Final Report

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Partnership Summary

Participant Number (Coordinating partner as participant N°1	Name of Participating Organization	Role in Project*
1	Uppsala University	LSF-IHP
2	Riso National Laboratory	LSF-TMR
3	Technical University Delft	OTHER
4	Council for the Central Laboratory of the Research Councils	LSF-IHP
5	Hahn Meitner Institute	LSF-IHP
6	Paul Scherrer Institute	LSF-OTH
7	Research Centre for Solid State Physics and Optics, Hungarian Academy of Sciences	LSF-IHP
8	Nuclear Physics Institute, Czech Academy of Sciences	LSF-OTH
9	INFM	OTHER

* LSF-IHP: a research infrastructure funded for access under the IHP programme
LSF-TMR: a research infrastructure funded for access under the TMR programme
LSF-OTH: a research infrastructure outside the IHP or TMR programmes
IND: an industrial or commercial enterprise
OTHER: other types of participant

1. Executive summary

The major focus of the SCANS project has been on the development of software for Monte Carlo simulation of neutron scattering instruments. In the project proposal efforts were to have been concentrated on developing the **McStas** program, which had previously been developed through projects within FP4 and FP5. However it rapidly became clear that it was more sensible to support the development of a variety of programs. In developing complex software and algorithms there is no single way to do things – end users have greater confidence in the results if different approaches can be benchmarked against each other and shown to produce the same results. The project was therefore modified to also support development of **VITESS** and **RESTRAX**. This has been highly successful. A benchmarking exercise was carried out during the project, also involving codes developed in the US. Some small problems were identified and fixed, but overall the results were very reassuring. The close interplay between the different code developments, enabled through regular SCANS meetings, has been enormously beneficial. Each code has its own particular specialisations, but there are large overlap areas and 'best practice' can be readily shared. In some cases modules developed for one program can be automatically converted for incorporation into another program.

Another key aspect has been the involvement of 'end-users', both passively and as active contributors to code development. Regular training workshops have been organised through SCANS. Regular code releases have made new developments immediately available to the community. These Monte Carlo simulation codes are now in routine use at essentially all neutron scattering facilities in Europe and are an integral part of the design process of any instrument, or of optical components of instruments. That is not to say that no further developments are required, since not all aspects are as comprehensive or sophisticated as is necessary (in particular regarding neutron polarisation). However all the basic requirements have essentially been covered.

SCANS has played a role in the development of the NeXus data format. This is an international collaboration, coordinated from the USA, to develop a standard format for (raw) neutron scattering data. Apart from the specific developments made through SCANS, the involvement has been helpful in maintaining the momentum of the collaboration, to the extent where NeXus is now gradually becoming as the standard for neutron scattering. SCANS has also supported the development of NeXus for muon spectroscopy.

The two other main tasks in SCANS have involved the development of advanced methods of data analysis, in particular reverse Monte Carlo (RMC) modelling, and methods for automated data analysis and 'intelligent control' of experiments. Development of the RMCPOW program has continued; this is at present the only software available for modelling disorder in magnetic crystalline materials. The RMCA code, which is the most commonly used RMC program worldwide, has been in use for more than 10 years but has become increasingly difficult to develop. The code has therefore been completely rewritten in an object oriented format as RMC++. Some preliminary work has been done on extending the RMC concept towards modelling the dynamics of materials, rather than just the structure, within the RMCt program.

In the area of intelligent control the ADAA program has been developed as a 'proof of concept'. ADAA has been demonstrated in two experiments – one involved the automatic optimisation of beam time use during a study of a crystal phase transition, the other involved the study of a liquid structure with fully automated data correction and structural (RMC) modelling. It is not to be

expected that these developments will be rapidly taken up across neutron scattering facilities; rather they are intended to push forward the frontiers.

Although the work done through SCANS has only concerned a small fraction of the wide variety of software relevant to neutron scattering, it has had a much broader impact. It was the first RTD collaborative project in the area of neutron scattering specifically focussed on software development, and its success has been important in demonstrating that (a) software collaboration can be highly effective and (b) this collaboration does not necessarily require the imposition of 'uniformity'. In addition the whole profile of software development has been raised throughout the neutron scattering community through the various dissemination activities, and among the neutron scattering facilities in particular through participation in the Neutron Round Table. Finally, the developments of Monte Carlo simulation software are already having, and will continue to have, a strong impact on the provision of high quality optimised instrumentation at European neutron scattering facilities, providing enhanced scientific opportunities for their users.

2. Project objectives

General objectives

- To develop software that enables more efficient and effective use of European neutron scattering facilities, either in terms of instrument design or experiment design and execution.
- To coordinate European efforts within this area, in order to avoid duplication of work.
- To disseminate the results of the project (that is the software produced) as widely as possible within the European neutron scattering community.

Specific objectives

- To develop, maintain and document general tools for Monte Carlo (MC) simulation of neutron scattering instruments, applicable to both steady state and pulsed neutron sources.
- To provide a range of kernels for these MC simulation tools describing different instrument components. Relevant instruments are diffractometers (powder, single crystal, liquids/amorphous, strain scanning, small angle scattering), spectrometers (triple axis, multirotor chopper, monochromator/chopper, inverse geometry, spin-echo) and reflectometers.
- To demonstrate the use of these tools in detailed simulations of particular instruments (liquids/amorphous diffractometer, strain scanning diffractometer, triple axis spectrometer, multirotor chopper spectrometer, inverse geometry spectrometer).
- To demonstrate the use of these tools in detailed simulations of particular experiments.
- To develop the use of advanced methods of data analysis (in particular RMC methods).
- To apply these methods to analysis of simulated (or real) data and demonstrate the automated control of an experiment based on monitoring of the analysed results (one demonstration for liquids/amorphous diffraction or strain scanning or quasielastic scattering).

Project methodology

The project is entirely devoted to the writing, testing and documentation of computer software. Most software will be based on Monte Carlo methods. However it is not intended to produce a single uniform software package. Partners responsible for particular tasks will be constrained in the precise methods used only by common agreements of compatibility (e.g. standard data format) and portability.

3. Project tasks

Task No.	Task (Technical Deliverables)
1	Development and maintenance of the McStas, VITESS and RESTRAX Monte Carlo simulation tools
2	Methodology transfer to/from synchrotrons
3	MC kernels for samples
4	MC simulation for single crystal, TOF and polarised neutron instruments
5	Virtual instruments (ESS)
6	NeXuS (data standard)
7	Inverse methods of data analysis
8	Data assessment/ information content
9	Dissemination of the results of the project.

4. Project partners

Partner No.		Acronym
1	Uppsala University, Sweden	UU
2	Riso National Laboratory, Denmark	Riso
3	Technical University Delft, Netherlands	TUD
4	Council for the Central Laboratory of the Research Councils, UK	CCLRC
5	Hahn Meitner Institute, Germany	HMI
6	Paul Scherrer Institute, Switzerland	PSI
7	Research Centre for Solid State Physics and Optics, Hungarian Academy of Sciences, Hungary	
8	Nuclear Physics Institute, Czech Academy of Sciences, Czech Republic	
9	INFM, Italy	INFM

4. Scientific and technical performance – details

Details of the progress in each task are summarised in the tables below.

Task 1. Development and maintenance of the McStas, VITESS and RESTRAX MC simulation tools

Partners involved: 2,5,6,8,9

Description of task:
(a) To develop, maintain and document the McStas, VITESS and RESTRAX software tools for MC simulation of neutron scattering instruments, in order to enable users to handle the complexity of specifying all relevant details of a modern instrument.
(b) To include the scattering kernels provided by other partners for instrument components, samples and sample environment.

Progress made: **Riso (partner 2) – McStas responsible**

McStas is a software package designed to perform simulation of neutron instruments. The first version of the package was released in 1998. McStas was first developed at Risø National Laboratory and is now developed there and at the ILL. This section presents a brief overview of the work carried out by McStas team members and contributors during the SCANS project.

EU Support has been given to development of the McStas package during the FP4 RTD programmes XENNI and Cool Neutrons, and the FP5 RTD programme SCANS. In FP6 McStas is involved in the MCNSI JRA within the NMI3 project.

During SCANS, McStas has been released 9 times by 5 different people, who together constitute the McStas development team.

McStas 1.3 (May 18th 2000) - KN/KL
McStas 1.4 (July 28th 2000) - KN/EF/KL
McStas 1.4.1 (March 16th 2001) - POA/EF/KN/KL
McStas 1.4.2 (April 6th 2001) - POA/EF/KN/KL
McStas 1.5 (September 18th 2001) - POA/EF/KL
McStas 1.6-ill (October 23rd 2001) - EF
McStas 1.6.1-ill (February 18th 2002) - EF
McStas 1.7 (May 20th 2003) - PW/EF/KL
McStas 1.8 (March 5th 2004) - PW/EF/KL

(KN = Kristian Nielsen, EF = Emmanuel Farhi, POA = Per-Olof Åstrand,
PW = Peter Willendrup, KL = Kim Lefmann)

After the emergence of McStas 1.5, differences of opinion resulted in a separate ILL release of McStas. The disagreements were eventually resolved, but because of a hacker attack on the Risø McStas website, the official Risø version of the package was more or less unsupported for approximately one year. As seen below, all of the problems have been resolved after the arrival of a new McStas administrator at Risø.

The original designer of McStas, Kristian Nielsen, worked as package administrator until August 1st 2000. The position was then vacant until filled by Per-Olof Åstrand who worked half-time as administrator during 2001. From January 1st to July 1st 2002 the position of McStas project administrator was again vacant. At that date the new McStas project administrator, Peter Willendrup, was employed at Risø.

Already before the beginning of SCANS, the McStas web site and mailing list was a well known forum for information and discussions. In October 2001 the mailing list was closed temporarily, but the hacker attack prevented a re-opening. Shortly after the employment of Peter Willendrup, the project website and mailing list were restored. Since then, the website has been modernised and has been updated frequently.

