Final Report

The eVERDI Project

IHP-ARI RESEARCH INFRASTRUCTURE RTD PROJECT

Contract Review Report

Contract N°	**HPRI-CT-2001-50020**
Network Title	eVERDI - Electron-Volt Energy Resonance Detector Instrument
Start date of contract	31st October 2001
End date of contract	31st October 2006 (a)
Contract value (EURO)	2 258 715 € (1 200 000 € will be provided by the Community)
Internet homepage	http://www.isis.rl.ac.uk/molecularspectroscopy/evs/index.htm
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(a) contract extension granted November 2004

Partnership Summary

Participant number (Co-ordinating partner as participant N°1)	Name of Participating Organisation	Name of Responsible Person	Role in network*
1	CLRC, UK	John TOMKINSON	LSF-TMR
2	INFM - UdR Roma Tor Vergata,Italy	Carla ANDREANI	OTHER
3	University of KENT at Canterbury, UK	Robert NEWPORT	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
USER: a research organisation representative of users of the facilities covered by the Round-Table
SOC: European scientific societies
IND: an industrial or commercial enterprise
OTHER: other types of participant

1 PROJECT OVERVIEW

The objectives of the eVERDI project are to **enhance the present performance** of ISIS and to **develop key technologies** for the next generation of electron volt (eV) neutron instruments. The proposed eVERDI project will enhance the performance of VESUVIO at ISIS and support the **R&D** efforts towards new instruments on the next generation neutron sources: the European Spallation Source (ESS) and the Spallation Neutron Source (SNS).

The eVERDI project is based around the following deliverables:

The construction of a high resolution and high count-rate forward scattering detector (**FSD)** bank for neutron scattering at high momentum transfer (10 $Å^{-1}$-100 $Å^{-1}$) and high energy transfer (1eV-20 eV).

The construction of a very low angle detector (**VLAD)** bank (1°< 2θ < 5°) for neutron scattering at low momentum transfer (3 $Å^{-1}$-10 $Å^{-1}$) and with very high-energy transfer, ω >1 eV.

The development and optimisation of novel γ **detectors,** to be employed in the VLAD bank, together with the associated high-count rate electronics and data acquisition systems, which will be required.

The **training of young scientists** in developing experimental techniques and data analysis procedures for eV neutron scattering.

In **summary**, the work of the fifth reporting period has proceeded as follows:

The exploitation of the VLAD detector was always the most ambitions objective of eVERDI. The final detector arrangements proved more difficult to achieve than expected and suffered from high levels gamma background. A gamma-ray survey of the experimental blockhouse was undertaken and showed higher levels of gamma than had been anticipated coming from all directions, the highest level was from the forward direction. In despite of this two experiments were performed, on water and on praseodymium. The signal from water is strong and it could be readily followed, the results have been published. The experiment on praseodymium was by far the most challenging since the signal falls off dramatically with angle and there can be but few detectors at the lowest angles. A preliminary analysis indicates that the results are compromised by the presence of small levels of Au impurities.

The new FSD detectors produced last year gave, with respect to the original detectors, significant improvements in signal-to-noise and resolution. Several experiments were performed, falling into two classes; total cross section measurements and conventional Neutron Compton Scattering measurements. The total cross section experiments proved to be very demanding of the instrument as a whole. This stemmed from the anomalous cross section determinations obtained for some samples. The short-fall in measured cross section became a major point of discussion at an international conference and significant work was undertaken to convince the user community that the spectrometer was performing correctly. This was achieved and anomalous cross section measurements are now a generally accepted aspect of high energy neutron scattering. These measurements exploited the signal-to-noise improvements obtained through the eVERDI Project.

Two measurements of the Neutron Compton profile of hydrogen in various salt/water solutions were less successful. Unexpected variations in profile were observed across the detector bank, giving an apparent resolution degradation to about 4.5 (compared to the value, 3, obtained from single detectors). This was finally traced to subtle crosstalk contamination. Despite this problem distinct changes in the Compton profile could be produced by varying the salt and the solution’s pH. The new software that was developed to analyse the data from the FSD was instrumental in detecting and understanding these detector problems. The contract amendment which enabled us to retain man-power for a further year was entirely justified by these events. The contamination is readily removed by a reorganisation of the detectors en-echelon, a development that will be undertaken after the eVERDI Project is closed. The overall success of the eVERDI Project can be judged by the fact that, based on the data it has provided, a new Neutron Compton scattering spectrometer has been provisionally approved for funding on SNS (USA) in the near future.

