AI-Based C++ Code Generation for Fitting Models in FITTER_WEB

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What is fitting?

- Process of optimizing model parameters to describe experimental data (spectra, particle distributions).
- Quality measured by χ^2 (chi-squared):

$$\chi^2 = \frac{1}{N - N_{par}} \sum_{i=1}^{N} \left(\frac{f(x_i) - y_i}{\Delta y_i} \right)^2$$

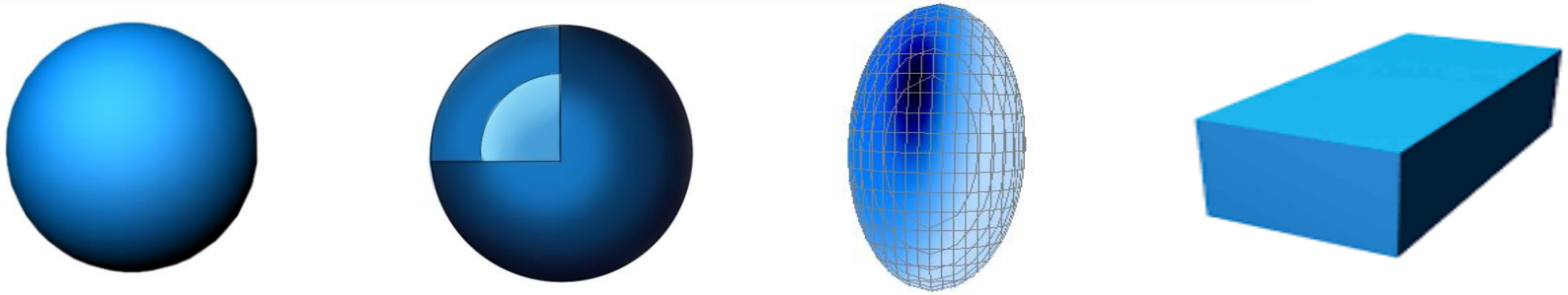
N	- Number of data points
N_{par}	- Number of model parameters
$f(x_i)$	- Model prediction
$y_i \pm \Delta y_i$	- Measured values with errors

How physicists use fitting?

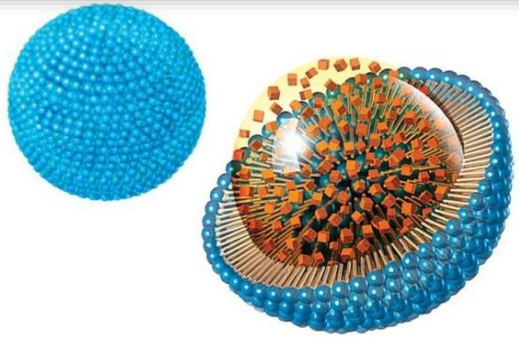
- Test hypotheses by comparing models with experimental data.
- Extract physical parameters (e.g., radii, amplitudes) from noisy data.
- Minimize χ^2 to ensure scientific accuracy.

Small-Angle Scattering: Key Model Types

Classical Form Factors integrated both in FITTER and FITTER_WEB



Vesicles & Membranes integrated in FITTER_WEB



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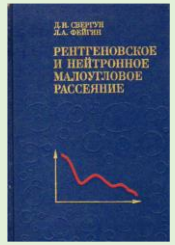
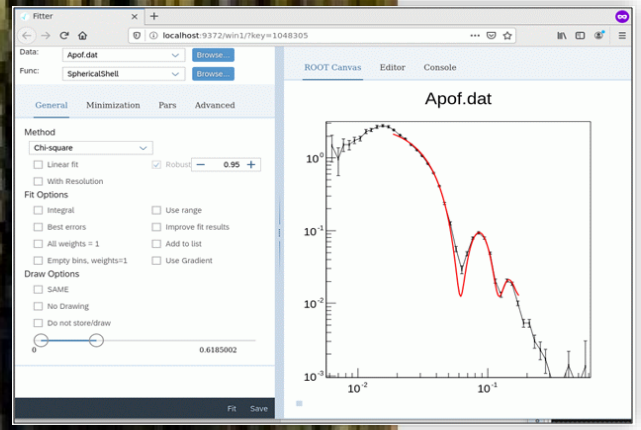
MORE MODELS

Рентгеновское и нейтронное малоугловое рассеяние / Дмитрий Иванович Свергун, Лев Абрамович Фейгин. – М. : Наука, 1986. – 279 с



History of FITTER application



- **2003-2008**

  Fitter is a standalone C++ program on Linux\Windows aimed to fit a chosen theoretical multi-parameter function through a set of data points. Respective theoretical models are implemented in it.

