High-Order Dependency Free Range Bounding for Validated Global Optimization

Martin Berz and Kyoko Makino

Department of Physics and Astronomy
Michigan State University

Fermi's Golden Rule

Fermi's Golden Rule

A sign near the entrance of Fermilab's Accelerator Simulation Department:

Fermi's Golden Rule

A sign near the entrance of Fermilab's Accelerator Simulation Department:

The difference between Theory and Practice
is greater in Practice than it is in Theory

A Simple 1D Example

Approximate the cos function by its power series to order 60:

$$f(x) = \sum_{i=0}^{30} (-1)^i \frac{x^{2i}}{(2i)!}.$$

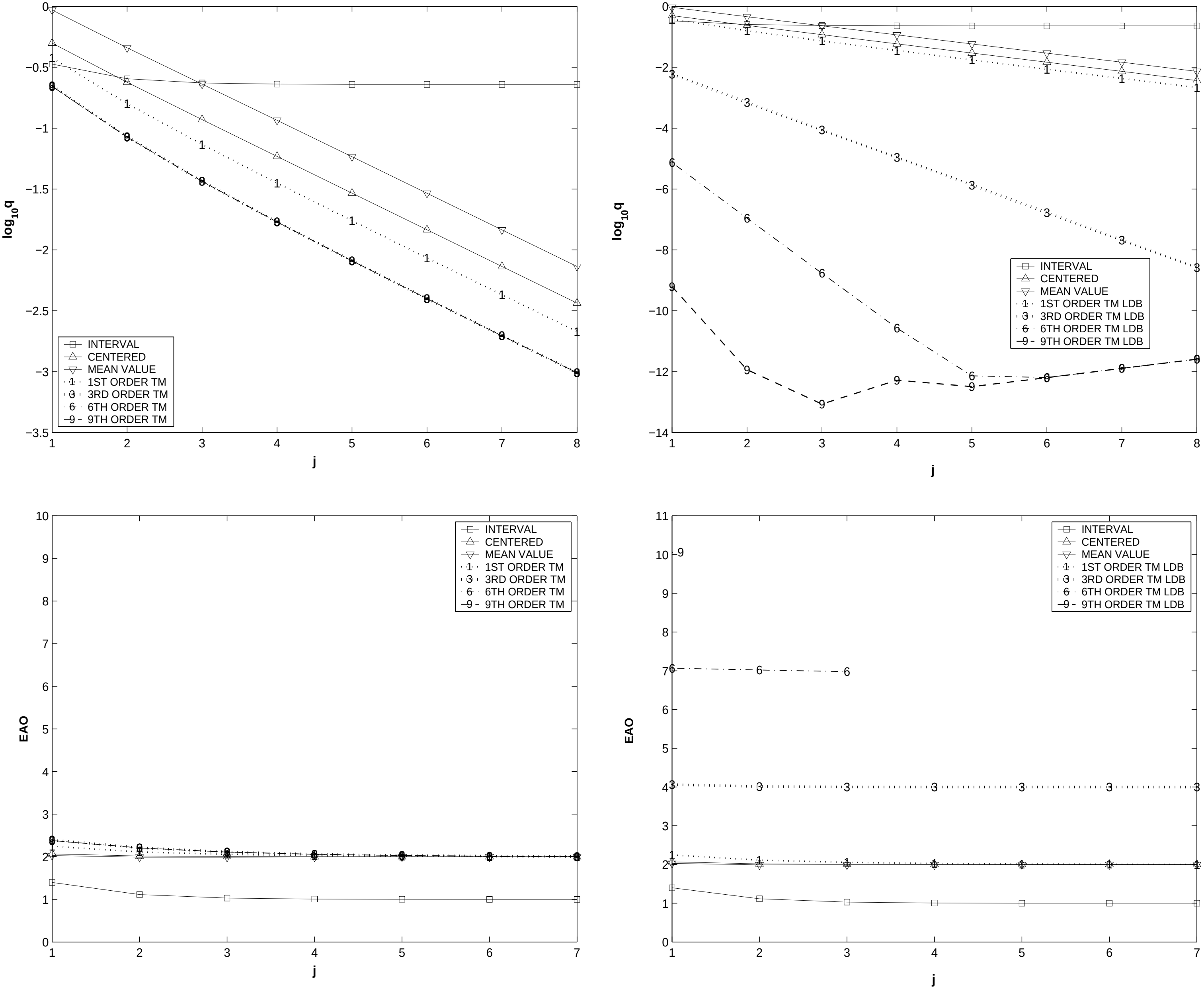
Several nice properties:

1. Properties of the function are well known
2. Dependency increases with x from very small to very large
3. Periodicity allows the study of the same functional behavior with varying amounts of dependency
4. Study at points with both non-stationary and stationary points is possible

Study results for expansion points $x_0 = n \cdot \pi/4$ for

$$n = 1, 5, 9, 13 \text{ and } n = 0, 4, 8, 12.$$

For each of these points, domains are $x_0 + [-2^{-j}, 2^{-j}]$ for $j = 1, ..., 8$.



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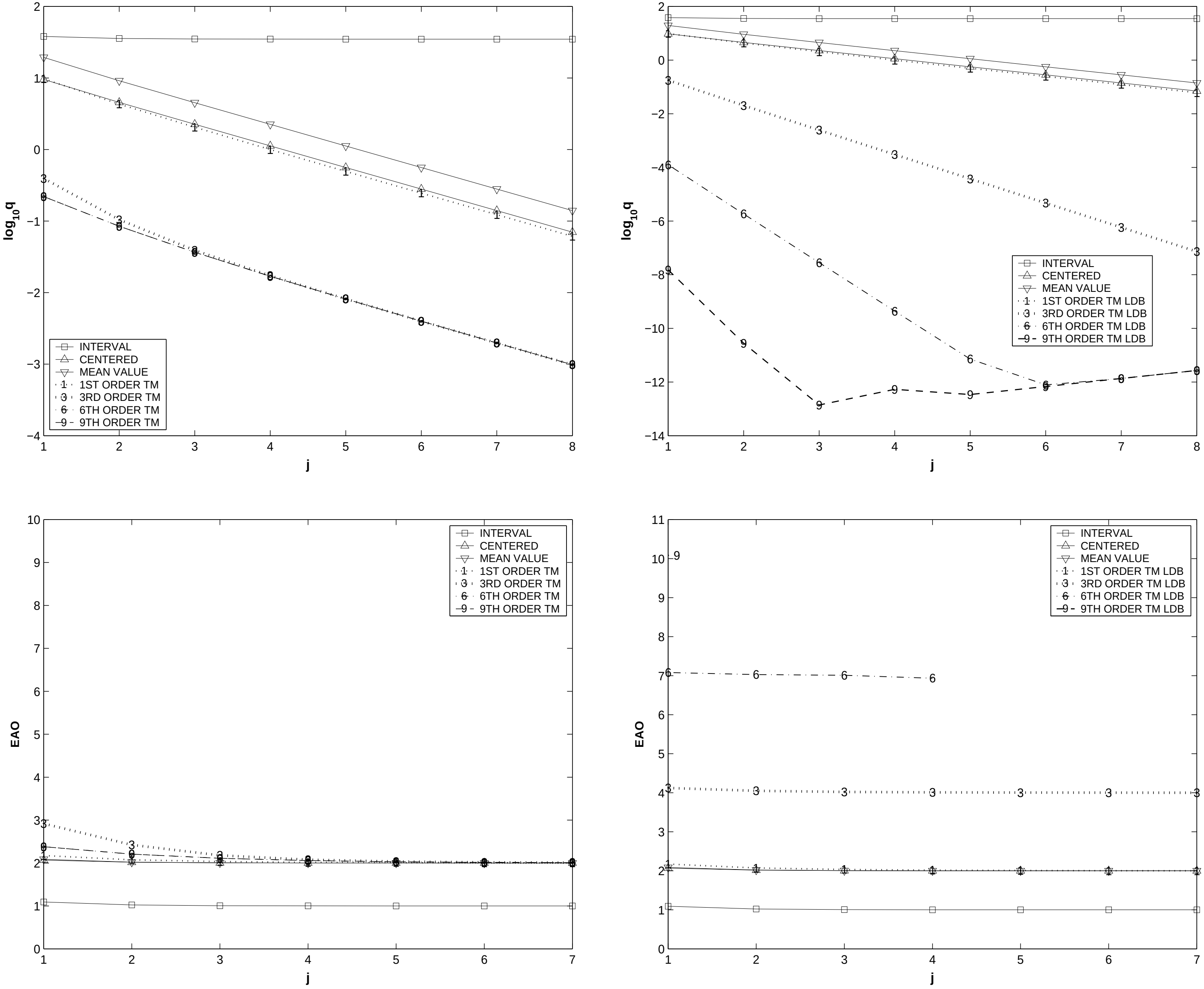
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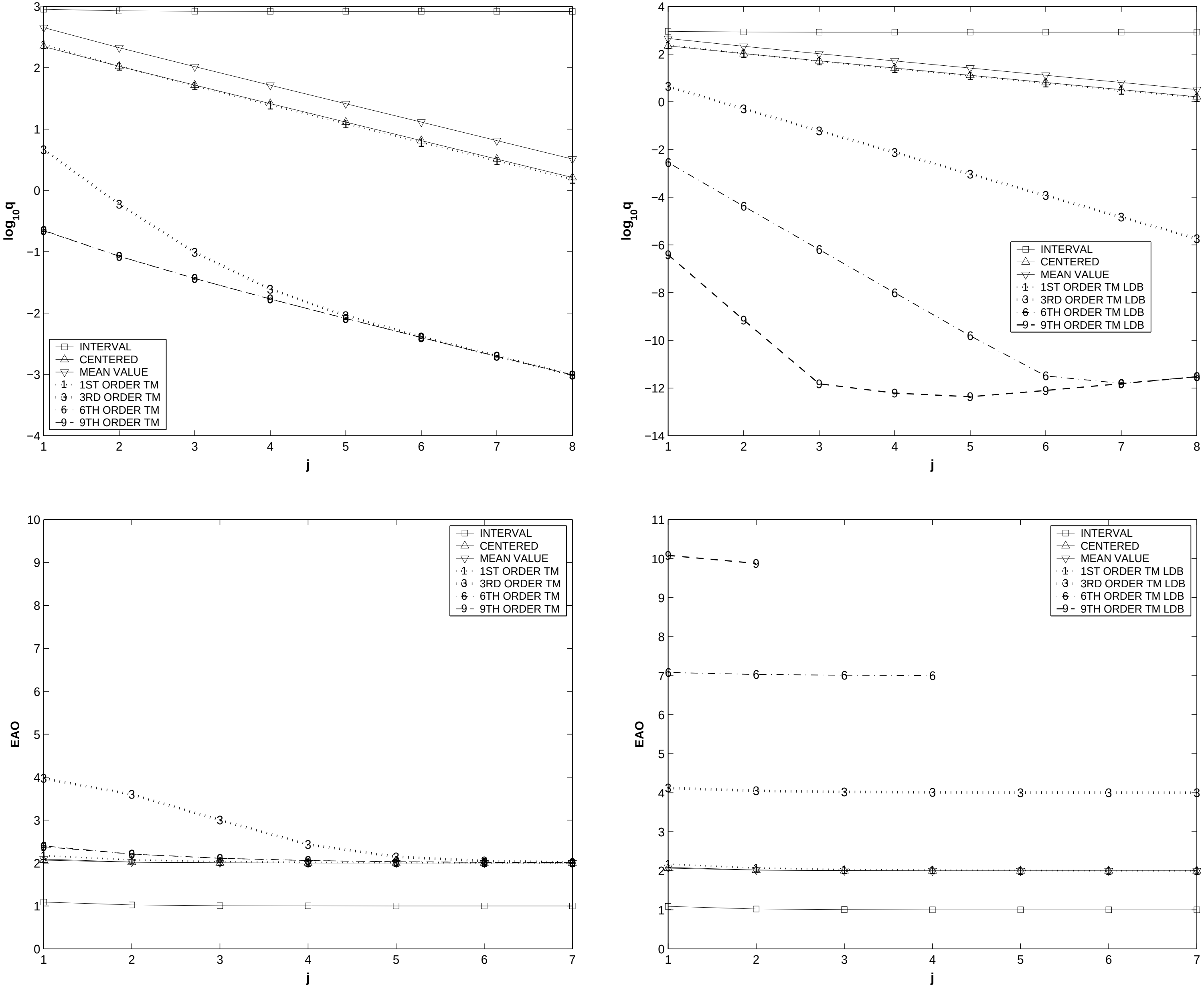
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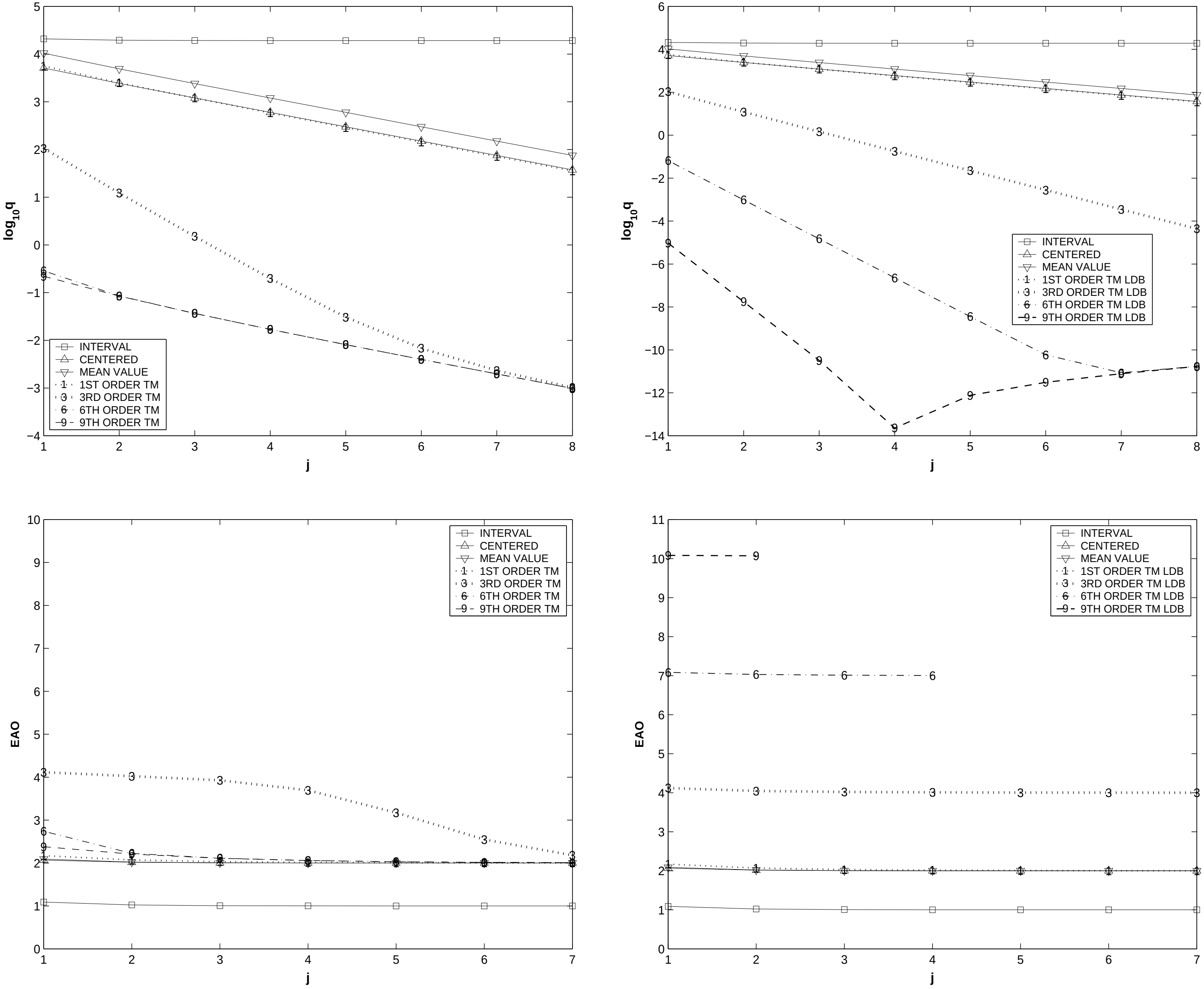
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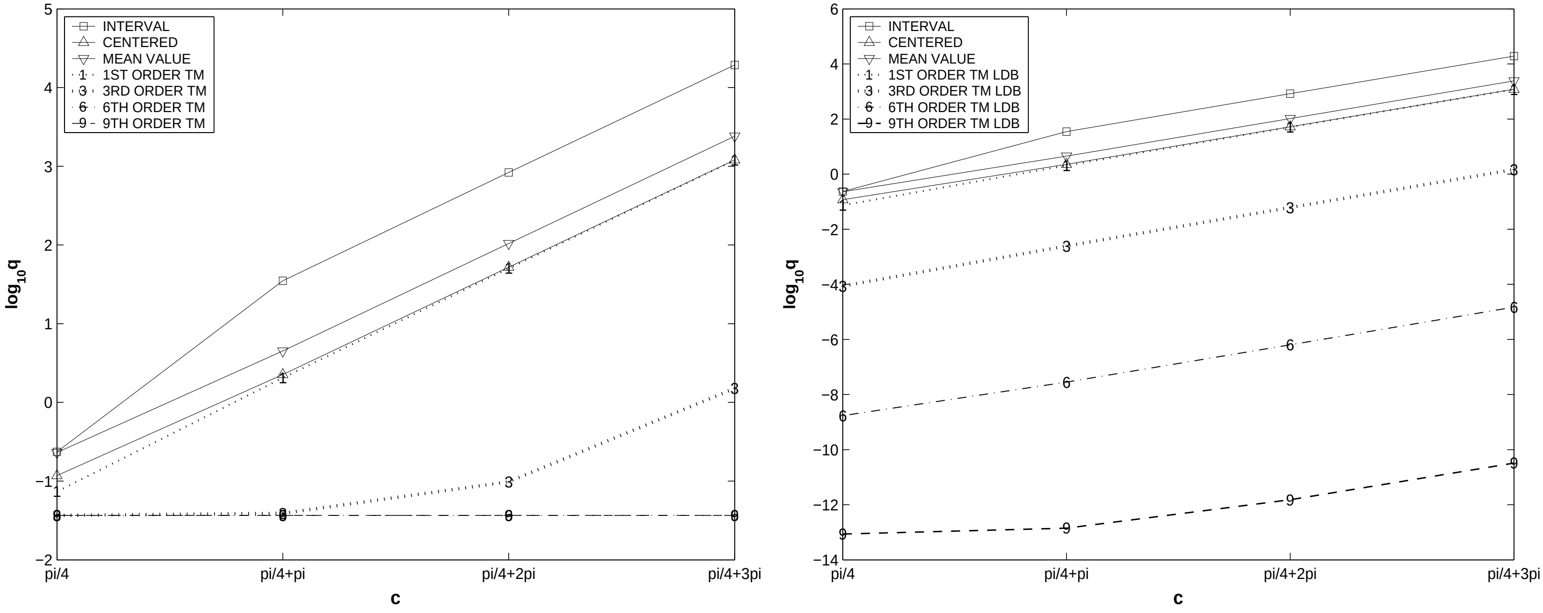
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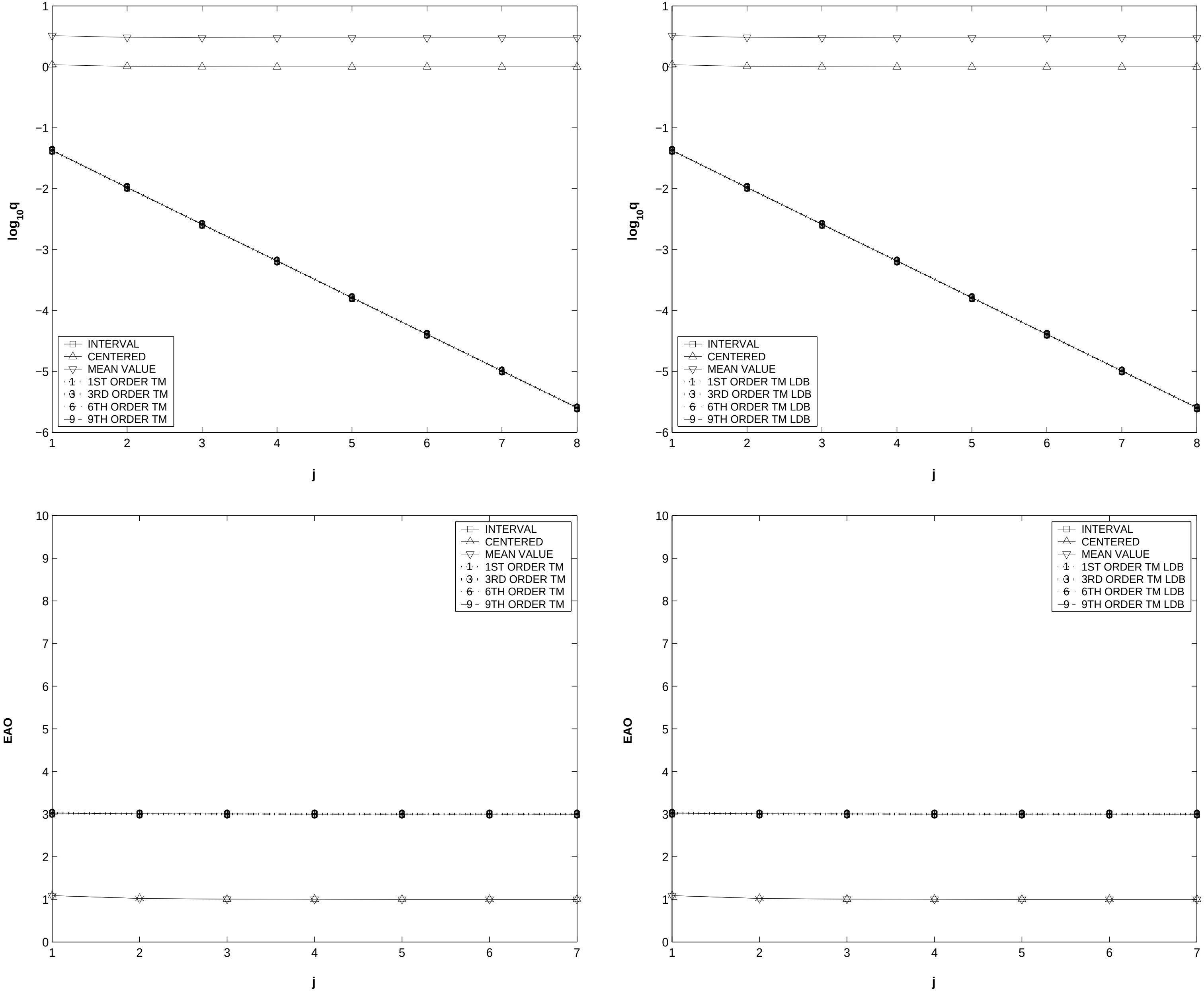

