

Muon JRA (WP 17) and Muon Outreach (WP 2)

Stephen Cottrell,
ISIS Facility, STFC

NMI3-II General Assembly
Copenhagen
15th October, 2015

Tasks in the Muon JRA

- Software development for Muon Data Analysis
- Concept studies for Future Muon Sources
- Detector Technologies for Pulsed Muon Sources

Tasks within the Outreach Work package

- Developing μ SR in High Magnetic Fields ...
Website development and publicity material
- Developing the community ...
Workshops on Functional Materials and Soft Matter

Project building on work during FP6, FP7 (NMI3-I) ...

A broad collaboration ...

Partners:

- STFC
- PSI

(PDRA at each facility)

Observers (muon JRA):

- Parma,
- Huddersfield,
- ESS
- RIKEN-RAL

Observers (Outreach):

- Coimbra,
- East Anglia,
- Orsay,
- Fribourg

Muon JRA

Software Development for Muon Data Analysis

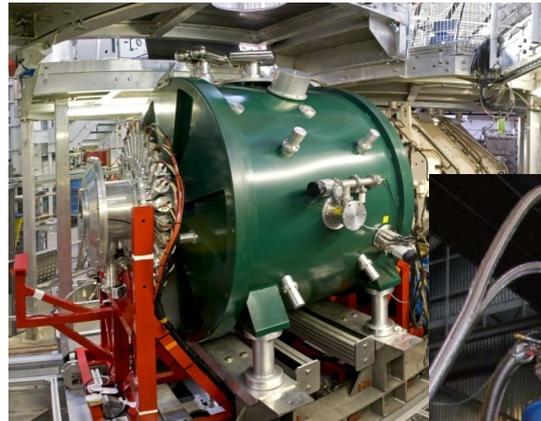
- Routines for efficient analysis of high field experiments
- Routines to link simulation with analysis codes
- Enhanced metadata for data storage

Analysis of High Field Experiments ...

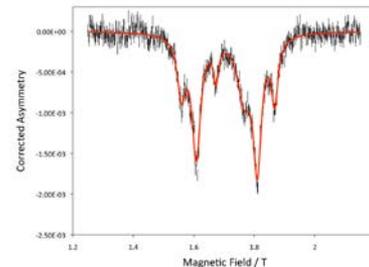
Both PSI and ISIS have recently developed novel high field spectrometers.

These instruments allow us to do new science ... but create new challenges for analysis codes ...

New software has been developed for efficient data analysis.

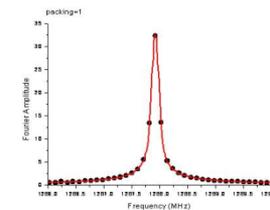
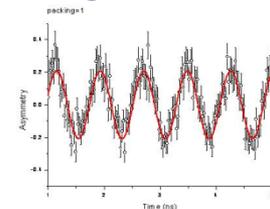


