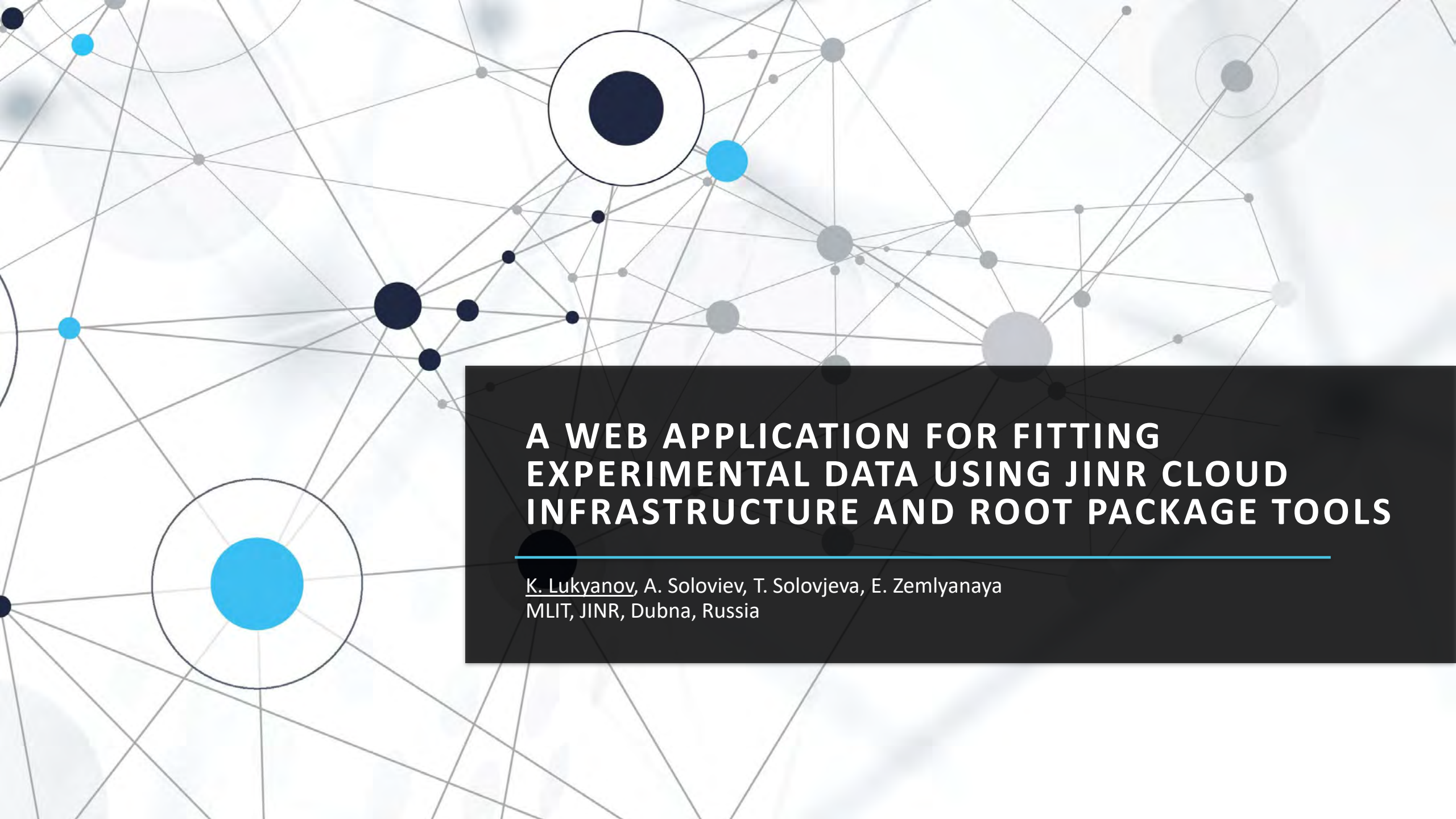


A WEB APPLICATION FOR FITTING EXPERIMENTAL DATA USING JINR CLOUD INFRASTRUCTURE AND ROOT PACKAGE TOOLS

K. Lukyanov, A. Soloviev, T. Solovjeva, E. Zemlyanaya
MLIT, JINR, Dubna, Russia

INTRODUCTION

FITTER

To find the parameters of a theoretical model, it is necessary to minimize the functional, which is a measure of the deviation between the theoretical curve and experimental data. Usually, this is done using the chi-square criterion