A new strategy for collaboration between McStas developers has been agreed and implemented. The new strategy ensures freedom for all participating developers to do modifications and provides means for testing the validity of all code changes as well as to preserve a full revision history of all code. The basis of the new collaboration strategy is a policy document and a CVS server, accessible by the full developer team, currently based at Risø and the ILL.

McStas releases during SCANS:

McStas 1.3 (released May 18th 2000)
USER LEVEL
- New facility `McDoc' for documentation of components, with automatic extraction of documentation from comment headers in the source code.
- The possibility in the graphical user interface `mcgui' to build instrument definitions using "point-and-click", based on McDoc.
- Much improved `mcrun' front-end, which now replaces the old `gscan' front-end and interfaces with `mcplot'.

COMPONENT LEVEL
- Optional component input parameters.
- New components Source_Optimizer and Monitor-nD, by Emmanuel Farhi.
- Improved Single_crystal component, now supports anisotropic mosaic, multiple scattering, extinction, absorbtion, and incoherent scattering.

RUNTIME/KERNEL LEVEL
- Instrument parameters may now also be of string type.

GENERAL
- Misc. minor bug fixes.

McStas 1.4 (released July 28th, 2000)
USER LEVEL
- Experimental mcstas2vitess conversion program to automatically translate a McStas component into a VITESS module.
- Option to clear the simulation output in mcgui.

RUNTIME/KERNEL LEVEL
- It is now possible to use arbitrary C expressions in the instrument definition, ie. to set rotations, component parameters, etc. Only works for SETTING parameters though, not DEFINITION parameters.
- Partial solution to the problem with name conflicts on component parameters.
- Partial NeXus support implemented, but not yet functional.

GENERAL

- Misc. minor bug fixes.

McStas 1.4.1 (released March 17th 2001)
COMPONENT LEVEL
- New components: ESS_moderator_long.comp and ESS_moderator_short.comp (by Kim Lefmann), Source_Maxwell (by Emmanuel Farhi). Gravity_guide.comp is included in the official version.
- Some support for the calculation of correlation functions in the components Monitor_nD and PreMonitor_nD (by Emmanuel Farhi)

RUNTIME/KERNEL LEVEL
- A signal handling system is included (by Emmanuel Farhi)

GENERAL
- Misc. minor bug fixes

McStas 1.4.2 (released April 6th, 2001)
(Information incomplete for this release, mainly small bugfixes)

McStas 1.5 (released October 10th, 2001)

COMPONENT LEVEL
- Corrected version of Arm.comp.
- Corrected version of Monitor_nD.comp by Emmanuel Farhi
- Rewritten version of Gravity_guide.comp by Emmanuel Farhi
- Handling of illumination in Source_flat, Source_div and Source_flat_lambda have been corrected.
- He3_cell.comp contributed by Trefor Roberts.
- Mon_2foc.comp contributed by Peter Link.
- Bender.comp contributed by Philipp Bernhardt.
- Powder_filter.comp contributed by Ben Fortescue.
- Source_Maxwell_3 component (source with three Maxwellian
- Various monitors have been added: EPSD_monitor, PSDcyl_monitor, PSDlin_monitor, TOF_cylPSD_monitor, TOFlog_mon, TOFLambda_monitor
- Guide_wavy
- Source_gen

KERNEL/RUNTIME LEVEL
- Initial infrastructure for polarisation added (not complete)
- New component level keywords: NAME_CURRENT_COMP, POS_A_CURRENT_COMP, ROT_A_CURRENT_COMP, ROT_R_CURRENT_COMP

McStas 1.6 (Never officially released. The list below includes various
code modifications from 1.6-ill and 1.6.1 versions)
USER LEVEL
- mcplot can now read a list of detector files, without a '.sim' file.
- 1D and 2D detectors compute signal statistics (min, max, mean, center and width of distributions). Stored in the detector file.
- mcplot generates PS, color PS and GIF output without display.

COMPONENT LEVEL
- Bug corrected (very small signal statistics) in Monitor_nD
- Renaming of components for easy sorting, e.g. Guide_..., Filter_...
- Monochromator_2foc and Monochromator_curved reads reflectivity table files
- The Virtual_input replaces the Source_file component, and can read text, Vitess and

binary float files of neutron events.
- The Gravity_guide now handles correctly the focusing multichannel guides.
- The Source_gen focuses uniformly, models rectangle, disk, gaussian, and Maxwellian
- We tried to lower the number of components by merging similar ones.

DEVELOPER LEVEL
- SHARE keyword followed by a C code block %{...}% acts the same as a DECLARE block, but is only included once in an instrument. Useful with many identical components
- EXTEND can be used to enrich behaviour of a standard compontent with special c code
- GROUP can be used to set up an exclusive group of components. Only one of the elements of the group acts on the neutron.

KERNEL/RUNTIME
- Improvements to the signal handler
- New MACROS for the component programmer:
  * mccompcurindex is the number (index) of the current component
  * RESTORE_NEUTRON(index, x, y, z, vx, vy, vz, t, sx, sy, sz, p) restores the neutron state to the one at the input of the component 'index'.
  * STORE_NEUTRON(index, x, y, z, vx, vy, vz, t, sx, sy, sz, p) stores the current neutron state in the trace-history table, in local coordinate system. This is automatically done when entering each component of an instrument.

GENERAL
- Misc. testing and bugfixing of components

McStas 1.7 (released May 20th 2003)

USER LEVEL
- Platform independence and less installation requirements (now works properly on Microsoft Windows)
- Update of the graphical tools, possibility to select different graphics backends
- Multiple data output formats for easier simulation data analysis (i.e. the availability of 8 different formats including, when relevant, their own embedded loading/plotting methods facilitates the choice, portability and accessibility of results from the simulations)
- Improved documentation

COMPONENT LEVEL
- Updates to existing components (new features/bug fixes), new contributed component (Guide_honeycomb)

DEVELOPER LEVEL
- Programming language extensions

GENERAL
- First official release incorporating massive work by Emmanuel Farhi from the unofficial McStas 1.6 series.

McStas 1.8 (released March 5th, 2004)

POLITICAL LEVEL
- Change of license; the GNU General Public License is now used to further encourage user contributions to the project

USER LEVEL
- Further improvemend support for Microsoft Windows
- Improvements to the built in editor (will receive further improvements with the next release)

- mcconvert, conversion between Matlab and Scilab datafiles
- Support for instrument scans directly from the main interface
- Support for scan plotting scan files with all graphical backends, single scan steps can be opened via the scan datafile
- First support for grid computing (extensions and improvements planned)
- Instruments can have default values (easy for first time users)
- New 'neutron site' menu for distribution of instrument files, categorised by institution (e.g. PSI, ILL, Brookhaven, ...) - gives the first time user a solid starting point
- New user tutorial (create your own triple axis instrument)
- Tutorial (html format) integrated with the main interface
- Various improvements to installation infrastructure

COMPONENT LEVEL
- Several user contributions included (components and instruments)

CONTRIBUTOR LEVEL
- First version of our new test suite, enables the developers and users to benchmark the package against older releases
- A few programming language extensions (PREVIOUS/RELATIVE)
- New version of Mersenne Twister algorithm
- Improvements to rectangular focusing

Collaboration policy of the McStas project:
McStas has a number of active contributors outside the core development team. Contribution and collaboration is warmly encouraged, because joint efforts increase the total amount of work done. The current number of components distributed with McStas 1.8 exceeds 100.

Recent contributions:
Uwe Filges, PSI:
- Guide_tapering (Focusing guide with user selectable tapering)
- Model of the PSI FOCUS instrument

Stuart Ansell & Dickon Champion, ISIS:
- ISIS_moderator (model of the ISIS 1st+2nd target stations)
- Test instrument for ISIS_moderator
- Model of the ISIS HET instrument

Ross Stewart, ILL:
- Guide_curved (Curved guide element model)

Chris Ling, ILL:
- Model of the ILL D9 instrument

Lise Arleth, Risø:
- Sans_spheres (Small Angle Neutron Scattering sample model)

Team member components:
- Powder2 (Powder sample, 2 broadened lines, incoherent scattering)
- Phonon_simple (Phonon generating sample)
- Test instrument for Phonon_simple

Contributions to be included in future releases:
Lucia Alianelli, ILL:
- Monochromator_reflect (Monochromator with reflectivity model)
- Advanced mosaic crystal component

Roberto Felici & Marina Defilici, INFM/OGG:

- Multiple powder line sample

Virgenie Hugovieux, U.de.Montpellier:

- General S(Q,w) sample

Strategic alliance with Vitess:

To further strengthen the collaboration between the McStas and Vitess packages, sharing of certain code parts has been proposed. Both of the packages would gain from such an arrangement, since each package can benefit from large work done by the other team.

Use of the McStas package:

Conferences: At ICNS 2001, more than 20 posters, many describing FRM-2 instruments, contained work related to McStas. Also a special mini-symposium on neutron simulation was held. At ECNS 2003, 8 posters were related to McStas.

Site presence:

McStas is running at all major instrument development projects including ISIS Target Station 2, ILL millenium programme, FRM-II and PSI.

Mailing list:

The neutron-mc@risoe.dk mailing list currently has about 100 users. Releases are also communicated to the more general neutron@lanl.gov mailing list.

Downloads of McStas 1.8:

Since March 5th 2004, downloads of the McStas package have been monitored. The data shows that McStas 1.8 is being used in 14 European countries:
Europe: DK, UK, FR, NL, DE, CZ, RU, ES, RO, SE, NO, HU, IT, GR

Future developments of McStas:

The McStas team intend to continue to develop the package under MCNSI in areas of

- Better grid computing support (for large scale simulations)
- Polarisation support (from Vitess collaboration)
- Concentric components (components inside other components)
- Further GUI and usability improvements
- Webserver front/backend for testing the package without installing
- Implement Triple Axis Spectrometer specific reciprocal space code, which will allow everyone to do virtual neutron scattering experiments without connecting an instrument control program

Progress made: **HMI (partner 5) – VITESS responsible**

VITESS versions 2.0 – 2.4 were released between 1st March 2000 and 29th February 2004. In this time, the set of modules was nearly completed to simulate the existing neutron scattering instruments.

