Optimization of the neutron spectrum unfolding algorithm based on Tikhonov regularization and shifted Legendre polynomials

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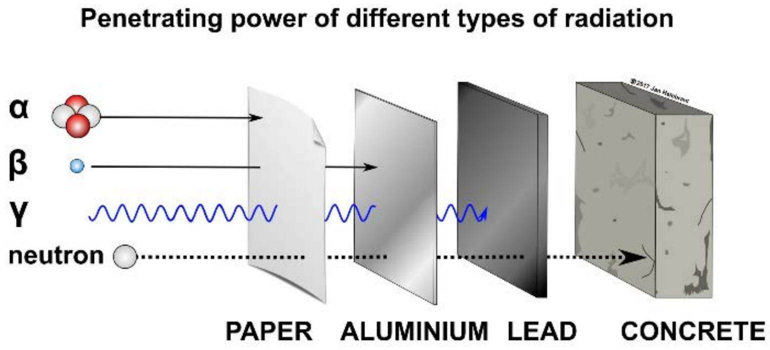
Mathematical Modeling and Computational Physics, Yerevan, Armenia, October 21-25, 2024

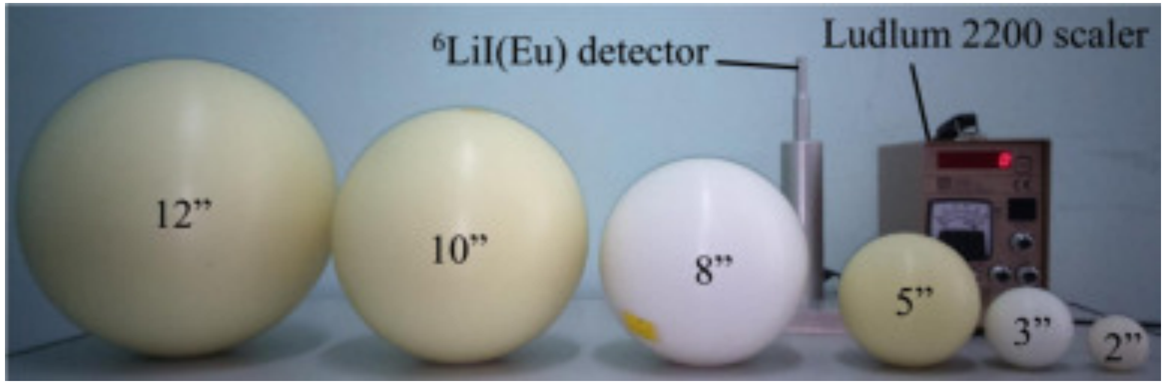
Introduction

- Radiation fields behind the protective shields of the JINR nuclear physics facilities (particle accelerator, nuclear reactors) are formed mainly by **neutrons** of a wide energy spectrum.
- Radiation monitoring at accelerators cannot be carried out using only standard dosimeters and neutron radiometers, since it operating range is limited by a maximum neutron energy of about **10 MeV**.
- **Bonner Multisphere Spectrometer** is a common used tool for radiation monitoring at accelerators.

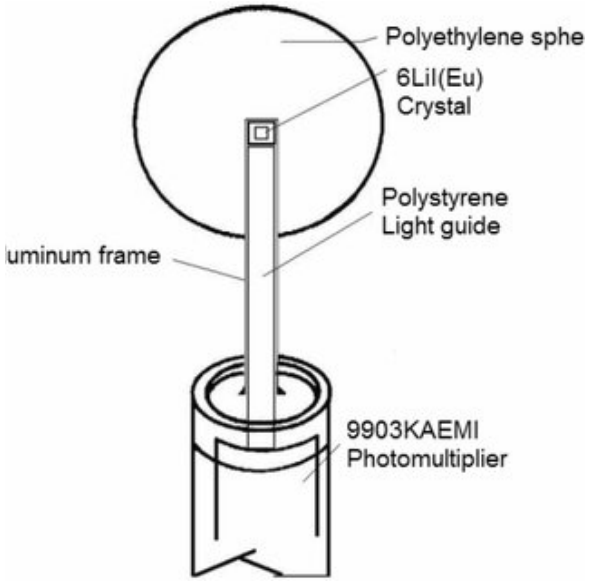


Bonner multisphere spectrometer

- A multisphere Bonner spectrometer is used to measure the neutron flux density.
- The measurement method is based on the moderation of fast neutrons in polyethylene spheres of various diameters.
- Various detectors are used to detect thermal neutrons, e.g., inorganic scintillators such as ^{6}LiI.



https://doi.org/10.1016/j.apradiso.2017.12.012.



Unfolding the neutron spectra

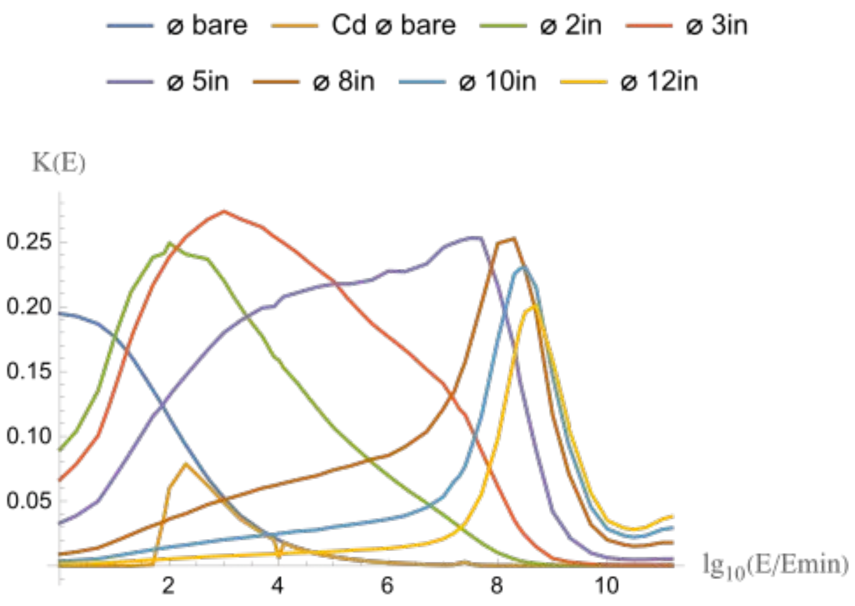
Fredholm integral equations of the 1st kind:

$$\begin{cases} \int\limits_{E_{\min}}^{E_{\max}} K_1(E)\varphi(E)dE = Q_1, \\ \vdots \\ \int\limits_{E_{\min}}^{E_{\max}} K_M(E)\varphi(E)dE = Q_M, \end{cases} \quad (1)$$

where:

