Mathematical Software

Digital Library of Mathematical Functions

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http://dlmf.nist.gov/

Scientific and engineering professionals need ready access to detailed technical data, including mathematical data. NIST has a solid reputation for serving this need with the publication of handbooks and, more recently, computer databases accessible from the World Wide Web.

The *NBS Handbook of Mathematical Functions*, published in 1964 with Milton Abramowitz and Irene Stegun as editors, is a particularly significant example of a mathematics handbook. The foundations for the analysis and modeling of scientific problems in mathematical terms that are covered in the NBS Handbook remain as valid today as when it was published, as evidenced by the fact that both sales and citations remain strong. These foundations have been added to since 1964 but hardly anything has become irrelevant. The NBS Handbook covers the major properties of selected special functions—definitions, graphs, derivatives and differential equations, integrals and integral representations, recurrence relations, power series and other convergent expansions, asymptotic expansions, interrelationships among different functions, and so on—as well as similar properties of the elementary functions. New special functions have come into importance in applications, and new applications as well as new properties have been found for the old ones since the Handbook was published. Examples are the nonlinear Painlevé transcendents and hyperasymptotic analysis. The NBS Handbook also contains approximations, algorithms and masses of tabular data for numerical evaluation of the functions. This material is badly out-of-date due to the dramatic rise of computational power.

The first objective of the Digital Library of Mathematical Functions (DLMF) Project is to determine current and anticipated future usage of special functions in applied mathematics, and to write a new DLMF Handbook. The new Handbook will supersede the original NBS Handbook, and in particular it will contain current information on computation. The DLMF Project has a second objective, which is to construct a free public web site at NIST that will offer the same information as the new Handbook, but in a form that can provide many advantages—downloading of formulas into word processors and computer algebra systems, generation of tables and graphs on demand, three-dimensional visualizations that can be rotated and viewed from any direction, mathematics-aware search, links to sources of computer programs at external sites, and simple symbolic transformations of formulas to accommodate notational or definitional characteristics of a particular application area. Some of these capabilities will exist in the initial release of the DLMF Web Site while others will be the subject of ongoing research and development efforts. For example, members of the NIST staff on the DLMF Project are participating in such external initiatives as the following.

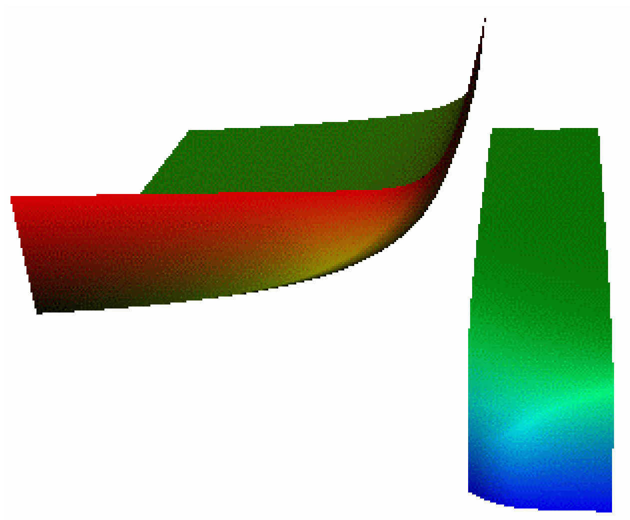
- OpenMath (www.openmath.org)
- MathML (www.w3.org/Math)
- Java Grande (www.javagrande.org)
- OMDoc (www.mathweb.org/omdoc)
- CEIC (www.ceic.math.ca).

The editorial leadership of the DLMF Project consists of four editors at NIST and nine associate editors from outside NIST. The DLMF Handbook will have approximately 40 chapters. Outside authors are writing most of the chapters under contract to NIST with funds provided by the NSF. The NIST staff is preparing the print and electronic versions. More than 15 members of the NIST staff have contributed to the project. The print edition will be finalized and marketed by an outside publisher in the third quarter of 2004, and the DLMF Web Site will be released simultaneously.

