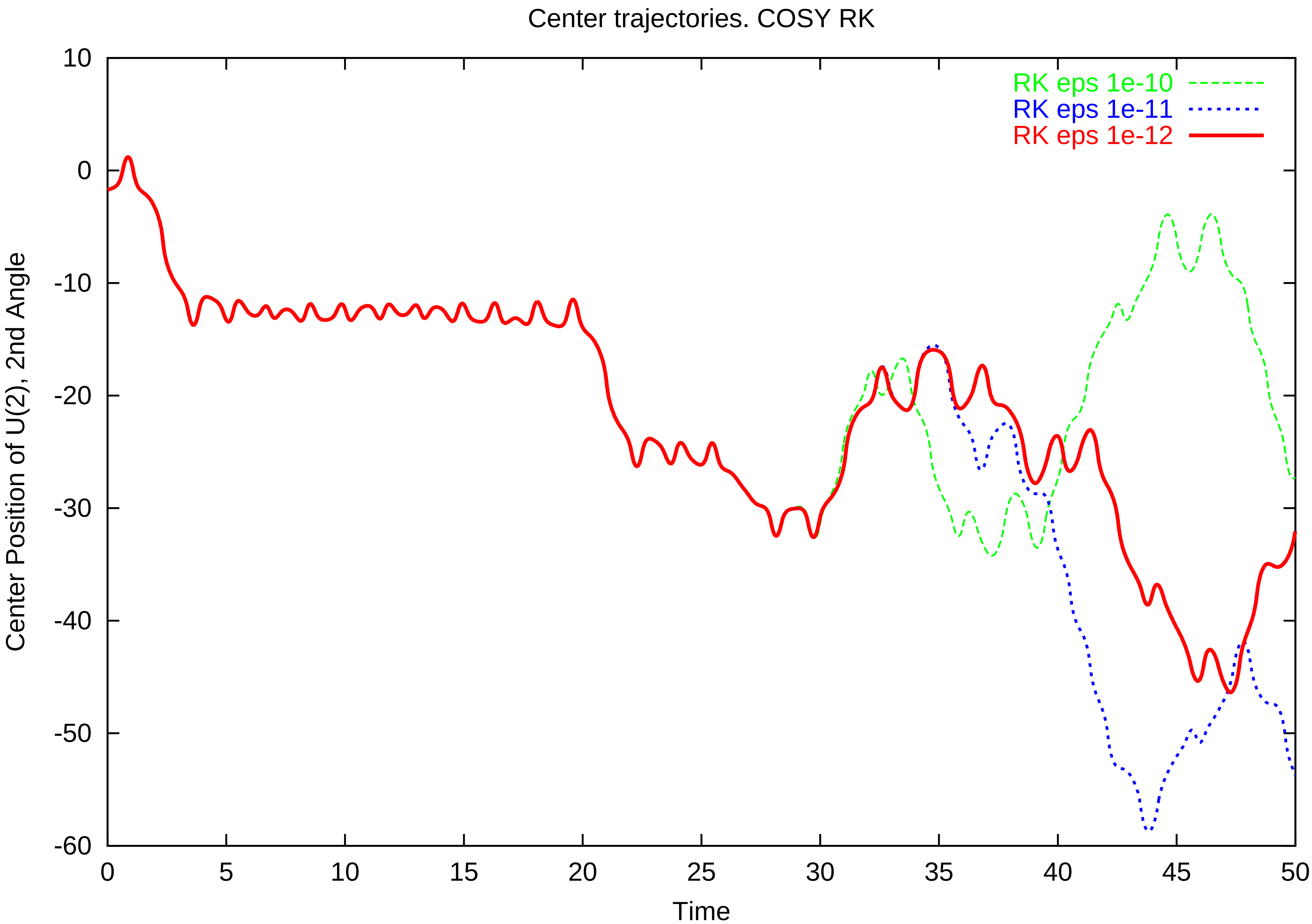
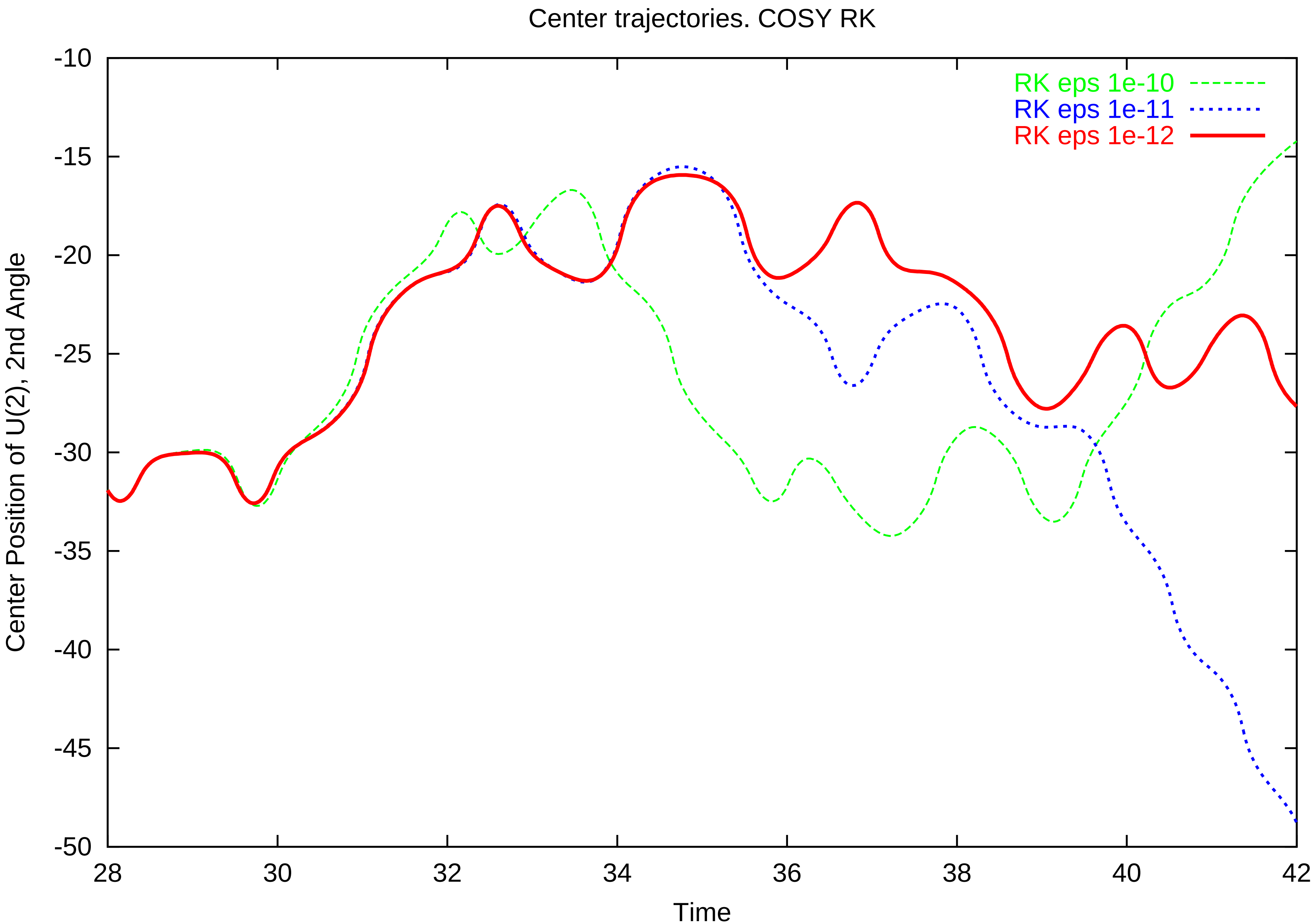
Center



Center trajectories. COSY RK
RK eps 1e-10
RK eps 1e-11
RK eps 1e-12
10
0
-10
-20
-30
-40
-50
-60
0
5
10
15
20
25
30
35
40
45
50
Time
Center Position of U(2), 2nd Angle

