INTRODUCTION TO THE MONTE CARLO METHOD

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George Krikelas
Hellenic Institute of Metrology / National Quality Infrastructure System (EIM/NQIS)
Electrical Measurements Dpt.-High Frequency Lab.
Industrial area of Thessaloniki, Sindos, 57022, Block 45
gkrik@eim.gr

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INTRODUCTION

Definition-Historical Background

“Definition”

- Multitude of definitions-lack of consensus
- “A computer-simulation technique that uses random samples and other statistical methods to find approximate solutions to mathematical and physical problems”
  - Broad class of computational algorithms (for pseudorandom generators, sampling, scoring, variance reduction-for example stratified sampling…)

Monte Carlo's "mathematical heart"

- **Law of large numbers**: the average of the results obtained from a **large number** of trials should be close to the expected value, and will tend to become closer as more trials are performed
- **Central limit theorem**: given certain conditions, the arithmetic mean of a sufficiently large number of iterates of independent random variables, each with a well-defined expected value and well-defined variance, will be approximately normally distributed, regardless of the underlying distribution.

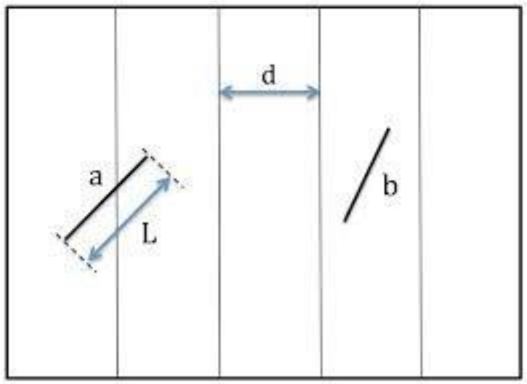
(estimate of the expected value / estimate of the uncertainty in the estimate!)

Pattern

- Generally varies
- Common steps:
  1. Define a domain of possible inputs.
  2. Generate inputs randomly from a probability distribution over the domain.
  3. Perform a deterministic computation on the inputs.
  4. Aggregate the results.

Historical Background

- Buffon's needle



(calculation of π-Georges-Luis Leclerc, Comte de Buffon, 1733)

What is the probability p, that a needle (length L), which randomly falls on a sheet, crosses one of the lines (distance d)?

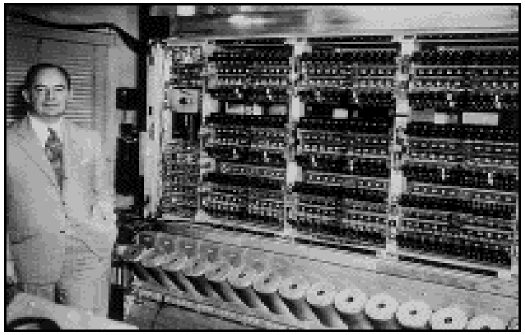
$$p_{L,d}(n) = \frac{2L}{d\pi} \quad \rightarrow \pi = \frac{2\mathrm{LN}}{\mathrm{dn}}$$

(N trials, n hits)

Historical Background

- Nuclear weapons project, Los Alamos (Manhattan)

Fermi: 1930s
Stanislav Ulam: modern MCMC, late 40s



John von Neumann: ENIAC

S. Ulam, J. von Neumann, N. Metropolis:
Markov Chain Monte Carlo
(Metropolis: Monte Carlo)

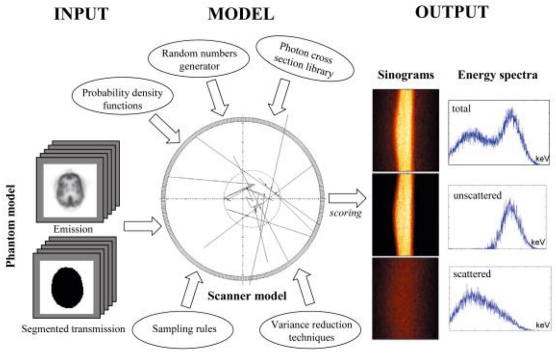
USE OF MCM

General and Metrological

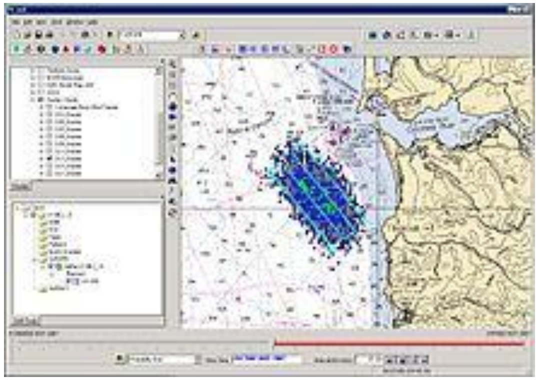
General usage

- Very broad range
  1. Physical sciences
  2. Engineering
  3. Climate change and radiative forcing
  4. Computation biology
  5. Computer graphics
  6. Applied statistics
  7. Artificial intelligence for games
  8. Design and visuals
  9. Search and rescue
  10. Finance and business

  (can be used to solve any problem having a probabilistic interpretation)



