

NRS Agent: An AI Agent for End-to-End Nuclear Resonant Scattering Data Analysis at HEPS



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Talk outline

1 Nuclear Resonant Scattering (NRS)

NRS Agent

2

3 Advantages of the NRS Agent

Example agent output

4

Nuclear Resonant Scattering (NRS):

Resonant interactions with nuclei excited by synchrotron X-ray pulses

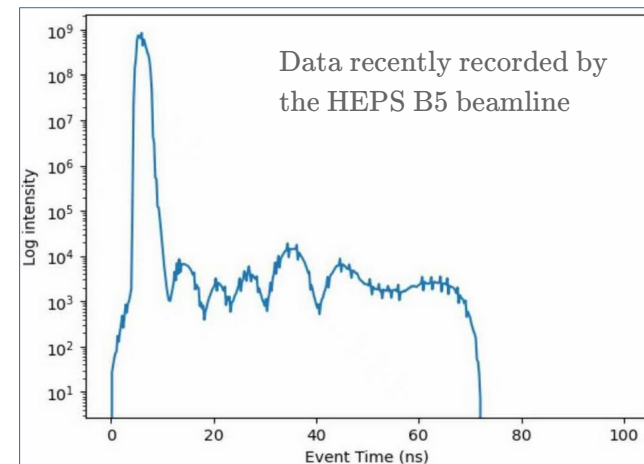
Two major NRS domains:

- **Coherent nuclear resonant scattering:**

Study hyperfine interactions (magnetic/electric fields at the nucleus)

- **Nuclear Resonant Inelastic Scattering (NRIXS):**

Find phonon density of states (DOS) and thermodynamic properties



Both domains supported by the NRS Agent

- **High complexity of NRS analyses**

Many steps, many configuration parameters, many intermediate files

- **High dimensionality of NRS analyses**

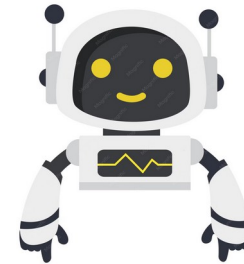
Many parameters involved in a single analysis

- **Time pressure**

Decisions must be made quickly

NRS Agent:

- **Reduces manual effort & errors**
- **Speeds up analysis**



NRS Agent

Data Analysis Agent System for Nuclear Resonant Scattering

+ Type your message here...



Three-tier architecture:

- **Frontend: OpenDrSai UI**

Multimodal chat: shows text + output plots

- **Backend: NRS Agent service**

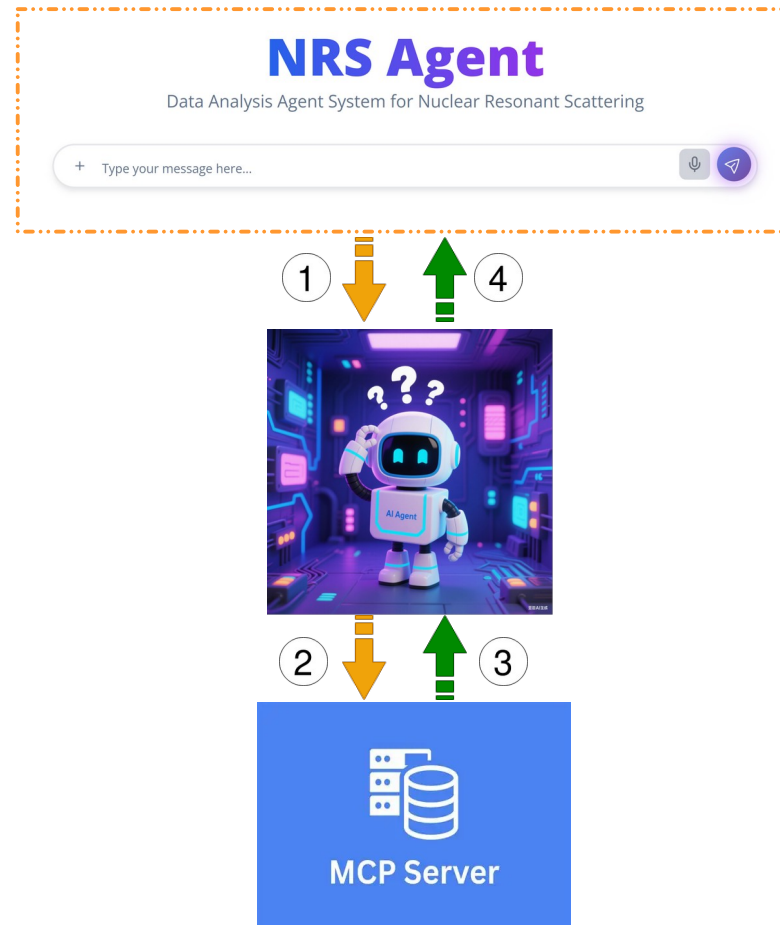
Based on DrSaiAgent; Addresses input tasks