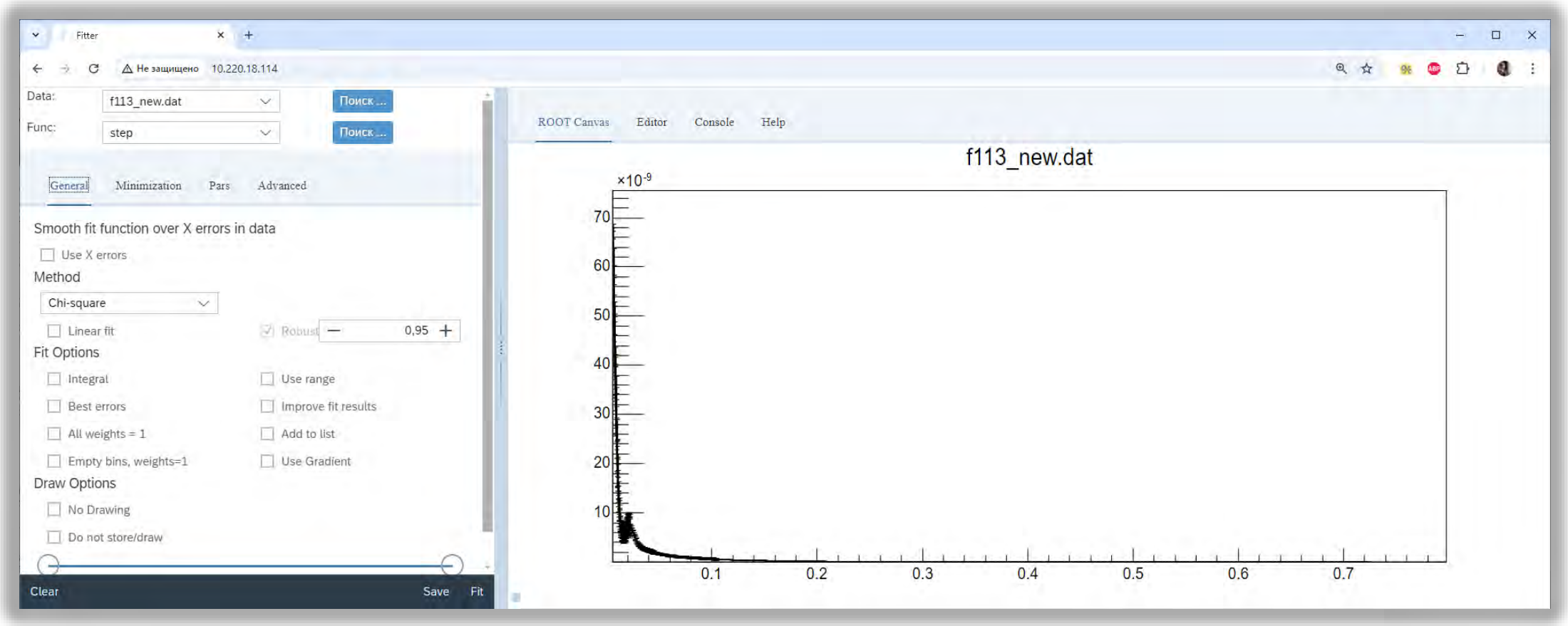
$$\chi^2 = \frac{1}{N - N_{parms}} \sum_{i=1}^{N} \left(\frac{f(x_i) - y_i}{\Delta y_i} \right)^2$$

Processing of data obtained on a small-angle neutron scattering spectrometer makes it possible to analyze the structure of the particles being studied. The shape of the particle is approximated by simple geometric bodies - ellipsoids, cylinders, prisms. The analytical equations for this bodies are part of the FITTER.

Soloviev A.G., Murugova T.N., Islamov A.H. and Kuklin A.I. FITTER. The package for fitting a chosen theoretical multiparameter function through a set of data points. Application to experimental data of the YuMO spectrometer. Journal of Physics: Conference Series, 2012, v. 351, № 12027, p.1-15.

WEB-BASED VERSION OF FITTER

http://fitter.jinr.ru/



Soloviev A.G., Solovjeva T.M., Lukyanov K.V. Deployment of a web application for fitting experimental data in the JINR cloud infrastructure // PEPAN, vol.55, issue 3, pp.627-631, 2024.

WEB-BASED VERSION OF FITTER

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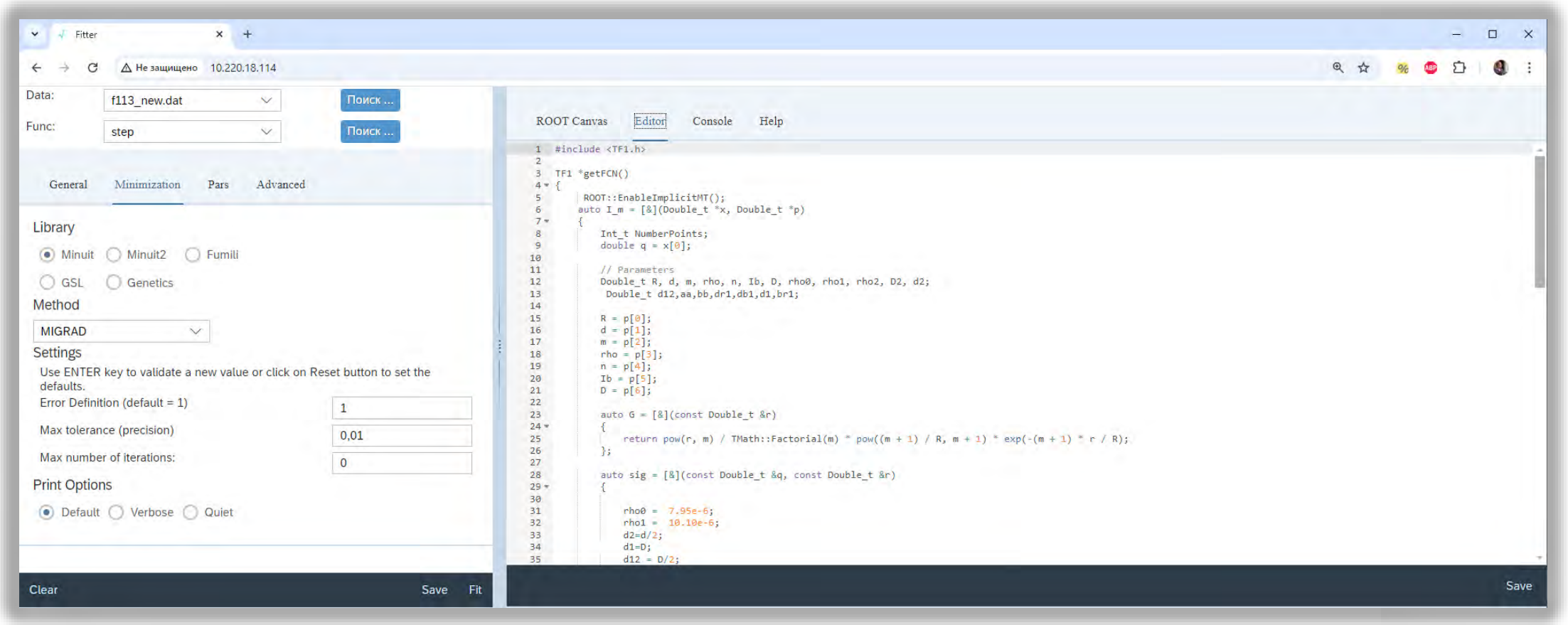

Soloviev A.G., Solovjeva T.M., Lukyanov K.V. Deployment of a web application for fitting experimental data in the JINR cloud infrastructure // PEPAN, vol.55, issue 3, pp.627-631, 2024.