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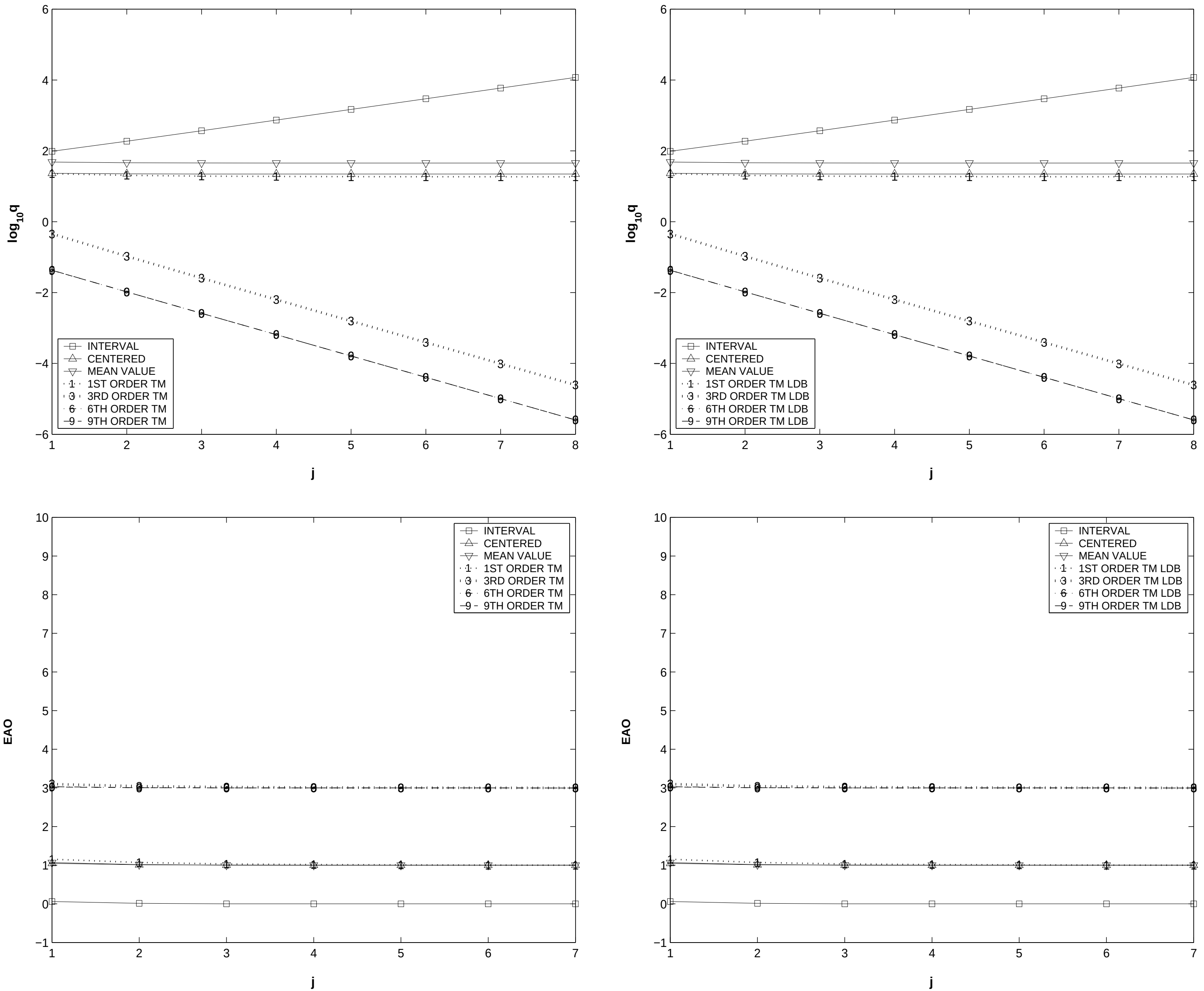
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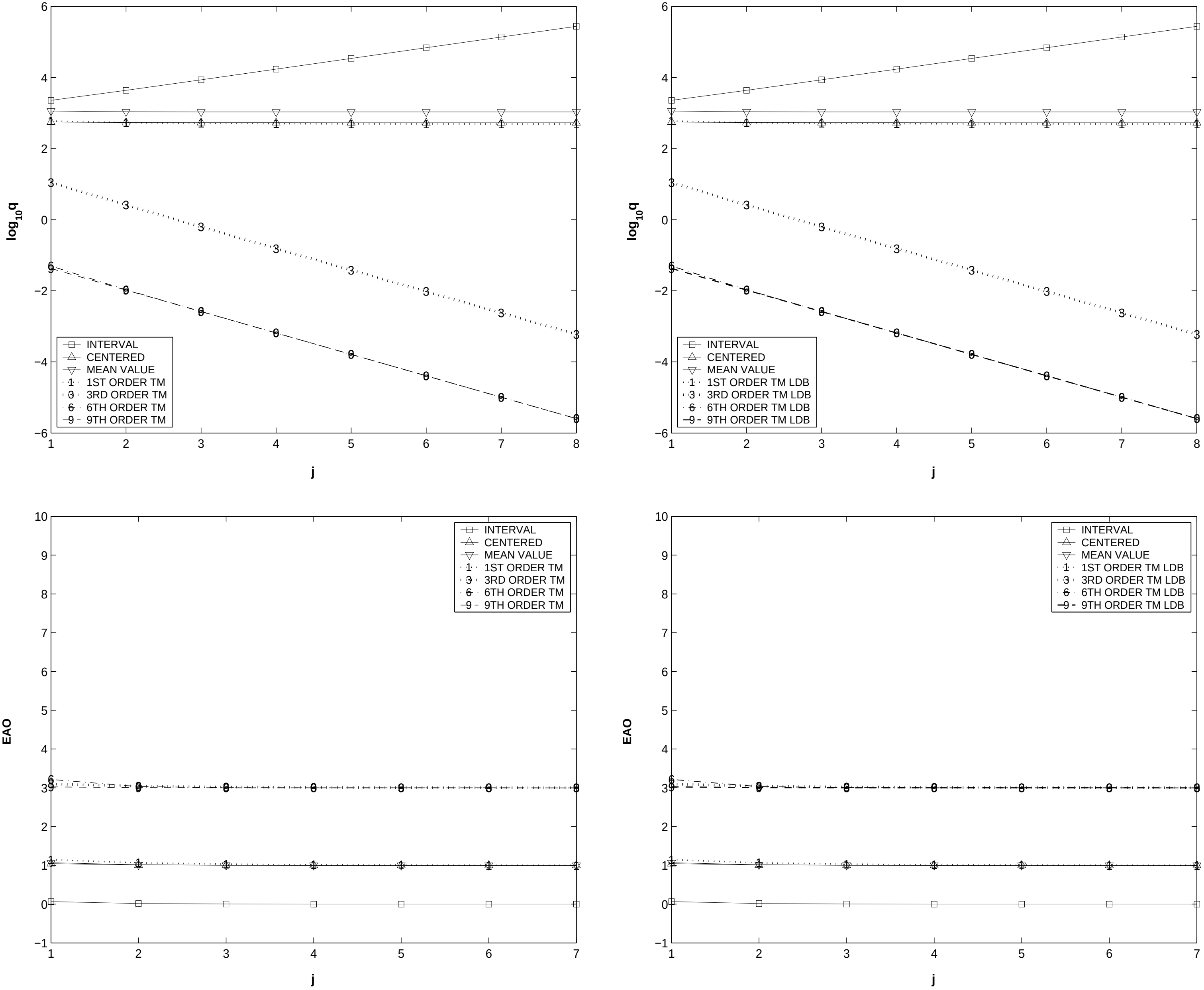

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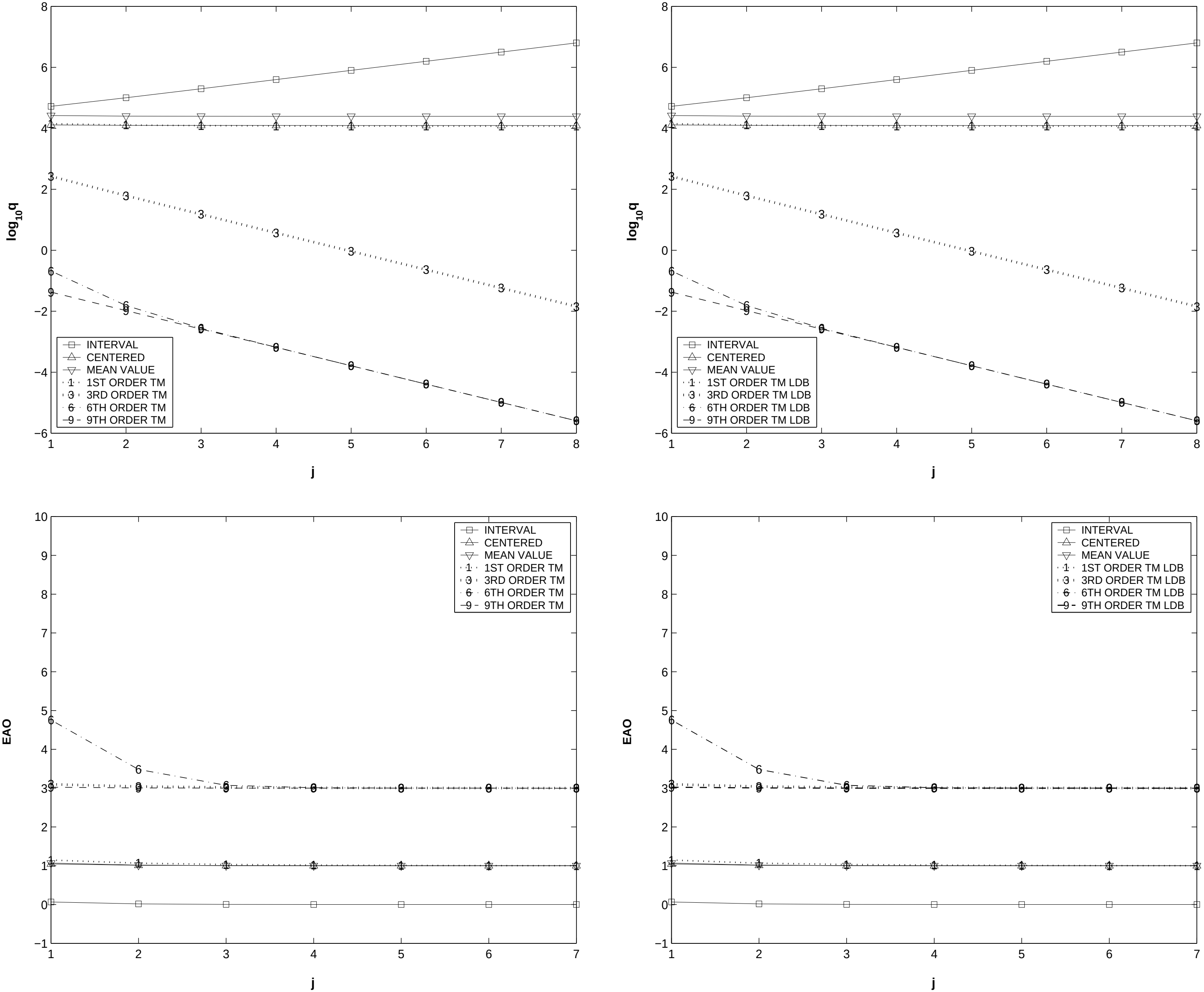
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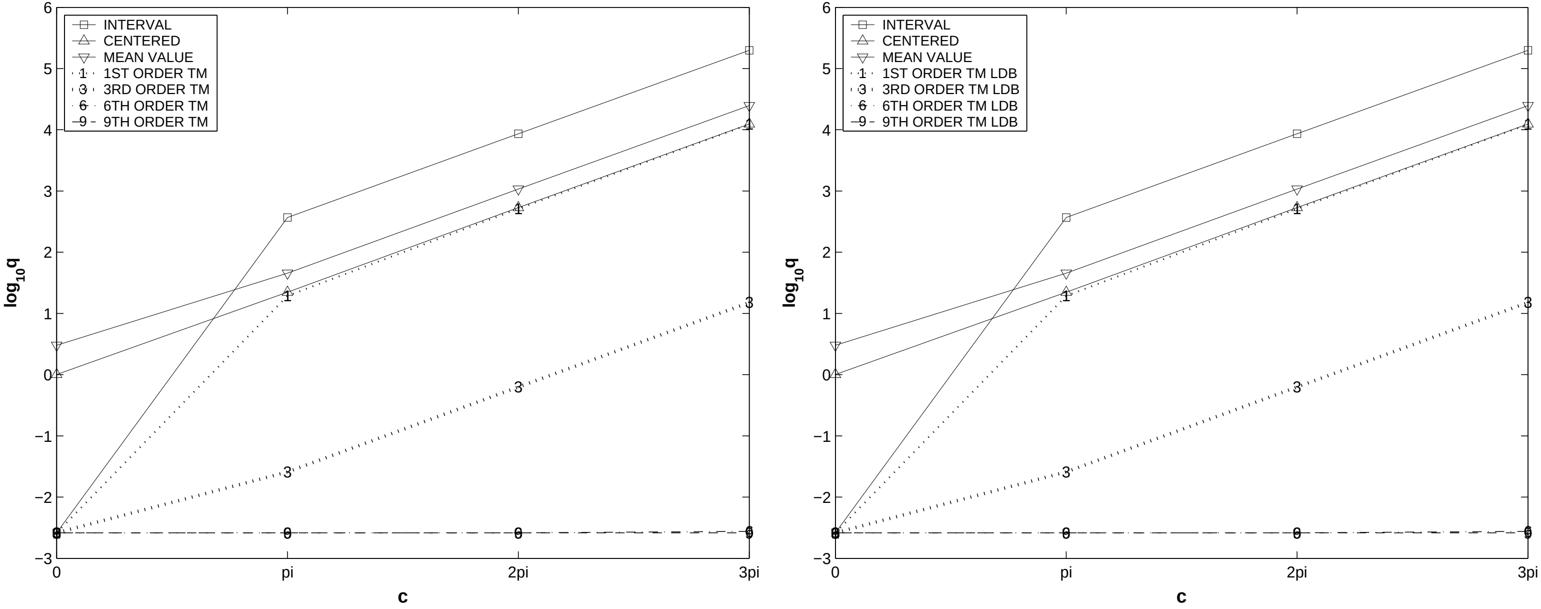

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Definitions - Taylor Models and Operations

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

Definition (Taylor Model) Let $f : D \subset R^v \to R$ 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

$$T_1 + T_2 = (P_1 + P_2, I_1 + I_2)$$
$$T_1 \cdot T_2 = (P_{1\cdot 2}, I_{1\cdot 2})$$

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

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

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.

Definitions - Taylor Model Arc Sine

Arcsine. Under the condition $\forall x \in D,\ B(P(x-x_0)+I) \subset (-1,1)$, using an addition formula for the arcsine, we re-write

$$\arcsin(f(x)) = \arcsin(c_f) + \arcsin\left(f(x)\cdot\sqrt{1-c_f^2} - c_f\cdot\sqrt{1-(f(x))^2}\right).$$

Utilizing that

$$g(x) \equiv f(x)\cdot\sqrt{1-c_f^2} - c_f\cdot\sqrt{1-(f(x))^2}$$

does not have a constant part, we have

$$\begin{aligned}\arcsin(g(x)) = g(x) + \frac{1}{3!}(g(x))^3 + \frac{3^2}{5!}(g(x))^5 + \frac{3^2\cdot 5^2}{7!}(g(x))^7 \\ + \cdots + \frac{1}{(k+1)!}(g(x))^{k+1}\cdot\arcsin^{(k+1)}(\theta\cdot g(x)),\end{aligned}$$

where

$$\arcsin'(a) = 1/\sqrt{1-a^2}, \qquad \arcsin''(a) = a/(1-a^2)^{3/2},$$

$$\arcsin^{(3)}(a) = (1+2a^2)/(1-a^2)^{5/2}, \ldots$$

Definitions - Taylor Model Arc Sine, Antiderivation

A recursive formula for the higher order derivatives of arcsin

$$\arcsin^{(k+2)}(a) = \frac{1}{1-a^2}\{(2k+1)a\arcsin^{(k+1)}(a) + k^2\arcsin^{(k)}(a)\}$$

is useful. Then, evaluating in Taylor model arithmetic yields the desired result, where again the terms involving θ only produce interval contributions.

Antiderivation. We note that a Taylor model for the integral with respect to variable i of a function f can be obtained from the Taylor model (P,I) of the function by merely integrating the part P_{n-1} of order up to $n-1$ of the polynomial, and bounding the n-th order into the new remainder bound. Specifically, we have

$$\partial_i^{-1}(P,I) = \left(\int_0^{x_i} P_{n-1}(x)dx_i\,,\ (B(P-P_{n-1})+I)\cdot(b_i-a_i)\right).$$

Thus, given a Taylor model for a function f, the Taylor model intrinsic functions produce a Taylor models for the composition of the respective intrinsic with f. Furthermore, we have the following result.

COSY

Design Features:

1. Uses two-stage coding, sparse storage of derivatives
2. All standard intrinsics as well as Derivation, Antiderivation
3. Highly optimized implementation
4. Can be called from F77 and C (subroutine calls), F95 and C++ (objects)
5. Language-Independent Platform - only one source code for four languages
6. Altogether nearly 1000 registered users, development almost 20 years, $5M in funding (DOE, NSF, URA)

Existing Application Packages:

1. COSY INFINITY (Beam Physics): Currently the main tool for simulation of nonlinear high-order effects in beam dynamics
2. COSY-VI: Validated Integrator, based on Taylor expansion in time AND initial condition
3. COSY-GO: Validated Global Optimizer, based on Taylor expansion for dependency suppression and domain reduction

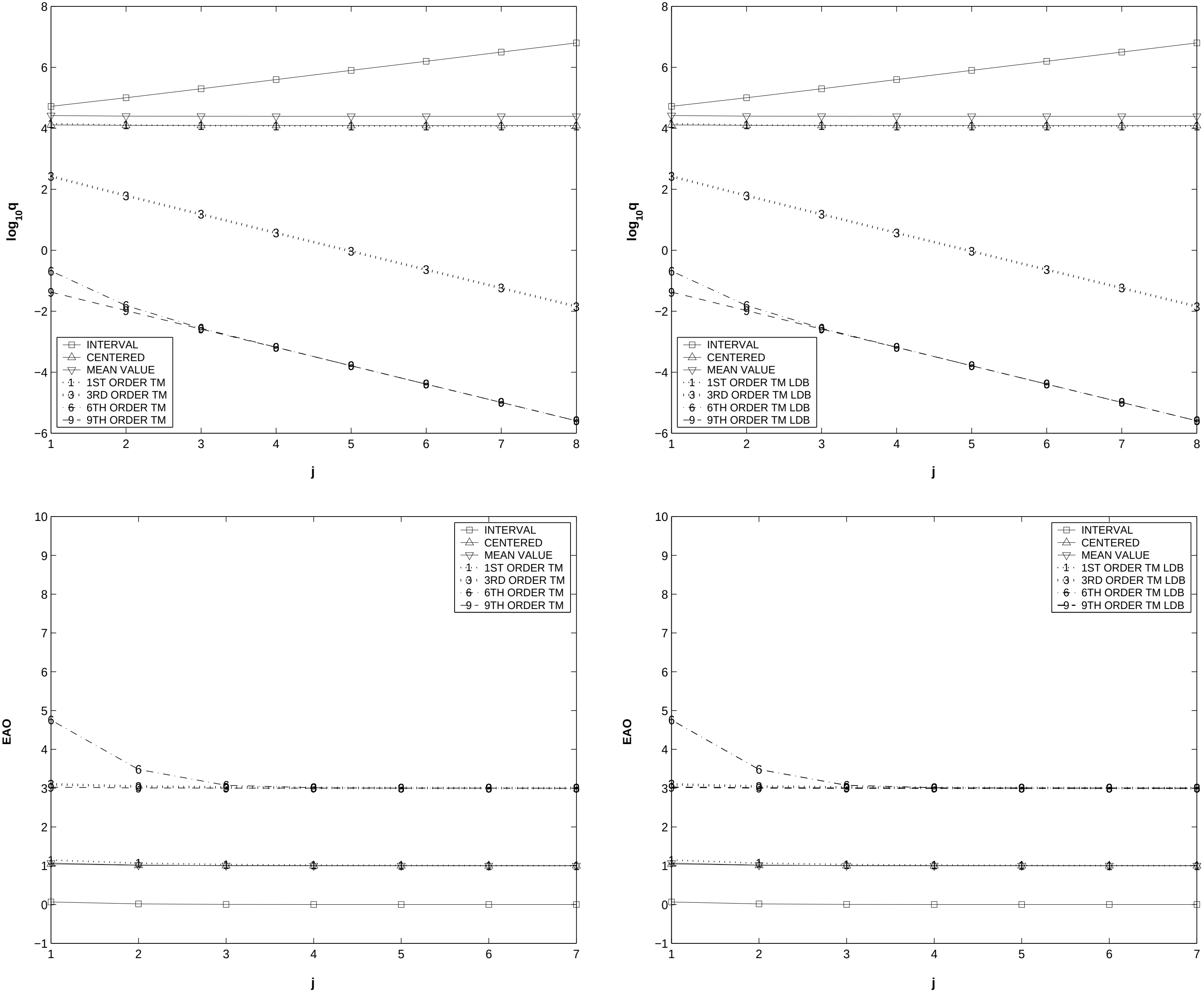
Implementation of TM Arithmetic

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++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Ordered LDL (Extended Cholesky) Decomposition

Given Quadratic Form with symmetric H

$$Q(x) = \frac{1}{2}x^t \cdot H \cdot x + a \cdot x + b$$

We determine Ordered LDL Decomposition (L: lower diagonal with unit diagonal, D: diagonal) as follows

1. Pre-sort rows and columns by the size of their diagonal elements
2. Successively execute conventional L^tDL decomposition step in interval arithmetic, beginning by representing every element of H by a thin interval; in step i:
   (a) If the $l(D(i,i)) > 0$ proceed to the next row and column.
   (b) If the $l(D(i,i)) < 0$,exchange row and column i with row and column $i+1$, $i_{-}+2$, ... If a positive element is found, increment i and repeat. If none is found, stop.

