

IC process optimization and modeling: a dedicated computer tool.

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July 15, 1988

1. Summary

Semiconductor device and process simulation programs make a wide use of analytical models with parameters extracted from experimental data fitting. It is quite obvious that process designer have to characterize these models to fit their own environment. Moreover it is a major task of process engineers to find process parameters which optimize designer and customer requirements.

Both these problems are substantially non linear, multi-dimensional regression problems. We have developed a computer tool which solves this kind of problems; it is based on the Levenberg-Marquardt algorithm, which is an efficient solver of non-linear, multi-dimensional constrained least square problems (Doganis,1981 and Ward, 1982). This algorithm has been enhanced by introducing several original features, to try to escape from local minimum when possible, and some statistical facilities which helps user in finding outliers and in monitoring the quality of the regression. The program will be able to drive various kind of simulators by forcing their inputs and reading their outputs with the appropriate interface. The present release is linked via a Remote Procedure Calls package with ST-SPICE 1.0-A, (Nagel,1975 and Profumo,1988) and ST-SUPREM-III (Hansen,1985). In this way it is possible to consider these simulators as "external" models to be characterized or optimized. Each variable that may appear in a simulator file can be optimized over a certain user-specified target; moreover the program can optimize parameters that appear in more than one simulator file. Referring to process optimization it is possible to vary any SUPREM-III variable or parameter (times, temperatures, fluxes, diffusivities, mobilities and so on) to fit one of these targets:

- Junction depths and sheet resistance of each layer,
- V-threshold as function of the V-substrate,
- Active and/or chemical concentration of any impurity at any depth,
- Net charge at any depth.

2. Software structure and simulation interface

The program SOBS 2.3-B is an optimizer built on the well known Levenberg-Marquardt algorithm as implemented in SUXES-IV, (Doganis,1985). The first release of SOBS has been linked with SGS-SPICE and was used since 1984 to extract model parameters for BJT, MOS device and other macro-models (Saporito,1984).

It is composed of the following modules :

- a compiler, that reads all files needed for the optimization, checks input syntax and compiles the optimization problem in an internal format that will be read by the algorithm module,
- the algorithm of minimization, the original Levenberg-Marquardt with an extension to search an optimal variation for each parameter to compute the gradient, that is to use a specific h_j^k for each parameter x_k to estimate the Jacobian J_{ij} , (see Algorithm section),
- the simulation interface that is cumbersed by a specific module, one for each external tool and a general module for every present or future linked tool,
- the external tools that has been modified with the needed RPC package for the communication, plus other routines to write output binary files of a format compatible with SOBS.

2.1 Simulation Interface

The algorithm and the external tool are two different executables linked via an RPC (Remote Procedure Calls) package that sincronizes them. Sincronous message is sent when the algorithm needs a new computation of data for the current value of parameters. An asincronous mailbox is used to trap every event as the unpredicted crash of one of the two executable.

The actions performed by the Simulation Interface (SI) can be summarized in a preliminary phase in which the capabilities to produce all needed output is verified. When the optimization loop starts the SI performs the following actions :

- current value of the parameters is written in the SUPREM-III input binary files as produced from GENII, the SUPREM-III preprocessor,
- SUPREM-III runs and produces binary output in SOBS format,
- output files are read, post-processed and associated with target.

Then SI stops and the algorithm computes the current value of the parameters. The Algorithm can call the SI with new values and this loop continues until one termination criteria is reached.

3. Algorithm

Here x is the vector of parameters to be optimized, the vector $f(x)$ consists of the error evaluated at each data point. The quantity to be minimized (the objective function) is the norm of the error vector, given by :

$$\|f(x)\|^2 = \sum_k f_k(x)^2 \equiv \sum_k \left(\frac{O_k(x) - T_k}{T_k} \right)^2$$

where O_k is the calculated function value, for example the concentration at the k -th point, that is the k -th depth and T_k is the desired value of concentration.

The program extracts the parameters in a user specified constrained region of operation. At each iteration of the algorithm, the model is evaluated at each data point and the error vector $f(x)$ is calculated, the parameter vector x is then adjusted to reduce the sum of the squares of the errors. The process converges when a termination criteria is reached. The heart of the method is the adjustment of x to minimize the error. Basically the Levenberg-Marquardt algorithm is used as implemented in SUXES-IV. The Jacobian (the matrix of partial derivatives of the errors with respect to the parameter values) is calculated numerically.