- **2012** Additional theoretical models implemented.

- **2022**

  Web-version of FITTER was developed as a standalone web-service.

- **2023-2024**

  Deploying and optimizing FITTER_WEB in JINR cloud infrastructure.

- **2025 – WHO WILL CODE THE MODELS?..**

How AI Simplifies Model Implementation

CORE IDEA:

Physicists describe models in LaTeX ⇒ AI generates optimized C++ code

User Input:

- LaTeX formula (e.g., scattering model)
- Parameter constraints

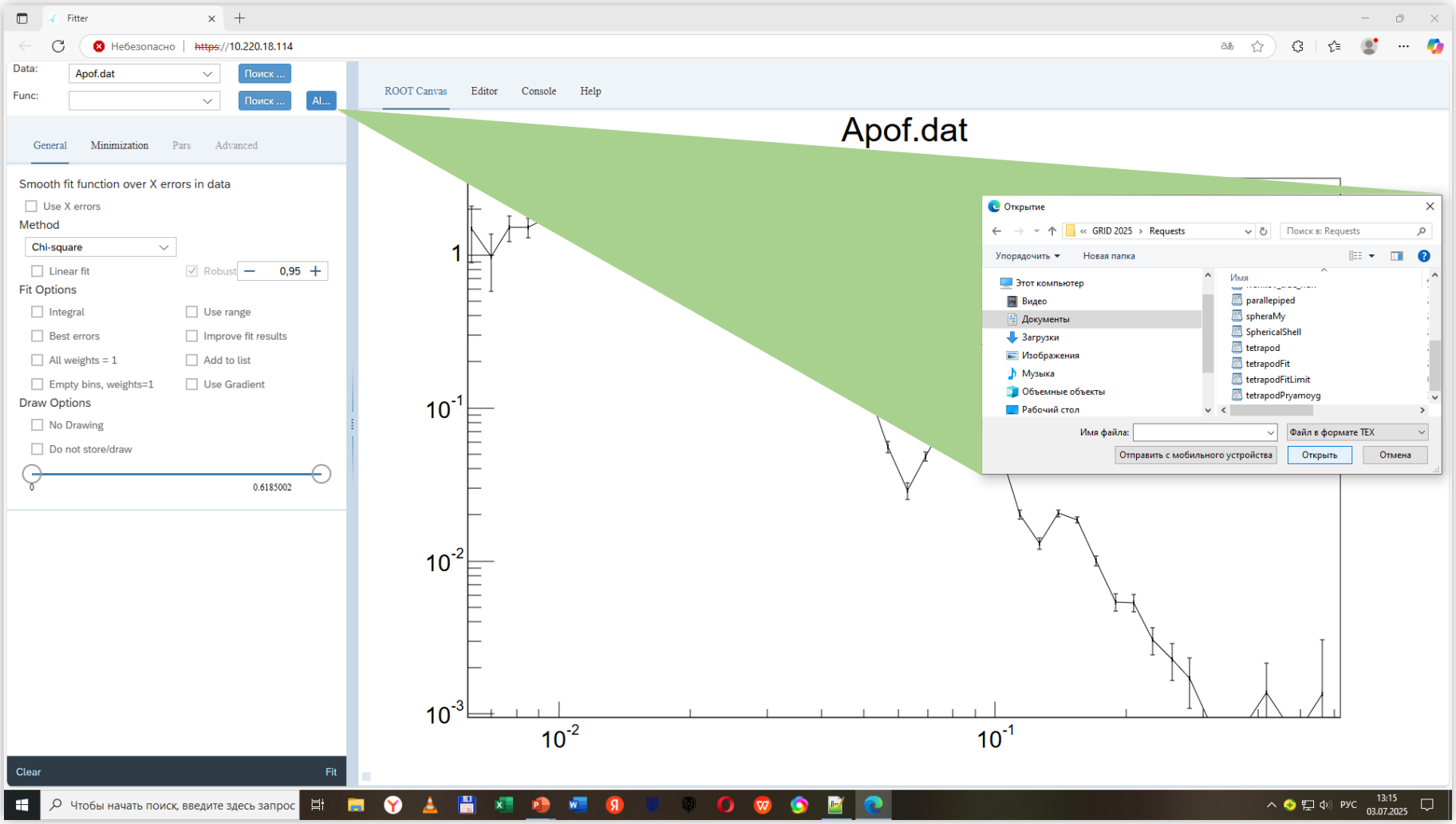
AI Output:

- Ready-to-use TF1 ROOT function
- or editable prototype

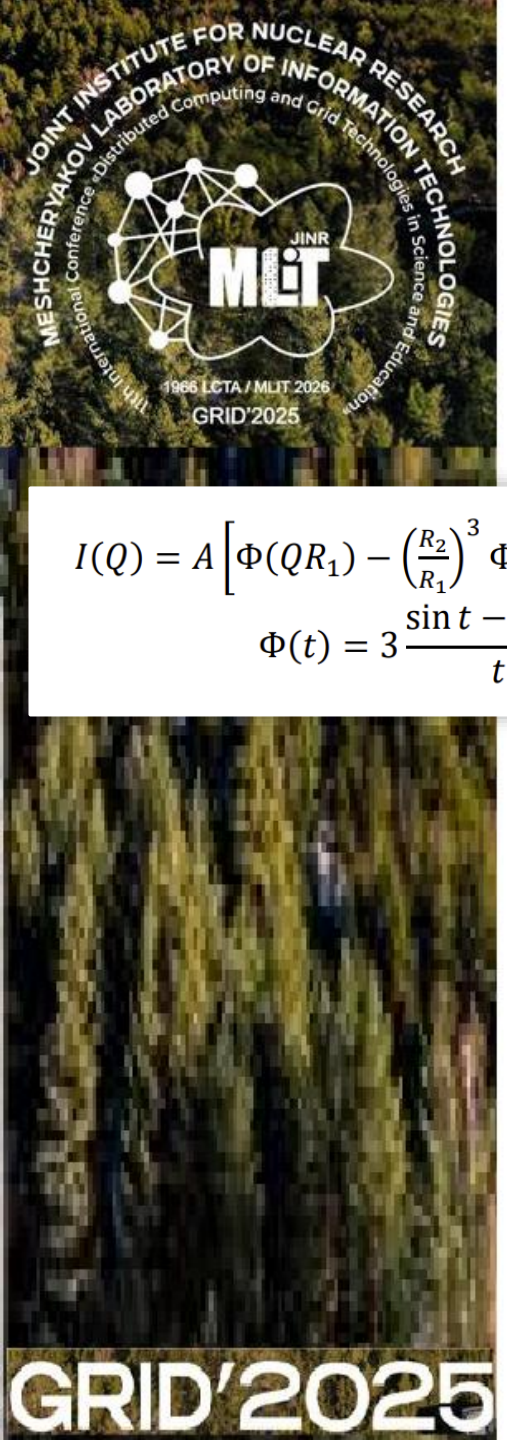
Current prompt (subject to further studying)

```
Convert the following LaTeX formulas to C++ code to create a TF1 function in ROOT:
The original LaTeX is unchanged as a comment
The function is strictly in the format 'TF1* getFCN()'
All auxiliary calculations are inside getFCN() as lambdas
For a one-dimensional integral, use ROOT::Math::Integrator
For a multidimensional integral, use ROOT::Math::IntegratorMultiDim
Detailed parameter comments
Here is the conversion formula: latex code of formula with parameters here
```

