G4-μSR: Towards a general instrument simulation program

JRA5 NMI3 – Launch Meeting
PSI Villigen, 30 March 2009

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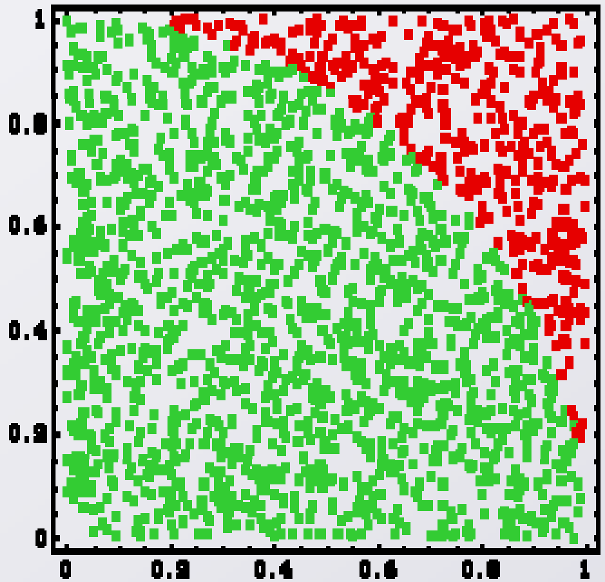
The Monte Carlo method

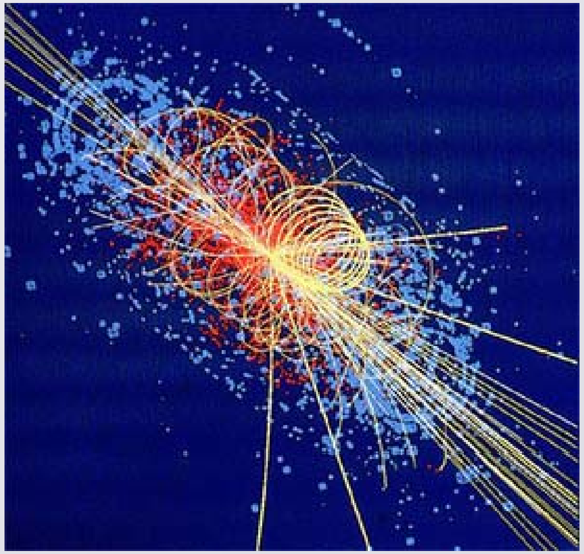
The use of MC simulations is crucial in addressing **complexity** and **intrinsic randomness**

Fundamental example



π calculation using Monte Carlo method

Advanced application



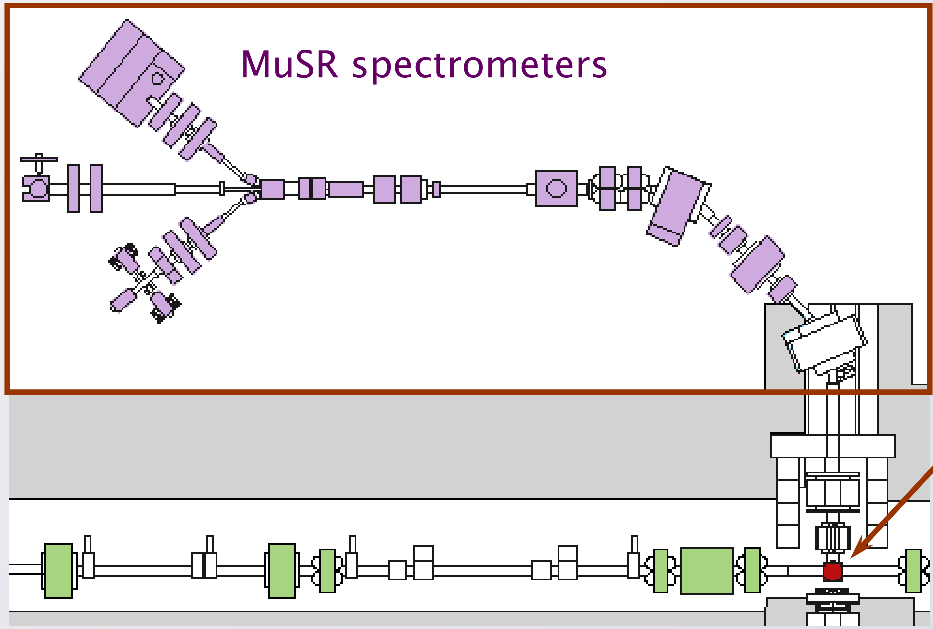
Monte Carlo simulation of Higgs boson search

Numerical simulations for μSR

Realistic experiment simulation involves two distinct domains:

- Muon production
- Positron detection

e^+ detection:
Low energies involved.
Focus on μ^+ and e^+ (and spin)



Muon beamlines at RAL

μ^+ production:
High energies involved.
Focus on p (C) and π^+.

GEANT4 and simulations in MuSR

What is GEANT4?

GEANT4 is a Monte Carlo radiation transport toolkit which includes a complete range of functionalities required to build flexible simulation frameworks

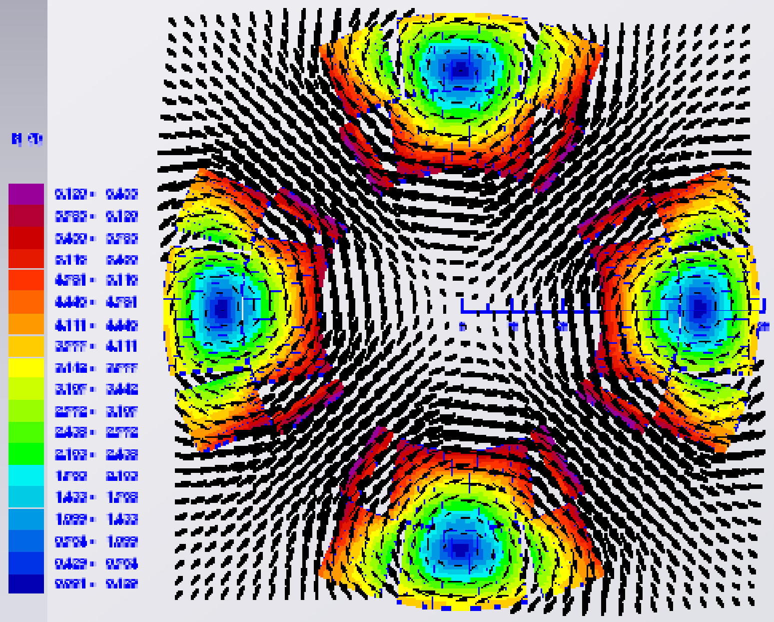
Why use G4 in μSR?

Taking advantage of its open architecture and OO design, we could develop a new software suite, able to model and simulate μSR experiments and instruments

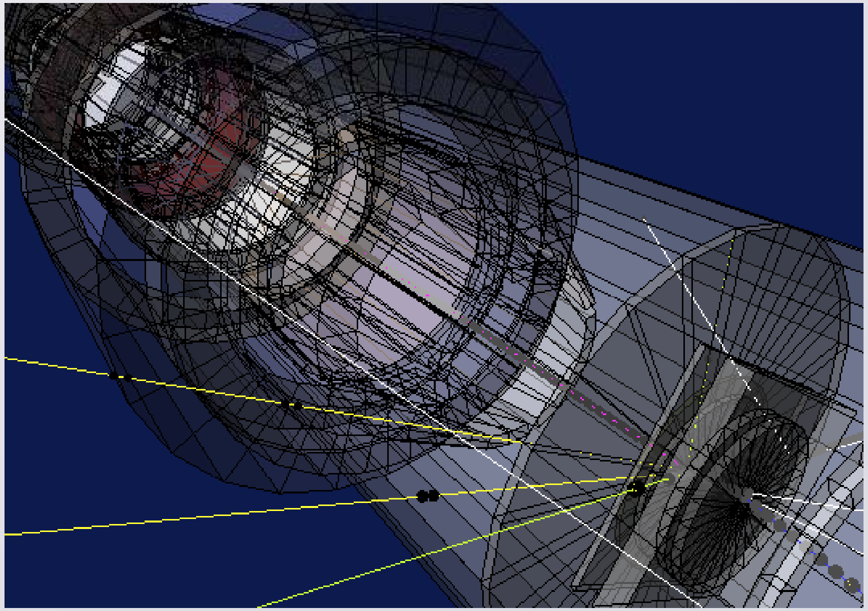
Basic paradigm for MuSR simulations

Philosophy: Use the best program for each task, then combine the results, i.e.:

Field **maps** by OPERA-3D or FemLab – Finite Element EM



Tracking, propagation and **physics** through Geant4



Ingredients of a GEANT4 simulation

- **Geometry**
  - Description of detectors, materials, positions, sensitivity, etc.

- **Physics**
  - Primary particle
    - Particle type, momentum, energy, spin, direction, beam type, etc.
  - Physical processes
    - Different processes for **each particle** (ionization, mult. scatt., etc.)
    - Different models for the **same process** (e.g. LowE, PENELOPE, etc.)

