Modeling and optimization of a wide aperture high-resolution neutron Fourier diffractometer as a system of independent detectors

NPCS-2017

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- Solution of the Euler-Lagrange equations for a point sample and zero-thickness detector

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Abstract

The Wide Aperture High-Resolution Neutron Fourier Diffractometer (HRFD) is designed for research in the area of solid state physics and materials science and is used as a detector in research nuclear reactors.

The purpose of HRFD shape optimisation is to increase their efficiency and reduce the cost of such detectors. Optimization of the HRFD configuration through the development of analytical and numerical methods made it possible to determine the contribution to the spectrometer response function both of the design characteristics and geometric characteristics associated with the spatial orientation of the spectrometer and its individual parts.

For definition of analytical surface form of the HRFD for a point target and target of finite dimensions, the variational procedure was used for representing the problem in the form of the Lagrange-Euler equation. This methodology was used earlier to find the shape of the detector, as a numerical solution of the Lagrange-Euler equations [1]. According to the results of calculations of the shape of the spoke for a point target, an analytical expression is obtained.

1. Application of the Monte-Carlo Methods and Variational Procedure for Optimization of Time-off-Flight Neutron Diffractometer Characteristics / A. A. Khrushchinsky, S. A. Kuten, K. A. Viarenich, P. A. Speransky // Physics of Particles and Nuclei Letters. - 2016. - Vol. 13. - No. 3. - pp. 390–405.

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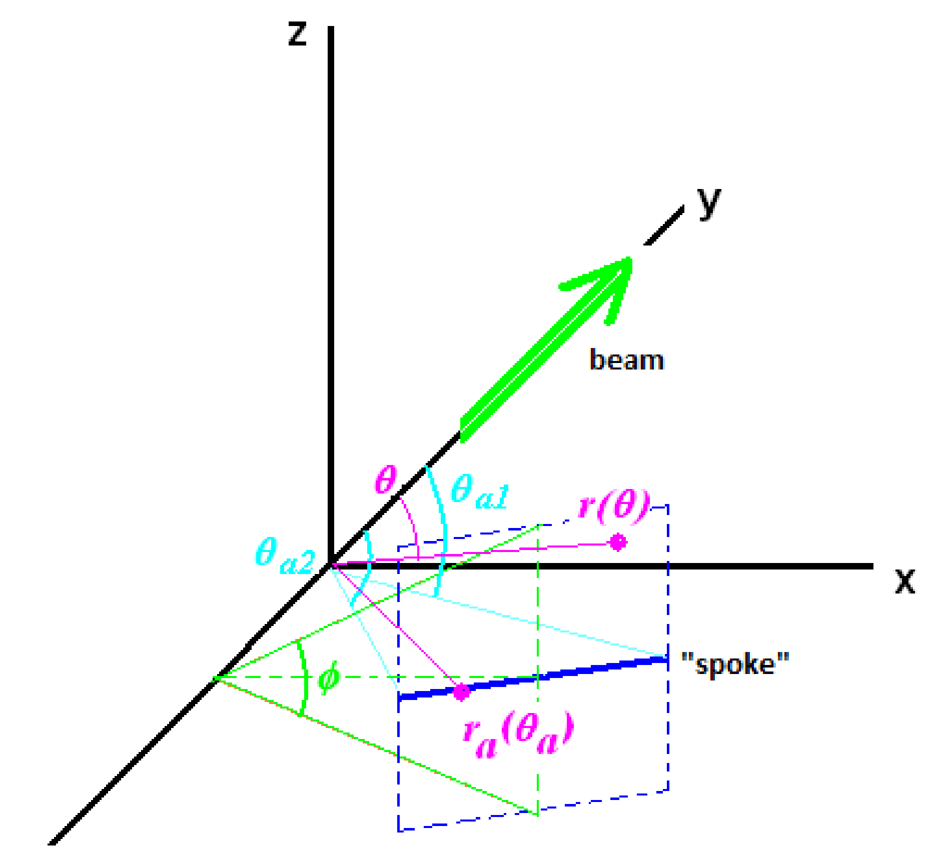
Formulation of the problem

- Fast neutrons from Impulse Fast Reactor IBR-2 are thermolysed in moderator.
- Thermal neutrons are captured by the mirror neutron guide and transported to and modulated by a chopper.
- Further, neutron flux is transported to the sample and, finally, after being scattered in air and parts of detector construction they are registered by the backscattering detector.
- Maximal value of scattering angle θ_2 defined by experimental conditions and equal to 172.7°.



Formulation of the problem

- The following approaches was used in the model:
  - The optimal approximation of TOF focusing surface is developed using a given technologically implementable class of the surfaces;
  - The problem is solved under ideal conditions: a point sample and zero thickness detector;
- Using Monte Carlo simulation with the selected optimal time of flight (TOF) focusing surface approximation, the dependence of resolution and relative aperture of diffractometer on the following parameters can be studied:
  - Sample sizes;
  - Nonzero detector thickness;
  - Neutron absorption in detector;
  - Neutron absorption in sample;
  - Energy spectrum;
  - Time width of the neutron pulse on the chopper.