Major accomplishments are the result of team efforts. In FY 2002 these include:

- The NIST editors are exercising strict control over the style and content of chapters. Substantial revisions of initial drafts have almost always been necessary. By the end of November 2002, satisfactory drafts of 27 chapters had been received. The remaining chapters are expected in the first quarter of 2003.
- Each chapter will be checked for accuracy by an outside validator under contract to NIST with funds provided by the NSF. The NIST editors have completed a written guide for the validators. The first validation contracts will be established in the first quarter of 2003.
- The NIST editors conduct a meeting with the associate editors once per year. This year's meeting was held at the University of Minnesota on July 27 and 28, 2002. All but one associate editor was present. NIST staff prepared two documents for discussion at the meeting: a 2-volume expanded printout of every chapter, showing all source material for the DLMF Handbook and Web Site; and a draft mini-handbook consisting of 7 chapters with front and back matter (title page, table of contents, and index) in the double-column large-page format that will be used in the eventual printed edition of the DLMF.
- A highly augmented version of AMS-LaTeX, under continuous development by NIST staff, is being used to store source material from the authors in a computer database. Prototypes of both the printed and Web versions of the DLMF have been produced from this database. Work is underway to improve the translation of database material into alternative electronic formats such as XML and HTML.
- The bibliography is an important part of the DLMF, both for identifying sources of proofs and for referring to extensions of material included in the DLMF. NIST staff is constructing and checking the bibliography with the aid of the Math Reviews (MR) and other bibliographic resources. The bibliography will include MR and Digital Object Identifier (DOI) links to reviews and full texts of articles wherever possible.
- Great attention is being paid to graphics and visualizations in the DLMF, some of which will be available only in the Web version. VRML is being used to construct 3D surfaces of functions that can be rotated and zoomed with a readily available free browser plug-in. Color is being used to represent height or, for complex functions, phase. The basic VRML capabilities are being extended in various ways to offer the user options for labeling, scaling, and viewing 2D slices. Currently there are more than 110 VRML figures, plus about 100 2D figures, including 25 other figure types (contour and density plots, bifurcation diagrams).

- Indexes are important for books but a search engine is needed also for the Web edition. The problem is that the search engine needs to work with mathematical queries. A NIST guest researcher has made good progress in developing a simple LaTeX-like system that allows interpretation of queries relevant to the DLMF. The system uses PLWeb, a publicly available search engine. The current interface displays all equations that satisfy the query, each with a link that can be followed to move to its occurrence in the DLMF.



Visualization of $\Pi(\alpha^2,k)$. View of the complete elliptic integral $\int^{\pi/2}_0 (1 - k^2\sin^2\theta)^{-1/2} (1 -\alpha^2\sin^2\theta)^{-1} d\theta$ for $-2 \le k^2 < 1$ and $-2 \le \alpha^2 \le 2$. Shown are the discontinuity of the surface at $\alpha^2 = 1$, the behavior of the surface as α approaches unity from below and above (left and right parts of the surface, respectively), and the behavior of the surface as $k^2 \uparrow 1$ (foreground). For fixed $k^2 < 1$, $\Pi(\alpha^2,k) \to + \infty$ as $\alpha^2 \uparrow 1$ but $\Pi(\alpha^2,k) \to K(k) - E(k)/\sqrt{(1 - k^2)}$ (finite) as $\alpha^2 \downarrow 1$, where $K(k)$ and $E(k)$ are complete elliptic integrals of the first and second kinds. As $k^2 \uparrow 1$, $\Pi(\alpha^2,k) \to + \infty$ for fixed $\alpha.^2 < 1$ and $\Pi(\alpha^2,k) \to - \infty$ for fixed $\alpha^2 > 1$; more specifically, $\Pi(\alpha^2,k) \sim (1-\alpha^2)^{-1} \ln(4/\sqrt{(1-k^2)})$. On the DLMF Web Site the user can rotate this view and see it from any angle.

Considerable external recognition of the DLMF has occurred because of the importance of its subject matter and because it is the first large effort to construct a widely accessible body of technical mathematics on the Web. For example, a two-week IMA Summer Workshop took place at the University of Minnesota from July 22 through August 2, 2002. The theme was *Special Functions in the Digital Age*. Observing that the traditional handbook format is becoming obsolete, the purpose of the workshop was to formulate, though concrete examples and experiences, the role and character of digital libraries in mathematics, and to forecast the mathematical and applied fields that would benefit from such libraries. Two of the NIST editors were on the organizing committee, and one of them gave the opening presentation. One-hour talks were given by most of the NIST editors and staff, as well as by many of the associate editors and authors.

