NRS Agent: Data Analysis Agent System for Nuclear Resonant Scattering

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Talk outline

- Motivation & problem statement
- NRS experiments & typical data products
- Analysis softwares: CONUSS & PHOENIX
- NRS Agent: architecture, agents, & end-to-end workflow
- Parameter control & high-throughput parallel analyses (core advantage)
- Example: HEPS ID33 (B5) beamline CONUSS kctl fit
- Next steps

Motivation: why we need NRS Agent

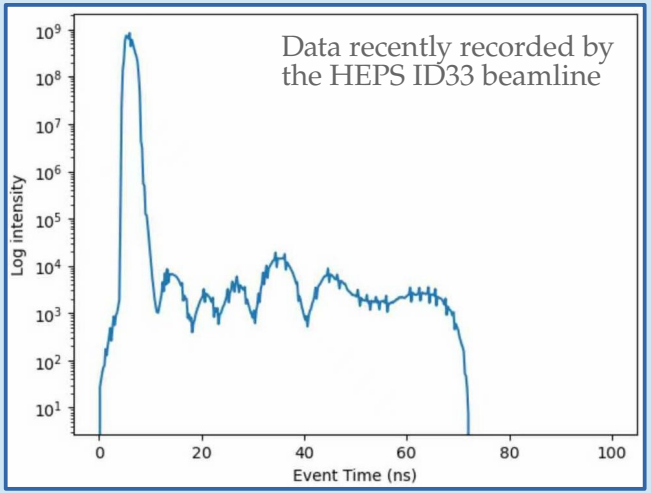
- **Constraints of beamline analysis:**
  - **Time pressure during beamtime:**
    Decisions must be made quickly
  - **High complexity:**
    Many steps, many configuration parameters, many intermediate files
  - **High-dimensional analyses:**
    Many coupled parameters; manual search is slow
- **Goal of NRS Agent:**
  - **Reduce manual effort & errors**
  - **Speed up analysis & model exploration**
  - **Standardize outputs for reproducibility & comparison**

NRS: what is measured?

Nuclear Resonant Scattering (NRS):
Resonant interactions with nuclei excited by synchrotron X-ray pulses.

Two major analysis domains supported in this project:

- Coherent nuclear resonant scattering (time/energy domain):
  Sensitive to hyperfine interactions, texture, thickness, instrumental resolution, time-zero shift, etc.
- Nuclear Resonant Inelastic X-ray Scattering (energy domain):
  Energy-domain spectra used to derive phonon density of states (DOS) & thermodynamic quantities



Why it is challenging:

- Many physical + instrumental effects involved → many fit parameters
- Data plausibly explained by many model variants

Analysis softwares: where CONUSS and PHOENIX fit

NRS Agent integrates two standard toolchains:

- CONUSS: coherent nuclear resonant scattering modeling and fitting
- PHOENIX: NRIXS pipeline → phonon DOS → derived physical quantities

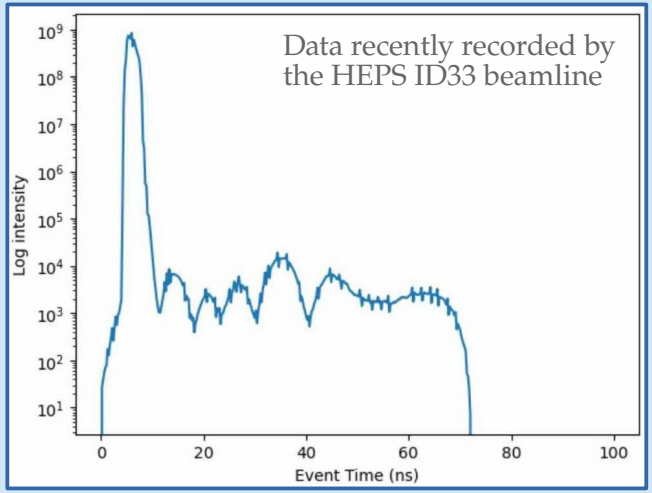
Why tool integration matters:

- Iteration & model comparison produce many artifacts that must be tracked consistently
- Both require structured configuration (SIF/MIF files) and multi-step execution

