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 μSR 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

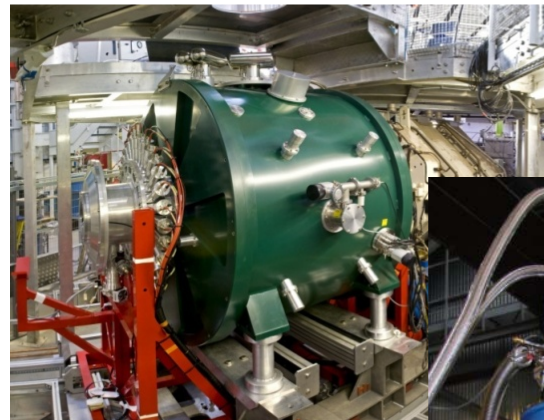
- Routines for efficient analysis of high field experiments
- Routines to link simulation with analysis codes
- Enhanced metadata for data storage

Analysis of High Field Experiments …

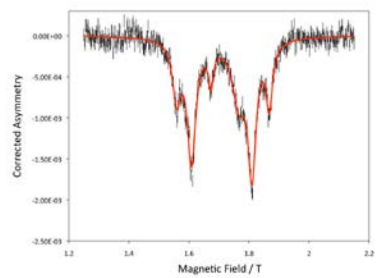
Both PSI and ISIS have recently developed novel high field spectrometers.

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

New software has been developed for efficient data analysis.