- Q_j — Bonner spectrometer reading for the *j*-th sphere,
- $\varphi(E)$ — neutron spectrum,
- $K_j(E)$ is the kernel of the *j*-th equation, which is a response function of the detector to neutrons of various energies,
- M —number of spheres used to measure the spectrum.
- The integration limits $E_{\min}$ and $E_{\max}$ are specified by the domain of definition of the neutron spectrum E and the set of detectors used for measurements.

This is an **ill-posed inverse problem**.

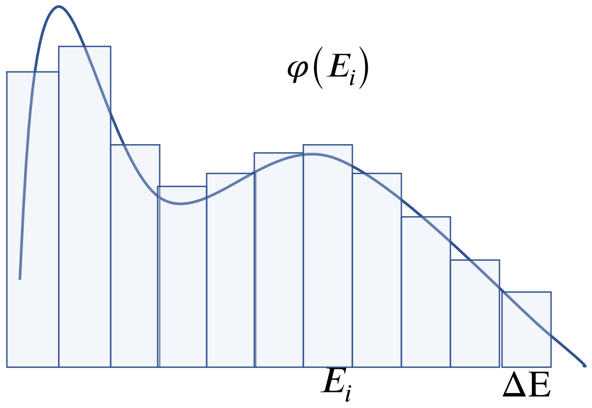


Martinkovic J., Timoshenko G. N. P16-2005-105 Calculation of Multisphere Neutron Spectrometer Response Functions in Energy Range up to 20 MeV, JINR preprint, 2005

Unfolding methods

- Reconstruction of the spectrum via a numerical solution of a system of Fredholm integral equations of the 1st kind with partitioning $\varphi(E)$ over a discrete grid and applying the Tikhonov regularization:

$$Q_j = \int_{E_{min}}^{E_{max}} K_j(E) \bullet \varphi(E) dE \approx \sum_{i=1}^{N} R_{ji} \Phi_i \Delta E, \quad j = 1, \dots, M, \qquad (2)$$



where $\Phi_i \equiv \varphi(E_i)$ is a vector that is a discrete analogue of a continuous quantity of $\varphi(E)$ being the neutron spectrum $(E_i,\ i = 1, \dots, N)$; R_{ji} is the matrix obtained from the kernel of the integral equations.

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- Representation of the spectrum in the form of a linear combination of L trial functions, when the expansion coefficients C_i are found by the formula:

$$\varphi(E) = \sum_{i=1}^{L} C_i \bullet F_i(E) \rightarrow \qquad Q_j = \sum_{i=1}^{L} A_{ji} \bullet C_i, \quad A_{ji} = \int_{E_{min}}^{E_{max}} K_j(E) \bullet F_i(E) dE \qquad (3)$$

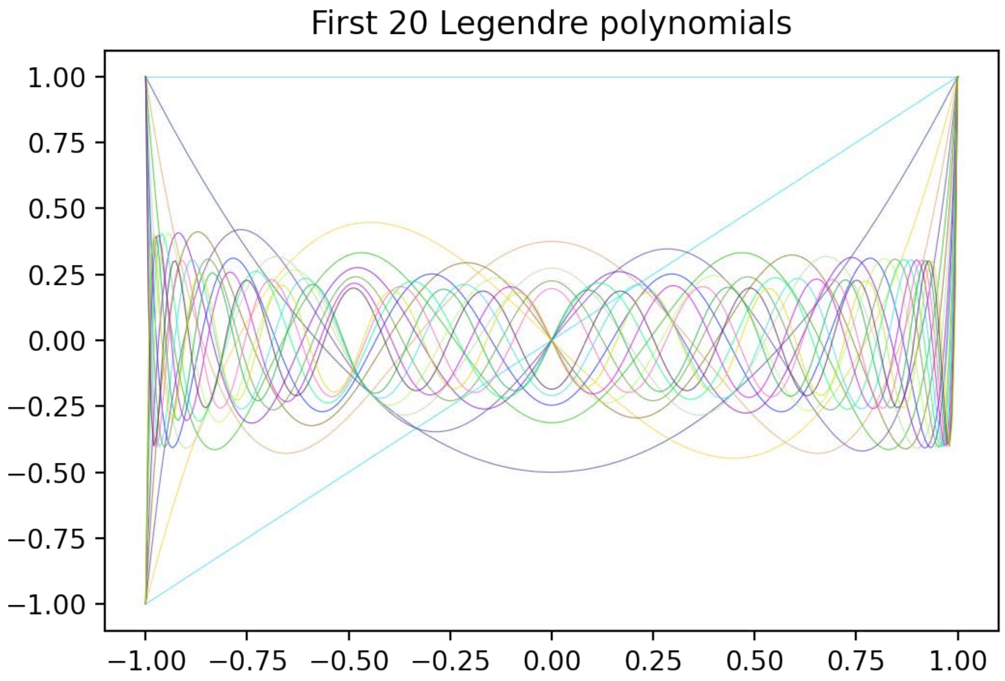
- other methods *(Brooks F. D., Klein H. Neutron spectrometry – historical review and present status, Nuclear Instruments and Methods in Physics Research, A 476, 2002, p.111)*.

