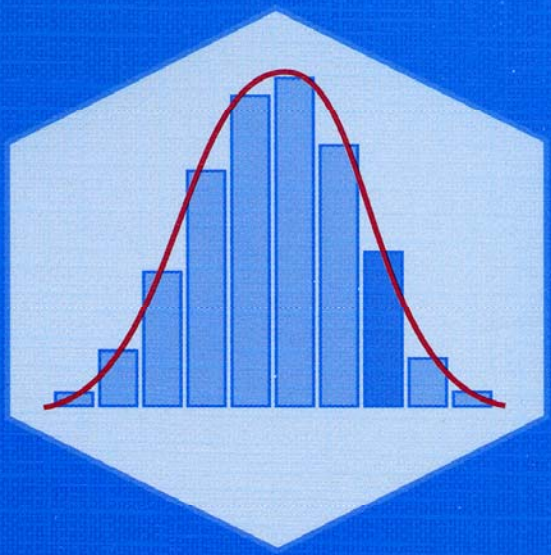
Erwin Achermann

MUSAC - a Tool for Evaluating Measurement Uncertainty



Verlag Dr. Kovač

Schriftenreihe

Forschungsergebnisse der Programmentwicklung

Band 13

ISSN 1435-6287

In der Schriftenreihe ***Forschungsergebnisse der Programmentwicklung*** werden neue wissenschaftliche Arbeiten zur Programmentwicklung veröffentlicht.

Verlag Dr. Kovač

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VERLAG DR. KOVAČ

Arnoldstraße 49 · 22763 Hamburg · Tel. 040 - 39 88 80-0 · Fax 040 - 39 88 80-55

E-mail vdk@debitel.net · Internet www.verlagdrkovac.de

Die Deutsche Bibliothek - CIP-Einheitsaufnahme

Achermann, Erwin:
MUSAC - a tool for evaluating measurement uncertainty /
Erwin Achermann. – Hamburg : Kovač, 2002
(Forschungsergebnisse der Programmentwicklung ; Bd. 13)
Zugl.: Zürich, Eidgenössische Techn. Hochsch., Diss., 2002

ISSN 1435-6287
ISBN 3-8300-0679-9

Umschlaggestaltung: Tia Thomas

Printed in Germany

Gedruckt auf säurefreiem, alterungsbeständigem Recyclingpapier RecyStar
(Nordic Environmental Label – Blauer Engel – DIN ISO 9706).

To Jil, Sandra and my family

Summary

MUSAC is a software project to assist the determination of measurement uncertainty in Analytical Chemistry and other fields. In order to satisfy the new ISO norms measurement laboratories must indicate the combined measurement uncertainties along with the measurement results. The software system MUSAC calculates the combined measurement uncertainty by automatically performing sensitivity analysis on a model description of the measurement method at hand.

This thesis introduces a new description language called M. It is intended to describe measurement procedures with a focus on uncertainty evaluation. The MUSAC-system analyzes the description and evaluates the combined standard uncertainty for a given measurement procedure according to ISO 17025 or by other methods such as Monte Carlo Simulations.

Zusammenfassung

MUSAC ist ein Software-Projekt, das die Ermittlung der Messunsicherheit im Bereich der analytischen Chemie oder auch in anderen Gebieten unterstützt. Neue ISO-Normen verlangen von Analysenlabors die Angabe der kombinierten Messunsicherheit zusammen mit den Messresultaten.

Diese Arbeit stellt eine neue Beschreibungssprache M vor. Sie beschreibt Messprozeduren mit einem speziellen Fokus auf anschliessende Unsicherheitsauswertungen. Das Computersystem MUSAC analysiert die Beschreibung für eine gegebene Messprozedur und wertet deren kombinierte Standardunsicherheit nach ISO 17025 oder auch nach anderen Methoden aus.

Oh Dear,
this was not my fault!

Acknowledgments

MANY persons have contributed to this work. It would never have come into existence without their initiative, their help and their patience. In 1997 Matthias Rösslein from EMPA, co-editor and member of the EURACHEM working group, asked Walter Gander of the Institute of Scientific Computing at ETH (IWR) for a problem of measurement uncertainty. Walter Gander handed the task over to me and it thus became my thesis. I am thankful and greatly indebted to both of them for initiating the project, offering me the possibility to work on it as I liked, introducing me to many interesting people and for pushing me gently towards a reasonable piece of work. I also thank Bruno Wampfler from EMPA and Walter Gander for supporting me on their budgets during the last years. Furthermore, this project was labeled by Eureka Project E!1910 MUSAC. And I thank the Kommision für Industrie und Technologie (KTI) for financial support in this project.

Whilst implementing the MUSAC-system many problems from a wide range of complexity revealed themselves. Some of them were easily solved, the solutions to others were not so obvious. Several questions were downright hard to understand at all. Once such questions were cleared, however, their solutions were often amazingly clear, too. Long-winded discussions with "non-computer scientists" taught me that the same concept can have more than one name. And it is sometimes even hard to recognize an accepted and agreed on concept in a foreign terminology.