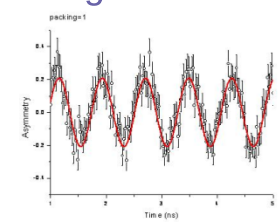
ISIS and PSI
High Field Instruments

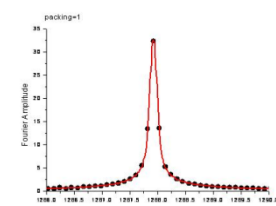


Complex spectra

Fast timing

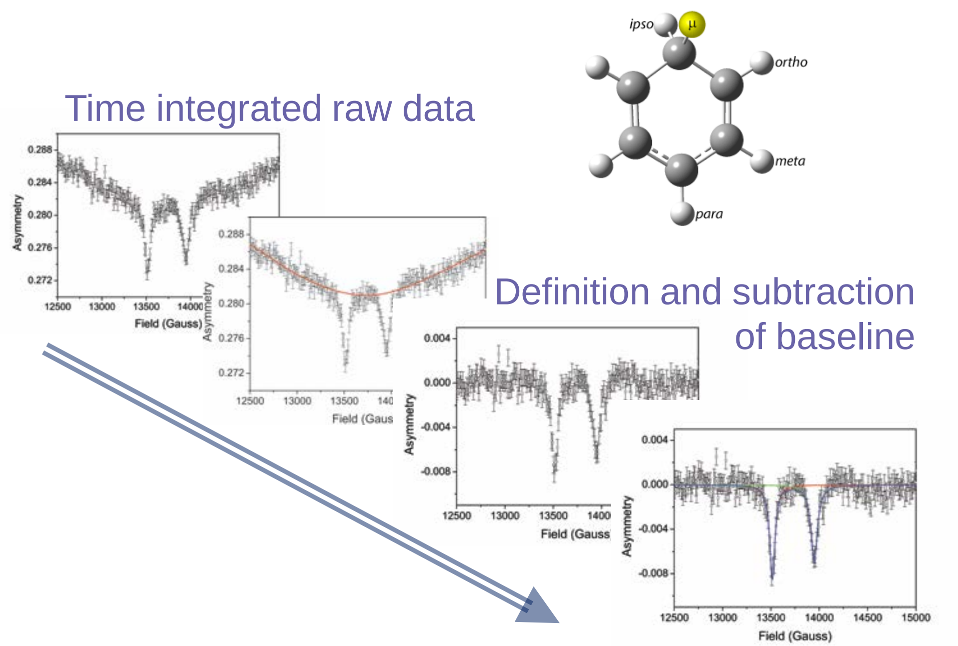
Large datasets



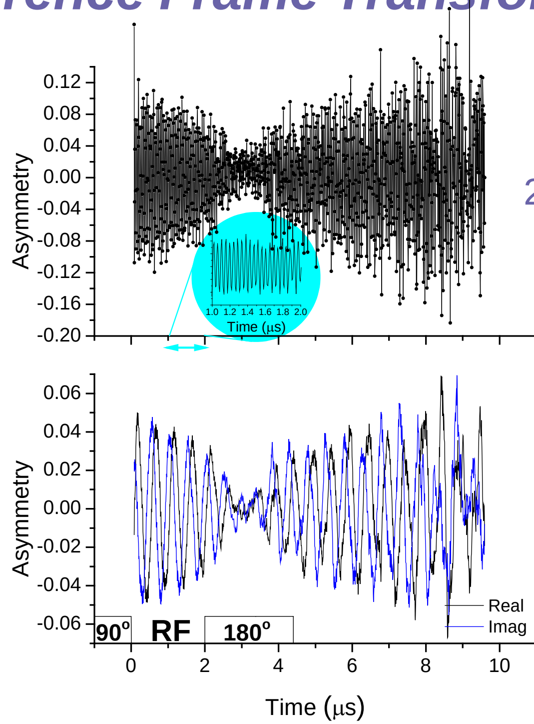


New Routines Developed for Data Analysis

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



Mantid Algorithm: Rotating Reference Frame Transform



22.7MHz signal

20 MHz RRF

For visualisation and analysis

Simulation codes for Data Analysis

Simulation codes are increasingly important for interpreting experimental results

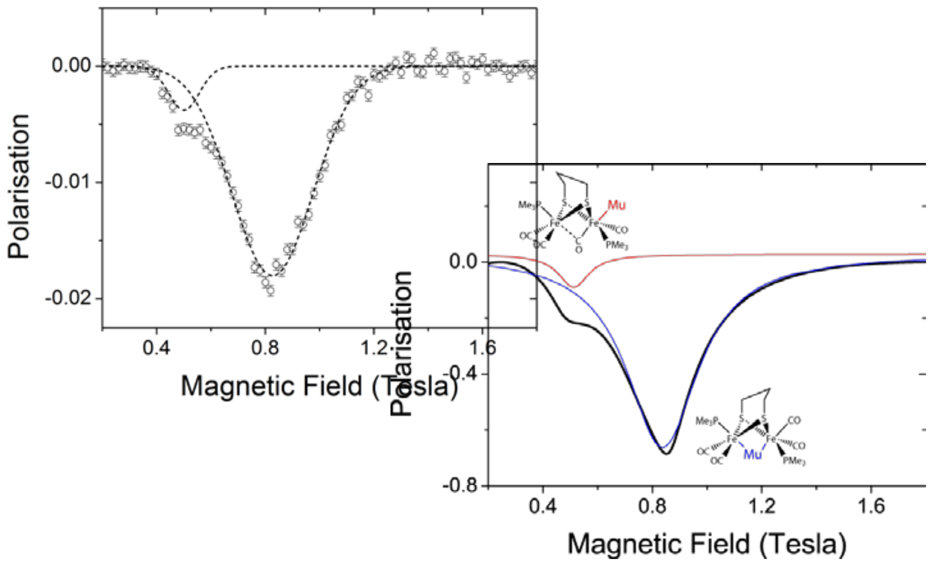
Examples developed during this project include:

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

Example – Understanding ALC Spectra

Identification of muonium addition site in artifical [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 μSR data analysis codes. This is motivated by the desire to provide users of the μSR technique with additional tools to help them better understand and interpret their data. The DFT method may be considered as complementary to the μSR 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 μSR relaxation and investigating the muon site