- **Tool layer: MCP Servers**

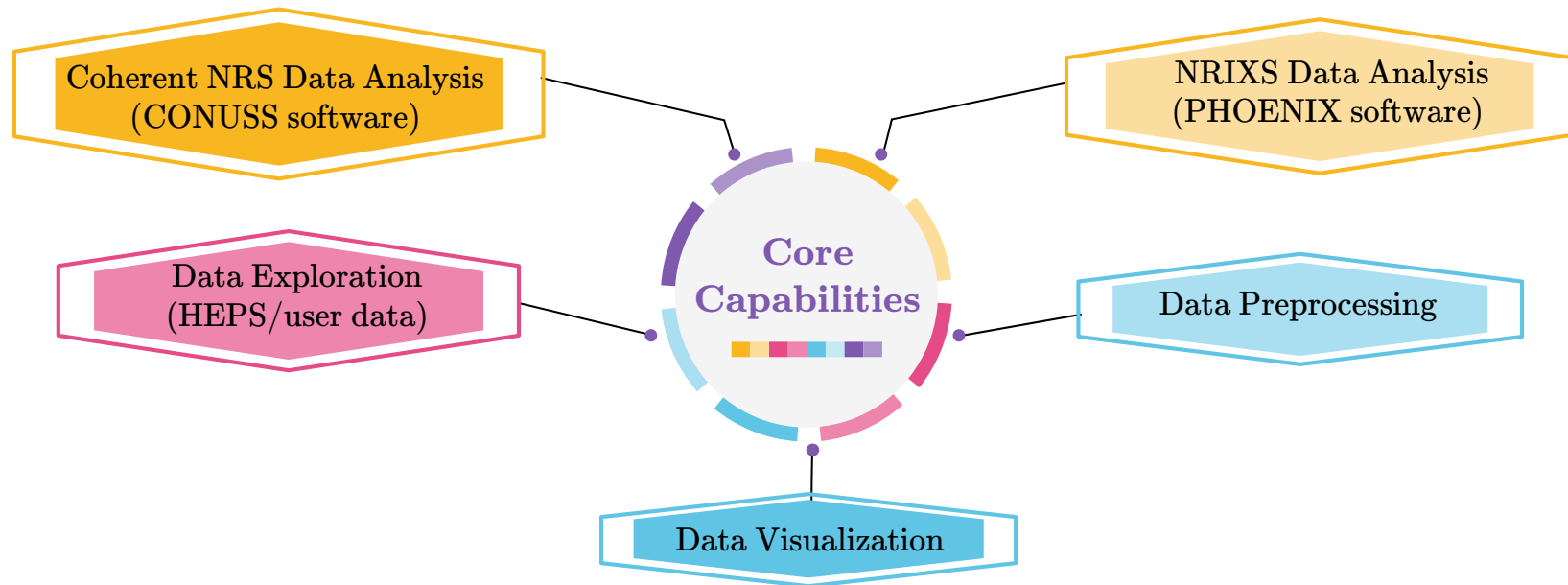
Analysis MCP server + HEPSDAS MCP server

Based on HaiMCP

Entirely based on Dr. Sai framework



NRS Agent: Multi-agent system that executes end-to-end NRS workflows



NRS Agent integrates CONUSS with PHOENIX toolchains:



CONUSS (COherent NUclear resonant Scattering by Single crystals)

Executables integrated in NRS Agent:

- **kfor** : Computes transmission amplitudes
- **kmix** : Computes scattered intensities
- **kfit** : Fits calculated intensities to measured data
- **kctl** : Orchestrates fit optimization



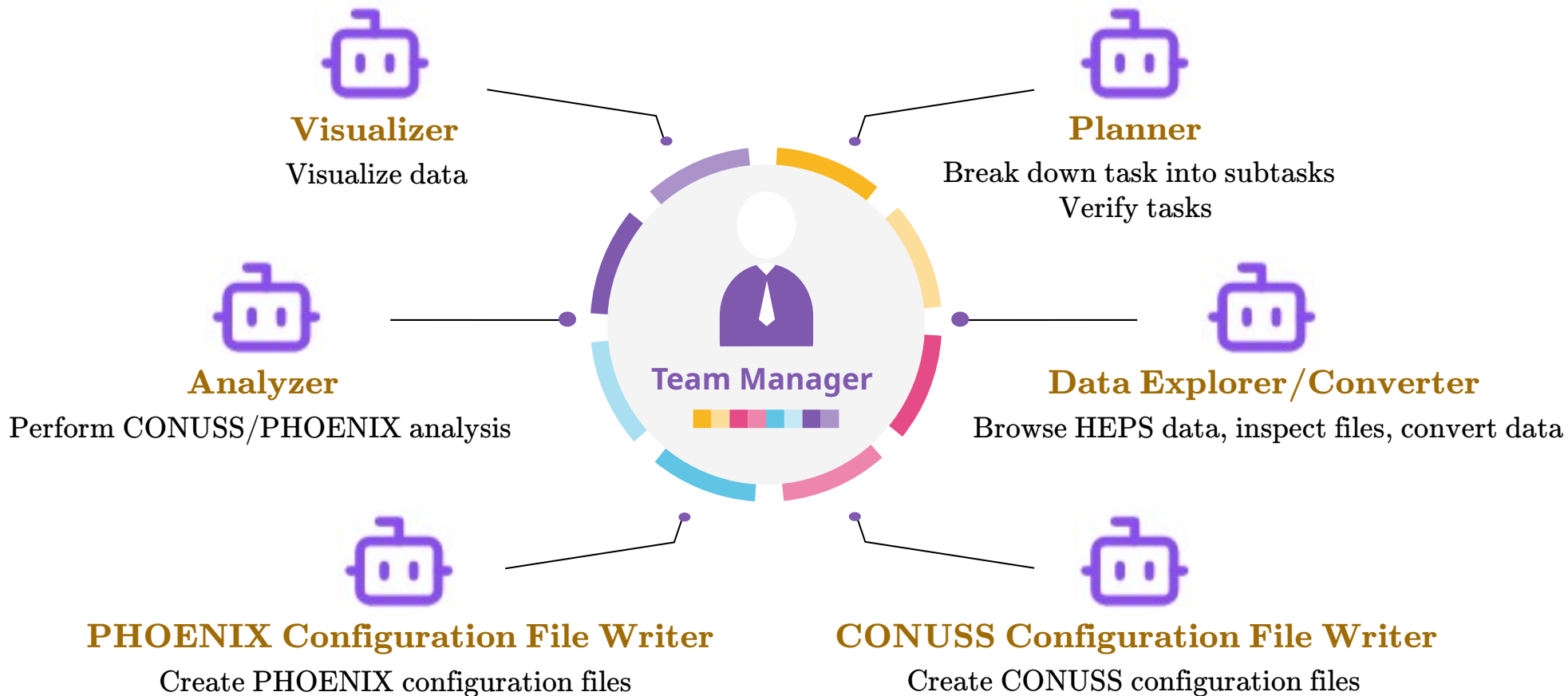
- Fit NRS data to physical models
- Extract physical quantities
- Quantify fit quality & correlations

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

Executables integrated in NRS Agent:

- **padd** : 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





Integration with HEPS Data Service Platform



NRS Agent



HEPS Data Service
MCP Server

HEPS Data Access

- System & Beamline Statistics (Public)
- Beamtime Management (Authorized users)
- Dataset & File Queries (Authorized users)
- File Directory Browsing (Authorized users)

OpenDrSai

NRS Agent

planner_agent

Here are the system overview statistics:

Field	Value
Dataset Count	101102
Proposal Count	2915
Download Data Volume	299TB
Beamline Count	15
Total Data Volume	748TB
File Count	41746271
Beamtime Count	807

Source: get_system_statistics

OpenDrSai

NRS Agent

hours	dataVolume	name	files	id	datasets	proposals
47	108GB	通用环境谱学线站	67753	80444	3687	185
106	60.3TB	生物大分子液晶衍射线站	4750173	ID02	8689	143
47	4.4TB	低维结构衍射线站	810854	ID05	6875	168
83	34.5TB	工程材料线站	170009	ID07	15542	386
55	4.3TB	粉光小角散射线站	67938	ID08	8706	204
18	23.1TB	硬X射线纳米衍射线站	457804	ID09	3181	90
4	21.2TB	硬X射线纳米探针线站	762185	ID19	14281	110
50	483.9TB	硬X射线成像线站	3022666	ID21	1719	159
40	34.4TB	结构动力学线站	25189882	ID23	1476	180
58	42.8TB	X射线显微成像线站	4659060	ID30	1413	189
65	5.0TB	高压线站	136990	ID31	1580	261
18	599GB	高分辨谱学线站	64149	ID33	14194	172
20	172GB	高分辨率电子结构线站	888	ID41	487	75
61	5.0TB	光学测试线	196710	ID42	11932	12
86	133GB	X射线吸收谱学线站	79131	ID46	4340	569

Parameter Coverage

CONUSS

95 parameters

composition	euler angle alpha (for efg=>xtal)	knix run mode	measured-data interpretation mode
density	euler angle beta (for efg=>xtal)	scan/tldi mode	output file prefix (+ optional output format)
isotope data file	euler angle gamma (for efg=>xtal)	time structure of synchrotron radiation	start of thickness/angle range
abundance	relaxation input file	incident x-ray degree of polarization	end of thickness/angle range
LM factor	distribution input file	incident x-ray mixing angle	start of time/energy range
Number of sites	weight is a fit parameter	incident x-ray canting angle	end of time/energy range
Site name	Bhf is a fit parameter	polarization filter efficiency	thickness/angle distribution function
sublattice weight	Bhf direction polar angle is a fit parameter	scattered x-ray mixing angle	time/energy distribution function
Bhf	Bhf direction azimuthal angle is a fit parameter	scattered x-ray canting angle	constant background
range of Bhf	isomer shift is a fit parameter	Debye-Waller factor	scaling factor
Bhf direction polar angle	quadrupole splitting is a fit parameter	non-ergodicity factor	shift of time or energy scale
range of Bhf direction polar angle	asymmetry parameter is a fit parameter	intensity distribution function width	thickness/angle distribution FWHM
Bhf direction azimuthal angle	euler angle alpha is a fit parameter	intensity distribution function shape	time/energy distribution FWHM
range of Bhf direction azimuthal angle	euler angle beta is a fit parameter	energy range of calculation	create rocking curves
texture coefficient	euler angle gamma is a fit parameter	material thickness	rocking curve position
range of texture coefficient	euler angle delta is a fit parameter	material thickness is a fit parameter	scaling factor is a fit parameter
isomer shift	texture coefficient is a fit parameter		shift of time or energy scale is a fit parameter
range of isomer shift			
quadrupole splitting			
asymmetry parameter			

PHOENIX

55 parameters

Operating X-ray Energy	Deconvolution Settings
Sample Temperature (PADD)	Fitting Parameters
Monochromator Lattice Constant	PSTH Transition Energy
Thermal Expansion Coefficient	PSTH Recoil Energy
First Monochromator Reflection	Temperature Range
Second Monochromator Reflection	Energy Range
Energy Axis Scaling Options	PSTH Output Prefix & Format
PADD Output Prefix & Format	PSTH Resolution FWHM
Comment Character	PSTH Resolution Shape
PADD Fit Range	PSTH Resolution Asymmetry
PADD Inelastic Background	PSTH Elastic Peak Strength
PADD Resolution Asymmetry	Resonant Isotope Mass
PADD Resolution Function	Sample Pressure
Measured Data File Format	Equation of State Type
Data Column Definitions	Ambient Density
PADD SIF Output Path	Bulk Modulus
PHOX Transition Energy	Bulk Modulus Pressure Derivative
PHOX Recoil Energy	Sound Velocity Window Start
PHOX Sample Temperature	Sound Velocity Window Width
Data Background Corrections	Fit Parameter p1
PHOX Output Prefix & Format	Fit Parameter p2
PHOX Fit Range	PSVL Fit Function Type
PHOX Inelastic Background	
PHOX Left/Right Asymmetry	
PHOX Resolution Function	