NRS Agent pipeline diagram

CONUSS: what it does

CONUSS (COherent NUclear resonant Scattering by Single crystals)



Executables integrated in NRS Agent:

- **Kfor :** Computes transmission amplitudes from material definition
- **Kmix** : Computes scattered intensities
- **Kfit** : Fits calculated intensities to measured data
- **Kctl** : Orchestrates fit optimization

What scientists typically use it for:

- Fit NRS data to physical models
- Extract parameters like thickness, hyperfine field, ...
- Quantify fit quality & uncertainties/correlations

PHOENIX: what it does

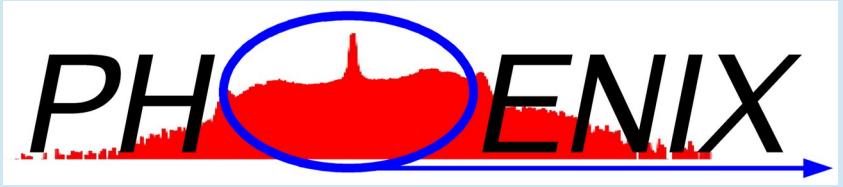
PHOENIX (PHOnon Excitation by Nuclear resonant Inelastic X-ray scattering)
NRIXS analysis

Pipeline integrated in NRS Agent:

- **padd** : Prepares/accumulates (energy, counts) data pairs
- **phox** : Computes phonon density of states (DOS)
- **psth** : Computes thermodynamic quantities from DOS (e.g., kinetic energy, vibrational entropy, etc.)
- **psvl :** Computes Debye sound velocity & related quantities

Key feature:

- Multi-step & configuration-heavy, like CONUSS



NRS Agent: goal and scope

NRS Agent:

Multi-agent assistant that executes end-to-end NRS workflows via analysis tools.
Entirely based on Dr. Sai framework

Core capabilities (today):

- HDF5/Nexus inspection + TXT inspection
- HDF5 → CONUSS-formatted TXT conversion
- CONUSS: SIF/MIF creation + kctl fitting + artifact collection
- PHOENIX: SIF creation + padd → phox → psth → psvl execution
- Plotting measured/fitted/residual data

Deployed architecture

Three-tier architecture:

- **Frontend: Dr. Sai UI**

  Multimodal chat: shows text + output plots

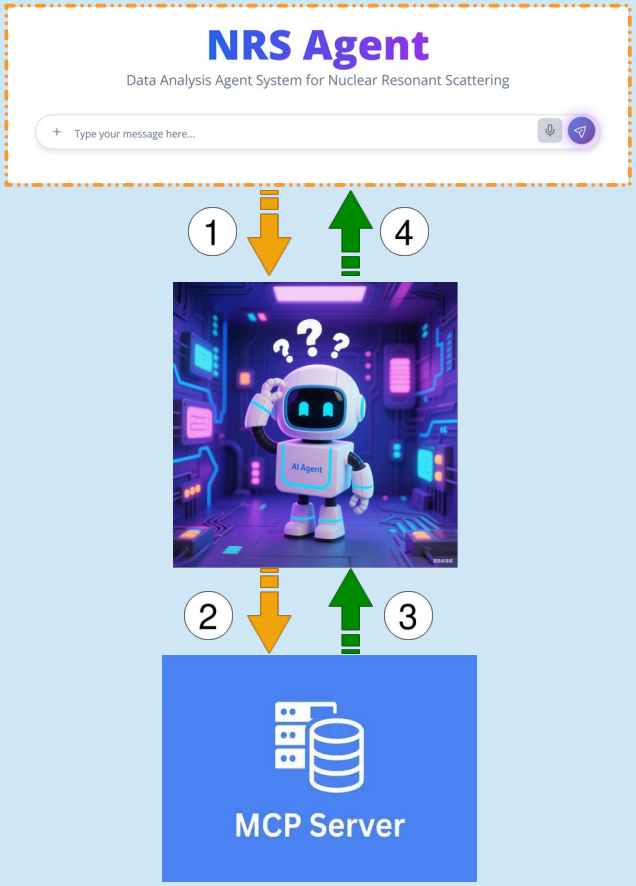
  Users can download produced files/plots