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

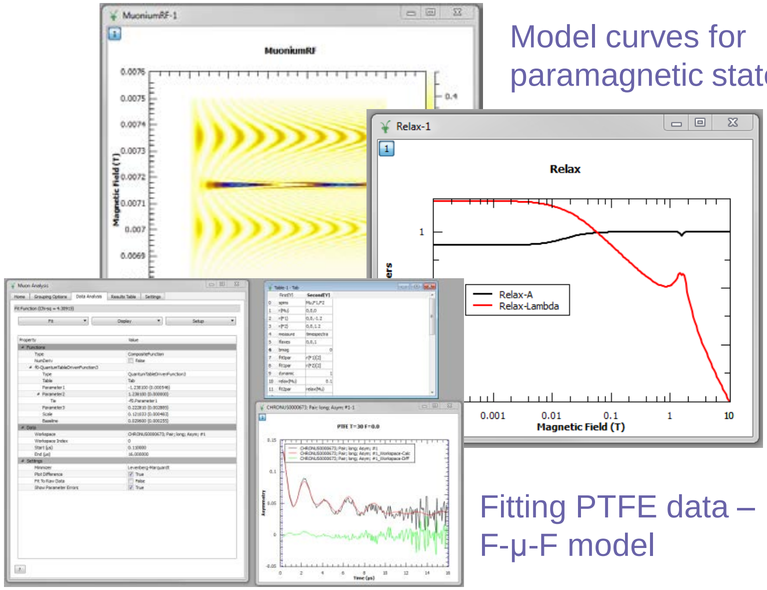
Example – Modelling Muon Data using the Density Matrix Method

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



Model curves for paramagnetic states

Fitting PTFE data – F-μ-F model

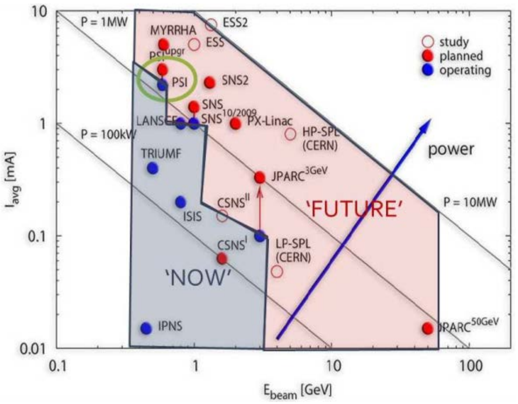
Concept Studies for Future Muon Sources

- 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 µSR / 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 mm^2 , best beam: size ~ 5 mm^2

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

Goal: Surface Muon Microbeam: with σ_x σ_y ~ 50 μm.

Advantages:

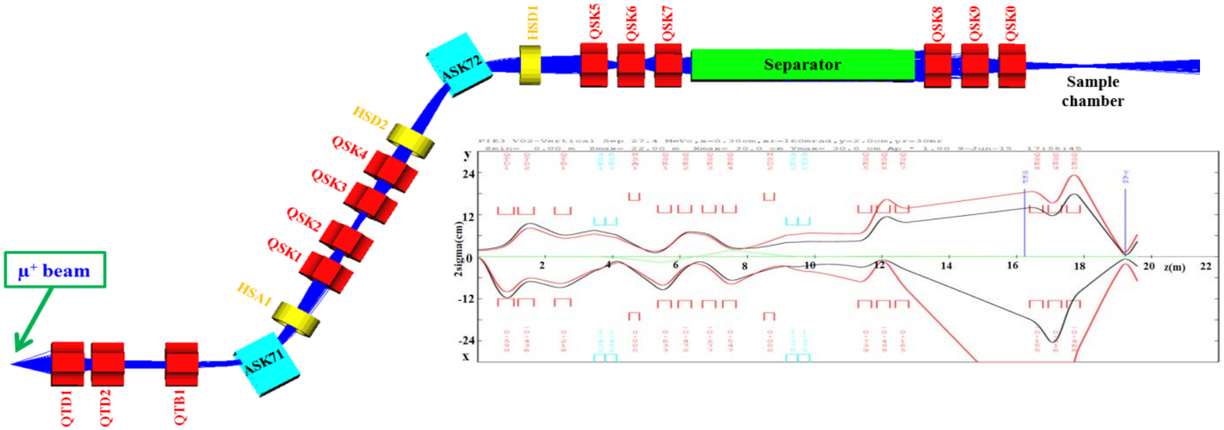
- μSR experiments on ~ micron size samples - many novel materials can be synthetized in good quality and as a crystal only in tiny quantities (reduction by more than 10^4 of required sample material)
- Study of inhomogeneities in larger samples (scanning beam)
- Multiple samples measurement
- Use of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