Nuclear medicine



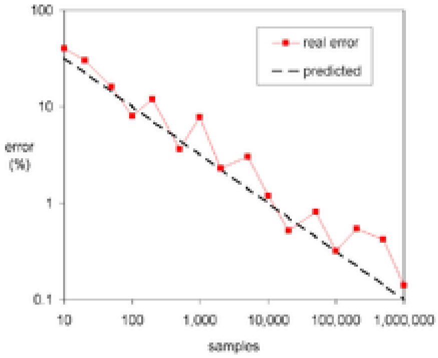
Search and rescue

General usage

- Mathematics

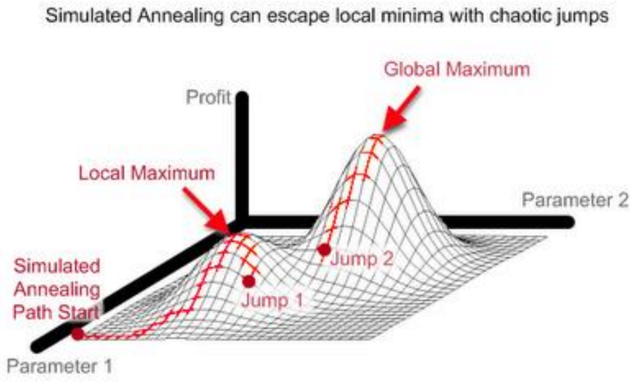
1. Integration

("curse of dimensionality". CLT: $\frac{1}{\sqrt{N}}$ convergence)



2. Simulation and optimization

(minimize or maximize functions)



3. Inverse problems

Metrological usage

- Measurement uncertainty → LPU: contains limitations
- Monte Carlo: versatile, broader class of problems can be addressed
- JCGM 101:2008 (supplement 1): guidance

Metrological usage

- Typical problems of LPU
  1. The contributory uncertainties are not of approximately the same magnitude
  2. It is difficult or inconvenient to provide the partial derivatives of the model, as needed by the LPU
  3. The PDF for the output quantity is not a Gaussian distribution or a scaled and shifted t-distribution
  4. An estimate of the output quantity and the associated standard uncertainty are approximately of the same magnitude
  5. The models are arbitrarily complicated and
  6. The PDFs for the input quantities are asymmetric

Metrological usage

- MC could be an alternative when
  1. Linearization of the model provides an inadequate representation, or
  2. The probability density function (PDF) for the output quantity departs from a Gaussian distribution or a scaled and shifted t-distribution, e.g. due to marked asymmetry

- Validation required
  - ✓ GUM uncertainty framework remains primary approach where it is applicable