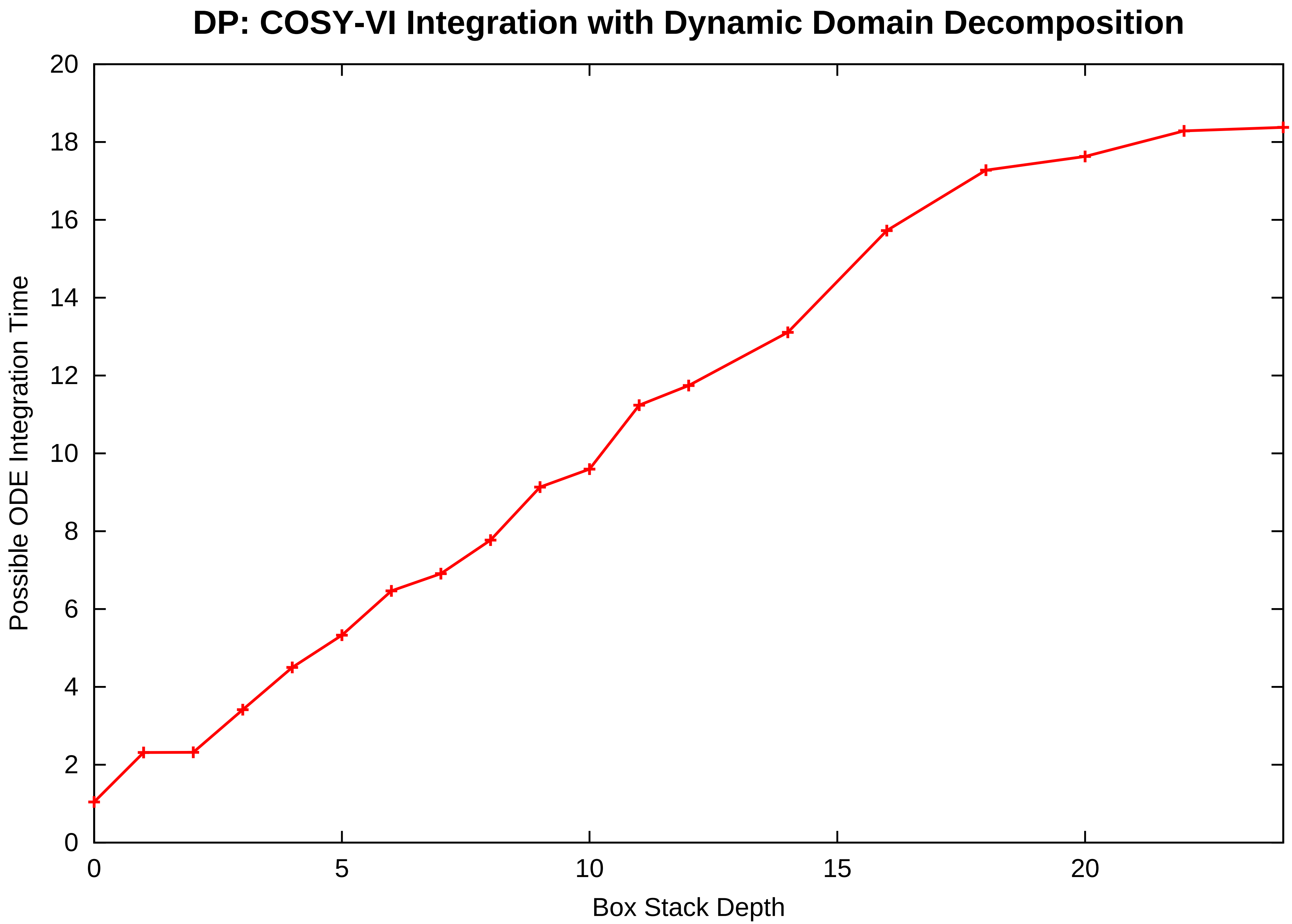

Center trajectories. COSY RK
RK eps 1e-10
RK eps 1e-11
RK eps 1e-12
Center Position of U(2), 2nd Angle
Time
-10
-15
-20
-25
-30
-35
-40
-45
-50
28
30
32
34
36
38
40
42

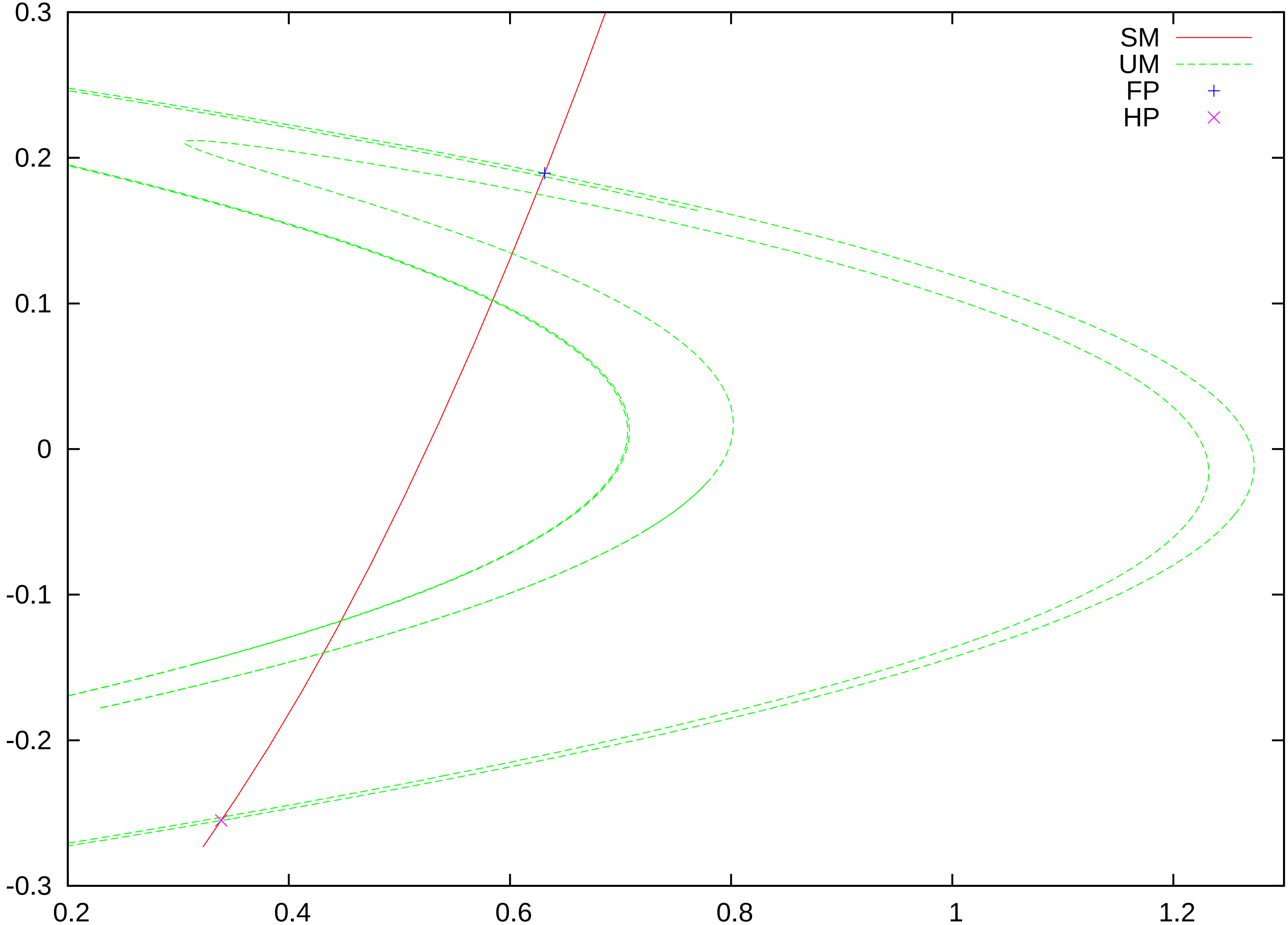
Long Term Behavior

We observe the following:

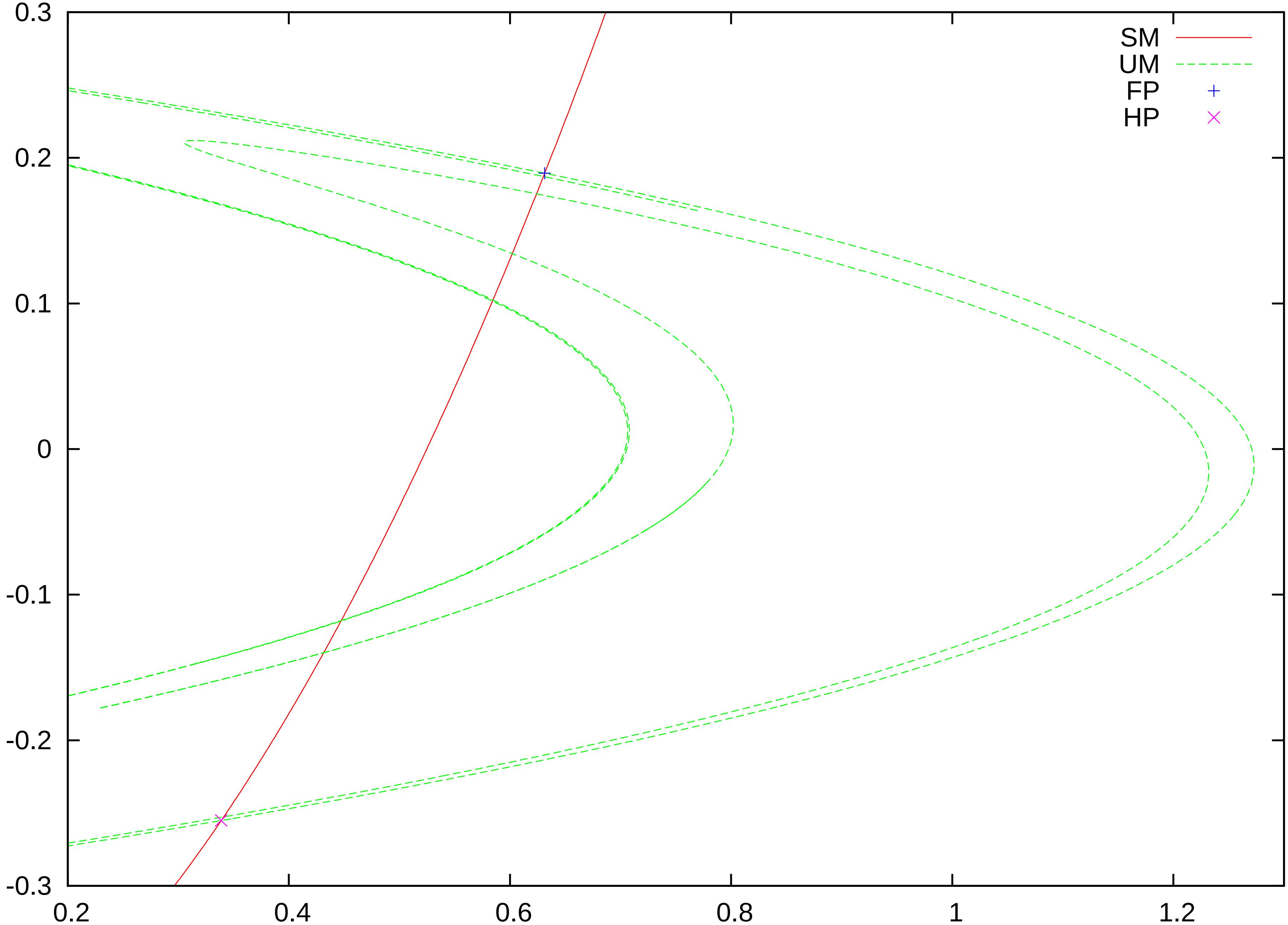
1. Around $t = 2$, initial condition range leads to noticeable broadening of ranges
2. Around $t = 5$, initial condition range leads to angle spread by $> 2\pi$, i.e. different full revolutions
3. Around $t = 30$, conventional non-verified integrators reach their accuracy limit

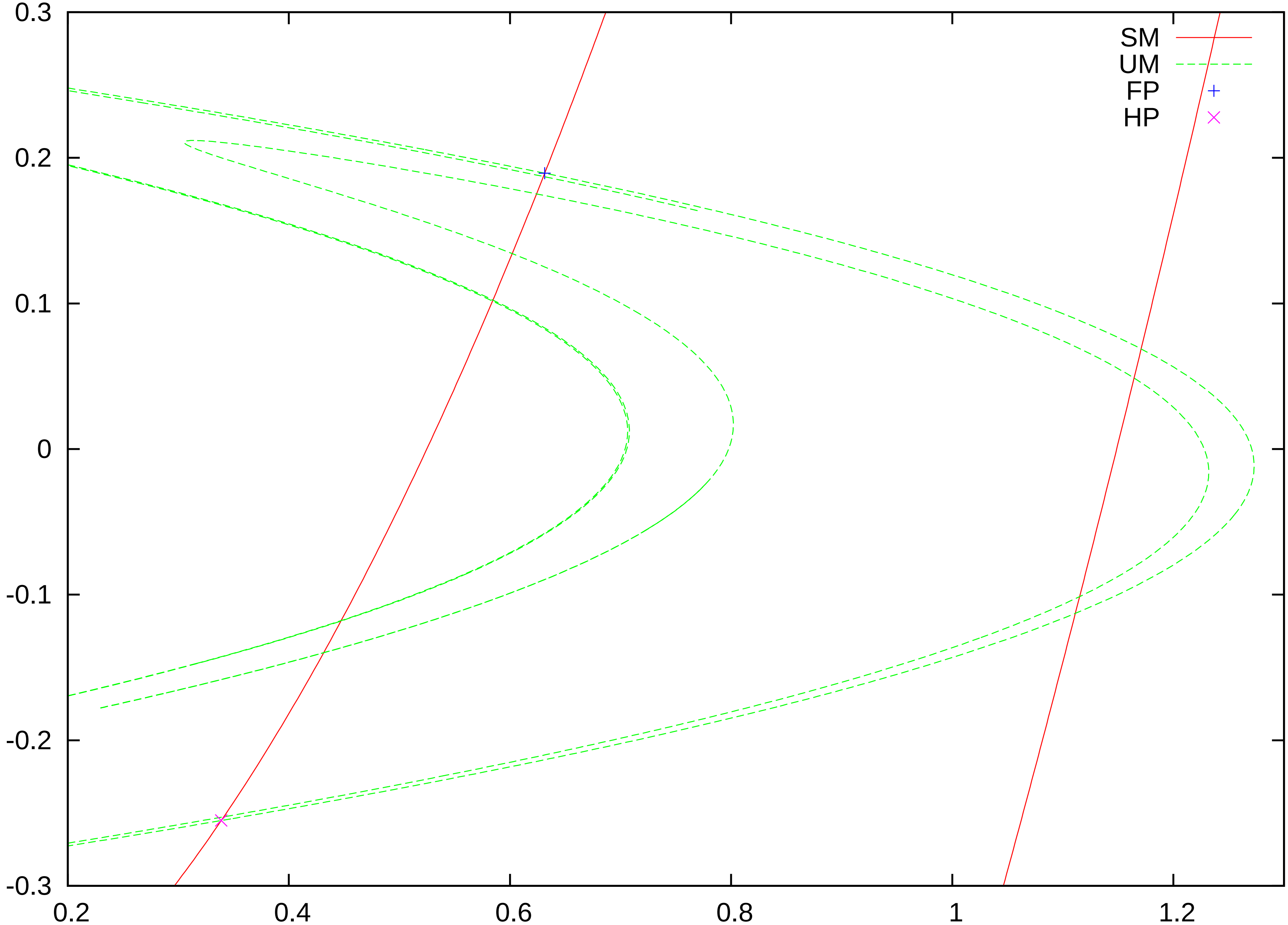
Question: How long can COSY integrate with dynamic domain decomposition?


DP: COSY-VI Integration with Dynamic Domain Decomposition
Possible ODE Integration Time
Box Stack Depth
0
2
4
6
8
10
12
14
16
18
20
0
5
10
15
20



SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2


SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2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UM
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HP
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0.4
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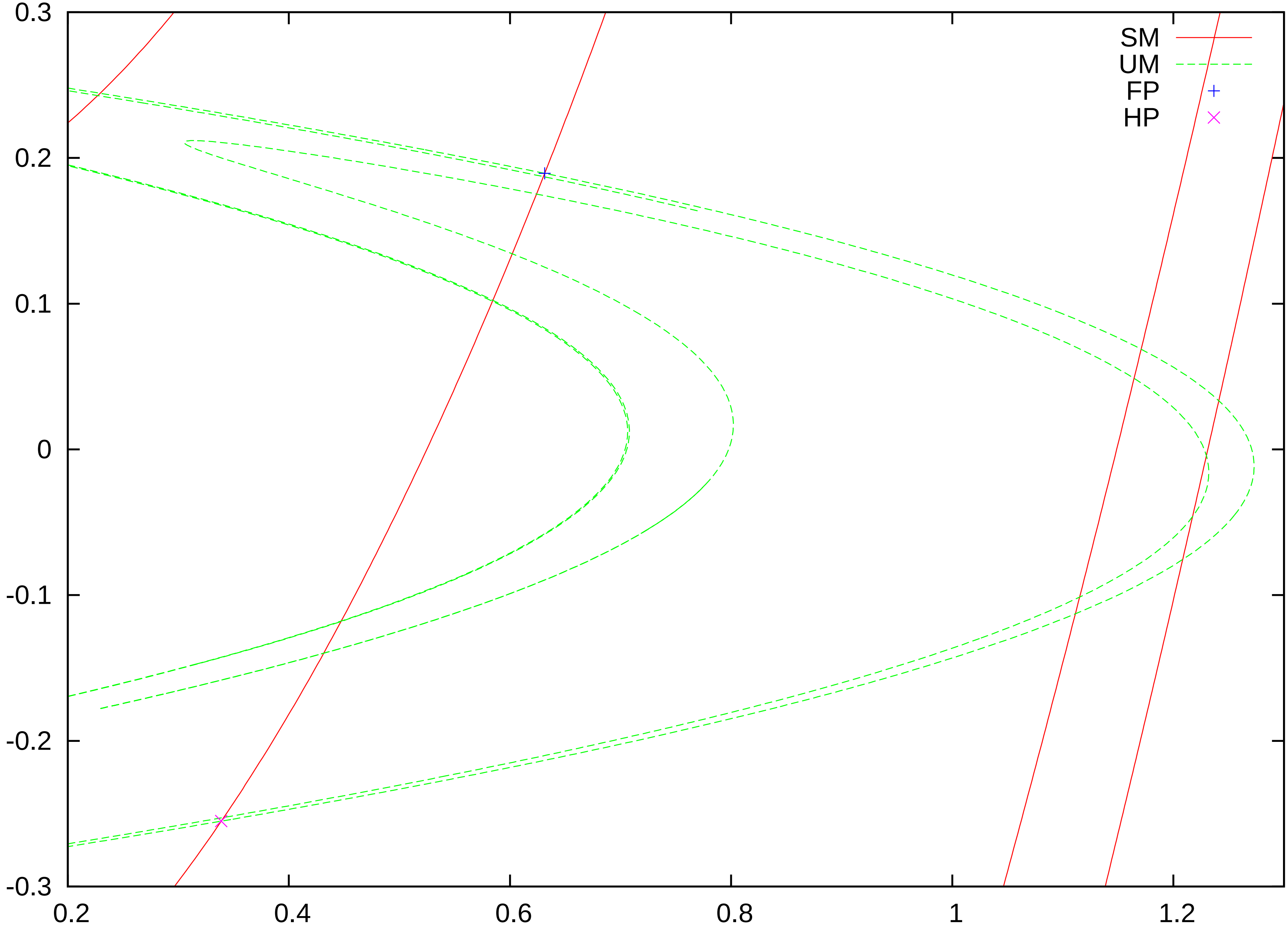
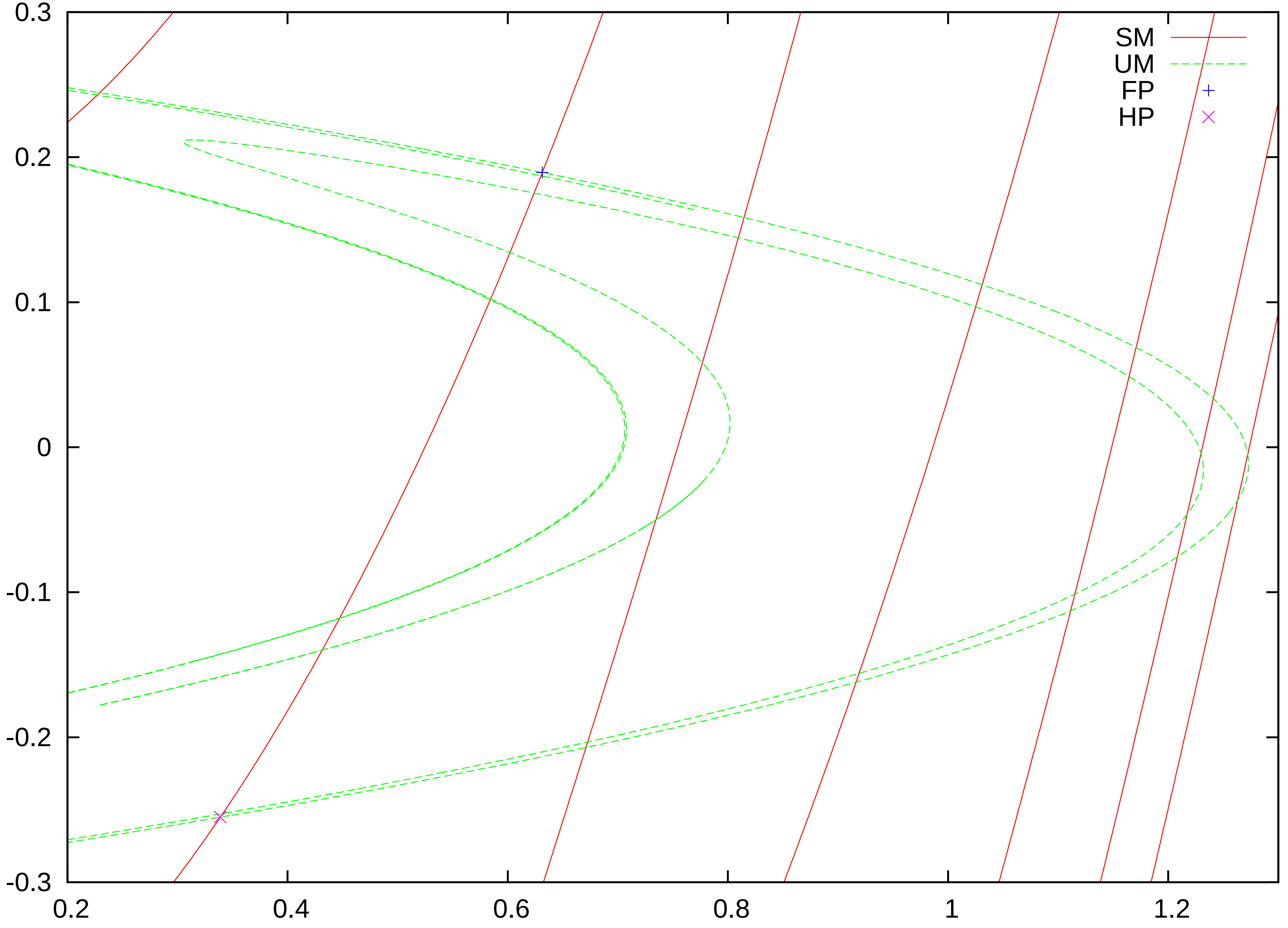
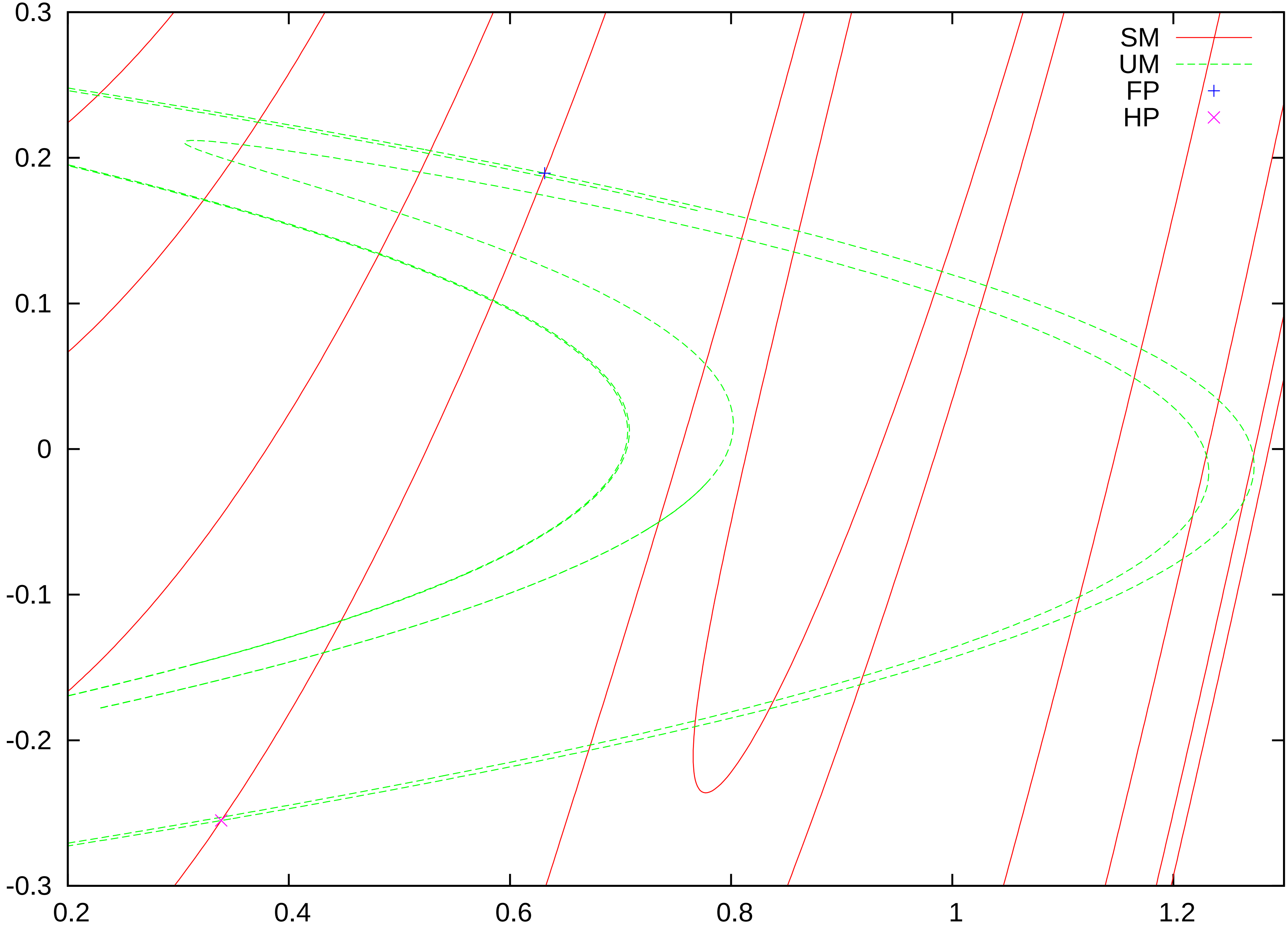
0.8
1
1.2



SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2



0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2
SM
UM
FP
HP



SM
UM
FP
HP
0.3
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0.4
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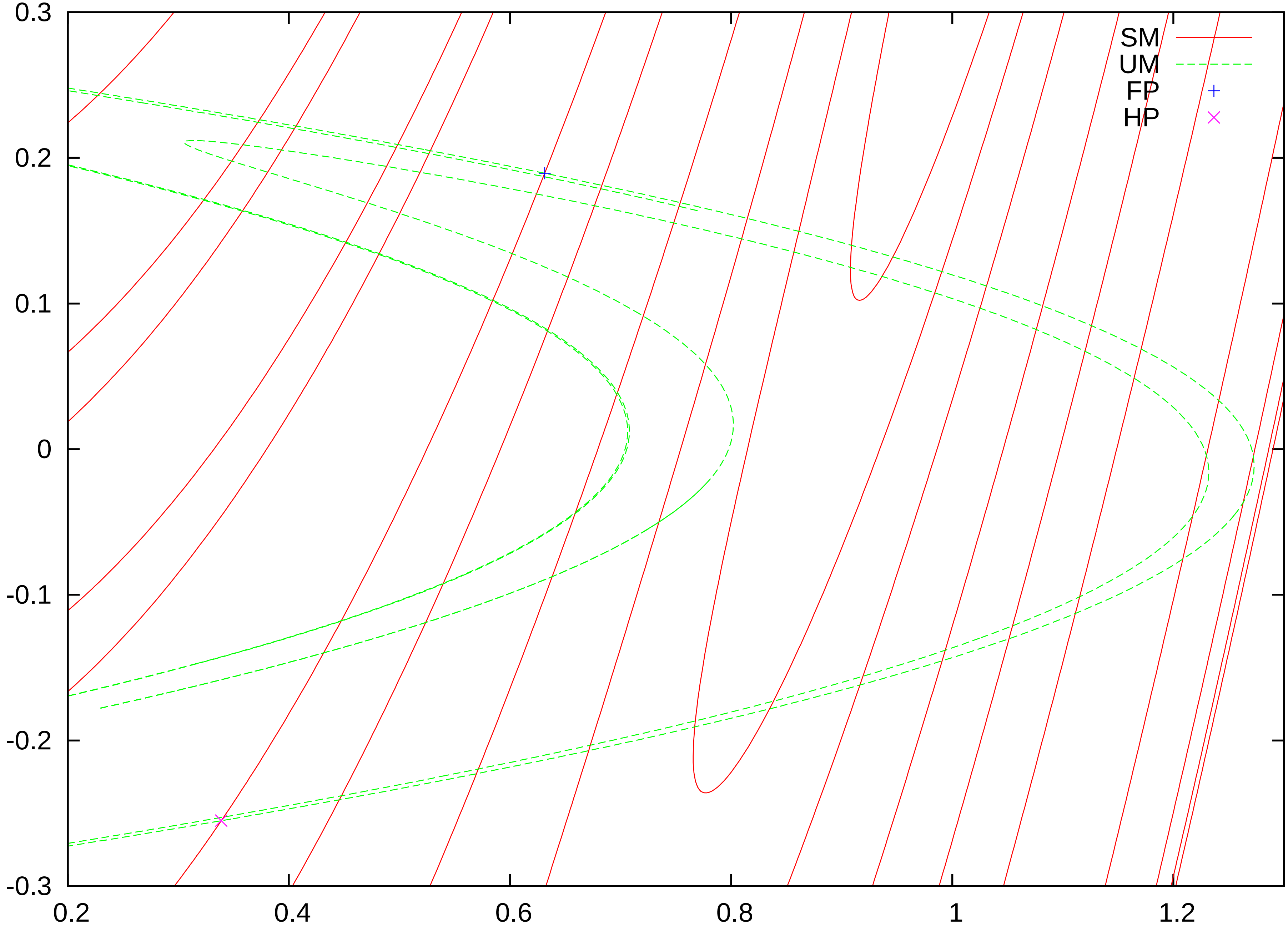
SM
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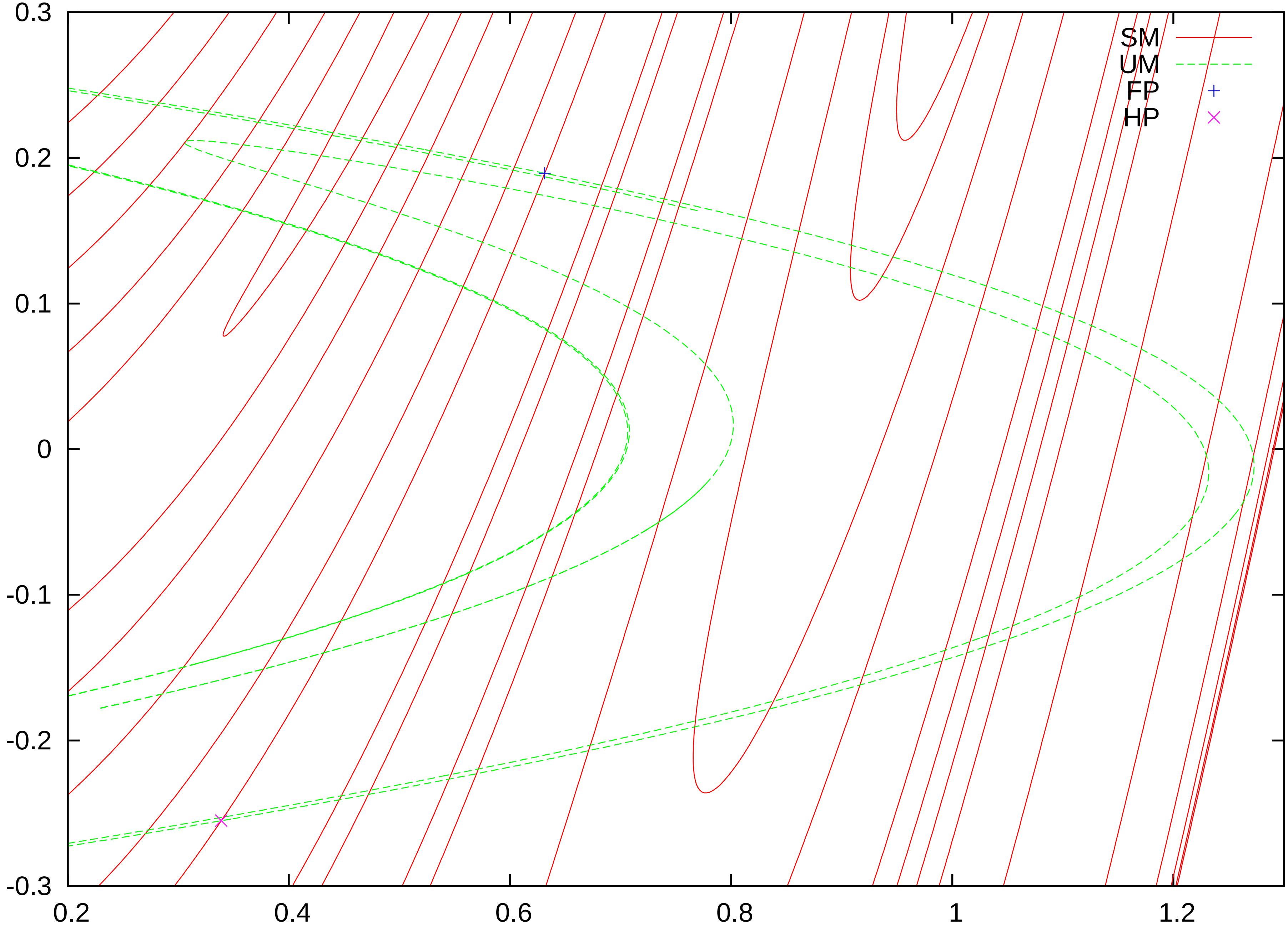

SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
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0.4
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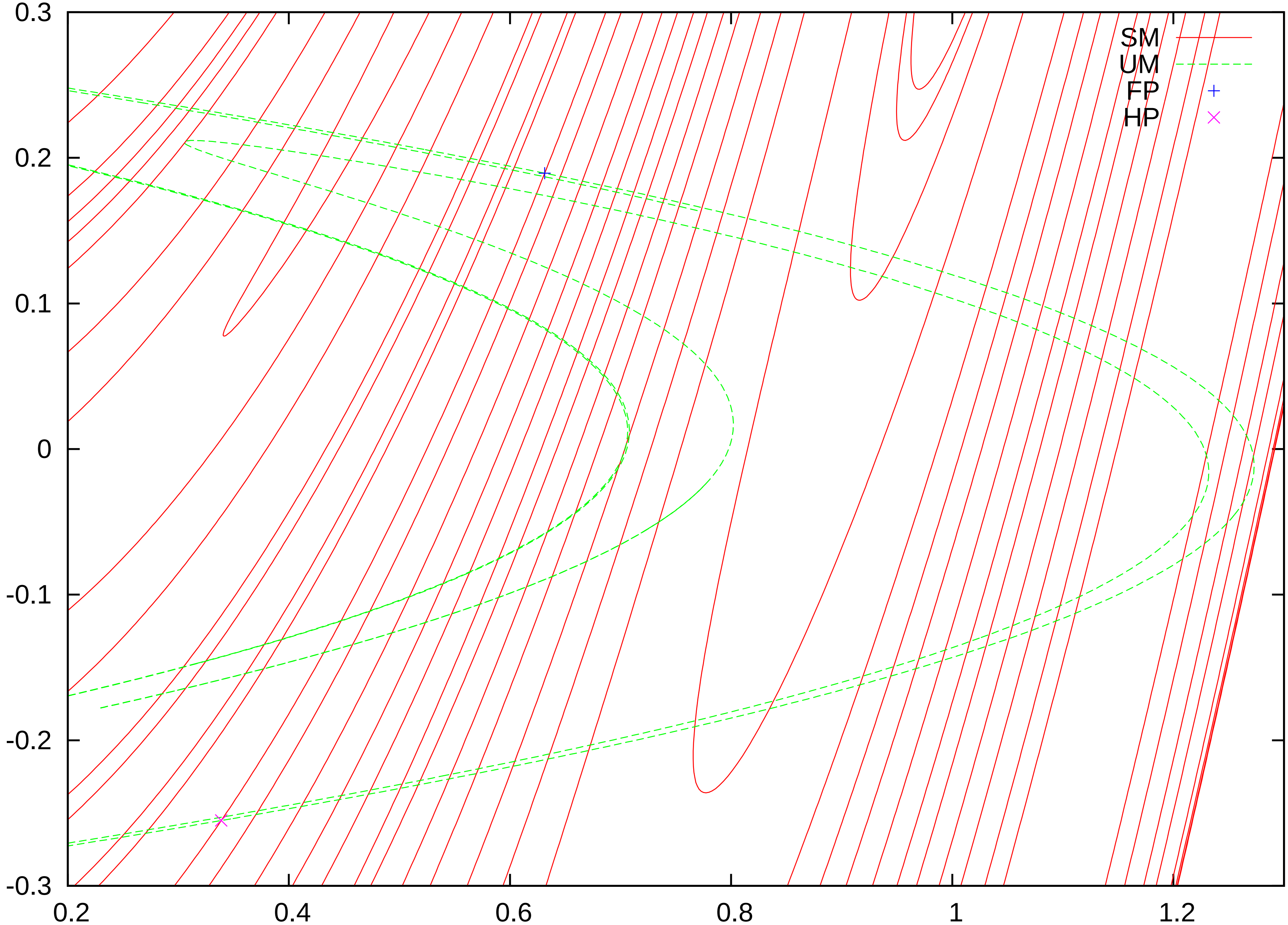
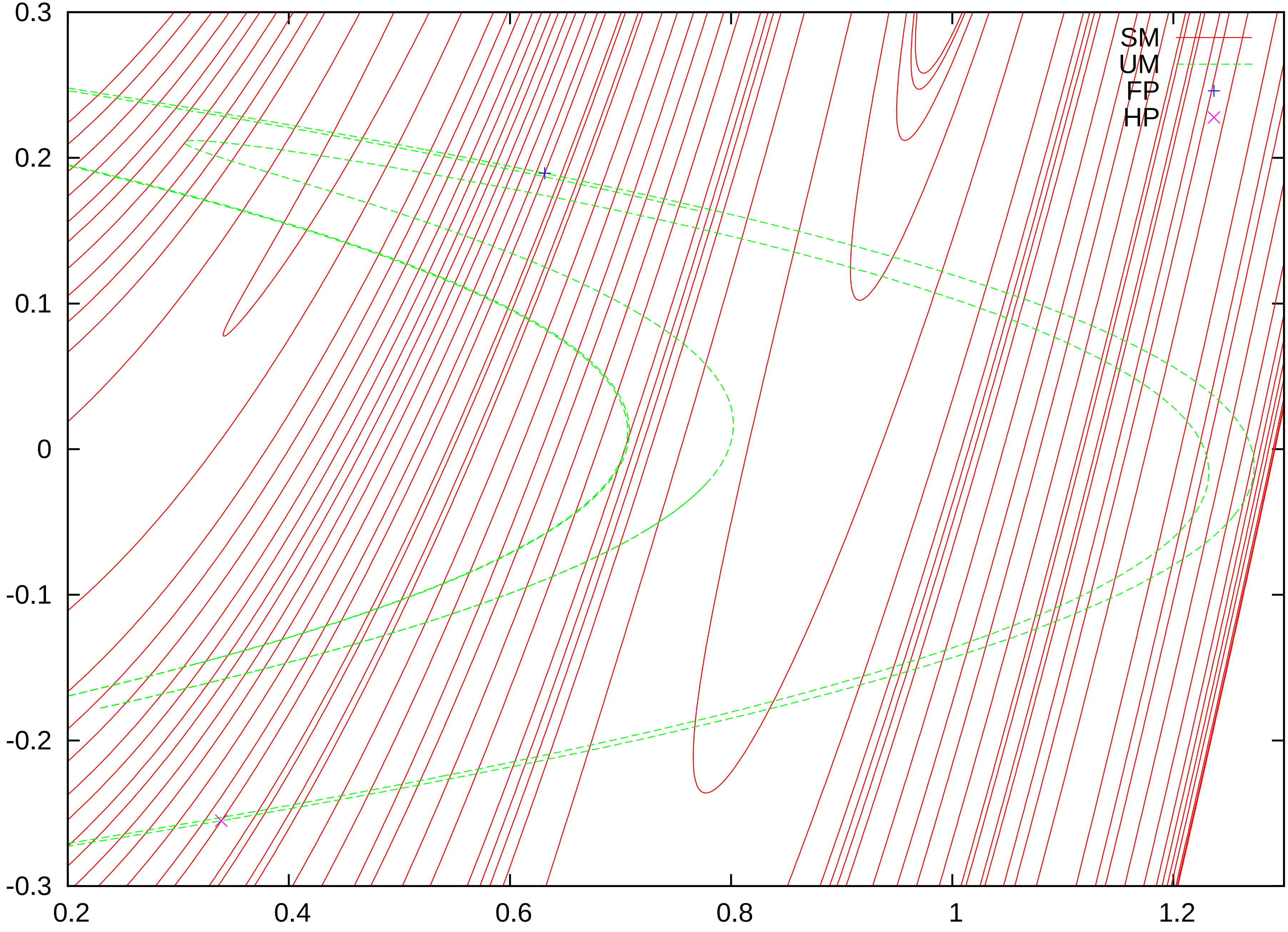
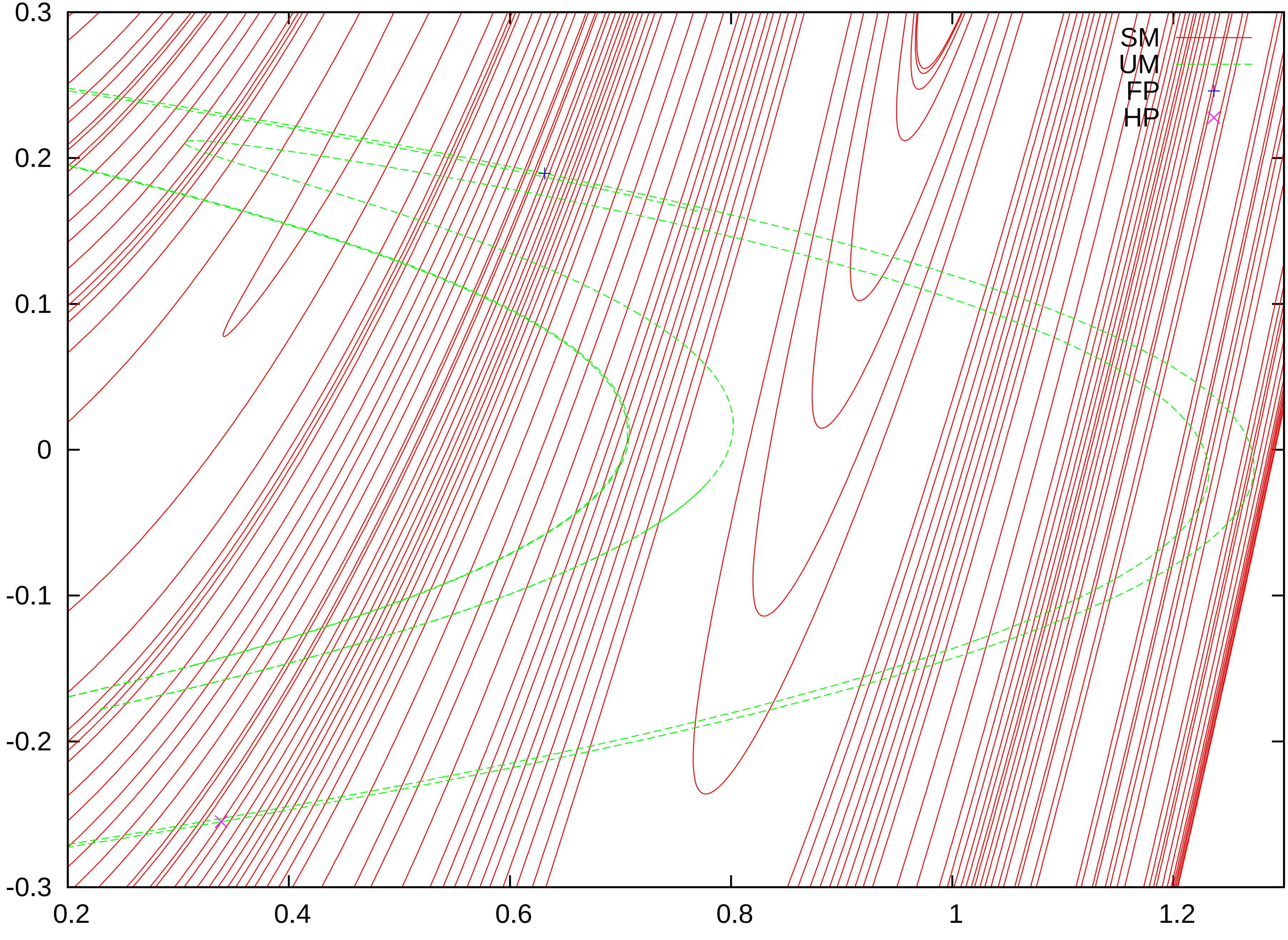
0.8
1
1.2