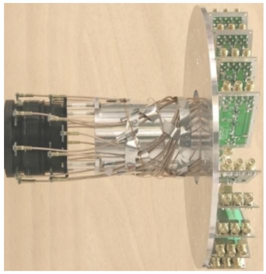
Outcome: A micro spot with ~ $2x10^4$ muons/sec at the sample position (comparable to existing continuous muon beam lines) … a plan for a future beamline

Detector Technologies for Pulsed Muon Sources

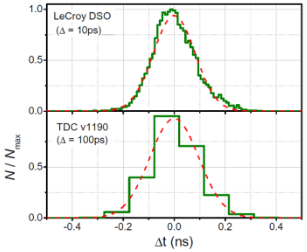
- Collaborative work between ISIS and PSI to develop G-APD technologies for Pulsed Muon beams
- Development of a prototype G-APD detector at ISIS for a performance assessment

Geiger mode Avalanche Photodiode Technologies

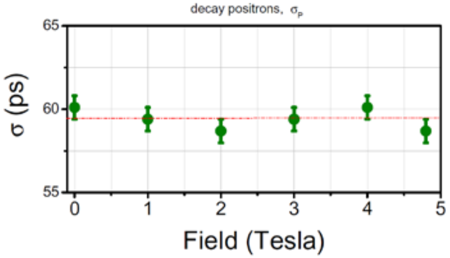
APD technologies developed at PSI during JRAs under FP6 and FP7
Required to meet the challenging requirements of the new High Field Instrument



APD Detector array



Detector resolution better than 100 ps



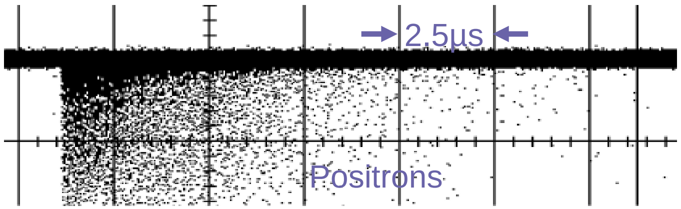
Resolution independent of field

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

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

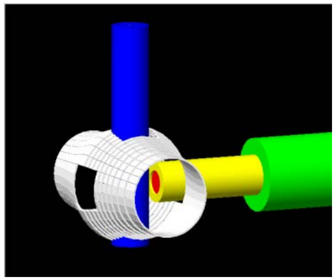
APD detectors for the ISIS Pulsed Source

Applying APD technology at ISIS
brings new challenges …



Very high instantaneous rates demand:

- High detector segmentation ✓
- Short detector deadtimes following each ‘hit’ ?

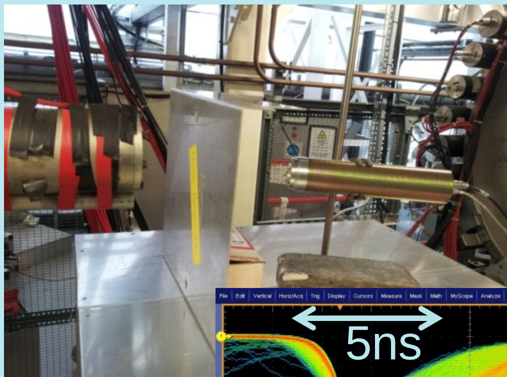


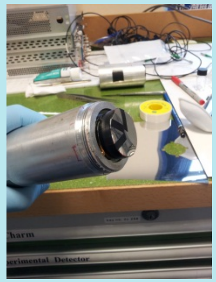
Future MuSR Detector Array

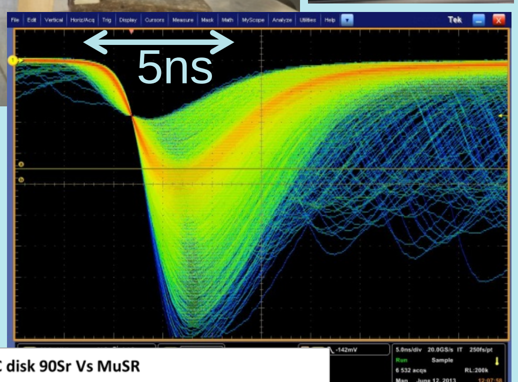
Currently studying the suitability of APD detectors for pulsed muon beams … focus on deadtimes