Note: Correction Matrix In case some $0 \in D(i,i))$ or $D(i,i)$ apply small correction C to H, i.e. study $H+C$ instead of H, such that all elements of D are clearly positive or negative. $|C|$ is lumped into the remainder bound of the original problem.

Ordered LDL Decomposition - Result

Have obtained representation of H as LDL composition

$$P^t H P = L^t D L$$

- First p elements of D satisfy $l(D(i,i)) > 0$
- Remaining $(n-p)$ elements of D will satisfy $u(D(i,i)) < 0$

Proposition: Sufficiently near a local minimizer, D will contain only positive elements. Furthermore, in the wider vicinity of the local minimizer, the number of negative elements in D will decrease as the minimizer is approached.

Simply follows from continuity of the matrix D as a function of position

The QDB (Quadratic Dominated Bounder) Algorithm

1. Let u be an external cutoff. Initialize $u = \min(u, Q(C))$. Initialize list with all 3^n surfaces for study.
2. If no boxes are remaining, terminate. Otherwise select one surface S of highest dimension.
3. On S, apply LDB. If a complete rejection is possible, strike S from the list and proceed to step 2. If a partial rejection is possible, strike the respective surfaces of S from the list and proceed to step 2.
4. Determine the definiteness of the Hessian of Q when restricted to S
5. If the Hessian is not p.d. strike S from the list and proceed to step 2.
6. If the Hessian is p.d., determine the corresponding critical point c.
7. If c is fully inside S, strike S and all surfaces of S from the list, update u $= \min(u, Q(c))$,and proceed to step 2
8. If c not inside S, strike S. If certain components of c lie between -1 and $+1$, strike the corresponding surfaces and proceed to step 2

The QDB Algorithm - Properties

The QDB algorithm has the following properties.

1. The quadratic bounder QDB has the third order approximation property.
2. The effort of finding the minimum requires the study of at most 3^n surfaces.
3. In the p.d. case, the computational effort requires at most the study of 2^n surfaces
4. Because of extensive box striking, in practice, the numbers of boxes to study is usually much much less.

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But still, it is desirable to have something **FASTER**.

The QFB (Quadratic Fast Bounder) Algorithm

Let $P+I$ be a given Taylor model. Idea. Decompose into two parts

$$P+I = (P-Q)+I+Q \text{ and observe}$$

$$l(P+I) = l(P-Q)+l(Q)+l(I)$$

Choose Q such that

1. Q can be easily bounded from below
2. $P-Q$ is sufficiently simplified to allow bounding above given cutoff.

First possibility: Let H be p.d. part of P, set

$$Q = x^t Hx$$

Then $l(Q)=0$. Removes all second order parts of P (!) Better yet:

$$Q_{x_0} = (x-x_0)^t H(x-x_0)$$

Allows to manipulate linear part. Works for ANY x_0 in domain. Still $l(Q_{x_0})=0$.

Which choices for x_0 are good?

The QFB Algorithm - Properties

Most critical case: near local minimizer, so H is the entire purely quadratic part of P.

Theorem: If x_0 is the (unique) minimizer of quadratic part of P on the domain of $P + I$, then the lower bound of the linear part of $(P - Q_{x_0})$ is zero. Furthermore, the lower bound of $(P - Q_{x_0})$, when evaluated with plain interval evaluation, is accurate to order 3 of the original domain box.

Proof: Follows readily from Kuhn-Tucker conditions. If x_0 inside, linear part vanishes completely. Otherwise, wlog if i-th component of x_0 is at left end, i-th partial there must be non-negative, so that we get non-negative contribution.

Remark: The closer x_0 is to the minimizer, the closer we are to order 3 cutoff.

Algorithm: (Third Order Cutoff Test). Let $x^{(n)}$ be a sequence of points that converges to the minimum x_0 of the convex quadratic part P_2 In step n, determine a bound of $(P - Q_{x_n})$ by interval evaluation, and assess whether the bound exceeds the cutoff threshold. If it does, reject the box and terminate; if it does not, proceed to the next point x_{n+1}.

The QMLoc Algorithm

Tool to generate efficient sequence $x^{(n)}$. Determine ”feasible descent direction”

$$g_i^{(n)} = \begin{cases} -\frac{\partial Q}{\partial x_i} & \text{if } x_i^{(n)} \text{ inside} \\ \min\left(-\frac{\partial Q}{\partial x_i}, 0\right) & \text{if } x_i^{(n)} \text{ on right} \\ \max\left(-\frac{\partial Q}{\partial x_i}, 0\right) & \text{if } x_i^{(n)} \text{ on left} \end{cases}$$

Now move in direction of $g^{(n)}$ until we hit box or quadratic minimum along line. Very fast to do, can change set of active constraints very quickly.

Result: Cheap iterative third order cutoff.

Use of QFB - Example

Let $f_1(x) = \frac{1}{2}x^t \cdot A_v \cdot x - A_v \cdot (a \cdot x) + \frac{1}{2}a^t \cdot A_v \cdot a$ with

$$A_v = \begin{pmatrix} 2 & 3 & \dots & 3 \\ -1 & 2 & \dots & 3 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \dots & 2 \end{pmatrix}$$

known to be p.d. with minimum a. Choose a random vector a, and 5^v boxes around it. Check box rejection with Interval evaluation, Centered Form, QFB. Output average number of QFB iterations.