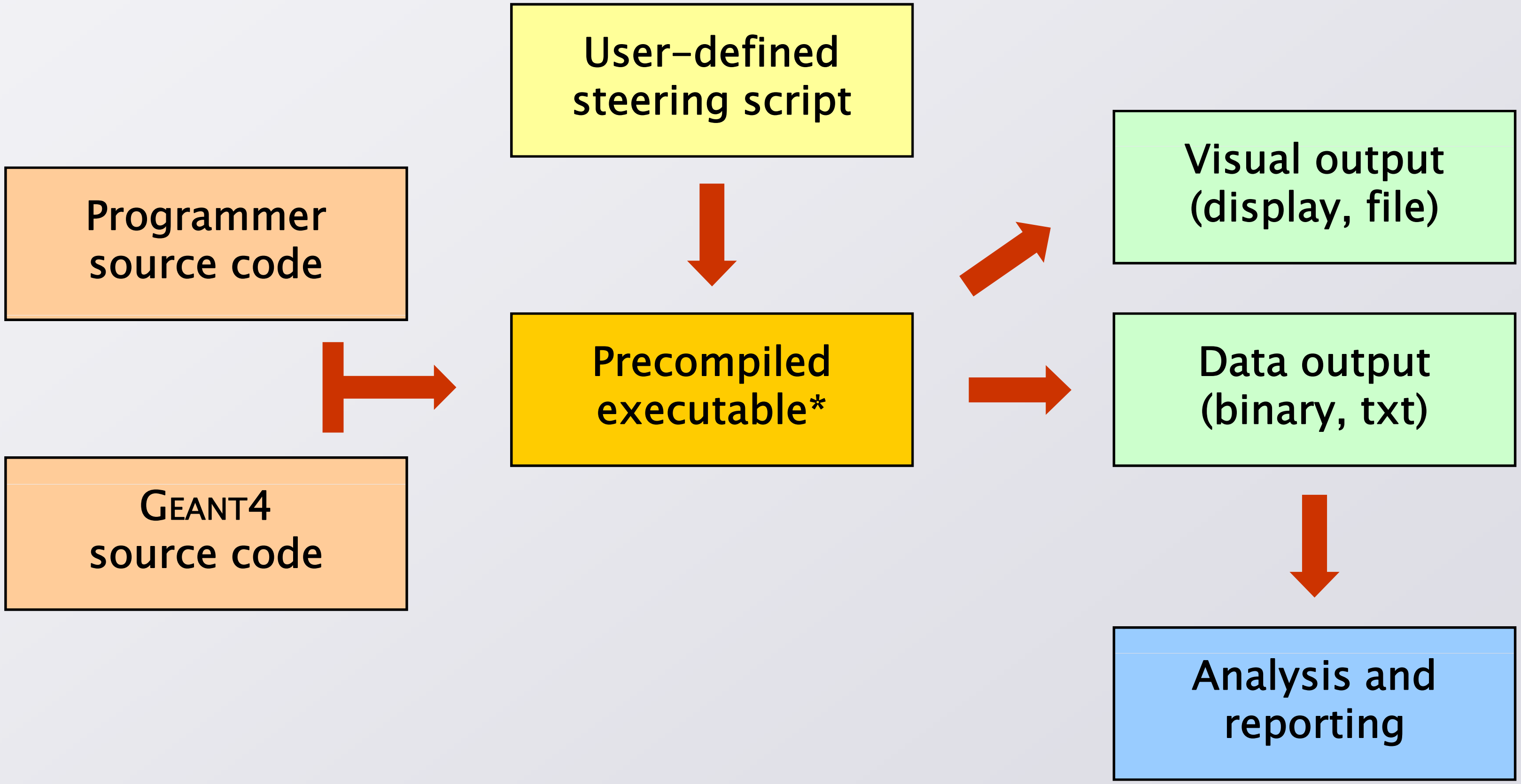
- **Tracking**
  - Propagation in matter, magnetic and electric fields
    - Account for spin, momentum, generation of secondary particles, etc.
  - Hits and digitization
    - Interaction with sensitive parts of detector:
      analog or digital output + recording and display

G4-µSR simulation – **New key features**

Extreme Flexibility

- Any geometry (even complex)
- Any EM field:
  - Electric or magnetic (recalcul.)
  - Field map or constant
  - 2D, 3D, axi-symmetric
  - Whatever field superposition
- Great user friendliness
  - No C++ knowledge required
  - Not even need to compile!
- root format output
- Platform / version independent
- \+ many other features …

G4-µSR simulation – **SW architecture**



Software architecture of the G4-based µSR simulation platform, optimized for maximum **flexibility** and end-user **friendliness**.

*) Running also in work-stations **without** GEANT4

Tuning GEANT4 for MuSR:

New developments and testing

Tuning GEANT4 for MuSR

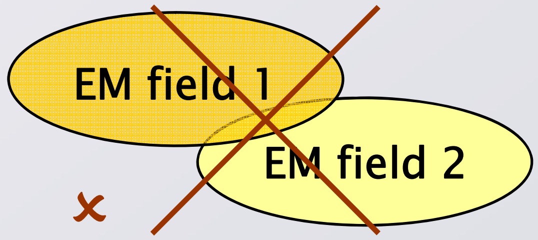
GEANT4 was conceived for use in high-energy physics. Using it in MuSR applications has required **significant tuning** efforts including:

- Redefining the **field overlap** concept in G4,
- Defining **muonium** as a new type of "particle".
- Introducing new **energy-loss** and **scattering** processes.
- Improving the concept of the **particle gun.**
- Improving user **interaction** and **friendliness**.

Overlapping fields in GEANT4

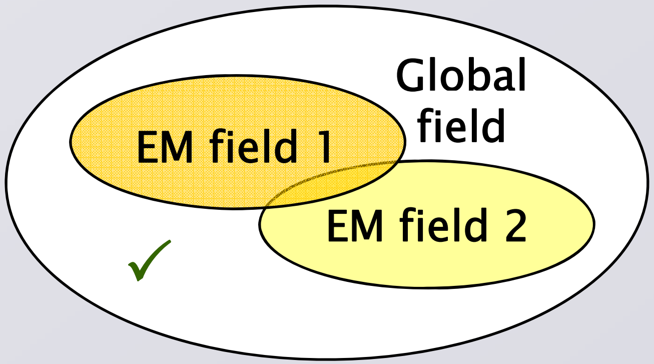
- By default G4 does **NOT** allow overlapping EM fields
- Electrostatic fields treated as "**secondary**" (privileged role for B)
- Changing existing model requires **considerable efforts** ("pushing G4 to the limits")

BEFORE



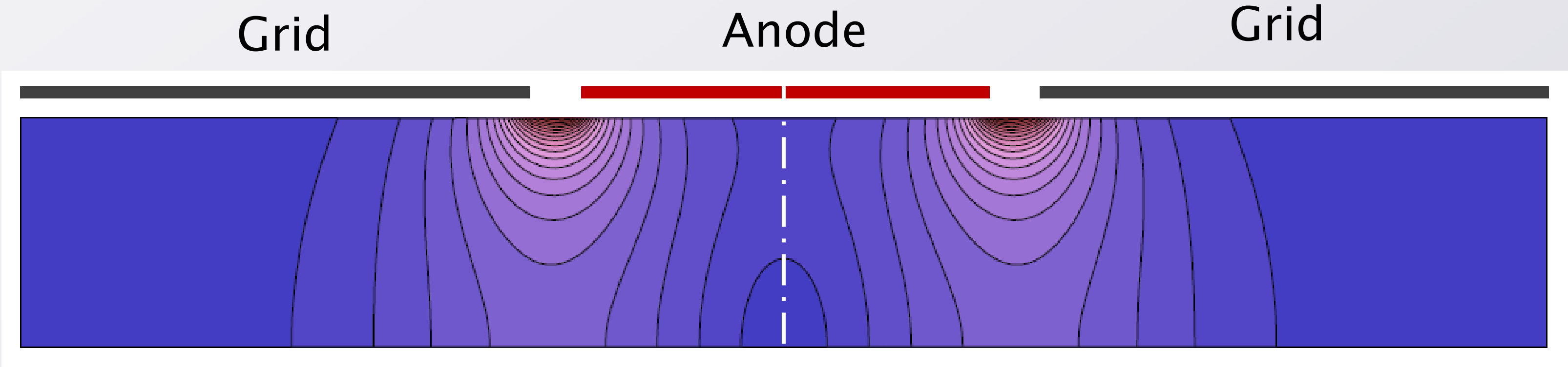
AFTER

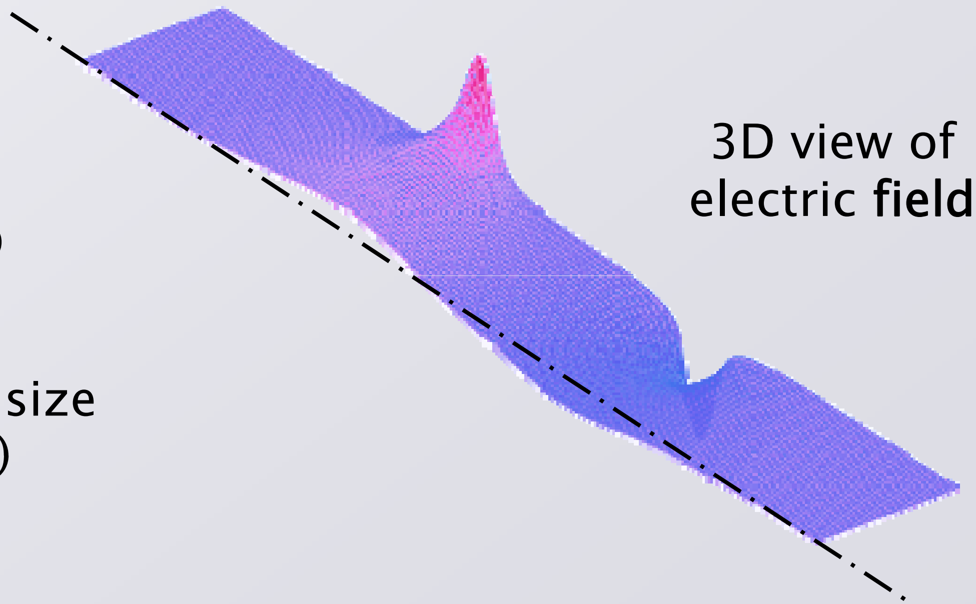
- Change in paradigm: Global field "contains" all the others
- In sample area up to 8 fields simultaneously overlapping!