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

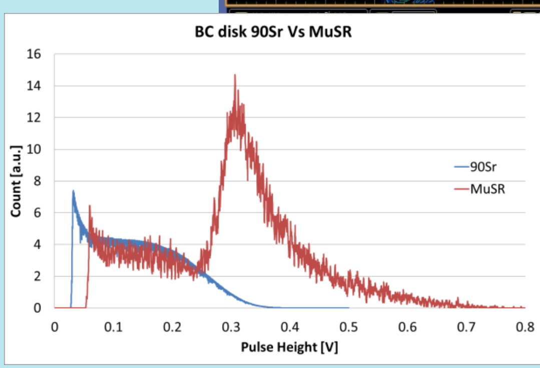
Comparing PMT and APD signals



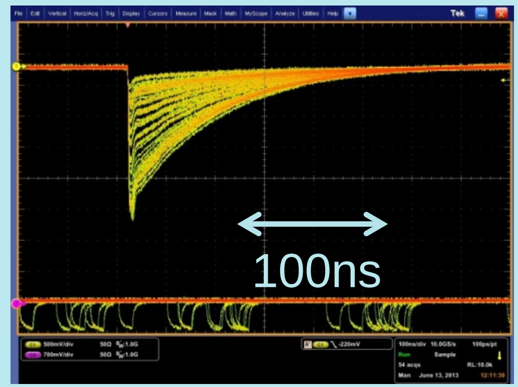


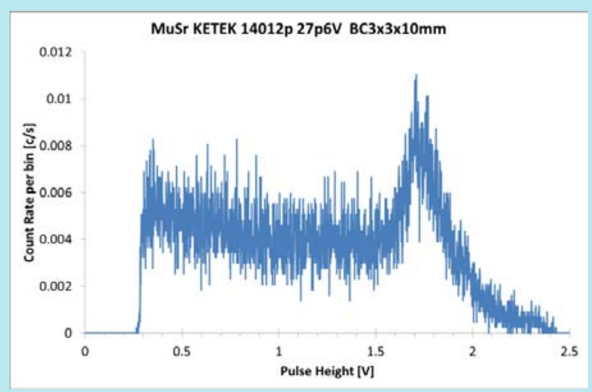


Signal from PMT



Ketek APD and Scintillator Rod 3x3x10mm





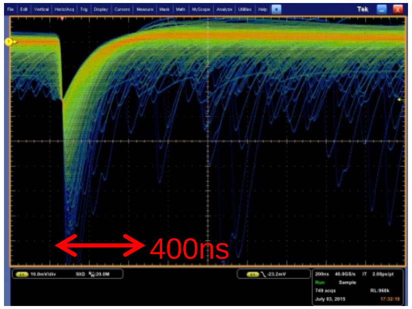
- **Good Signal Amplitude**
- **Low Noise**
- **Extended ‘recovery’**

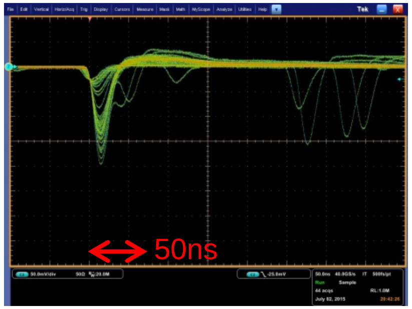
Studying APD Deadtimes

Work ongoing to determine/characterise device deadtimes...

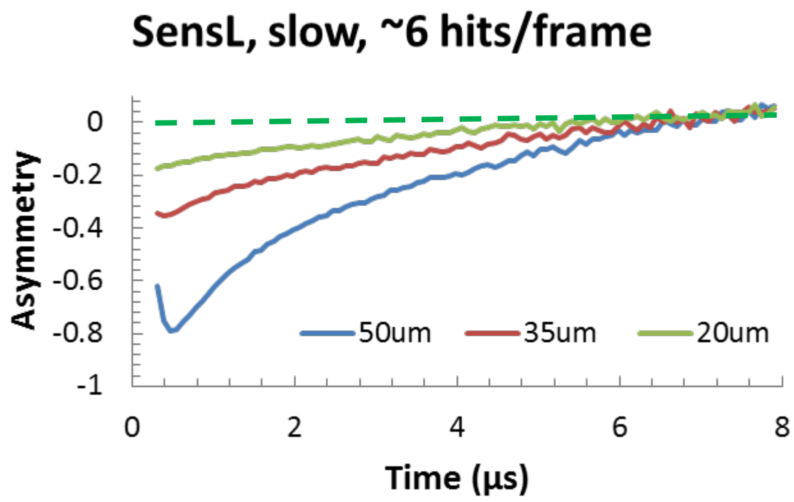
Comparing different microcell sizes: 50µm, 35µm, 20µm