A module to simulate (straight and curved) Fermi choppers was added to complete the set of components for monochromatisation that already existed: velocity selector, disk chopper, crystal (ensembles).

Most kinds of samples now exist (see task 2). Modules were written to build or describe optical devices: bender, (super)mirror ensemble or multiple holes.

Polarisation was included and several modules written to describe components used for polarised neutrons: polarisers, flippers and monitors. Additionaly, modules were written to simulate the neutron precession in constant and rotating magnetic fields (for details see task 4).

Apart from that, more realistic simulations were enabled by adding gravity effects or properties like waviness in guides and benders.

Absolute flux values are calculated at each point of the instrument to allow for a comparison of instruments at different sources or to compare experiment and simulation.

Visualisation was improved and a module added to watch neutrons paths or place of arrival during a run. Ten tools were added to facilitate the generation of input data or view simulation results.

Progress made: **PSI (partner 6) – McStas contributor**

The developers of the McStas simulation tool are interested in a common output format in order to facilitate the exchange and the analysis of McStas simulation results. Furthermore a common output format gives the opportunity to use an increasing number of available analysis tools. For this reason the McStas developers decided to integrate NeXus into McStas as an additional output format. In practice the McStas user can choose to optionally produce an additional NeXus-XML file. This file is generated through the NXdict-API which was designed at PSI. The NXdict-API reads all file structure information from a dictionary data file and creates the NeXus structure automatically. Thus the handling of NeXus is simplified drastically. The decision to generate a NeXus-XML output file was taken because the standard NeXus-HDF output file requires a lot of additional libaries. These libaries must be compiled with the McStas kernel which results in a more complicated installation procedure of McStas. But the goal of the McStas developers is to simplify the installation and to minimise the McStas kernel. The co-operation between McStas developers and PSI-NeXus team has resulted in a development version of McStas which includes the NeXus-XML output format.

Focusing techniques play an increasingly important role in neutron scattering due to the rather low flux of the neutron sources and the advent of modern materials that can often only be produced in small quantities. Usually, doubly focusing monochromators in combination with doubly focusing guide tubes with linear tapering are used. The disadvantage of linear tapering is a very inhomogeneous phase space at the sample position and that the flux is decreasing with increasing distance from the exit of the guide tube. In order to investigate the problem a new guide component Guide_tapering.comp was developed and released in McStas version 1.8. The new guide component allows simulation of advanced guide geometries like parabolic and elliptic tapered guides. In addition any tapering given by an arbitrary function can be simulated.

Progress made: **NPI (partner 8) – RESTRAX responsible**

RESTRAX has been developed in two modifications. One is dedicated to three-axis spectrometers (TAS) and provides simplified ray-tracing code for simulation of TAS resolution functions and additional tools for data analysis. The second, called SIMRES, provides more flexible (and more realistic) ray-tracing code useful for simulation of newly designed or upgraded instruments and optimisation of their configuration. The development has proceeded in two directions: (1) improvement of Monte Carlo ray-tracing code and (2)

support for instrument optimisation and data analysis.

1. Monte Carlo ray-tracing code

Particular attention has been paid to the improvement of software equivalents of **neutron-optical components**, which are used in various modifications of three-axis spectrometer (TAS) arrangement. They included:

- **"Polymorphic" collimator segments**. This component permits to simulate neutron transport through the class of components derived from a simple collimator: apertures, Soller collimators (including convergent and/or oscillating ones), neutron guides/mirrors and polarising benders.

- **Mosaic & gradient crystals**. Reflecting and focusing properties of crystals used as monochromators and analysers at TAS instruments influence essentially both the flux and momentum-space profile of a neutron beam. Therefore, their simulation has to be as realistic as possible, particularly in the cases of high-resolution arrangements or studies involving assessment of absolute neutron intensities. As a result of necessary trade-off between accuracy and computational efficiency, we have developed a single software component simulating diffraction of neutrons in three types of materials: mosaic crystals, elastically bent perfect crystals and deformed mosaic crystals. Secondary extinction is realistically simulated by *random-walk* code for neutron transport. The component also permits to simulate focusing arrays of crystals and/or sandwich of elastically bent crystals including multiple reflections between different crystal segments.

Although RESTRAX was conceived as a tool for simulation of TAS instruments, its code has been upgraded to allow for simulations of other **arrangements derived from classical TAS**. By using appropriate configuration parameters and commands, RESTRAX can simulate

- powder diffractometers either with a position-sensitive detector or a multidetector bank
- strain-scanner (involves special features like mapping of gauge volume in real and momentum spaces)
- other segments of TAS beamline (neutron guides or the whole primary spectrometer)
- phase-space maps of neutron beam at each of the basic TAS component

Partially, effort has been spent on improving **optimisation of the Monte Carlo sampling strategy**. The three main features resulting in fast simulations of neutron trajectories include:

- **Variance reduction**. Initially, correlations can be estimated since the basic arrangement is known at the compilation time. Subsequent optimisation is automated, based on covariance matrix estimations.
- **Up-stream simulation** between source and sample. This is particularly efficient for small sample gauge volumes (e.g. strain scanner).
- **Splitting of the ray-tracing procedure** to the monochromator and analyser parts (efficient for multiplexed analyser/detector systems, step-by-step measurements).

2. Instrument optimisation & data analysis

Numerical optimisation of instrument parameters has been implemented in RESTRAX. The procedure uses ray-tracing Monte Carlo method to simulate a selected figure of merit (flux at the sample, energy resolution, and phonon or diffraction peak parameters) and to find its maximum with respect to any instrument parameter (e.g. crystal curvatures, neutron energy etc.).

Non-linear least squares fitting tool implemented in RESTRAX permits to use simulated resolution functions in convolution with a scattering function. This feature has been substantially upgraded since the start of the project. In the present version, the program can

handle multiple data sets measured on the same specimen under different conditions ($\boldsymbol{Q}$,ω-range, neutron energy, collimation etc.). The scattering model is separated in shared library, which provides sufficient flexibility for users to define large variety of scattering models in 4-dimensional ($\boldsymbol{Q}$,ω) space and to use this model in data analysis. The default model provided with the package can serve as a template for other user-written code.

User support
Information about RESTRAX, documentation and download links have been made available at the RESTRAX home page, http://omega.ujf.cas.cz/restrax. Recent releases of the program include

- Build and installation scripts for easy installation
- Support of Linux (in addition to Digital UNIX)
- Distribution of binary files for Linux/i386 and Digital UNIX/Alpha platforms - easy installation and use (just unpack & run)
- Server-based scripts (PHP) for creation and editing of instrument configuration files

Progress made: **INFM (partner 9) – McStas contributor**

The INFM staff has contributed to the development of new McStas components. In particular we have implemented our crystal simulation programs into the McStas package as new components able to describe the reflectivity from perfect and imperfect crystals.

Imperfect_crystal.comp allows for detailed simulations of a large variety of imperfect crystals. This component is useful for monochromators, analysers and crystal samples.
Monochromator_reflect.comp is an upgrade of the Monochromator_curved component. The improvement consists in a better description of the crystal reflectivity. The component uses a reflectivity database created with the REF.pro IDL program. The role of gradient crystal monochromators can now be accurately simulated with this component. The IDL program is being translated to C and will be better interfaced to McStas in the next months. Several papers and reports have been written on the use of these new programs. The Monochromator_reflect component has been fully benchmarked against results of other codes. In particular, we found a good agreement between simulations of gradient crystal monochromators efficiency using Monochromator_reflect, Imperfect_crystal and RESTRAX data (provided by J. Saroun). The comparison results can be found in the ILL technical report ILL03AL05T.

Monochromator_reflect.comp has been used to simulate the D19 crystal diffractometer at the ILL (L. Alianelli). The simulation aimed at estimating the gain in flux with increasing the instrument source size (i.e. the beam tube size) and the monochromator size and bending.

Moreover a new component able to fully describe powder samples as been developed: **Filter_sy.comp**. This routine computes the full transport of neutrons inside a powder materials properly taking into account multiple scattering, incoherent scattering and absorption. This module will be extremely useful to optimize the performance of instruments and to optimize sample dimensions.

Task 2. Methodology transfer to/from synchrotrons

Partners involved: 9

Description of task:
(a) To collaborate with the synchrotron community on development of MC kernels for neutron/X-ray optical elements, transferring appropriate methodology to the SCANS project.
(b) Comparison of results of simulation using the X-ray program SHADOW and McStas.

Progress made: **INFM (partner 9) – task responsible**

The NOP package, built on the top of the XOP package developed for synchrotrons, has been developed and released. The main utilities are: neutron cross-section databases; calculation of material properties, neutron refractive index, neutron reflectivity; calculation of imperfect crystal reflectivity.

The IMD (Windt) software, that is widely used in the x-ray synchrotron and astrophysics community, has been adapted to the calculation of neutron reflectivity from multilayers. Several experimental reflectivity profiles have been successfully compared to those produced by IMD for neutrons.

The Imperfect_Crystal component for McStas has been developed from a code that has been used for both x-ray and neutron crystal diffraction. The simulation results (neutron and x-ray) have been compared in detail to experiments on several kinds of imperfect crystals (mosaic as graphite and copper, assembled as germanium, perfectly bent as mica, silicon and quartz). This code has been recently used to predict the performance of a novel gamma lens (made of an assembly of mosaic crystals) that is being designed for astrophysics research.

Task 3. MC kernels for samples and sample environment

Partners involved: 2,5,8

Description of task: To provide MC kernels describing the scattering from a number of generic types of samples.

Progess made: **Riso (partner 2) – McStas responsible**

See Task 2.