Use of QFB - Example

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```
v     N=5^v     NI         NC    NQFB Avg. Iter
2        25        25         8   1      1.1
4       625       625       308   1     0.31
```

Use of QFB - Example

Let $f_1(x) = \frac{1}{2}x^t \cdot A_v \cdot x - A_v \cdot (a \cdot x) + \frac{1}{2}a^t \cdot A_v \cdot a$ with

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 4       625        625        308   1      0.31
 6    15,625     15,625     12,434   1      0.31
 8   390,625    390,625    372,376   1      0.43
10 9,765,625 9,765,625 9,622,750   1      0.55
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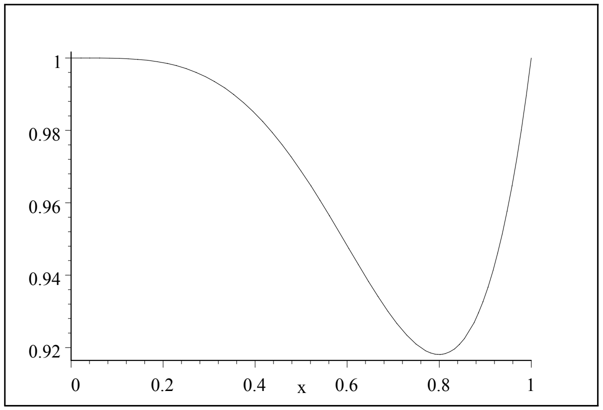
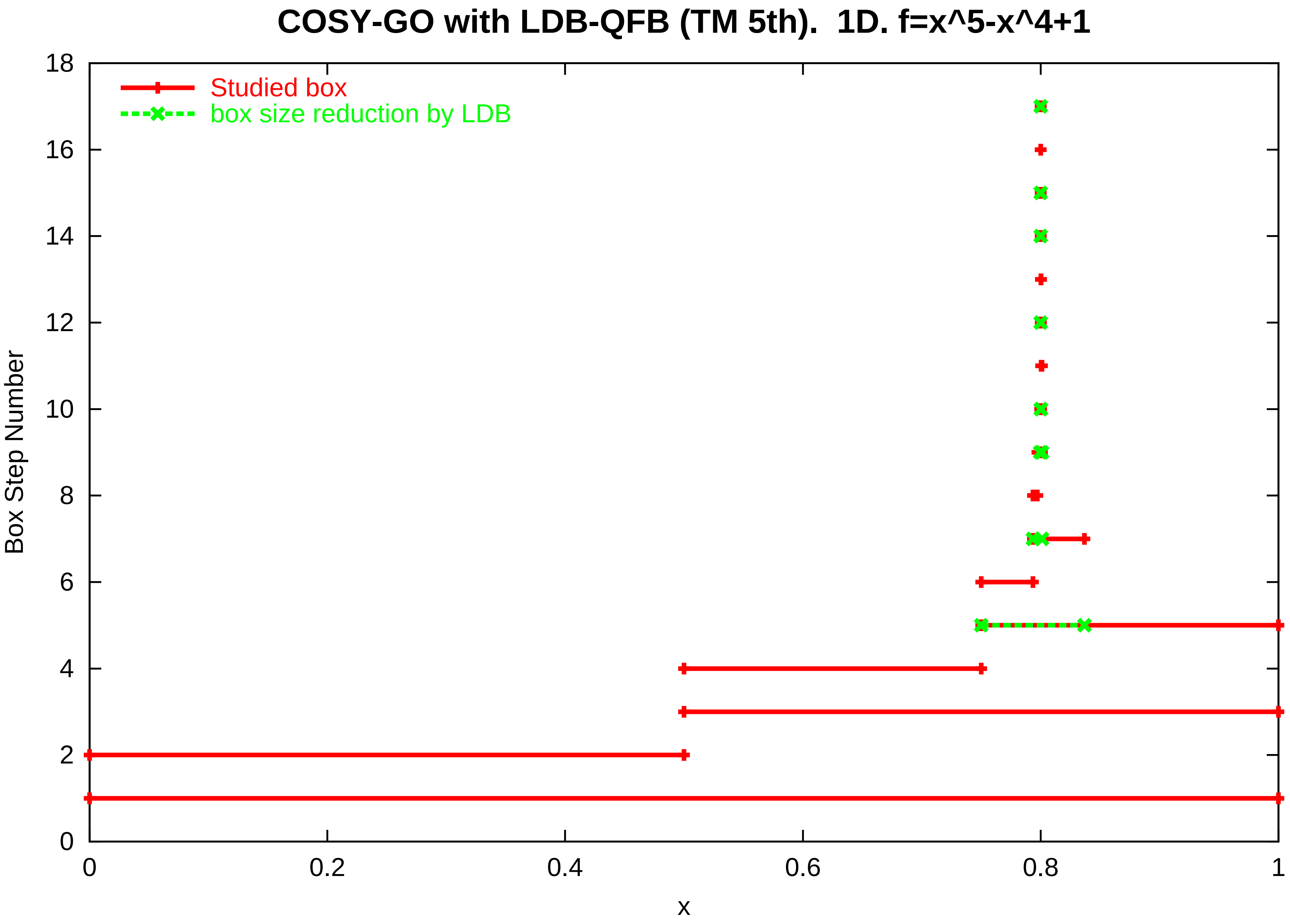
Moore's Simple 1D Function

$$f(x) = 1 + x^5 - x^4.$$

Study on $[0, 1]$. Trivial-looking, but dependency and high order. Assumes shallow min at 0.8.




COSY-GO with LDB-QFB (TM 5th). 1D. f=x^5-x^4+1
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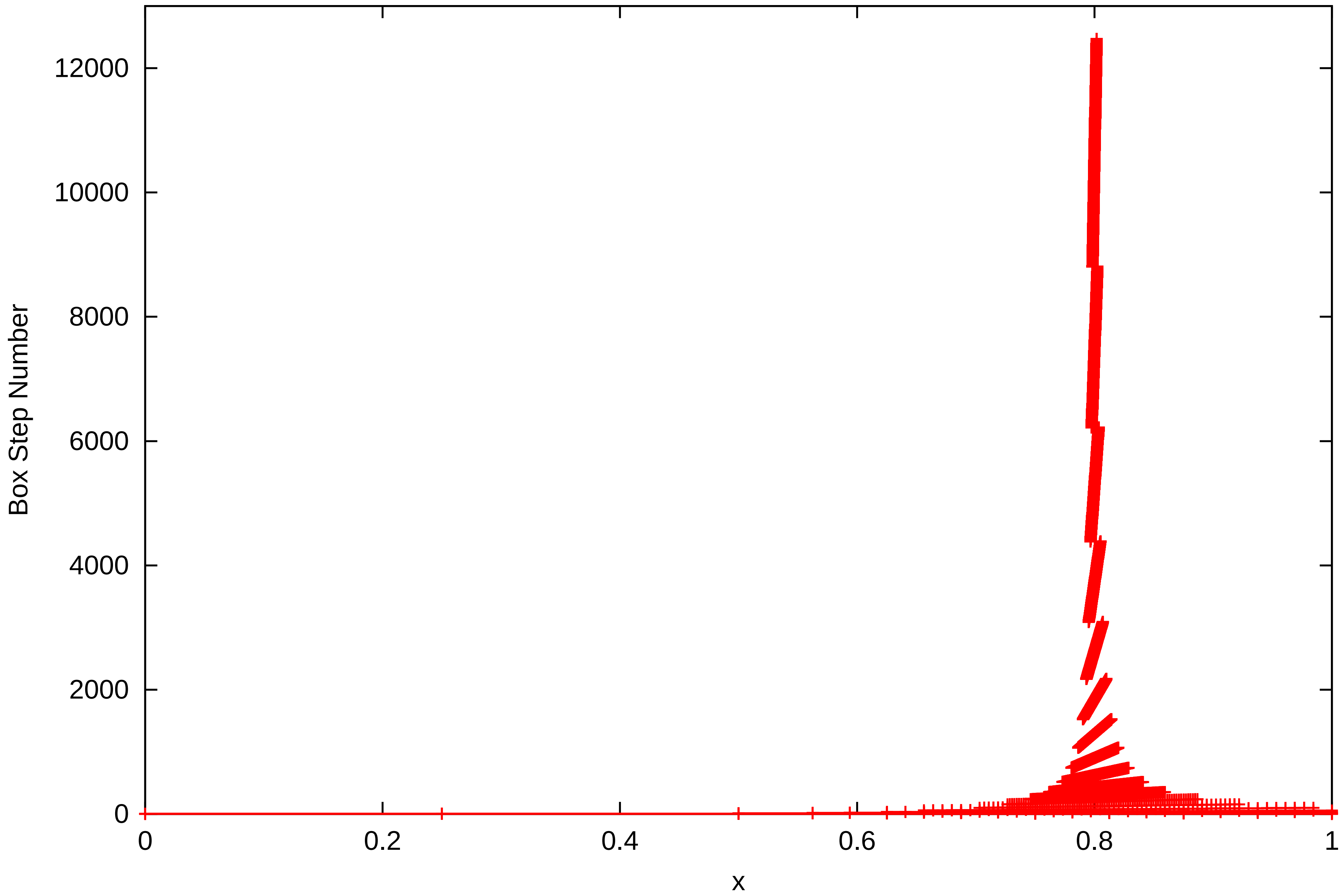
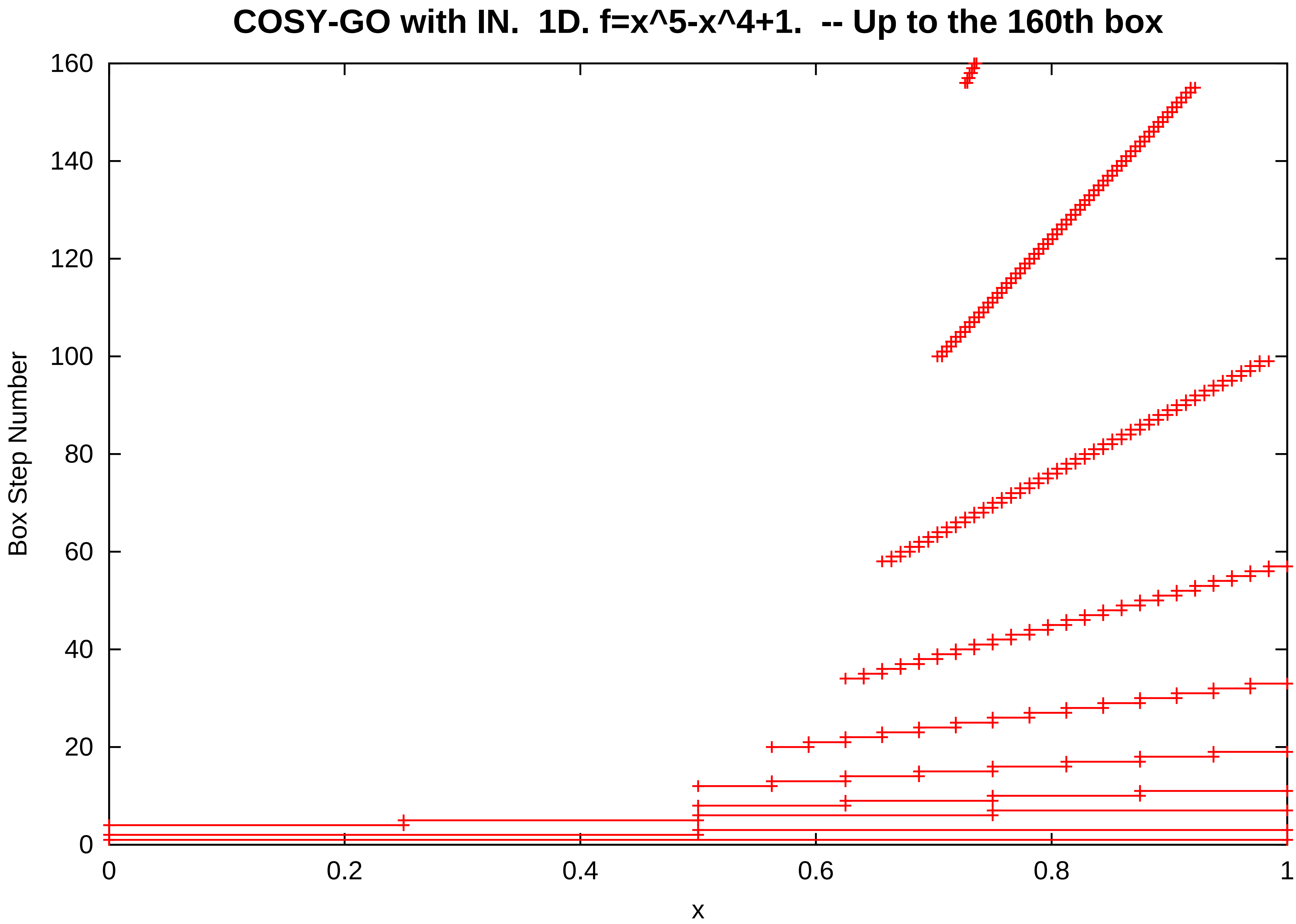
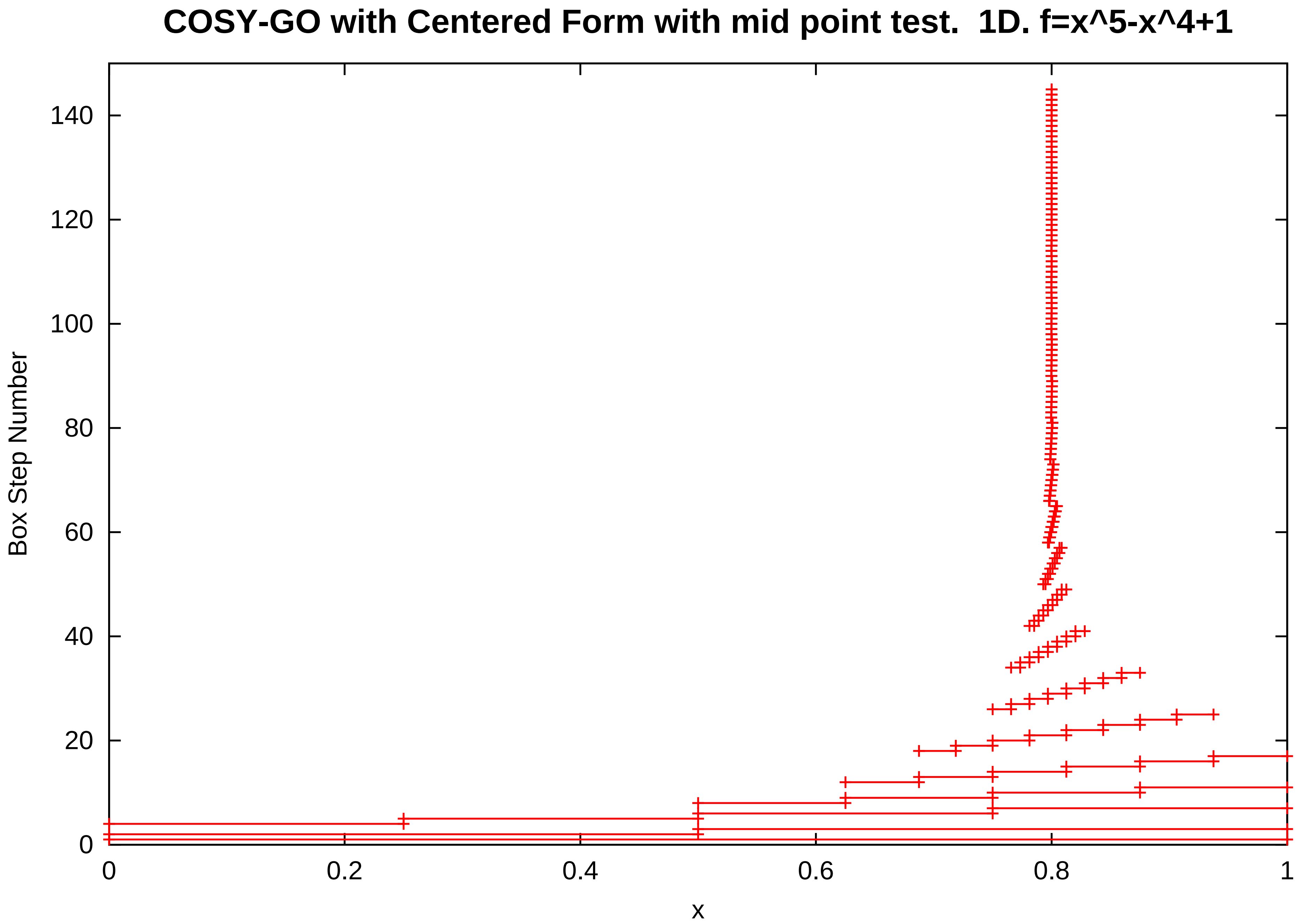
16
18
0
0.2
0.4
0.6
0.8
1

COSY-GO with naive IN with mid point test. 1D. f=x^5-x^4+1




COSY-GO with IN. 1D. f=x^5-x^4+1. -- Up to the 160th box
Box Step Number
0
20
40
60
80
100
120
140
160
0
0.2
0.4
0.6
0.8
1
x


COSY-GO with Centered Form with mid point test. 1D. f=x^5-x^4+1
Box Step Number
0
20
40
60
80
100
120
140
x
0
0.2
0.4
0.6
0.8
1

Beale's 2D and 4D Function

$$f(x_1, x_2) = (1.5 - x_1(1 - x_2))^2 + \big(2.25 - x_1(1 - x_2^2)\big)^2 + \big(2.625 - x_1(1 - x_2^3)\big)^2$$

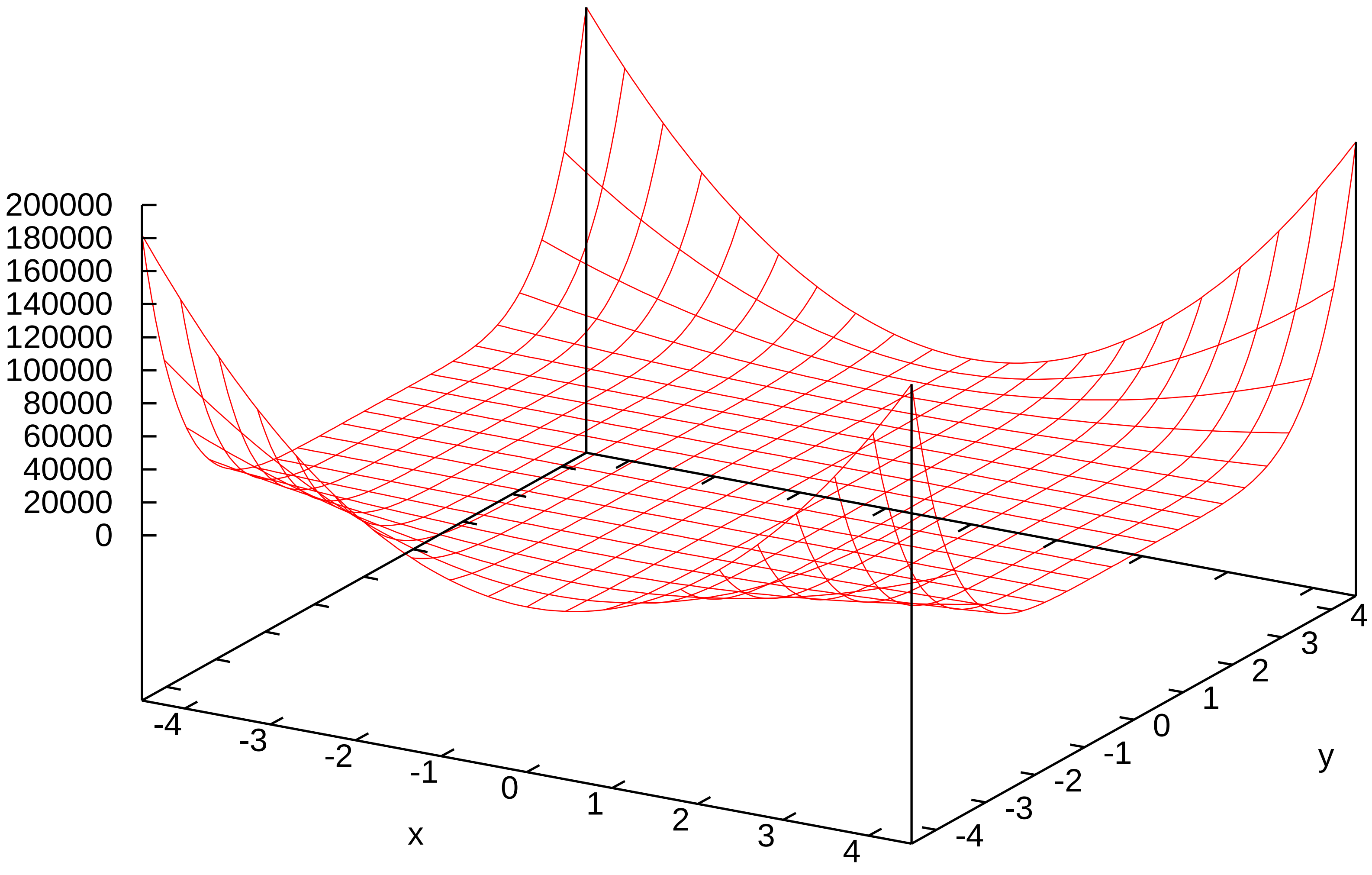
Domain $[-4.5, 4.5]^2$. Minimum value 0 at $(3, 0.5)$.

Little dependency, but tricky very shallow behavior.
Generalization to 4D:

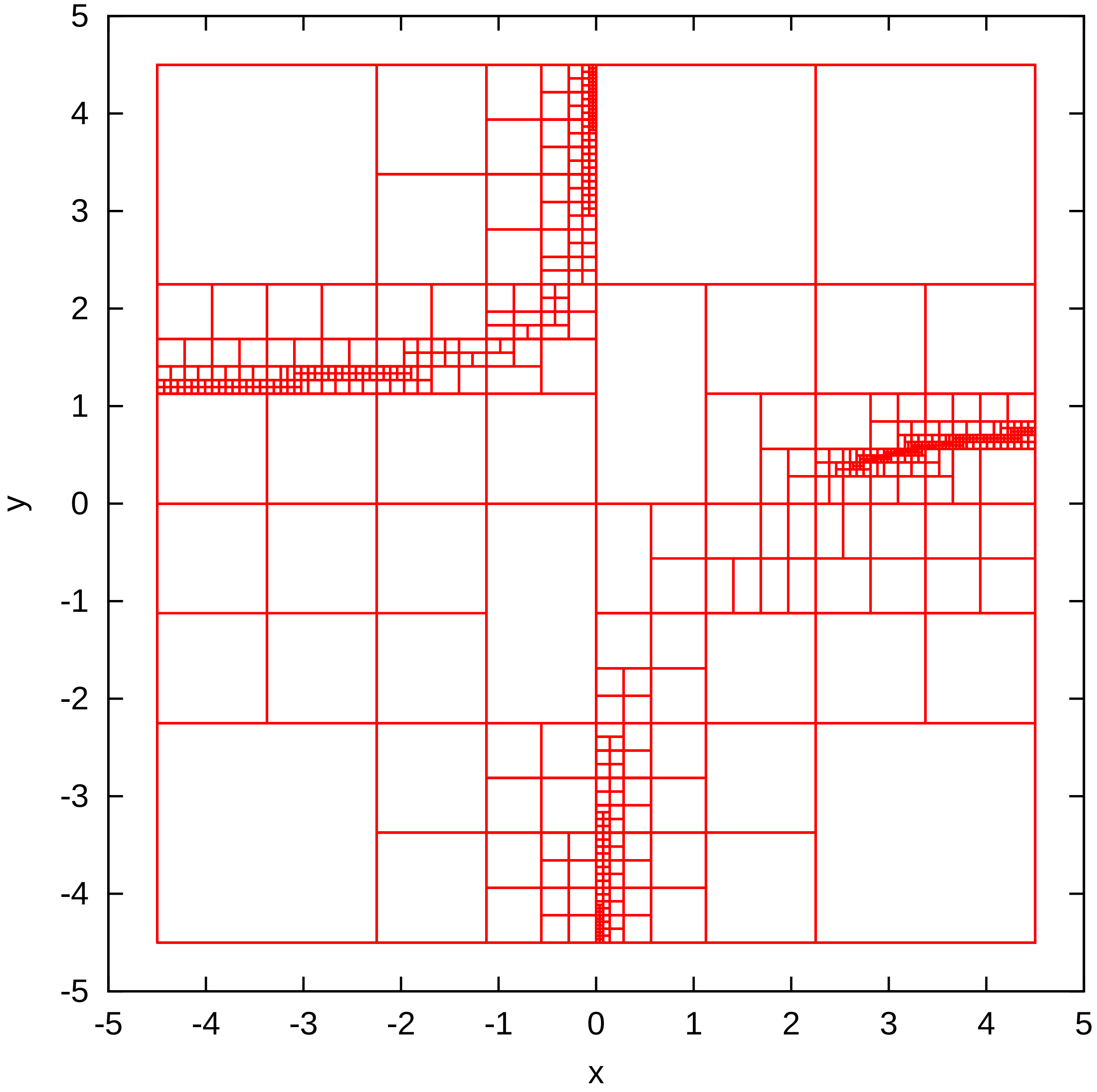
$$\begin{aligned} f(x_1, x_2, x_3, x_4) = {} & (1.5 - x_1(1 - x_2))^2 + \big(2.25 - x_1(1 - x_2^2)\big)^2 + \big(2.625 - x_1(1 - x_2^3)\big) \\ & + (1 + x_3(1 - x_4))^2 + \big(3 + x_3(1 - x_4^2)\big)^2 + \big(7 + x_3(1 - x_4^3)\big)^2 \\ & + (3 + x_1(1 - x_4))^2 + \big(9 + x_1(1 - x_4^2)\big)^2 + \big(21 + x_1(1 - x_4^3)\big)^2 \\ & + (0.5 - x_3(1 - x_2))^2 + \big(0.75 - x_3(1 - x_2^2)\big)^2 + \big(0.875 - x_3(1 - x_2^3)\big) \end{aligned}$$

Domain $[0, 4]^4$. Minimum value 0 at $(3, 0.5, 1, 2)$

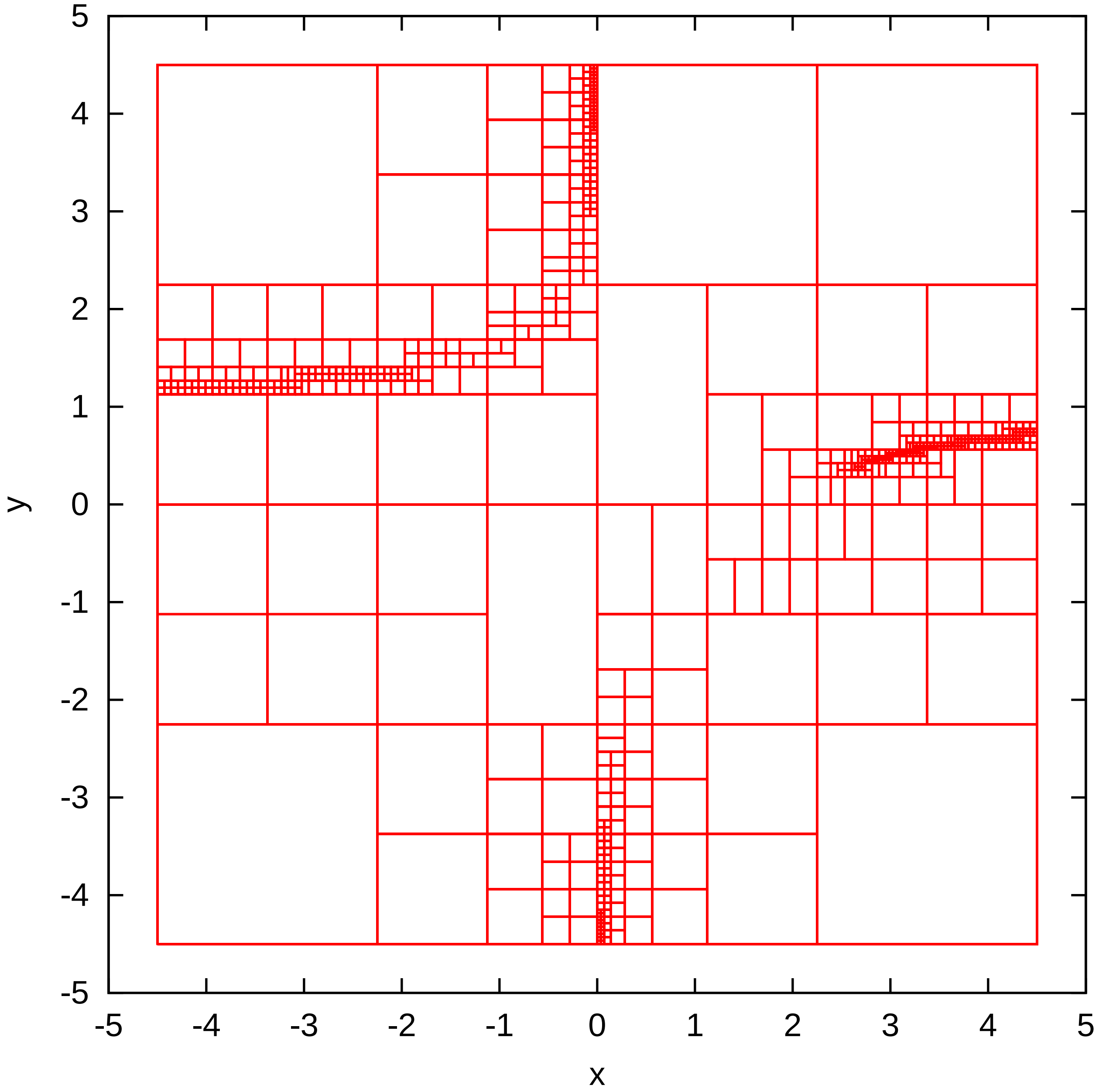