ISIS and PSI High Field Instruments



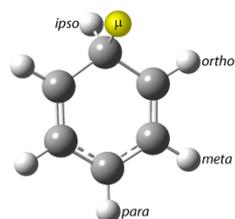
Complex spectra

Fast timing
Large datasets

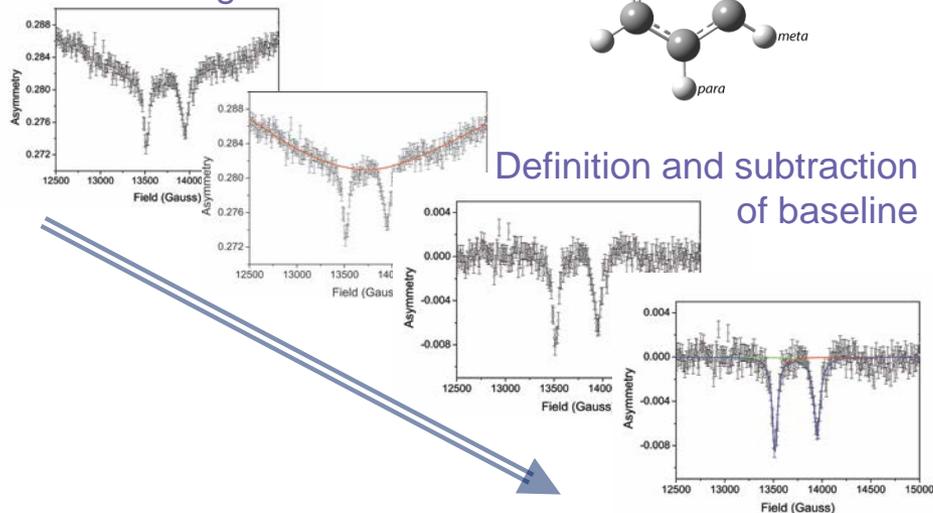


New Routines Developed for Data Analysis

Mantid Interface: Analysis of Avoided Level Crossing (ALC) spectra

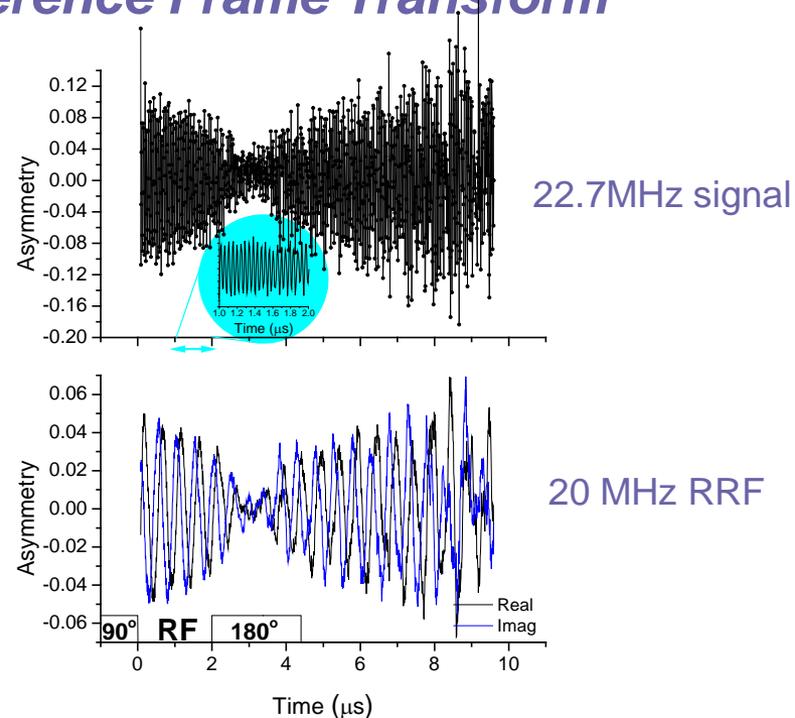


Time integrated raw data



Peak fitting of reduced data

Mantid Algorithm: Rotating Reference Frame Transform



For visualisation and analysis

Simulation codes for Data Analysis

Simulation codes are increasingly important for interpreting experimental results

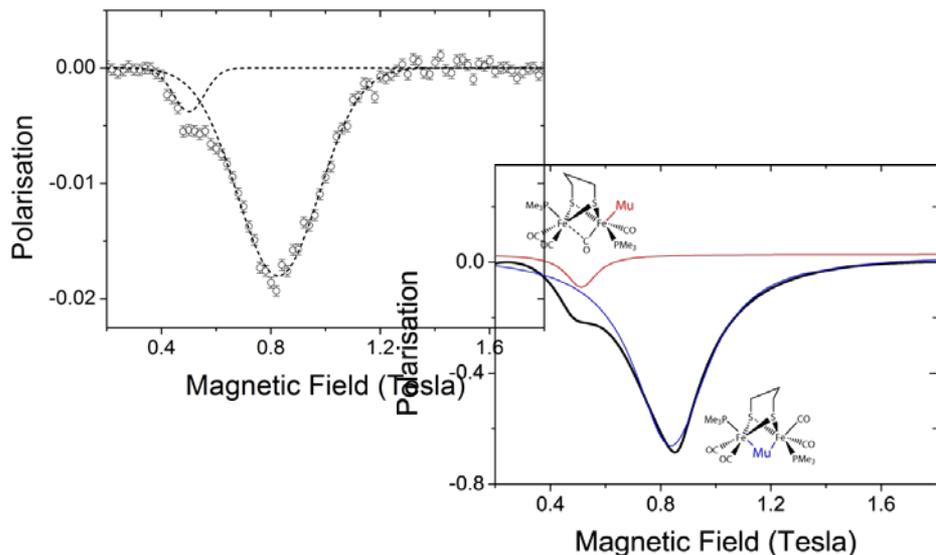
Examples developed during this project include:

- Applying Density Functional Theory for interpreting Avoided Level Crossing spectra
- Using Monte Carlo methods for modelling μ SR instruments and experiments

Example – Understanding ALC Spectra

Identification of muonium addition site in artificial [FeFe]hydrogenase

Measured ALC spectrum



DFT ⇒ *simulated curves*
 ⇒ *Candidate structures*

Extended study of molecular DFT methods by Jamie Peck

Highlights benefits, discusses limitations and considers future work

Simulating hyperfine coupling constants of muoniated radicals using density functional theory calculations

Abstract

In this work we consider potential benefits, and limitations of linking *ab initio* Density Functional Theory (DFT) methods with existing μ SR data analysis codes. This is motivated by the desire to provide users of the μ SR technique with additional tools to help them better understand and interpret their data. The DFT method may be considered as complementary to the μ SR technique. It is essential for interpreting muonium chemistry type experiments, where it provides the experimenter with an indication of the appropriate field regions where resonances are likely to be found, and can also help assign resonances to nuclei and identify the muonium binding sites during data analysis. A link between data analysis and DFT simulation codes is therefore likely to be highly beneficial in making efficient use of beamtime.