MCM WITHIN THE GUM

Stages, conditions, pros & cons-Examples

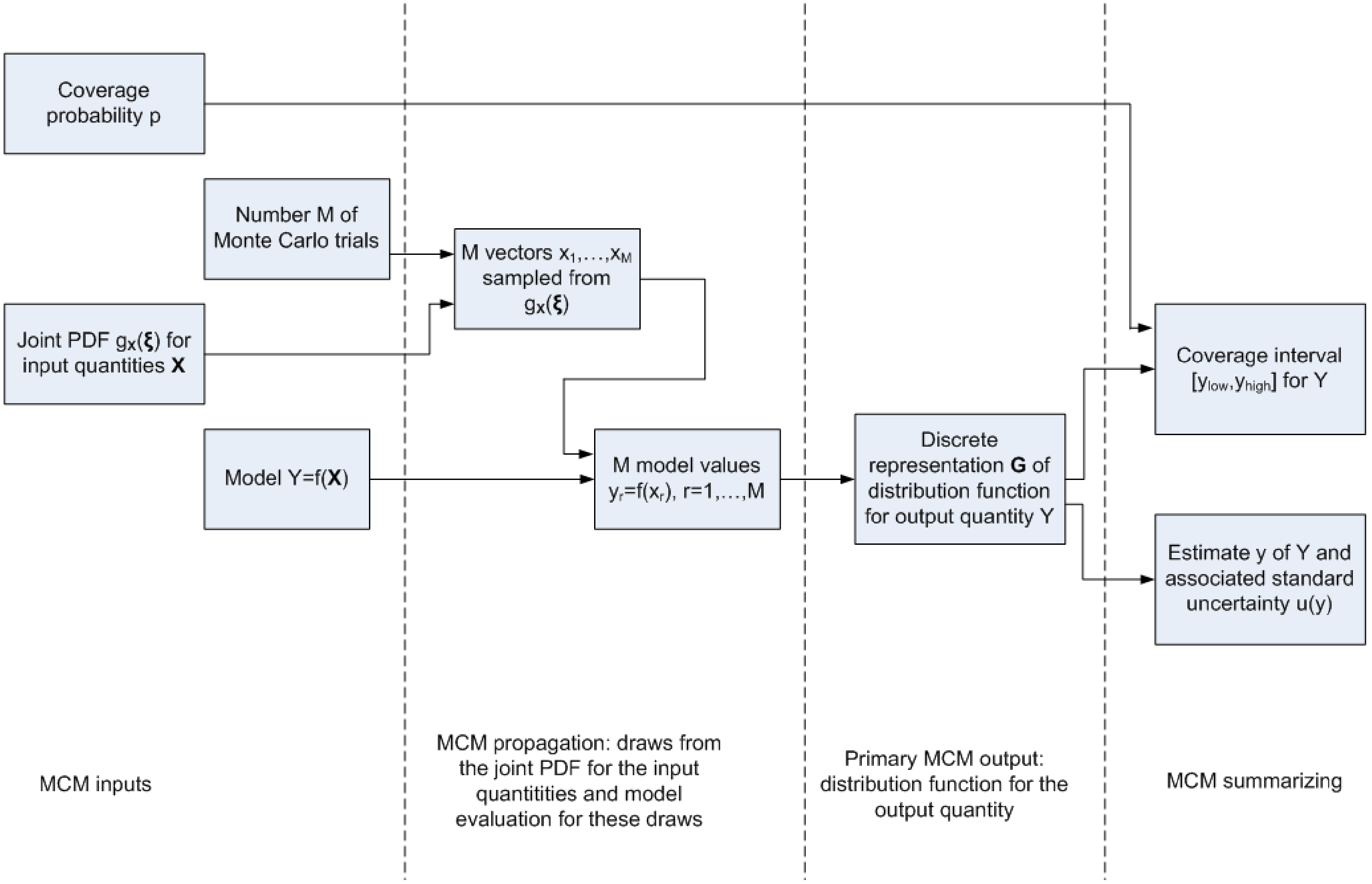
Main stages of uncertainty evaluation

- Formulation:
  1. Define the output quantity Y, the quantity intended to be measured.
  2. Determine the input quantities **X**=$(X_1,\ldots,X_N)^T$ upon which Y depends.
  3. Develop a model relating Y and **X**.
  4. on the basis of available knowledge assign PDFs to the X_i (joint PDF to those not independent).
- Propagation:
  1. Propagate the PDFs.
- Summarizing: use the PDF for Y to obtain
  1. The expectation of Y, taken as an estimate y of the quantity.
  2. The standard deviation of Y, taken as the standard uncertainty u(y).
  3. A coverage interval containing Y with a specified probability.

Main stages: Monte Carlo

- Propagation
  1. Select the number M of MC trials to be made.
  2. Generate M vectors, by sampling from the assigned PDFs, as realizations of the (set of N) input quantities X_i.
  3. For each such vector, form the corresponding model value of Y, yielding M model values.
  4. sort these M model values into strictly increasing order, using the sorted model values to provide **G** (distribution function).
- Summarizing
  1. Use **G** to form an estimate y of Y and the standard uncertainty u(y) associated with y.
  2. Use **G** to form an appropriate coverage interval for Y, for a stipulated coverage probability p.

Main stages (schematically)



Coverage probability p

Number M of Monte Carlo trials

M vectors $x_1,\dots,x_M$ sampled from $g_X(\xi)$

Joint PDF $g_X(\xi)$ for input quantities **X**

Model Y=f(**X**)

M model values $y_r=f(x_r)$, r=1,…,M

Discrete representation **G** of distribution function for output quantity Y