The Beale function. f = [1.5-x(1-y)]^2 + [2.25-x(1-y^2)]^2 + [2.625-x(1-y^3)]^2

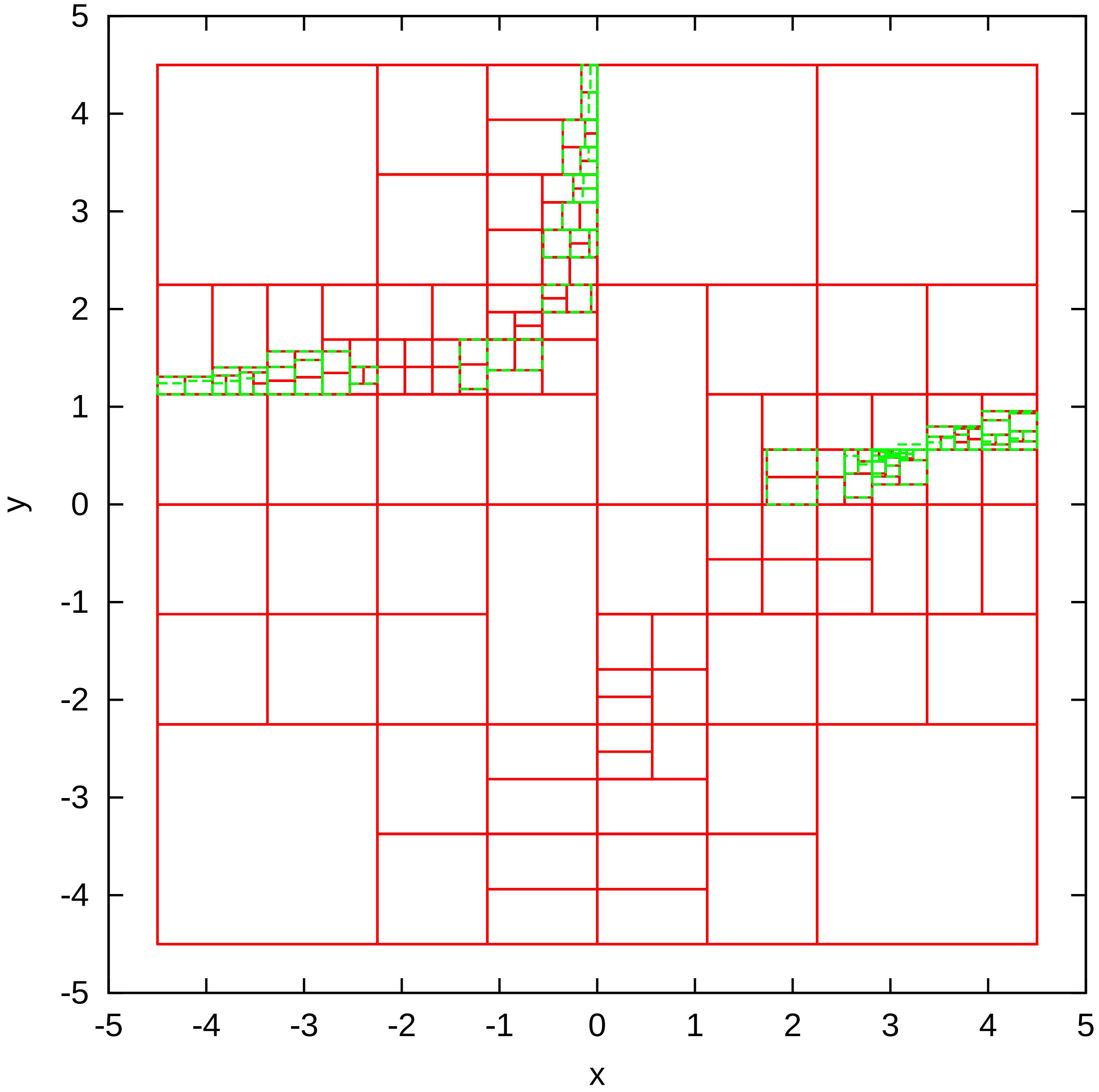


COSY-GO with IN. The Beale function



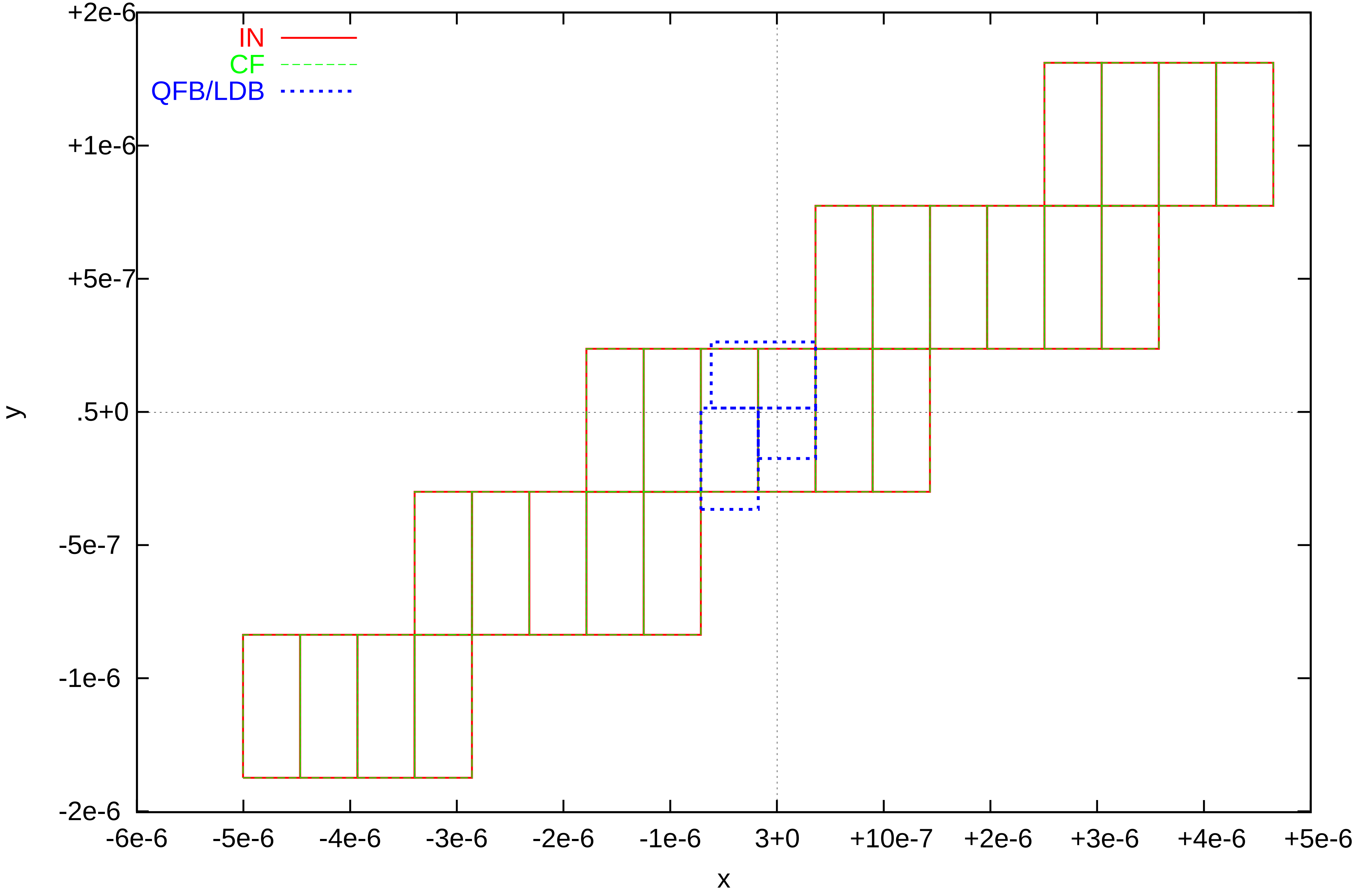
COSY-GO with CF. The Beale function

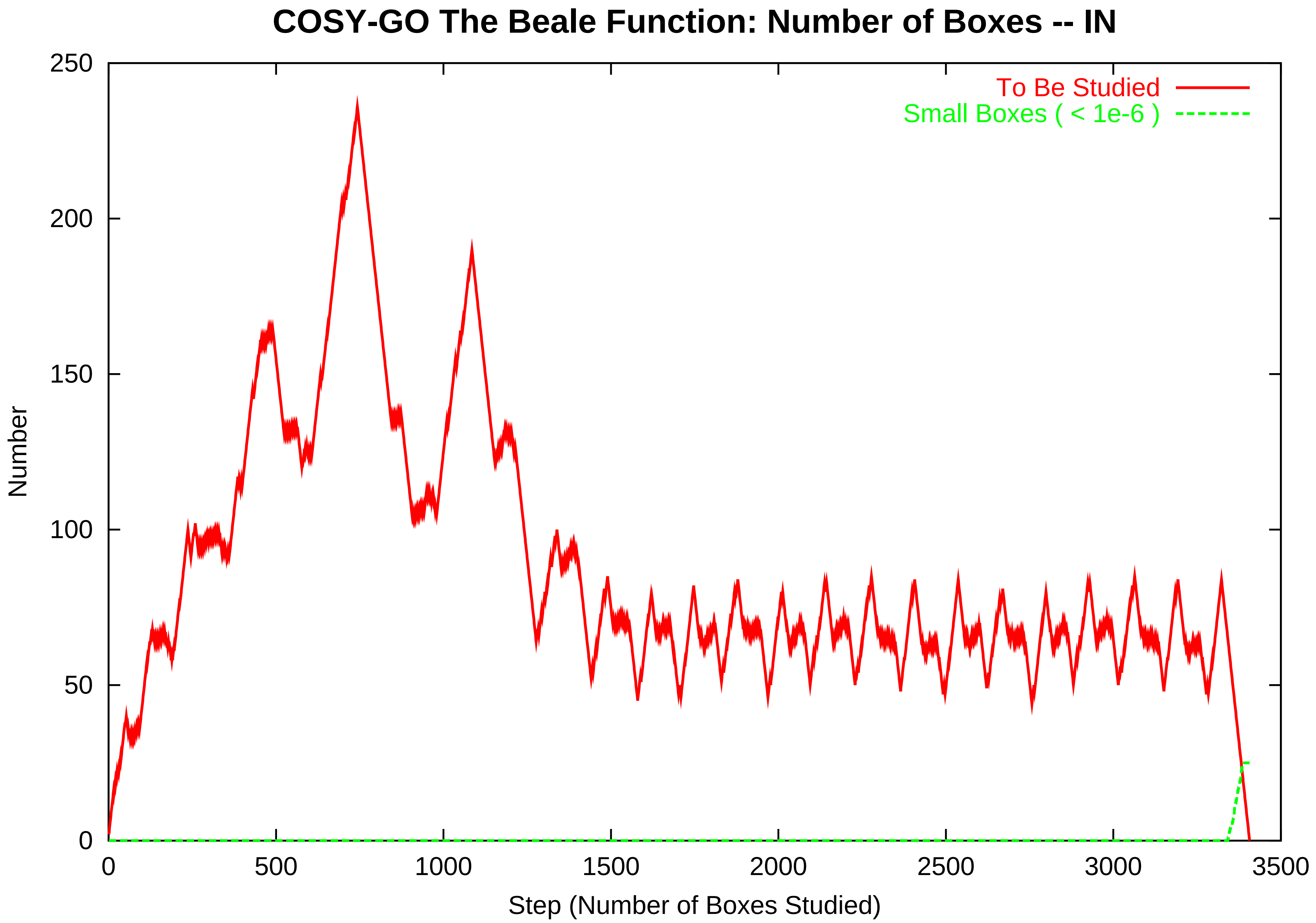


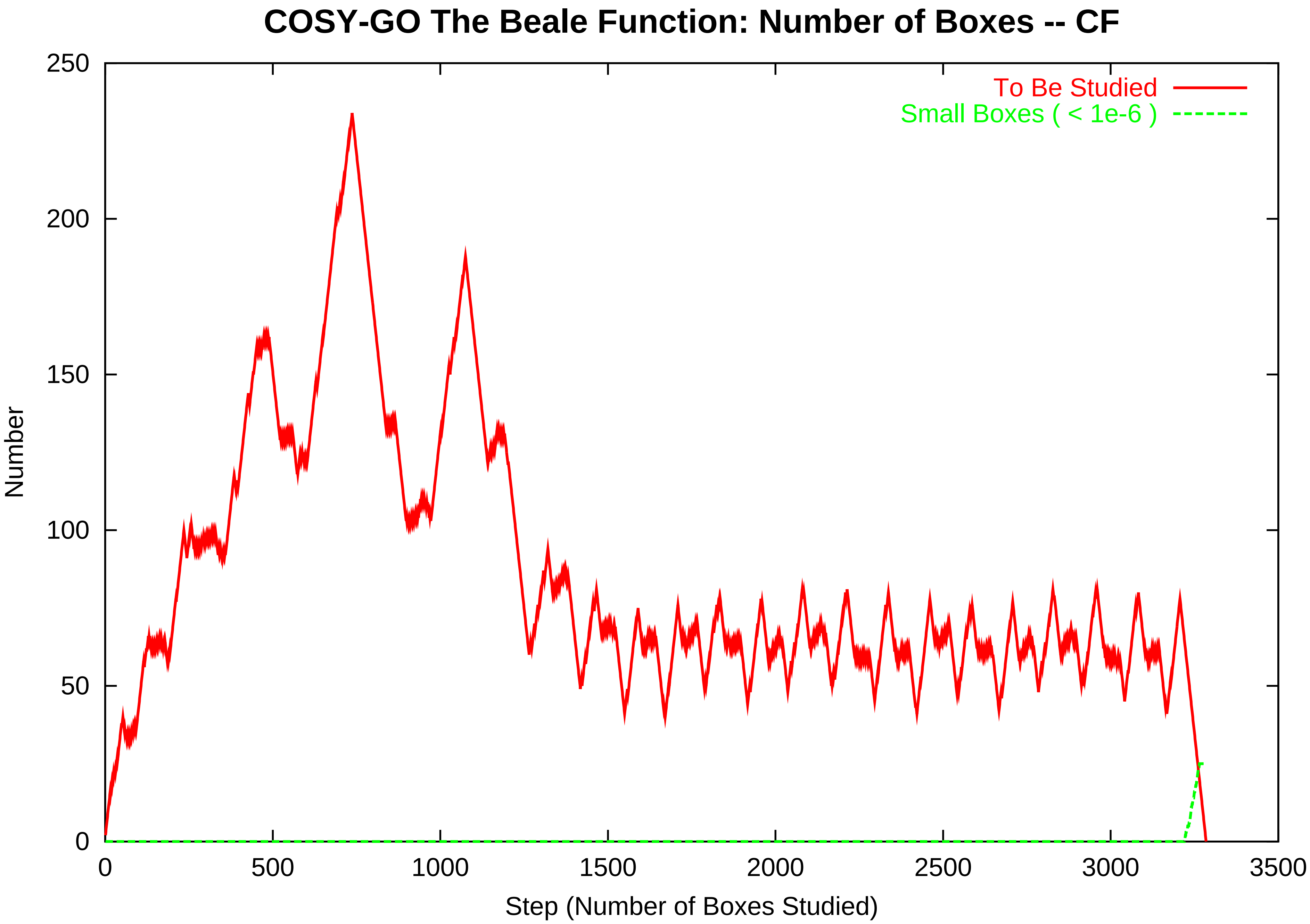


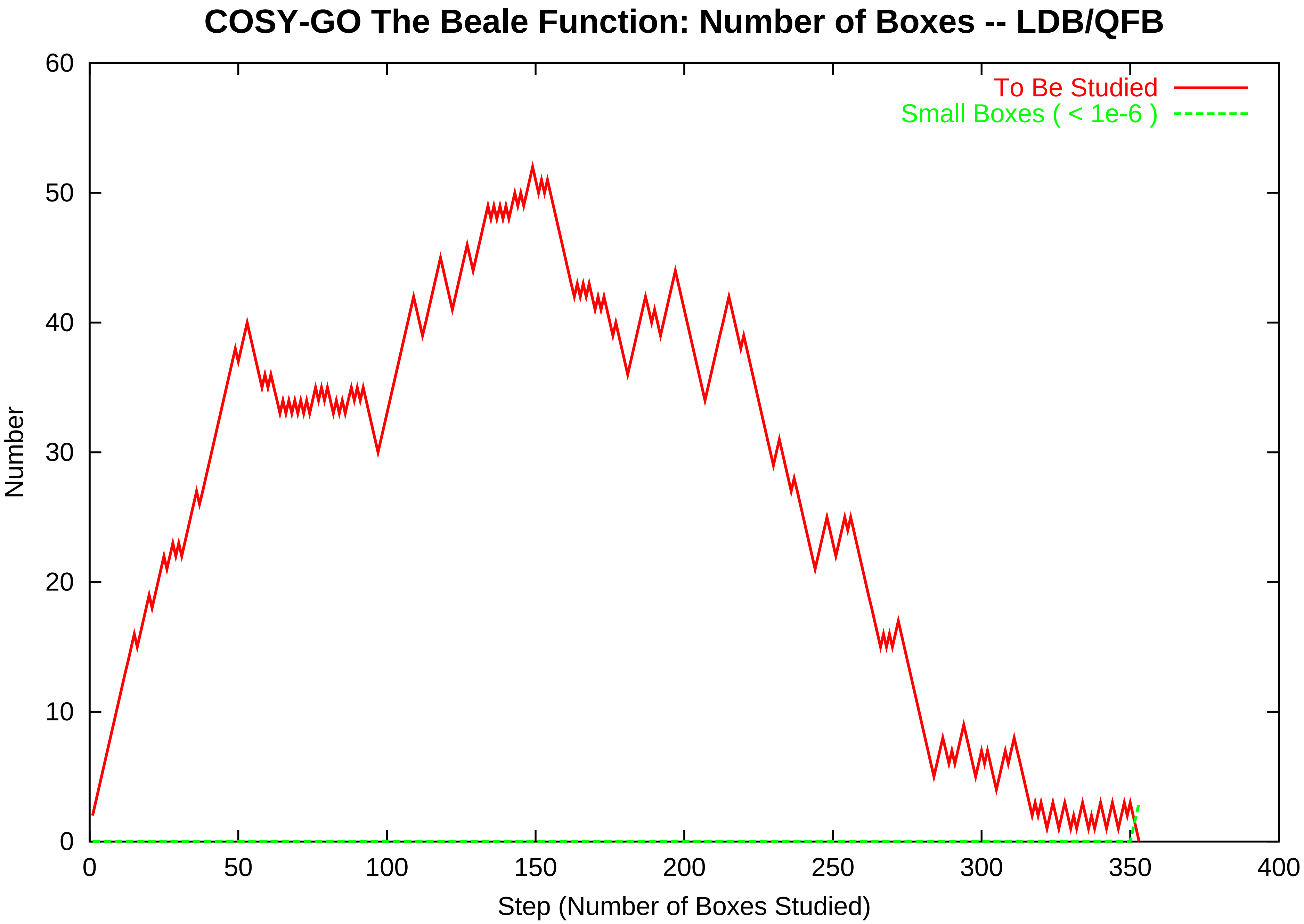
COSY-GO with LDB/QFB. The Beale function

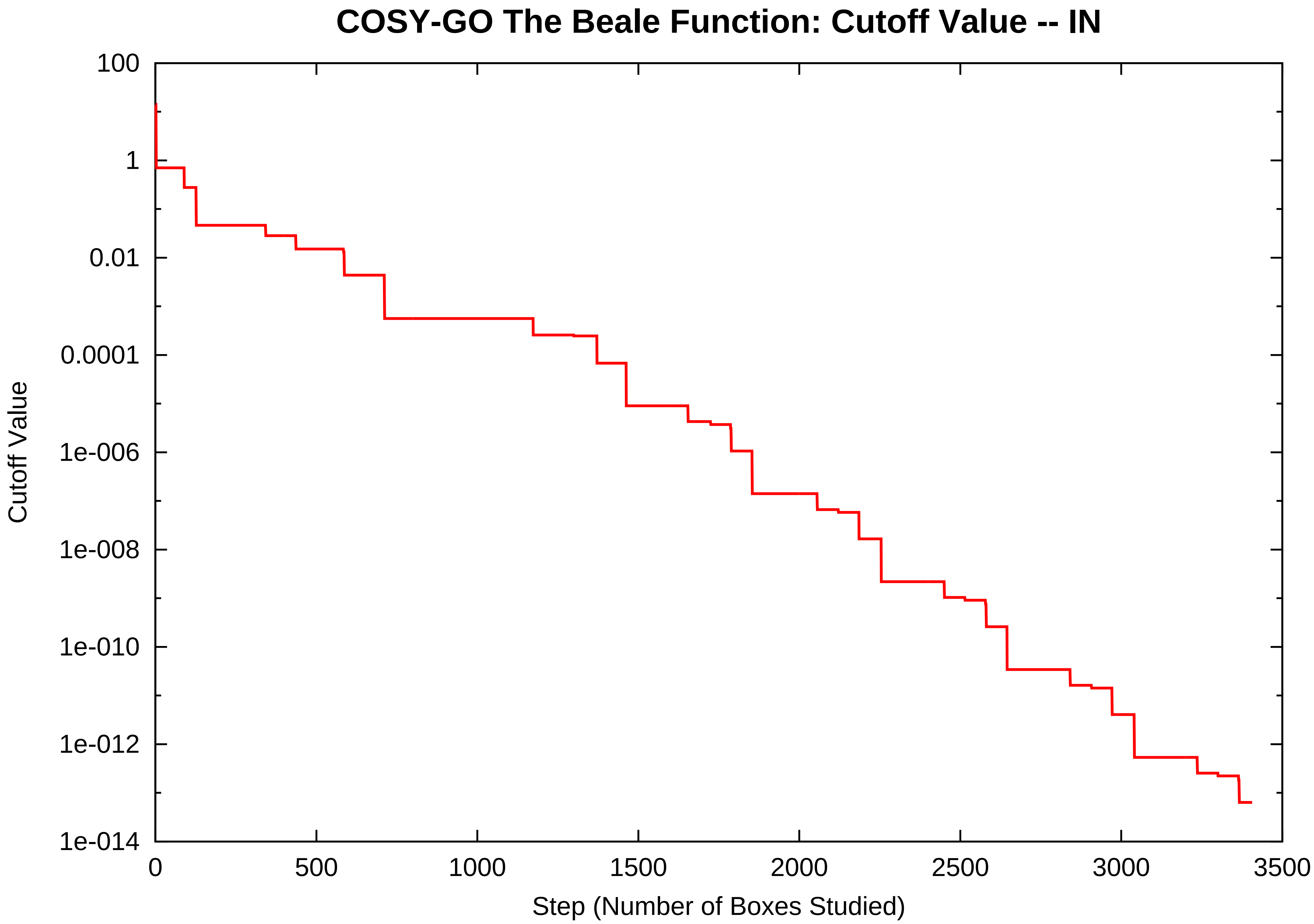
COSY-GO. The Beale function. Remaining Boxes (< 1e-6) around (3,0.5)

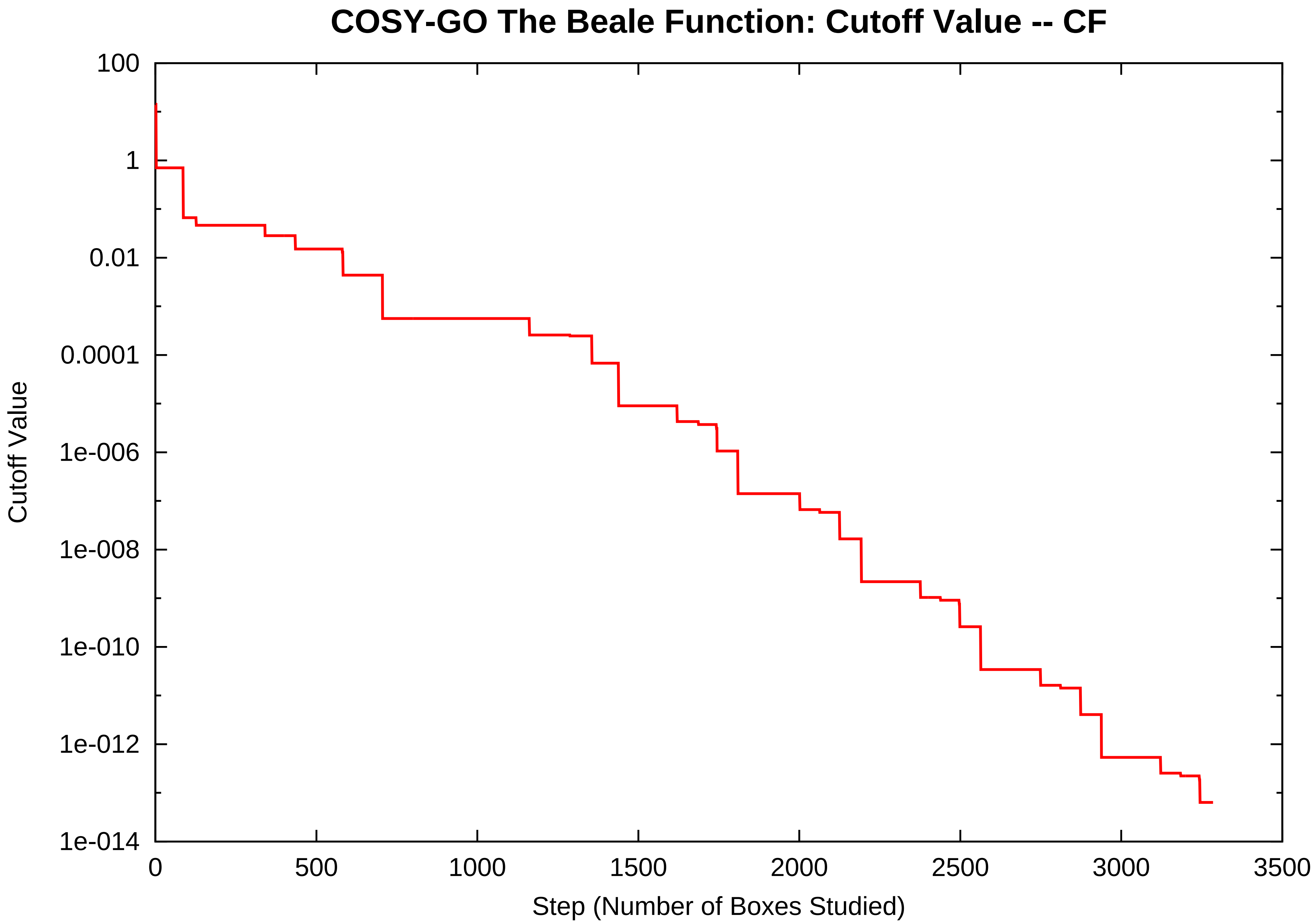


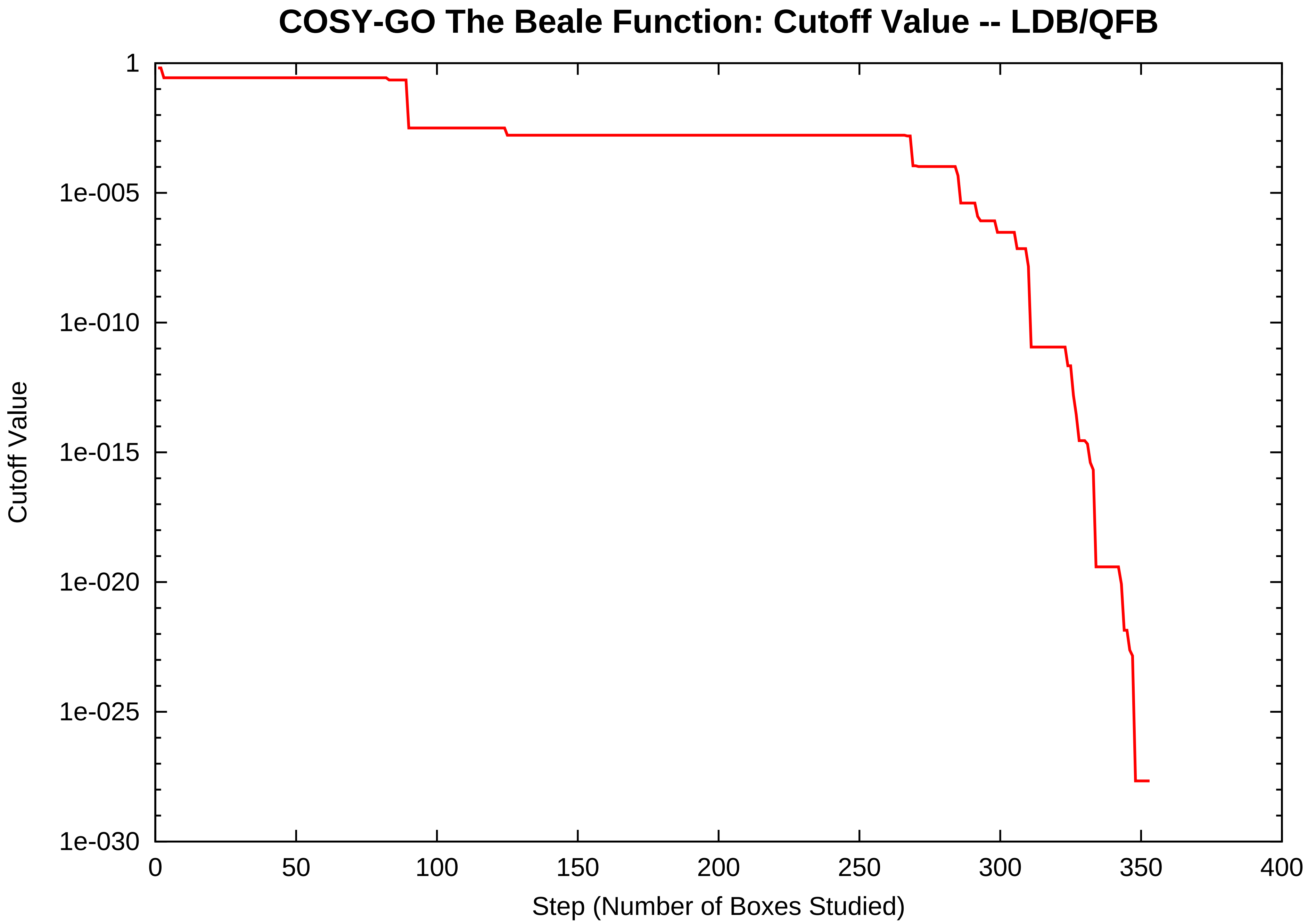

COSY-GO The Beale Function: Number of Boxes -- IN
To Be Studied
Small Boxes (< 1e-6)
Number
250
200
150
100
50
0
0
500
1000
1500
2000
2500
3000
3500
Step (Number of Boxes Studied)

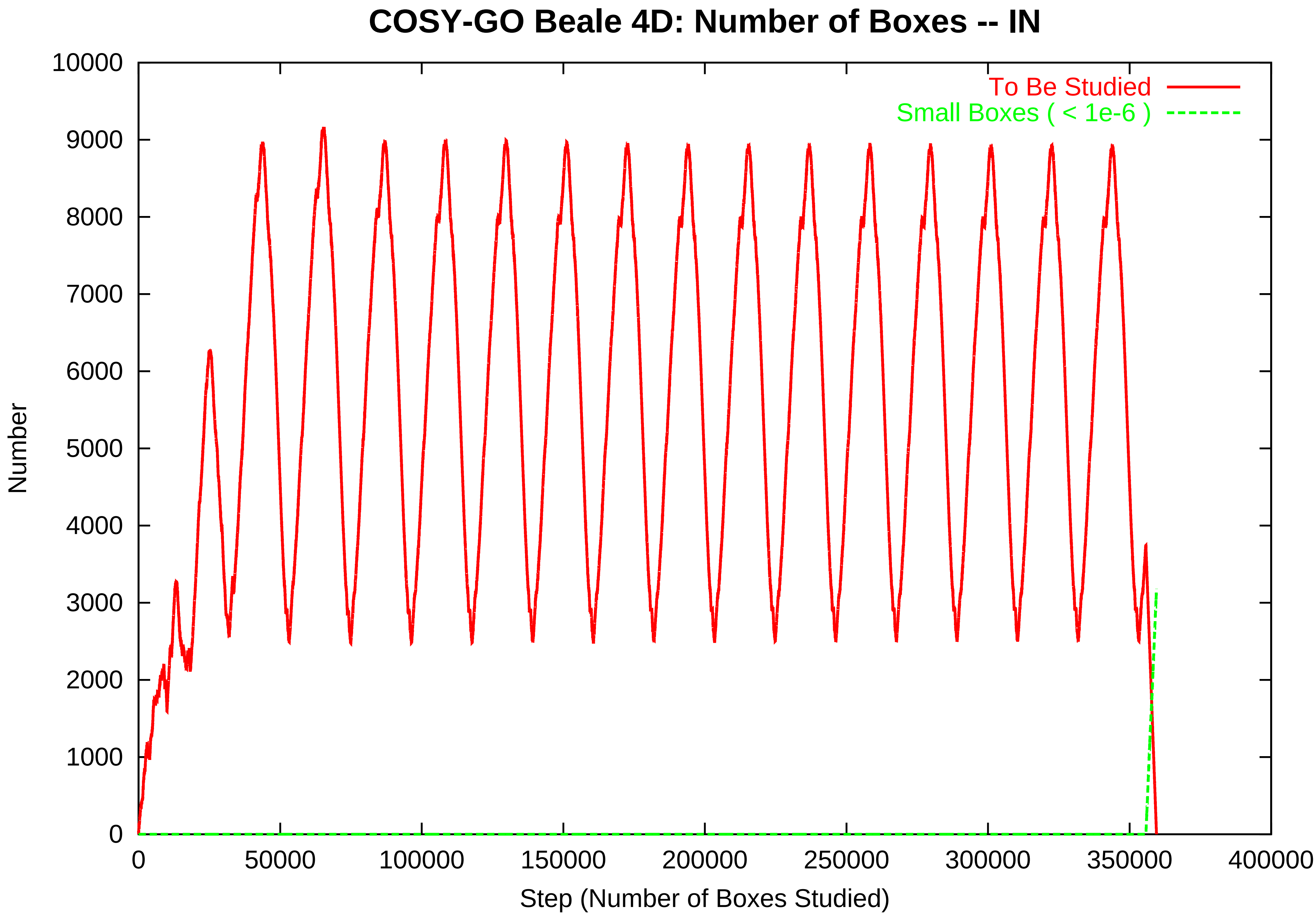

COSY-GO The Beale Function: Number of Boxes -- CF
To Be Studied
Small Boxes (< 1e-6)
Number
Step (Number of Boxes Studied)
0
50
100
150
200
250
0
500
1000
1500
2000
2500
3000
3500

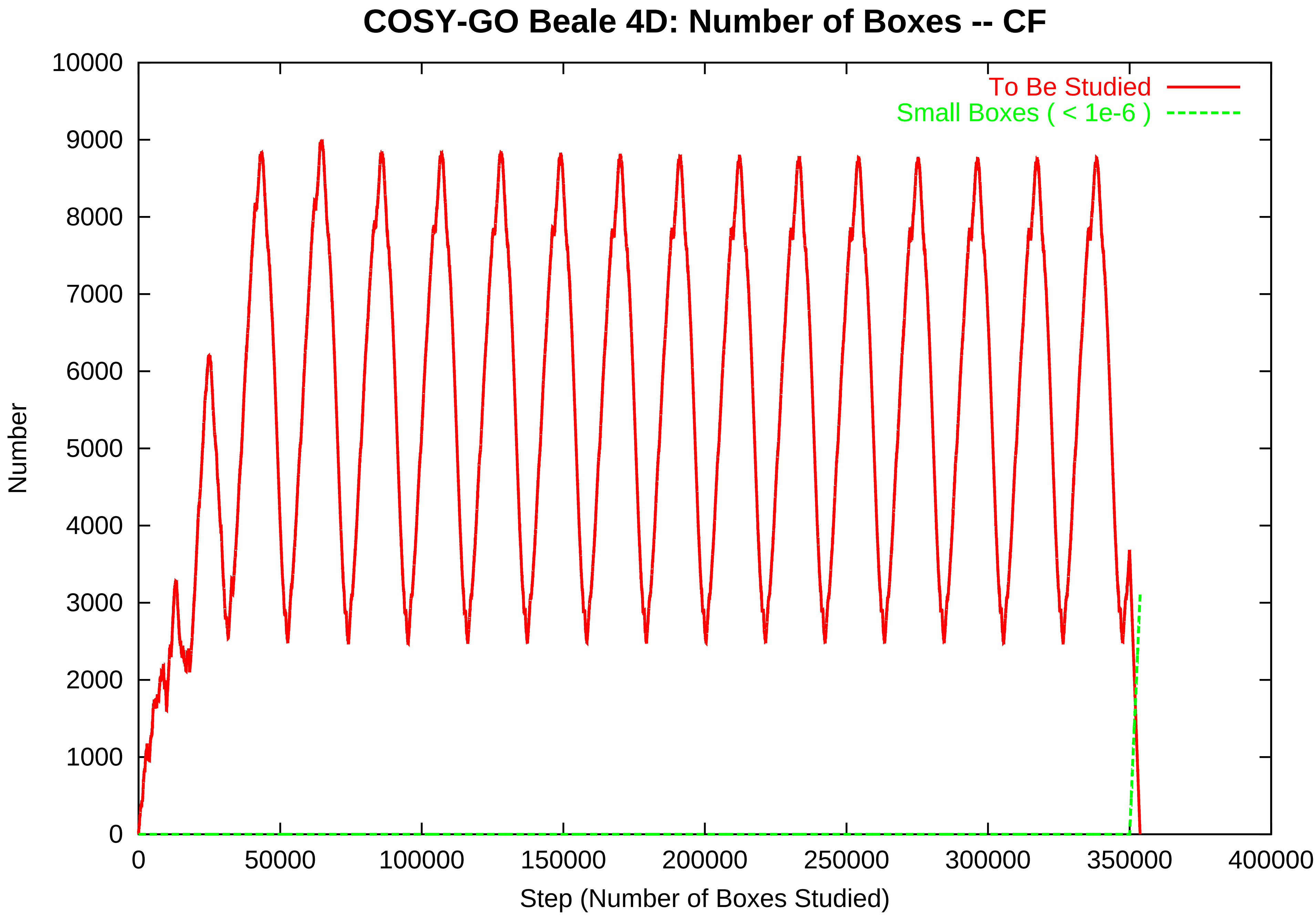

COSY-GO The Beale Function: Number of Boxes -- LDB/QFB
To Be Studied
Small Boxes (< 1e-6)
Number
0
10
20
30
40
50
60
0
50
100
150
200
250
300
350
400
Step (Number of Boxes Studied)

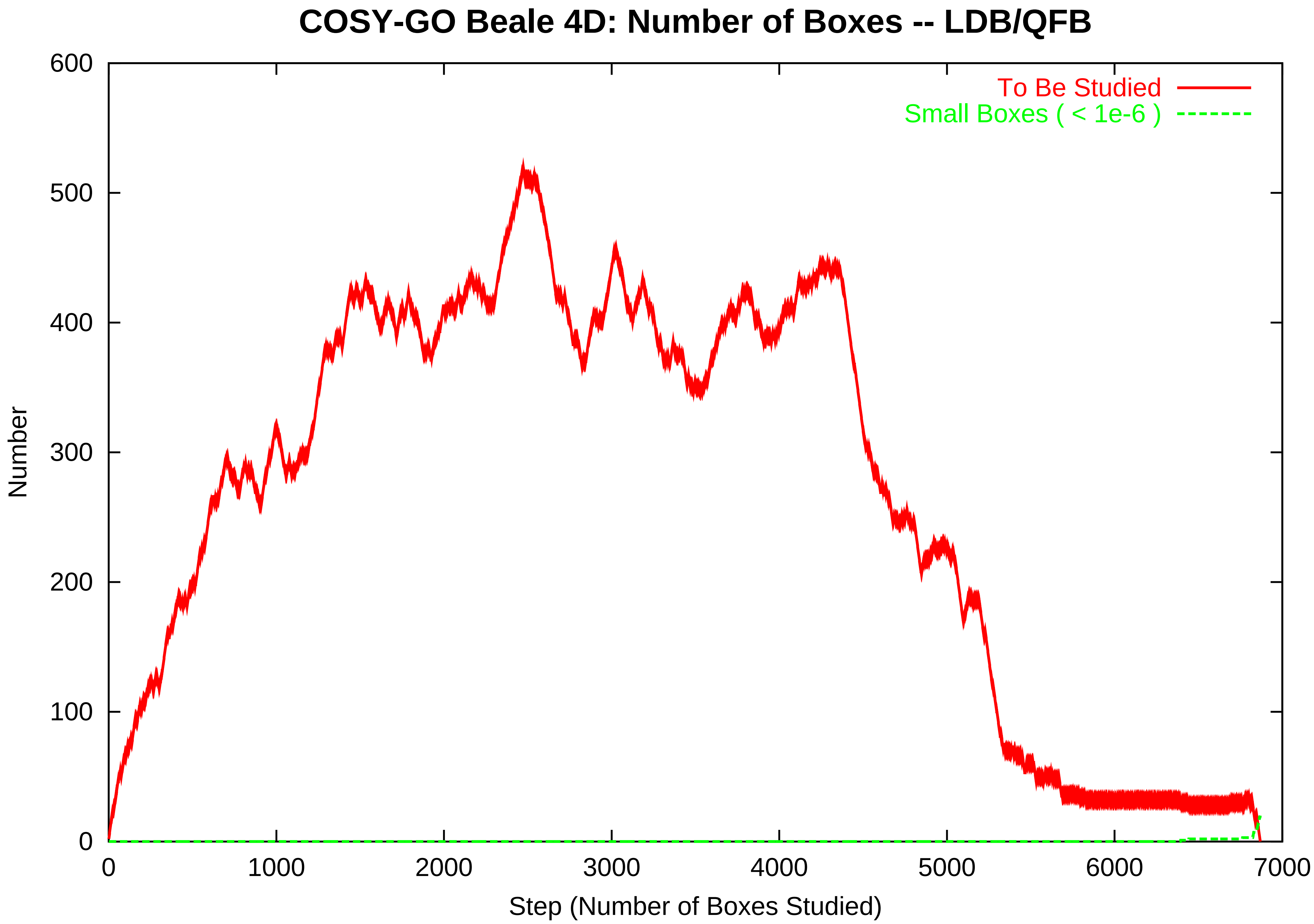

COSY-GO The Beale Function: Cutoff Value -- IN
Cutoff Value
100
1
0.01
0.0001
1e-006
1e-008
1e-010
1e-012
1e-014
0
500
1000
1500
2000
2500
3000
3500
Step (Number of Boxes Studied)

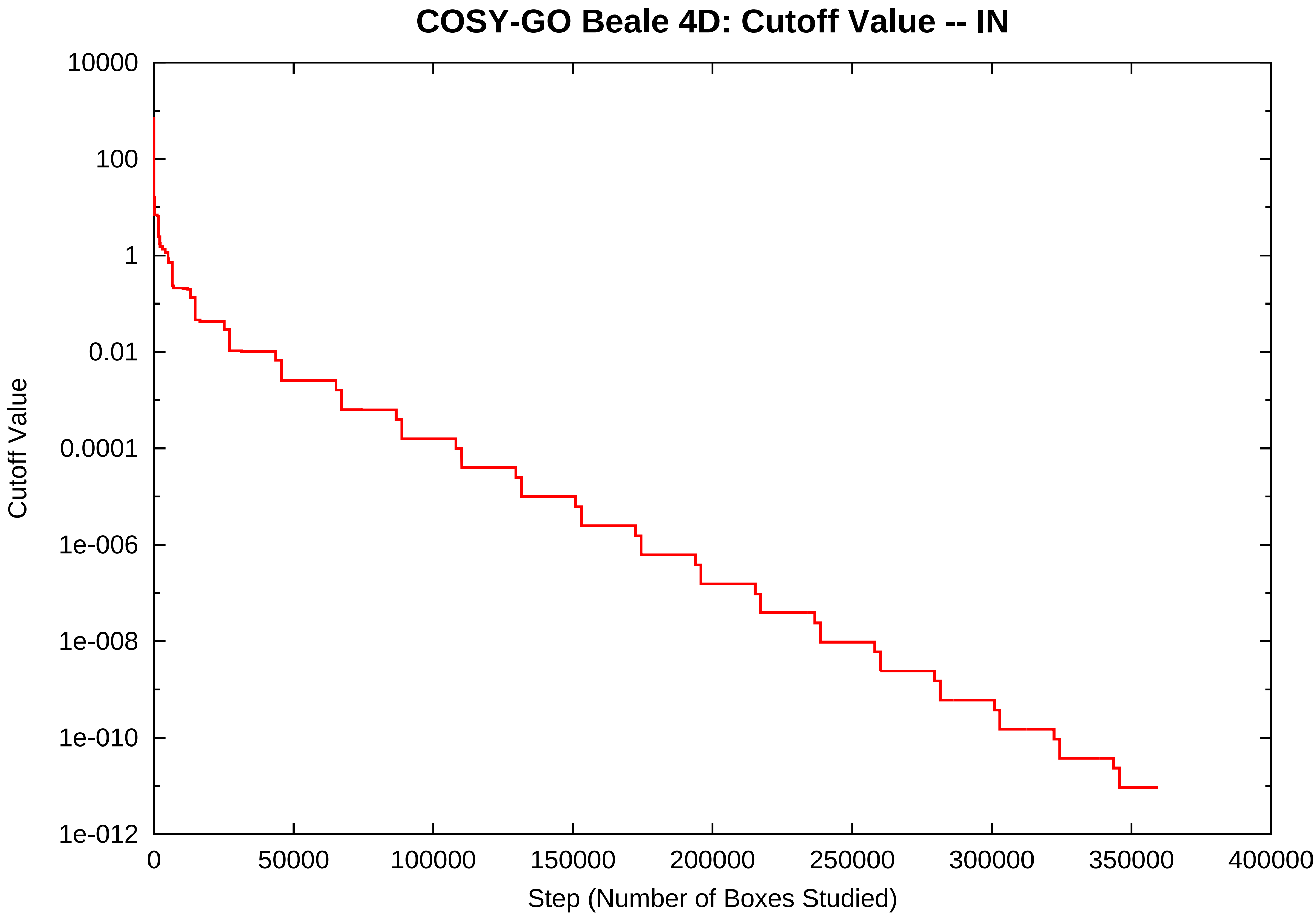

COSY-GO The Beale Function: Cutoff Value -- CF
Cutoff Value
Step (Number of Boxes Studied)
100
1
0.01
0.0001
1e-006
1e-008
1e-010
1e-012
1e-014
0
500
1000
1500
2000
2500
3000
3500

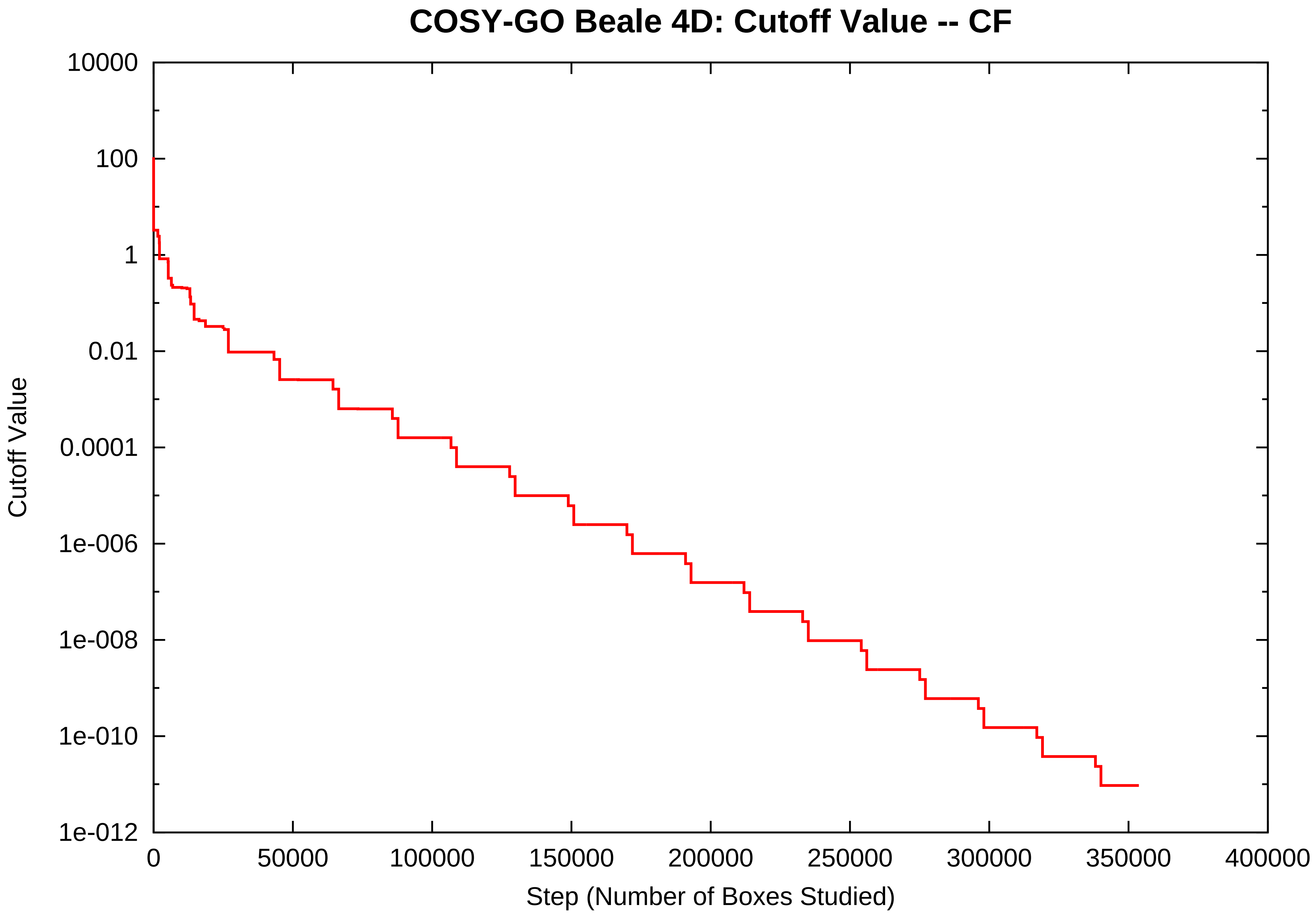

COSY-GO The Beale Function: Cutoff Value -- LDB/QFB
Cutoff Value
1
1e-005
1e-010
1e-015
1e-020
1e-025
1e-030
0
50
100
150
200
250
300
350
400
Step (Number of Boxes Studied)

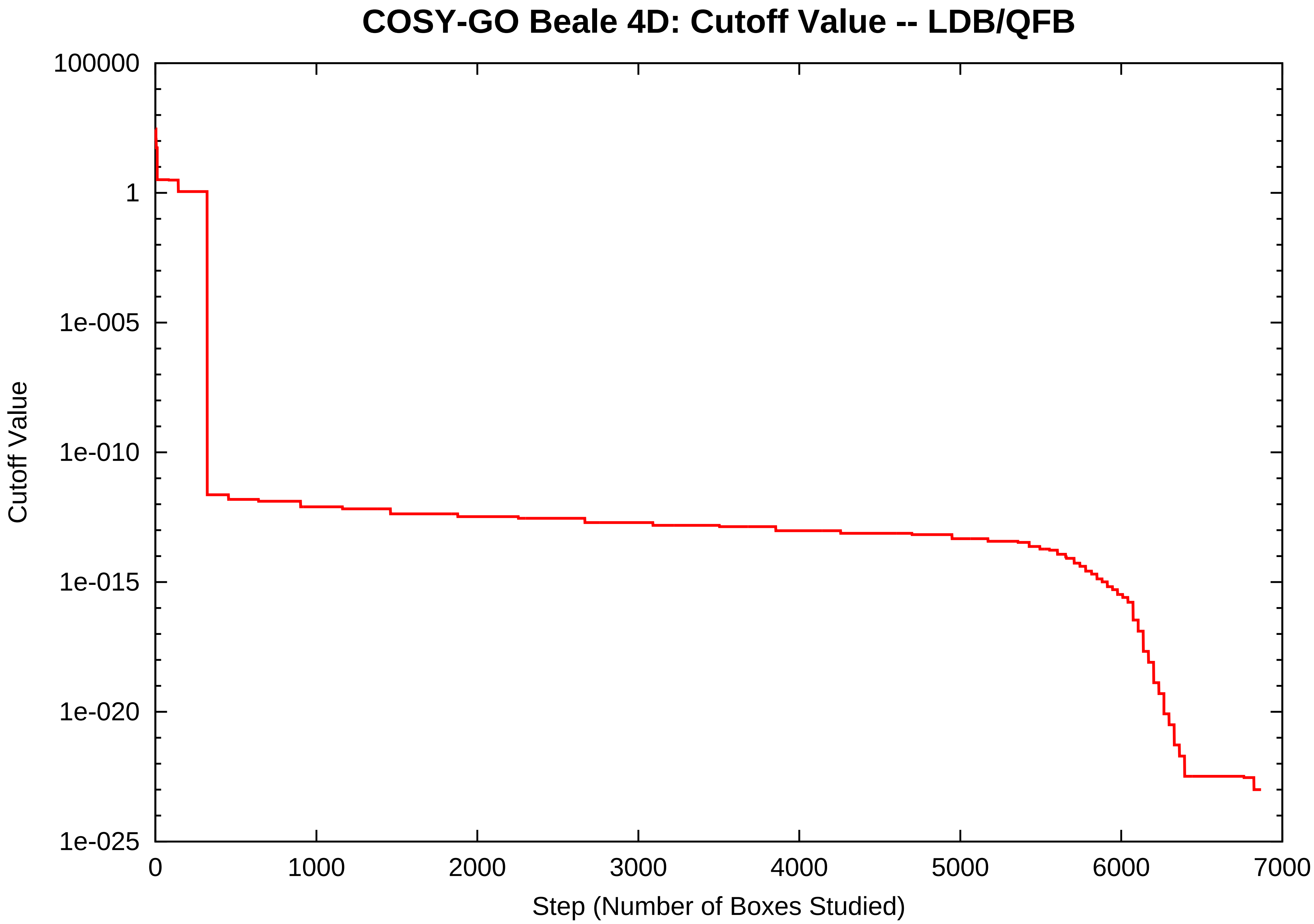

COSY-GO Beale 4D: Number of Boxes -- IN
To Be Studied
Small Boxes (< 1e-6)
Number
Step (Number of Boxes Studied)
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
0
50000
100000
150000
200000
250000
300000
350000
400000


COSY-GO Beale 4D: Number of Boxes -- CF
To Be Studied
Small Boxes (< 1e-6)
Number
Step (Number of Boxes Studied)
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
0
50000
100000
150000
200000
250000
300000
350000
400000


COSY-GO Beale 4D: Number of Boxes -- LDB/QFB