New FITTER_WEB workflow



A LaTex file with example formula

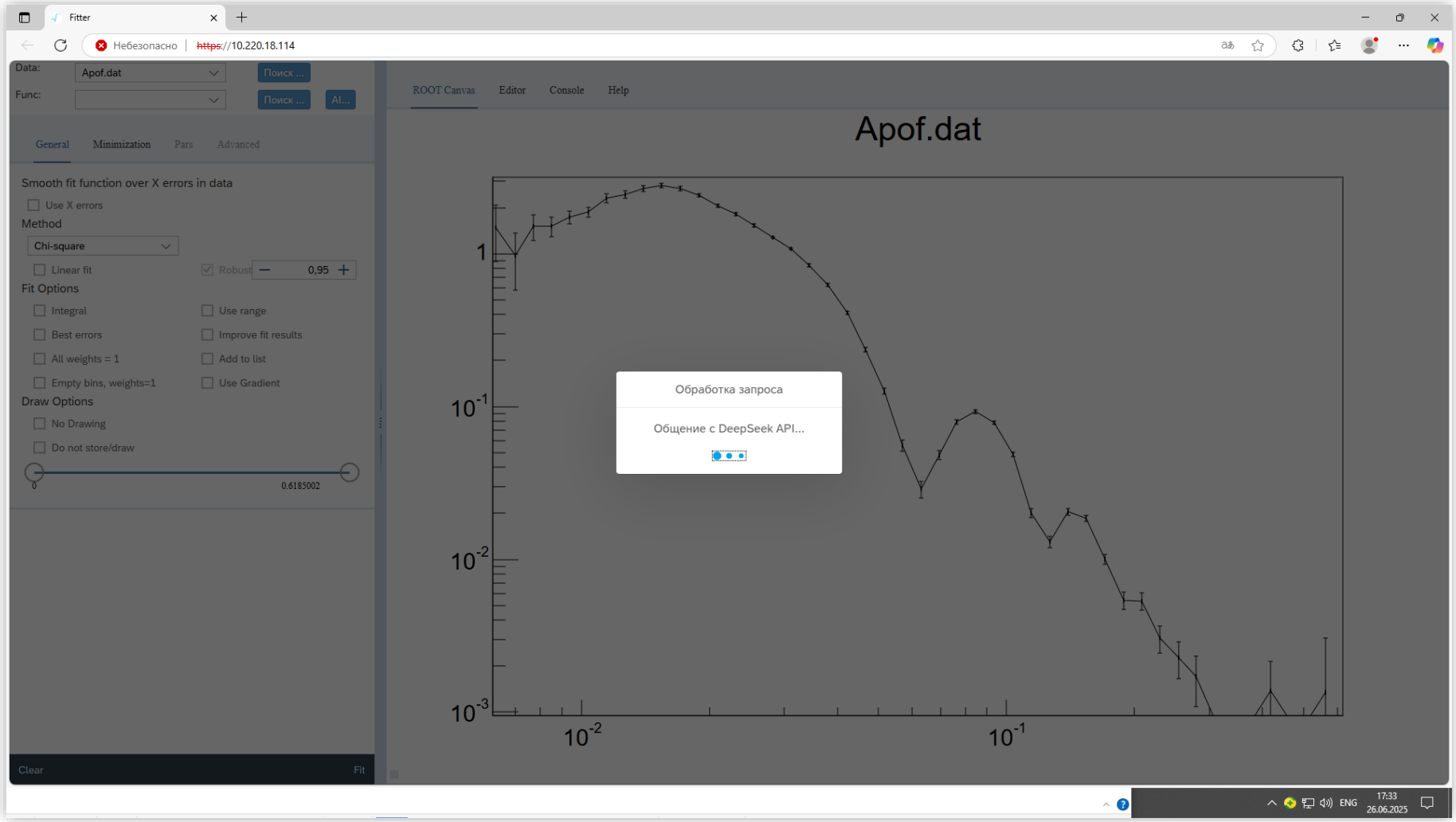


$$I(Q) = A\left[\Phi(QR_1) - \left(\frac{R_2}{R_1}\right)^3 \Phi(QR_2)\right]^2 + B$$