New and improved field maps

Electrostatic **potential**



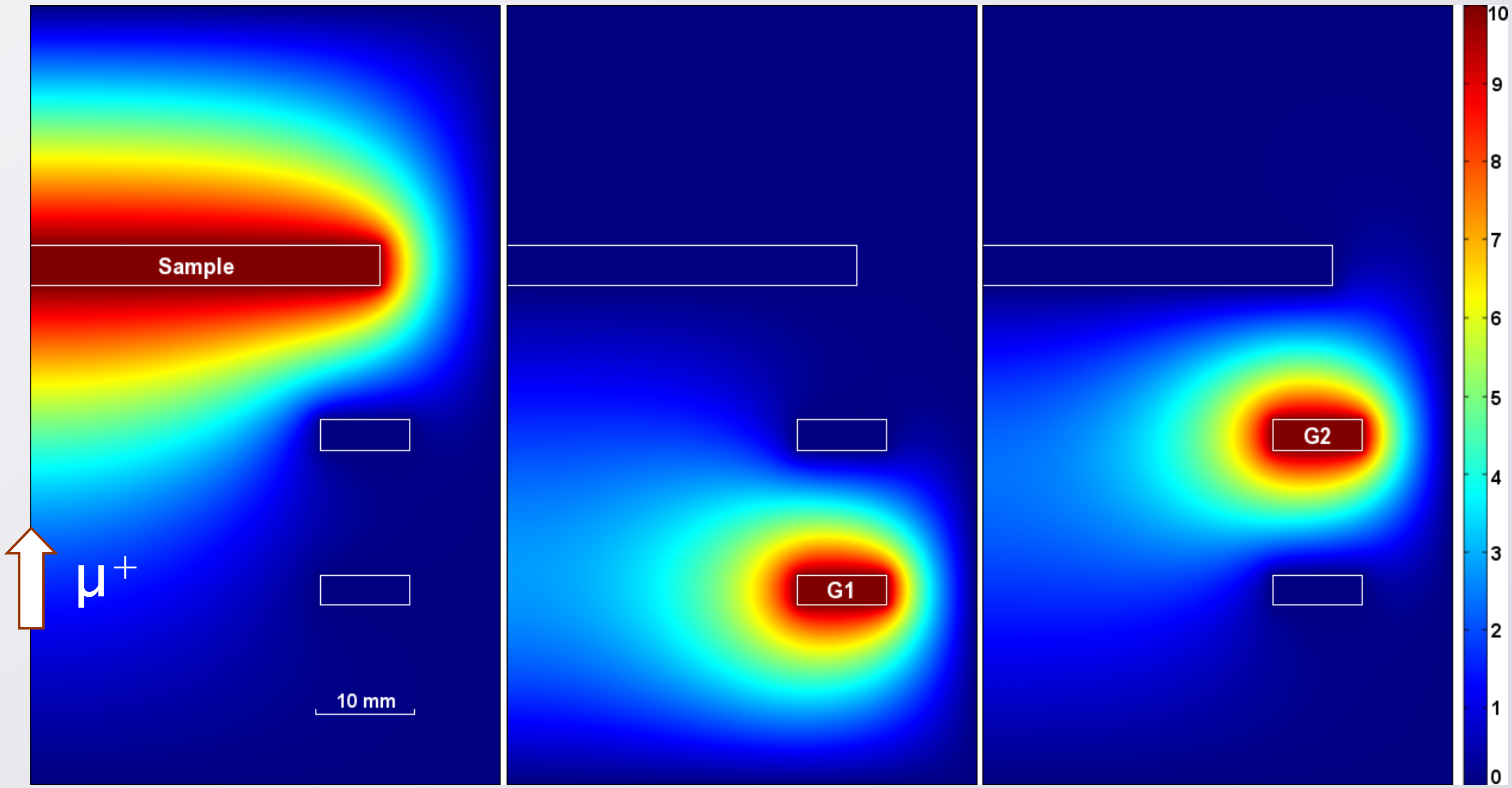


3D view of electric **field**

- Perfectly smooth 2D axi-symmetric field
- Extremely small file size (64 kB vs. ~100 MB!)

Electric field map at sample area

- Arbitrary E–field configuration obtainable by superposition



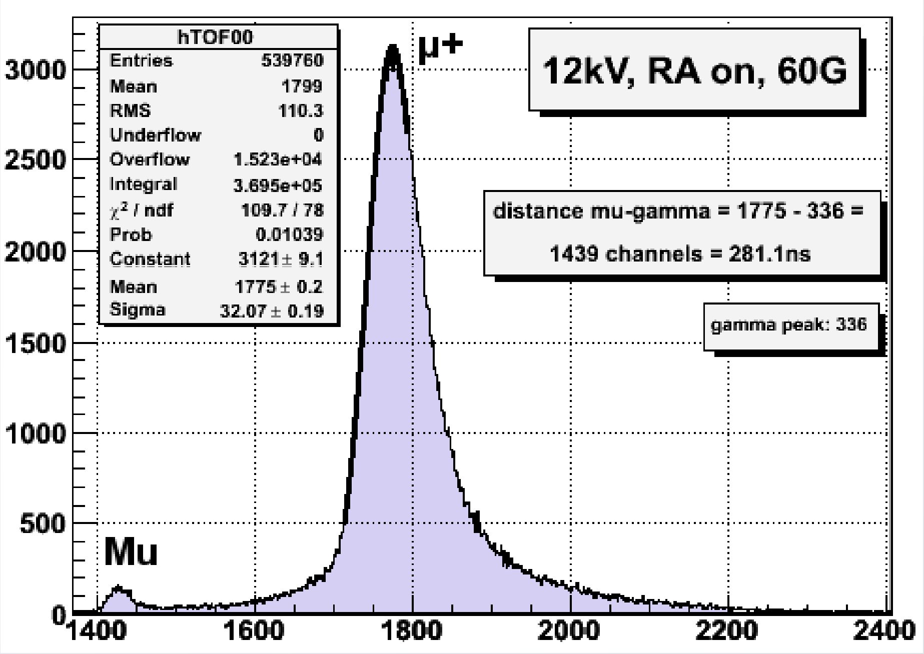
Sample Grid 1 Grid 2

New particles – Muonium

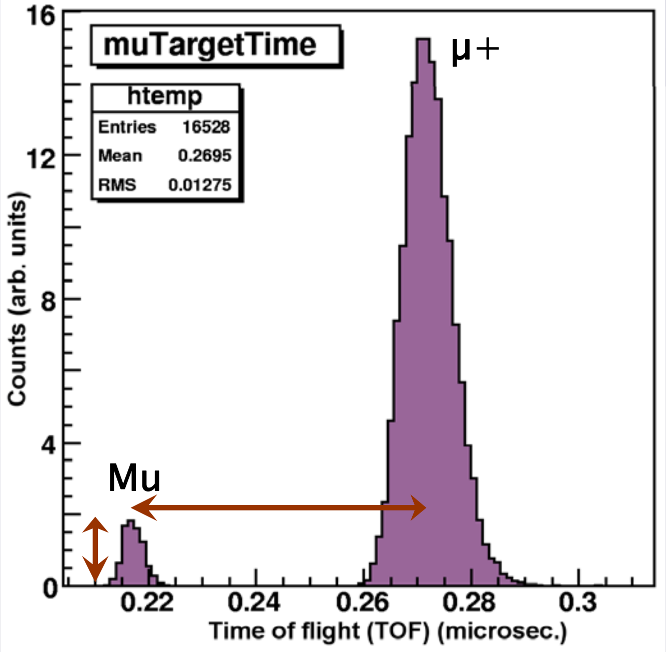
Results of Mu simulations in good agreement with experimental data*

*) Details depend on EM field map precision

- Peak **height** (production efficiency)
- Peak **TOF** (type of particle, i.e. Mu)