Possible outgrowths of the DLMF Project, in addition to maintenance tasks such as errata and Web improvements, include a second edition, reference algorithms for the validated computation of special functions, a digital library in another field of mathematics, R&D in issues related to mathematics and the Web, and R&D in issues related to formalization of mathematics using computers.

NIST Strategic Focus Areas. *Emerging Industries:* Information and Knowledge Management.

DLMF Editors meeting at the Institute for Mathematics and Its Applications, Minneapolis, July 2002. From left to right: F. Olver, C. Clark, I. Olkin, M. Berry, W. Gautschi, D. Lozier, N. Temme, W. Reinhardt, P. Paule, R. Askey.

Information Services for Computational Science

Ronald Boisvert
Joyce Conlon
Marjorie McClain
Bruce Miller
Roldan Pozo

http://math.nist.gov/
http://gams.nist.gov/
http://math.nist.gov/MatrixMarket/

MCSD continues to provide Web-based information resources to the computational Science research community. The first of these is the Guide to Available Mathematical Software (GAMS), a cross-index and virtual repository of some 9,000 mathematical and statistical software components of use in science and engineering research. Both public domain and commercial software supported for use on NIST central computers is cataloged, as well as software assets distributed by *netlib*. GAMS users locate software via several search mechanisms. The most popular is the GAMS Problem Classification System, which provides a tree-structured taxonomy of standard mathematical problems solvable by extant software. Major math software library vendors have also adopted it.

A second resource provided by MCSD is the Matrix Market, a visual repository of matrix data used in the comparative study of algorithms and software for numerical linear algebra. The Matrix Market database contains more than 400 sparse matrices from a variety of applications, along with software to compute test matrices in various forms. A convenient system for searching for matrices with particular attributes is provided. The web page for each matrix provides background information and visualizations.

Web resources developed by MCSD continue to be among the most popular at NIST. The MCSD Web server at math.nist.gov has serviced more than 50 million Web hits since its inception in 1994 (12 million of which have occurred in the past year!). The Division server regularly handles more than 11,000 requests for pages each day, serving more than 411,000 distinct hosts on a yearly basis. Altavista has identified more than 8,500 external links to the Division server. Seven MCSD sites are listed in ITL's top 10:

1. NIST Math Portal, http://math.nist.gov/
2. Matrix Market, http://math.nist.gov/MatrixMarket/
3. Guide to Available Mathematical Software: http://gams.nist.gov/
4. Division home page: http://math.nist.gov/mcsd/
5. ACM Transactions on Mathematical Software: http://math.nist.gov/toms/
6. Digital Library of Mathematical Functions: http://dlmf.nist.gov/
7. Template Numerical Toolkit: http://math.nist.gov/tnt/

The GAMS home page is downloaded more than 28,000 times per month by some 18,000 hostnames. The Matrix Market has distributed more than 42 Gbytes of matrix data, including nearly 120,000 matrices, since its inception.

NIST Strategic Focus Areas. *Emerging Industries:* Information and Knowledge Management.

Java Numerics

Ronald Boisvert
Roldan Pozo
Bruce Miller

http://math.nist.gov/javanumerics/
http://math.nist.gov/scimark/

Java, a network-aware programming language and environment developed by Sun Microsystems, has already made a huge impact on the computing industry. Recently there has been increased interest in the application of Java to high performance scientific computing. MCSD is participating in the Java Grande Forum (JGF), a consortium of companies, universities, and government labs who are working to assess the capabilities of Java in this domain, and to provide community feedback to Sun on steps that should be taken to make Java more suitable for large-scale computing. The JGF is made up of two working groups: the Numerics Working Group and the Concurrency and Applications Working Group. The former is co-chaired by R. Boisvert and R. Pozo of MCSD. Among the institutions participating in the Numerics Working Group are: IBM, Sun, SAS Institute, Visual Numerics, Waterloo Maple, Florida State University, the University of Tennessee at Knoxville, and the University of Manchester.

Earlier recommendations of the Numerics Working Group were instrumental in the adoption of a fundamental change in the way floating-point numbers are processed in Java. This change will lead to significant speedups to Java code running on Intel microprocessors like the Pentium. The working group also advised Sun on the specification of elementary functions in Java, which led to improvements in Java 1.3. The specification of the elementary functions was relaxed to tolerate errors of up to one unit in the last place, permitting more efficient implementations to be used. A parallel library, java.lang.StrictMath, was introduced to provide strictly reproducible results. The Numerics Working Group continues to advise Sun on issues related to floating-point computation.