Coverage interval $[y_{low},y_{high}]$ for Y

Estimate y of Y and associated standard uncertainty u(y)

MCM inputs

MCM propagation: draws from the joint PDF for the input quantitities and model evaluation for these draws

Primary MCM output: distribution function for the output quantity

MCM summarizing

Conditions for valid application

a) f is continuous with respect to the elements X_i of $\mathbf{X}$ in the neighborhood of the best estimates x_i of the X_i

b) The distribution function for Y is continuous and strictly increasing

c) The PDF for Y is: 1) continuous over the interval for which this PDF is strictly positive, 2) udimodal (single-peaked) and 3) strictly increasing (or zero) to the left of the mode and strictly decreasing (or zero) to the right of the mode

d) E(Y) and V(Y) exist

e) A sufficiently large value of M is used

(less restrictive than those for GUM uncertainty framework)

Features of MCM-pros

a) Reduction in the analysis effort required for complicated or non-linear models, especially since the partial derivatives of first- or higher-order used in providing sensitivity coefficients for the law of propagation of uncertainty are not needed

b) Generally improved estimate of Y for non-linear models

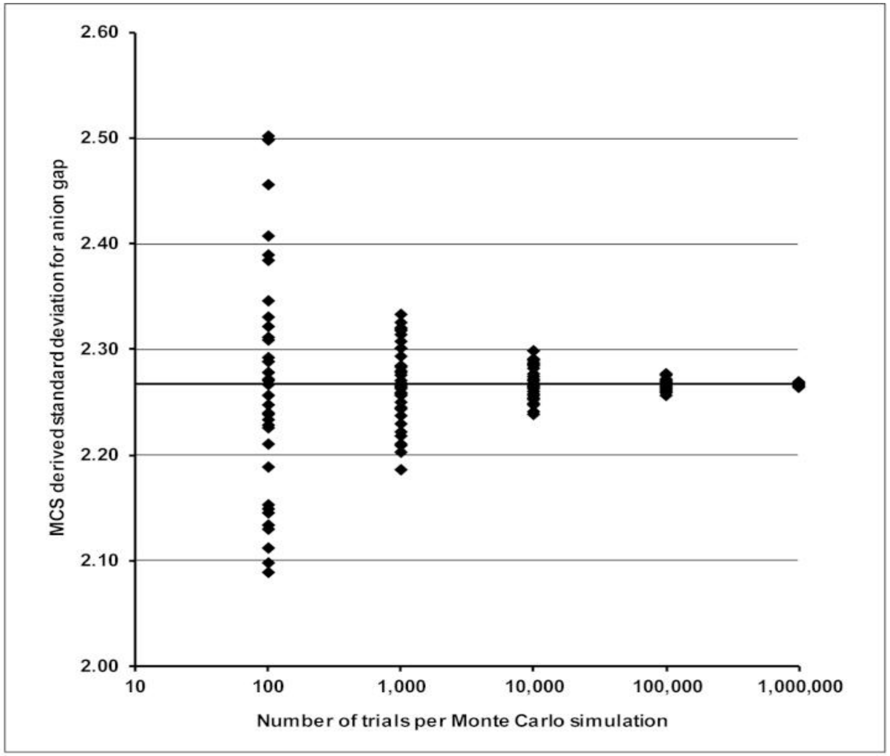
c) Improved standard uncertainty associated with the estimate of Y for non-linear models, especially when the Xi are assigned non-Gaussian (e.g. asymmetric) PDFs, without the need to provide derivatives of higher order

d) Provision of a coverage interval corresponding to a stipulated coverage probability when the PDF for Y cannot adequately be approximated by a Gaussian distribution or a scaled and shifted t-distribution, i.e. when the CLT does not apply.