Broad parameter control

- Enhanced Flexibility and Customization
- Unbiased, Globally Optimized Fitting
- Automated contextual calibration
- Seamless Cross-Module Consistency
- Adaptive file and format management

```

0 Weight1 := 1.0
% 0 Bhf1 := 32.4
% 0 [0.0-90.0] Theta1 := 83.0
% 0 [-90.0-90.0] Phi1 := 64.0
% 0 [0.0-100.0] Texture1 := 26.0
% 0 Iso1 := 0.0
% Weight2 := 1.0
% 0 Bhf2 := 32.4
% 0 [0.0-90.0] Theta2 := 83.0
% 0 [-90.0-90.0] Phi2 := 64.0
% 0 [0.0-100.0] Texture2 := 26.0
% 0 Iso2 := 0.0
(1) Composition :: Fe
(2) Density (g/cm^3) :: 8.0
(3) ME data file :: fe57.mbt
(4) Abundance of the ME atom :: 0.95
(5) Lamb-Mössbauer factor :: 0.796
(6) Number of sites of the ME atom :: 2
(7.1.1) Memo name for the site :: sites1
(7.1.2) Weight of the sublattice :: @Weight1
(7.1.3) Isomer shift (mm/s) :: @Iso1
(7.1.4) Bhf (T) :: @Bhf1
(7.1.5) Bhf angle theta (deg) :: @Theta1
(7.1.6) Bhf angle phi (deg) :: @Phi1
(7.1.7) Quadrupole splitting (mm/s) :: 0.0
(7.1.8) Asymmetry parameter :: 0.0
(7.1.9) Euler angle alpha (deg) :: 0.0
(7.1.10) Euler angle beta (deg) :: 0.0
(7.1.11) Euler angle gamma (deg) :: 0.0
(7.1.12) Relaxation input file ::
(7.1.13) Distribution input file ::
(7.1.14) Texture coefficient (%) :: @Texture1
(7.2.1) Memo name for the site :: sites2
(7.2.2) Weight of the sublattice :: @Weight2
(7.2.3) Isomer shift (mm/s) :: @Iso2
(7.2.4) Bhf (T) :: @Bhf2
(7.2.5) Bhf angle theta (deg) :: @Theta2
(7.2.6) Bhf angle phi (deg) :: @Phi2
(7.2.7) Quadrupole splitting (mm/s) :: 0.0
(7.2.8) Asymmetry parameter :: 0.0
(7.2.9) Euler angle alpha (deg) :: 0.0
(7.2.10) Euler angle beta (deg) :: 0.0
(7.2.11) Euler angle gamma (deg) :: 0.0
(7.2.12) Relaxation input file ::
(7.2.13) Distribution input file ::
(7.2.14) Texture coefficient (%) :: @Texture2
    
```

```

(1) Project name :: NIS data analysis
(2) Material data input file :: A1_fe57.mf
(3) Transmission data output file :: A1_trsm.dat
(4) X-ray direction coordinates :: 0 0 1
(5) Energy range :: 5000
% (6) Material thickness :: 12

(1) Transmission data input file :: A1_trsm.dat
(2) Intensity data output file :: A1_ints.dat
(3) knix run mode :: time
(4) Scan/tldi mode ::
(5) Time structure of SR :: 72
(6) Unused ::
(7) X-ray polarization degree (%) :: 100
(8) Incident X-ray mixing angle (deg) :: 0
(9) Incident X-ray canting angle (deg) :: 0
(10) Polarization filter efficiency (%) :: 0
(11) Scattered X-ray mixing angle (deg) :: 0
(12) Scattered X-ray canting angle (deg) :: 0

(1) Intensity data input file :: A1_ints.dat
(2) Measured data input file :: A1_input_data.txt T1 C2
(3) Output file prefix :: AL_grace_grace
(4) Start of thickness/angle range ::
(5) End of thickness/angle range ::
(6) Start of time/energy range ::
(7) End of time/energy range ::
(8) Thickness/angle distribution function ::
(9) Time/Energy distribution function :: exponential 2 0.3
(10) Constant background :: 0
% (11) Scaling factor :: 5000
% (12) Shift of time/energy scale :: 5.0
% (13) Thickness/angle distribution FWHM :: 0
% (14) Time/Energy distribution FWHM :: 0.08
(15) Thickness/angle position :: 0
(16) Create rocking curves [yes/no] :: no
(17) Rocking curve position :: 10

(1) kfor sif :: A1_kfor.sif
(2) knix sif :: A1_knix.sif
(3) kfit sif :: A1_kfit.sif
(4) Reference file ::
(5) Iteration steps :: 50
(6) Iteration stop quality :: 0.001
(7) Prior correlation file ::
    
```

High-throughput batch analyses (advantage)

NRS Agent supports parallel analyses

- Analyze multiple physical configurations
- Collect standardized outputs
- Compare results
- Report the most supported configuration

Why this matters:

- Facilitates “model selection”
- Speeds up decision-making

CONUSS_analysis_agent

All referenced CONUSS kctl analyses were completed successfully.

Analysis ID	normalized χ^2	Label text (verbatim)
A1	153.00 +- 0.84	Normalized χ^2 value:
A2	153.02 +- 0.84	Normalized χ^2 value:
A3	153.12 +- 0.84	Normalized χ^2 value:
A4	153.12 +- 0.84	Normalized χ^2 value:
A5	153.03 +- 0.84	Normalized χ^2 value:

Configuration Files

CONUSS_SIF_MIF_writer_agent

analysis number | path to created SIF/MIF

```
A1 | /home/agent/A1_Fe57_Fe_v2.mif | N/A
A1 | /home/agent/A1_kfor_v2.sif | kfor
A1 | /home/agent/A1_kmix_v2.sif | kmix
A1 | /home/agent/A1_kfit_v2.sif | kfit
A1 | /home/agent/A1_kctl_v2.sif | kctl

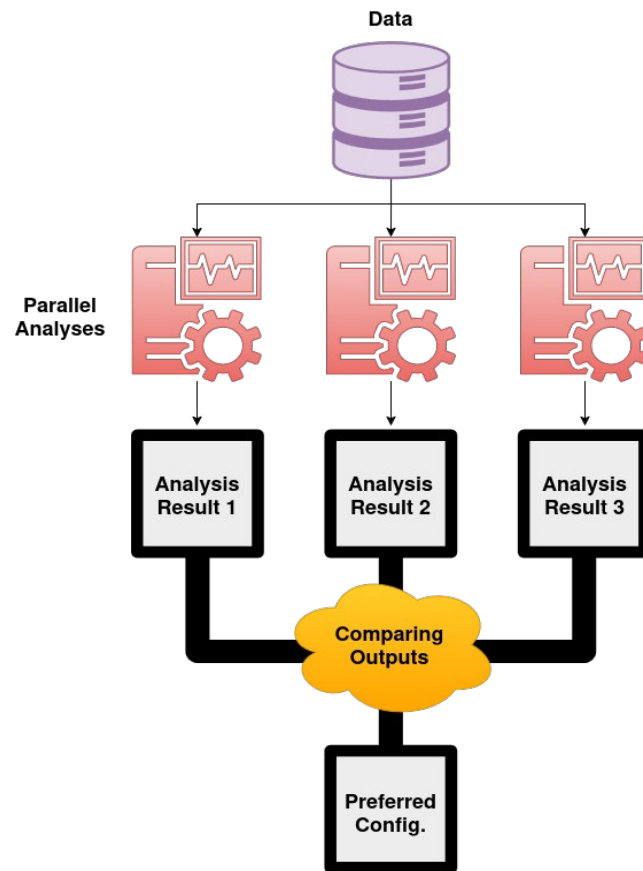
A2 | /home/agent/A2_Fe57_Fe_v2.mif | N/A
A2 | /home/agent/A2_kfor_v2.sif | kfor
A2 | /home/agent/A2_kmix_v2.sif | kmix
A2 | /home/agent/A2_kfit_v2.sif | kfit
A2 | /home/agent/A2_kctl_v2.sif | kctl

A3 | /home/agent/A3_Fe57_Fe_v2.mif | N/A
A3 | /home/agent/A3_kfor_v2.sif | kfor
A3 | /home/agent/A3_kmix_v2.sif | kmix
A3 | /home/agent/A3_kfit_v2.sif | kfit
A3 | /home/agent/A3_kctl_v2.sif | kctl

A4 | /home/agent/A4_Fe57_Fe_v2.mif | N/A
A4 | /home/agent/A4_kfor_v2.sif | kfor
A4 | /home/agent/A4_kmix_v2.sif | kmix
A4 | /home/agent/A4_kfit_v2.sif | kfit
A4 | /home/agent/A4_kctl_v2.sif | kctl

A5 | /home/agent/A5_Fe57_Fe_v2.mif | N/A
A5 | /home/agent/A5_kfor_v2.sif | kfor
A5 | /home/agent/A5_kmix_v2.sif | kmix
A5 | /home/agent/A5_kfit_v2.sif | kfit
A5 | /home/agent/A5_kctl_v2.sif | kctl
```

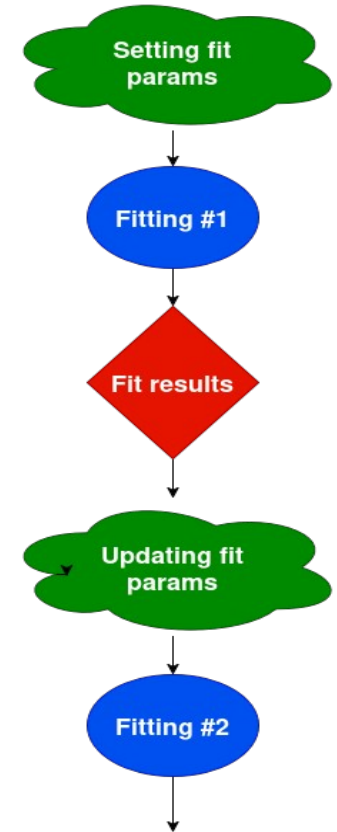
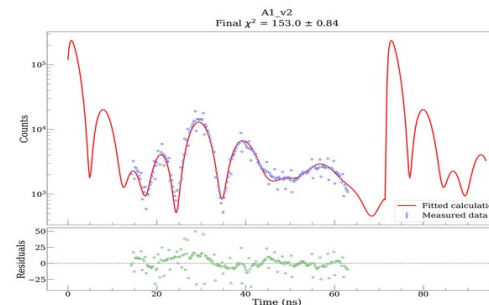
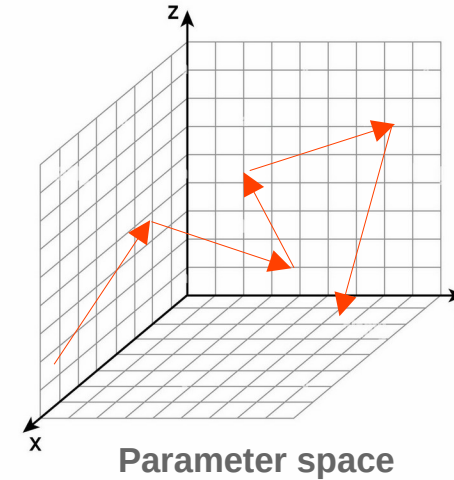
Outputs of parallel fits



“Wise” iteration: not random trial-and-error (advantage)

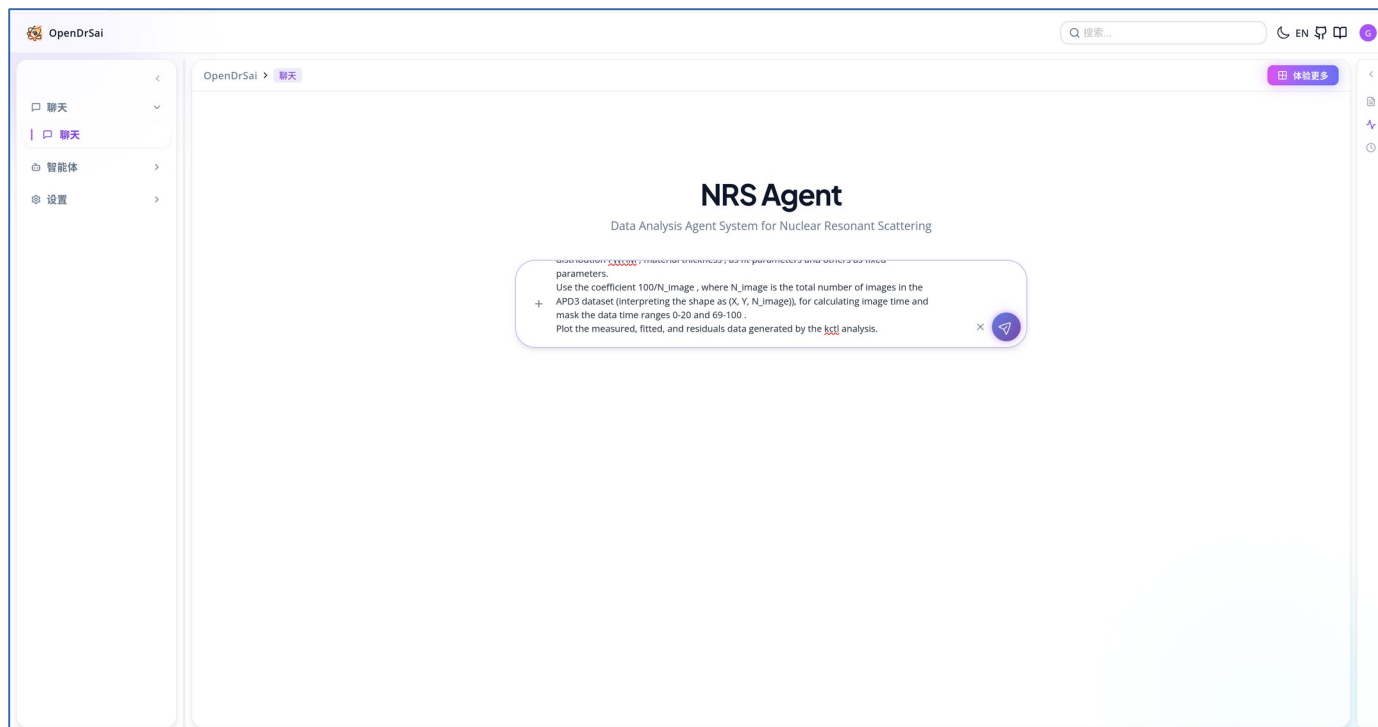
A key feature during fitting / model exploration

