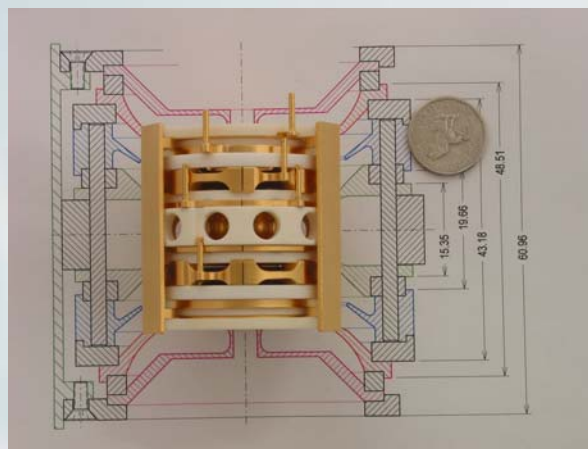


SOMA, Excel and Data Analysis



Ryan Ringle, NSCL

ringle@nscl.msu.edu

From Detection to Analysis

Online

Timing Control

-CS Server/Mass Measure

Signal Detection

-MCP

Signal Collection

-scope

Data Archival/Discrimination

-Mass Measure

Offline

TOF/Fit Analysis

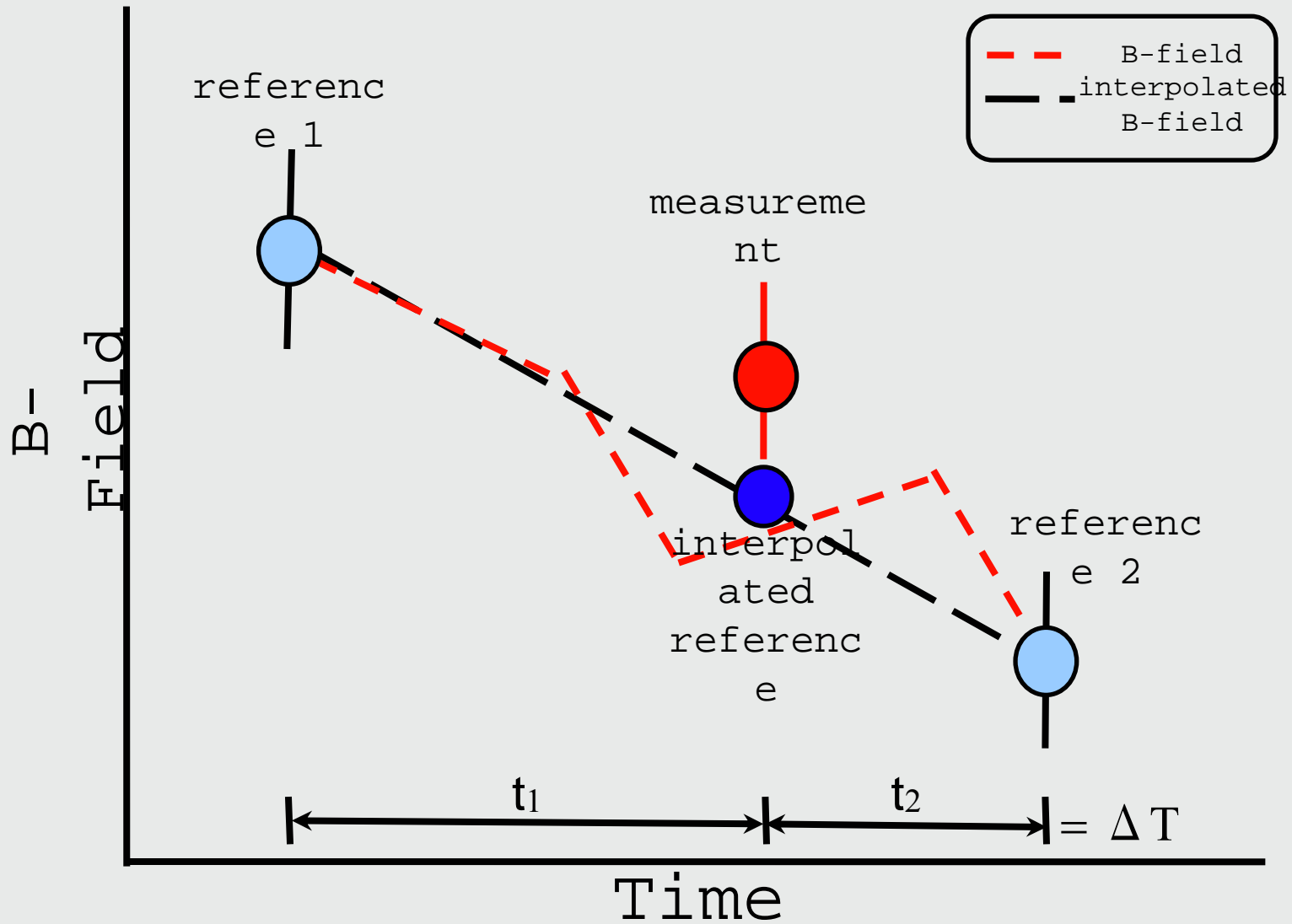
-Eva

Mass Analysis

-Excel

-SOMA

Single Measurement Procedure



Single Measurement Procedure Cont.

Step 1

- calculate error in interpolated slope

$$err_{slope} = \frac{\sqrt{(err_{ref1} t_1)^2 + (err_{ref2} t_2)^2}}{\Delta T}$$

Step 2

- calculate ratio of cyclotron frequencies

$$ratio = \frac{(v_c)_{interp} q_{meas}}{(v_c)_{meas} q_{ref}}$$

Step 3

- calculate error in ratio

$$err_{ratio} = ratio \sqrt{\left(\frac{err_{slope}}{(v_c)_{interp}}\right)^2 + \left(\frac{err_{meas}}{(v_c)_{meas}}\right)^2}$$

Step 4

- calculate corrected ratio error

$$err_{corr_ratio} = \sqrt{err_{ratio}^2 + \left(\Delta T \left(\frac{dB}{dt}\right)_{err} ratio\right)^2}$$

Multiple Measurement Procedure

Step 5

- calculate the mean ratio

$$ratio_{mean} = \frac{\sum_{meas} \frac{ratio}{err_{corr_ratio}^2}}{\sum_{meas} \frac{1}{err_{corr_ratio}^2}}$$

Step 6

- calculate the inner error

$$err_{inner} = \sqrt{\frac{1}{\sum_{meas} \frac{1}{err_{corr_ratio}^2}}}$$

Step 7

- calculate the corrected ratio

$$ratio_{corr} = ratio_{mean} + shift_{mass} (A_{meas} - mass_{ref_amu})$$

Step 8

- calculate corrected mass

$$mass_{corr} = ratio_{corr} mass_{ref_amu} + q_{meas} mass_{electron}$$

Multiple Measurement Procedure Cont.