To Be Studied
Small Boxes (< 1e-6)
Number
0
100
200
300
400
500
600
0
1000
2000
3000
4000
5000
6000
7000
Step (Number of Boxes Studied)


COSY-GO Beale 4D: Cutoff Value -- IN
10000
100
1
0.01
0.0001
1e-006
1e-008
1e-010
1e-012
Cutoff Value
0
50000
100000
150000
200000
250000
300000
350000
400000
Step (Number of Boxes Studied)

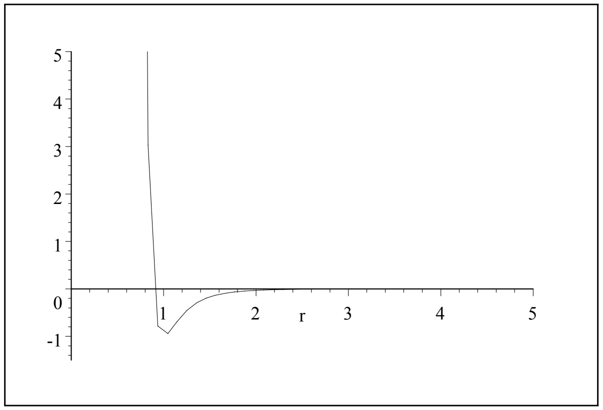

COSY-GO Beale 4D: Cutoff Value -- CF
Cutoff Value
10000
100
1
0.01
0.0001
1e-006
1e-008
1e-010
1e-012
0
50000
100000
150000
200000
250000
300000
350000
400000
Step (Number of Boxes Studied)


COSY-GO Beale 4D: Cutoff Value -- LDB/QFB
Cutoff Value
100000
1
1e-005
1e-010
1e-015
1e-020
1e-025
0
1000
2000
3000
4000
5000
6000
7000
Step (Number of Boxes Studied)

Lennard-Jones Potentials

Ensemble of n particles interacting pointwise with potentials

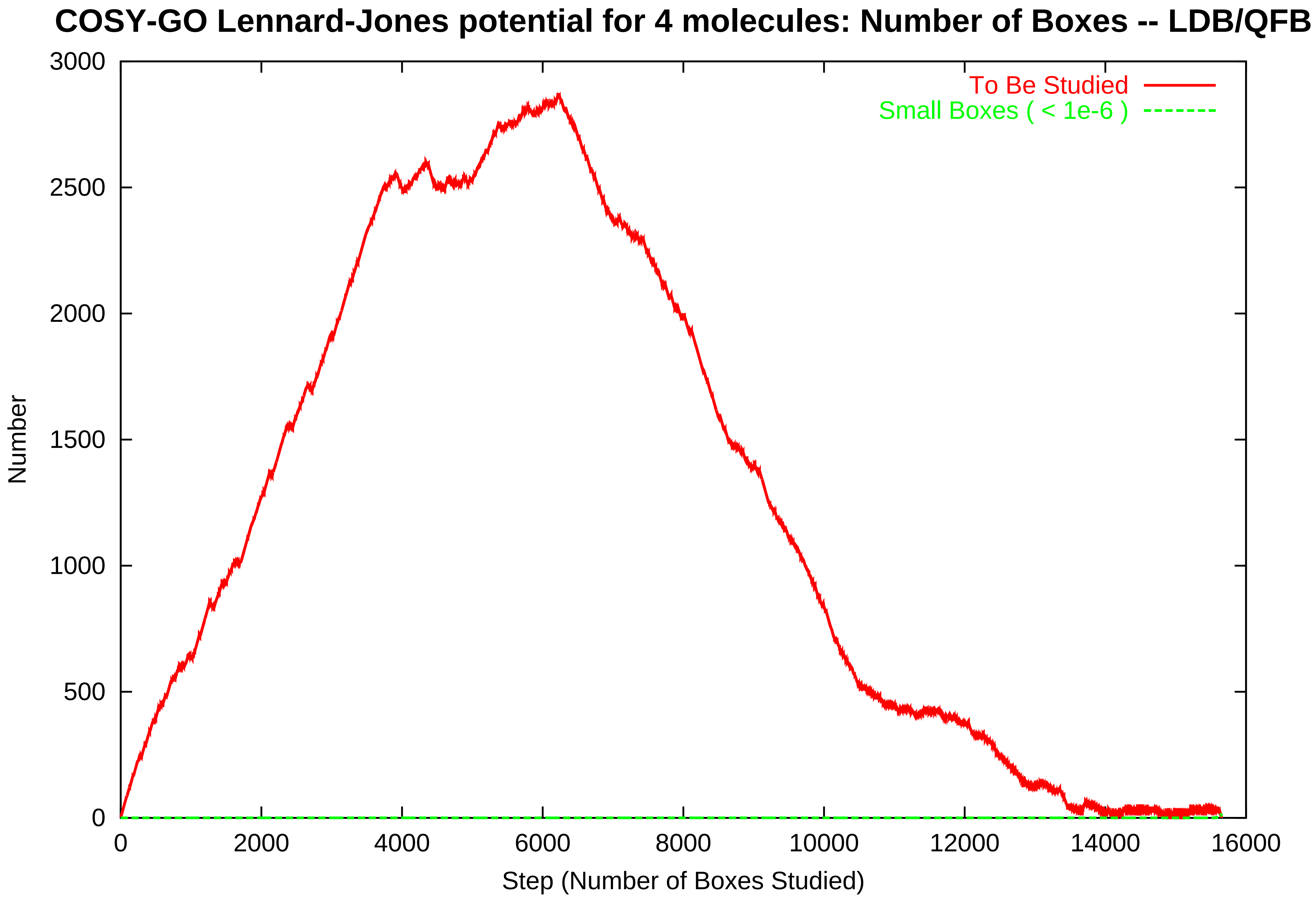
$$V_{LJ}(r) = \frac{1}{r^{12}} - 2 \cdot \frac{1}{r^6}$$



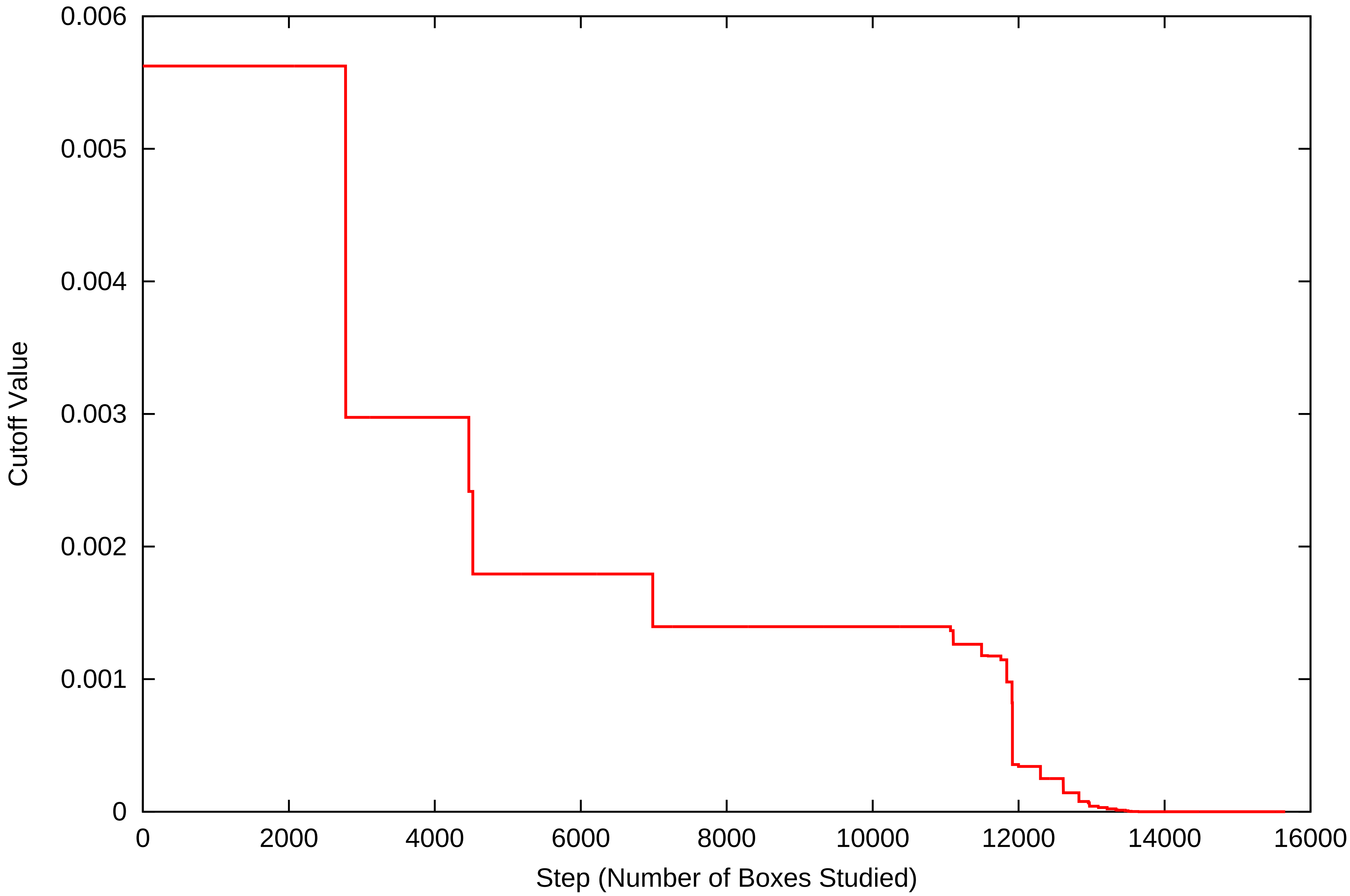
Has very shallow minimum of -1 at $r = 0$. Very hard to Taylor expand. Extremely wide range of function values: $V_{LJ}(0.5) \approx 4000$, $V_{LJ}(2) \approx 0.03$

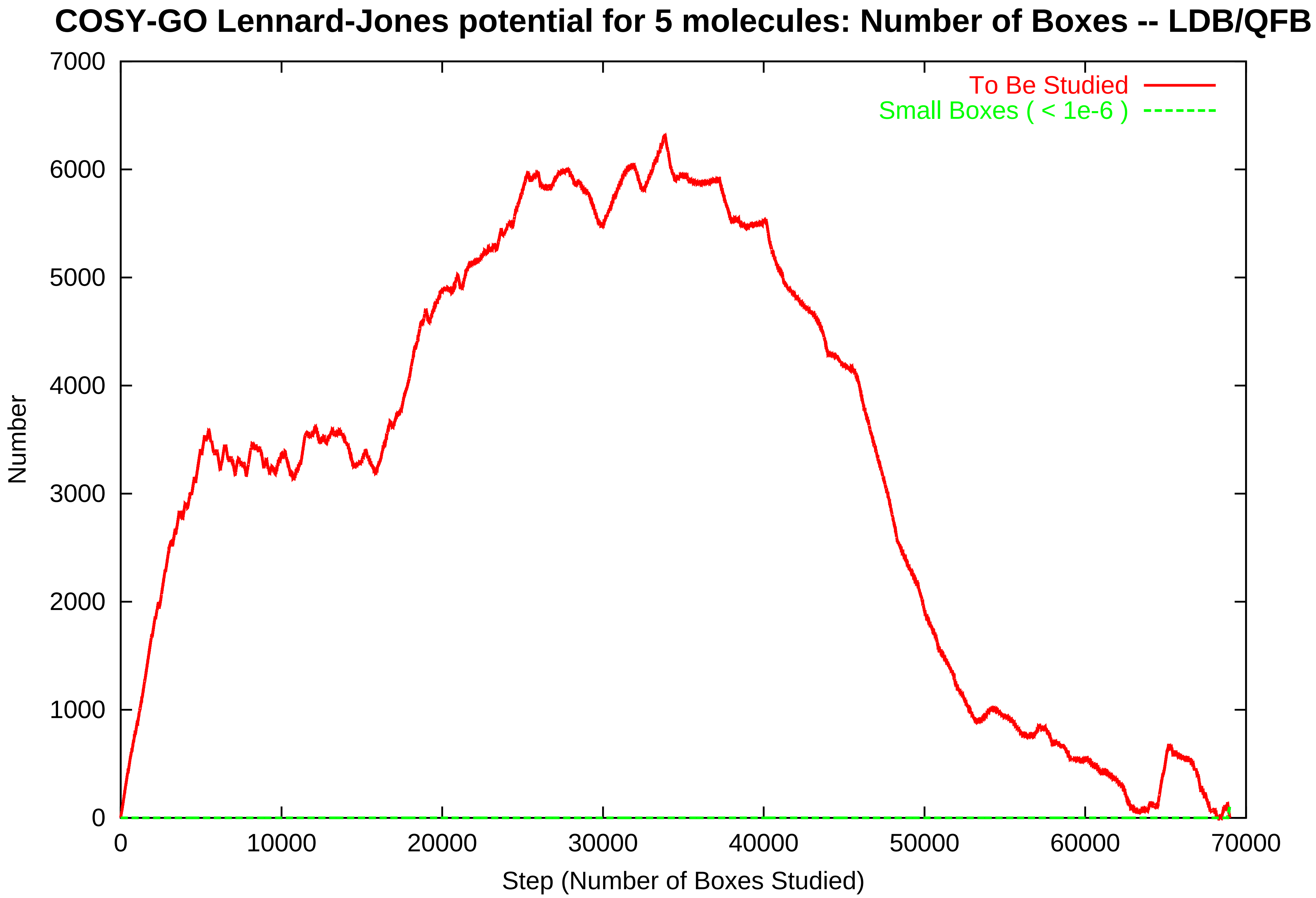
$$V = \sum_{i<j}^{n} V_{LJ}\left(r_i - r_j\right)$$

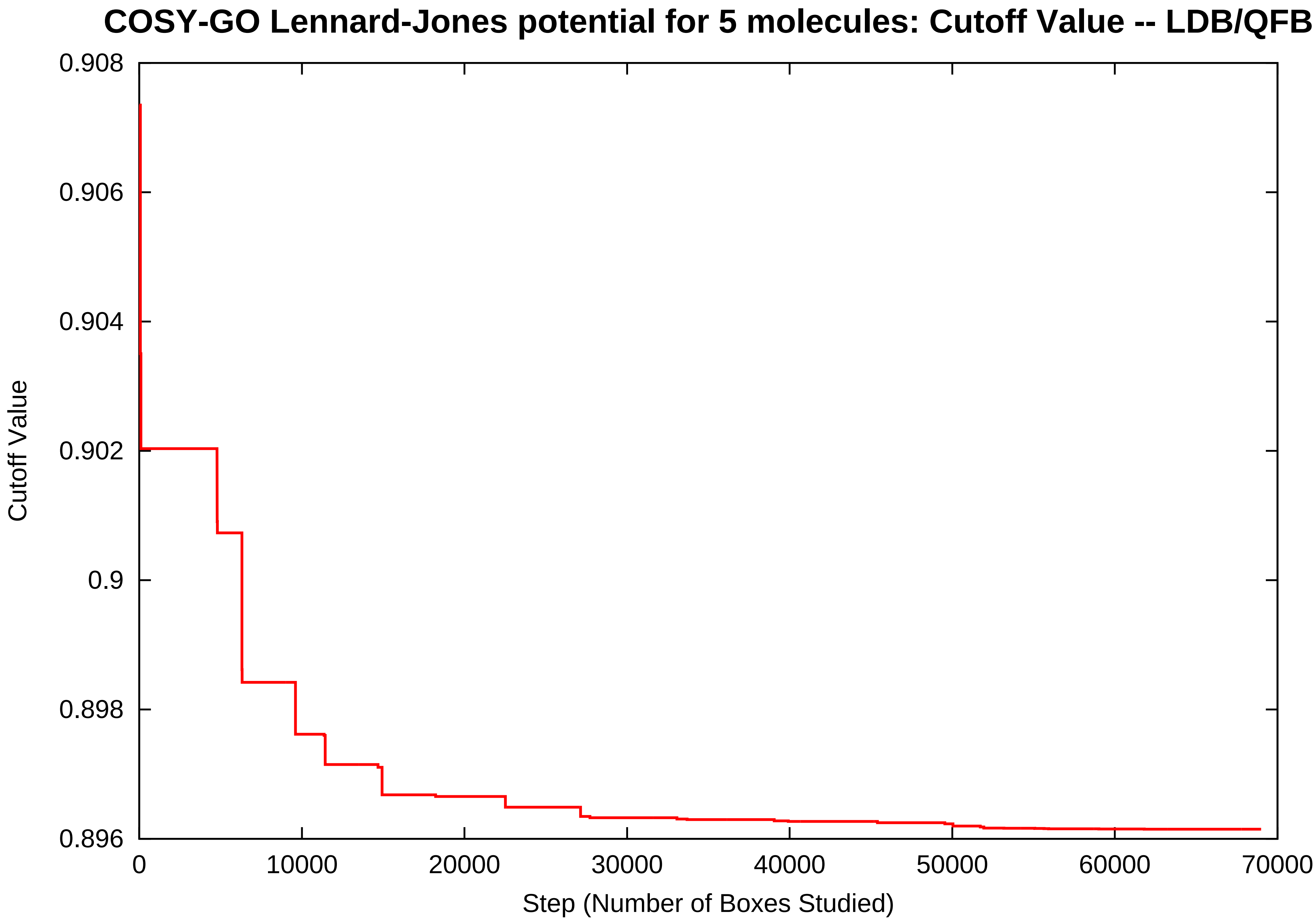
Study $n = 3$, 4, 5. Pop quiz: What do resulting molecules look like?


COSY-GO Lennard-Jones potential for 4 molecules: Number of Boxes -- LDB/QFB
Number
Step (Number of Boxes Studied)
To Be Studied
Small Boxes (< 1e-6)
0
500
1000
1500
2000
2500
3000
0
2000
4000
6000
8000
10000
12000
14000
16000

COSY-GO Lennard-Jones potential for 4 molecules: Cutoff Value -- LDB/QFB




COSY-GO Lennard-Jones potential for 5 molecules: Number of Boxes -- LDB/QFB
To Be Studied
Small Boxes (< 1e-6)
Number
0
1000
2000
3000
4000
5000
6000
7000
0
10000
20000
30000
40000
50000
60000
70000
Step (Number of Boxes Studied)


COSY-GO Lennard-Jones potential for 5 molecules: Cutoff Value -- LDB/QFB
Cutoff Value
0.908
0.906
0.904
0.902
0.9
0.898
0.896
0
10000
20000
30000
40000
50000
60000
70000
Step (Number of Boxes Studied)

Lennard-Jones Potentials - Results

Find minimum with COSY-GO and Globsol.
Use TMs of Order 5, QFB&LFB.
Use Globsol in default mode.

Problem	CPU-time needed	Max list	Total # of Boxes
n=4, COSY	89 sec	2,866	15,655
n=5, COSY	1,550 sec	6,321	69,001

Lennard-Jones Potentials - Results

Find minimum with COSY-GO and Globsol.