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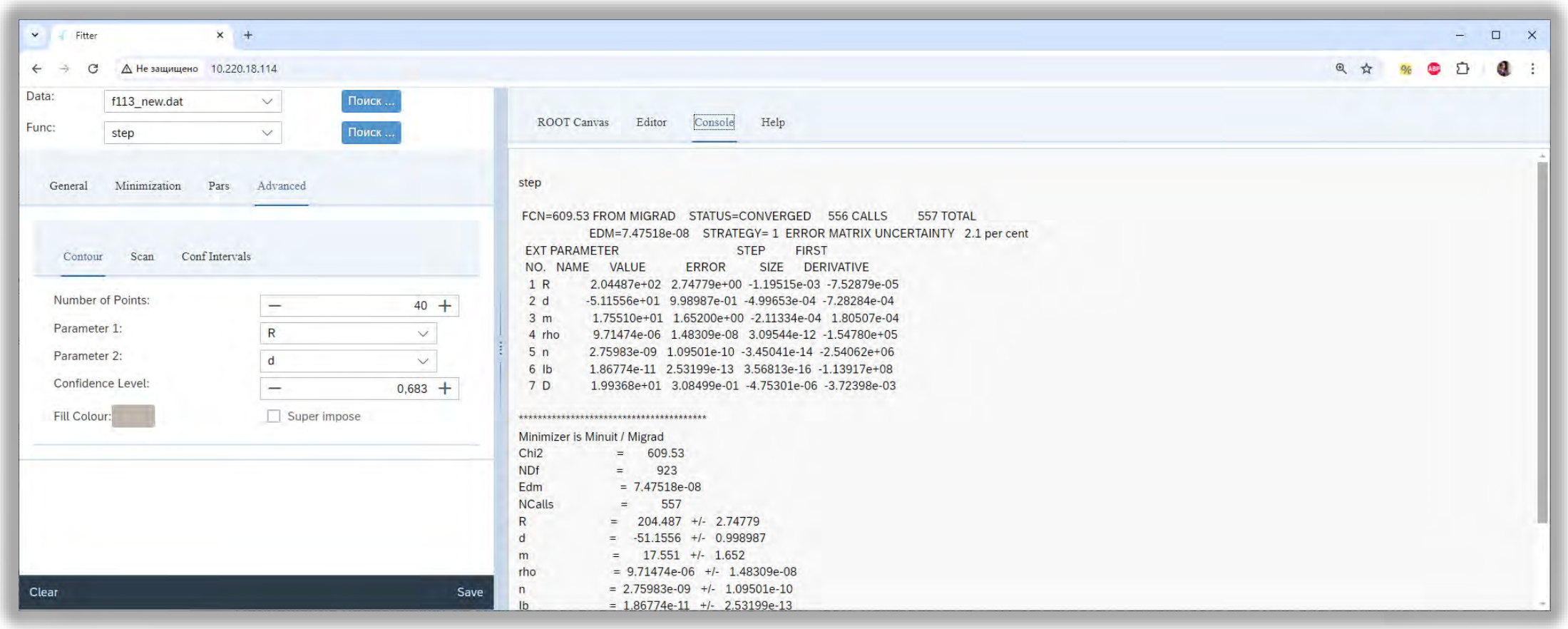
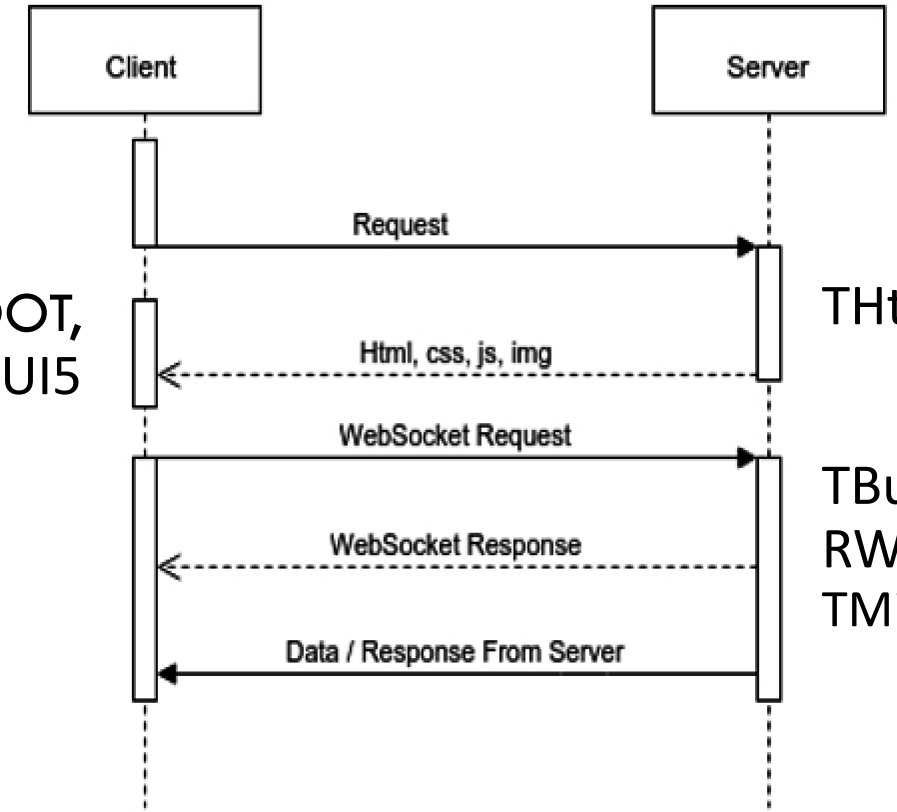


Soloviev A.G., Solovjeva T.M., Lukyanov K.V. Deployment of a web application for fitting experimental data in the JINR cloud infrastructure // PEPAN, vol.55, issue 3, pp.627-631, 2024.