Method of functional expansion of flux density using shifted Legendre polynomials with the Tikhonov regularization

Method for decomposing the neutron flux density using shifted Legendre polynomials defined on the interval $[0, l]$:

$$P_n^*(x) = P_n\left(\frac{2x}{l} - 1\right), \quad (4)$$

where $P_n(x) = \frac{1}{2^n n!} \bullet \frac{d^n}{dx^n}\left(x^2 - 1\right)^n$ is the Legendre polynomial of n-th order defined on the interval $[-1,1]$.



Method of functional expansion of flux density using shifted Legendre polynomials with the Tikhonov regularization

$$Q_j = \int_{E_{\min}}^{E_{\max}} K_j(E) \bullet \varphi(E) dE, \quad j = 1, \ldots, M, \tag{5}$$

Wide energy range from **10^{-8} to 10^{3} MeV**, proceed to integration over lethargy $\mathbf{u(E) = lg(E/}\boldsymbol{E}_{\mathbf{min}}\mathbf{)}$**:**

$$Q_j = \ln 10 \bullet \int_{0}^{l_E} K_j(u) \bullet \varphi(u) E(u) du, \quad j = 1, \ldots, M, \ \ l_E = \lg\left(E_{\max}/E_{\min}\right) \tag{6}$$

In our method, the problem of reconstructing the spectrum is reduced to finding expansion coefficients C_i using shifted Legendre polynomials:

$$\Phi(u) \equiv \varphi(u) E(u) = \sum_{i=1}^{N} C_i \, P_{i-1}\left(2u/l_E - 1\right), \quad u \in \left[0, l_E\right] \tag{7}$$

$$\boldsymbol{AC = Q}, \tag{8}$$

where N - number of Legendre polynomials, the matrix elements **A** are defined as:

$$A_{ji} = \ln 10 \bullet \int_{0}^{L_E} K_j(u) \bullet P_{i-1}\left(2u/l_E - 1\right) du \tag{9}$$

Tikhonov regularization with m^th derivative

Solution of the $\boldsymbol{AC} = \boldsymbol{Q}$ with the Tikhonov regularization.

Stabilizing functional with m^th derivative:

$$M^\alpha[C] = \left\|\mathbf{AC} - \mathbf{Q}\right\|^2 + \alpha \times \int_0^{l_E} \left\{\Phi^2(u) + \left[\Phi'(u)\right]^2 + \ldots + \left[\Phi^{(m)}(u)\right]^2\right\} du \;=\; \sum_{j=1}^{M} \left[\sum_{i=1}^{N} A_{ji} C_i - Q_j\right]^2 + \alpha \times Z, \quad (10)$$

$$Z = \sum_{i,k=1}^{N} C_i C_k \int_0^{l_E} \left[\begin{array}{l} P_{i-1}\left(2u/l_E - 1\right) P_{k-1}\left(2u/l_E - 1\right) + \\ + P'_{i-1}\left(2u/l_E - 1\right) P'_{k-1}\left(2u/l_E - 1\right) + \ldots + P^{(m)}_{i-1}\left(2u/l_E - 1\right) P^{(m)}_{k-1}\left(2u/l_E - 1\right) \end{array}\right] du \,. \quad (11)$$

From the condition of the minimum of the stabilizing functional $\dfrac{\partial M^\alpha[C]}{\partial C_i} = 0$, we get a regularized system of linear algebraic equations relative to the new expansion coefficients $\boldsymbol{C}^\alpha$ of the neutron spectrum and regularization parameter $\alpha > 0$:

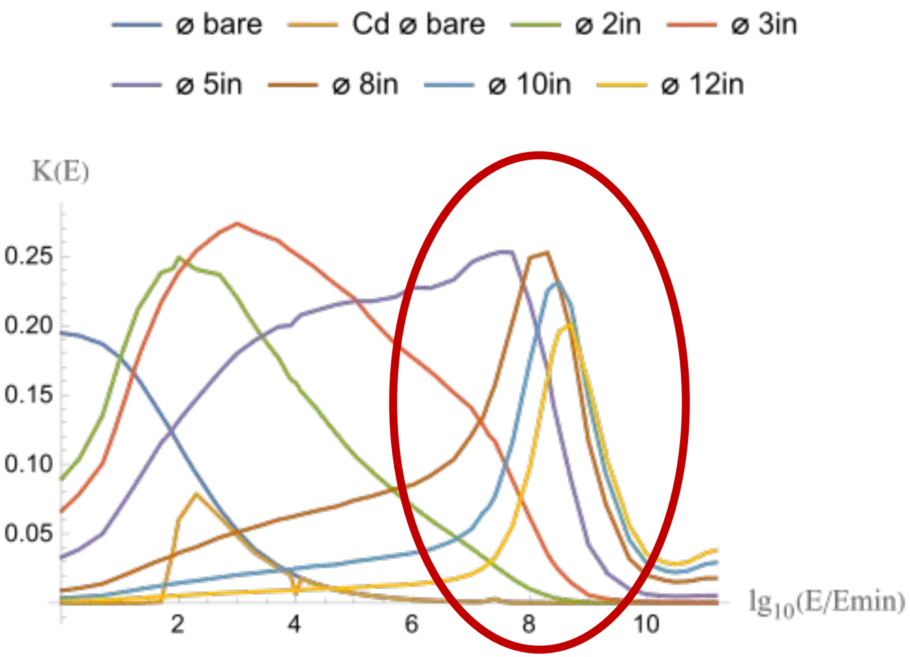
$$\left(\boldsymbol{A}^T \boldsymbol{A} + \alpha \boldsymbol{B}\right) \boldsymbol{C}^\alpha = \boldsymbol{A}^T \boldsymbol{Q} \quad (12)$$