Step 9

- calculate the absolute final error

$$err_{abs_final} = \sqrt{err_{inner}^2 + (err_{sys} ratio_{mean})^2}$$

Step 10

- calculate the final mass error

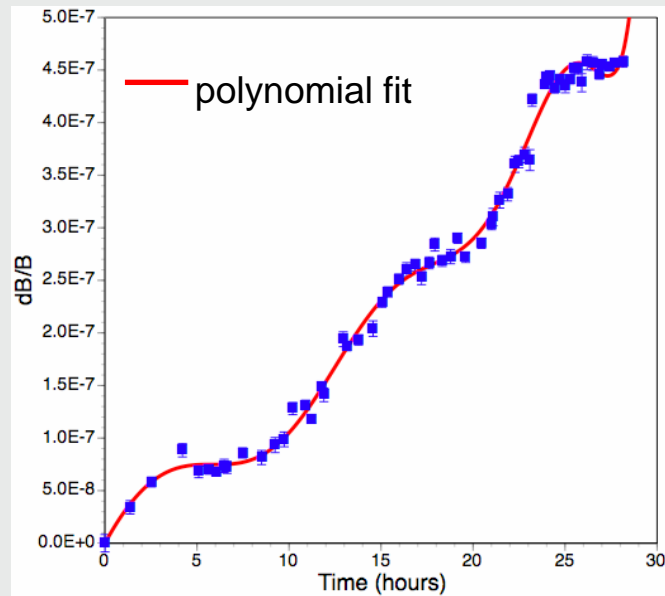
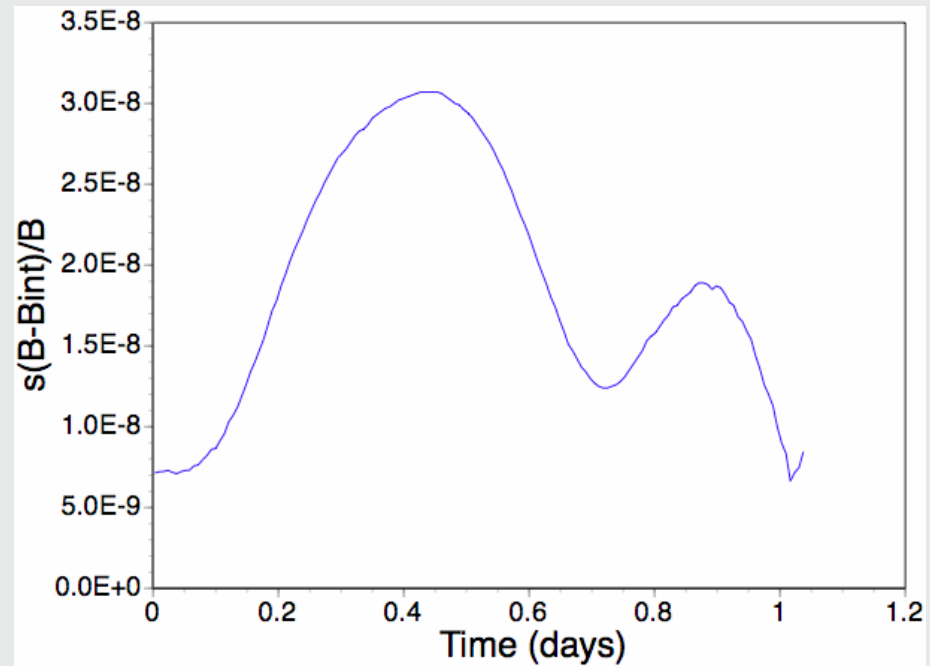
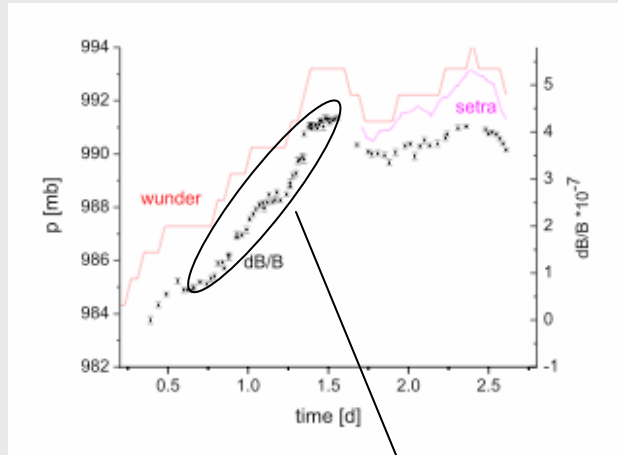
$$err_{final_mass} = \sqrt{(mass_{ref_amu} err_{abs_final})^2 + (ratio_{corr} err_{ref_mass})^2}$$

Currently **NOT** accounted for:

- Electron binding energies (future SOMA update)
- Error in mass dependent shift correction

Nonlinear Magnetic Field Strength Effects

A. Kellerbauer et al., "From direct to absolute mass measurements: A study of the accuracy of ISOLTRAP", Eur. Phys. J. D 22 (2003) 53



Generate evenly distributed data using fit

Introducing SOMA

calibration
area

Simple Online Mass Analysis v.1

Calibration Menu

Manual Calibration

Load File

Delete Row(s)

	Date	Time	Center (Hz)	Error (Hz)	File
1	Sat Jun 18 2005	10:38:12	7583447.0830	0.0431	050618
2	Sat Jun 18 2005	11:48:18	7583447.2652	0.0503	050618
