Development of Python-based tools for modeling the dynamics of systems based on Josephson junctions

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Joint Institute for Nuclear Research

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MLIT - BLTP Joint projects

Main directions

Meshcheryakov Laboratory of Information Technologies, JINR

Rahmonova A. R.
Bashahin M. V.
Balashov N. A.
Zemlyanaya E. V.
Zuev M. I.
Nechaevskiy A. V.
Streltsova O. I.
Sokolov I. A.

Development of algorithms for spintronics problems and high-performance computing

Development of cloud services for mathematical modeling of a system of coupled Josephson junctions

Development of Python tools for mathematical modeling of Josephson structures

Bogoliubov Laboratory of Theoretical Physics, JINR

Shukrinov Yu. M.
Abdelgani M. A.
Kulikov K. B.
Mazanik A.A.
Rahmonov I.R.

ML/DL/HPC Ecosystem in HybriLIT platform

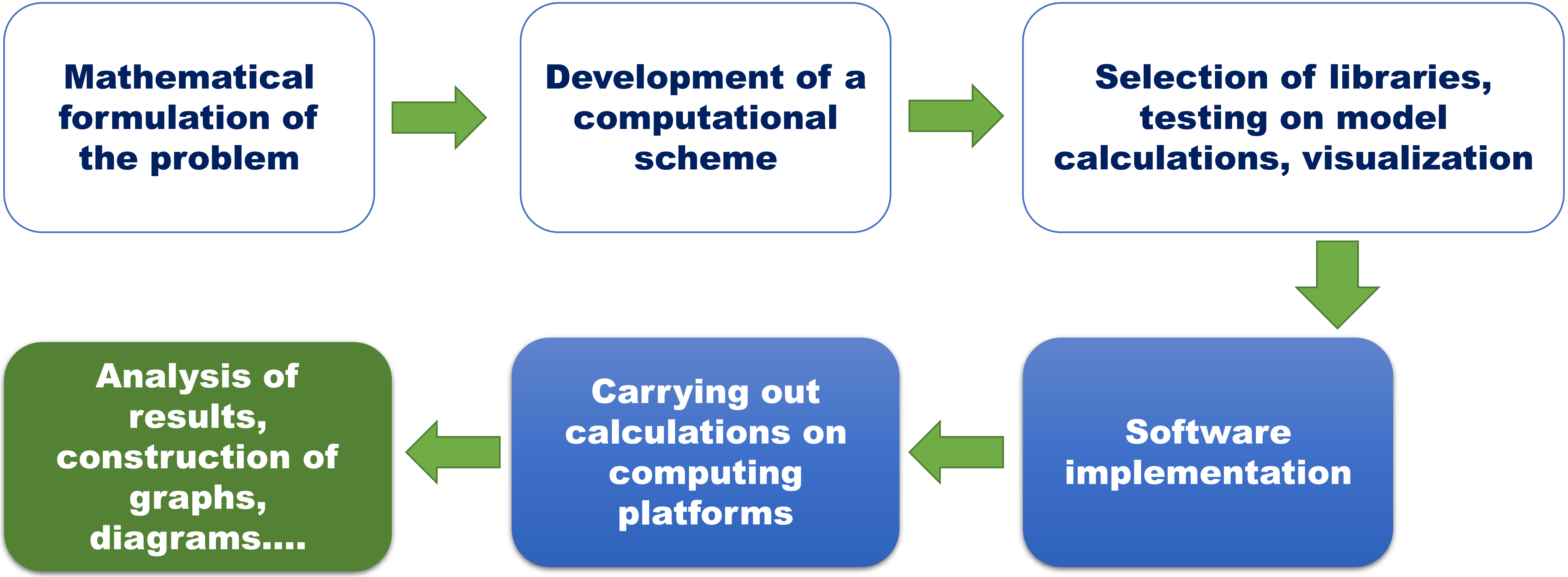
HPClab component
VM with JupyterHub and SLURM [**https://jlabhpc.jinr.ru**]
- ❑ Intel Xeon Gold 6126 (24 Cores @ 2.6 GHz)
- ❑ 32 GB RAM