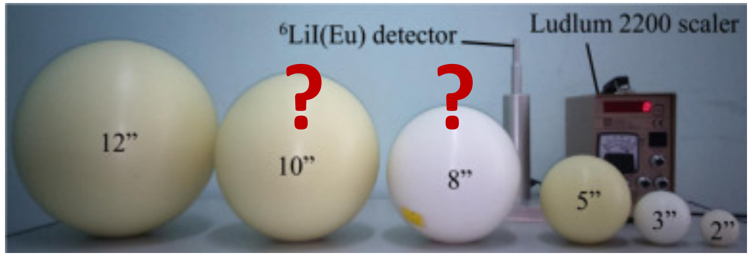
$$B_{ik} = \frac{2 l_E}{2i - 1} \delta_{ik} + \sum_{n=1}^{m} 4^{1-n} \left(\frac{2}{l_E}\right)^{2n-1} \times \sum_{j=1}^{[N/2]-1} (-1)^{j-1} (n - j)!\,(n + j - 1)\,! \left\{\begin{array}{l} \binom{i+n-j}{n-j} \binom{i}{n-j} \binom{k+n+j-1}{n+j-1} \binom{k}{n+j-1} \delta_{k-i,2(j-1)} + \\ + \binom{k+n-j}{n-j} \binom{k}{n-j} \binom{i+n+j-1}{n+j-1} \binom{i}{n+j-1} \delta_{i-k,2j} \end{array}\right\} \quad (13)$$

Considering the importance of the detector with the selected moderator

Correlation in response functions can worsen the result of spectrum unfolding.

Taking into account the "importance" of the detector, we introduce a stabilizing functional with a **weight matrix,** *W*:





Generalized Tikhonov regularization with weight matrix

Stabilizing functional with m[th] derivative with **weight matrix** W:

$$M_W^{\alpha}[C] = (\mathbf{AC}-\mathbf{Q})^T W (\mathbf{AC}-\mathbf{Q}) + \alpha \times \int_0^{l_E} \left\{ \Phi^2(u) + [\Phi'(u)]^2 + \ldots + [\Phi^{(m)}(u)]^2 \right\} du = \sum_{j=1}^{M} W_{jj} \left[\sum_{i=1}^{N} A_{ji} C_i - Q_j \right]^2 + \alpha \times Z, \quad (14)$$

$$Z = \sum_{i,k=1}^{N} C_i C_k \int_0^{l_E} \left[P_{i-1}(2u/l_E - 1) P_{k-1}(2u/l_E - 1) + P'_{i-1}(2u/l_E - 1) P'_{k-1}(2u/l_E - 1) + \ldots + P_{i-1}^{(m)}(2u/l_E - 1) P_{k-1}^{(m)}(2u/l_E - 1) \right] du .$$

α – regularization parameter.

The elements of the diagonal weight matrix $W = \{W_{jj}\}$ are constructed on the *condition numbers* of the matrices $\mathbf{A}_j$ (j=1,…,M), obtained from the matrix $\mathbf{A}_{M\times N}$ by deleting the j-th row

$$W_{jj} = \mathrm{cond}(\mathbf{A}_j) = \sqrt{\lambda(\mathbf{A}_j \mathbf{A}_j^T)_{\max} / \lambda(\mathbf{A}_j \mathbf{A}_j^T)_{\min}}, \quad (15)$$

where $\lambda(\mathbf{A}_j \mathbf{A}_j^T)$ are the eigenvalues of the symmetrical matrix $\mathbf{A}_j \mathbf{A}_j^T$.

$$\begin{pmatrix} A_{11} & A_{12} & \ldots & A_{1j} & \ldots & A_{1N} \\ A_{21} & A_{22} & \ldots & A_{2j} & \ldots & A_{2N} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ A_{j1} & A_{j2} & \ldots & A_{jj} & \ldots & A_{jN} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ A_{M1} & A_{M2} & \ldots & A_{Mj} & \ldots & A_{MN} \end{pmatrix}$$

From $\dfrac{\partial M_W^{\alpha}[C]}{\partial C_i} = 0$, we get:

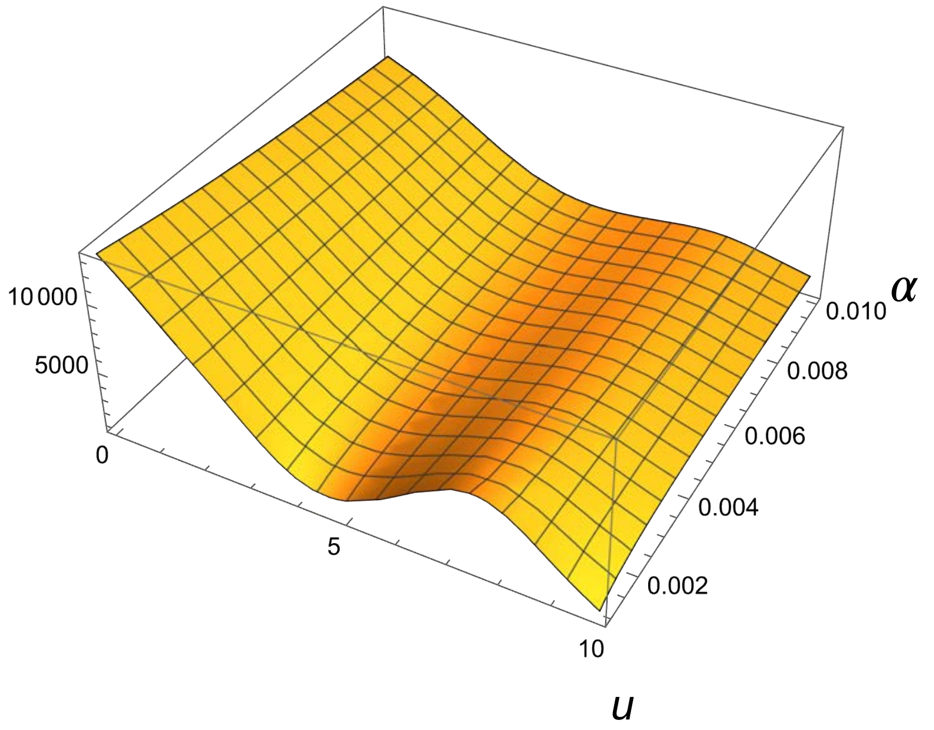
$$(\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A} + \alpha \boldsymbol{B}) \boldsymbol{C}^{\alpha}(\boldsymbol{W}) = \boldsymbol{A}^T \boldsymbol{W} \boldsymbol{Q} \quad (16)$$