Linking Simulation with Analysis Codes

Linking analysis programs with simulation codes for new methods of working and new insight

Examples developed during this project include:

- Modelling muon data using the density matrix formalism
- Dipolar field calculations for modelling μ SR relaxation and investigating the muon site

More of this in **SINE2020...**

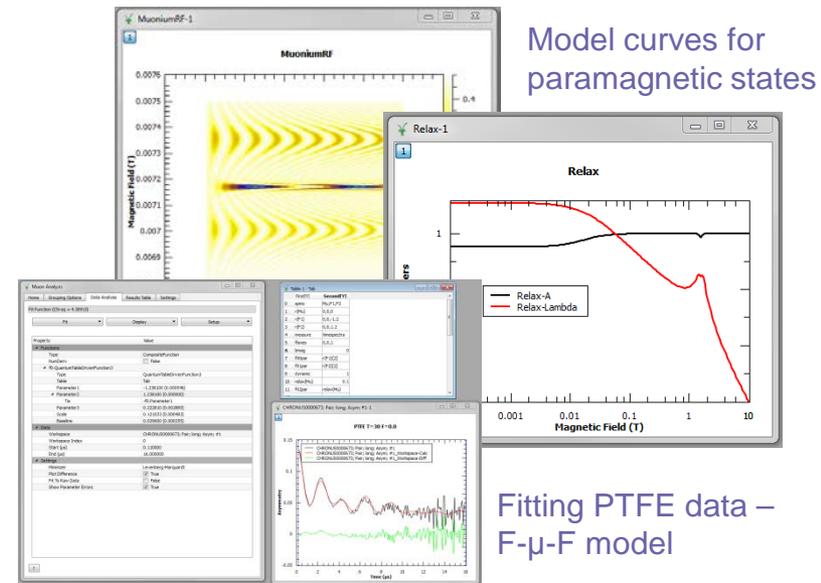
Example – Modelling Muon Data using the Density Matrix Method

Original FORTRAN code rewritten in Python and implemented as a series of Mantid Algorithms.

Model spectra can be generated within Mantid

or...

Use package as a fit function in Mantid to refine model parameters based on experimental data



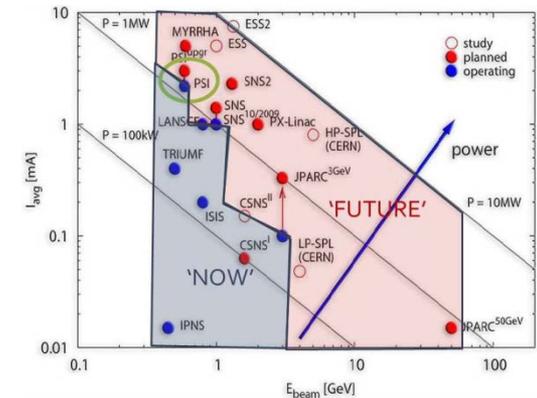
Concept Studies for Future Muon Sources

- Concept study for advanced muon beams
- Workshop discussing future high intensity muon sources

Considering 'Next Generation' Muon Experiments...

For example...

- High-Intensity Low Energy Muon Source
 - Nanometer scale implantation depths
 - Study of thin films, multilayers and surfaces
- Muon micro-beams
 - micron size samples
 - Study of inhomogeneities in larger samples (scanning beam)
 - Measurement of multiple samples
- High pressure studies (anvil cell)



These Require Advanced High-Intensity Beams!

Workshop held discussing Future Muon Sources

Aim: To bring together scientists and engineers involved in developing and using accelerator-based muon sources to discuss ideas about future facilities



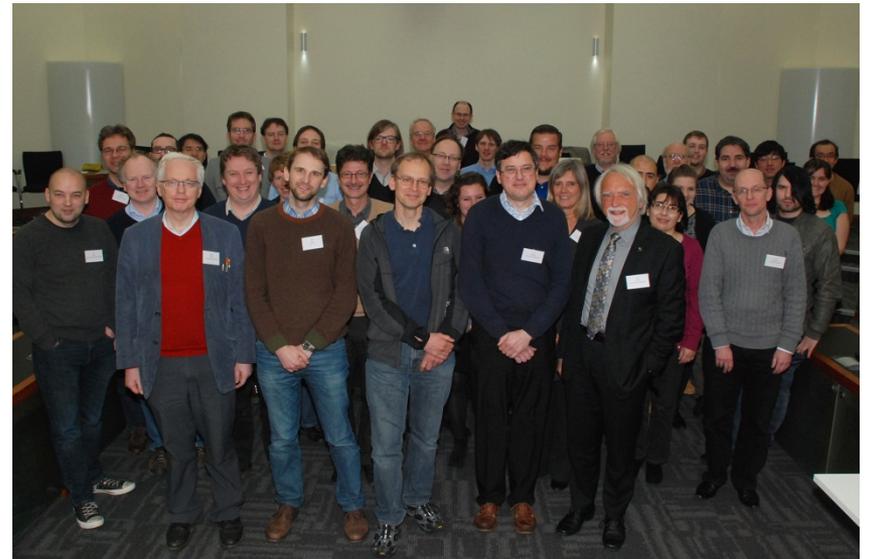
Hosted by Bob Cywinski at the University of Huddersfield, January 2015