Progess made: **HMI (partner 5) – VITESS responsible**

In Vitess there are several modules to simulate the scattering in different kind of samples. During the time of the contract, the following sample modules were added:
- isotropic elastic sample
- reflectometer sample
- S(Q) sample
- single crystal sample

On 1st March 2000, the following samples already existed:
- inelastic sample
- powder sample
- SANS sample

So the set of samples is nearly complete now.

Progess made: **NPI (partner 8) – RESTRAX responsible**

Basic MC kernel for samples was developed to simulate scattering on Vanadium and four basic types of resolution functions:
- $R(Q,\omega)$ – isotropic inelastic scattering (all energy transfers)
- $R(Q)\delta(\omega)$ – isotropic elastic scattering
- Powder diffraction
- Single crystal (Bragg) reflection

The resolution functions are then used in convolution with an arbitrary scattering function defined in a shared library. It permits users to define large variety of samples by linking their own module to the program. The generic scattering model provided with the package describes up to 6 dispersion branches as a quadratic form in 4-dimensional ($\boldsymbol{Q}$,ω) space. The branches can have both zero and finite width in energy. Other models were written by users:
- antiferromagnetic magnons
- phonons in diamond
- bond-charge model describing complete system of phonons in Ge and Si

Task 4. MC simulation for single crystal, TOF and polarised neutron instruments

Partners involved: 2,3,5,6,8,9

Description of task:
(a) To provide MC kernels describing the scattering from the components of single crystal / TOF / polarised instruments and generic samples.
(b) To perform MC simulations of such instruments and validate the results where possible by experiment.
(c) To use these results to provide an analytic/numerical description of the incident beam on the sample as a function of the instrument set-up.

Progess made: **Riso (Partner 2) – McStas responsible**

See Task 2.

Progess made: **PSI (Partner 6) – McStas contributor**

PSI has used Monte Carlo simulations to investigate the properties of optical beam line components for SINQ instruments. The main object was to investigate the use of focusing devices in order to increase the neutron intensity. Candidates were the powder diffractometer DMC and the triple axis spectrometer TASP at SINQ. Another topic was to study the possibilities of guide improvements using advanced guide geometries.

A. DMC simulations

The Monte Carlo program McStas was chosen for the simulation of the cold neutron powder diffractometer DMC. Especially the influence of a linear focusing supermirror device (trumpet) was investigated. The trumpet was positioned between monochromator and sample position. The goal was to find out an optimized parameter set yielding maximal intensity but with no substantial loss of instrumental resolution. The investigations were carried out for small sample sizes (about 21 mm^3). Before starting a real measured data set was compared with a simulation without a focusing device. The calculated and measured data agree very well. Afterwards the focusing device was integrated into the McStas simulations. In a first step only horizontal supermirrors had been considered for the trumpet. The vertical walls were modeled with absorbing material. In this state the parameters entrance and exit height of the focusing device were optimized in the 'scan'- mode of McStas. For the reflectivity of the horizontal walls m(y) a value of three was used. The simulations had been shown that a focusing device which covers only vertical focusing increases the intensity at the sample position up to a factor of 1.5 (Fig. 1).

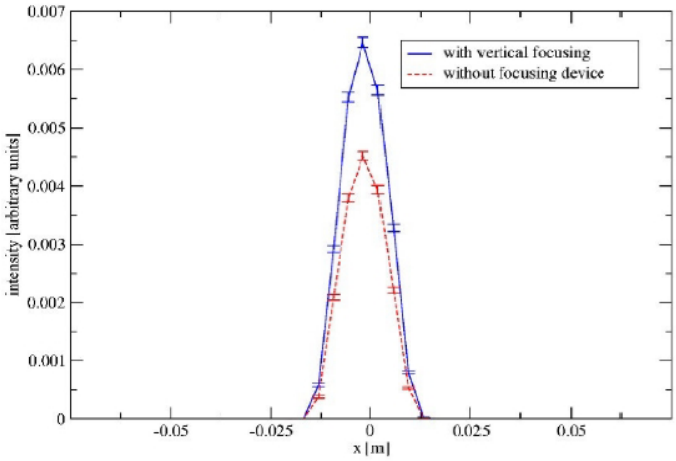

Fig. 1: Comparison of peak resolution/gain with and without vertical focusing device

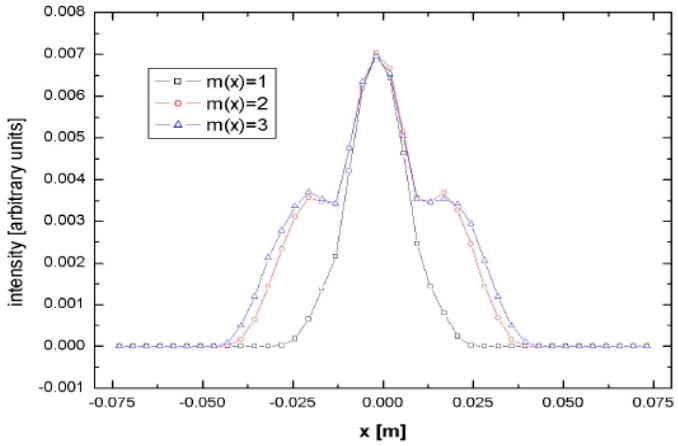

Fig. 2: Comparison of peak resolution for different reflectivity values of the vertical walls

After the optimal heights of the focusing device had been determined the vertical walls were changed to reflecting supermirrors. Different reflectivity values m(x) were tested (Fig. 2). The entrance width of the focusing device was set to the width of neutron beam (2 cm) and kept fixed. In opposite the width of the trumpet exit has essential influence on the intensity at the sample position. The simulations had been shown that the intensity can be increased up to a factor of 4 (vertical and horizontal focusing, m(x) = m(y) = 3). But horizontal focusing degrades the peak shape and resolution. With higher values of reflectivity m(x) the resolution decreases (Fig. 2). Therefore the optimal result can be reached using a combination of supermirrors with reflectivity values m(x) = 1 for horizontal focusing and m(y) = 3 for vertical focusing. In this case the intensity of DMC can be increased by a factor of 2.14 at sample position without significant loss of instrument resolution.

B. TASP simulations

For the triple axis spectrometer TASP at SINQ McStas simulations were done. The TASP instrument is positioned at the end of the cold neutron guide RNR14. The distance between TASP monochromator and cold neutron source is approx 54 m. The dimension of neutron guide is 3.5 cm (width) x 12 cm (height). The present vertical focusing monochromator

(PG002) covers a neutron energy range of 2.1 to 25 meV. Figure 3 shows the comparison of calculated and measured wavelength spectrum at the TASP monochromator position.

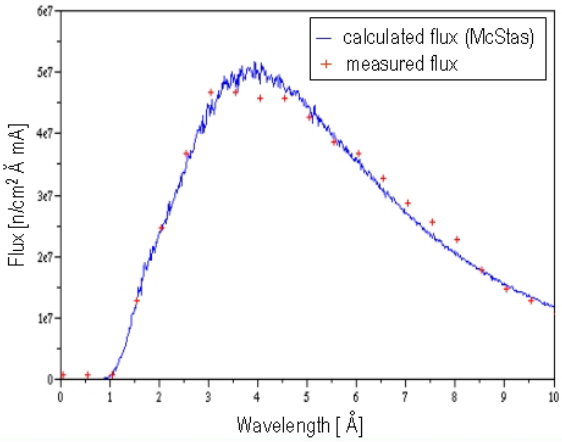

Fig. 3: Available wavelength spectrum at the TASP monochromator position; comparison of calculated and measured spectrum

The aim was to study the effect of a parabolic trumpet situated between monochromator and sample position. The investigations were done for the cases of horizontal, vertical and horizontal/vertical focusing of the neutron beam. The sample size, the distance between monochromator and sample position and the trumpet length were further investigated parameters. In general the parameter study was performed for different wavevectors k_i. Of course, through a horizontal focusing supermirror device, the divergence of the neutron beam is increased. The consequence is that the q-resolution will be coarser. The calculated parameter sets cover the real conditions for TASP at the spallation source SINQ at PSI.

Generally the McStas simulations have shown that the flux at sample position can be increased significantly using a parabolic tapering focusing guide. Figure 4a and 4b show the beam spot at sample position (1.8 m far away from the monochromator position). In the case of focusing (2a) the beam maxima is higher and the area of maxima flux is smaller as without focusing (2b). The dimensions of the calculated trumpet are: length 1.3 m; entry height 0.12 m; entry width 0.035 m; focal point 0.3 m far away from the guide exit.

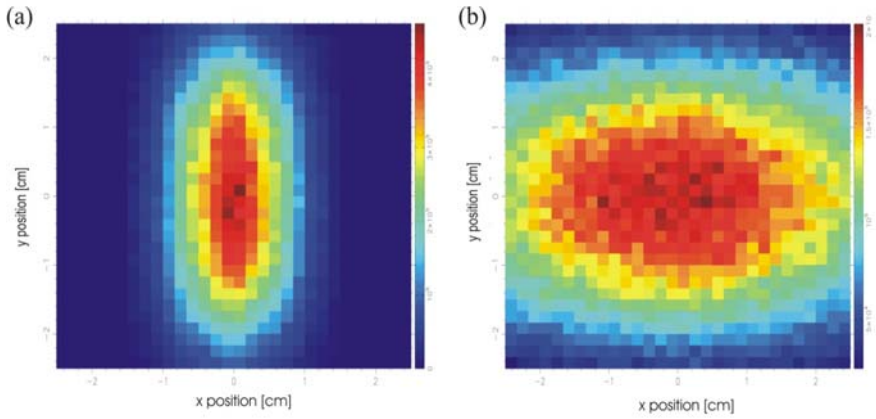

Fig. 4: Comparison of the beam spot at the sample position; (a) with vertical/horizontal parabolic trumpet; (b) without trumpet

In principle the focusing effect could be obtained also by linear focusing. The special effect of parabolic focusing is displayed in figure 5a. The figure shows that the flux maxima is located at the focal point, 0.3 m away from the trumpet exit. In case of linear focusing the flux is decreasing with increasing distance from the trumpet exit.