To minimize the objective function :

$$F(x) = f^T f = \sum_{i=1}^m [f_i(x)]^2 \quad x \in R^n, f : R^n \rightarrow R^m$$

it is necessary to find an x^* such that the gradient g of F equal zero :

$$g = 2J^T(x^*)f(x^*) = 0$$

where :

$$J_{ij} = \frac{\partial f_i(x)}{\partial x_j}$$

is the Jacobian of f . The Newton step x for improving an approximate solution x is obtained by solving the normal equations :

$$\left[J^T J + \sum_{i=1}^m f_i(x) N^{(i)} \right] \Delta x = -J^T f(x)$$

where the term in brackets represent the Hessian matrix, and :

$$N_{kj}^{(i)} = \partial^2 f_i(x) / \partial x_k \partial x_j$$

for $i = 1, \dots, m$ and $k, j = 1, \dots, n$.

The Levenberg-Marquardt (L-M) method approximates the second term into the square bracket with : $\lambda_k (J^T J)_{ii}$, where λ_k is a "weighting" parameter between the steepest descent and Gauss-Newton methods, and requires evaluation of the Jacobian of the residual vector $f(x)$ and solution of normal equations at each iteration step. The Jacobian J_{ij} is estimated numerically by means of either a forward difference approximation :

$$J_{ij}(x_k) \simeq \frac{f(x_k + h_j^k u_j) - f(x_k)}{h_j^k}$$

or a central difference approximation :

$$J_{ij}(x_k) \simeq \frac{f(x_k + h_j^k u_j) - f(x_k - h_j^k u_j)}{h_j^k}$$

where u_j is the j unit column vector and h_j^k is a small increment in the x_k direction.

4. Optimizable parameters, data and targets

Four types of files are required to run SOBS :

- input file with an initial estimate of the parameters to be optimized.
- data files with the targets.
- Suprem files that must be able to produce output consistent with the target.
- command files with the list of the previous files, and of the parameters to be optimized.

4.1 Optimizable parameters and input file

The parameters that can be optimized are process parameters as Time, Temperature, Implanted Dose, Energy, etc. or fitting parameters for new physical model for diffusion, deposition, oxidation etc. Every input variable in a Suprem file can be optimized; it is considered to be an optimizable parameter if it is present in the input file, with the syntax :

```
<prefix \ parameter> <initial value> <lower bound> <upper bound>
```

and in the Suprem file with the syntax :

```
# prefix # parameter
```

A parameter can be present in more than one suprem file and different parameters must have the same values :

```
<prefix1 \ parameter1> <prefix2 \ parameter2> ... <prefixn \ parametern>
<initial> <lower> <upper>
```

Example of input file and suprem file :

```
* input file
&parameter          initial  lower  upper
time1\time time2\time   100    90    120
time3\time           200    180    240

* suprem file 1
.diffusion temp = 950 #time1# time = 100
.diffusion temp = 900 #time2# time = 100

* suprem file 2
.diffusion temp = 850 #time1# time = 100
.diffusion temp = 950 #time3# time = 200
```

4.2 Data files and targets

To associate each data files to the related suprem files the command file must have the following two lines :

```
.datafiles   data1  data2  data3
.supremfiles  suprem1  suprem2  suprem2
```

The outputs of suprem1 will be associated to the targets if the file data1. The suprem2 file will be forced to produce two different type of outputs to be associated with data2 and data3, because the same suprem file can be associated to several data files.

Each data file must have in the heading the field *model* followed by an integer. Each model number is associated with a different type of Suprem output.

Each data file has one column that is the target, and one column that is the independent variable. An additional column is present to specify the sub-type of the target.

Example of data file to optimize active concentrations of Boron and Phosphorus.

```
model = 2
depth  trgtyp  target
0.2000   5      1.0e17
0.3000   5      2.0e17
0.2000   6      1.7e17
0.3000   6      2.7e17
```

The available models are :

- model = 1, the threshold voltage as computed from SUPREM-III is the target, the independent variable is the base-substrate voltage,
- model = 2, every active and/or chemical concentration, as well as the total net concentration can be the target. The target types are : BO-Active, BO-chemical, PH-A, PH-C, SB-A, SB-C, AS-A, AS-C, NET-chemical.
- model = 3, sheet resistance and/or junction depth of each layer,

Several models can be present and optimized at the same time.