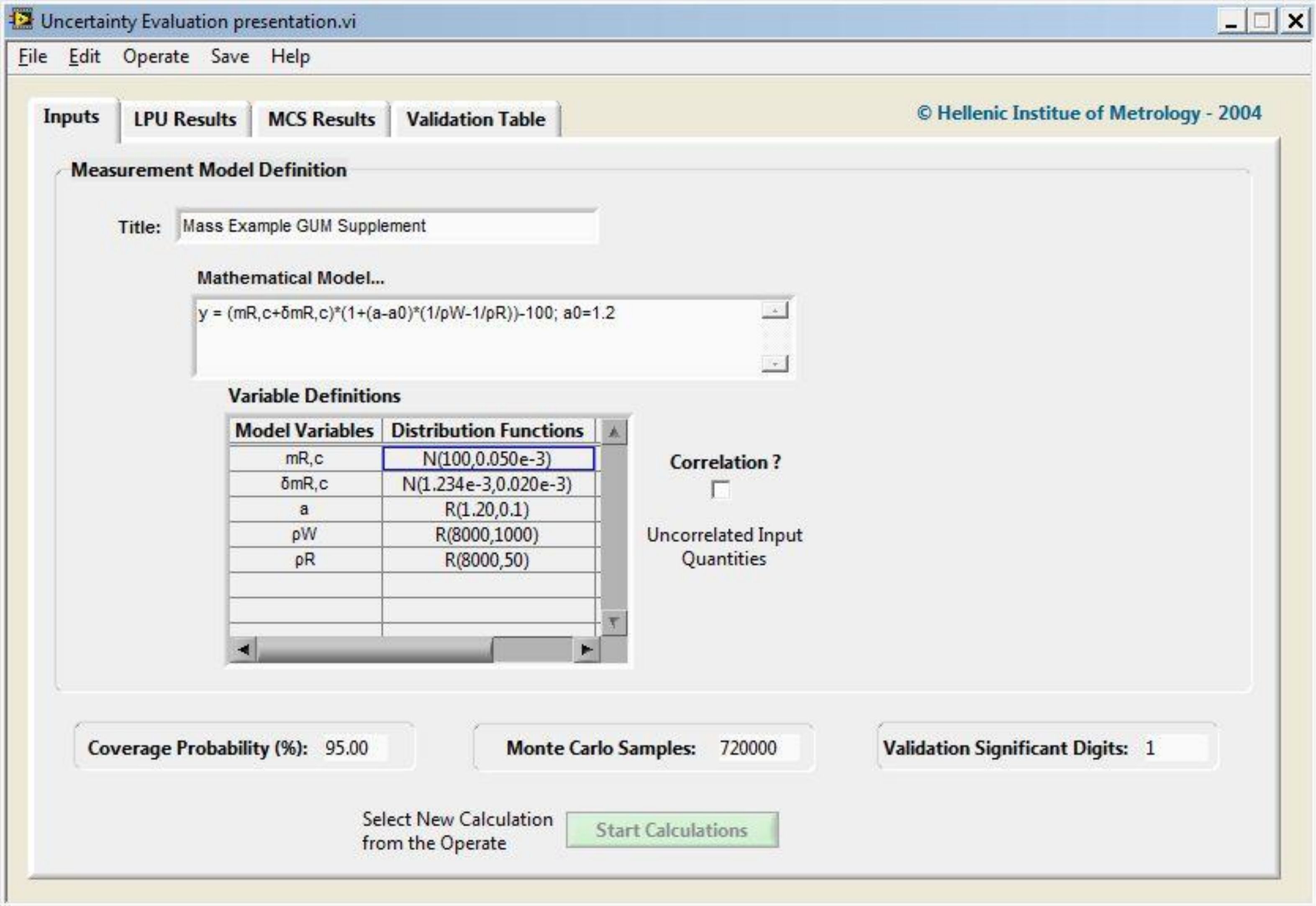
e) A coverage factor is not required when determining a coverage interval

Features of MCM-cons

- a single run of trials does not indicate by itself the reliability of the results
- Criterion for the number of trials: when standard deviation “stabilizes” (alternative: adaptive MC)
- Other possibilities:
  - Pre-assigned value (for example $M=10^6$)
  - Choice of M compared to 1/(1-p) (for example: $M>10^4*1/(1-p)$)



Example: mass calibration



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Measurement Model Definition

Title: Mass Example GUM Supplement

Mathematical Model...

y = (mR,c+δmR,c)*(1+(a-a0)*(1/ρW-1/ρR))-100; a0=1.2

Variable Definitions

Model Variables	Distribution Functions
mR,c	N(100,0.050e-3)
δmR,c	N(1.234e-3,0.020e-3)
a	R(1.20,0.1)
ρW	R(8000,1000)
ρR	R(8000,50)