Joint meeting between **NMI3** and the **Accelerator Applications Network of EuCARD-2** (both FP7 activities)

Future Muon Sources Workshop...

Sessions included:

- Muon production and accelerator technologies
- Specialised beams
- Condensed matter μ SR / New Techniques
- Update and outlook from the Facilities
- Novel applications of muons



A report of the meeting is available on the NMI3 website

Concept study for a Muon Microbeam

Background:

Present muon beams are generally used for bulk studies.

Typical beam size: 10 - 300 mm² , best beam: size ~ 5 mm²

No lateral resolution (LEM beam at PSI has depth resolution ~10 nm).

Goal: Surface Muon Microbeam: with $\sigma_x \sigma_y \sim 50 \mu\text{m}$.

Advantages:

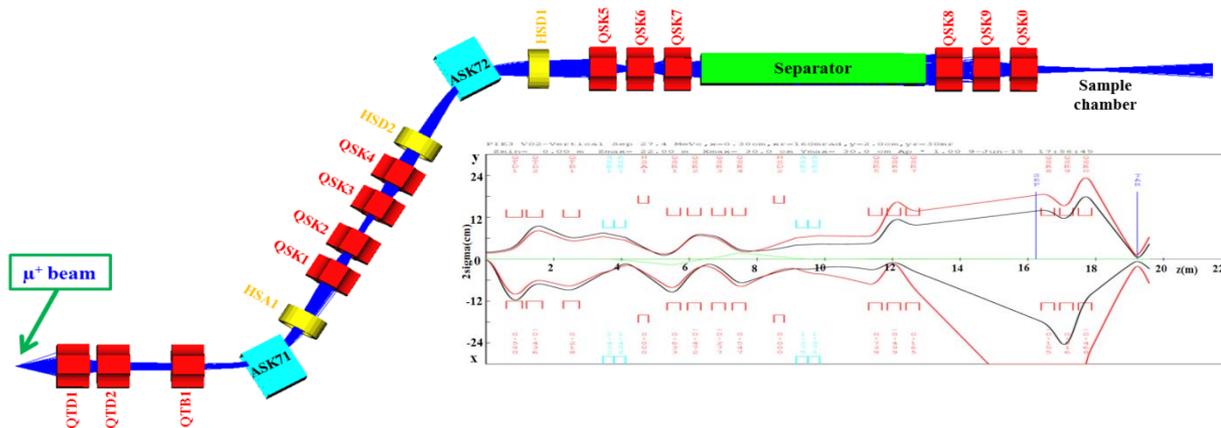
- μSR experiments on ~ micron size samples - many novel materials can be synthesized in good quality and as a crystal only in tiny quantities (reduction by more than 10^4 of required sample material)
- Study of inhomogeneities in larger samples (scanning beam)
- Multiple samples measurement
- Use of anvil cells allowing higher pressures

Muon Microbeam Study

Elvezio Morenzoni, PSI

First step: Investigate how an existing beam line (e.g. the PSI line, piE3) could be modified to accommodate a muon microbeam.

(minimum impact; spin rotator for LF/TF pol; realistic beam parameters)



Simulation:
TRANSPORT,
TURTLE,
GEANT4
gives consistent results

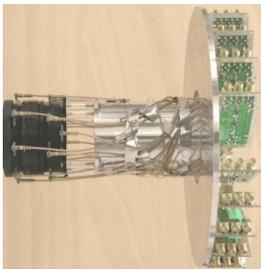
Outcome: A micro spot with $\sim 2 \times 10^4$ muons/sec at the sample position (comparable to existing continuous muon beam lines) ... a plan for a future beamline

Detector Technologies for Pulsed Muon Sources

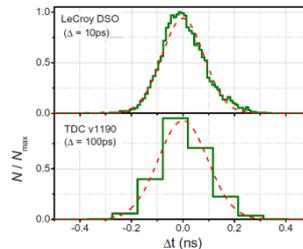
- Collaborative work between ISIS and PSI to develop G-APD technologies for Pulsed Muon beams
- Development of a prototype G-APD detector at ISIS for a performance assessment