2 COMPARISON WITH THE PROJECT PROGRAMME

2.1 Scientific and Technical Performance

In Table 1 below is the list of the four areas of research to be undertaken by eVERDI and the associated technical objectives deliverable over the (originally four but now) five years of the project .

<table>
<tr><th colspan="3">TABLE 1</th></tr>
<tr><th></th><th>Research Task</th><th>Technical Objectives (Deliverables)</th></tr>
<tr><td>1</td><td>Design a detector assembly suitable for measurement of protons.</td><td>Construction of a high resolution and count rate forward scattering detector (FSD).
completed</td></tr>
<tr><td>2</td><td>Develop a theoretical understanding of the FSD data.</td><td>Write and issue a FSD data analysis package.
completed</td></tr>
<tr><td>3</td><td>Develop the gamma-detector technologies to a point such that they can be compared and contrasted.</td><td rowspan="2">Construct a very low angle detector (VLAD) based on the most promising system(s).
completed</td></tr>
<tr><td>4</td><td>Develop the fast counting electronics need to support the VLAD</td></tr>
<tr><td>5</td><td>Develop a theoretical understanding of the VLAD data.</td><td>Write and issue a VLAD data analysis package.
completed in part – insufficient data was obtained from VLAD.</td></tr>
</table>

An overview of the technical progress made is given in Table 2 below. This table is taken form the lists of tasks defined in the Annex to the eVERDI contract.

2.2 Deliverables

The deliverables are listed in Table 2, condensed from the original specification in the Annex of the eVERDI contract.

TABLE 2			
1. Forward Scattering Detector			
1.1	**CONSTRUCTION SUBTASK**		
			Comment
1.1.1	RAL	The FSD for NCS measurements on hydrogen containing systems. The geometric contributions to the final resolution and the saturation problems will both be reduced, by decreasing the size of individual detector elements and positioning them along the annulus associated with the Debye-Scherrer cone. The FSD bank will consist of scintillator detectors at angles about $35° < 2\theta < 55°$.	The installed detector has a slightly reduced geometric contribution to its resolution (see also 1.1.2, below). The saturation problem has been eliminated by exploiting the new technology. The (relevant) data collection rate has effectively tripled.
1.1.2		The new analyser foil arrangement of eVERDI will improve resolution by a factor of about three.	The installation of the new technology resulted in a dramatic improvement in the line-shape (Lorentzian to Gaussian) and a two-fold reduction in the full-width-at-half-height. We believe this represents an effective improvement in the resolution by a factor four.
1.2	**DATA ANALYSIS SUBTASK**		
			Comment
1.2.1	UNI KENT	In principle, proton wave functions and potential-energy surfaces can be reconstructed from FSD data in a model independent way.	Model independent data analysis is now routine on the spectrometer. Copies of the data analysis manual are available.
1.2.2		The reconstruction of the wave function in the relatively simple and well understood metal hydride system to provide verification of the data analysis procedures used on eVERDI-FSD.	Achieved using the well understood metal hydride MnH (with low energy quantum tunneling states and classical higher energy states). The derived potential is completely in line with published spectroscopic data.