ARCHITECTURE

http://fitter.jinr.ru/



JSROOT,
OpenUI5

THttpServer

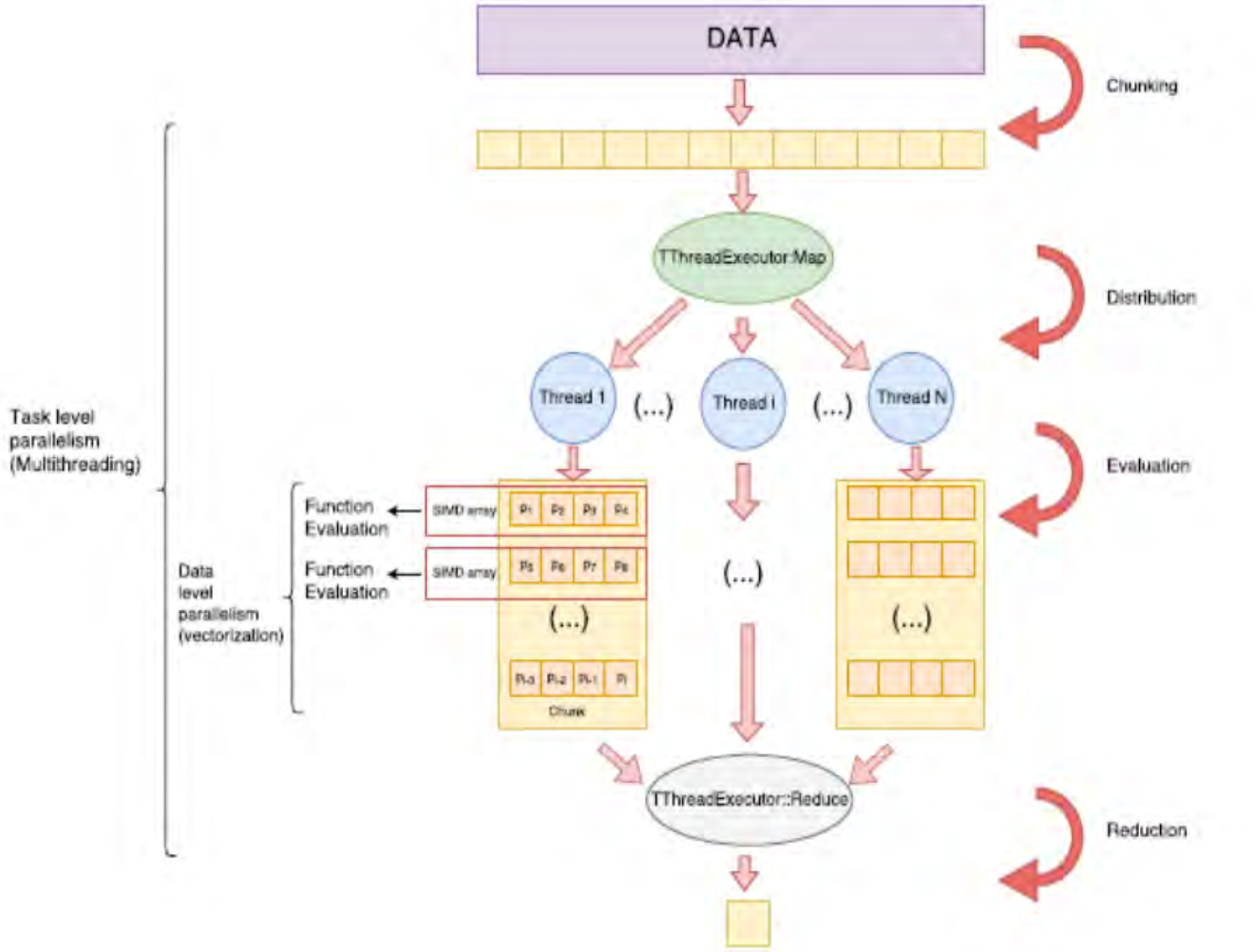
TBufferJSON,
RWebWindow
TMinuit

```
↑ 10:10:0:READY=
↓ 1:10:1:SHOWPANEL:localapp.view.Main
↑ 1:10:1:PANEL_READY
↓ 1:10:1:OPTIONS:{ "_typename" : "ROOT::Experimental::RFitPanelModel", "fTitle" : "", "fDataSet" :
↑ 1:10:0:KEEPALIVE
↑ 0:9:0:KEEPALIVE
↑ 0:8:1:OPTIONS:{"_typename":"ROOT::Experimental::RFitPanelModel","fTitle":"","fDataSet":[{"_type
↑ 0:7:1:DATA: 6.4707398e-03 5.7622315e-08 9.7453739e-09 6.5988727e-03 5.8733149e-08 9.9395
↓ 4:10:1:DATA:{ "_typename" : "TGraphErrors", "fUniqueID" : 0, "fBits" : 1032, "fName" : "f113_new
↓ 0:9:1:OPTIONS:{ "_typename" : "ROOT::Experimental::RFitPanelModel", "fTitle" : "", "fDataSet" : [{
↑ 2:10:0:KEEPALIVE
```

```
1   0:7:1:DATA:   6.4707398e-03   5.7622315e-08   9.7453739e-09
2     6.5988727e-03   5.8733149e-08   9.9395164e-09
3     6.7270063e-03   5.8177527e-08   9.8922512e-09
4     6.8551399e-03   5.6085984e-08   9.6427664e-09
5     6.9832735e-03   5.4336522e-08   9.5603091e-09
6     7.1114071e-03   5.1121204e-08   9.2211981e-09
7     7.2395399e-03   4.9306049e-08   8.9781282e-09
8     7.3676735e-03   4.8772709e-08   8.9811363e-09
9     7.4958071e-03   4.7488745e-08   8.8890914e-09
10    7.6239407e-03   4.5697627e-08   8.6491182e-09
11    7.7520743e-03   4.4534891e-08   8.5005185e-09
12    7.8802072e-03   4.3626876e-08   8.3913524e-09
```

Adamczewski-Musch J., Bellenot B., Linev S. THttpServer and JavaScript in ROOT. GSI Report 2015-1, 508 p. (2015)