The choice of the regularization parameter (α)

The choice of the regularization parameter α is carried out in accordance with the *generalized residual principle*

$$\left(\mathbf{A}\mathbf{C}^{\alpha}(\boldsymbol{W}) - \mathbf{Q}\right)^{T}\left(\mathbf{A}\mathbf{C}^{\alpha}(\boldsymbol{W}) - \mathbf{Q}\right) - \delta^{2}\mathbf{Q}^{T}\mathbf{Q} - \mu^{2}\left(\mathbf{Q}, \mathbf{A}\right) = 0, \quad (17)$$

- δ is the relative error in measurements of the neutron spectrum $\varphi(E)$
- μ (**Q**,**A**) is a measure of incompatibility (physical restrictions on the spectrum form)



Dose assessment

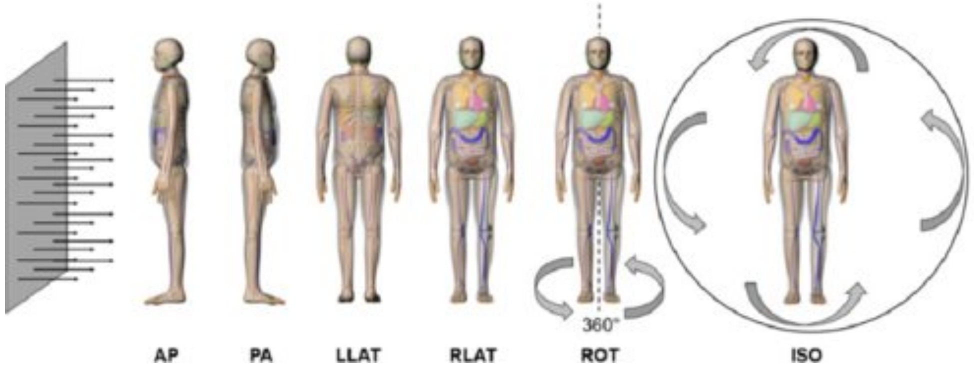
The Bonner multisphere spectrometer is used to measure neutron spectra in stationary fields to assess exposure of personnel.

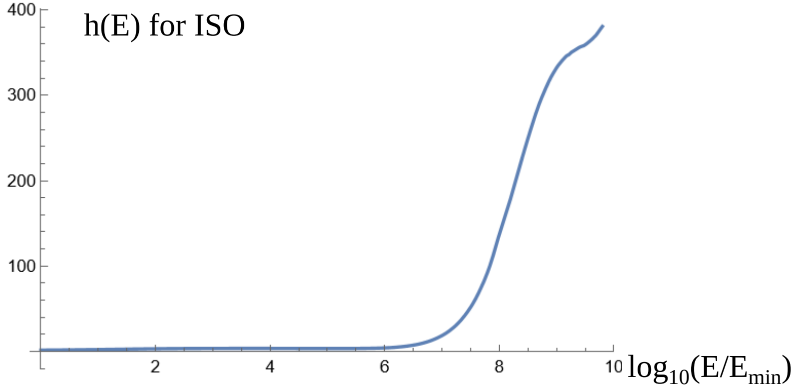
$$\Phi^{\alpha}(u) \equiv \varphi^{\alpha}(u) E(u) = \sum_{i=1}^{N} C_i^{\alpha} \bullet P_{i-1}\left(2u/l_E - 1\right), \qquad (18)$$

$$\dot{H}^{\alpha} = \int_{E_{\min}}^{E_{\max}} h(E) \bullet \varphi^{\alpha}(E) dE = \ln 10 \times \int_{0}^{l_E} h(u) \bullet \Phi^{\alpha}(u) du, \qquad (19)$$

where $h(E)$ [pSv•cm2] is the *dose conversion coefficient* for mono energetic particles in various irradiation geometries (up to 20 MeV from NRB 99/2009; up to 10 GeV from ICRP116), for different irradiation types: *AP, PA, LLAT, RLAT, ROT, ISO*.

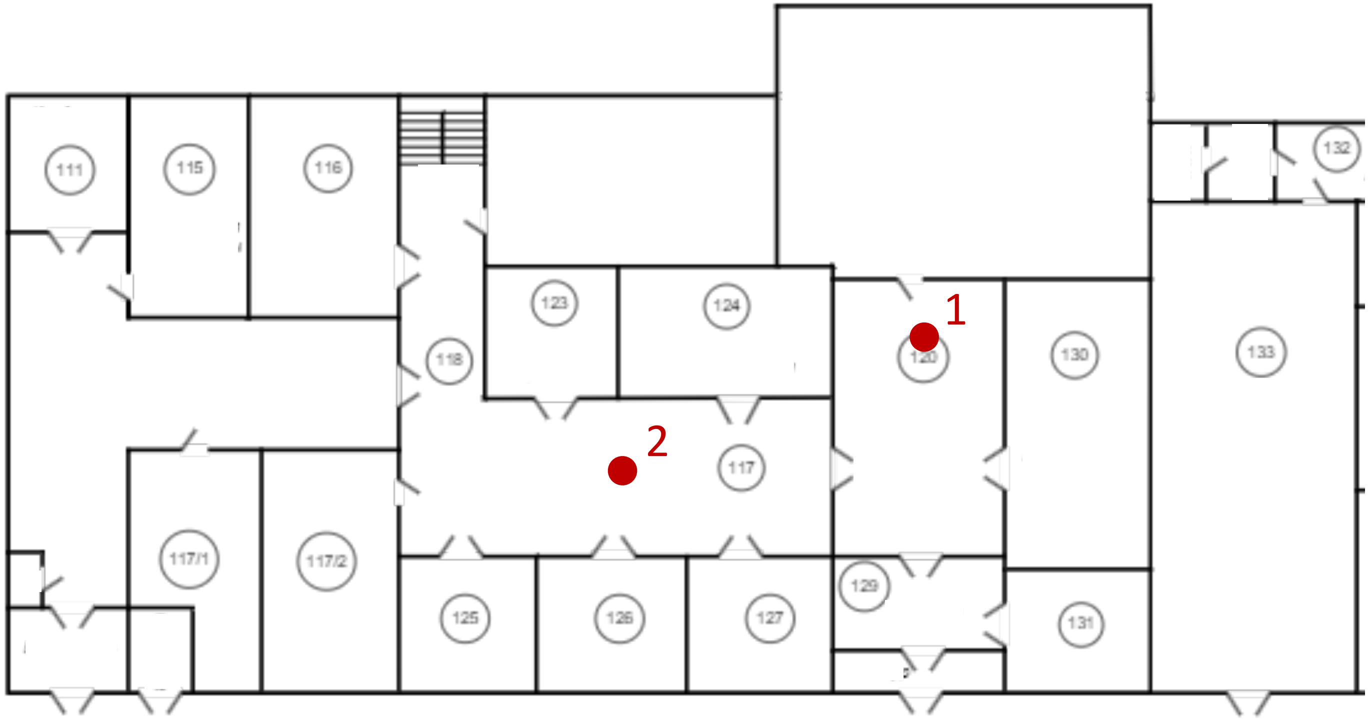
$\dot{H}^{\alpha}$ - Dose rate ($\dot{E}_{\text{eff\_AP}}$,$\dot{E}_{\text{eff\_ISO}}$, $\dot{H}^{*}(10)$, $\dot{H}_{\text{p}}(10,0^{\circ})$)