TABLE 2. CONTINUED			
2. Very Low Angle Detector			
2.1	**VLAD DEVELOPMENT AND FAST ELECTRONICS SUBTASK**		
			Comment
2.1.1	INFM	The VLAD bank will require the use of the Resonance Detector Technique (RDT). The RDT measures the energy of scattered neutrons. Prototype detector devices will be assessed and the final choice will be based on its performance in realistic experimental conditions.	The YAP technology finally selected proved robust and effective.
2.1.2		The tests will be used to select detectors with the best efficiency, resolution and γ background suppression. This chosen technology will be used in the final assembly.	
			Comment
2.1.3.	INFM	Associated with the VLAD; fast, high count-rate electronics and data acquisition systems will be developed.	The data acquisition system has been installed and is operating well.
2.2	**VLAD COLLIMATION SUBTASK**		
			Comment
2.2.1	RAL	Access to very low angles is required for VLAD, and yet the γ detectors must lie beyond the penumbra of the transmitted neutron beam to suppress background.	New collimation was installed and was a much easier and cheaper solution to the problem than that originally proposed. The improvement has exposed an underlying γ background that will be tackled in due course.
2.2.2		The present neutron beam stop assembly will not be reorganised. A suitable in beam collimation device will be constructed	
2.3	**VLAD CONSTRUCTION SUBTASK**		
			Comment
2.3.1	INFM	A VLAD bank (1°< 2θ < 5°), equipped with the selected γ detectors, will be constructed	The detector bank was constructed and installed based on YAP technology.
2.3.2	INFM	Final selection of VLAD technology.	
2.4	**VLAD DATA ANALYSIS SUBTASK**		
			Comment
2.4.1	UNI KENT	VLAD will require new data analysis procedures.	But little data has been obtained to date and analysis is none routine. The analysis processes are currently insufficiently robust to use a ‘manual’ as the only support for their understanding.
2.4.2			
2.4.3		Initial versions of the analysis programs released.	These were tested by the Italian partner.
2.4.4		Verification tests of VLAD detector and analysis programs using suitable calibration samples.	Measurements on a Pr sample have been performed, they demonstrated that the γ background from the sample itself is a serious problem.

2.3 Exploitation and Dissemination

The project has been delivered to specification and within budget but somewhat late. The components provided will be fully exploited at ISIS on a scheduled basis from October 2007.

Dissemination efforts included, both, aspects of design and scientific output and a steady stream of high profile papers appeared in the relevant scientific literature. To underline the common thread relating these publications to the project, their details were annexed to the yearly reports. Our efforts here can already be judged successful in terms of recent dissemination events, most especially at the International Conference on Neutron Scattering. At this venue there was a major session dedicated to ‘Femtosecond dynamics’ (see, http://www.icns2005.org/programme.html).

As a direct result of this, and other similar events, the new American neutron source, SNS, has provisionally approved the building of a spectrometer that will exploit the eVERDI technological advances. This is such an important a step that we have taken the liberty of publishing, on our web page, the text of the letter of intent that was greeted so positively by the SNS board.

The web page was regularly updated:
http://www.isis.rl.ac.uk/molecularspectroscopy/evs/index.htm,
(also, http://www.fisica.uniroma2.it/infm/vesuvio/dins/index.html).

The CORDIS web page will be brought up to date after this report is finalised.

2.4 Management and Coordination

The eVERDI project was co-ordinated by Dr J Tomkinson at the Rutherford Appleton Laboratory, where he is the Head of the ISIS Molecular Sciences Group. The Rutherford Appleton Laboratory provided much of the necessary technical direction and leadership required for the project, together with the secretarial support necessary to service the management meetings and information dissemination.

The project was steered and progress monitored by the *eVERDI Project Management Committee* (PMC) with representatives from all of the participating groups in the eVERDI programme. The PMC was chaired by the coordinator, Dr. J Tomkinson, and met twelve times since the start of the project, seven times face-to-face and otherwise by videoconference. These meetings were used to set and refine objectives, define priorities and to review progress. The minutes of these meetings were circulated to the participating groups and appeared annexed to the yearly reports. During installation, towards the end of the project, when all the participating members were present for several days continuosuly, formal meetings were abandoned and no records kept of the day-to-day decisions.

Each of the research tasks was assigned a *task-leader*. This person was responsible for managing the progress of the research, preparing written reports, and reporting the progress of the research to the PMC. Detailed technical co-ordination was achieved by meetings between the *task-leader* and the relevant partners, as appropriate.

The coordinator was in close contact by email with all participants during the whole period and considerable technical interaction through technical meetings or correspondence occurred with the INFM partners, at Rome and Milan.

Management and Coordination

TABLE 5-1 The **per task & per partner** Manpower allocation, based on the scheduled requirements of the contract as amended.

Three events shaped the general form of the project's progress. 1) the late start of many of its aspects, due to difficulties in securing post-doc staff, which necessitated a contract extension; 2) the switch to a novel technology for task#1, which made many of the original manpower estimates unreliable; and 3) the change to a short collimation device, which made the original consumables estimates of CCLRC irrelevant. Fortunately, this freed budgetary resources, enabling a virement among the partners and increasing the manpower resources for the data analysis of both tasks.