- **Read/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 fitted/fixed
 - ✓ Update initial guesses based on previous fitted values
 - ✓ Tighten/relax constraints and ranges when appropriate
 - ✓ Run multiple configurations in parallel and find the best



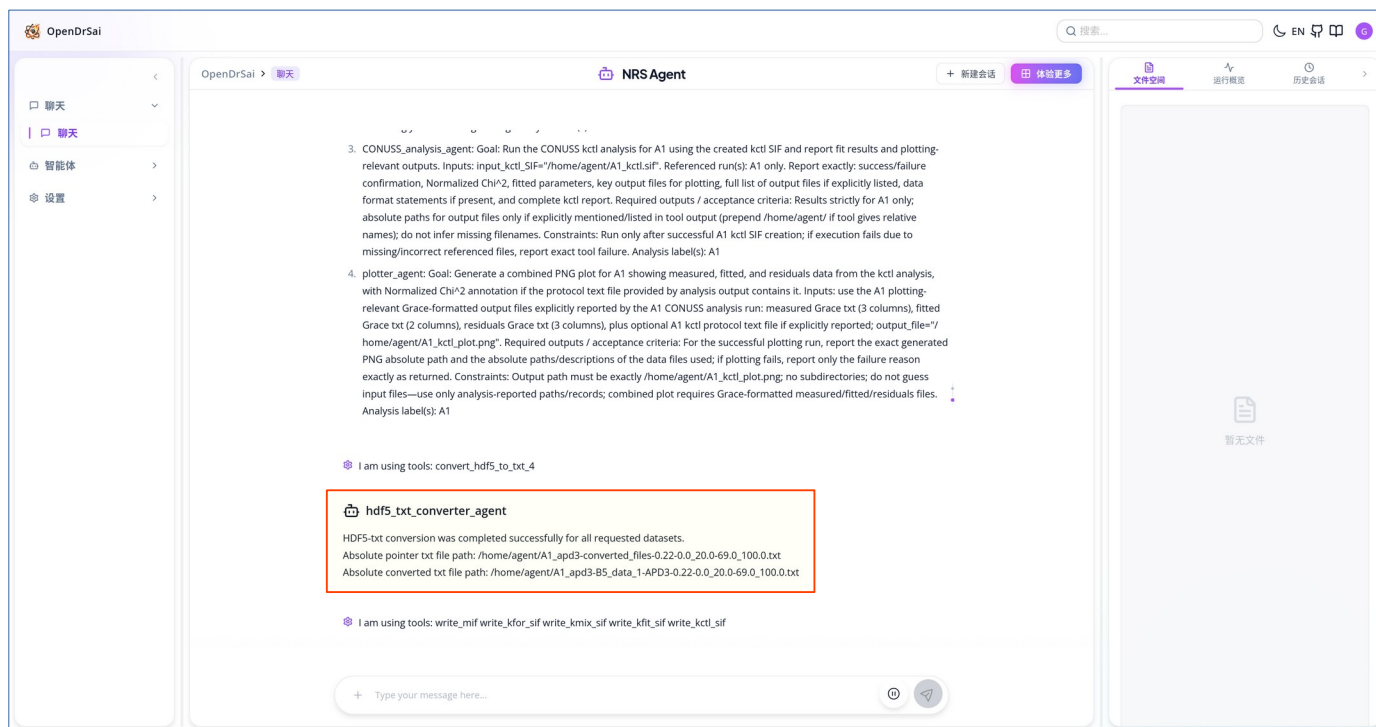
Task submitted to NRS Agent:

- Convert B5 data to analysis-ready data
- Perform CONUSS fit
- Report/plot best fit



Task submitted to NRS Agent:

- Convert B5 data to analysis-ready data
- Perform CONUSS fit
- Report/plot best fit



The screenshot displays the NRS Agent interface within the OpenDrSai environment. The main content area shows a list of tasks:

- 3. CONUSS_analysis_agent: Goal: Run the CONUSS kctl analysis for A1 using the created kctl SIF and report fit results and plotting relevant outputs. Inputs: input_kctl_SIF="/home/agent/A1_kctl.sif". Referenced run(s): A1 only. Report exactly: success/failure confirmation, Normalized $\chi^2/2$, fitted parameters, key output files for plotting, full list of output files if explicitly listed, data format statements if present, and complete kctl report. Required outputs / acceptance criteria: Results strictly for A1 only; absolute paths for output files only if explicitly mentioned/listed in tool output (prepend /home/agent/ if tool gives relative names); do not infer missing filenames. Constraints: Run only after successful A1 kctl SIF creation; if execution fails due to missing/incorrect referenced files, report exact tool failure. Analysis label(s): A1
- 4. plotter_agent: Goal: Generate a combined PNG plot for A1 showing measured, fitted, and residuals data from the kctl analysis, with Normalized χ^2 annotation if the protocol text file provided by analysis output contains it. Inputs: use the A1 plotting-relevant Grace-formatted output files explicitly reported by the A1 CONUSS analysis run: measured Grace txt (3 columns), fitted Grace txt (2 columns), residuals Grace txt (3 columns), plus optional A1 kctl protocol text file if explicitly reported; output_file="/home/agent/A1_kctl_plot.png". Required outputs / acceptance criteria: For the successful plotting run, report the exact generated PNG absolute path and the absolute paths/descriptions of the data files used; if plotting fails, report only the failure reason exactly as returned. Constraints: Output path must be exactly /home/agent/A1_kctl_plot.png; no subdirectories; do not guess input files—use only analysis-reported paths/records; combined plot requires Grace-formatted measured/fitted/residuals files. Analysis label(s): A1

Below the tasks, the agent reports tool usage:

- I am using tools: convert_hdf5_to_txt_4

A red box highlights the following tool output:

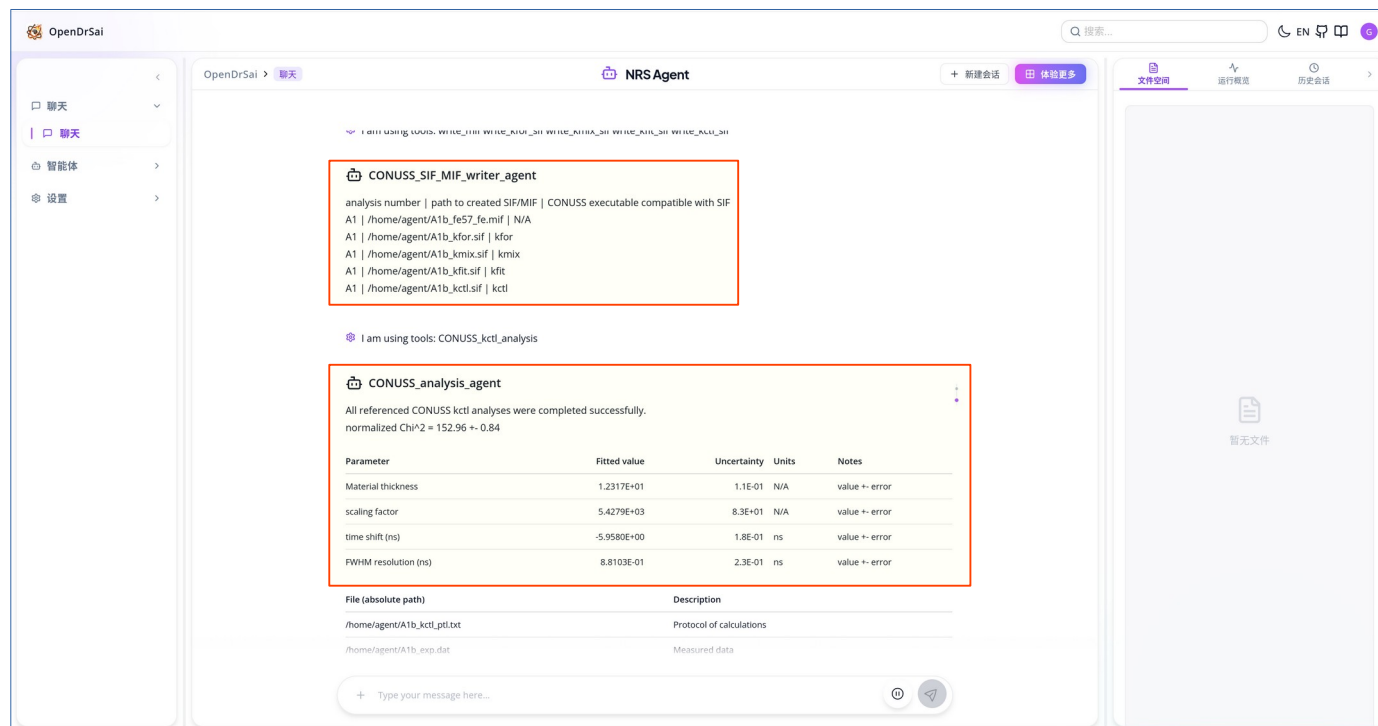
```
🔗 hdf5_txt_converter_agent
HDF5-txt conversion was completed successfully for all requested datasets.
Absolute pointer txt file path: /home/agent/A1_apd3-converted_files-0.22-0.0_20.0-69.0_100.0.txt
Absolute converted txt file path: /home/agent/A1_apd3-B5_data_1-APD3-0.22-0.0_20.0-69.0_100.0.txt
```

- I am using tools: write_mif write_kfor_sif write_kmix_sif write_kfit_sif write_kctl_sif

The interface includes a search bar, navigation icons, and a file management sidebar on the right.

Task submitted to NRS Agent:

- Convert B5 data to analysis-ready data
- Perform CONUSS fit
- Report/plot best fit



The screenshot displays the NRS Agent interface within the OpenDrSai environment. The main content area shows the output of a CONUSS fit analysis, which includes a list of generated SIF/MIF files and a table of fitted parameters.