The variation of the gain factor depending of the neutron energy is a second point of interest. With the chosen TASP configuration and a sample size of 1 cm^2 a gain factor of 1.6 to 2.4 was calculated for wavevectors k_i between 2.3 and 1.1 $Å^{-1}$ (Fig. 5b

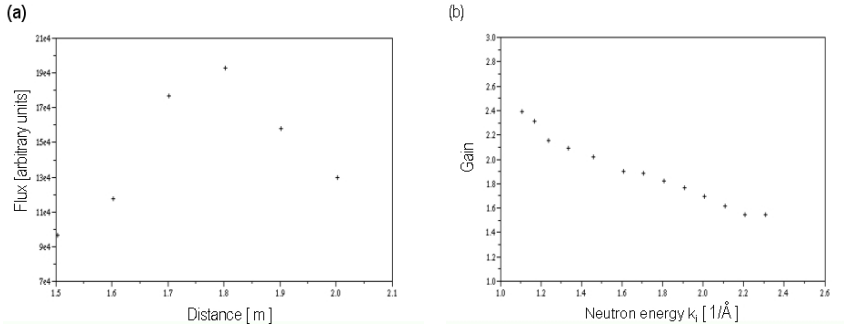

Fig. 5: (a) neutron intensity behind guide exit – focal point at 1.8 m after monochromator; (b) gain with focusing guide over a setup without trumpet for different neutron energies

C. Comparison of advanced neutron guides

Sophisticated neutron guide systems take advantage of supermirrors to increase the neutron flux. However, the finite reflectivity of supermirrors becomes a major loss mechanism when a large number of reflections occur, e.g. in long neutron guides and for long wavelengths. In order to reduce the number of reflections, ballistic neutron guides have been proposed. Usually linear tapered sections are used to enlarge the cross section and finally focus the beam to the sample. The disadvantages of linear tapering are an inhomogeneous phase space at the sample position and a decreasing flux with increasing distance from the exit of the guide. We investigated various guide geometries by means of the Monte-Carlo simulation program McStas in order to improve the neutron flux density as well as the homogeneity of the phase space. Four types of neutron guides were compared (table 1): i) a conventional straight guide with supermirror coating $m = 2$, ii) a ballistic guide with linearly tapered divergent/convergent sections, iii) a ballistic guide where the divergent/convergent sections are parabolically shaped in two dimensions and iv) a neutron guide of elliptical shape in two dimensions. Parameters of the neutron guide 1RNR14 at SINQ (Swiss spallation source) are used for source to guide distance, cross section at guide entry etc. representing typical conditions for neutron guides.

	Straight	Ballistic, linearly tapered	Ballistic, parabolically tapered	Elliptical
Cross section at entrance	35 x 120 mm²	35 x 120 mm²	35 x 120 mm²	35 x 120 mm²
Cross section at exit	35 x 120 mm²	23 x 80 mm²	39 x 135 mm²	33 x 112 mm²
Largest cross section	--	76 x 233 mm²	105 x 360 mm²	102 x 250 mm²
Guide length	46.8 m	46.8 m	46.8 m	46.8 m
Length of divergent section	--	12 m	12 m	--
Length of convergent section	--	8 m	8 m	--
Coating (at all sides)	SM, m = 2	SM, m = 3 / 1 / 3[a]	SM, m = 3 / 1 / 3[a]	SM, m = 3
Distance focal point to guide entrance	--	--	1.5 m	1.5 m
Distance focal point from guide exit	--	--	1.3 m	1.3 m
Distance source to guide entrance	1.5 m	1.5 m	1.5 m	1.5 m

Table 1: Geometry of the simulated neutron guides. The dimensions are similar as for the guide 1RNR14 at SINQ, PSI

Figure 6 shows the wavelength dependence of the intensity of the various guide geometries normalized to the intensity of the straight supermirror guide at distances of a) 1.3 m and b) 0.5 m from the guide exit. The intensities are integrated over an area of 10 x 40 mm² and the full divergence. The distance of 1.3 m corresponds to the position of the monochromator of the TASP instrument at 1RNR14 and to the nominal focal point positions of the elliptical and parabolic geometries. At this position the ballistic guide with linearly tapered sections yields only in the range of about 1.5 Å < λ < 5.5 Å. For shorter wavelengths neutrons are lost in the final convergent section as for a significant number of neutrons the angle of incidence is too steep compared to the maximum reflection angle of the coating. For λ > 5.5 Å the divergence of the beam becomes so high that the monitored area is only illuminated incomplete by the ballistic guide compared to the straight guide.

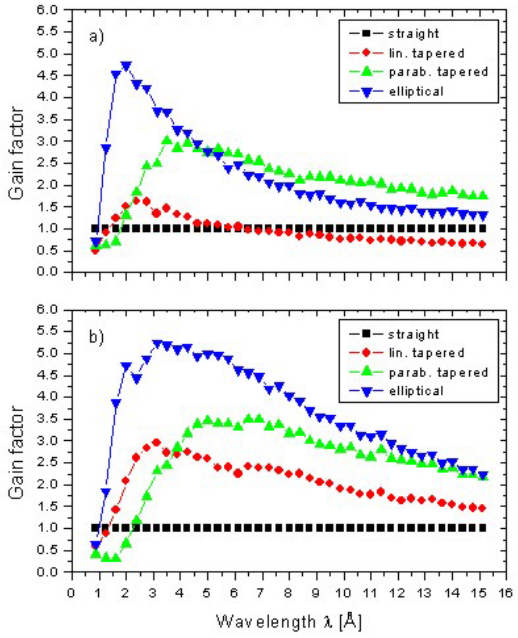

Fig. 6: Gain factors of various guide geometries normalised again a straight supermirror guide (m = 2). Gain factors are calculated from integrated intensities (10 x 40 mm²) at a distance of a) 1.3 m and b) 0.5 m from the guide exit.

The ballistic guide with parabolically shaped divergent and convergent sections exhibit gains for about $\lambda > 2.5$ Å. Below $\lambda = 2.5$ Å, neutrons again hit the convergent section too steeply. The largest gain factors can be obtained the elliptical guide. A maximum gain of about 4.5 at $\lambda \approx 2$ Å can be realised. Even at low wavelengths the gain is significant. This is due to the particular input acceptance and transmission function of the elliptical geometry.

In neutron experiments not only the intensity of the neutron beam but also the phase space distribution (divergence) is important too as the measured signal is a convolution of the phase space with the structure of the sample. In order to identify features of the sample a homogeneous phase space distribution of the neutron beam is desired. Figure 7 shows the intensity distribution versus the vertical and horizontal divergence of different guide geometries at selected wavelengths. It can be seen that the intensity profile is rather inhomogeneous for the linear and parabolic ballistic guides. It breaks down into a structure of peaks because of a mismatch of the phase space delivered by the straight "ballistic" section to the acceptance profile of the convergent part. The phase space of the elliptical guide is very homogeneous only for medium wavelengths (e.g. $\lambda = 4$ Å) a weak peak structure exists in the vertical direction where the focusing of the beam is larger then in the horizontal direction.

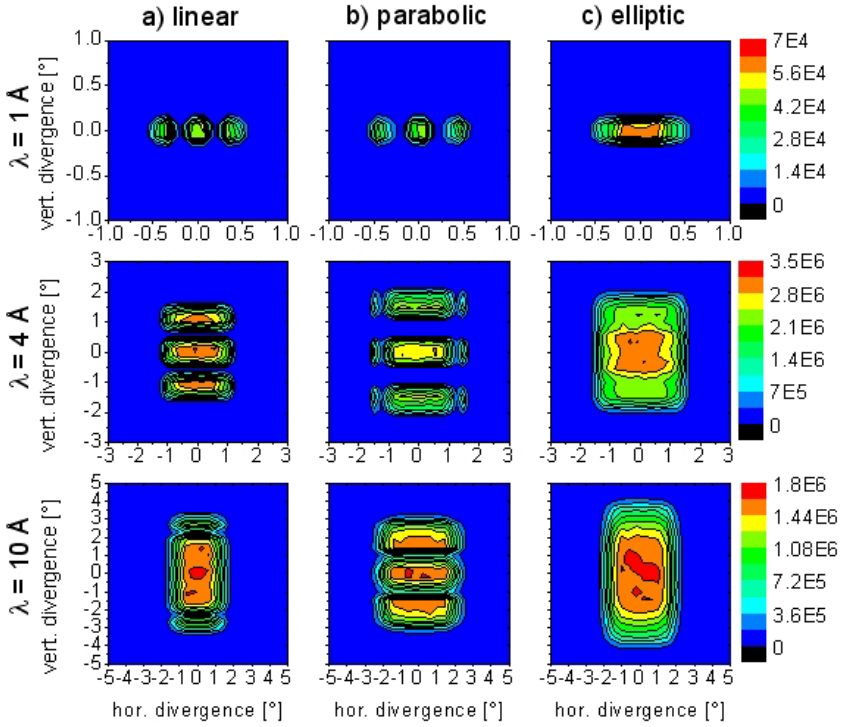

Fig. 7: Vertical and horizontal intensity distribution versus the divergence for wavelengths λ = 1 Å, 4 Å, 10 Å of a) ballistic guide with linearly tapered divergent and convergent sections, b) ballistic guide with parabolic divergent and convergent sections, c) elliptic guide.

We can summarise our results as follow. The transmission of neutron guides can be improved rather dramatically by means of non-linearly tapered ballistic guides. The replacement of the conventional $m = 2$ guide 1RNR14 at SINQ by a ballistic elliptic guide with coatings $1 \leq m \leq 3$ yields a flux gain of the order of 5, while maintaining a very homogenous divergence.