3	Sat Jun 18 2005	11:52:17	7583447.1568	0.0421	050618
4	Sat Jun 18 2005	11:57:46	7583447.2041	0.0656	050618

B-Field Decay
1.50069e-08 hr⁻¹

Chi²
2.49402e-10

Measurement Menu

Mass Tab

Add Tab

Remove Tab

Delete Row(s)

Manual Add

Load File

Results 1Ca38

	Date	Time	Center (Hz)	Error (Hz)	A	Species	Charge (e)	F
1	Sat Jun 18 2005	11:13:45	7595520.7350	0.1084	38	1Ca38		20
2	Sat Jun 18 2005	13:01:09	7595521.2600	0.1700	38	1Ca38		20
3	Sat Jun 18 2005	14:02:30	7595520.7323	0.0822	38	1Ca38		20
4	Sat Jun 18 2005	14:39:01	7595521.2082	0.0947	38	1Ca38		20
5	Sat Jun 18 2005	22:44:47	7595521.8210	0.0804	38	1Ca38		20
6	Sat Jun 18 2005	23:28:11	7595521.9061	0.0689	38	1Ca38		20

Error

Mass Dependent Error: 0

Systematic Error: 0

dB/dt (hours) 0

1 Reference Choice

Calculate

Show Scatter Plot

Open (%O)

error
area

measurement
area

Manual Calibration Data

The screenshot shows a software window titled "Calibration Data" with three main sections: "Nucleus Info", "Molecular Calibration", and "Manual Calibration Data".