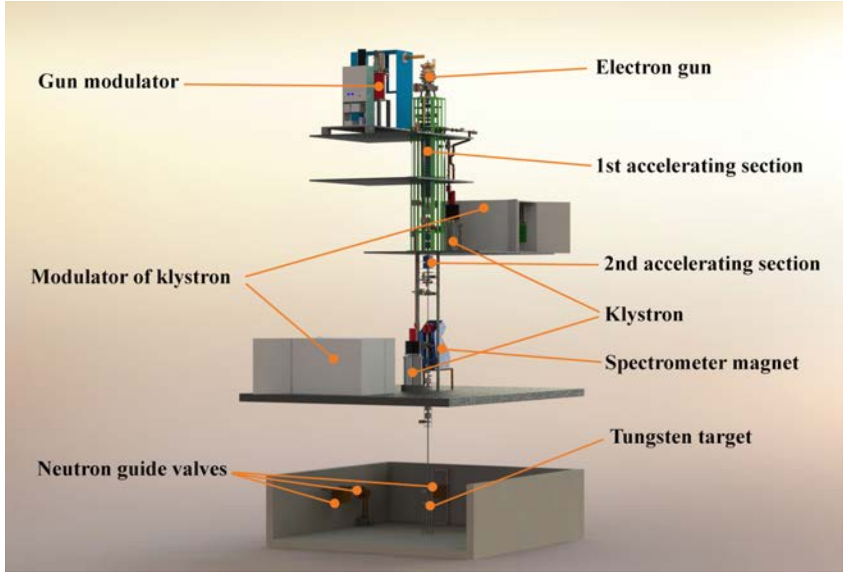




IREN facility (Intense Resonance Neutron Source)

Spectrum unfolding for IREN facility accelerator and target halls.





https://flnp.jinr.int/en-us/main/facilities/iren

IREN facility (Intense Resonance Neutron Source)

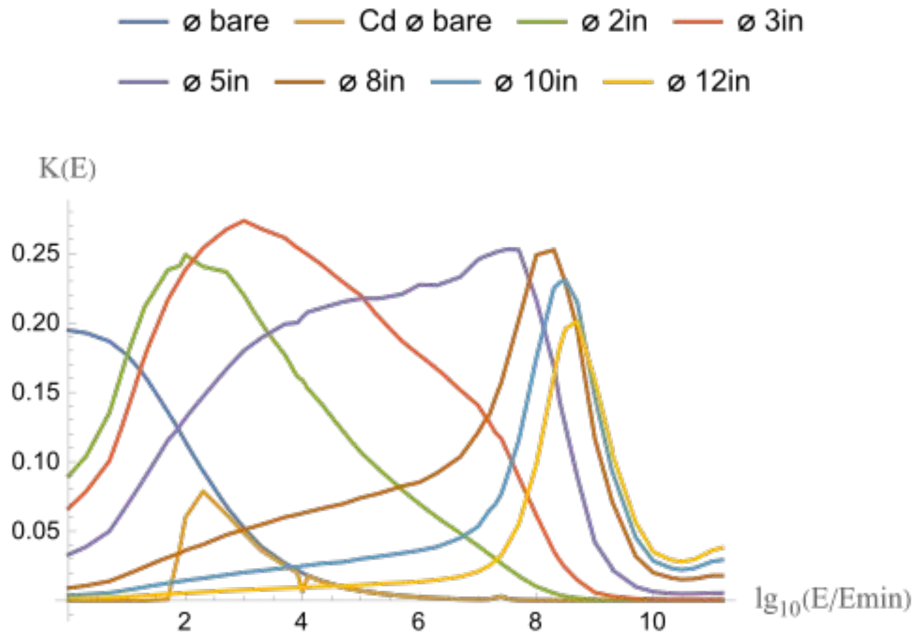
M = 8 measurements with Bonner spheres
i = 15 Legendre polynomials

Weight matrix for JINR Multisphere Bonner spectrometer:

$W = \{1.0,\ 0.997,\ 0.746,\ 0.516,\ 0.349,\ 0.200,\ 0.191, 0.287\}$

Comparison cases:

- without taking into account the weight matrix,
- taking into account the weight matrix,
- without the 6th and 7th detectors.