Progress made: **HMI (partner 5) – VITESS responsible**

(a) During the time of the contract, a module simulating straight and curved Fermi choppers was written. Now, all components in a usual TOF instrument can be simulated. Also, a module 'single crystal sample' was written.
(b) Polarisation was included during the time of the contract. The following modules simulating the behaviour of polarised neutrons existed on 29th February 2004:
- ^{3}He polariser
- supermirror polariser
- (polarising) bender
- coil flipper
- gradient flipper (but not yet included in the released version 2.4)
- precession field
- rotating field
- Drabkin resonator (but not yet included in the released version 2.4)
- monitor for polarisation

(c) A single crystal experiment at IPNS was simulated and the results were compared to experimental data.
(d) Many time-of-flight instruments at pulsed sources (e.g. IRIS at ISIS, NSE instrument at SNS) and continuous sources (e.g. NEAT and EXED at HMI) were simulated. Simulations of the chopper spectrometer HET at ISIS were performed (in conjunction with CCLRC) and the results were compared with real data.
(e) NSE instruments at pulsed and continuous sources were simulated, especially IN11 at ILL. The NRSE instrument ZETA and NSE instruments with foils (rotating field) with different configurations (SESANS, SERGIS) were simulated. Simulations of Drabkin resonators and double Drabkin resonators were performed.

Progress made: **NPI (partner 8) – RESTRAX responsible**

RESTRAX has been used in several projects of **instrument development** to assess future instrument performance and/or to optimise parameters of some components (monochromators, collimators, and guides) at ILL Grenoble,
- IN20B (focusing Heusler monochromator, collimator design, flat-cone multianalyser)
- IN14 (design of convergent supermirror guide)
- D2B (study an option with bent perfect Si monochromator)
- SALSA (strain scanner design - neutron guide, monochromators, collimators)
- H22 (supermirror neutron guide)

and elsewhere (e.g. diffractometer E3 at HMI Berlin, design of Si monochromator for strain measurements)

A series of simulations of the three-axis spectrometer H8 at Brookhaven was carried out with RESTRAX in the frame of the ray-tracing **code intercomparison** project.

Progress made: **INFM (partner 9) – McStas contributor**

The Monte Carlo and analytical codes have been benchmarked against experiments for the following classes of imperfect crystals:

- isotropic and anisotropic mosaic crystals. The analysis of mosaic crystal reflectivity has allowed the study of primary extinction effects, presence of inhomogeneities and the

estimation of the total attenuation coefficient. Some of these effects have been successfully implemented in the simulations. The measurement of copper anisotropic mosaic crystal reflectivity has allowed estimating the peak and integrated reflectivity of these crystal versus the azimuthal angle with high accuracy.

- elastically and plastically bent crystals, assembled germanium wafers. A comparison between measured and simulated reflectivity has been performed with neutrons and synchrotron radiation.

The developed routines allow for a detailed estimation of the travel time inside these optical components. Then they are crucial for a detailed simulation of TOF instrumentation.

Task 5. Virtual instruments (ESS)

Partners involved: 2,5

Description of task: To undertake a series of MC design studies of possible instruments for the ESS project, integrating these with other parts of the SCANS project to enable a series of virtual 'ESS experiments' and to document the results to demonstrate the scientific possibilities of the ESS.

Progress made: **Riso (partner 2) – McStas responsible**

See Task 2

Progress made: **HMI (partner 5) – VITESS responsible**

The ESS moderator characteristics were implemented. Several instruments planned for the ESS were simulated:

- reflectometers at LPTS and SPTS with different repetition rates (results published)
- SANS instruments at LPTS and SPTS (publication ongoing)
- backscattering spectrometers at different moderators (results published)
- single crystal spectrometers at different moderators (results published)
- ultra-high resolution powder spectrometer at LPTS (results published)
- a magnetic powder instrument at LPTS and SPTS (publication ongoing)

In many cases, the results were compared to comparable instruments at existing sources to valuate the possibilities of ESS. In other cases, the performance at different target stations and moderators was compared. Also, pulse shaping by (disk) chopper systems on a long pulse target station or at a coupled moderator was simulated and the results compared to the performance using decoupled (poisoned and unpoisoned) moderators.

Task 6. NeXus (data standard)

Partners involved: 4,6

Description of task: Development of the NeXus data standard, in particular of the NeXus dictionary for instrument definition, and provision of assistance to other partners in the use of NeXus.

Progress made: **CCLRC (partner 4)**

The newly formed NeXus International Advisory Committee (NIAC) met for the first time in September 2003 and began the process of ratifying the base classes. This discussion has continued since then, with matters being debated online with the whole neutron community via the NeXus SWIKI http://www.neutron.anl.gov:8080/NeXus/. In addition instrument editors for the various instrument types have now been nominated and they will begin consulting on key definitions once voting on the base classes has been finished (estimated to be early summer 2004).

ISIS has been involved with the NeXus project since its inception, helping to formulate initial classes, producing the FORTRAN77 and Windows bindings, and maintaining the central CVS source code repository. For the NIAC meeting above ISIS consulted with staff members and produced a document detailing its proposed new NeXus based RAW file format; a copy of which can be viewed at
http://www.isis.rl.ac.uk/computing/nexus/isis_nexus_016.pdf.

The ISIS muon group has taken the lead within its community and produced an internationally agreed muon standard for data storage based on the NeXus format; this standard is currently being revised to incorporate changes that have occurred during the base class voting.

In addition ISIS has also contributed to:

- A re-organisation of the CVS repository to provide a better structure for the increasing number of applications and bindings
- The production of a Linux NeXus RPM install kit.

A key tool in the ISIS NeXus project is the Open GENIE software package, which can readily read, write and manipulate NeXus data files. Using Open GENIE a basic ISIS (VMS) RAW data to NeXus file converter has been produced.

Progress made: **PSI (partner 6)**

NeXus is a common data format for both the neutron and synchrotron community. The aim is to provide an efficient and platform independent data exchange format.
The NeXus proposal has five different levels:

- A physical file format. This is the Hierarchical Data Format HDF (http://hdf.ncsa.uiuc.edu) as developed by the National Center for Supercomputer Application, USA.
- An API for accessing NeXus-HDF files
- A structure for organising data in a NeXus file
- Rules for storing individual data items.

- A dictionary of variable names and definitions of valid NeXus file formats for different instrument types.

More information about NeXus can be found at http://lns00.psi.ch/NeXus.

Within the SCANS project the following projects were realized:

- Extensions to the ANSII-C NeXus core API.
- Development of software adapters to make the NeXus-API usable from a plethora of further programming platforms.
- A NeXus tutorial was written.

A. Extensions to the NeXus core API

NeXus uses the Hierarchical Data Format HDF from the National Center for Supercomputing Applications NCSA as its physical file format. This is a binary, platform independent, self describing data format. HDF is well supported by a lot of data analysis packages. The HDF libraries are public domain software and are available for the ANSI-C, Fortran77 and Java programming languages for all important operating systems. Using the HDF library is fairly complex and covers a wide range of functionality. On this account a common NeXus Application Programmer Interface (API) was defined which facilitates access to NeXus-HDF files. The original NeXus-API based on the HDF version 4.1 (HDF-4).

After intense discussions at the 2001 joint NeXus/SCANS meeting a new NeXus-API version 1.3.3. was released in 2001. This new version included a new function NXflush, to flush data to the output file, and the new Java NeXus-API as part of the standard distribution. Furthermore the API was extended to support unlimited dimensions.

Since 2000 the developers of HDF promote mainly the new HDF5 library, which is incompatible to the HDF-4 version. The HDF5 version has a much cleaner interface. Further improvements are that HDF5 also supports file sizes larger then 2GB and an unlimited number of objects in a file. As next generation source need these enhanced features, it became necessary to provide a NeXus-API for HDF5 as well. For the implementation of this new API we strived to achieve two main goals:

- maximum compatibility at the API level in order to minimize changes to existing code
- support for both HDF-4 and HDF5.

These requirements made the implementation of the new API a little tricky but since June 2001 a new version of the new NeXus-API is available. The new NeXus-API version 2.0.0. can be downloaded from http://lns00.psi.ch/NeXus/NeXus_API.html#Install .

The new API can be built to support HDF-4 or HDF5 or both. The main goal of maximum API compatibility was achieved. Only one new API function became necessary for the creation of compressed datasets due to limitations in the HDF5 library. The new NeXus-API is written in the ANSII-C programming language. The C-API was interfaced to both the Fortran77 and Java programming languages.
If the measured data are stored in the NeXus data file format the next logical steps are viewing, editing and analysing the data. In this direction the well-tried NXbrowse viewer has also been adapted to work with the new API version. Shortly after the release of the new NeXus API the first data files based on HDF5 were collected at the Single Crystal Neutron Diffractometer (TriCS) and Amor reflectometer at the SINQ spallation source. HDF5 support was integrated into PSI's instrument control software and about 20,000 files have already been

written with the new NeXus-API.

B. Porting the NeXus API to more Programming Systems

Java is an important new programming platform. One of its strong features is platform independence and this makes Java a valuable tools for the development of general purpose NeXus applications. However, Java does not support HDF or NeXus out of the box. Moreover Java has an own incompatible system for the representation of numbers internally. Both problems were solved through a software adapter written using the Java Native methods Interface. Binary packages for a couple of important platforms and documentation is available from http://lns00.psi.ch/NeXus/jnexus/index.html

Scripting languages are an extremely valuable programming tool. They can be used for quick application development or as a software glue to combine separate software packages in a creative way. In order to broaden the NeXus user base it would be valuable to have a NeXus interface to scripting languages. Most scripting languages have a C-interface which allows to extend them through library code. The problem is that there are too many scripting languages with different calling conventions for the C-language extension API. This problem can be solved through a tool named SWIG, the Simplified Interface and Wrapper Generator (http://www.swig.org). SWIG generates interface code for a variety of scripting languages including perl, tcl, python from an interface definition file. Such an interface description file for the NeXus-API and a dataset interface were developed and tested with the scripting languages Tcl and mzScheme.