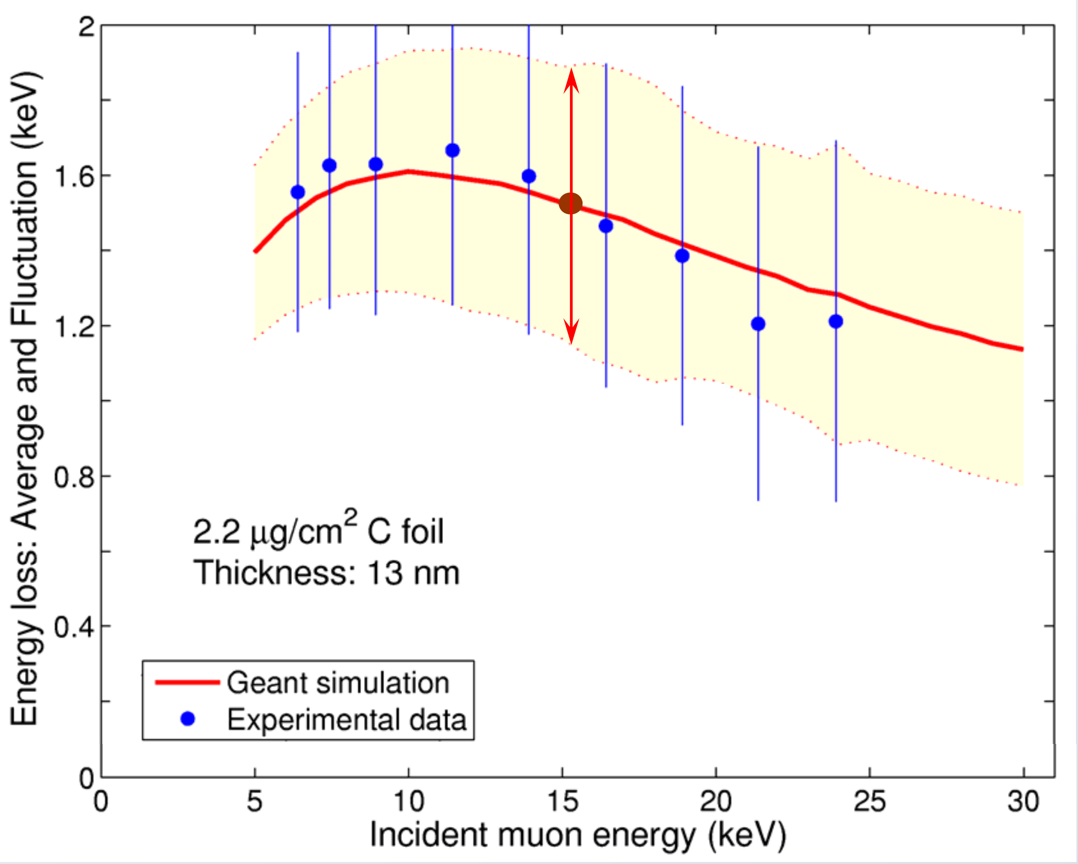
Time-of-flight: **Experiment**

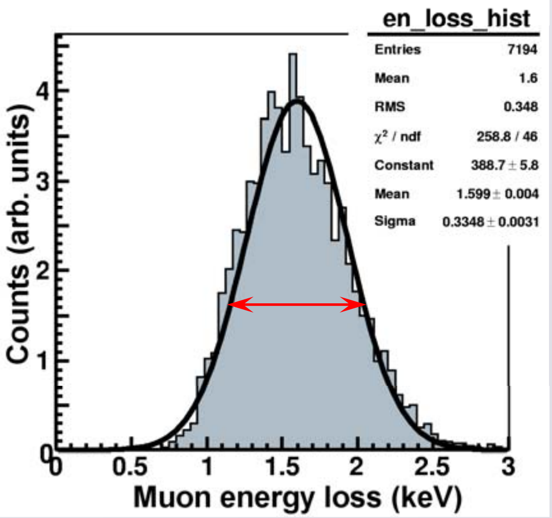


Time-of-flight: **Simulation**

Energy loss processes

Energy loss and straggling at Trigger both satisfactorily described by G4 (error ~ 7%)

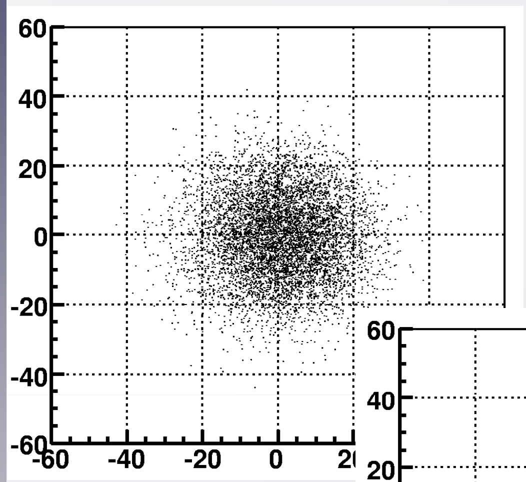




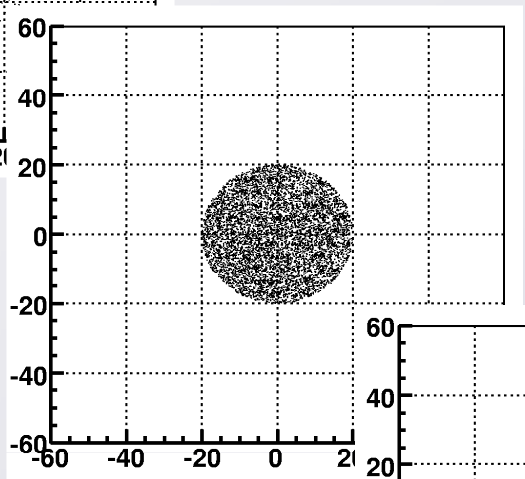
Energy loss and straggling for E_0 = 15 keV muons

Flexibility aspects – Particle gun choice

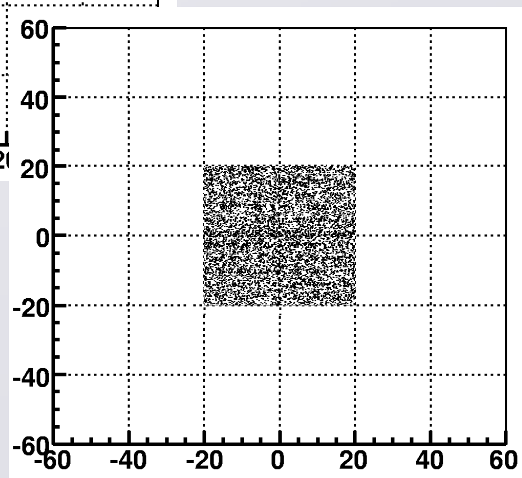
~~G4 default beam is **point-like**~~



Gaussian



Elliptic/Circular
(or point-like)



Square or
Rectangular

Different **beam profile** choices for testing:

- Shape
- Dimension
- Position
- Momentum
- Randomness

All dimensions in mm

G4 inner workings (not so simple)

```
…
typedef G4THitsCollection<TargetHit> TargetHitsCollection;

extern G4Allocator<TargetHit> TargetHitAllocator;
inline void* TargetHit::operator new (size_t) void *aHit;
  {
  aHit = (void *) TargetHitAllocator.MallocSingle();
  return aHit;
  }
inline void TargetHit::operator delete(void *aHit)
  {
  TargetHitAllocator.FreeSingle((TargetHit*) aHit);
  }
#endif
```

User's task much easier: NO need to know neither GEANT4, nor C++!

Simplified user's interaction with G4

Constructing detector geometry:

```
construct tubs target 0 25 1.5 0 360 MCPglass 0 0 108 log_MCPV norot dead 032 nofield
```

keyword dimensions position

Setting the electromagnetic fields:

B E

```
globalfield Trigg1_field 0 0 -1130 uniform  log_TriggE1 0 0 0 0 0 -0.02375
globalfield Lens3_field  0 0 -567. fromfile 2DE L3_Erz.map log_L3VA 6.78
```

Checking field values, setting visual attributes, etc. (optional):

```
globalfield printFieldValueAtPoint 0. 0. -35.0
visattributes log_MCPV invisible
```

Setting parameters, processes, etc:

```
/gun/particle mu+
/gun/kenergy 12 keV
/lem/command typeofprocesses lowenergy
```

Interface architecture
by K. Sedlak

Applying G4-μSR to real-life cases

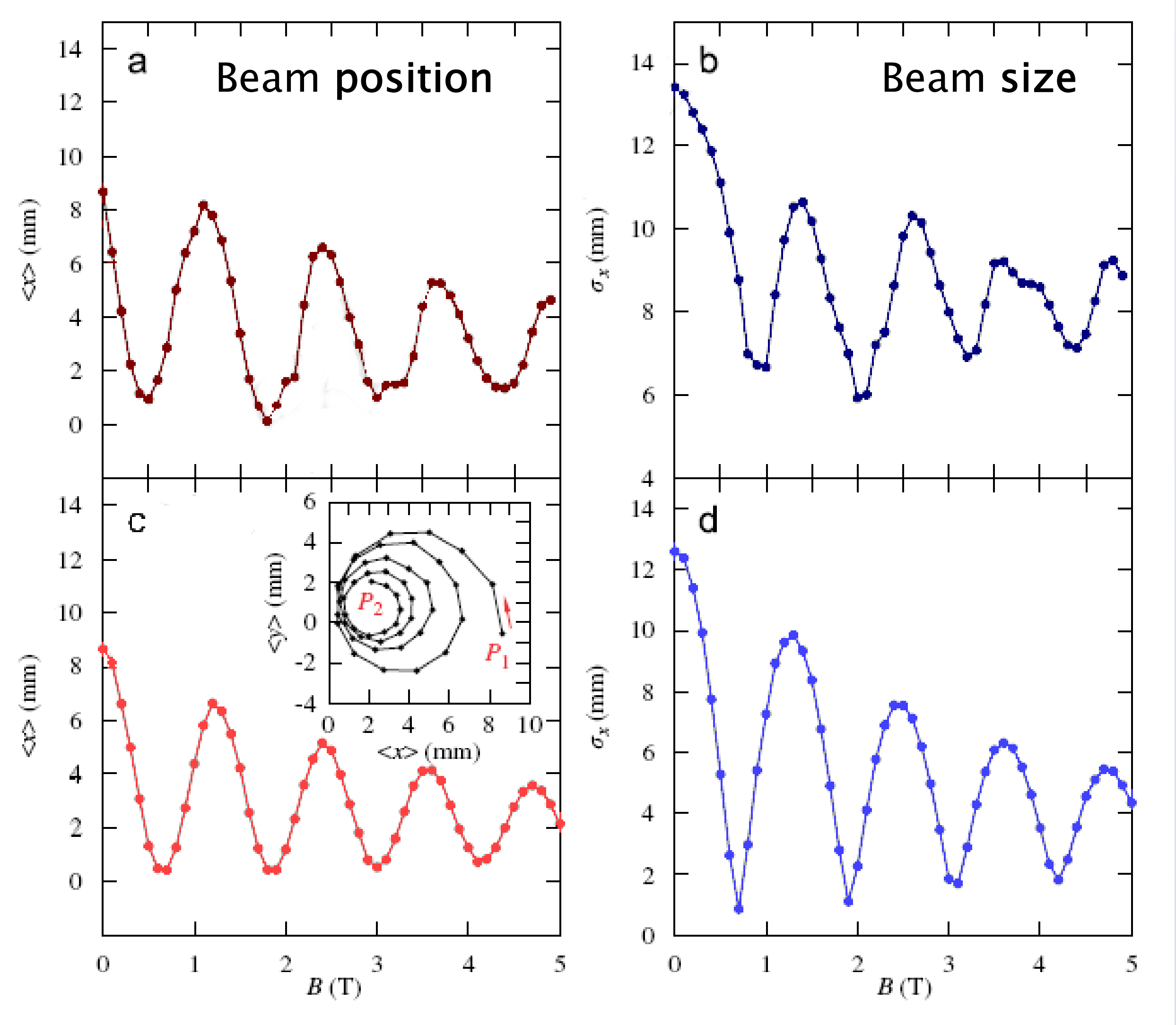
The newly developed G4-μSR simulation toolkit offers several advantages:

- New insights into the **basics** of the μSR.
- A better understanding of the **existing** spectrometers, and the development and optimization of **new ones**.