Correlation ? ☐

Uncorrelated Input Quantities

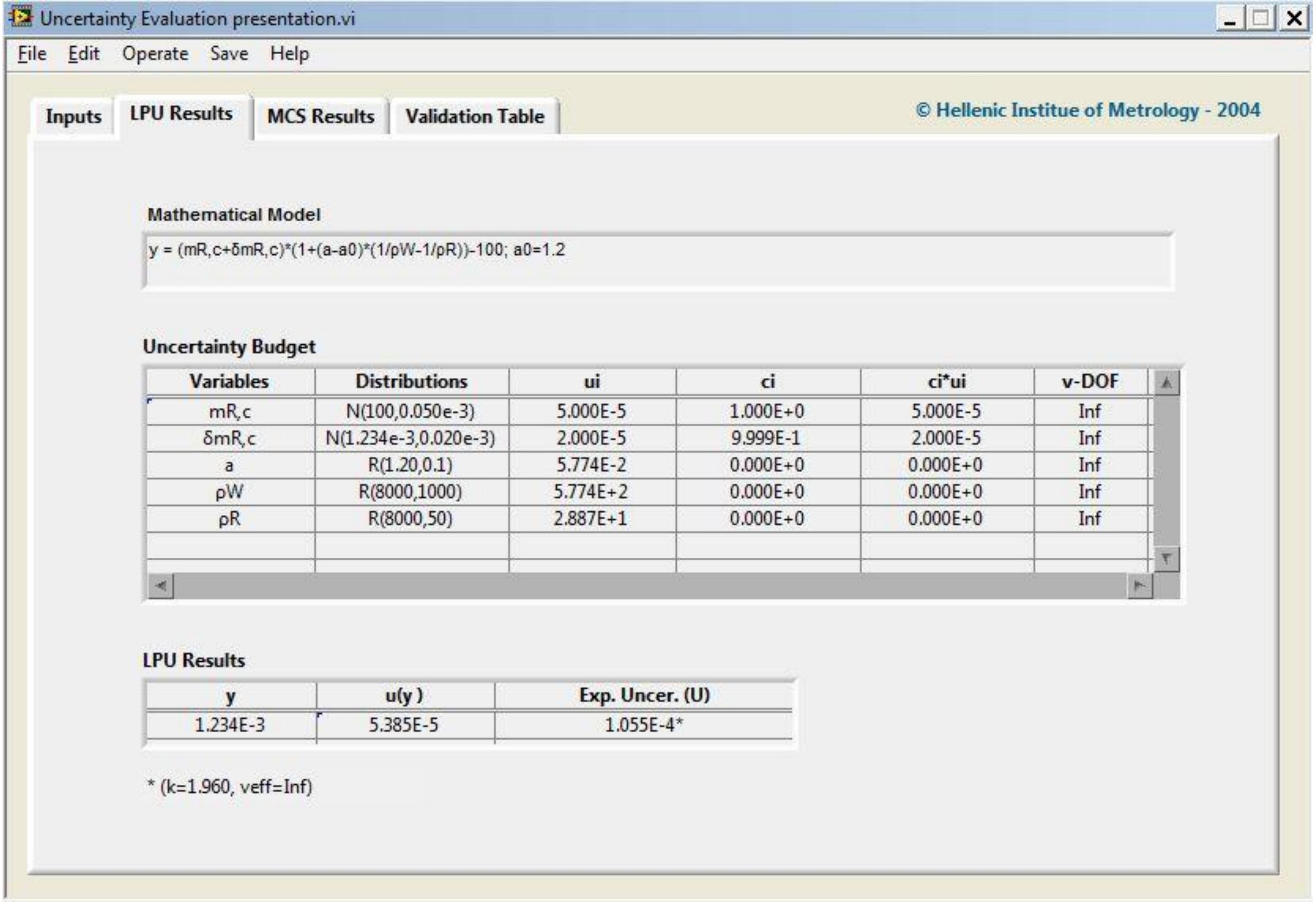
Coverage Probability (%): 95.00

Monte Carlo Samples: 720000

Validation Significant Digits: 1

Select New Calculation from the Operate

Example: mass calibration



Mathematical Model

y = (mR,c+δmR,c)*(1+(a-a0)*(1/ρW-1/ρR))-100; a0=1.2

Uncertainty Budget

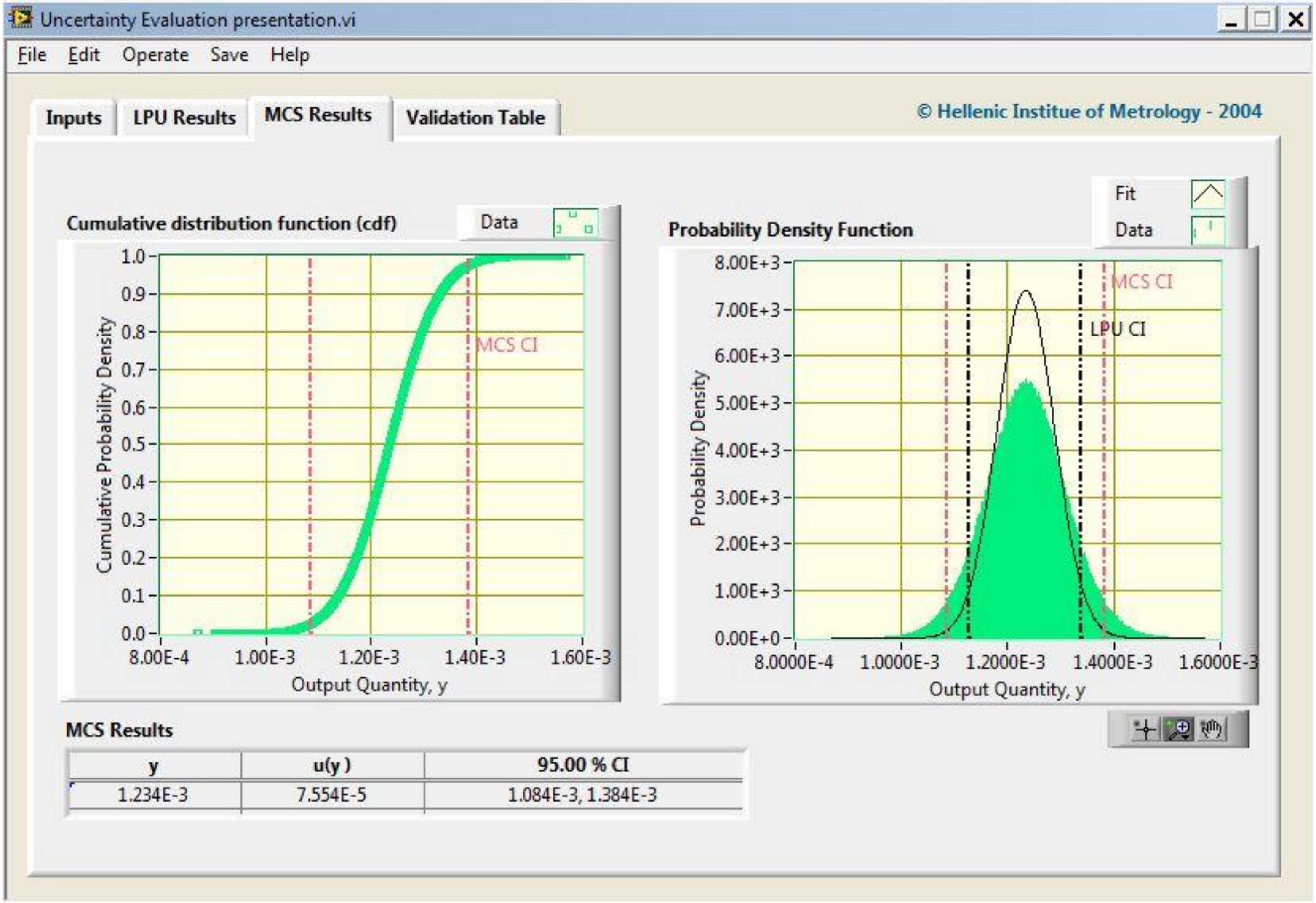
Variables	Distributions	ui	ci	ci*ui	v-DOF
mR,c	N(100,0.050e-3)	5.000E-5	1.000E+0	5.000E-5	Inf
δmR,c	N(1.234e-3,0.020e-3)	2.000E-5	9.999E-1	2.000E-5	Inf
a	R(1.20,0.1)	5.774E-2	0.000E+0	0.000E+0	Inf
ρW	R(8000,1000)	5.774E+2	0.000E+0	0.000E+0	Inf
ρR	R(8000,50)	2.887E+1	0.000E+0	0.000E+0	Inf

LPU Results

y	u(y)	Exp. Uncer. (U)
1.234E-3	5.385E-5	1.055E-4*

* (k=1.960, veff=Inf)