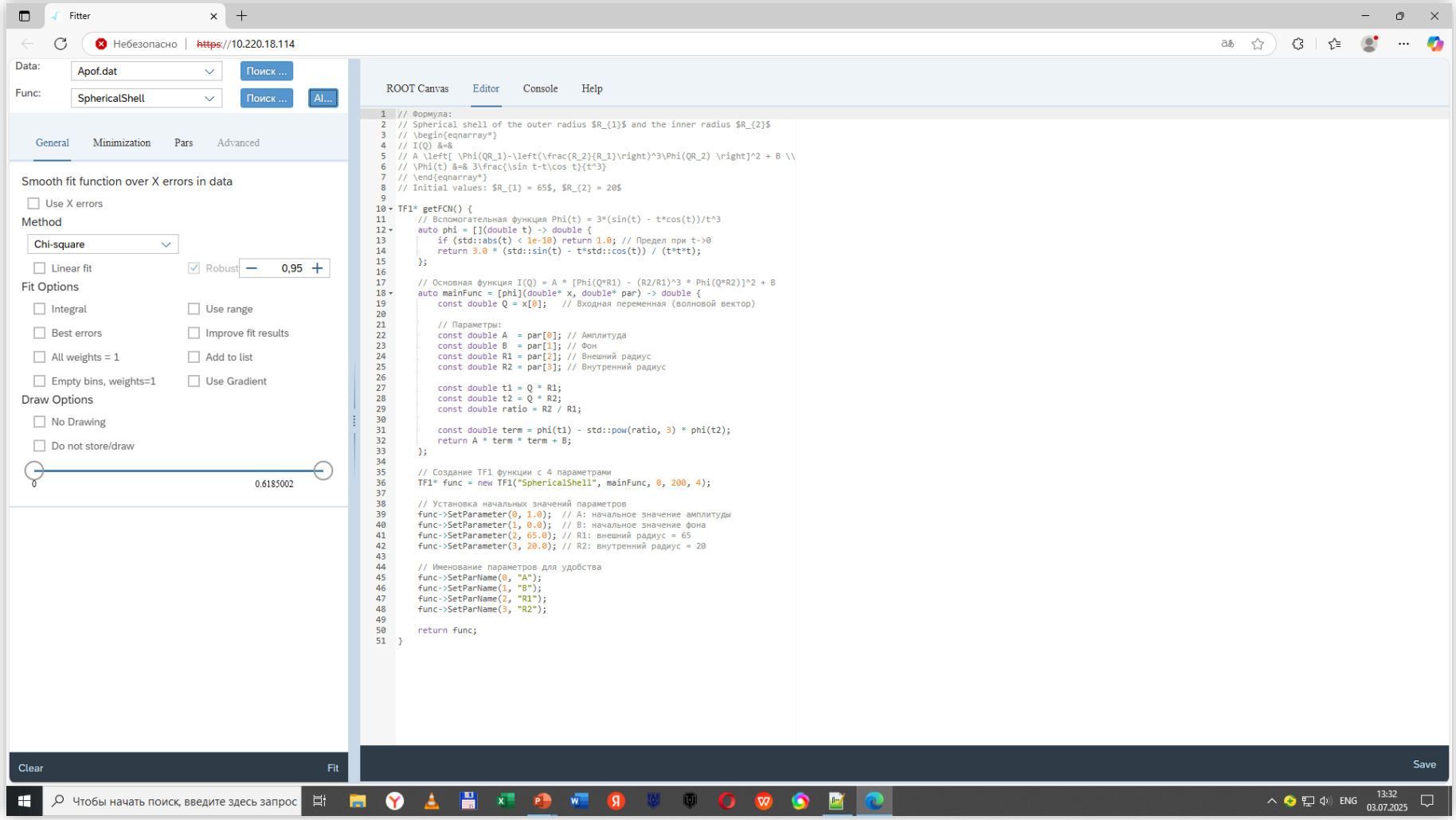
$$\Phi(t) = 3\frac{\sin t - t\cos t}{t^3}$$

```
{\bf Spherical shell} of the outer radius $R_{1}$ and the inner
radius $R_{2}$

\begin{eqnarray*}
I(Q) &=& A \left[ \Phi(QR_1)-
\left(\frac{R_2}{R_1}\right)^3\Phi(QR_2) \right]^2 + B \\
\Phi(t) &=& 3\frac{\sin t-t\cos t}{t^3}
\end{eqnarray*}

Initial values for the parameters are: $R_{1} = 65$, $R_{2} = 20$
The parameter values  $R_{1}$,    $R_{2}$  and  A  are strictly
greater than zero.
```