Use TMs of Order 5, QFB&LFB.
Use Globsol in default mode.

Problem	CPU-time needed	Max list	Total # of Boxes
n=4, COSY	89 sec	2,866	15,655
n=5, COSY	1,550 sec	6,321	69,001
n=4, Globsol	5,833 sec		243,911
n=5,□Globsol□	>60,530□sec (not finished yet)		

Fermi's Golden Rule

A sign near the entrance of Fermilab's Accelerator Simulation Department:

The difference between Theory and Practice
is greater in Practice than it is in Theory

Fermi's Golden Rule - Corollary I

A sign near the entrance of Fermilab's Accelerator Simulation Department:

The difference between Theory and Practice
is greater in Practice than it is in Theory

...but the difference between Validated Computing
and Theory is often greater yet!

Fermi's Golden Rule - Corollary II

A sign near the entrance of Fermilab's Accelerator Simulation Department:

The difference between Theory and Practice
is greater in Practice than it is in Theory

...but the difference between Validated Computing
and Theory is often greater yet!

...however, both these differences will be safely contained
in the validated error bounds.

The Normal Form Defect Function

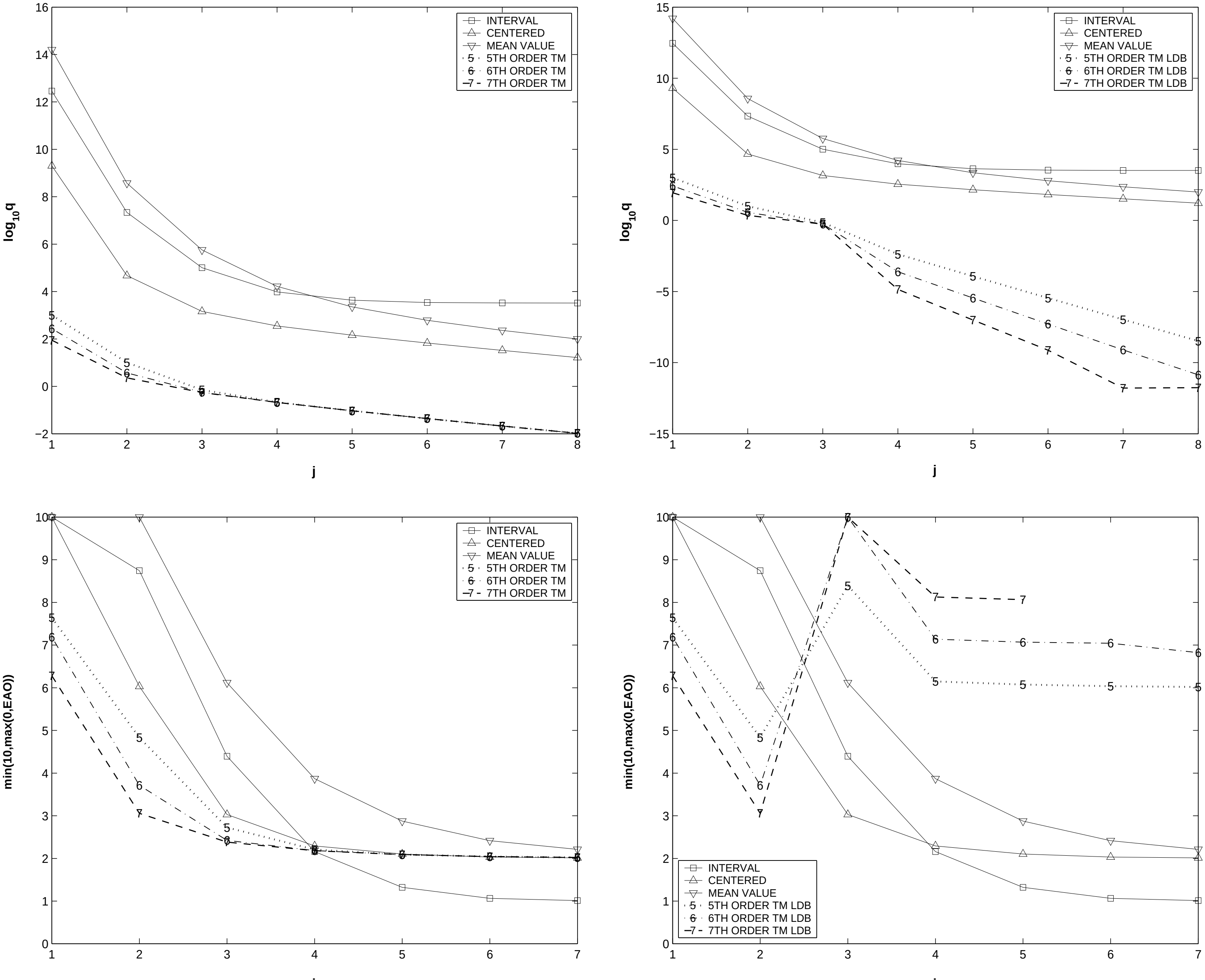
- **Extreme cancellation**; one of the reasons TM methods were invented
- Six-dimensional problem from dynamical systems theory
- Describes invariance defects of a particle accelerator
- Essentially composition of three tenth order polynomials
- The function vanishes identically to order ten
- Study for $a\cdot\ (1,1,1,1,1,1)$ for $a = .1$ and $a = .2$
- Interesting **Speed observation**: on same machine,

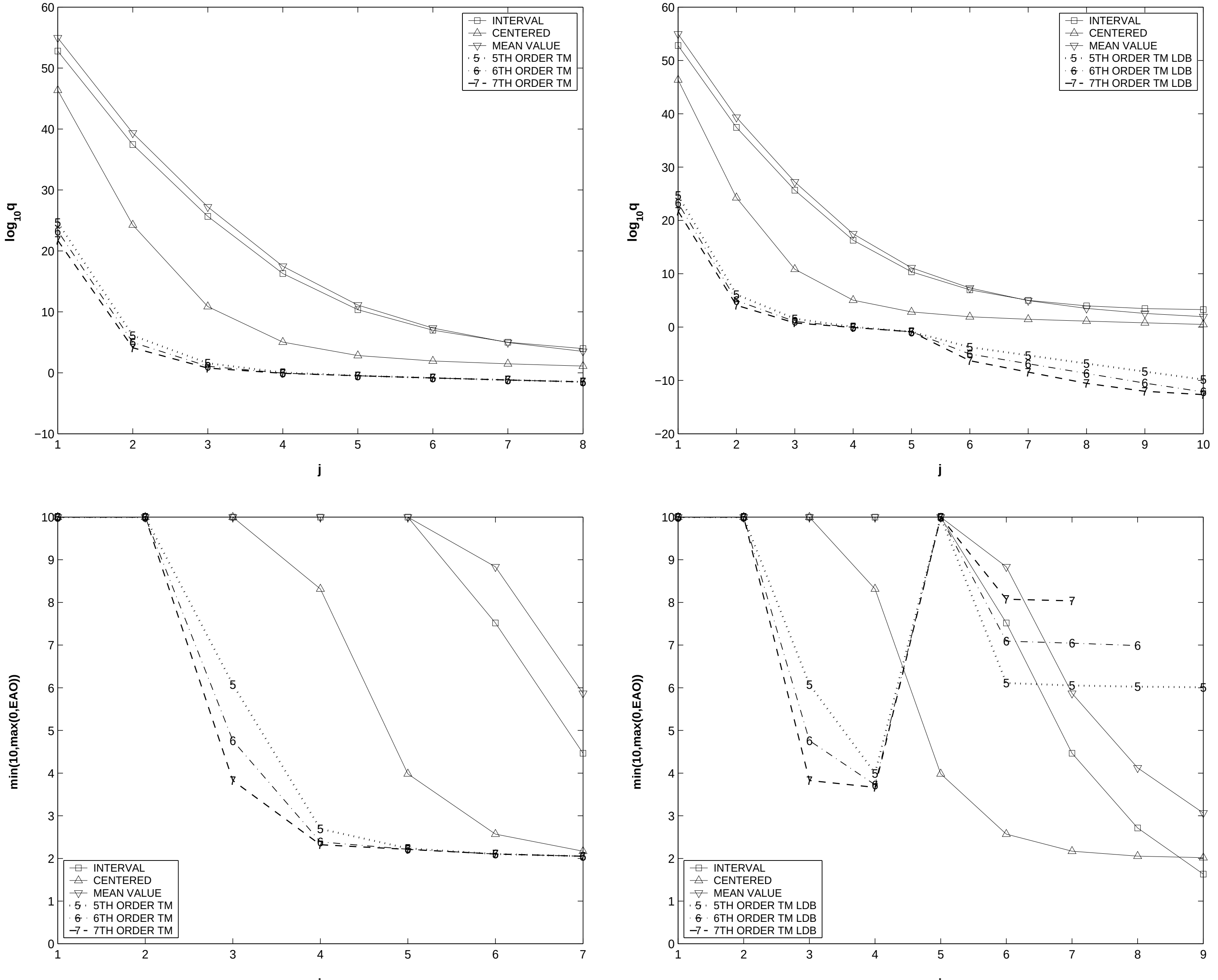
  * one CF in INTLAB takes 45 minutes

  * one TM of order 7 takes 10 seconds

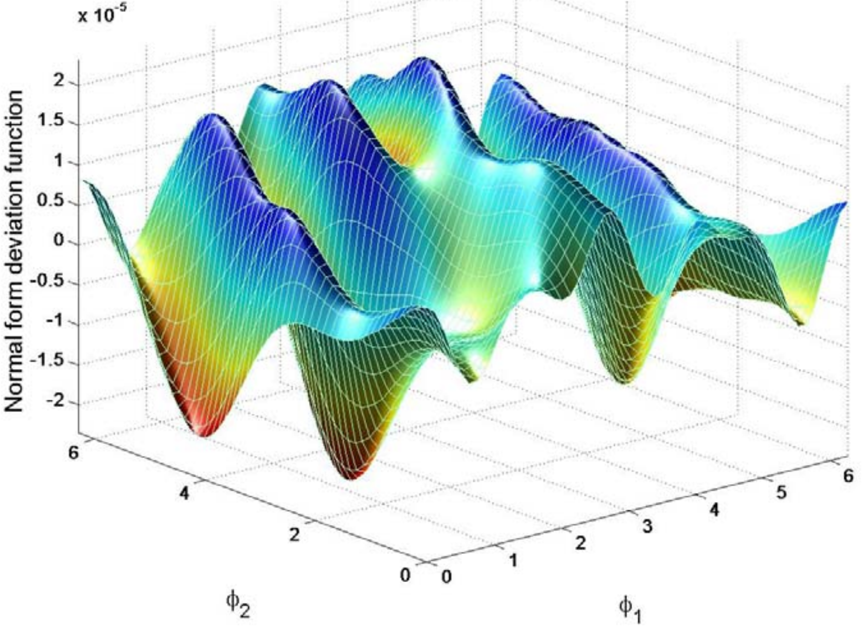
$$f_4(x_1, .., x_6) = \sum_{i=1}^{3} \left(\sqrt{y_{2i-1}^2 + y_{2i}^2} - \sqrt{x_{2i-1}^2 + x_{2i}^2} \right)^2$$

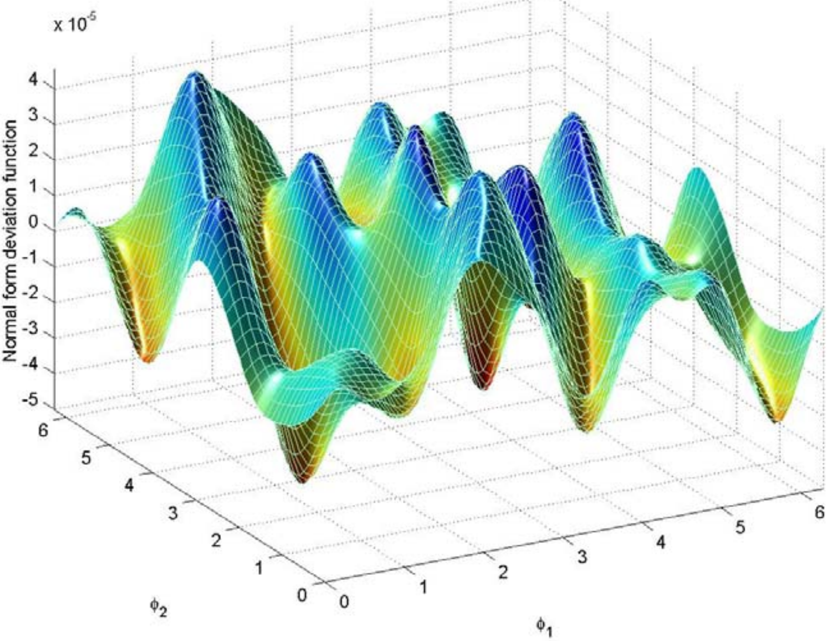
$$\text{where } \vec{y} = \vec{P}_1 \left(\vec{P}_2 \left(\vec{P}_3(\vec{x}) \right) \right)$$


16
14
12
10
8
6
4
2
0
−2
1
2
3
4
5
6
7
8
log10q
j
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM
6TH ORDER TM
7TH ORDER TM
15
10
5
0
−5
−10
−15
log10q
j
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM LDB
6TH ORDER TM LDB
7TH ORDER TM LDB
10
9
8
7
6
5
4
3
2
1
0
min(10,max(0,EAO))
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM
6TH ORDER TM
7TH ORDER TM
min(10,max(0,EAO))