PARALLELIZATION



TASK-LEVEL PARALLELISM

- data fragmentation
- distribution and evaluation
- reduction

ACTIVATION

ROOT::EnableImplicitMT()

DATA-LEVEL PARALLELISM

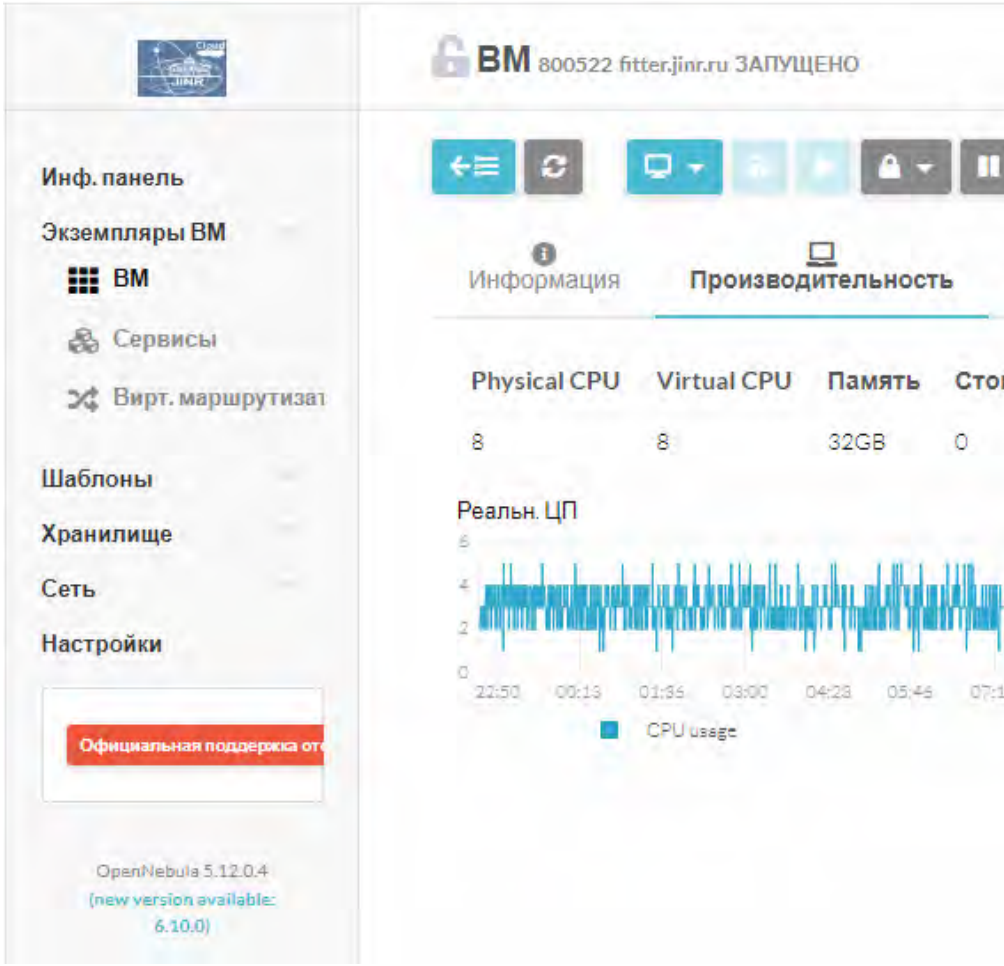
- vectorization of the model function during evaluation

VM AT THE JINR CLOUD INFRASTRUCTURE

- **HARDWARE**
  - 8 cores (CPU Intel Xeon E5-2650 v4 @ 2,20 GHz)
  - 32 Gb RAM
  - 20 Gb SSD

- **SOFTWARE**
  - Ubuntu 22.04.1
  - ROOT 6.24.06
  - FITTER_WEB from https://git.jinr.ru/yumo/fitter-next

- **SECURITY**
  - Public key auth
  - Standart JINR security tests for web-sites passed



COMPARISON OF FITTING CPU TIME

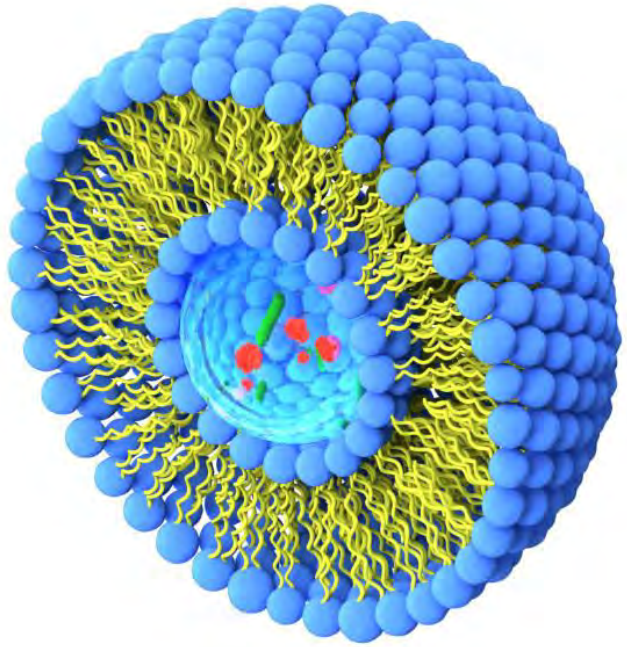
Models of particles of ferromagnetic liquid sample	fitter.jinr.ru 8 cores local	fitter.jinr.ru 8 cores web	hybrilit.jinr.ru 6 cores local	hybrilit.jinr.ru 6 cores web	computer Intel Core™ i9 10 cores local	computer Intel Core™ i9 10 cores web
BallPolydispersity	**0.21** +/- 0.02	**0.22** +/- 0.02	**0.28**+/-0.03	**0.29** +/- 0.05	**0.07**+/-0.01	**0.07** +/- 0.01
Ellipsoid	**39.3** +/- 0.2	**41.5** +/- 0.2	**51.4** +/-0.2	**54.5** +/- 0.3	**19.83** +/- 0.05	**19.97** +/- 0.08
Parallelepiped	**374** +/ -3	**475** +/- 3	**490** +/- 1	**527** +/- 2	**188** +/- 0.5	**186** +/- 0.5