Geiger mode Avalanche Photodiode Technologies

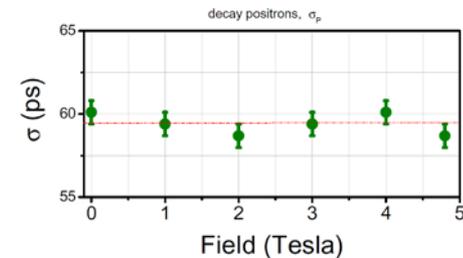
APD technologies developed at PSI during JRAs under FP6 and FP7
 Required to meet the challenging requirements of the new High Field Instrument



APD Detector array



Detector resolution better than 100 ps



Resolution independent of field

Very successful for measuring at PSI with a *continuous* beam structure

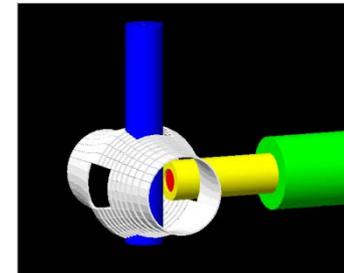
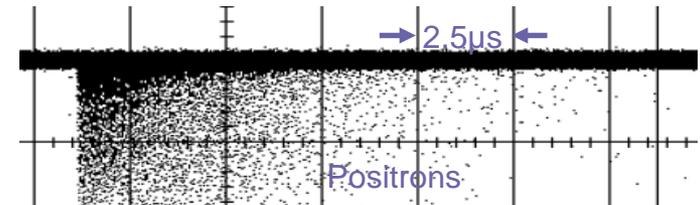
Can the same technology be applied at the ISIS *Pulsed* Source?

APD detectors for the ISIS Pulsed Source

Applying APD technology at ISIS
brings new challenges ...

Very high instantaneous rates demand:

- High detector segmentation ✓
- Short detector deadtimes following each 'hit' ?

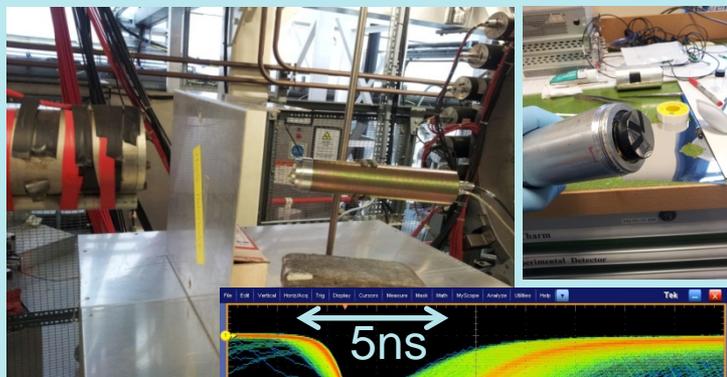


Future MuSR Detector Array

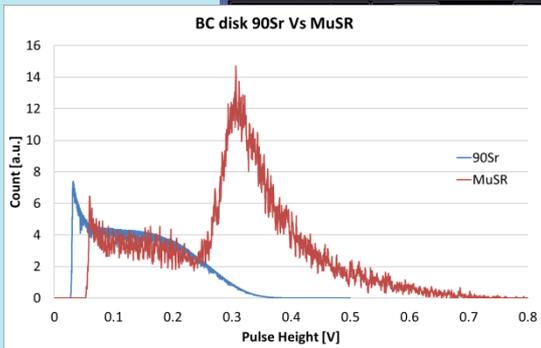
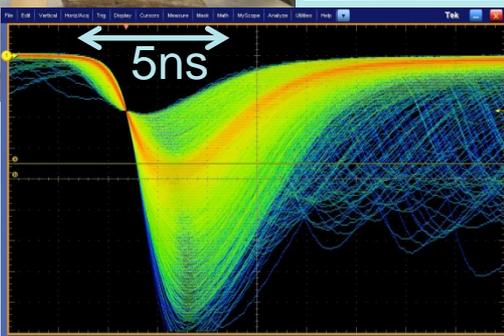
**Currently studying the suitability of APD detectors
for pulsed muon beams ... focus on deadtimes**

Work led by the ISIS detector group, including Myron Huzan and Dan Pooley

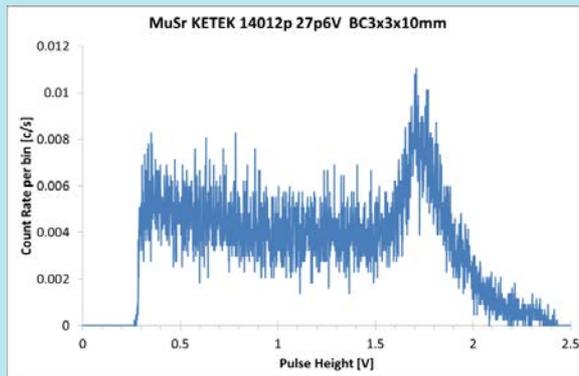
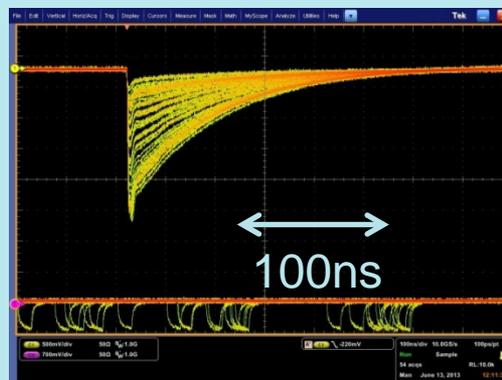
Comparing PMT and APD signals