A popular tool for analysing data is the commercial package IDL. For example, IDL is the programming language used for the general analysis tool LAMP. IDL does not support HDF5 directly. Therefore a NeXus-API for IDL (Interactive Data Language) was developed which uses IDL's native method support. Thus both HDF-4 and HDF5 NeXus files can be accessed in IDL as well.

In 2003 the McStas developers have redesigned the graphical output interface of McStas. One of the possible output format is SCILAB, a public domain graphical data analysis tool like Matlab. This triggered us to provide NeXus support for SCILAB, because this would simplify the NeXus integration into McStas.
Moreover, SCILAB as powerful analysis tool in itself deserves NeXus support. An advantage of SCILAB is that external tools/libaries can be included easely as dynamic link libraries. Using this feature a suitable dynamic link library was developed which allows SCILAB to read and write NeXus files. This interface could also be used to convert standard ASCII-McStas data into NeXus files through a SCILAB program. The new NeXus-SCILAB interface is already tested for the TRU64 and LINUX platforms. The extension to other platforms can be done without big effort by linking the standard NeXus API on the target platform. A data analysis program REDAS using the NeXus-SCILAB interface is used for the reflectometer AMOR at SINQ. The GUI of the program is realized through the SCILAB-TCL interface.

C. NeXus Instrument Definitions

The specification of the NeXus instrument definitions has made same progress. A NeXus Advisory Committee was founded to oversee future developments of the NeXus format including the NeXus instrument definitions. The definitions will be expressed in the form of XML-DTD's. The present state is documented on the webpages:
http://lns00.psi.ch/NeXus/NeXus_metaformat.html

and
http://www.neutron.anl.gov:8080/NeXus

D. NeXus Tutorial

In order to support the NeXus user community a two-part Tutorial was written and is available on http://lns00.psi.ch/NeXus/nxtutorial.ps. The first part covers the installation of NeXus and its basic usage. The second part covers advanced topics of the NeXus API and an introduction to the NeXus dictionary API.

Task 7. Inverse methods of data analysis

Partners involved: 1,4,7

Description of task:
(a) Development of inverse methods of analysis, in particular Bayesian analysis (maximum entropy) / MC based methods (e.g. RMC).
(b) Investigate the possibility of on-line monitoring of the accuracy of derived parameters in order to maximise experimental efficiency.

Progress made: **UU (partner 1)**

The work started in 2002 to include angular (triplets) constraints in the **RMCA** code has finished. The new constraint has been tested successfully on simulations of nano-porous carbon. The structure of carbon atoms is supposed to consist to a large extent of sp^2 bond which give bond-bond angles of 120^o. Without angular constraints in the RMC modelling, it was impossible to simulate a structure that fitted measured data without producing unrealistic bond-bond angles of 60^o. The new constraint solved this problem. The user can select to model any combination of atom types in a triplet.

The work on RMCt, an inverse method for producing dynamical models (‘movies') based on inelastic neutron scattering data, was started and a test version of the programme produced and tested. The method works. More work is needed to finish.

The RMC code for powder diffraction data, RMCPOW, can combine neutron and X-ray powder diffraction data and some steps have been made towards including single crystal data. RMCPOW has also been tested successfully for ab-initio determination of magnetic structures. Within the time-frame of the SCANS project development of the RMCPOW code has included adding more flexibility for experimental data input, e.g. data can be read not only as a function of scattering vector (Q) but also angle (2θ) or time-of-flight (TOF) and need not be equidistantly binned. More resolution profiles have been added. The non-linear minimisation parameter minimisation step has been revised, and now also wavelength and the 2θ zero-point (or corresponding for TOF) can be refined. Linear constraints on parameters refined using non-linear least-squares are now applicable.

Complete teaching examples are available for RMCA and RMCPOW programs. All RMC and related programs, including CONFPLOT graphics, are available as a single package called WinNFLP.

Progress made: **CCLRC (partner 4)**

No development has been made in the area of Bayesian methods due to the unavailability of a key expert. However this did not have any knock-on effect on other parts of the project.

Progress made: **SzFKI (partner 7)**

1. Code developments

A new Reverse Monte Carlo code has been written for modelling disordered (liquid and amorphous) structures. The new code, RMC++, can replace the existing RMCA programme, as the format of all input files are identical to those required for RMCA. RMC++ has been

written in C++, for providing a framework for modular development (which possibility is missing from the existing RMCA code).

At present, RMC++ is best suited for modelling the structure of atomic/ionic and molecular liquids. It is now possible to move entire flexible molecules, a feature which was missing from all previous versions of RMC. The new code has been tested for one- and multi-component atomic(/ionic) systems, as well as for several molecular liquids (including Cl_2, CCl_4, C_2Cl_4 and water). Experience gained during the testing period shows that RMC++ is about two to three times faster than RMCA.

RMC++ has been officially released in October, 2003; few months later, the first bug-fix followed. The programme is available at http://www.szfki.hu/~nphys. Full support is provided for Windows and Linux based platforms, whereas the original Apple Macintosh version (still available on the above website) is not going to be maintained.

As a separate development, the RMCA programme has been extended to be able to deal with quadratic backgrounds (very much like it is done in MCGR version 2.15). This feature is expected to provide valuable help when neutron diffraction data on hydrogeneous materials. Our own testing ground was CBr_3H, for which the approach proved rather successful: neutron diffraction data can now be successfully reproduced.

2. Novel applications of the Reverse Monte Carlo method

2.1. The application of the Reverse Monte Carlo method for modelling the structure of *aqueous elecrolyte solutions* has been re-examined. According to the new approach, one neutron and one X-ray total structure factor are modelled simultaneously: the neutron S(Q) reflects mostly the water (sub-)structure, whereas the X-ray data carry more information on the hydration shells of the ions. Instead of involving more experimental total structure factors for a given compostion (by using, e.g., the method isotopic substitution in neutron diffraction), structural changes as a function of the elctrolyte concentration are monitored.

The first two examples were aqueous lithium-chloride (LiCl) and hydrogen-chloride (HCl) solutions. For both materials, neutron and X-ray difraction measurements are available over a rather wide concentration range. It could be concluded that for selected atom(/ion) pairs, the two total structure factors provide sufficient basis for discussing the water (sub-)structure and even the structure of the hydration shells in detail.

2.2. Understanding the microscopic processes that accompany *chemical reactions* is of utmost importance. Diffraction methods, that proved to be extremely successful in describing microscopic structure, have hardly been applied for direct investigations of chemical reactions in the fluid phase. The main objective of our study was to assess the capability of these methods, when combined with Reverse Monte Carlo, for providing new details concerning structural relations in equlibrium chemical reactions.

Our strategy can be summarised as follows: first, (equilibrium) molecular dynamics simulations have been carried out on systems containing monomers and dimers of a fictious species A (dimers will be noted as A_2). Average structural quantitites like the (site-site) pair correlation function (pcf) and its Fourier transform, the (site-site) structure factor (sf) have been calculated and applied as input quantities for Reverse Monte Carlo (RMC) calculations. It was inspected that how well the mole fraction of the monomers(/dimers) could be retrieved on the basis of particle configurations in case where no extra information was included in

addition to the 'diffraction' data. As a further (more realistic) attempt, the extra piece of information that dimers are formed (but not their concentration!) was added as a constraint in the RMC calculations.

From a sizeable set of calculations (most important varying parameters: density and intramolecular A-A distance), it could already be concluded that liquid-like densities and a clear separation of intra- and intermolecular distances are necessary pre-requisites for reproducing the concentration of dimers within about 5 %.

2.3. The possibility of (RMC) modelling of structures with more than one characteristic length-scale was investigated. For this purpose, the structure factors of *computer-built models of aerogels* have been simulated by the Reverse Monte Carlo method. The 'experimental' structure factors contained a distinct small angle scattering part, in addition to the usual 'wide angle' part.

It was found that at not too low densities (but still well within the 'aerogel' range), the full structure factors could be well fitted and the resulting models possessed all key features (like porosity) of the original structures. It was shown that fitting the the small angle scattering part only is not sufficient even for the good reproduction of the pair correlation function. This finding may serve as a warning against over-interpreting data from small angle neutron/X-ray scattering.

Task 8. Data assessment/ information content

Partners involved: 1,4

Description of task:
(a) Investigate methods for assessment of raw data quality (statistics and systematics).
(b) Investigate methods for estimation of analysed data information content.

Progress made:

M. Johnson has developed a simple expression to quantify the information content in a diffraction pattern for residual stress determination. This has been used for optimising new instrumentation at the ISIS facility and in preliminary design studies for ESS instrumentation.

R. McGreevy has investigated the information content of diffraction data in PDF form as a function of the statistical accuracy of the structure factor, i.e. the measured data. This has conclusively shown that data measured in the time frame for a typical crystallographic study (e.g. 10-15 minutes on the GEM instrument at ISIS) cannot be reliably used for a PDF analysis – counting times an order of magnitude greater (e.g. several hours on GEM) are required.

Task 9. Dissemination of the results of the project.

Partners involved: 1

Description of task: Disseminate the results of the project to neutron scattering facilities and users via the Neutron Round Table.

Progress made: The results of the project have been presented to the Neutron Round Table at all meetings during the timeframe of the project.

Sections 4.1, 4.3 and 5.1 give full details of all dissemination activities.

- 45 papers published or in press (to date).
- More than 40 conference contributions.
- 8 special meetings, workshops, symposia etc.
- 4 major web sites and contributions to others.

5. Exploitation and dissemination of results

5.1 Publications, conference proceedings etc.

Papers

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- Highly Frustrated Magnetism 2003 Conference. Budapest, Hungary. (2003)
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- Joint McStas-Vitess workshop. ISIS, UK. (2004)
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5.2 Patentable results.