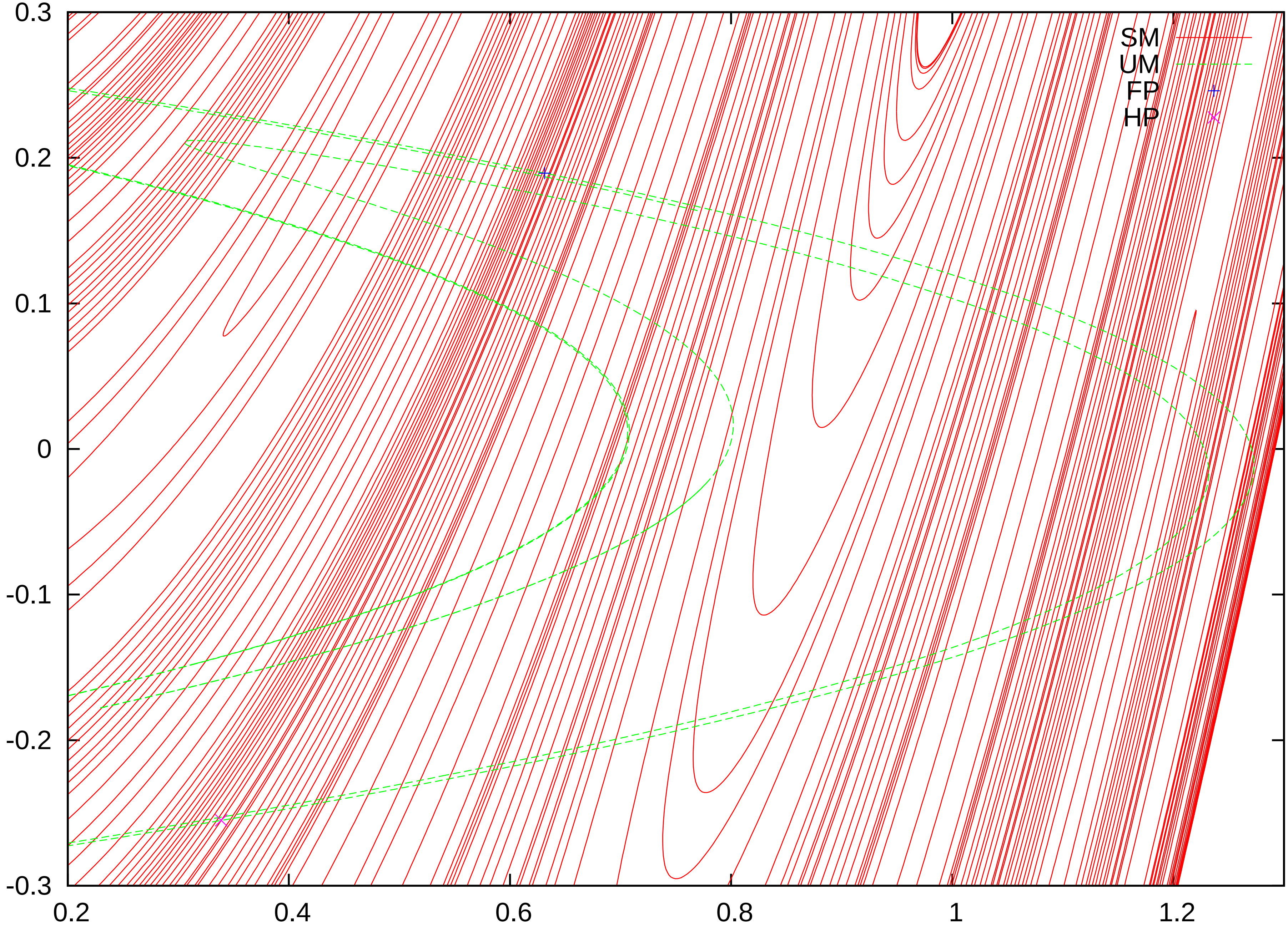
SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2



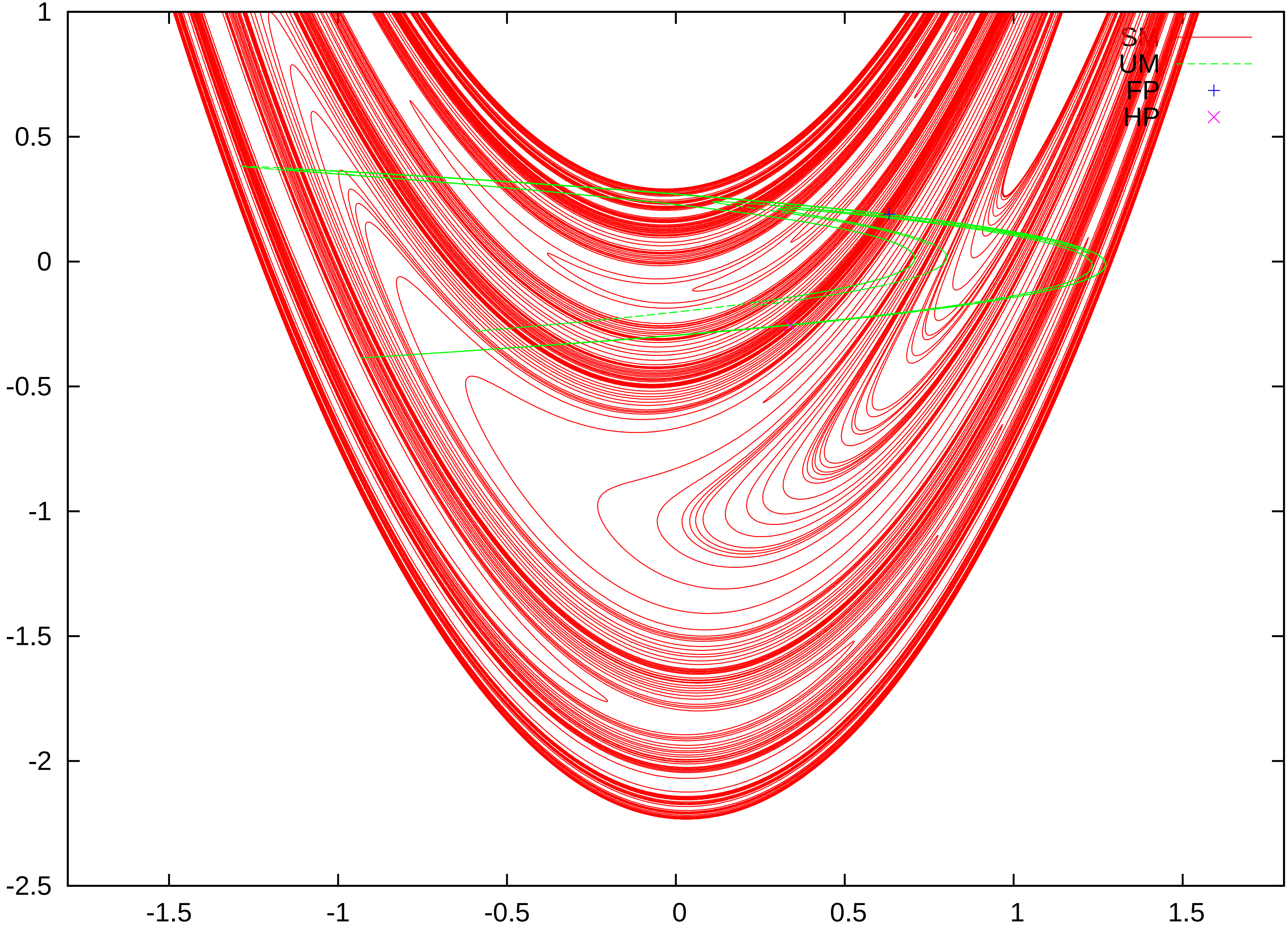
SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2