Signal from PMT



Ketek APD and Scintillator Rod 3x3x10mm



- Good Signal Amplitude
- Low Noise
- Extended 'recovery'

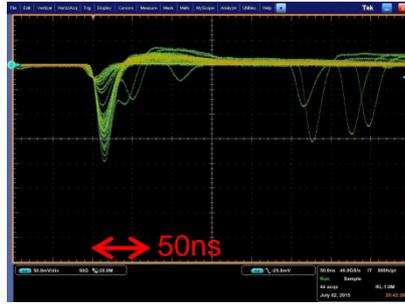
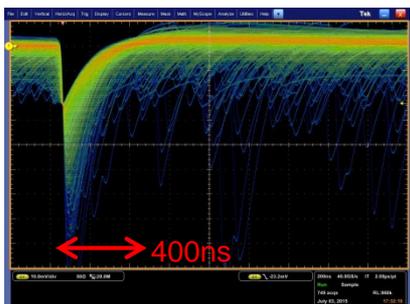
Studying APD Deadtimes

Work ongoing to determine/characterise device deadtimes...



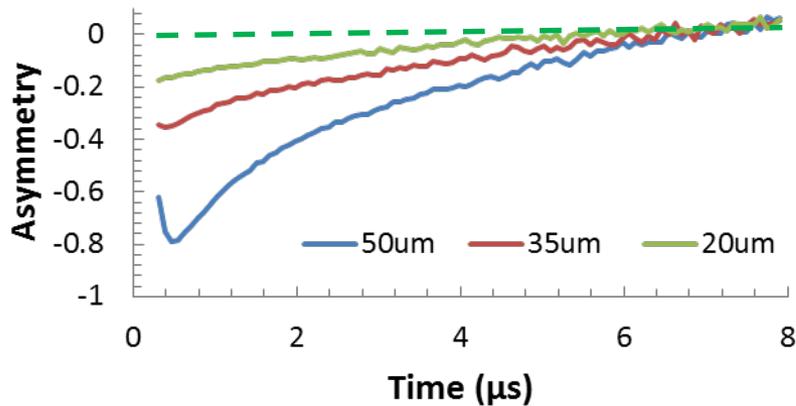
Comparing different microcell sizes:
 $50\mu\text{m}$, $35\mu\text{m}$, $20\mu\text{m}$