4.3 Command file

The command file is composed of control cards as in that example :

```
.inputfile  initial
.iteration  time1\time time2\time
.datafile   data1   data2
.supremfile suprem1 suprem2
.outputfile file=output
```

The meaning of inputfile, datafile, supremfile is known, the iteration card asks for the extraction only of :

```
time1\time  time2\time
```

and the optimized value of parameters will be written in file output.dat.

5. Limits of the program and final consideration

The example showed is a fitting of the net concentration after seven steps. The optimizable parameter are three : thickness of the first deposition, temperature and time of the first diffusion. The target cannot be reached with greater accuracy, because the initial region, of 0.3 micron, is flat, and the output cannot be flattened with that parameters. The region deeper than 0.3 micron is very accurate. The initial mean error (131.204 %) has been reduced of ten times (11.614 %), in 7 minutes of elapsed time of a VAX 8650. The figure shows graphically the same information listed in the error file. The optimization flow is reported and it is possible to see the number of iterations performed.

The number of optimizable parameters, either of the data (or suprem) files and of the targets data has hardware and software limitation. The physical limits of the

system : page file quota, or working set of the main process (algorithm) and the detached one (SUPREM-III) must be taken into account before the compilation of the source code because the program is all written in Fortran and it needs a static definition of the work space.

The dimension of the problem that can be solved also depends from the good formulation of the minimization problem. The knowledge of the physical models implemented in SUPREM-III will avoid the formulation of unreachable problems. If the User knows what are the parameters sensitive to solve the minimization problem then SOBS can help him to find the optimal value in less time then by hand.

In the following figure is shown the initial, the final and the target profile.

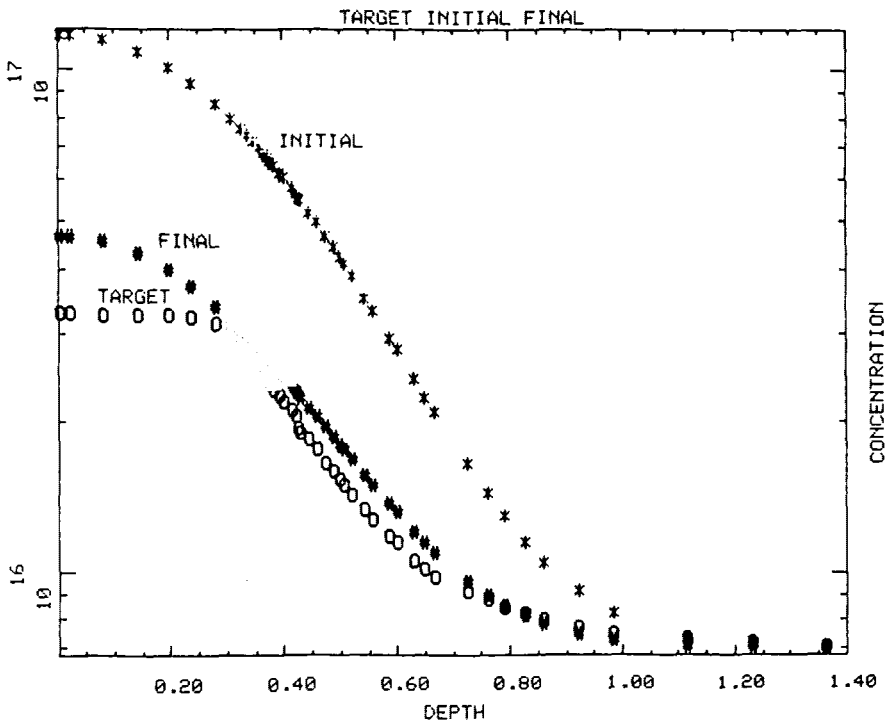


Fig 1. Final result compared with initial and target.

6. Example

example of input file with initial values of parameters, lower and upper bounds :

```
*
&PARAMETERS      INITIAL/EXTRACTED          LOWER          UPPER
THI1\THICKNESS    0.0050                0.0010         0.0100
TEM1\TEMPER       1000.000              950.000        1100.000
TIM1\TIME         90.000                10.000         100.000
*
```