New insights into the basics of μSR

- Modelling of the incoming **muon** beam
- Study of the outgoing **positrons'** behaviour
- Investigation of the **geometrical** effects, etc.

Muon behaviour in a magnetic field

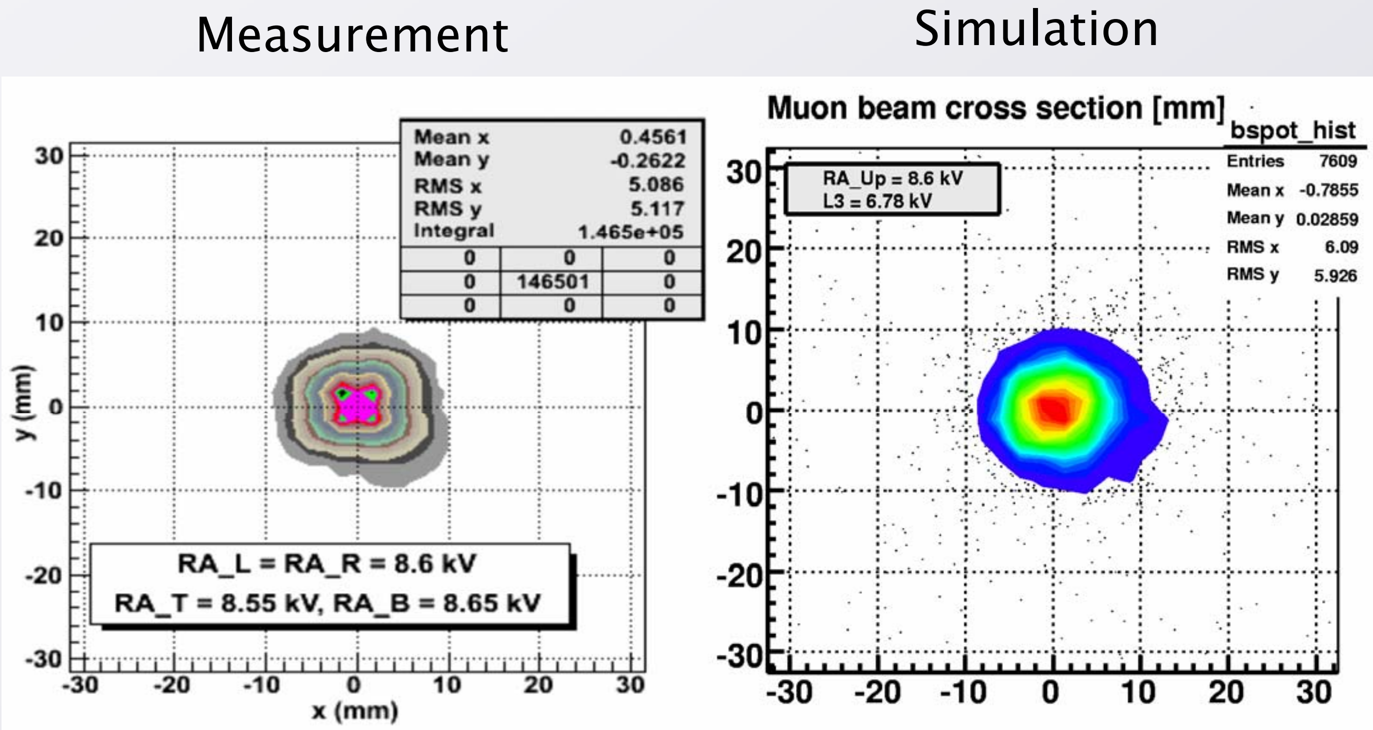


⬅ Measurement

⬅ Simulation

T. Lancaster, et al., *Nucl. Inst. Meth. A.* **580** (2007) 1578

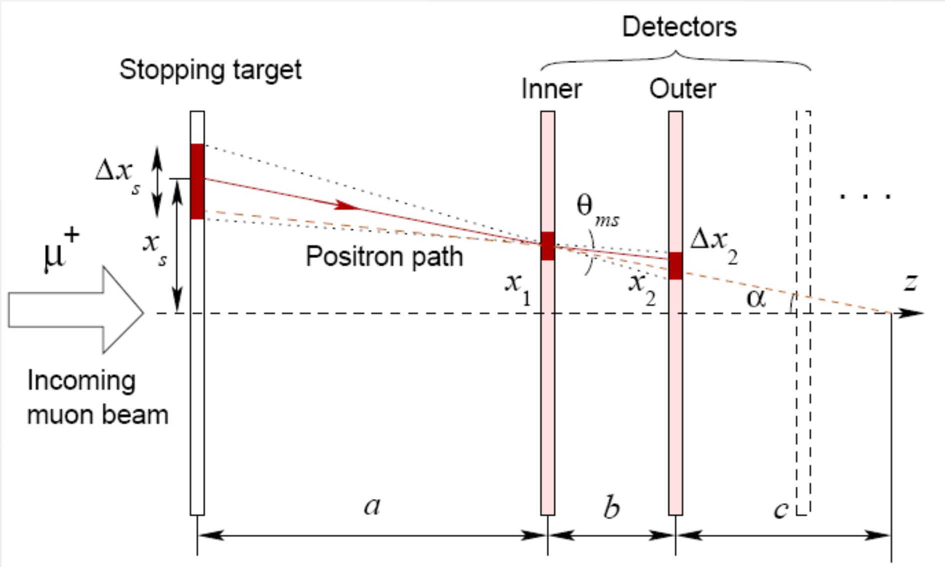
Muon beam spot (LE-μSR)



Beam spot of a low-energy muon beam at $z = 0$.

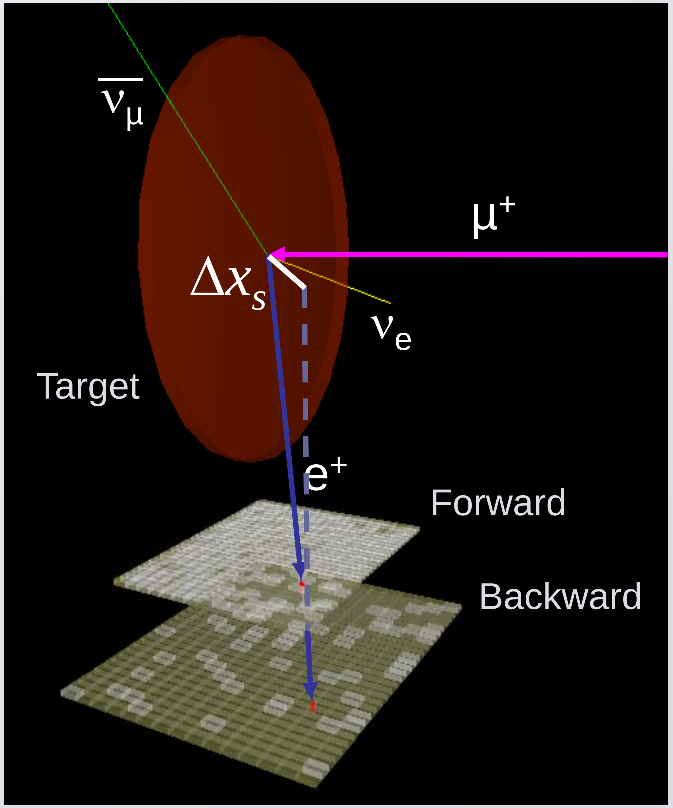
Beam spot accounts for the cumulative propagation effects in various EM fields. A correct spot reproduction indicates good predictive capabilities of the simulation package.