Comparing different manufactures:
SensL and Hamamatsu



Comparing signal conditioning:
slow (left), fast/differentiated outputs

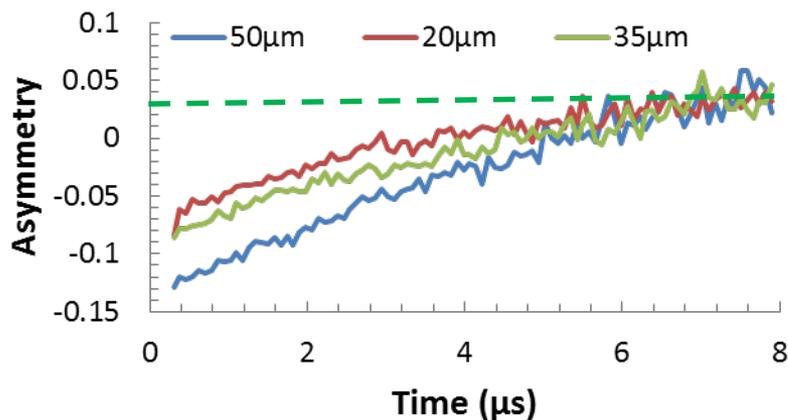
SensL, slow, ~6 hits/frame



Example data measured for SensL devices of differing Microcell size

Distortion at early times arises from lost counts due to detector deadtime

SensL, fast/diff, ~6 hits/frame



Currently analysing/modelling data to quantify deadtime

Parallel work off-beam to characterise devices

Outreach

Developing the Muon User Community was an important part of our work

Focus was on High Field μ SR,
an area of facility development

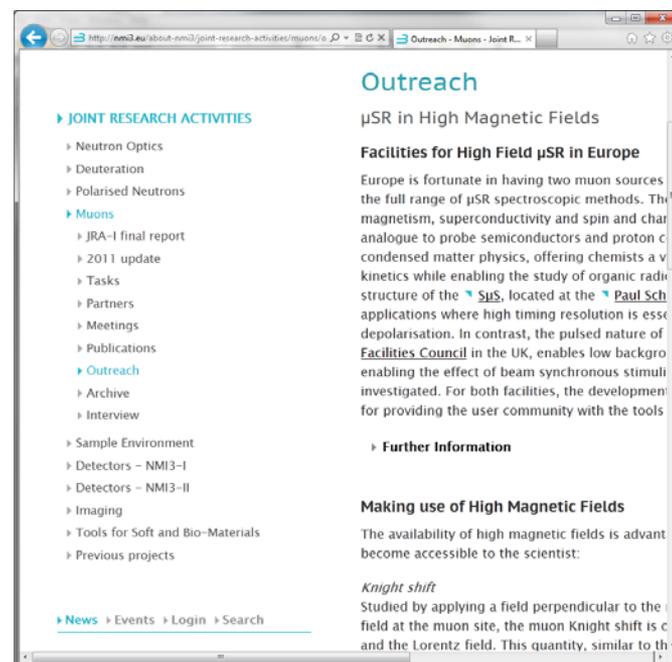


What we've done ...

Publicising the High Field facilities at PSI and ISIS ...

A Website...

Making scientists aware of the facilities, and applications of High Field μ SR



<http://nmi3.eu/about-nmi3/joint-research-activities/muons/outreach.html>

Publicity material ... applications of High Field μ SR

Avoided
Level
Crossing

What can LCR tell us about free radicals?

Structure

The structure of a free radical can be inferred from the muon and nuclear hyperfine couplings.

¹³C-Mu radical: The ¹³C hyperfine couplings can be determined from the positions of the resonances. They indicate that the unpaired electron is covalently bonded to a carbon atom in a substituted benzene ring.

P.W. Perle et al., Chem. Phys. Lett. 248 (1995) 90

Molecular dynamics

The resonance line shape provides information about molecular dynamics in the solid state.

The linewidth indicates that reorienting radicals rotate around an axis parallel to C3-C5.

M. Acopi et al., Phys. Lett. A 179 (1994) 193; J. Borner et al., Chem. Soc. Rev. 22 (1993) 337

Reaction rates

Radical reaction rates can be measured from the broadening of resonances, as a function of reactant concentration.

Reaction of cyclohexanone radical with an anisotropic N₂.

J. Ollier et al., Physica 9 334-375 (1966) 377

Muon LCR: the basic idea

Once implanted inside a material, muons interact with their local atomic environment. The interaction can be particularly strong when an energy level in the muon system matches one within the environment. The system matches one when the muon is put on resonance terms, and this can strongly affect the muon's behaviour.

Such resonances – called level crossing resonances, LCR (or, sometimes, 'avoided level crossing resonance') – between the muons and their environment can be produced by changing the applied magnetic field in a muon experiment. The resonances can be detected by observing the muon polarisation as they are seen as a dip in the polarisation as the applied field is changed. Observation of such resonances gives an additional information about the muon's atomic environment.

High resolution muon spectroscopy: the basic idea

Once implanted inside a material, muons interact with their local atomic environment. In some cases the interaction can be strong, and fast timing resolution is required to follow the evolution of the muon spin polarization. For example, in magnetic systems, large internal fields give rise to fast precession frequencies, while broad internal field distributions will lead to a rapid decay of the muon polarisation. In chemical systems, the measurement of detailed spectroscopic information requires large precessing fields which, in turn, give rise to energy level splittings of the order of hundreds of MHz.

The beam structure of the SPS, located at PSI, Switzerland is ideal for these type of measurements. Here, muons are implanted into the sample one by one, allowing accurate timing of the interval between muon arrival and the detection of the decay positron. With careful instrument design and specialist detector technologies, timing resolutions of ~80ps are possible.

This is illustrated by the transverse field experiment, where fast applied perpendicular to the muon spin polarisation. In this case the muon response and the corresponding shape of the Fourier transform reflects the microscopic field distribution sensed by the muon.

Example applications of High Resolution μ SR

Superconductivity

The vortex state induced in a type-II superconductor when a strong magnetic field is applied can be studied using muons. The technique probes the magnetic field on a length scale much shorter than the inter-vortex distance, enabling information about the internal vortex structure and interactions to be obtained.

Field distribution data modelled by a vortex lattice (vortex spacing a) and a central field of 100G.

Anderson & Chouhan et al., Phys. Lett. 161 (1994) 205

Muons are now routinely used to determine characteristic length scales, such as the magnetic penetration depth and coherence length, and the muon technique enables vortex lattice topology to be investigated. Muons are also playing a key role in the search for experimental evidence for exotic vortex states. For example, a change in the spatial field distribution around the vortex cores has been predicted for clean superconductors at low temperatures and at fields close to the upper critical field. Measurements capable of extended temperature and field measurements promise to bring a new insight to these studies.