QUESTIONS

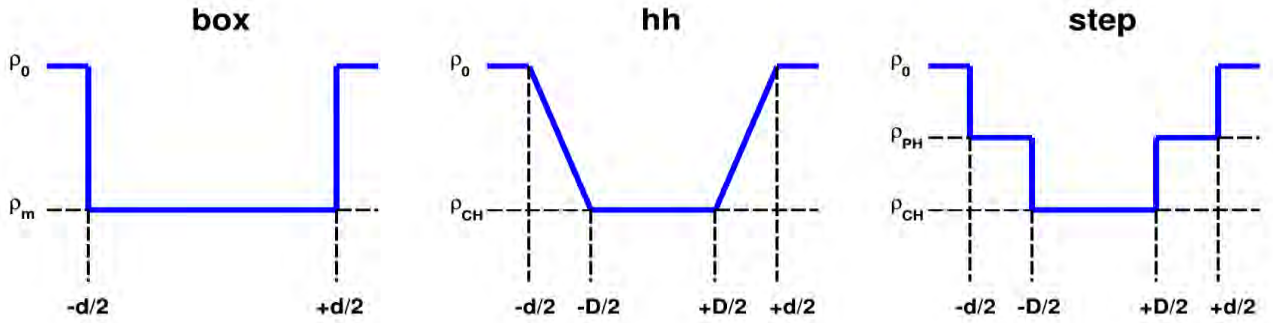
1. Is 8 cores enough? How much cores needed to obtain maximum efficiency?
2. How much memory needed in current and “optimal” configuration? *
3. How multiuser calculations affects the fitter application?
4. What is the balance solution between computing time and the amount of allocated by VM resources?

* N. Balashov, I. Kuprikov, N. Kutovskiy, A. Makhalkin, Ye. Mazhitova, I. Pelevanyuk, R. Semenov, and D. Shpotya. Changes and Challenges at the JINR and Its Member States Cloud Infrastructures. Physics of Particles and Nuclei, 2024, Vol. 55, No. 3, pp. 366–370

METHODOLOGICAL TASK



THE STRUCTURE OF VESICULAR SYSTEMS



Some of parameters:

R – radius of the vesicle
d – bilayer thickness
m – polydispersity coefficient
n – number of vesicles

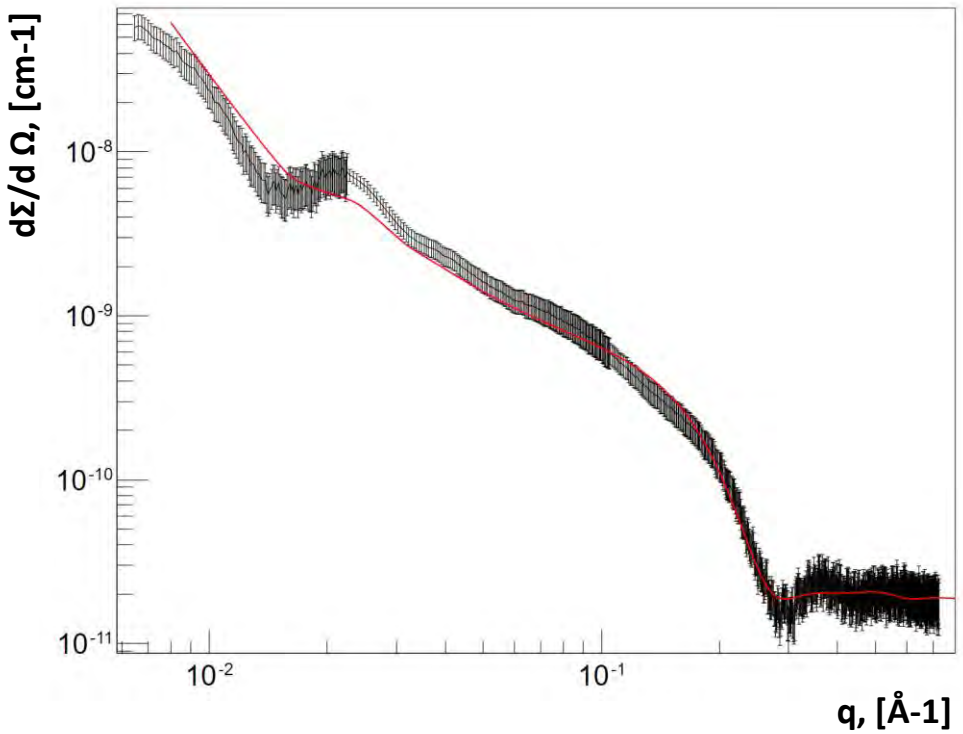
ρ_m – membrane density
ρ_{PH} – density in the area of polar heads
D –hydrophobic thickness