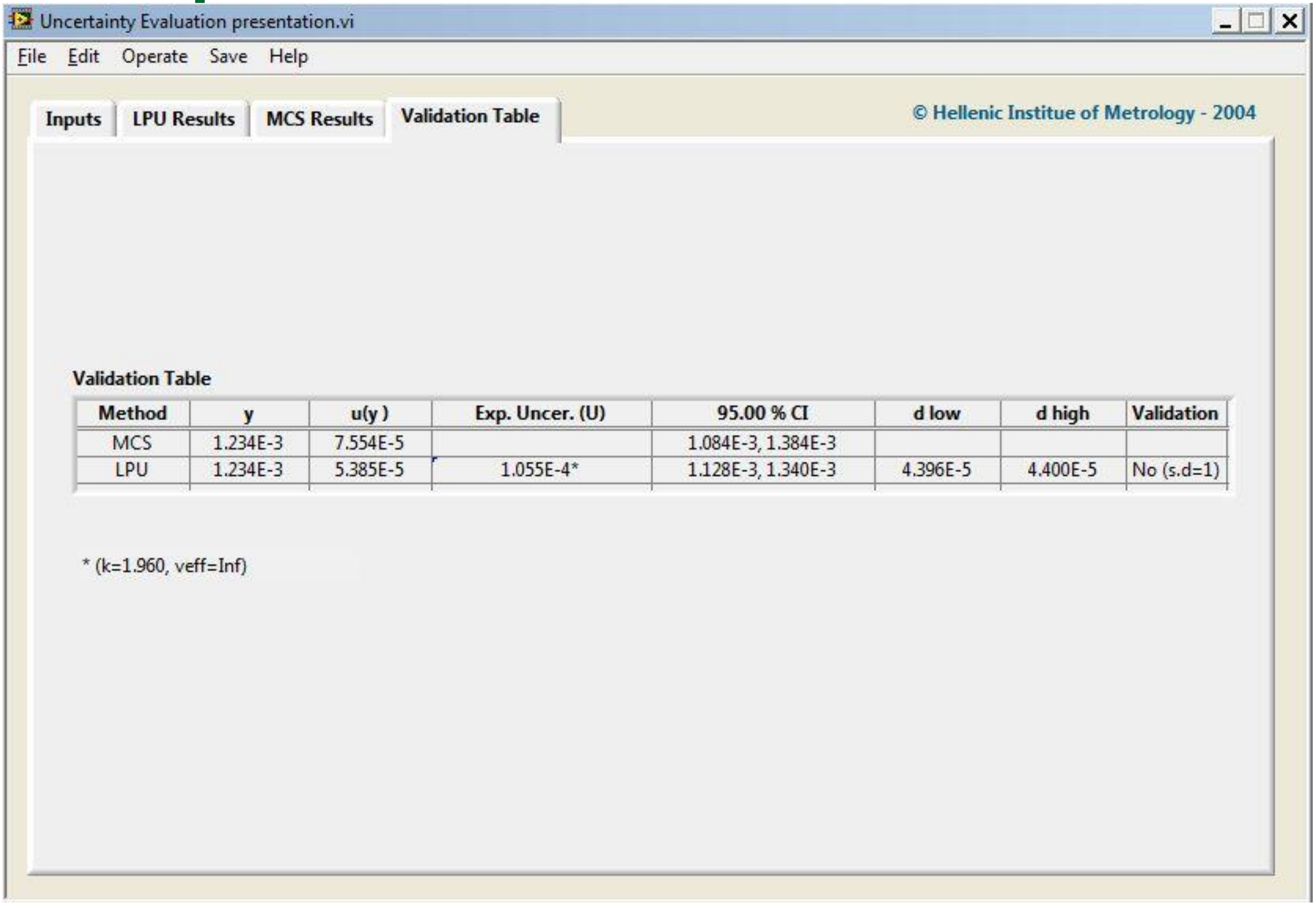
Example: mass calibration



MCS Results

y	u(y)	95.00 % CI
1.234E-3	7.554E-5	1.084E-3, 1.384E-3

Example: mass calibration



Validation Table

Method	y	u(y)	Exp. Uncer. (U)	95.00 % CI	d low	d high	Validation
MCS	1.234E-3	7.554E-5		1.084E-3, 1.384E-3			
LPU	1.234E-3	5.385E-5	1.055E-4*	1.128E-3, 1.340E-3	4.396E-5	4.400E-5	No (s.d=1)

* (k=1.960, veff=Inf)

Example: VNA, 1-port measurements

Calibration equations

$$\begin{bmatrix} \Gamma_n^{O} & 1 & -\Gamma_n^{O}\Gamma_m^{O} \\ \Gamma_n^{S} & 1 & -\Gamma_n^{S}\Gamma_m^{S} \\ \Gamma_n^{L} & 1 & -\Gamma_n^{L}\Gamma_m^{L} \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} \Gamma_m^{O} \\ \Gamma_m^{S} \\ \Gamma_m^{L} \end{bmatrix}$$