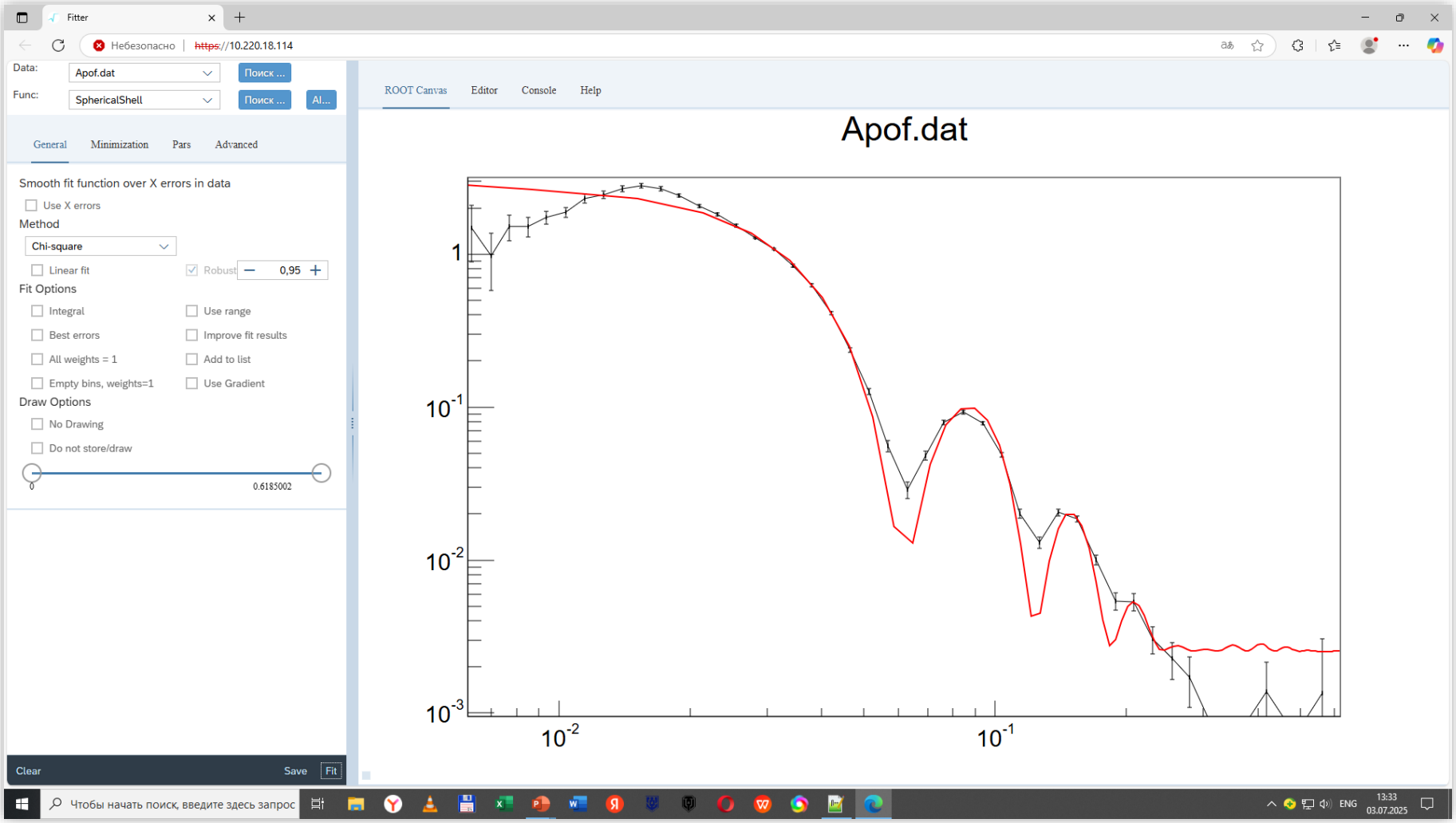
AI request processing



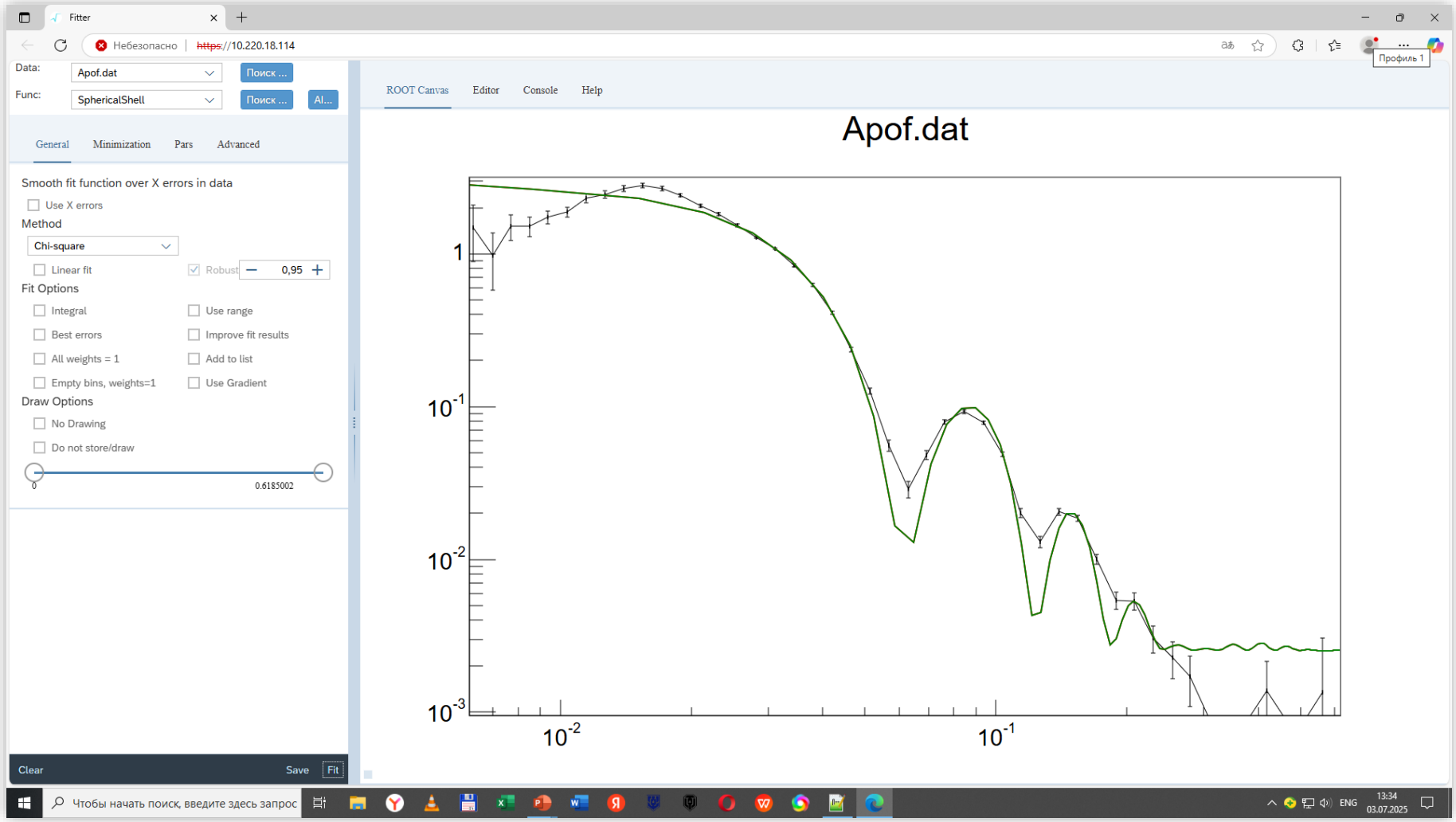
The code appears in the Editor tab



Fitting by function from AI



Fitting a function written by the user



Fitting Results

Fitting a function generated by AI

```
**********************************************
Minimizer is Minuit / Migrad
Chi2                      =     688.425
NDf                       =          42
Edm                       =  9.55216e-09
NCalls                    =         215
R1                        =     61.1049   +/-   0.190481
R2                        =     39.2687   +/-   0.256541
A                         =     5.34815   +/-   0.0950282
B                         =   0.00253013   +/-   0.000207522
```