BCS model $T=0$

GL limit of BCS $T=0$

Models for conventional (BCS) and exotic (right vortex states) can be investigated using muon techniques.

A. Huxley et al., Phys. Rev. B 63 (2001) 20120

High
Resolution
 μ SR

Themed Science Workshops ...

Function Materials

Held at PSI (part of JUM@P '13)
September 2013

Soft Matter, Excitations and Muon Induced Perturbations



New Application of μ SR: Studies of Soft Matter and Spectroscopy of Excited States

** Registration for the meeting has now closed, but it may still be possible to attend the meeting. Please contact Steve Cottrell if interested in attending. **

3-4 September: Queen Mary, University of London

A workshop is planned with a focus on introducing new applications of μ SR.

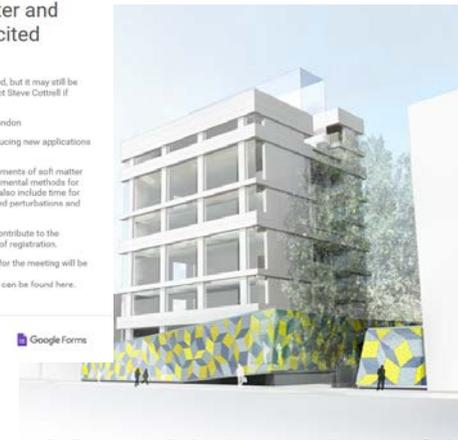
Sessions are anticipated discussing measurements of soft matter systems and the development of novel experimental methods for studying excited states. The programme will also include time for discussion of the phenomena of Muon induced perturbations and their impact on the muon experiment.

There will be an opportunity for students to contribute to the programme; abstracts are invited at the time of registration.

An up to date programme and abstract book for the meeting will be sent by email.

The meeting instructions including directions can be found here: <http://tinyurl.com/MuSR2013MeetingDirections>

This form was created using Google Forms. [Create your own](#)

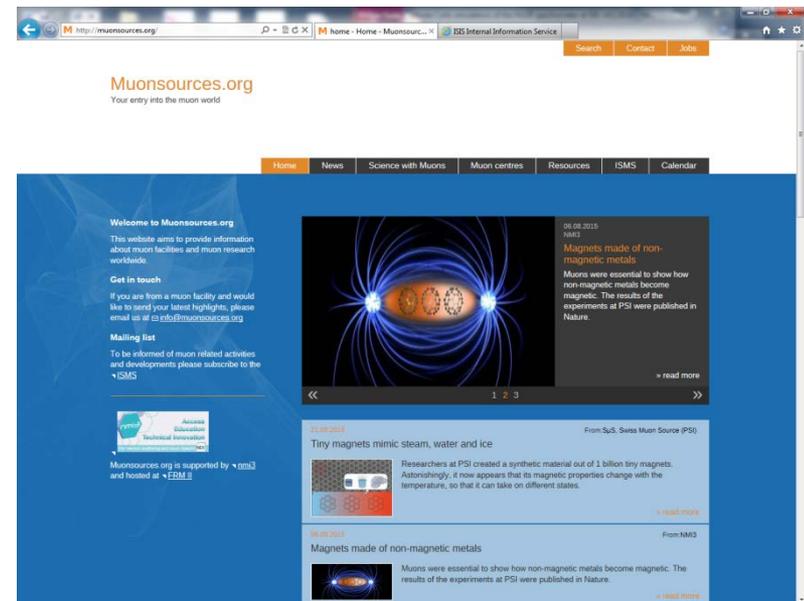


Held at Queen Mary University of London,
September 2015

Hosted by Alan Drew, ERC grant holder
developing laser stimulated μ SR at ISIS

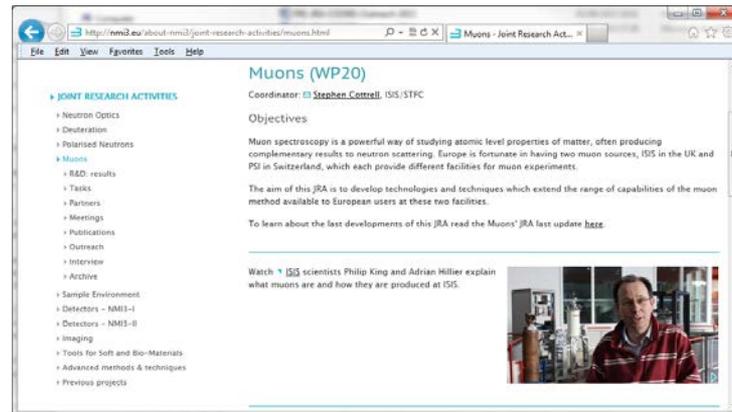
Developing muonsources.org ...

- A Portal for Scientists Using Muon Techniques
- A companion website to neutronsources.org



Watch our page on the NMI3 website...

<http://nmi3.eu> ...



where we are posting project news and results