Position sensitive detection in µSR



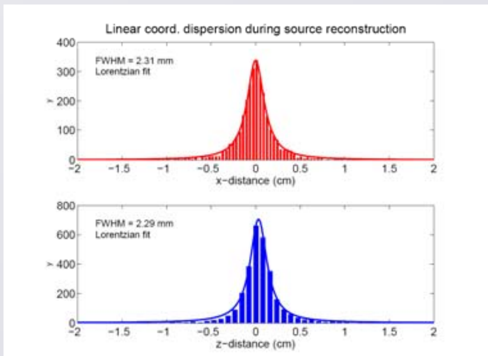
T. Shiroka, et al.,
Nucl. Inst. Meth. A.
589 (2008) 136

… GEANT4 Simulation



Detector schematics and …

Statistical analysis

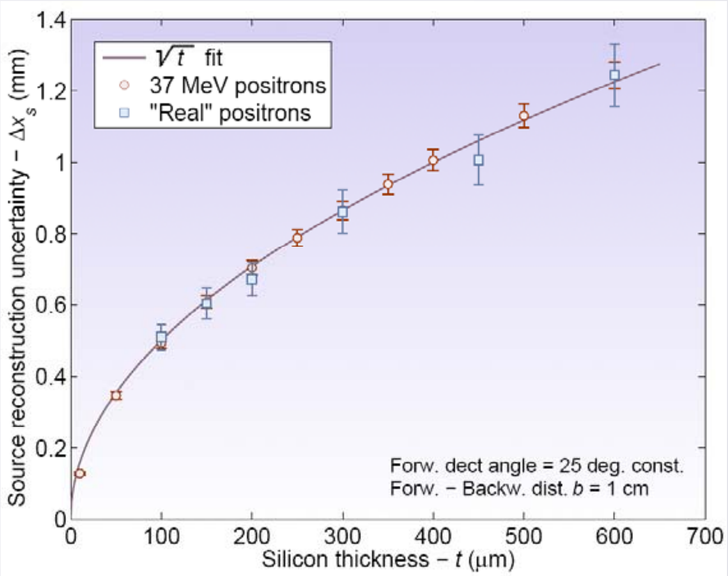


Multiple scattering and geometrical effects

An **increased** error expected for thicker detectors, with large mult. scatt.: $\theta \sim \sqrt{t}$

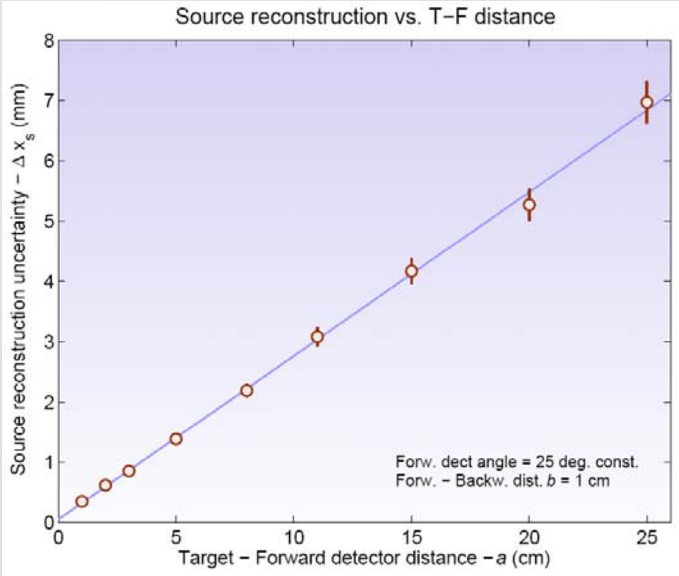
If: $\Delta x_s = a \cdot \theta \cdot 1/\cos^2\alpha$

$$\Delta x_s \sim \sqrt{t}$$



A **linear** error is expected with the first detector-to-source distance:

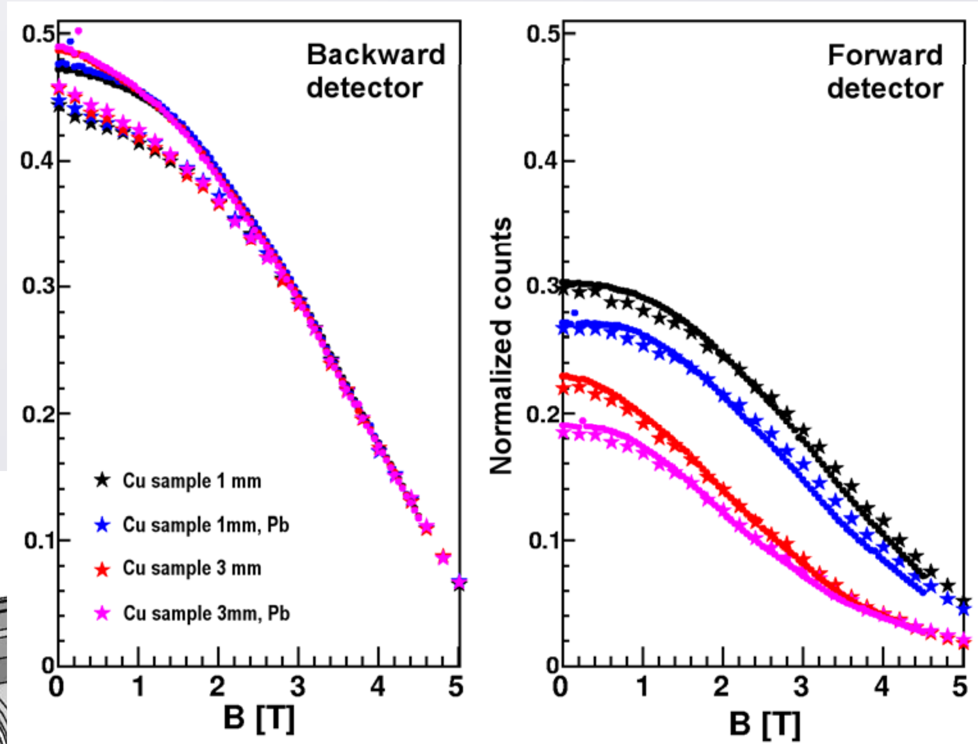
$$\Delta x_s = \mathbf{a} \cdot \theta \cdot 1/\cos^2\alpha$$

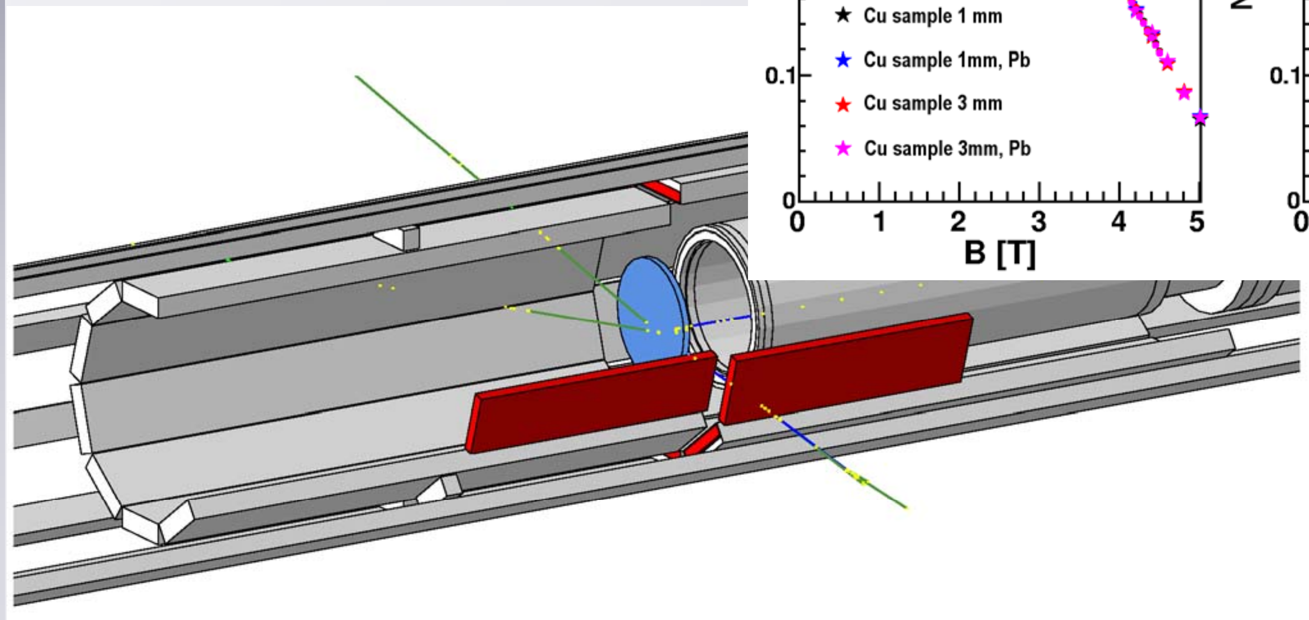


Improving existing and building new μSR instruments

Improving existing μSR spectrometers: ALC

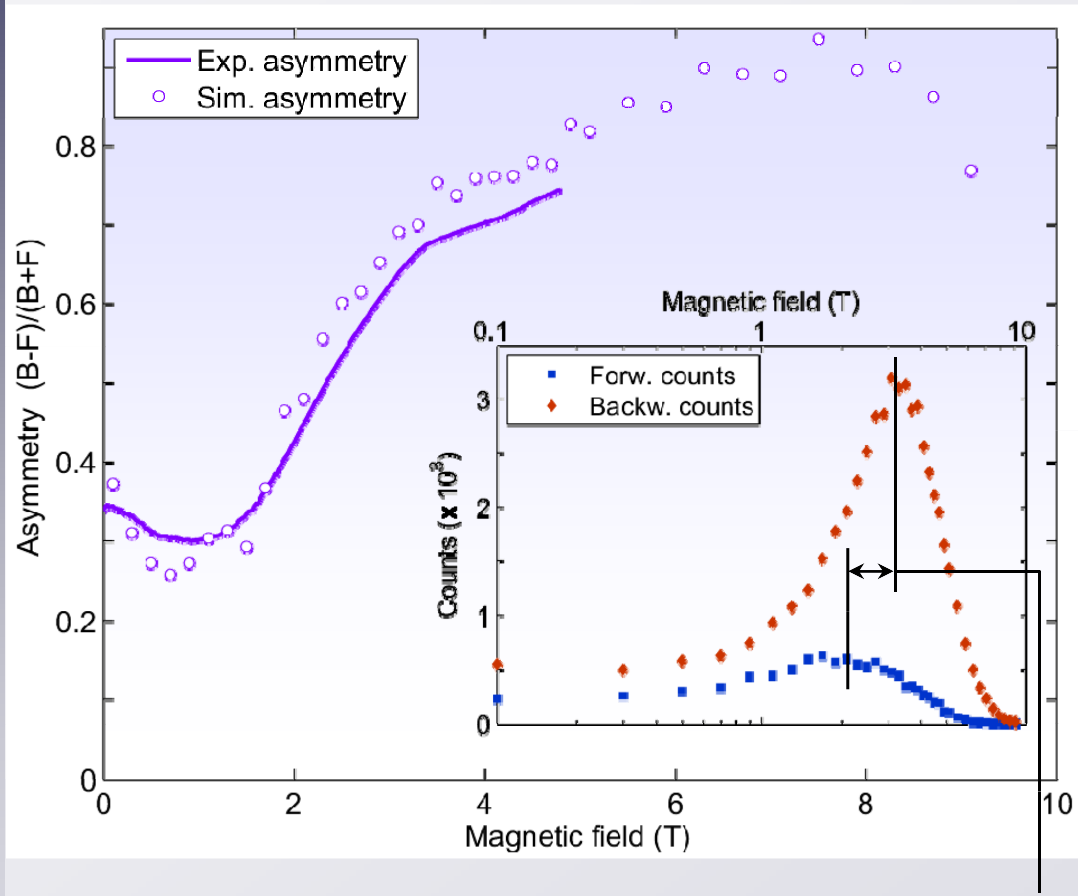
- ALC instrument simulation to eliminate/simplify **baseline counts** interfering with measurements
  - Good agreement with exp.
  - Control over the causes