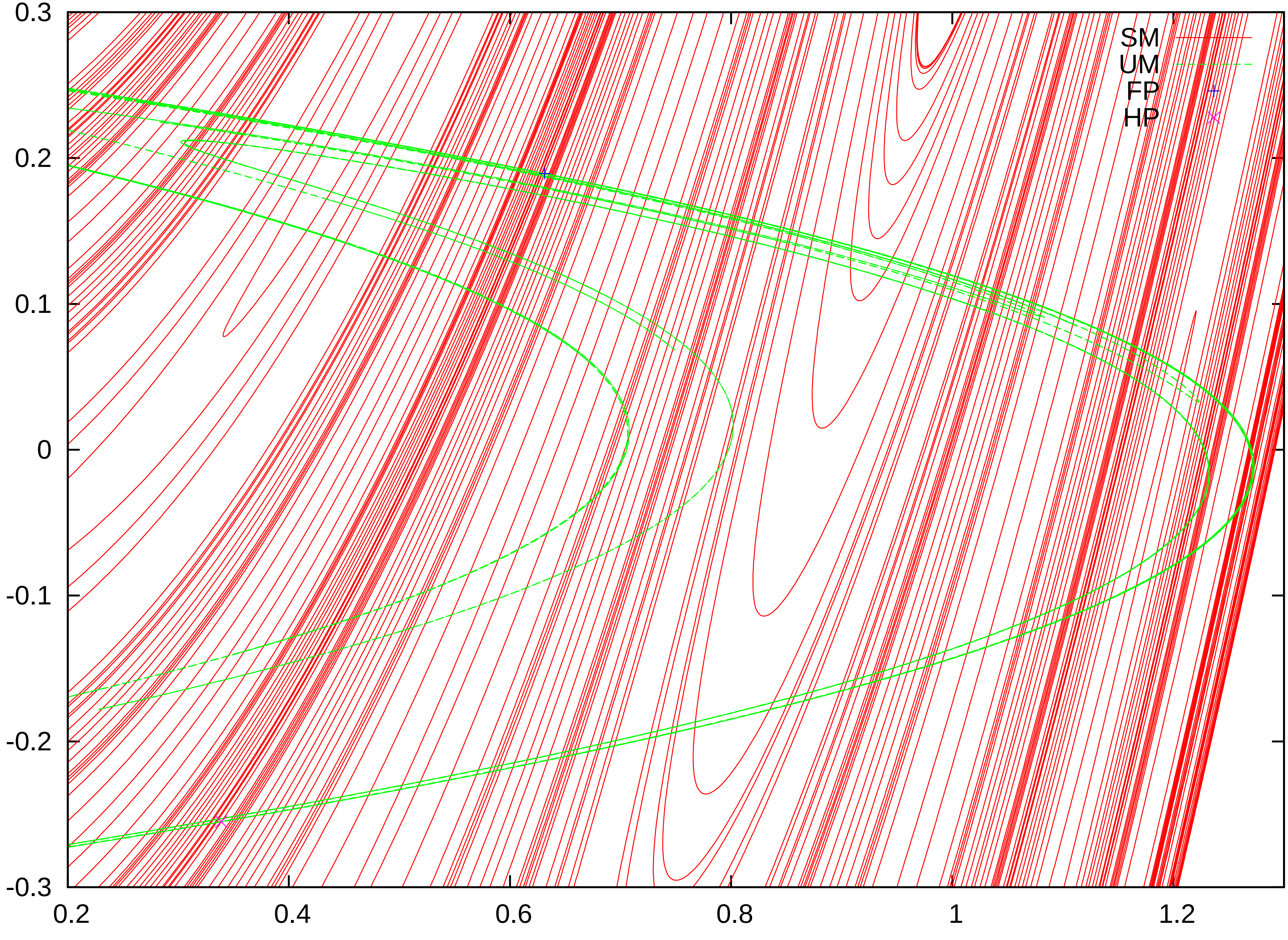
SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2



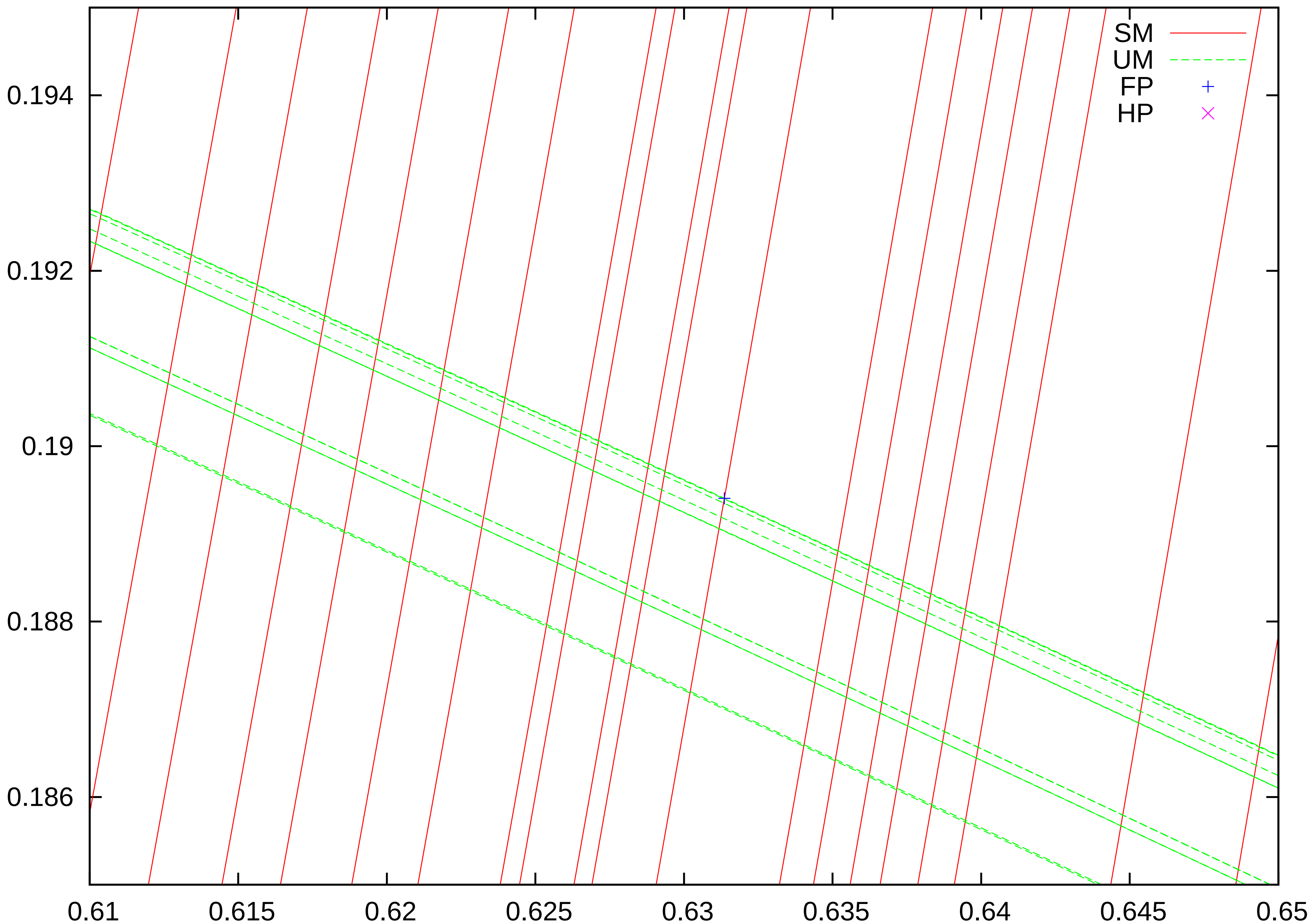
SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2



SM
UM
FP
HP
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-1.5
-1
-0.5
0
0.5
1
1.5



SM
UM
FP
HP
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.2
0.4
0.6
0.8
1
1.2


SM
UM
FP
HP
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0.192
0.19
0.188
0.186
0.61
0.615
0.62
0.625
0.63
0.635
0.64
0.645
0.65


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Boca Raton, Florida
December 16-19, 2006
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Automatic Differentiation
Differential Algebraic Tools
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Constraint Satisfaction
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Support: Department of Energy
Michigan State University