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Variational method of optimization

The Lagrangian

$L(r, \dot{r}, \theta) =< J_1(r, \dot{r}, \theta; \Gamma) > +\lambda^* < J_1(r, \dot{r}, \theta; \Gamma) >;$

were $J_1 = \int \delta t(r, \dot{r}, \theta) d\Gamma$, $J_2 = \int \delta t^2(r, \dot{r}, \theta) d\Gamma$.

$\delta t\ (r, \dot{r}, \theta) = t(r, \dot{r}, \theta) - t_0$.

$d\Gamma$ presented below has the mining of surface integration and can be written as:

$d\Gamma = ds \frac{|(n_s \cdot l_n)|}{r^2(\theta)}$.

The solution of variational problem is the task of searching the form of the function $r_a(\theta_a)$ which minimizes functional L.

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Variational method of optimization

System of coordinates:

$$x = r\sin(\theta)\cos(\varphi) = r_a sin\ (\theta_a)$$

$$y = r\cos(\theta) = r_a\cos(\theta_a)$$

$$z = r\sin(\theta)\, sin(\varphi) = r_a sin\ (\theta_a) tg(\varphi)$$

$$\theta\ (\theta_a, \varphi_a) = arctg\,\frac{tg\ (\theta_a)}{cos\ (\varphi_a)}$$

$$tg(\theta_a) = tg(\theta)\cos(\varphi)$$

Taking into account initial conditions Lagrangian function can be written as:

$$L(r_a, \theta_a) = \int_{-\varphi_0/2}^{\varphi_0/2} [\left(\frac{a_0 + nu(\theta_a,\varphi) r_a(\theta_a)}{\nu(\theta)} - t_0\right)^2 + \ \lambda(\frac{a_0 + nu(\theta_a,\varphi) r_a(\theta_a)}{\nu(\theta)} - t_0)]\, \frac{sin(\theta_a) d\varphi}{nu^3(\theta_a,\varphi) cos^2(\varphi)}$$

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Solution of the Euler-Lagrange equations for a point sample and zero-thickness detector

The solution of variational problem is the solution of Euler-Lagrange equations that was found and has the following view:

$$r_a(\theta_a) = \frac{1}{K_0 \overline{b^2nu^2}}\left[\frac{v_0 t_0}{s_a} K_s \overline{bnu} - a_0\left(\overline{b^2nu} - \frac{K_b}{S_a}\overline{bnu}\right)\right],$$

where

$$K_s = f(\theta_{a2}, \varphi_0) - f(\theta_{a1}, \varphi_0),\ f(x, \varphi_0) = \sqrt{2}\frac{\cos(x)}{\sqrt{1+tg^2(\varphi_0/2)sin^2(x)}} arctg\left(\frac{\sqrt{1+tg^2(\varphi_0/2)sin^2(x)}}{tg(\varphi_0/2)|\cos(x)|}\right),$$

$$K_b =< \left(\frac{\overline{bnu}\ \ \overline{b^2nu}}{\overline{b^2nu^2}} - \bar{b}\right)s_a \sin(\theta_a) >,\ K_0 =< \frac{(\overline{bnu})^2}{\overline{b^2nu^2}} \sin(\theta_a) >,\ < f > = \int_{\theta_{a1}}^{\theta_{a2}} f(\theta_a)d\theta_a,$$

$$\overline{b^2nu} = \frac{1}{\sin(\theta_a)sin^2(\theta_a/2)}\left(arctg(u) - \frac{u\cos(\theta_a)}{\sqrt{1+u^2}}\right),\ \overline{b^2nu^2} = \frac{1}{\sin(\theta_a)sin^2(\theta_a/2)}(arcsh(u) - arctg(u)\cos(\theta_a)),$$

$$u = \sin(\theta_a)\, tg(\varphi_0/2).$$

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Solution of the Euler-Lagrange equations for a point sample and zero-thickness detector

Numerical calculations demonstrate low dependence of $\overline{bnu}(\theta_a)$ of θ_a angle parameter.

Final spoke function view for point target can be written analytically as follows:

$$\boxed{r_a(\theta_a) = \frac{1}{arcsh(u) - \cos(\theta_a) arctg(u)} \left[2u(a_0 + r_\pi) \sin\left({}^{\theta_a}/_2\right) - a_0 \left(arctg(u) - \frac{u\cos(\theta_a)}{\sqrt{1+u^2}} \right) \right].}$$

For the small angles θ upper equation limiting case has the form of the surface of ideal time-of-flight focusing surface:

$$r_a(\theta_a) = \frac{a_0 + r_n}{\sin(\frac{\theta_a}{2})} - a_0.$$

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Thank you for your attention!

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