example of supremfile in which to optimize :

```
#THI1#THICKNESS #TEM1#TEMPERATURE #TIM1#TIME
```

```
TITLE            BOXER ISOLATION
INITIALIZE       <100> SILICON BORON CONCENTRATION=7E15
+               THICKNESS=4 DX=0.02
```

```
$ Deposition of a thin oxide
DEPOSITIO OXIDE #THI1# THICK=0.005
```

```
$ Deposition of a doped oxide
DEPOSITIO OXIDE CONCEN=1.184E20 BORON THICK=0.20 TEMP=390
PRINT LAYERS
```

```
$ Diffusion for the impurities throught the thin oxide
DIFFUSION #TEM1# TEMPERAT=1000 #TIM1# TIME=50
PRINT LAYERS
```

```
$ Etch oxide
ETCH        OXIDE ALL
```

```
$ Deposition oxide
DEPOSIT     OXIDE THIC=0.5
```

```
$ Diffusion for the impurities
DIFFUSION  TEMPERAT=1100 TIME=30 DRYO2
```

```
$ Etch oxide
ETCH        OXIDE ALL
```

```
$ Save the file
PRINT      LAYERS
SAVEFILE   FILENAME=BOX.EXP EXPORT
STOP
```

Example of flow of the optimization, the first 7 numbered lines are the cards of the command file. The flow has the same format of SUXES-IV.

```

1 ... .INPUTFILE BOXIEF
3 ... .ITERATION &EXTRACT &ALL
4 ... .SUPREMFIE BOX
5 ... .DATAFILES BOX
6 ... .IOPTIONS LIST=ERR OUT=2 AUTO=Y
7 ... .OUTPUT FILE=BOXOUT

```

JACOBIAN EVALUATION

SSQNEW = 109.133 SSQOLD = 120.376

ITERATION COMPLETED

```

THI1\THI 4.945429166E-03 IN.CHG % -1.09142 IT.CHG % -1.09142
TEM1\TEM 991.673167 IN.CHG % -0.832683 IT.CHG % -0.832683
TIM1\TIM 93.5319975 IN.CHG % 3.92444 IT.CHG % 3.92444
ITER= 1 EVAL= 12 ABSSSQ= 109.133 AL= 2.500000E-02 GRAD=14216.3
ERMAX % = 252.399 ERMIN % = 5.661878E-02 RMS % = 124.407
XSIGN= 1.42294 RELSSQ= 109.133 SEARCH# = 1

```

BROYDENS RANK ONE UPDATE

SSQNEW = 93.9632 SSQOLD = 109.133

ITERATION COMPLETED

```

THI1\THI 4.897361237E-03 IN.CHG % -2.05278 IT.CHG % -0.961359
TEM1\TEM 983.416167 IN.CHG % -1.65838 IT.CHG % -0.825700
TIM1\TIM 91.8476916 IN.CHG % 2.05299 IT.CHG % -1.87145
ITER= 2 EVAL= 13 ABSSSQ= 93.9632 AL= 1.095850E-02 GRAD=12463.2
ERMAX % = 240.682 ERMIN % = 5.658808E-02 RMS % = 114.806
XSIGN= 1.73665 RELSSQ= 93.9632 SEARCH# = 1

```

BROYDENS RANK ONE UPDATE

SSQNEW = 85.2525 SSQOLD = 93.9632

ITERATION COMPLETED

```

THI1\THI 4.814017241E-03 IN.CHG % -3.71966 IT.CHG % -1.66688
TEM1\TEM 971.836941 IN.CHG % -2.81631 IT.CHG % -1.15792
TIM1\TIM 93.6789483 IN.CHG % 4.08772 IT.CHG % 2.03473
ITER= 3 EVAL= 14 ABSSSQ= 85.2525 AL= 3.278762E-03 GRAD=7457.92
ERMAX % = 235.658 ERMIN % = 5.678760E-02 RMS % = 108.678
XSIGN= 1.70889 RELSSQ= 85.2525 SEARCH# = 1

```


BROYDENS RANK ONE UPDATE

SSQNEW = 1.87419 SSQOLD = 85.2526

ITERATION COMPLETED

THI1\THI 5.565533074E-03 IN.CHG % 11.1107 IT.CHG % 14.8303
 TEM1\TEM 966.536016 IN.CHG % -3.34640 IT.CHG % -0.530092
 TIM1\TIM 87.9543931 IN.CHG % -2.27290 IT.CHG % -6.36062
 ITER= 4 EVAL= 15 ABSSSQ= 1.87419 AL= 8.196905E-04 GRAD=3499.19
 ERMAX %= 47.9332 ERMIN %= 5.663412E-02 RMS %= 14.8541
 XSIGN= 0.874605 RELSSQ= 1.87419 SEARCH# = 1