K. Sedlak, et al.,
IEEE Trans. Nucl. Sci.
manuscript in prep.

Positron behaviour in a magnetic field



Simulation maxima at ~ 3 T

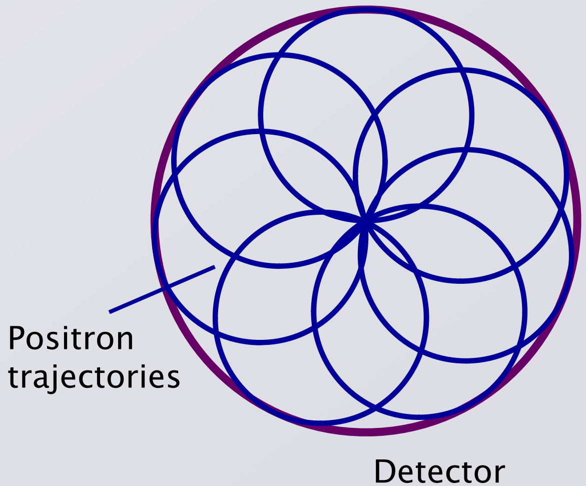
$B = mv/qR$

$B\,[\mathrm{T}] = 3.3 \cdot E\,[\mathrm{MeV}]\ /\ R\,[\mathrm{mm}]$

Detect diam. $D = 4R$ and mean pos. energy $<E_p>$ ~ 37 MeV/ 2

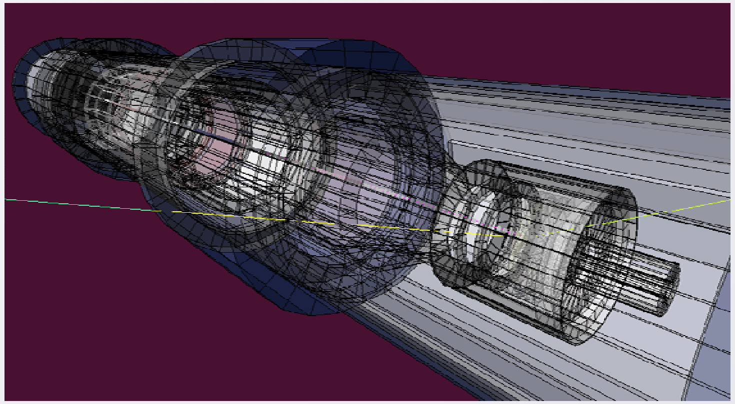
⬇

Expected. Max at 3 T!

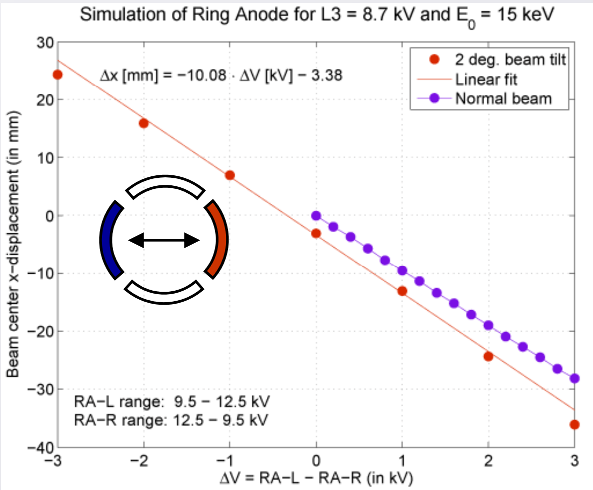


Shift in max. positions, due to different emission energy in F and B, accounts for the field-dependent asymmetry

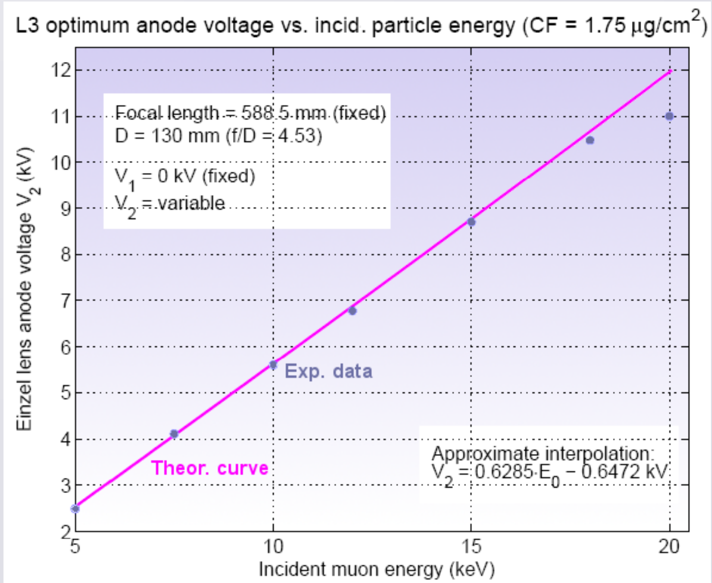
Improving existing μSR spectrometers: LEM



- The simulation of LE-μSR spectrometer allows to:
  - Check optimum settings
  - Investigate spurious effects



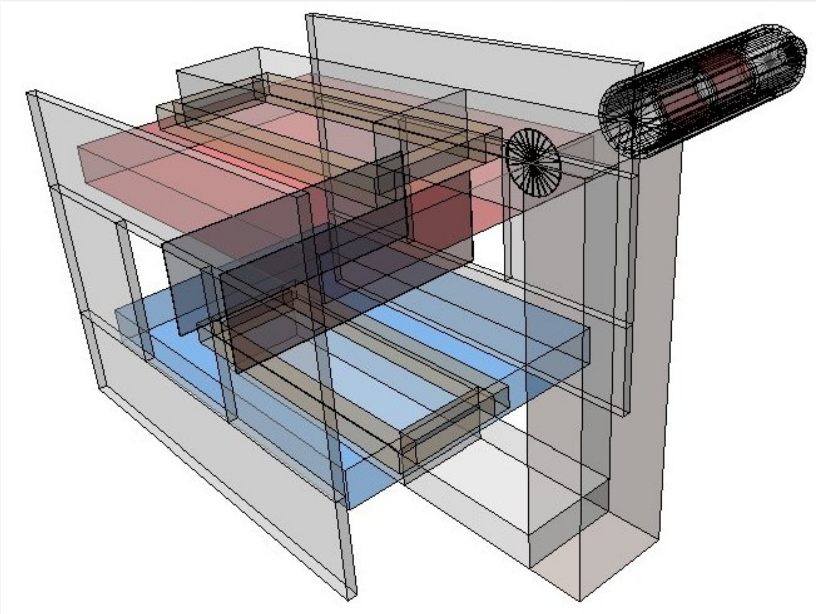
Simulating muon beam steering



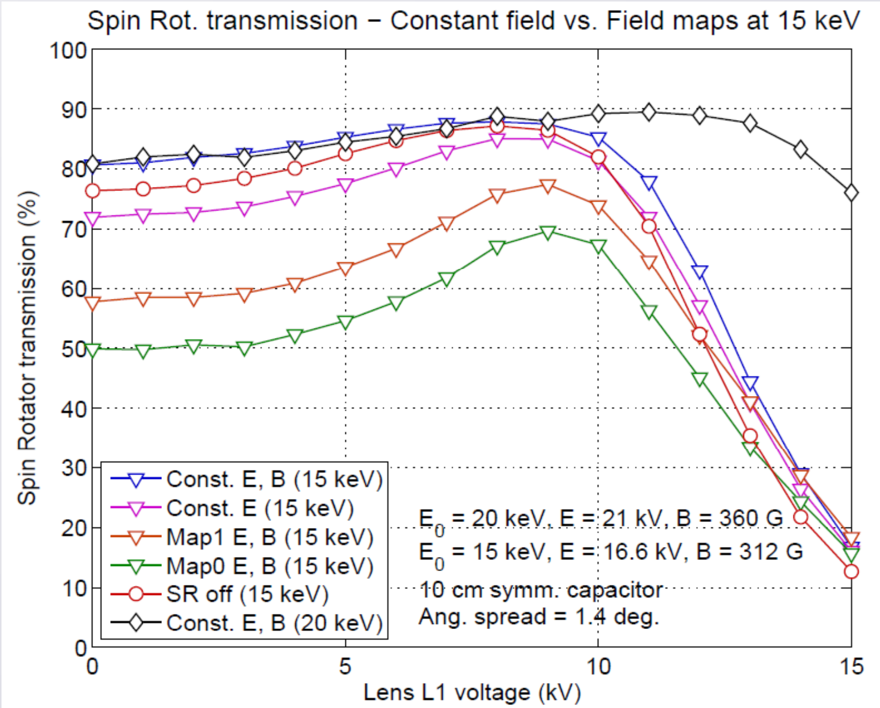
Einzel lens focussing: setting optimum voltage