This year, MCSD presented the findings of the Working Group in a variety of forums, including

- Joint Workshop of the Organisation Associtave du Parallelisme (ORAP), and the Swiss Forum for High-Performance Computing (SPEEDUP), Lyon, France (October 2001).
- Seminar, University of Tennessee at Knoxville (February 2002)
- Seminar, Sandia National Laboratoies, Albuquerque (March 2002)
- Java Grande / ISCOPE Conference, Seattle (November 2002)

MCSD staff also worked on the organization of a number of events related to Java.

- Ronald Boisvert was a member of the Program Committee of the ACM Java Grande / ISCOPE conference, which was held in conjunction with ACM's OOPSLA Conference in Seattle in November 2002.
- Ronald Boisvert and Roldan Pozo co-chaired a half-day meeting of the Java Numerics Working group, which was held in conjunction with the Java Grande Conference in Seattle in November 2002.

The NIST SciMark benchmark continues to be widely used. SciMark includes computational kernels for FFTs, SOR, Monte Carlo integration, sparse matrix multiply, and dense LU factorization, comprising a representative set of computational styles commonly found in numeric applications. SciMark can be run interactively from Web browsers, or can be downloaded and compiled for stand-alone Java platforms. Full source code is provided. The SciMark result is recorded as megaflop rates for the numerical kernels, as well as an aggregate score for the complete benchmark. The current database lists results for more than 1,500 computational platforms, from laptops to high-end servers.

As of December 2002, the record for SciMark is 380 Mflops, a 38% improvement over the best reported one-year ago (275 Mflops).

NIST continues to distribute the JAMA linear algebra class for Java that it developed in collaboration with the MathWorks several years ago. More than 4,500 copies of this software were downloaded by 3,100 hosts during the last 12 months.

NIST Strategic Focus Areas. *Emerging Industries:* Information and Knowledge Management.

TNT: Object Oriented Numerical Programming

Roldan Pozo

http://math.nist.gov/tnt/

MCSD maintains an active research program in the design of object-oriented mathematical software libraries. A by-product of this work has been some of the most highly used object-oriented linear algebra packages, including Lapack++, Iterative Methods Library (IML++), Sparse Matrix Library (SparseLib++), Matrix/Vector Library (MV++), and most recently the Template Numerical Toolkit (TNT). The latter package was downloaded more than 9,000 times during the past 12 months, for example, and is currently in use in a variety of industrial and commercial applications. This year saw two major software releases and new web site configuration.

TNT incorporates many of the ideas we have explored with previous designs, and includes new techniques that were difficult to support before the implementation of ANSI C++ compilers. The package includes support for both C and Fortran multidimensional array layouts, array sections, and application modules, such as linear algebra, which includes fundamental algorithms (LU, Cholesky, SVD, QR, and eigenvalues) as well as basic support for sparse matrices.

With the latest releases of TNT (version 1.1) we have designed a separation of the interface specification from the actual implementation. Thus, TNT formally defines a numeric interface that can be incorporated into several implementations. This allows library developers to develop specialized modules that take advantage of particular hardware platforms, utilize vendor-specific libraries, or implement different C++ strategies, such as expression templates, or instrumented versions for debugging sessions. The TNT web site provides a basic implementation for testing and development, as well as links to other library packages that utilize the TNT interface. Full documentation and source code for all TNT components are available on-line.

NIST Strategic Focus Areas. *Emerging Industries:* Information and Knowledge Management.

Matwrap: A Fortran 95 Wrapper for Matrix Operations

G. W. Stewart

Matrix-oriented languages like MATLAB provide an extremely convenient user interface for matrix computations. But when high-performance is necessary, users must still resort to traditional programming languages like Fortran. In this project we are exploring library designs that can make programming linear algebra algorithms in traditional Fortran nearly as painless as in MATLAB.