- **Backend: NRS Agent service**

  Based on DrSaiAgent; Addresses input tasks

- **Tool layer: MCP Server**

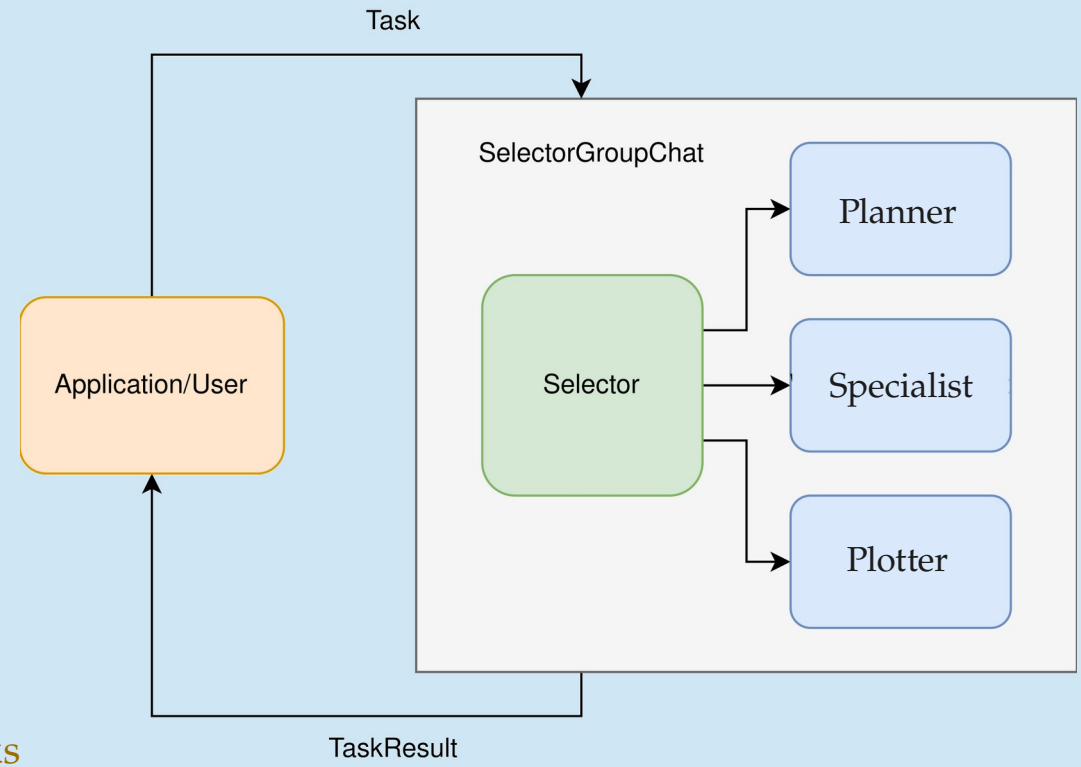
  Based on HaiMCP



NRS Agent internal structure

Current agents:

1. Planner Agent
2. File Inspection Agent
3. HDF5-TXT Converter Agent
4. CONUSS SIF/MIF Writer Agent
5. CONUSS Analysis Agent
6. PHOENIX SIF Writer Agent
7. PHOENIX Analysis Agent
8. Plotter Agent



Division of labor:

- Planner decides steps
- Specialists execute tool-grounded subtasks
- Plotter standardizes visualization for rapid interpretation

Parameter control & reproducibility

A key project outcome: broad parameter control.