TASK #1, FSD					
	Manpower time, months				
Manpower type	Scheduled	Actual	Variance	Remains	Comment
CCLRC-RAL-UK					Band 4 & 5 resources were poorly estimated in the original proposal, which aimed to work with established technology. The move to new technology (years 1,2) demanded much more Band 4 & 5 input. Although Band 3 work remains to be done to fully complete the detectors no Band 4 or 5 resources were available in the final year.
Band 3	27.8	26.7	-1.1	+1.1	
Band 4	1.1	3.4	+2.3	-	
Band 5	2	10.2	+8.2	-	
Uni-Canterbury-UK					After a late start, caused by the need to find appropriate personnel, this aspect of the project went smoothly. Although the analysis procedure became well established it was only after several data sets were available, late on in the project. Funds were vired from CCLRC to extend the original 18 months to 24.
Prof. Physics	1.5	1.5	-	-	
Post -Doc Fellow	24	24	-	-	
INFM-IT					
Prof Physics	5.5	7.6	+2.1	-	
Lecturers and					The young research effort needed for this task was poorly estimated in the original proposal, which aimed to work with established technology. The move to new technology (years 1,2) demanded more of this type of input. This was exacerbated by the difficulty in securing sufficiently well trained post doc's. Taken together these problems delayed the project start (9 months), slowed progress and required a contract extension.
Senior Researchers	0.0	2.1	+2.1	-	
Researchers and					
Post Doc	18.5	32.9	+14.4	-	

TASK #2, VLAD					
	Manpower time, months				
Manpower type	Scheduled	Actual	Variance	Remains	Comment
CCLRC-RAL-UK					
Band 3	25.8	23.9	-1.9	+1.9	Band 4 & 5 resources were poorly estimated in the original proposal, which aimed to work with a different collimation method. The change (year 1) produced a need for further Band 4 & 5 input, over and above that proposed.
Band 4	1.1	5.1	+4.0	-	
Band 5	2	11.7	+9.7	-	
Uni-Canterbury-UK					After a late start, caused by the need to find appropriate personnel, this aspect of the project went slowly. Due to the delays imposed by the lack of Post Doc. personnel few data-sets were available from which to generate a robust analysis process (see below). Funds were vired from CCLRC to extend the original 18 months to 24 in an attempt to mitigate these effects.
Prof. Physics	1.5	1.5	-	-	
Post -Doc Fellow	24	24	-	-	
INFM-IT					
Prof Physics	14.5	15.7	+1.2	-	
Lecturers and					The estimates in the original proposal were realistic in respect of this task, which always involved the introduction of new technology. However, staff shortages still appeared but here they were due to competition from other work. The modest effort remaining in the last year of the project was insufficient to cover the delicate, manually intensive, setting-up of the VLAD detectors. Data collection was delayed and only a few data-sets were obtained.
Senior Researchers	7.0	9.7	+2.7	-	
Researchers and					
Post Doc	80.5	84.8	+4.3	-	

TABLE 5-2 The **per item & per partner** Budgetary allocation. All values are given in Euros.

CCLRC-RAL-UK				
	Budget			
Budget item	Scheduled	Actual	Variance	Comment
Personnel costs	1,245,997	422,880	-823,117	A combination of factors arising from changes in CCLRC accounting procedures and the difference between the technological routes proposed and finally implemented.
Travel and Subs	12,600	4,104	-8,396	The UK partners travelled little once the effectiveness of videoconferencing was established.
Consumables	170,940	236,070	+65,130	The final year consumables costs were greater than expected. They could have easily been covered by the amended contract if this had been foreseen.

Uni-Canterbury-UK				
	Budget			
Budget item	Scheduled	Actual	Variance	Comment
Personnel costs	229,178	171,001	-58,177	The quality of staff employed at Kent, although adequate, failed to attract the salaries for which provision had been made.

INFM-IT				
	Budget			
Budget item	Scheduled	Actual	Variance	Comment
Personnel costs	389,922	282,697	-107,225	The Italian partner always found problems obtaining adequate manpower and effectively ran some of their sub-tasks somewhat short handed.
Travel and Sub's.	40,666	38,411	-2,255	Trips to UK from Italy were essential to have access to the neutron beam during installation. This cost was well estimated in the original proposal.
Consumables	169,412	176,995	+7,583	This cost was well estimated in the original proposal.