JACOBIAN EVALUATION

SSQNEW = 1.32485 SSQOLD = 1.87419

ITERATION COMPLETED

THI1\THI 5.551397416E-03 IN.CHG % 11.0279 IT.CHG % -8.271316E-02
 TEM1\TEM 963.939456 IN.CHG % -3.60605 IT.CHG % -0.259656
 TIM1\TIM 84.3886626 IN.CHG % -6.23482 IT.CHG % -3.96192
 ITER= 5 EVAL= 20 ABSSSQ= 1.32485 AL= 2.049226E-04 GRAD=874.004
 ERMAX %= 42.7316 ERMIN %= 5.663412E-02 RMS %= 12.0657
 XSIGN= 1.37414 RELSSQ= 1.32485 SEARCH# = 1

BROYDENS RANK ONE UPDATE

SSQNEW = 1.36351 SSQOLD = 1.32485
 SSQNEW = 1.27923 SSQOLD = 1.32485

ITERATION COMPLETED

THI1\THI 5.553356236E-03 IN.CHG % 11.0671 IT.CHG % 3.917639E-02
 TEM1\TEM 962.609491 IN.CHG % -3.73905 IT.CHG % -0.132997
 TIM1\TIM 87.6739929 IN.CHG % -2.58445 IT.CHG % 3.65037
 ITER= 6 EVAL= 22 ABSSSQ= 1.27923 AL= 6.659928E-04 GRAD=710.122
 ERMAX %= 42.1773 ERMIN %= 5.651134E-02 RMS %= 11.8138
 XSIGN= 1.42629 RELSSQ= 1.27923 SEARCH# = 2

JACOBIAN EVALUATION

SSQNEW = 1.25021 SSQOLD = 1.27923

ITERATION COMPLETED

THI1\THI 5.533843343E-03 IN.CHG % 10.6769 IT.CHG % -0.390258
 TEM1\TEM 959.902488 IN.CHG % -4.00975 IT.CHG % -0.270700
 TIM1\TIM 87.4682947 IN.CHG % -2.81301 IT.CHG % -0.228554
 ITER= 7 EVAL= 28 ABSSSQ= 1.25021 AL= 1.36395 GRAD=229.684
 ERMAX %= 42.1514 ERMIN %= 5.664180E-02 RMS %= 11.6142
 XSIGN= 2.45271 RELSSQ= 1.25021 SEARCH# = 1

ERROR CONDITION:

THE MARQUARDT PARAMETER (1396.69)
 EXCEEDED THE MAXIMUM (1000.00)

----- SOBS END -----

Example of output result with termination criteria before the optimization, initial error, and after the optimization :

```

*
*      STATISTIC SUMMARY
*
*      DATE AND TIME
*
*      Start :  9-JUL-1988 10:36:24.03
*      End   :  9-JUL-1988 10:40:59.63
*
*      ----- MINIMIZATION RESULTS -----
*
*      RESIDUAL SUM OF SQUARES      =  120.376
*      NORM OF THE GRADIENT          =  14216.3
*      MARQUARDT SCALING PARAMETER   =  0.000000E+00
*      NO. OF SIGNIFICANT DIGITS     =    4
*      NO. OF FUNCTION EVALUATIONS   =   18
*      NO. OF ITERATIONS             =    0
*      THE MAX ERROR IS              =  259.568      %
*      THE RMS ERROR IS              =  131.204      %
*
*      -----
*
*      &PARAMETERS  INITIAL/EXTRACTED  LOWER  UPPER
*      TH11\THICKNESS  5.000000E-03  5.000000E-03  5.000000E-03
*      TEM1\TEMPER  1000.00  1000.00  1000.00
*      TIM1\TIME  90.0000  90.0000  90.0000
*
*
*      STATISTIC SUMMARY
*
*      DATE AND TIME
*
*      Start :  9-JUL-1988 11:23:30.53
*      End   :  9-JUL-1988 11:30:26.01
*
*      ----- MINIMIZATION RESULTS -----
*
*      RESIDUAL SUM OF SQUARES      =  1.25021
*      NORM OF THE GRADIENT          =  608.691
*      MARQUARDT SCALING PARAMETER   =  1.36395
*      NO. OF SIGNIFICANT DIGITS     =    4
*      NO. OF FUNCTION EVALUATIONS   =   39
*      NO. OF ITERATIONS             =    7
*      THE MAX ERROR IS              =  42.1514      %
*      THE RMS ERROR IS              =  11.6142      %
*
*      -----
*
*      &PARAMETERS  INITIAL/EXTRACTED  LOWER  UPPER
*      TH11\THICKNESS  5.533843E-03  1.000000E-03  1.000000E-02
*      TEM1\TEMPER  959.902  950.000  1100.00
*      TIM1\TIME  87.4683  10.0000  100.000