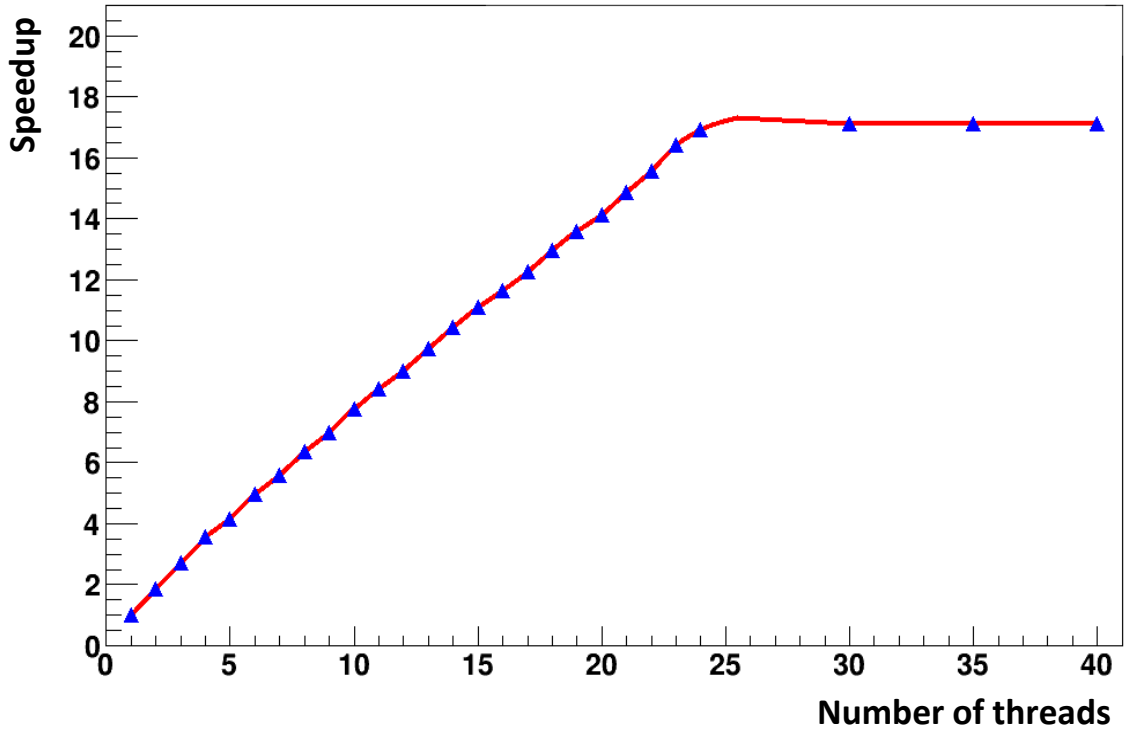
1000 experimental points, ~50 minutes CP in single-threaded mode.

Soloviev A.G., Solovjeva T.M., Zemlyanaya E.V. Proceedings of Parallel computational technologies (PCT'2024), p.158. https://doi.org/10.14529/pct2024

QUESTION 1: NUMBER OF CORES

HARDWARE: 24 cores, 120 Gb RAM. **SOFTWARE – the same**





M. Bashashin, E. Zemlyanaya, M. Kiselev, K.Lukyanov, and K. Turapbay. SFF Analysis of Small Angle Scattering Data from Phospholipid Vesicle Systems: Parallel Implementation and Online Interface. Physics of Particles and Nuclei Letters, 2022, Vol. 19, No. 5, pp. 554–557.

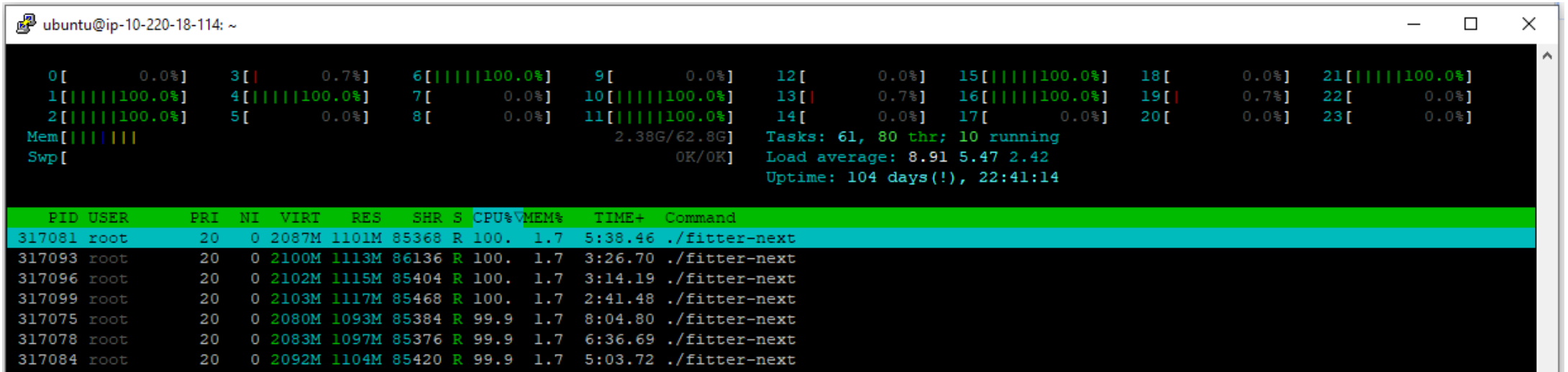
QUESTION 2: MEMORY

	N=230	N=460	N=930
VIRT, MB	**2108**	**2109**	**2114**
RES, MB	**1127**	**1129**	**1136**
CP_1, SEC	**459**	**1494**	**2980**

Each process takes the same amount of memory – about 1GB RAM.

Max number of processes for single fitting procedure = number of cores (24)