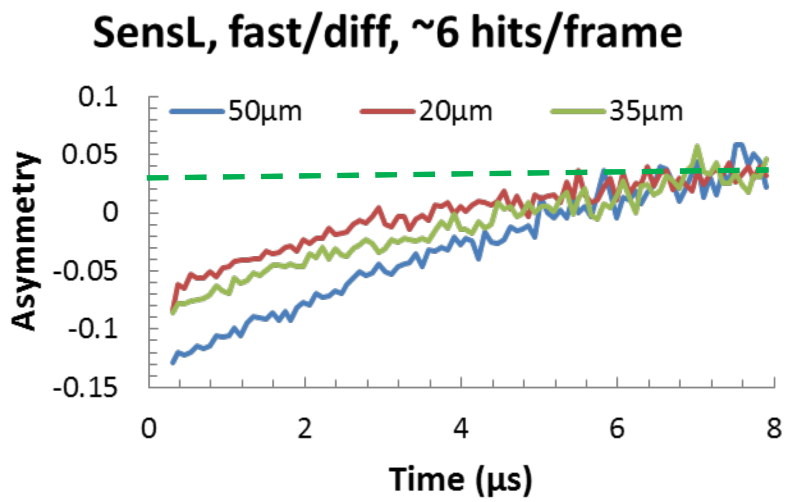
Comparing different manufactures: SensL and Hamamatsu





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





Example data measured for SensL devices of differing Microcell size

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

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

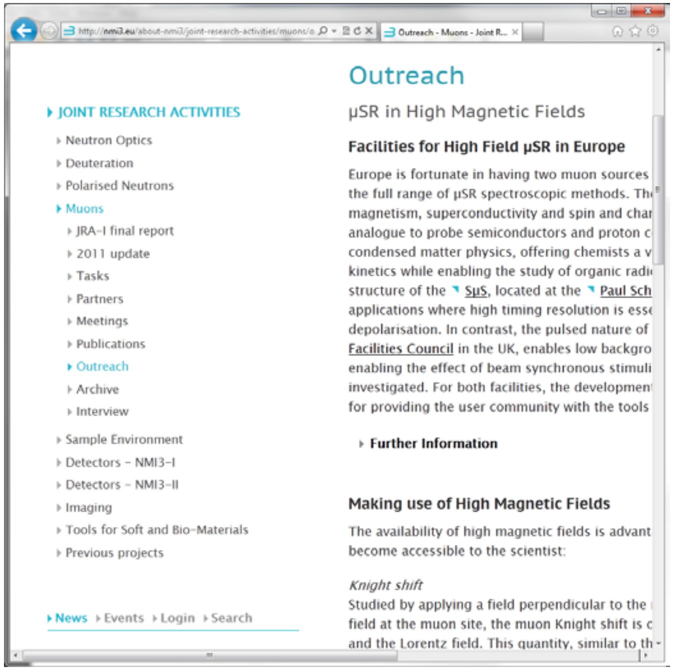
Focus was on High Field μSR, an area of facility development

What we've done …

Publicising the High Field facilities at PSI and ISIS …

A Website...