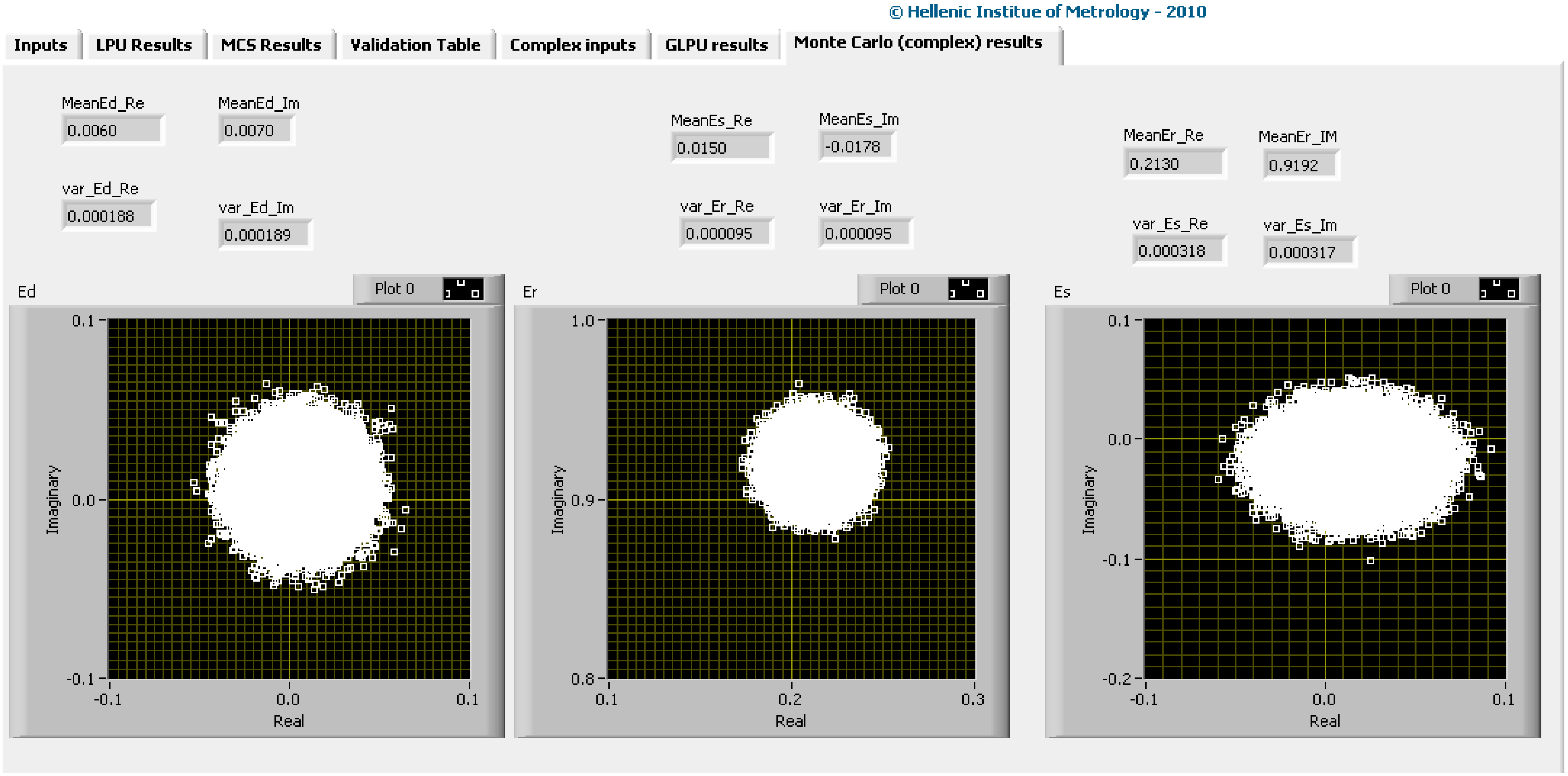
Remaining errors

$$\boldsymbol{E}_D = \boldsymbol{B}$$

$$\boldsymbol{E}_S = -\boldsymbol{C}$$

$$\boldsymbol{E}_R = \boldsymbol{A} - \boldsymbol{BC}$$

Example: VNA, 1-port measurements



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MeanEd_Re 0.0060
MeanEd_Im 0.0070
var_Ed_Re 0.000188
var_Ed_Im 0.000189

MeanEs_Re 0.0150
MeanEs_Im -0.0178
var_Er_Re 0.000095
var_Er_Im 0.000095

MeanEr_Re 0.2130
MeanEr_IM 0.9192
var_Es_Re 0.000318
var_Es_Im 0.000317

Calculation of mean value and covariance matrix using Monte Carlo

Example: VNA, 1-port measurements

E_D	GLPU	MC (10^3)	MC (10^4)	MC (10^5)
Re(E_D)	0.0060	0.0058	0.0059	0.0061
Im(E_D)	0.0070	0.0067	0.0067	0.0070
u[Re(E_D)]	1.89xE-4	1.87xE-4	1.91xE-4	1.90xE-4
u[Im(E_D)]	1.89xE-4	1.84xE-4	1.95xE-4	1.89xE-4

E_S	GLPU	MC (10^3)	MC (10^4)	MC (10^5)
Re(E_S)	0.0150	0.0156	0.0155	0.0151
Im(E_S)	-0.0177	-0.0180	-0.0177	-0.0177
u[Re(E_S)]	3.19xE-4	3.01xE-4	3.26xE-4	3.20xE-4
u[Im(E_S)]	3.19xE-4	3.23xE-4	3.22xE-4	3.18xE-4

Compare results from GLPU and Monte Carlo simulation

SOFTWARE

Commercial-freeware-proprietary

Software implementation for MC

- Commercial software

1. Goldsim: http://www.goldsim.com/Home/
2. Oracle Crystall Ball: http://www.oracle.com/technetwork/middleware/crystalball/
3. Palisade @Risc: http://www.palisade.com/risk/
4. Vose ModelRisk Standard: http://www.vosesoftware.com/
5. Front Line Risk Solver: http://www.solver.com/

Software implementation for MC

- Freeware
  1. http://excelmontecarlo.com/ (tutorial, linux)
  2. Gnumeric: https://projects.gnome.org/gnumeric/
  3. MCS: https://sourceforge.net/projects/mcsimulations/
  4. MonteCarlito: http://www.montecarlito.com/
  5. SimTools: http://home.uchicago.edu/~rmyerson/addins.htm
  6. SimulAr: http://www.simularsoft.com.ar/SimulAr1e.htm
  7. Tukhi: http://tukhi.com/
  8. Xlsim: http://xlsim.com/xlsim/index.html
  9. Yasai: http://www.yasai.rutgers.edu/index.html

Software implementation for MC

- Software of direct metrological interest

1. NIST: http://www.nist.gov/itl/sed/gsg/metrology-for-microsoft-excel.cfm
2. NPL: http://www.npl.co.uk/science-technology/mathematics-modelling-and-simulation/mathematics-and-modelling-for-metrology/software-for-measurement-uncertainty-evaluation
3. GUM Workbench (commercial): http://www.metrodata.de/products_en.html
4. QMsys GUM (commercial): http://www.qsyst.com/qualisyst_en.htm
5. Measurement Software Toolkit (freeware): http://www.msl.irl.cri.nz/services/specialist-user-groups/measurement-software-toolkit/mst-software

- Self-developed solutions

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Magazine articles

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Conference proceedings

- Hall B. D., “A computational technique for evaluating and propagating the uncertainty of complex valued quantities”, Proc. 60th ARFTG, Washington DC, USA, 5-6 December 2002, pp 19-28

References

International Standards and Guidelines

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- JCGM 101:2008, "Evaluation of measurement data-Supplement 1 to the "Guide to the expression of uncertainty in measurement"-Propagation of distributions using a Monte Carlo method", 2008, electronic form
- JCGM 102:2009, "Evaluation of measurement data-Supplement 2 to the "Guide to the expression of uncertainty in measurement"-Models with any number of output quantities", 2009 (draft), electronic form

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Books

- Lira I., "Evaluating the measurement uncertainty: Fundamentals and practical guidance", I*o*P, 2002
- William L. Dunn, J. Kenneth Shultis-Exploring Monte Carlo Methods-Academic Press (Elsevier), 2011
- Victor (Wai Kin) Chan, "Theory and applications of Monte Carlo simulations", Intech, 2013 (open access: http://www.intechopen.com/books/theory-and-applications-of-monte-carlo-simulations)

CONCLUSIONS

Conclusions

- Monte Carlo method: versatility, can replace GUM uncertainty framework where it fails
- Care must be taken concerning choice of M, random generators.
- Multitude of available tools: which one to choose? Is a combination advisable?

Thank
You
For
Your
attention