CONUSS coverage:

- **User controls 86 CONUSS parameters across kfor / kmix / kfit / kctl / Fe.mif**
- **Supports 18 fit-promotable parameters:**

  Thickness, Bhf, theta/phi, texture, background, …

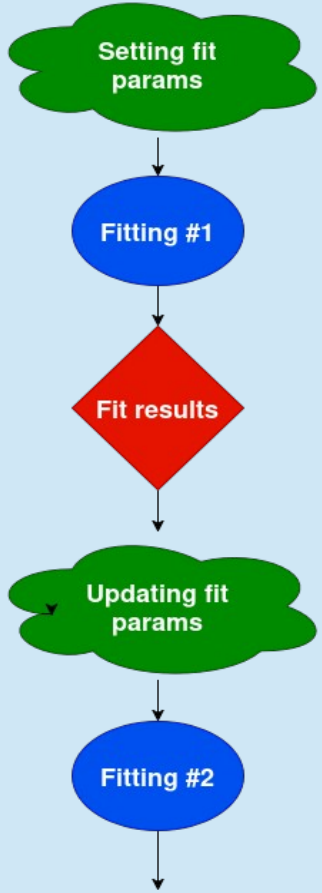
Impact:

- **Controlled, repeatable studies by changing a defined subset of parameters.**
- **Automated comparison across many configurations / datasets.**

“Wise” iteration: not random trial-and-error

A key feature during fitting/model exploration:

- Read and interpret fit outputs from each iteration
- Detect lack of improvement or instability
  (e.g., strong correlations, unrealistic parameter jumps)
- Decide the next configuration intentionally:
  - adjust which parameters are promoted to fit parameters vs kept fixed
  - update initial guesses based on previous fitted values
  - tighten/relax constraints and ranges when appropriate
  - run multiple candidate configurations in parallel and select the best



High-throughput batch analyses (main advantage for scientists)

NRS Agent supports parallel orchestration of:

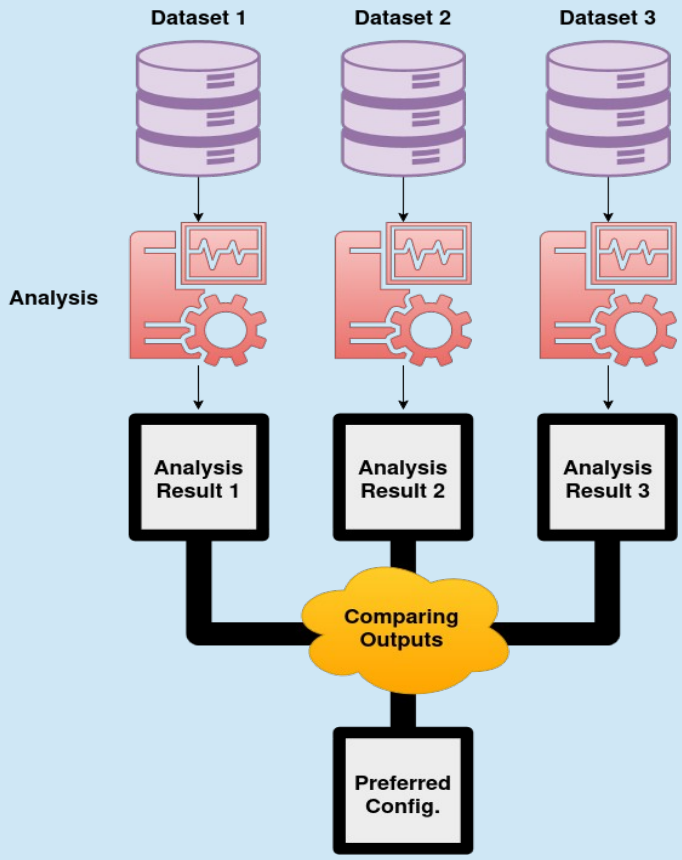
- Multiple datasets
- Multiple physical configurations

Then it can:

- Collect standardized outputs
- Compare configurations across datasets
- Report the most supported physical configuration(s)

Why this matters:

- Facilitates “model selection by comparison”
- Speeds up decision-making & reduces operator bias