Matwrap is a collection of defined types and subprograms in Fortran 95 that implements matrix operations and computes matrix functions and decompositions. Although Matwrap is not based on formally defined matrix language, the results of using Matwrap are akin to coding in a subset of matrix-oriented languages like MATLAB and OCTAVE. By using routines from LAPACK and the BLAS, Matwrap allows the user to obtain the computational advantages of these packages with minimal fuss and bother.

Matwrap defines types for real and complex matrices (currently only real) and operators for the common matrix operations (addition, multiplication, and multiplication by an inverse). It also provides operations for combining matrices and extracting submatrices. Common matrix functions, like norms, are also included. Matwrap provides types for the following decompositions: pivoted LU decomposition, Cholesky decomposition, pivoted and unpivoted QR decompositions, spectral decomposition of a symmetric matrix, eigenvalue-eigenvector decomposition of a general matrix, and singular value decomposition. Matwrap provides means of reusing decompositions, as, for example, when one wishes to solve several linear systems all having the same matrix.

Matwrap is modularized at a fine-grained level. This means that the programmer can pick and choose among Matwrap's capabilities without linking to the entire package. Storage management in Matwrap requires only a minimal assist from the user. However, the package also provides means by which the user can choose reuse storage already allocated, thus reducing calls to the allocator.

Matwrap is an open package in the sense that its modules and types have no private components. This means that the programmer can use the resources Fortran 95 to manipulate matrices in ways not provided by Matwrap. This ability is especially important for matrix computations, since the number of things people want to do with matrices far exceeds the number of functions that a closed, object-oriented package can provide.

A preliminary version of Matwrap will be released this spring.

NIST Strategic Focus Areas. *Emerging Industries:* Information and Knowledge Management.

Sparse BLAS Standardization

Roldan Pozo

http://math.nist.gov/spblas
http://www.netlib.org/blas/blast-forum/

MCSD is playing a leading role in the new standardization effort for the Basic Linear Algebra Subprograms (BLAS). The BLAS are kernels for computational linear algebra. If the interfaces to such kernels, is standardized, computer manufacturers or software vendors can provide high-performance implementations especially suited to each given hardware platform. By developing their applications in terms of the BLAS, then, computational scientists can achieve high levels of both portability and performance for their applications. The original BLAS, which were developed from the late 1970s through the early 1990s achieved this goal very well. Recently, there has been renewed interest in extending this success to new areas. The BLAS Technical Forum (BLAST) is coordinating this work. BLAST is an international consortium of industry, academia, and government institutions, including Intel, IBM, Sun, HP/Compaq/Digital, SGI/Cray, Lucent, Visual Numerics, and NAG.

One of the most important components of the new BLAS standard is support for sparse matrix computations. Roldan Pozo served as chair of the Sparse BLAS subcommittee during the standardization process, and NIST was the first to develop and release a public domain reference implementation in ANSI C for early versions of the standard, which helped shape the final specification. The standard was formally approved and accepted in early 2002, with publication of the complete specification, as well as a special issue of the ACM Transactions of Mathematical Algorithms (TOMS) devoted to the new BLAS standard and implementations. A paper devoted solely to the Sparse BLAS was included in the latter.

This year we are continuing our development of an ANSI C reference implementation for public release. In addition, we are beginning work on an alternate C++ binding to augment the official standard.

NIST Strategic Focus Areas. *Emerging Industries:* Information and Knowledge Management.

William Mitchell (center) of MCSD explains the operation of his PHAML software for the parallel solution of elliptic boundary value problems to ITL staff members Jim Filliben (left) and Nader Moyeri (right) during an MCSD Open House in May 2002.

Parallel Adaptive Refinement and Multigrid Finite Element Methods

William F. Mitchell

http://math.nist.gov/phaml/
http://www.cs.sandia.gov/Zoltan/

Finite element methods using adaptive refinement and multigrid techniques have been shown to be very efficient for solving partial differential equations on sequential computers. Adaptive refinement reduces the number of grid points by concentrating the grid in the areas where the action is, and multigrid methods solve the resulting linear systems in an optimal number of operations. W. Mitchell has been developing a code, PHAML, to apply these methods on parallel computers. The expertise and software developed in this project are useful for many NIST laboratory programs, including material design, semiconductor device simulation, and the quantum physics of matter.