Fitting a function written by the user

```
**********************************************
Minimizer is Minuit / Migrad
Chi2                      =     688.425
NDf                       =          42
Edm                       =  9.5182e-09
NCalls                    =         215
Outer radius              =     61.1049   +/-   0.190485
Inner radius              =     39.2687   +/-   0.256545
Amplitude                 =     5.34815   +/-   0.0950293
Background                =   0.00253013   +/-   0.000207522
```

Code comparison

```
TF1* getFCN() {
    auto phi = [](double t) -> double {
        if (std::abs(t) < 1e-12) return 1.0; // Предел при t→0
        double sin_t = std::sin(t);
        double cos_t = std::cos(t);
        return 3.0 * (sin_t - t * cos_t) / (t * t * t);
    };
// Основная функция I(Q) = A [Φ(QR₁) - (R₂/R₁)³ Φ(QR₂)]² + B
    auto mainFunc = [phi](double* x, double* p) -> double {
        // Параметры:
        // p[0] = A (амплитуда)
        // p[1] = B (фон)
        // p[2] = R1 (внешний радиус)
        // p[3] = R2 (внутренний радиус)
        double Q = x[0]; // Переменная Q
        double QR1 = Q * p[2];
        double QR2 = Q * p[3];
        double ratio = p[3] / p[2];
        double ratio3 = ratio * ratio * ratio;
        double term = phi(QR1) - ratio3 * phi(QR2);
        return p[0] * term * term + p[1];
    };
    // Создание TF1 функции с 4 параметрами
    TF1* func = new TF1("SphericalShell", mainFunc, 0, 100, 4);
    // Установка начальных значений параметров
    func->SetParameter(0, 1.0); // A = 1.0 (временное значение)
    func->SetParameter(1, 0.0); // B = 0.0 (временное значение)
    func->SetParameter(2, 65.0); // R1 = 65
    func->SetParameter(3, 20.0); // R2 = 20
    // Именование параметров для удобства
    func->SetParName(0, "A");
    func->SetParName(1, "B");
    func->SetParName(2, "R1");
    func->SetParName(3, "R2");
    return func;
}
```

user

```
#include <TF1.h>
TF1* getFCN(){
auto fcn = [] (Double_t * x, Double_t * p)
 {
 auto phi = [] ( const Double_t & x )
  {
   Double_t res = 1;
    if ( x )            res = 3 * ( sin(x) - x * cos(x) ) / ( x * x * x );
    return res;
 };
 Double_t q = x[0];
 Double_t r2r1 = p[1]/p[0];
 Double_t res =  phi ( q * p[0] ) - phi ( q * p[1] ) * ( r2r1 * r2r1 * r2r1 );
return p[2] * res * res + p[3];
 };
  TF1* modelFCN = new TF1("SphericalShell", fcn, 0, 1, 4);
  modelFCN->SetParNames("Outer radius", "Inner radius", "Amplitude",
"Background");
 modelFCN->SetParameters(65, 20, 1, 0);
 return modelFCN;}
```

AI

Possible benefits of AI in our app

- Reduced time and resource costs.
- Physicists and biologists can focus on the challenges of scientific problems without spending their time learning C++.
- Artificial intelligence analyze large amounts of data, so it offers optimal approaches for coding. Its work is based on trained models that recognize patterns in millions of lines of code.
- Fewer errors: typos and syntax issues.
- Quick prototyping.

Current problems to be solve

- Switch to the home neural network deployed on the LIT servers.
- Select the optimal LLM (large language model).
- Optimize the prompt to ensure the repeatability of the generated model code.
- Extend the fitter so that it can accept files with the extension .pdf.
- Develop an interface so that the user can add additional instructions to the prompt located inside the fitter.

Thanks for your attention