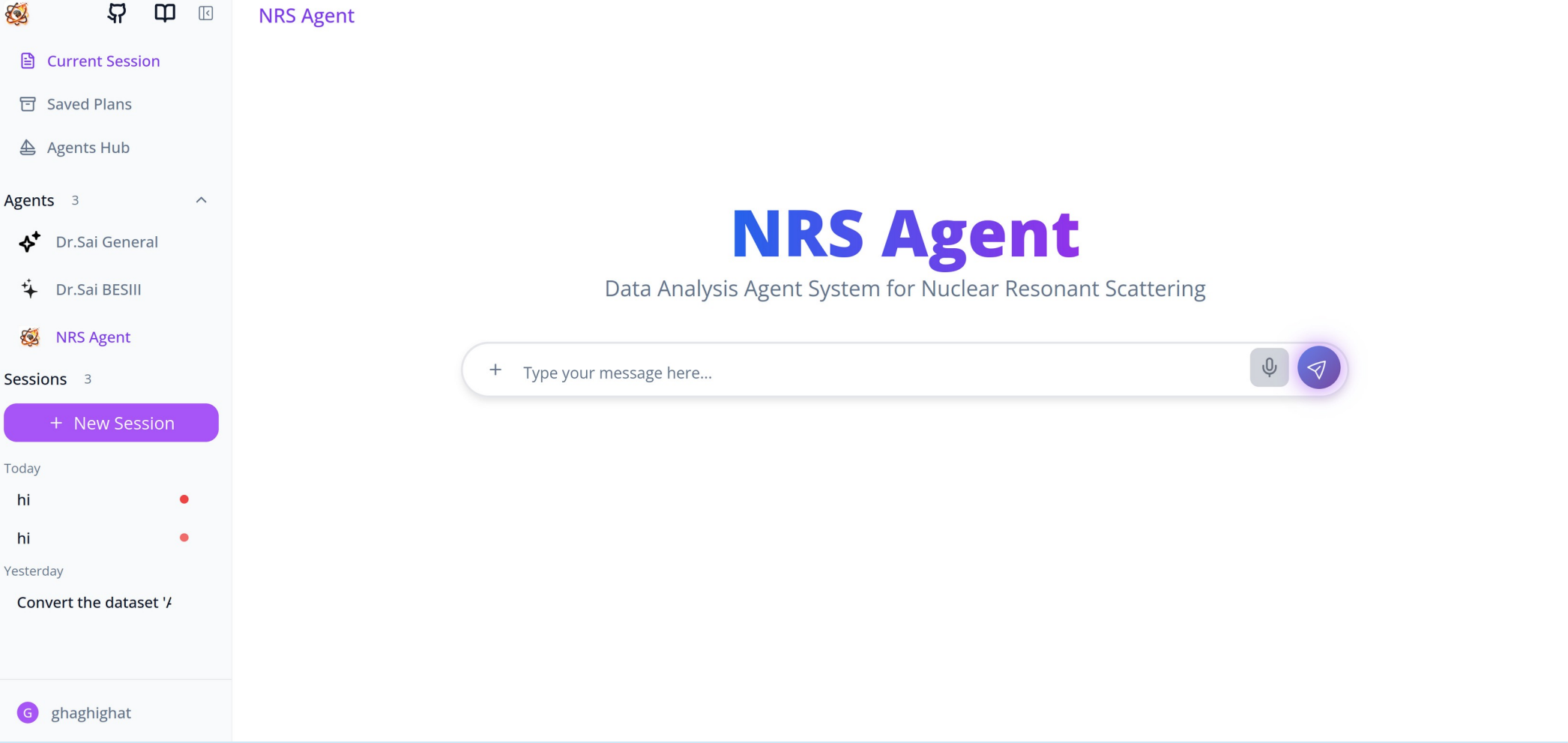
Example: HEPS ID33 (B5) CONUSS kctl fit

Task to NRS Agent:

- Convert HDF5 data to TXT
- Perform time calibration using ...
- Mask time ranges ...
- Promote ... as fit parameters
- Run CONUSS kctl with defaults except ...
- Report / plot output

Representative output:

- $Chi^2 \approx$ ...
- Fitted values: ...
- Outputs: logs, iteration, exp/fit/residual, best-fit SIF/MIF


NRS Agent
Current Session
Saved Plans
Agents Hub
Agents 3
Dr.Sai General
Dr.Sai BESIII
NRS Agent
Sessions 3
New Session
Today
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Convert the dataset '/
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NRS Agent
Data Analysis Agent System for Nuclear Resonant Scattering
Type your message here...