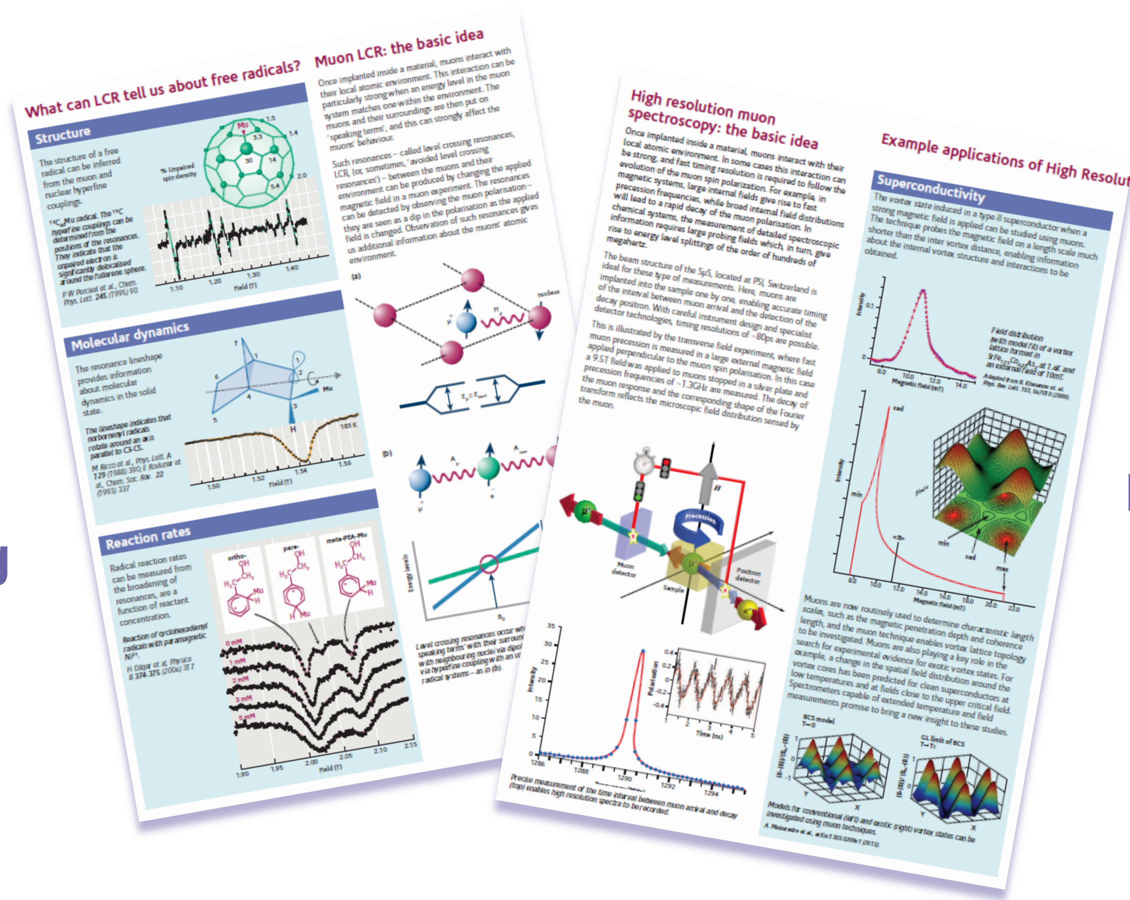
Making scientists aware of the facilities, and applications of High Field µSR