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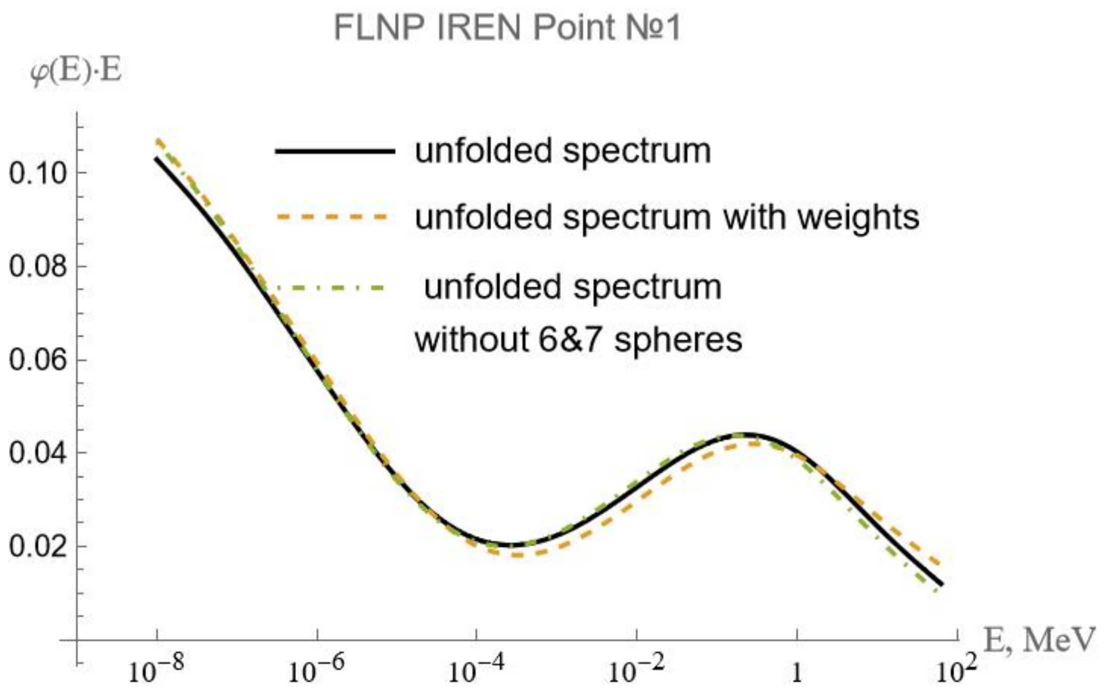
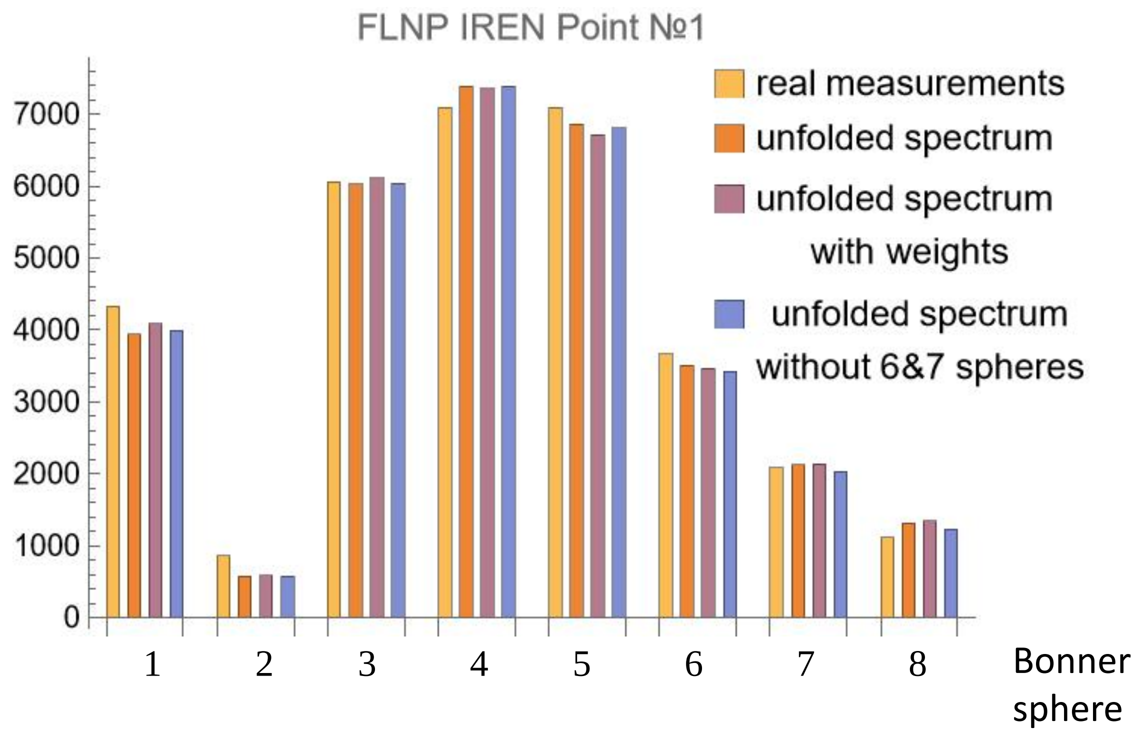
IREN facility (Intense Resonance Neutron Source)

Point 1:





Unfolded neutron spectra (left) and detector readings (right) with a relative measurement error of δ=0.05 (5%).