This year we pursued three major activities on this project. The first is collaboration with Sandia National Laboratories to develop and support Zoltan, a dynamic load-balancing library that was released to the public in 2001. NIST's contributions to Zoltan are the implementation of a Fortran 90 interface to the library, and the implementation of the K-Way Refinement Tree (RTK) partitioning method, which was developed as part of PHAML. This year's work concludes NIST's participation in the Zoltan project, except for continued support of the released software. Our second activity is the public release of an initial version of the PHAML software. In the coming year, robustness and documentation will be improved so that a more broadly announced release can be made. Third is the application of PHAML to solve Schrödinger's equation for eigenvalues and eigenstates relevant to optical traps for neutral atoms. This work is being done in collaboration with the Quantum Processes Group of NIST's Atomic Physics Division, who are modeling such systems for the development of quantum-based information processors and memory. These are challenging computations, as the interactions of adjacent atoms involve computing multiple eigenvalues in the middle of the spectrum, with eigenstates that have very sharp gradients.

The specific accomplishments for this fiscal year include the following.

- Modified the REFTREE code in Zoltan to handle heterogeneous architectures and number of partitions not equal to number of processors
- Proved that one can always find a path through the elements of a triangle or tetrahedron grid which passes from element to element through vertices, and implemented an algorithm in Zoltan to find such a path (when it exists) in grids consisting of any shape of element
- Improved to PHAML, wrote documentation, and released the software
- Determined how to use the parallel version of ARPACK with PHAML to use parallel computers to solve Schrödinger's equation
- Experimented with several eigensolver approaches to get closer to the desired eigenvalues for models of neutral atoms relevant to quantum gates.

NIST Strategic Focus Areas. *Emerging Industries:* Information and Knowledge Management (virtual measurements).

OOF: Finite Element Analysis of Material Microstructures

Stephen Langer
Andrew Reid
Andrew Roosen (NIST MSEL)
Edwin Fuller (NIST MSEL)
Seung-Ill Haan (U. Maryland, Baltimore County)
Craig Carter (MIT)
Edwin Garcia (MIT)
Kevin Chang (Montgomery Blair High School)

http://www.ctcms.nist.gov/oof/

The OOF Project, a collaborative effort of MCSD, MSEL's Ceramics Division and the Center for Theoretical and Computational Materials Science, and MIT, is developing software tools for analyzing real material microstructure. The microstructure of a material is the (usually) complex ensemble of polycrystalline grains, second phases, cracks, pores, and other features occurring on length scales large compared to atomic sizes. The goal of OOF is to use data from a micrograph of a real material to compute the macroscopic behavior of the material via finite element analysis.

OOF is composed of two programs, oof and ppm2oof, which are available as binary files and as source code on the OOF website. From December 2001 through November 2002, ppm2oof was downloaded about 1500 times and oof was downloaded approximately 2100 times. The source code was downloaded 1800 times, and a conversion program, oof2abaqus, was downloaded 100 times. The OOF mailing list numbers 300. These are roughly equal to the previous year's, except for source code downloads, which increased by a factor of three.

Work during FY02 concentrated almost exclusively on OOF2, a completely new version of OOF that will handle a wider variety of physical problems and be much more easily extended. The core finite element and material property classes for OOF2 were constructed in FY01. In FY02 the OOF team worked on the graphical user interface, new methods of mesh construction (in collaboration with UMBC), and improvements to the material property code (including support for plasticity modeling). An initial version of OOF2 is expected to be released during FY03.

Kevin Chang, a student at Montgomery Blair High School, worked on incorporating automatic grain boundary detection code into OOF2. The algorithm, which detects the often indistinct borders of grains in a micrograph, was developed the previous summer by another student from the same school, Robert Kang-Xing Jin. Jin's project earned him a semi-finalist's place in the nationwide Intel Science Talent Search. (http://www.sciserv.org/sts/61sts/02semis.asp.)

Steve Langer began collaborating with a group from Penn State University and Ford. The group, funded by an NSF-ITR grant, will be developing software for multiscale modeling of materials, incorporating atomistic models, thermodynamics, phase field models (continuum models of microstructure evolution) and finite elements. The idea is to create an integrated computational environment to model all aspects of material development. OOF will serve as the project's finite element tool, without losing its ability to run as a stand-alone program. PSU will fund a post-doc to work at NIST.

NIST Strategic Focus Areas. *Existing Industries:* Materials processing. *Emerging Industries:* Information and Knowledge Management (virtual measurements).