Current Session
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NRS Agent

Sessions 1
+ New Session

Today
Convert the data

Convert the dataset 'APD3' in the measured data file /home/hossein/exp_data/B5_data.nxs to txt and perform a CONUSS kctl analysis on the converted data assuming that the scatterer material is iron. For the parameters of the kctl analysis, use default values except for shift of the time scale = -5.9582E+00, scaling factor = 5.4279E+03, time or energy distribution FWHM = 8.8108E-01, material thickness = 1.2317E+01, Bhf = 3.2465E+01, Bhf angle theta range = [0,90], Bhf angle theta = 8.2990E+01, Bhf angle phi range = [-90,90], Bhf angle phi = 6.4229E+01, Texture coefficient range = [0,100], Texture coefficient = 2.6001E+01. Treat the parameters: shift of the time scale, scaling factor, time or energy distribution FWHM, material thickness, as the fit parameters and others as the fixed parameters. Use the coefficient 100/450 for calculating image times and mask the data time ranges 0-20 and 69-100. Plot the measured, fitted, and residuals data generated by the CONUSS kctl analysis.

planner_agent

1. file_inspection_agent: Inspect `/home/hossein/exp_data/B5_data.nxs` to find the exact internal HDF5 path of dataset `APD3` (and confirm it is 3D with shape (X,Y,Z)).
2. hdf5_txt_converter_agent: Convert the `APD3` 3D dataset in `/home/hossein/exp_data/B5_data.nxs` to txt using:
   - `coefficient_to_calculate_image_time = 100/450`
   - `masked_ranges = [[0,20],[69,100]]`
   - output prefix: `B5_APD3_masked`
3. CONUSS_SIF_MIF_writer_agent: Create a full CONUSS **kctl** input set (Fe MIF + kfor/kmix/kfit/kctl SIFs) using default values except:
   - kfit SIF: `shift_of_time_or_energy_scale = -5.9582E+00` (fit parameter=True)
   - kfit SIF: `scaling_factor = 5.4279E+03` (fit parameter=True)
   - kfit SIF: `time_or_energy_distribution_FWHM = 8.8108E-01` (fit parameter=True)

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暂无文件事件（message_files / FilesEvent）

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NRS Agent

Sessions 1
+ New Session

Today
Convert the datas

CONUSS_analysis_agent

Created (grace-format) CONUSS kctl outputs:

- Protocol: **/home/agent/APD3_kctl_ptl.txt**
- Measured: **/home/agent/APD3_exp.dat**
- Best fit: **/home/agent/APD3_fit.dat**
- Residuals: **/home/agent/APD3_rsd.dat**
- Results/iterations: **/home/agent/APD3_kctl.csv**

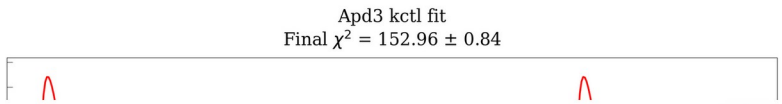
Fit results (fit parameters):

- Material thickness = **1.2317E+01 ± 1.1E-01**
- Scaling factor = **5.4279E+03 ± 8.3E+01**
- Time shift (ns) = **-5.9580E+00 ± 1.8E-01**
- FWHM resolution (ns) = **8.8103E-01 ± 2.3E-01**

Normalized Chi² = **152.96 ± 0.84**

I am using tools: plot_MFR_data

Here is the generated plot:



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source: plotter_agent type: FilesEvent time: 4/14/2026, 7:55:22 PM