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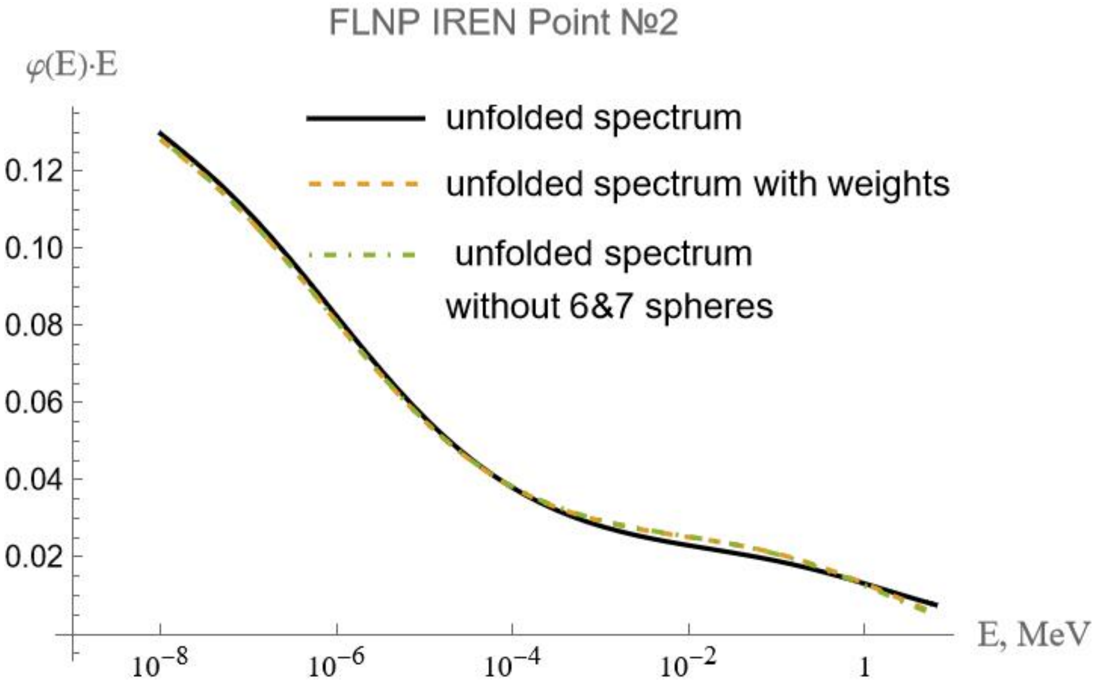
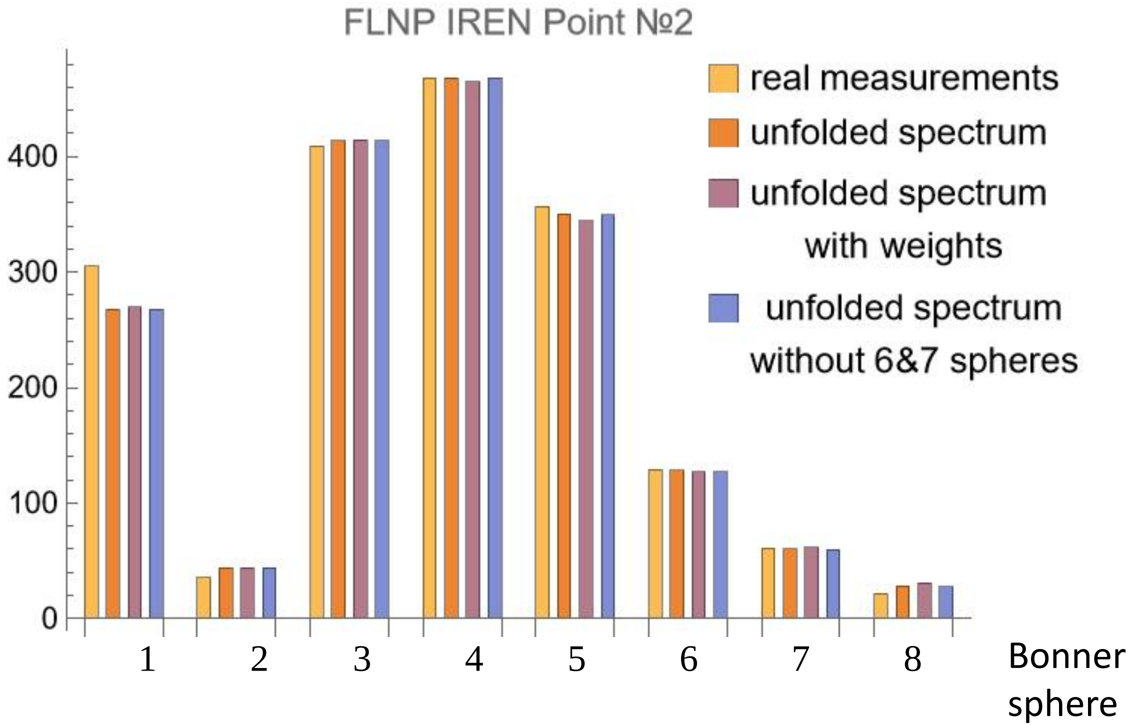
Point 2:





Unfolded neutron spectra (left) and detector readings (right) with a relative measurement error of δ=0.05 (5%).

Advantages of the method

1. The introduction of a weight matrix allows one to reduce the number of measurements, thereby reduce doses on personnel.
2. The unfolded spectrum can be used to obtain values for excluded spheres with good accuracy.

Constrains

1. The method is suitable for unfolding spectra in stationary fields.
2. Set of Bonner spectrometer spheres limits the energy range of unfolded spectrum.
3. The reliability of the reconstructed neutron spectra significantly depends on the quality of the response functions.

Conclusions

1. A method has been developed for reconstructing the energy spectra of neutron flux density by decomposing the spectrum into Legendre polynomials using Tikhonov regularization.
2. The developed method made it possible to unfold the neutron spectra for two locations at the IREN based on actual measurements.
3. Taking into account the weight matrix $\boldsymbol{W}$ in the regularization algorithm of A.N. Tikhonov ensures statistical alignment of contributions from measurements with spheres of different diameters, which allows theoretically determining optimal sets of Bonner spheres (their sizes and number) for effective practical measurements.

Thank you!

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Chizhov K, Beskrovnaya L, Chizhov A, “Neutron spectra unfolding from Bonner spectrometer readings by the regularization method using the Legendre polynomials”, *Physics of Elementary Particles and Atomic Nuclei*, 2024 3 (**55)**, 532–534