Uncountable discussions with Matthias Rösslein, Rolf Strebel and Oscar Chinellato, both from IWR, were the source of ideas implemented in the presented MUSAC-system. Guys, it was fun and I enjoyed very much arguing with you. I thank you for letting me reject some of your ideas, and I thank you even more for letting me use and implement ideas that sometimes were clearly not mine. I would also like to include my colleagues at IWR Oliver Bröker, Leonhard Jaschke and Roman Geus into this round of thanks for the

many fruitful and vivid discussions we had during the last few years about life, the universe and everything; and Leo, thanks for all the Knigge!

During the development of MUSAC the so called "MUSAC core group" gathered on a regular basis. I thank all the members of this group for patiently explaining and clarifying things to me. In particular I would like to thank Wolfhard Wegscheider from Montanuniversität Leoben in Austria and Arnold Cziurlok from Metrohm on this behalf.

The MUSAC-implementation described in this text is only half of the story, the other half is the user interface. It was implemented and designed by people at *creasoft ag*. I thank Stefan Matt, Marco Wolf and Martin Müller for giving an attractive look and feel to my dry machinery and for their fruitful and seamless cooperation. Especially, I congratulate Martin Müller from TU München for his successful diploma thesis on "Drawing Cause and Effect Diagrams".

It was a fun piece of work for me to implement the MUSAC-system. But it was less fun to write the text presented here. I bored several persons with intermediate versions of this manuscript and they helped me streamline my jolty English considerably. I cordially thank on this behalf Walter Gander, Wolfhard Wegscheider, Matthias Rösslein, Rolf Strebel, Oscar Chinellato and Lisa von Boehmer CS-student at ETH. I especially thank Marc Salit from NIST in USA and Alfred Jacob, the Spiez Laboratory representative in the "MUSAC core group", for providing the data and the protocols needed for real life examples.

I also wish to thank Wolfram Bremser from BAM for the friendly invitation to Berlin, Maurice Cox for the hospitality at NPL in London, Alex Williams, former head of LGC, chairman and co-editor of the EURACHEM working group and "father of INC-1", for the interesting discussion about calibration and means, as well as Franz Achermann, my brother, for analyzing an early version of my code. My apologies to all those that have supported or helped me in any way over the past years and that I have forgotten to mention here.

Last but not least, I express my gratitude to my parents for all that they have done for me; and finally thanks to my wife Sandra for giving me her patience and her impatience and a big hug to my little daughter Jil for trustfully counting on me.

Contents

1 Measurement Uncertainty **1**
1.1 Historical review . . . 3
1.2 Goal of this Work . . . 5
1.3 What's new . . . 6

2 Mathematical Concepts **9**
2.1 What is a Measurement . . . 9
2.1.1 Definitions . . . 9
2.2 Different Approaches . . . 13
2.2.1 Random variables . . . 13
2.2.2 Mathematical Model . . . 22
2.2.3 ISO Guide: First Order Approximation . . . 27
2.2.4 Simple Rules . . . 27
2.2.5 Monte Carlo Simulation . . . 28
2.3 Calibration . . . 30
2.3.1 Calibration and Measurement . . . 30
2.3.2 Calibration Models . . . 31
2.3.3 Computations . . . 36
2.3.4 Measurement . . . 43
2.3.5 Truncated SVD Solver . . . 44
2.3.6 Numerical Comparisons and Simulations . . . 48
2.3.7 Final remarks on Regression . . . 54

3 M description **57**
3.1 Compiling and Interpreting . . . 58
3.2 Language M . . . 59

3.2.1 Extended Backus-Naur Form (EBNF) . . . 59
3.2.2 Grammar of M . . . 61
3.2.3 Token definitions for M . . . 63
3.2.4 Example: Grammar for Units . . . 63
3.2.5 Complete Grammar of M . . . 65

4 Semantics of M **69**
4.1 Expression . . . 69
4.1.1 Equation . . . 70
4.1.2 Leaf . . . 70
4.1.3 Units . . . 72
4.2 Attribute List . . . 74
4.3 Functions . . . 75
4.3.1 Predefined Functions . . . 78
4.4 Measurement . . . 85

5 Implementation **93**
5.1 General Architecture . . . 93
5.2 COM Interface . . . 95
5.3 Several Modules . . . 99
5.3.1 SI-Units . . . 99
5.3.2 Parser . . . 113
5.3.3 Visitor Pattern . . . 116
5.3.4 Drawing Cause and Effect Diagrams . . . 122
5.3.5 The program *Uncertainty Manager* . . . 123

6 Real Life Application **127**
6.1 Certification of Bismuth content in SRM 3106 . . . 129
6.1.1 NIST SRM Program . . . 129
6.1.2 High Performance ICP-OES . . . 130
6.2 Measuring calcium content in spring water . . . 136

7 Conclusion **169**