There are no patentable results. All of the results of the project have been or will be made publicly available.

5.3 Contacts with potential users.

Web sites:
Monitoring downloads shows that software produced as part of the SCANS project is in use by hundreds of users in more than 20 European countries, and many others worldwide.
http://www.studsvik.uu.se/software/scans/scans.htm
http://neutron.risoe.dk/mcstas/
http://www.hmi.de/projects/ess/vitess/
http://omega.ujf.cas.cz/restrax/index.html
http://www.studsvik.uu.se/Software/rmc/rmc.htm
http://www.esrf.fr/computing/scientific/xop2.1/extensions.html#NOP
http://www.neutron.anl.gov/nexus/

Mailing lists:
scans@risoe.dk
mcstas@risoe.dk
vitess@hmi.de

Neutron News Volume 13 Issue 4 (2002) was edited by the SCANS coordinator and devoted to Monte Carlo simulation of neutron scattering instrumentation. It featured several papers by SCANS participants.

The results of the SCANS project have been presented at all meetings of the Neutron Round Table held during the period of the contract.

The results of the SCANS project have been presented at numerous international conferences, workshops etc. See section 4.1 for conference contributions by SCANS participants. There have also been many conference contributions using software produced as part of the SCANS project, but not involving SCANS participants. See Section 5.1 for special meetings, workshops, held under the auspices of SCANS.

6. Management and coordination aspects

6.1 Project coordination activities

2000	May	1st general meeting.	Institut Laue Langevin, Grenoble.
2000	October	Special meeting 'Requirements for Monte Carlo simulation of polarised neutron scattering instruments'. Joint meeting with members of the ENPI Network (European Neutron Polarisation Initiative).	Institut Laue Langevin, Grenoble.
2001	January	Workshop 'Monte Carlo simulation of neutron scattering instruments using McStas'. Organised with support from the Neutron Round Table.	Risø National Laboratory, Denmark.
2001	March	2nd general meeting. Organised in conjunction with the NeXus 2001 workshop.	Paul Scherrer Institute, Switzerland
2001	June	Workshop on VITESS 2 and other Packages for Simulations of Neutron Scattering.	Hahn-Meitner-Institut, Berlin
2001	September	Mini-symposium organised at the International Conference on Neutron Scattering.	Munich, Germany.
2001,	September	Special symposium at the 7th ESS general meeting.	Graz, Austria.
2001	October	3rd general meeting.	Budapest, Hungary.
2002	March	Common workshop on MC simulation packages.	Institut Laue Langevin, Grenoble.
2002	15 May	4th general meeting. Held as a satellite to the ESS European Conference.	Bonn, Germany.
2002	May	Joint RTD network meeting (organized by,the SCANS coordinator).	Bonn, Germany.
2002	October	5th general meeting.	Abingdon, UK.
2003	April	6th general meeting.	Prague, Czech Republic.
2003	Sept	7th general meeting.	Nykoping, Sweden.
2003	October	2nd Reverse Monte Carlo Conference**.** The preparation of a proceedings volume, based on the oral and poster presentations, is underway.	Budapest, Hungary.
2004	February	8th general meeting.	Abingdon, UK.
2004	February	ISIS Joint McStas-VITESS training course	ISIS, Didcot, UK.

6.2 Manpower allocation.

See Table 6.2.1. The total manpower allocated to the project was significantly larger than funded by the contract. The only task for which proportionately (i.e allocated/planned) there has been any significant lack of effort has been task 8. However this was a small task (less than 2% of the total planned manpower for the whole project), which did not affect the rest of the project, and which was assigned lower priority mainly due to the unavailability of key expertise, and the impossibility to bring in appropriate expertise purely for such a small task.

6.3 Budget Information.

See Table 6.3.1.
Some changes were made to the budget during the course of the project, via contract amendments. The major change concerned the reallocation of resources following the withdrawal of Technical University Delft from the project.

6.4 Management of the project

The contract was amended twice during the project. The amendments concerned:

1. Extension of the contract due to personnel problems encountered by Technical University Delft.
2. Subsequent withdrawal of Technical University Delft from the project due to the same personnel problems.
3. Re-allocation of tasks and resources following (2).
4. Some re-allocation of tasks and resources following the move of the coordinator between institutions.

These changes had no significant effect on the overall scope of the project.

Manpower allocation (man months)											
		1	2	3	4	5	6	7	8	9	
Task		McStas	Shadow	Samples	Inst.	VITESS	NeXus	Inverse	Data	Results	Total
Partner		Whole project (actual)									
1	UU	0	0	0	0	0	0	63	0	1.6	64.6
2	Risoe	18	0	2	5	0	0	0	0	0	25
3	TUD	3.5	0	0.5	11	0	0	0	0	0	15
4	CCLRC	3	0	2	4	2	7.2	0	0.7	1	19.9
5	HMI	22	0	9	35	52	0	0	0	0	118
6	PSI	4	0	0	13	0	18	0	0	0	35
7	SzFKI	0	0	0	0	0	0	35	0	0	35
8	NPI	6	0	3	9	0	0	0	0	0	18
9	INFM	24	31.6	4	4	0	0	0	0	0	63.6
	Total	**80.5**	**31.6**	**20.5**	**81**	**54**	**25.2**	**98**	**0.7**	**2.6**	**394.1**

Manpower allocation (man months)											
		1	2	3	4	5	6	7	8	9	
Task		McStas	Shadow	Samples	Inst.	VITESS	NeXus	Inverse	Data	Results	Total
Partner		Whole project (planned - from 2003 contract modification)									
1	UU	0	0	0	0	0	0	21	2	1	24
2	Risoe	12	0	0	4.4	0	0	0	0	0	16.4
3	TUD	1	0	1	16	0	0	0	0	0	18
4	CCLRC	3	0	0	3	0	0	12	3	0	21
5	HMI	6	0	0	6	41.2	0	0	0	0	53.2
6	PSI	8.5	0	1	19	0	6	0	0	0	34.5
7	SzFKI	3	0	3	0	0	0	12	0	0	18
8	NPI	2	0	1	2	0	0	0	0	0	5
9	INFM	11	33	0	15	0	0	0	0	0	59
	Total	**46.5**	**33**	**6**	**65.4**	**41.2**	**6**	**45**	**5**	**1**	**249.1**

Manpower allocation (man months)										
		1	2	3	4	5	6	7	8	9	
Task		McStas	Shadow	Samples	Inst.	VITESS	NeXus	Inverse	Data	Results	Total
Partner		Whole project (actual-planned)									
1	UU	0	0	0	0	0	0	42	-2	0.6	40.6
2	Risoe	6	0	2	0.6	0	0	0	0	0	8.6
3	TUD	2.5	0	-0.5	-5	0	0	0	0	0	-3
4	CCLRC	0	0	2	1	2	7.2	-12	-2.3	1	-1.1
5	HMI	16	0	9	29	10.8	0	0	0	0	64.8
6	PSI	-4.5	0	-1	-6	0	12	0	0	0	0.5
7	SzFKI	-3	0	-3	0	0	0	23	0	0	17
8	NPI	4	0	2	7	0	0	0	0	0	13
9	INFM	13	-1.4	4	-11	0	0	0	0	0	4.6
	Total	**34**	**-1.4**	**14.5**	**15.6**	**12.8**	**19.2**	**53**	**-4.3**	**1.6**	**145**

Table 6.2.1. Manpower allocation – actual, planned and difference.

Total Budget (modified Mar 2003)										
	UU	Risoe	TUD	CCLRC	HMI	PSI	SzFKI	NPI	INFM	TOTAL-PSI
Personnel	0.00	73049.00	158285.00	86626.00	66793.00	76000.00	0.00	0.00	57000.00	441753.00
Durable equipment	0.00	0.00	2000.00	0.00	0.00	4000.00	1000.00	0.00	0.00	3000.00
Travel and subsistence	15000.00	4943.00	3000.00	7500.00	6900.00	5000.00	4000.00	5000.00	5104.00	51447.00
Consumables	5994.00	0.00	1000.00	0.00	0.00	0.00	0.00	0.00	0.00	6994.00
Overheads	3601.00	84008.00	0.00	151333.00	7307.00	0.00	1000.00	1000.00	12301.00	260550.00
TOTAL	24595.00	162000.00	164285.00	245459.00	81000.00	85000.00	6000.00	6000.00	74405.00	763744.00
EU contribution	24595.00	81000.00	46000.00	81000.00	81000.00	0.00	6000.00	6000.00	74405.00	400000.00
%	100.00%	50.00%	28.00%	33.00%	100.00%	0.00%	100.00%	100.00%	100.00%	52.37%

(Year 1 +Year 2 + Year 3) accepted costs + Year 4 cost statement										
	UU	Risoe	TUD	CCLRC	HMI	PSI	SzFKI	NPI	INFM	TOTAL
Personnel	0.00	105396.40	154583.29	95844.87	69881.73	0.00	0.00	0.00	58360.69	484066.98
Durable equipment	0.00	946.32	0.00	0.00	0.00	0.00	1000.00	0.00	0.00	1946.32
Travel and subsistence	16545.82	11104.45	3992.28	12480.89	4069.63	0.00	4196.66	4506.63	6413.02	63309.38
Consumables	3306.25	0.00	0.00	0.00	441.70	0.00	0.00	0.00	0.00	3747.95
Overheads	3176.61	117964.60	2429.99	141573.36	7376.07	0.00	1039.33	901.33	12954.75	287416.04
TOTAL	23028.68	235411.77	161005.56	249899.12	81769.13	0.00	6235.99	5407.96	77728.46	840486.67
EU contribution (req)	23028.68	117705.89	45081.75	82465.21	81769.13	0.00	6235.99	5407.96	77728.46	439423.07
EU contribution (max)	24595.00	81000.00	46000.00	81000.00	81000.00	0.00	6000.00	6000.00	74405.00	400000.00

Table 6.3.1. Project budget – planned and actual.