```

DEPTH	TARGET	INITIAL		FINAL	
		RESULT	ERROR	RESULT	ERROR
3.372E-03	3.258E+16	1.170E+17	-259.	4.627E+16	-42.0
2.047E-02	3.256E+16	1.171E+17	-260.	4.628E+16	-42.2
8.006E-02	3.251E+16	1.149E+17	-253.	4.540E+16	-39.7
0.140	3.248E+16	1.090E+17	-236.	4.308E+16	-32.6
0.197	3.231E+16	1.006E+17	-211.	3.977E+16	-23.1
0.238	3.203E+16	9.328E+16	-191.	3.696E+16	-15.4
0.281	3.119E+16	8.481E+16	-172.	3.371E+16	-8.09
0.305	3.026E+16	7.990E+16	-164.	3.185E+16	-5.22
0.324	2.926E+16	7.591E+16	-159.	3.034E+16	-3.69
0.336	2.774E+16	7.341E+16	-165.	2.940E+16	-5.97
0.346	2.692E+16	7.137E+16	-165.	2.864E+16	-6.40
0.355	2.616E+16	6.940E+16	-165.	2.790E+16	-6.64
0.363	2.570E+16	6.788E+16	-164.	2.734E+16	-6.36
0.370	2.543E+16	6.640E+16	-161.	2.679E+16	-5.34
0.375	2.485E+16	6.541E+16	-163.	2.643E+16	-6.33
0.375	2.394E+16	6.539E+16	-173.	2.642E+16	-10.3
0.382	2.319E+16	6.389E+16	-176.	2.586E+16	-11.5
0.394	2.254E+16	6.146E+16	-173.	2.497E+16	-10.8
0.399	2.187E+16	6.048E+16	-177.	2.461E+16	-12.5
0.413	2.122E+16	5.761E+16	-172.	2.357E+16	-11.1
0.421	2.044E+16	5.618E+16	-175.	2.305E+16	-12.8
0.426	1.945E+16	5.522E+16	-184.	2.270E+16	-16.7
0.430	1.907E+16	5.429E+16	-185.	2.237E+16	-17.3
0.445	1.847E+16	5.156E+16	-179.	2.138E+16	-15.7
0.457	1.764E+16	4.934E+16	-180.	2.059E+16	-16.7
0.474	1.658E+16	4.631E+16	-179.	1.951E+16	-17.7
0.486	1.592E+16	4.421E+16	-178.	1.877E+16	-17.9
0.498	1.539E+16	4.219E+16	-174.	1.806E+16	-17.4
0.505	1.490E+16	4.099E+16	-175.	1.764E+16	-18.4
0.520	1.418E+16	3.869E+16	-173.	1.685E+16	-18.8
0.544	1.328E+16	3.506E+16	-164.	1.560E+16	-17.5
0.558	1.270E+16	3.303E+16	-160.	1.491E+16	-17.4
0.587	1.179E+16	2.924E+16	-148.	1.364E+16	-15.7
0.599	1.142E+16	2.779E+16	-143.	1.316E+16	-15.3
0.630	1.052E+16	2.432E+16	-131.	1.203E+16	-14.3
0.650	1.008E+16	2.241E+16	-122.	1.141E+16	-13.2
0.666	9.733E+15	2.087E+16	-114.	1.093E+16	-12.3
0.724	9.083E+15	1.649E+16	-81.6	9.576E+15	-5.43
0.760	8.751E+15	1.437E+16	-64.2	8.944E+15	-2.21
0.791	8.431E+15	1.286E+16	-52.5	8.508E+15	-0.911
0.827	8.166E+15	1.145E+16	-40.3	8.113E+15	0.657
0.861	7.966E+15	1.041E+16	-30.7	7.828E+15	1.74
0.920	7.689E+15	9.069E+15	-17.9	7.477E+15	2.77
0.983	7.462E+15	8.193E+15	-9.80	7.260E+15	2.70
1.11	7.307E+15	7.337E+15	-0.415	7.066E+15	3.30
1.23	7.155E+15	7.099E+15	0.770	7.018E+15	1.91
1.36	7.056E+15	7.023E+15	0.464	7.004E+15	0.737
3.74	6.996E+15	7.000E+15	-5.657E-02	7.000E+15	-5.664E-02
3.96	6.987E+15	7.000E+15	-0.180	7.000E+15	-0.180

7. References

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