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

Publicity material … applications of High Field µSR

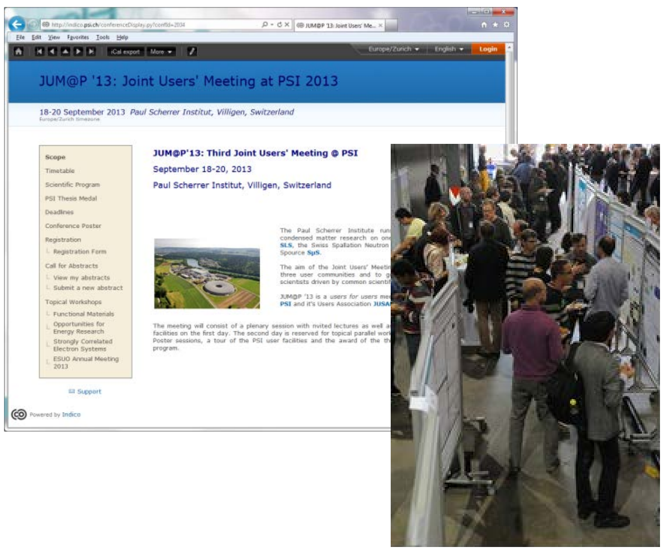
Avoided Level Crossing



High Resolution µSR

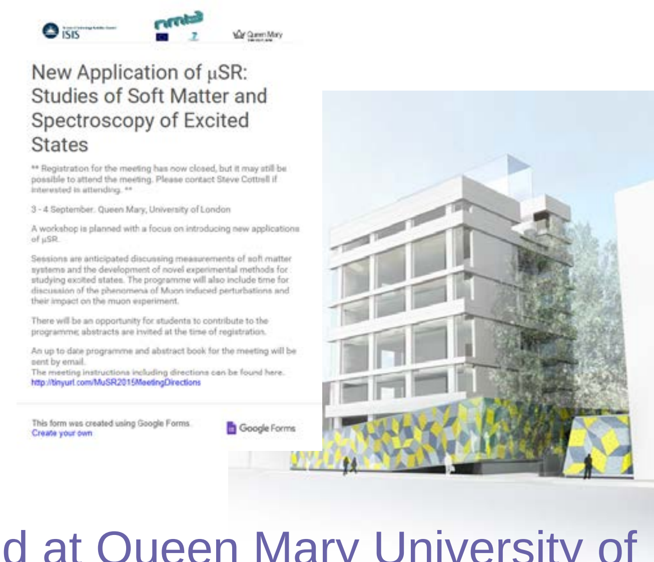
Themed Science Workshops …

Function Materials



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

Soft Matter, Excitations and Muon Induced Perturbations

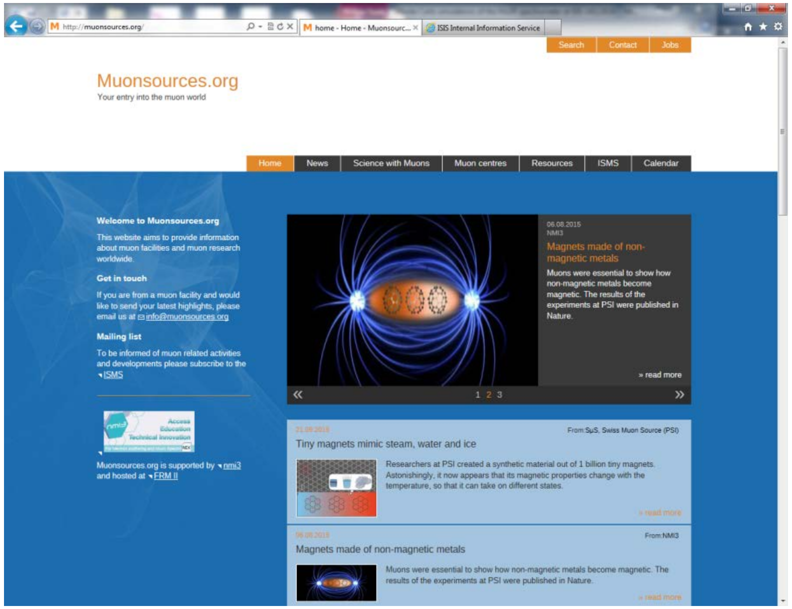


Held at Queen Mary University of London, September 2015

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

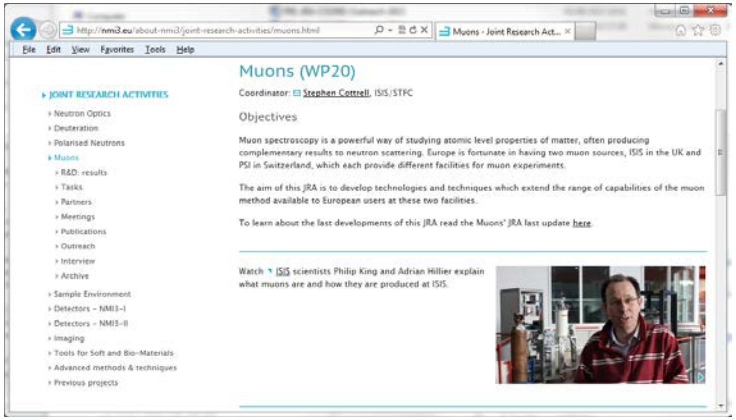
Developing muonsources.org …

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



Watch our page on the NMI3 website…

http://nmi3.eu …



where we are posting project news and results