Max RAM for single fitting procedure: 24cores * 1GB ~ 24GB



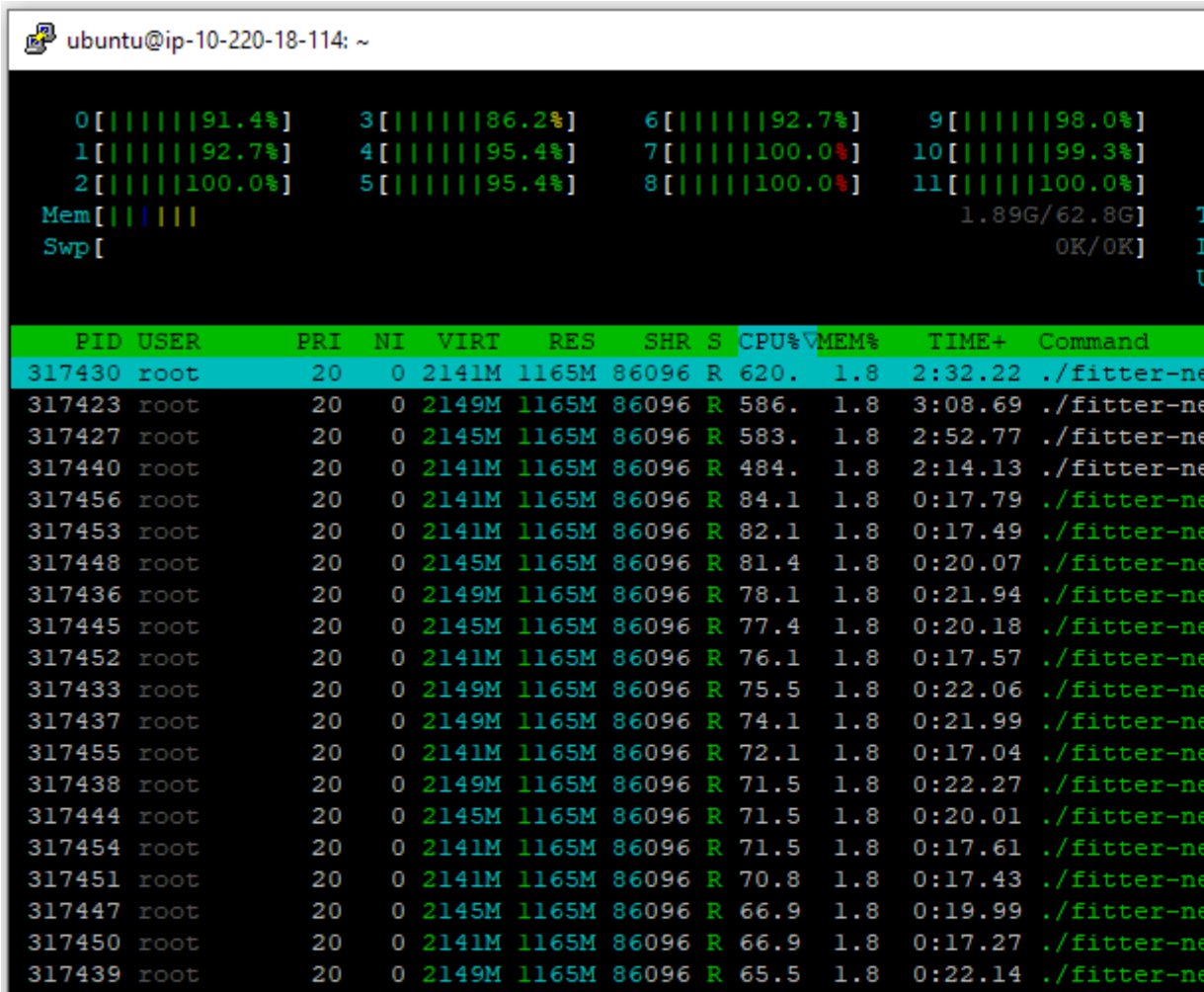
QUESTION 3: MULTIUSER CALCULATIONS

- THttpServer limitation: 10 simultaneous web-threads by default.
- Each web-thread can run the fitting procedure on all cores

  => 240 processes

  => 240GB RAM

  => Unreal, need limitations



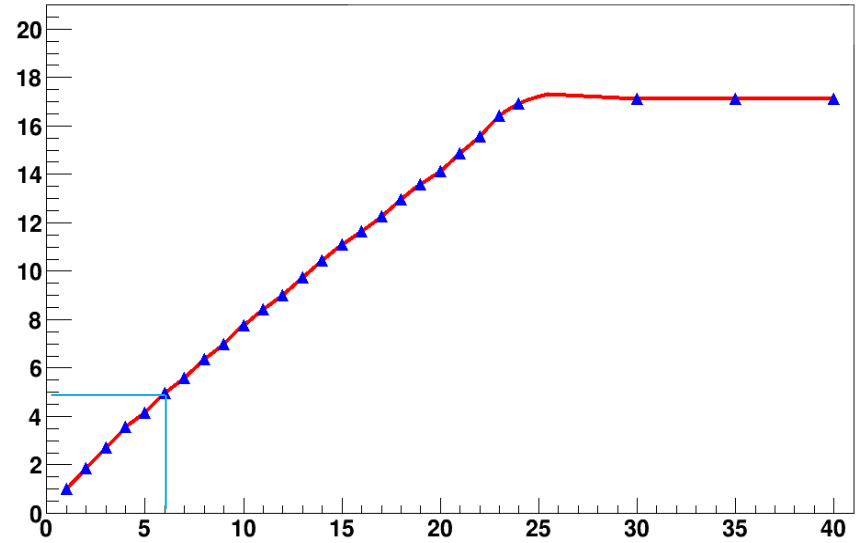
DISCUSSION

LIMITING ASSUMPTIONS:

1. Maximum 2 simultaneous fittings (current usage stats)
2. Calculation time limit of 10 minutes for 1 user

RESOURCE LIMITATIONS (PROJECT):

1. 1-core fit takes about 3000 sec CP (50min)
2. 10 minutes requires 5x speedup => 6 cores; **12 cores** for 2 users
3. 2 parallel fits = 24 server processes => **24 GB RAM (+4GB for operating system)**
4. Limit THttpServer number of **web-threads to 2 (+ 1 reserve)**



R	=	204.487	+/- 2.74779
d	=	-51.1556	+/- 0.998981
m	=	17.551	+/- 1.65201
rho	=	9.71474e-06	+/- 1.48309e-08
n	=	2.75983e-09	+/- 1.09501e-10
lb	=	1.86774e-11	+/- 2.532e-13
D	=	19.9368	+/- 0.308499

Real time 0:04:28, CP time 3021.250

Real time 0:08:57, CP time 3119.410

CONCLUSION

Both methodological calculations and approbation for fitting data in real physical tasks were made using the presented web application. Some links were listed in the footnotes of the slides.

Based on the results of methodological calculations, the following can be stated:

1. A web application implements parallelization quite well, which gives it a certain "margin of safety", allowing it to use processors with a larger number of cores.
2. The minimum amount of memory per 1 process required under different operating conditions of the application is determined.
3. Estimation of the required number of resources (CPU cores and RAM memory) based on the desired time of calculation and number of users is demonstrated.