Improving existing μSR spectrometers: LEM

- The addition of a Spin Rotator to LE-MuSR would allow:
  - New LF experiments
  - Background reduction



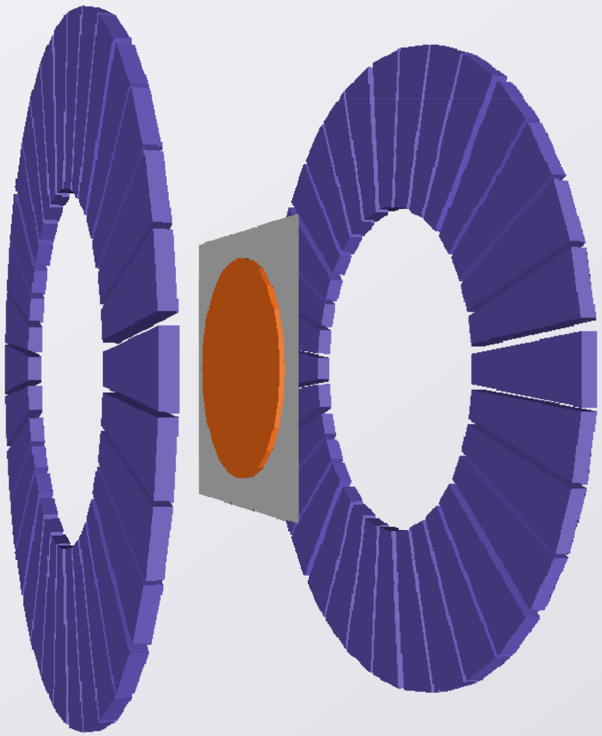
LEM cross-field spin rotator

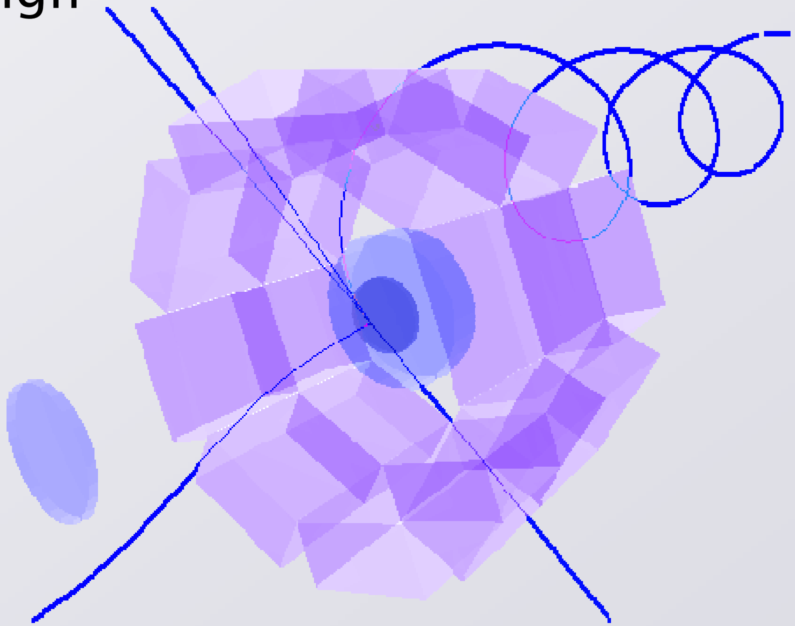


Building new μSR spectrometers

Simulation-based instrument design

High-field spectrometer for
LF-μSR planned at RAL (Z. Salman)





High-field spectrometer for
TF-μSR being built at PSI (K. Sedlak)

G4-μSR toolkit dissemination

- Widespread dissemination of the work:
  - 5 conference talks/posters (of which 2 invited)
  - Dedicated web site: http://lmu.web.psi.ch/simulation
  - 11 scientific papers

GEANT4 as a simulation framework in μSR ☆

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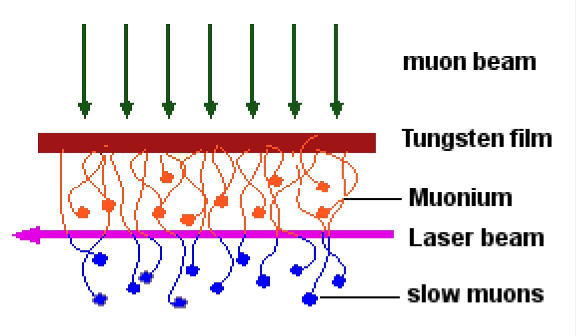
ABSTRACT

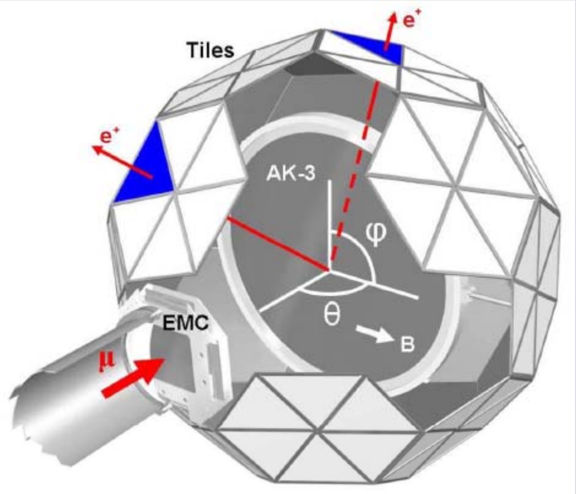
GEANT4 is a Monte Carlo radiation transport toolkit which includes a complete range of functionalities required to build flexible simulation frameworks. Taking advantage of its open architecture and object-oriented design, we could develop a software suite, able to simulate μSR experiments and instrumentation. The versatility offered by this new tool has permitted us to model the existing instruments, thus allowing a fuller understanding of their operation. It has guided also the design and construction of new types of spectrometers, as those equipped for high-field μSR, where numerical simulations proved decisive in understanding the complex behaviour of the incoming muon beam and of the outgoing positrons in a high magnetic field environment. The developed μSR simulation framework, with its fully flexible and customizable design, will allow potential users not familiar with programming to focus exclusively on physics, by building and running their own applications without the need to modify the source code.

G4-μSR toolkit is already a success

- Already in use in advanced simulations at the new low-E μSR beamline at RIKEN-RAL (UK, P. Bakule).
  - Epithermal muons by Mu ionisation



- Potential interest also from the MuLAN (Muon Lifetime Analysis) particle physics experiment (USA, K.R. Lynch).
  - Determine μ^+ lifetime to <1 ppm. High precision test of Fermi coupling constant G_F and hence of the Standard Model.



Summary and future developments

- We could build a **complete simulation framework** dedicated to μSR applications, characterised by a high degree of flexibility, modularity, and a simple user interface.

- The reported examples show that numerical simulations carried out with the new platform:
  - Provide a deeper understanding of the physics of the μSR experiment.
  - Are crucial in designing and building new, sophisticated μSR instruments.

Future uses and developments

G4-μSR could be also used in:
- Feasibility **analysis**,
- Experiment **planning**,
- Interactive **teaching**.

New developments could include:
- Simplified **graphical** interface,
- Implement material **specificity**,
- Open to **suggestions** from users …

Acknowledgements

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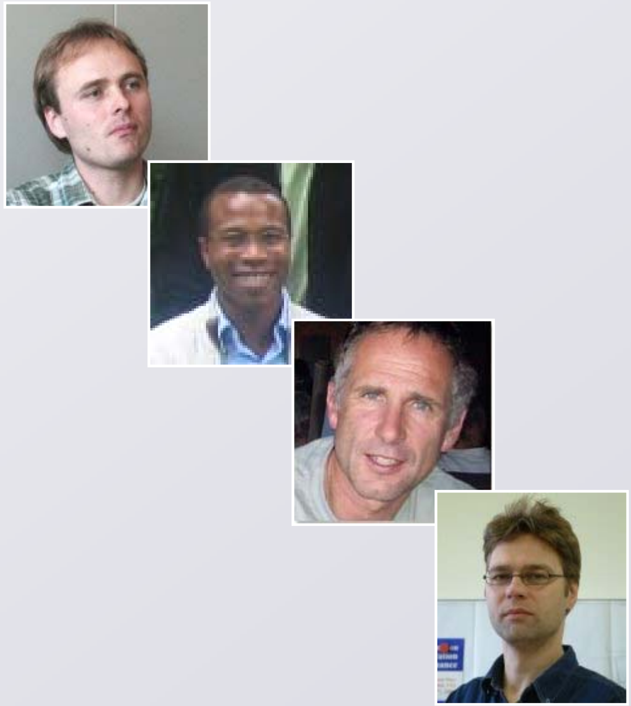
  Laboratory of Quantum Optoelectronics,
  EPFL, Lausanne, Switzerland

- **P. Gumplinger**
  TRIUMF, Vancouver, BC, Canada

- **T. Prokscha**
  Laboratory for Muon-Spin Spectroscopy,
  PSI, Villigen, Switzerland

  Also: **T. Lancaster, Z. Salman**



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