- Nucleus Info:** Contains input fields for Z (18), N (22), and charge state (1). A "Choose" button is next to the N field. Below these are fields for Symbol (^{40}Ar), Mass Excess (-35550.9), and Mass Error (0.00268).
- Molecular Calibration:** Features a table with columns "Number", "Z", and "N". Below the table are fields for "species" (0) and "charge state" (1), along with a "Choose" button.
- Manual Calibration Data:** Includes "Date and Time" (12/02/2005 12:28:23), "Center (Hz)", and "Error (Hz)" input fields, and a "Submit" button. To the right, a table displays calculated values: Symbol (Ar40), Charge (e) (1), Mass (amu) (39.9618345), and Mass Error (amu) (2.877e-09).

Annotations with arrows point to specific elements:

- "single ion calibration" points to the Nucleus Info section.
- "molecular calibration" points to the Molecular Calibration section.
- "data entry" points to the Date and Time input fields.
- "additional info" points to the table of calculated values.

Data Conversion Tool

The screenshot shows a software window titled "ft2 Conversion Tool". On the left, there is a section titled "ft2 Entry Selection" containing a list of parameters, each with a numeric input field and a small up/down arrow button. The parameters and their values are: Filename (2), Element/Molecule (3), A (4), q (5), Start Date (6), Start Time (0), End Date (7), End Time (0), Low Freq (8), High Freq (9), SpF (10), Number of Ions (11), Frequency (18), and Error (19). To the right of this list is a large empty rectangular box. Below this box is a "Clear" button. Further down, there are two rows of controls: "delimiter" set to "Comma" and "file type" set to "log", each with a dropdown arrow. To the right of these are three buttons: "delete row(s)", "delete col(s)", and "insert col(s)". At the bottom, a section titled "Main Window Control" contains three buttons: "reference", "measurement", and "new tab".

Parameter	Value
Filename	2
Element/Molecule	3
A	4
q	5
Start Date	6
Start Time	0
End Date	7
End Time	0
Low Freq	8
High Freq	9
SpF	10
Number of Ions	11
Frequency	18
Error	19

ft2 Conversion Tool

ft2 Entry Selection

Filename 2

Element/Molecule 3

A 4

q 5

Start Date 6

Start Time 0

End Date 7

End Time 0

Low Freq 8

High Freq 9

SpF 10

Number of Ions 11

Frequency 18

Error 19

Clear

delimiter Comma

file type log

delete row(s)

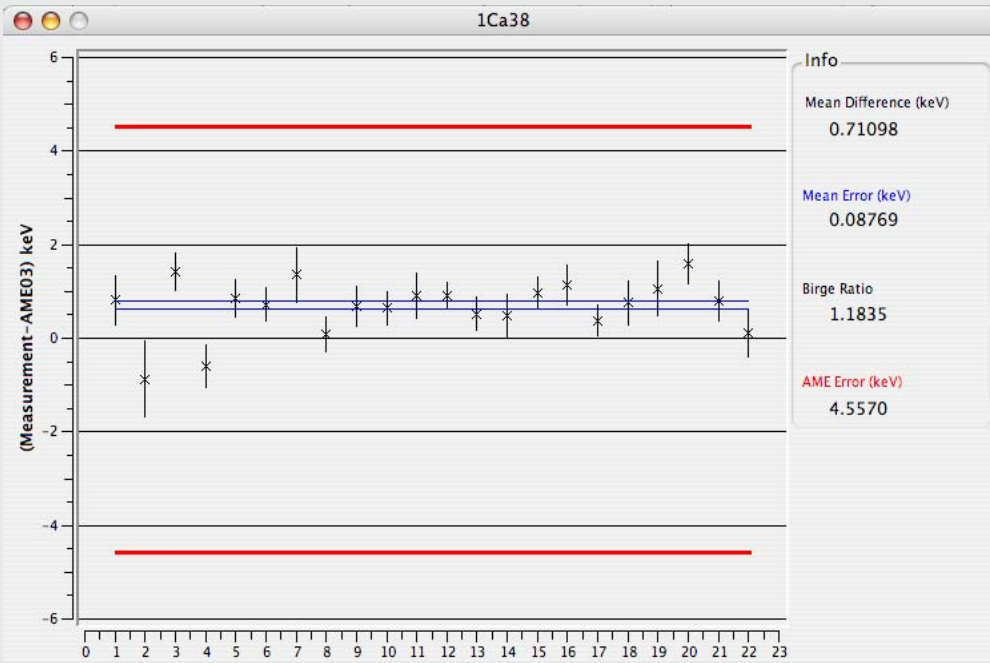
delete col(s)