Output file
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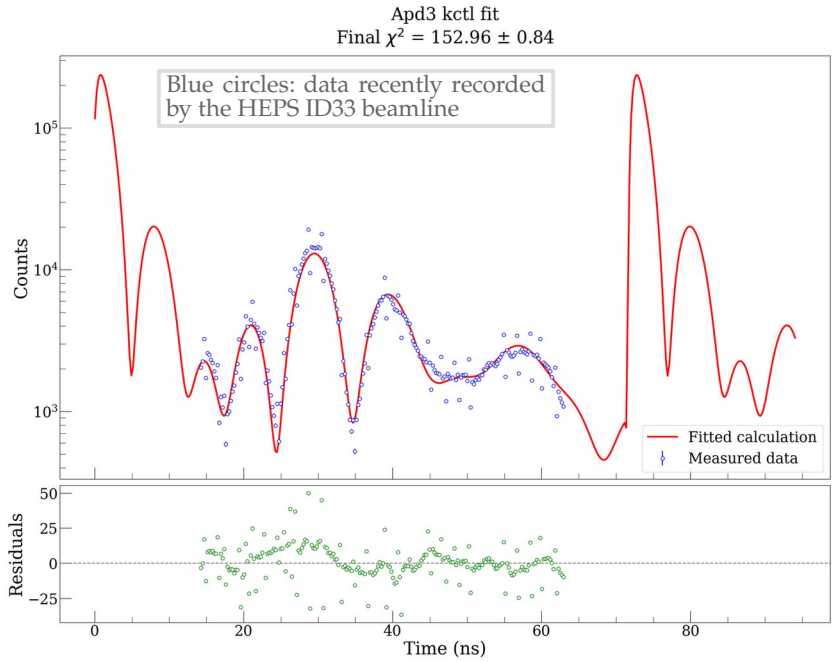
Today
Convert the datas

Here is the generated plot:



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source: plotter_agent type: FilesEvent time: 4/14/2026, 7:55:22 PM

Output file
Generated by Agent
URL
打开 / 下载

Current status

- Integrated with Dr. Sai UI (multimodal outputs; plots displayed; files downloadable)
- End-to-end tool execution via MCP, with improved validation and error handling
- Supports both HDF5 inputs and user-provided TXT measured data
- Supports batch preparation of multiple SIF/MIF sets for parallel CONUSS kctl analyses
- Supports PHOENIX pipeline with SIF generation for padd/phox/psth/psvl

Heading to the initial user acceptance test

Next steps

- Add new capabilities based on scientists' needs: enrich material library, add tools, ...
- OAuth 2.0 authorization for MCP service
- Further extend the batch mode

Many thanks to
the IHEP AI group for providing the software infrastructure and assistance
and
the HEPS ID33 (B5) beamline for the data and all the fruitful comments.

And special thanks to you for your attention!
Feel free to ask questions

Backup Slides

BACKUP SLIDE A — CONUSS outputs captured by the agent

- kctl protocol/log file
- Measured (exp), fitted (fit), residual (rsd) files
- Power spectra files (exp/fit/rsd)
- Iteration/results table
- Error ellipse outputs + correlation matrices
- Best-fit snapshots of SIFs and MIFs

BACKUP SLIDE B — Fit-promotable parameters (18 supported)

- Isomer shift
- Magnetic hyperfine field (Bhf)
- Magnetic field direction angles (theta, phi)
- Quadrupole splitting
- Asymmetry parameter
- Euler angles alpha/beta/gamma
- Texture coefficient
- Thickness of the material
- Time structure of SR
- Scaling factor
- Shift of energy/time scale
- Constant background
- Energy/time resolution FWHM
- Thickness distribution FWHM
- Center of thickness/angle distribution

BACKUP SLIDE C — HDF5→TXT conversion details (B5-style)

- Read 3D dataset (X, Y, Z)
- Integrated intensity per image: sum over spatial axes → length Z
- Time for image N: time = N × coefficient
- Output TXT: header + two columns (time, intensity)
- Masked time ranges supported
- Parallelization at file level

BACKUP SLIDE D — OAuth plan for MCP

Goal: protect tool execution and data access when deployed for multiple users.

Standards to comply with:

- RFC 9728: OAuth 2.0 Protected Resource Metadata
- RFC 8707: OAuth 2.0 Resource Indicators
- RFC 7662: OAuth 2.0 Token Introspection

Flow summary:

- Client obtains token from AS
- Client calls RS (MCP resources) with token
- RS introspects token with AS before granting access

BACKUP SLIDE E — References

- MCP: https://modelcontextprotocol.io/
- RFC 7662: https://www.rfc-editor.org/rfc/rfc7662
- RFC 8707: https://www.rfc-editor.org/rfc/rfc8707
- RFC 9728: https://www.rfc-editor.org/rfc/rfc9728