CONUSS_SIF_MIF_writer_agent

analysis number | path to created SIF/MIF | CONUSS executable compatible with SIF
A1 | /home/agent/A1b_fe57_fe.mif | N/A
A1 | /home/agent/A1b_kfor.sif | kfor
A1 | /home/agent/A1b_kmix.sif | kmix
A1 | /home/agent/A1b_kfit.sif | kfit
A1 | /home/agent/A1b_kctl.sif | kctl

I am using tools: CONUSS_kctl_analysis

CONUSS_analysis_agent

All referenced CONUSS kctl analyses were completed successfully.
normalized $\chi^2 = 152.96 \pm 0.84$

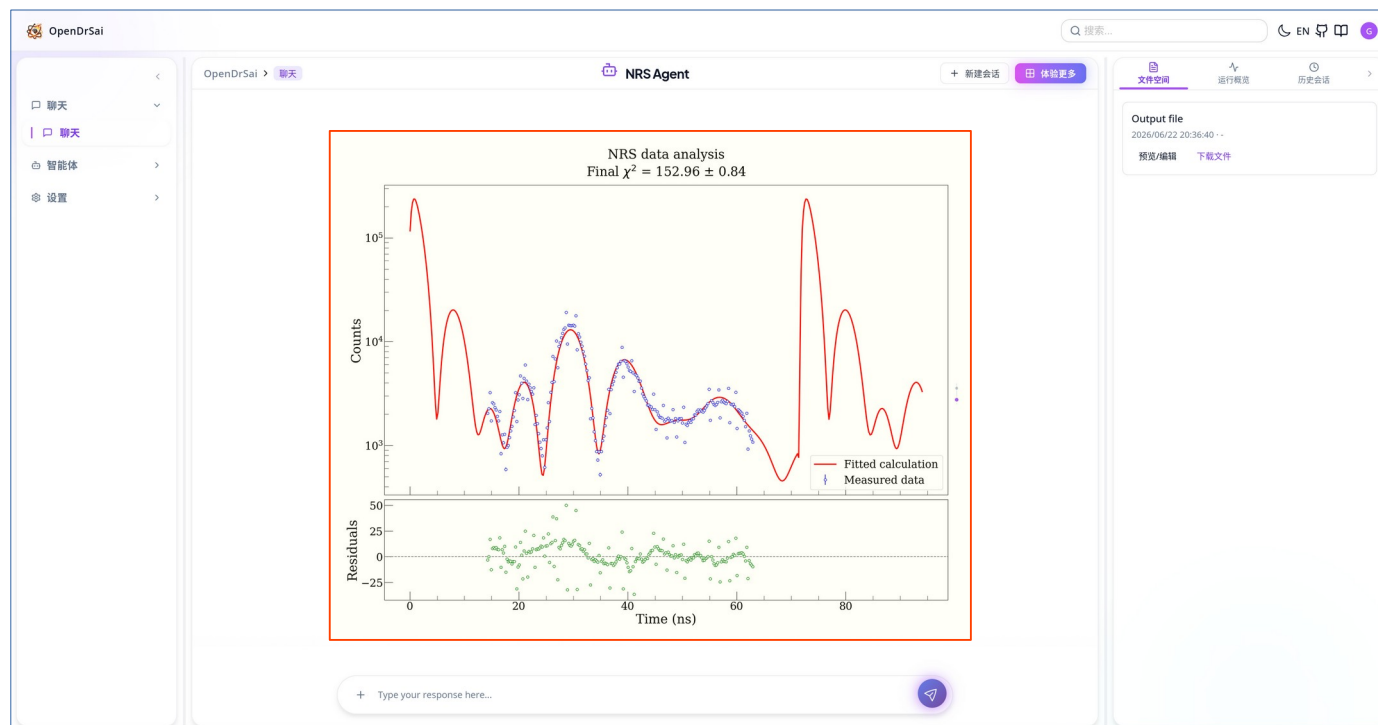
Parameter	Fitted value	Uncertainty	Units	Notes
Material thickness	1.2317E+01	1.1E-01	N/A	value +- error
scaling factor	5.4279E+03	8.3E+01	N/A	value +- error
time shift (ns)	-5.9580E+00	1.8E-01	ns	value +- error
FWHM resolution (ns)	8.8103E-01	2.3E-01	ns	value +- error

File (absolute path) | Description

/home/agent/A1b_kctl_ptt.txt	Protocol of calculations
/home/agent/A1b_exp.dat	Measured data

Task submitted to NRS Agent:

- Convert B5 data to analysis-ready data
- Perform CONUSS fit
- **Report/plot best fit**



- **Core architecture:** complete and stable
- **End-to-end processing:** verified for HEPS Nuclear Resonant Scattering data
- **Integration:** fully connected with existing backends
- **Output generation:** complete and operational
- **Authorization:** under final implementation
- **Performance testing:** ongoing (success/failure rate, time per dataset, concurrent job throughput, large datasets handling)

Heading to public deployment upon completion of performance testing

How to access the NRS Agent



The screenshot shows the OpenDrSai web interface. The browser address bar displays `opendr.sai.ihep.ac.cn/?menu=agent_square&view=chat`. The page title is "OpenDrSai" and the current view is "智能体广场" (Agent Square). A search bar is present with the text "搜索名称 / 描述 / 创建人". There are buttons for "+ 连接远程", "全部", "我的", "本地", "按最近使用", and "刷新".

The interface is divided into two main sections: "最近使用" (Recently Used) and "全部" (All). The "最近使用" section contains two cards:

- NRS Agent** (ghaghighat@ihep.ac.cn): Data Analysis Agent System for Nuclear Resonant Scattering. Button: 开始对话
- Rongzai Agent** (wanghao96@ihep.ac.cn): {"en": "Rongzai-Your neutron scattering data analysis assistant by CSNS data...". Button: 开始对话

The "全部" section contains five cards:

- NRS Agent** (ghaghighat@ihep.ac.cn): Data Analysis Agent System for Nuclear Resonant Scattering. Button: 开始对话
- Rongzai Agent** (wanghao96@ihep.ac.cn): {"en": "Rongzai-Your neutron scattering data analysis assistant by CSNS data...". Button: 开始对话
- Dr.Sai Synchrotron** (xiangdb@ihep.ac.cn): A general assistant for Synchrotron. Button: 开始对话
- DrSai_BESIII_v3.0** (zhangbolun@ihep.ac.cn): The AI agent for BESIII analysis. Button: 开始对话
- YuanYuan_Agent** (liqm@ihep.ac.cn): 源源——光源中子源衍射数据精修助手. Button: 开始对话

A large red arrow points to the "开始对话" button of the NRS Agent card in the "全部" section.



THANK YOU



Backup Slides

- **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**

- 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

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