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM LDB
6TH ORDER TM LDB
7TH ORDER TM LDB



log10q
60
50
40
30
20
10
0
−10
1
2
3
4
5
6
7
8
j
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM
6TH ORDER TM
7TH ORDER TM
log10q
60
50
40
30
20
10
0
−10
−20
1
2
3
4
5
6
7
8
9
10
j
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM LDB
6TH ORDER TM LDB
7TH ORDER TM LDB
min(10,max(0,EAO))
10
9
8
7
6
5
4
3
2
1
0
1
2
3
4
5
6
7
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM
6TH ORDER TM
7TH ORDER TM
min(10,max(0,EAO))
10
9
8
7
6
5
4
3
2
1
0
1
2
3
4
5
6
7
8
9
INTERVAL
CENTERED
MEAN VALUE
5TH ORDER TM LDB
6TH ORDER TM LDB
7TH ORDER TM LDB


x 10^-5
Normal form deviation function
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
6
4
2
0
ϕ2
0
1
2
3
4
5
6
ϕ1


x 10^-5
4
3
2
1
0
-1
-2
-3
-4
-5
Normal form deviation function
6
5
4
3
2
1
0
φ2
0
1
2
3
4
5
6
φ1

GlobSol Results

For the computations, GlobSol's maximum list size was changed to 10^6, and the CPU limit was set to 10 days. All other parameters affecting the performance of GlobSol were left at their default values.

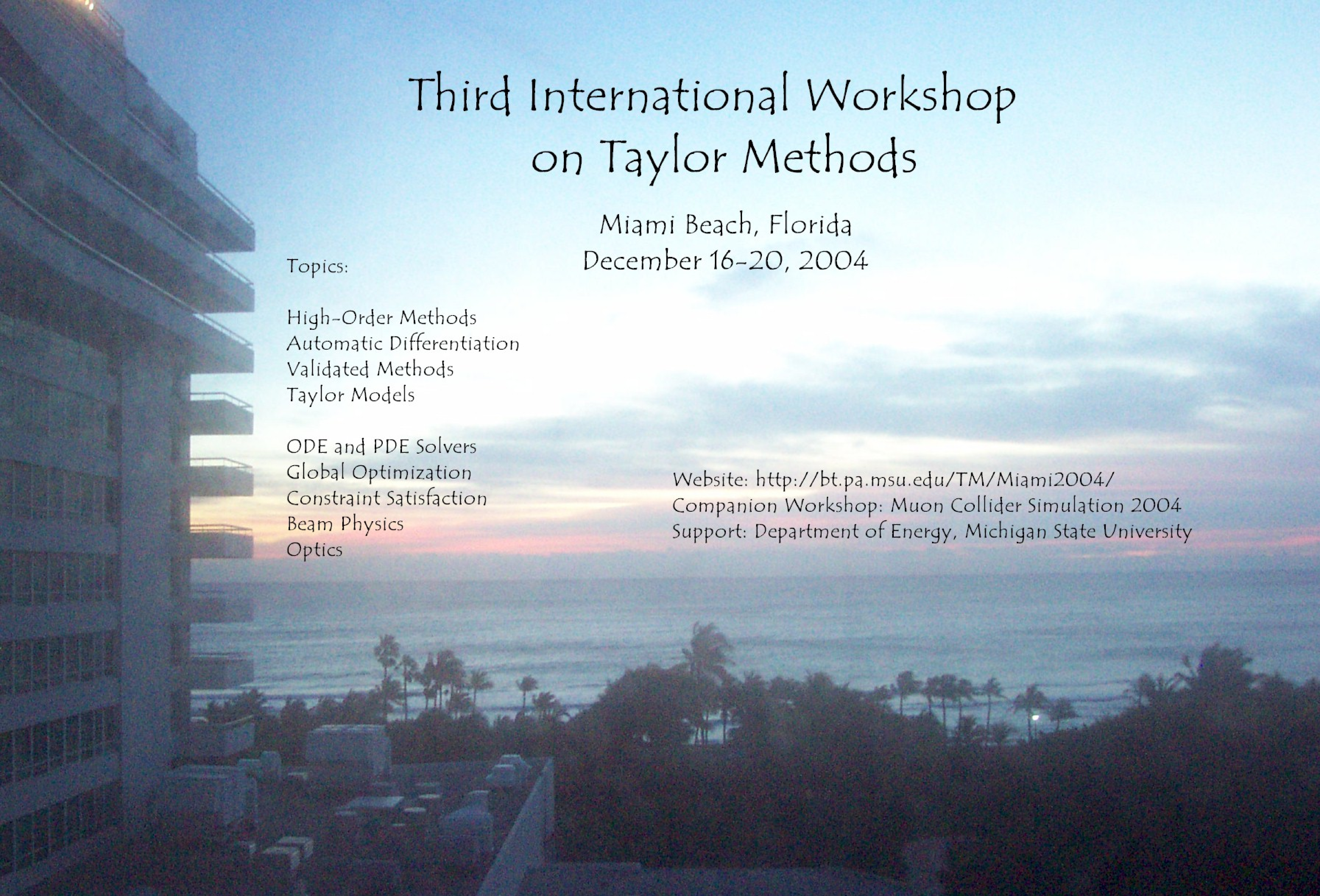
Dimension	CPU-time needed	Max list	Total # of Boxes
2	18810 sec		4733
3	>562896 sec (not finished yet)		
4	>259200 sec (could not finish)		63446 (remaining)
5	> 86400 sec (could not finish)		21306 (remaining)
6	not attempted		

We observe that in this example, COSY outperforms GlobSol by many orders of magnitude. However, we are not completely sure if a different choice of parameters for GlobSol could result in better performance.

COSY-GO Results

Tolerance on the sharpness of the resulting minimum is 10^{-10}.For the evaluation of the objective function, Taylor models of order 5 were used. For the range bounding of the Taylor models, Makino's LDB with domain reduction was being used.

Dimension	CPU-time needed	Max list	Total # of Boxes
2	5.747071 sec	11	31
3	38.48828 sec	44	172
4	346.8604 sec	357	989
5	3970.746 sec	2248	6641
6	57841.94 sec	17241	49821



Third International Workshop on Taylor Methods

Miami Beach, Florida
December 16-20, 2004

Topics:

High-Order Methods
Automatic Differentiation
Validated Methods
Taylor Models

ODE and PDE Solvers
Global Optimization
Constraint Satisfaction
Beam Physics
Optics

Website: http://bt.pa.msu.edu/TM/Miami2004/
Companion Workshop: Muon Collider Simulation 2004
Support: Department of Energy, Michigan State University