insert col(s)

Main Window Control

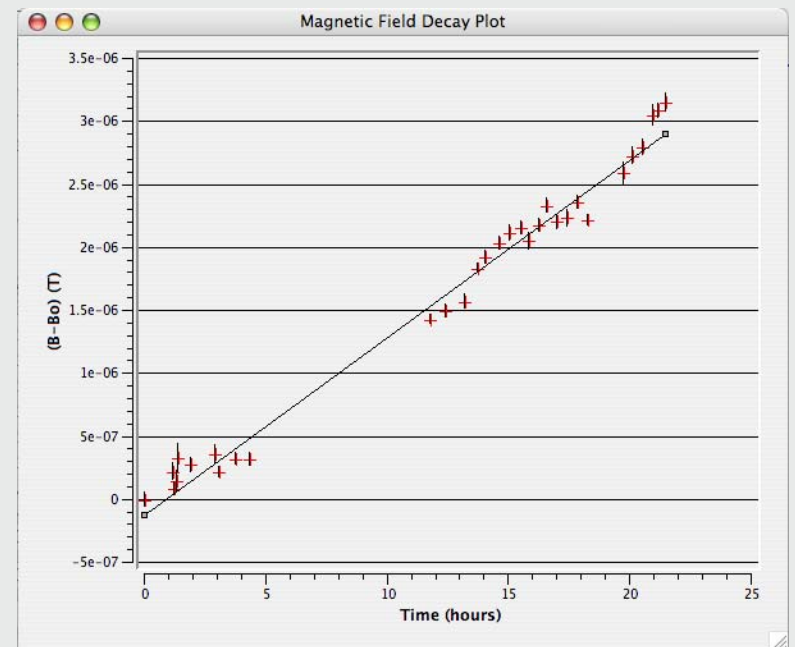
reference measurement new tab

Data Visualization



magnetic field plot with linear fit

measurement scatter plot



Under the Hood

- Built using QT3, a well-known C++ software design framework.
- Multi-platform: Tested on Windows and OSX. Should work on Linux.
- Saved “parameter files” in user editable text format.

SOMA vs. Excel

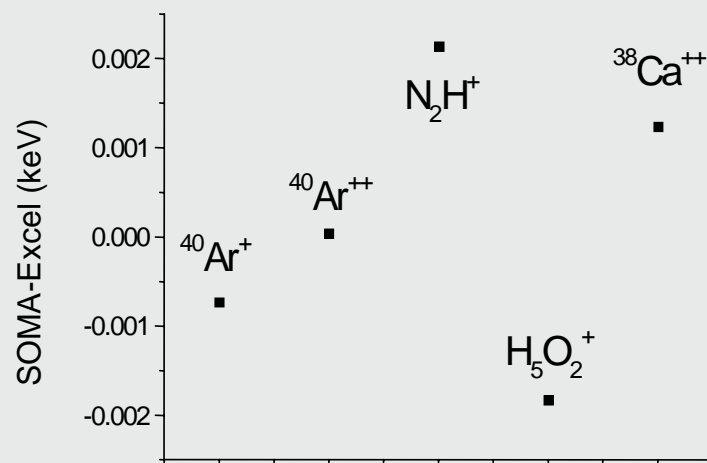
Pros

- immediately useable, small learning curve
- fast data input
- number crunching hidden
- same results given same data files
- quick alterations and immediate results
- Has yet to lock to any systems or been targeted by malicious code.

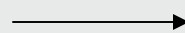
Cons

- number crunching hidden
- constants hard coded and (currently) inaccessible
- code is slightly convoluted and difficult to interpret
- technical support slow and inefficient

SOMA vs. Excel Cont.



- Same fit files used in both tests
- Same constant values
- Same mass values (AME03)



Difference < 7×10^{-11}