Educational component
JupyterLab Server [**https://studhub.jinr.ru**]
[**https://studhub2.jinr.ru**]
- ❑ 2x Intel Xeon Gold 6152 (22 Cores @ 2.1 GHz)
- ❑ 512 GB RAM

Computation component
Server with NVIDIA Volta [**https://jhub1.jinr.ru**]
[**https://jhub2.jinr.ru**]
- ❑ 2x Intel Xeon Gold 6148 (20 Cores @ 2.4 GHz)
- ❑ 4x NVIDIA Tesla V100 SXM2 32 GB HBM2
- ❑ 512 GB RAM

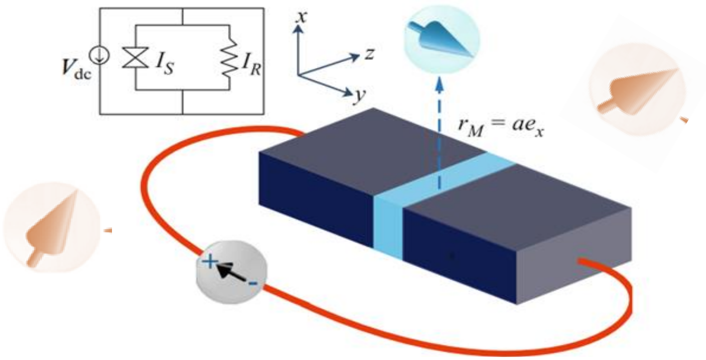
[**https://jhub3.jinr.ru**]
- ❑ 2x Intel Xeon E5 2698v4 (20 Cores @ 2.2 GHz)
- ❑ 8x NVIDIA Tesla V100 SXM2 16 GB HBM2
- ❑ 512 GB RAM

Process of numerical research



Investigation of systems, based on Josephson junctions

Block of Symbolic calculations

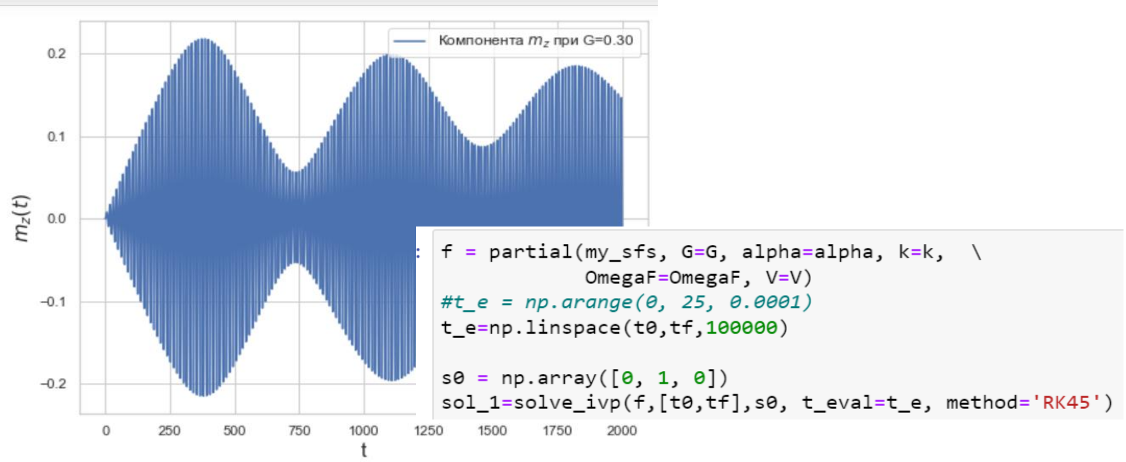


$$\gamma_{m_i} \quad = \quad = -\frac{\mu_0}{2\Phi_0}\int d\mathbf{r}_i \frac{\mathbf{M}_i \times \mathbf{r}_i}{r^3}$$

$$B_{12}(r_{12}, m_1) = \frac{\mu_0}{4\pi}\left(\frac{3(m_1 \cdot \hat{r})\hat{r}}{b^5} - \frac{m_1}{b^3}\right)$$

SymPy is a Python library for symbolic mathematics.

Block of numerical calculations and analysis



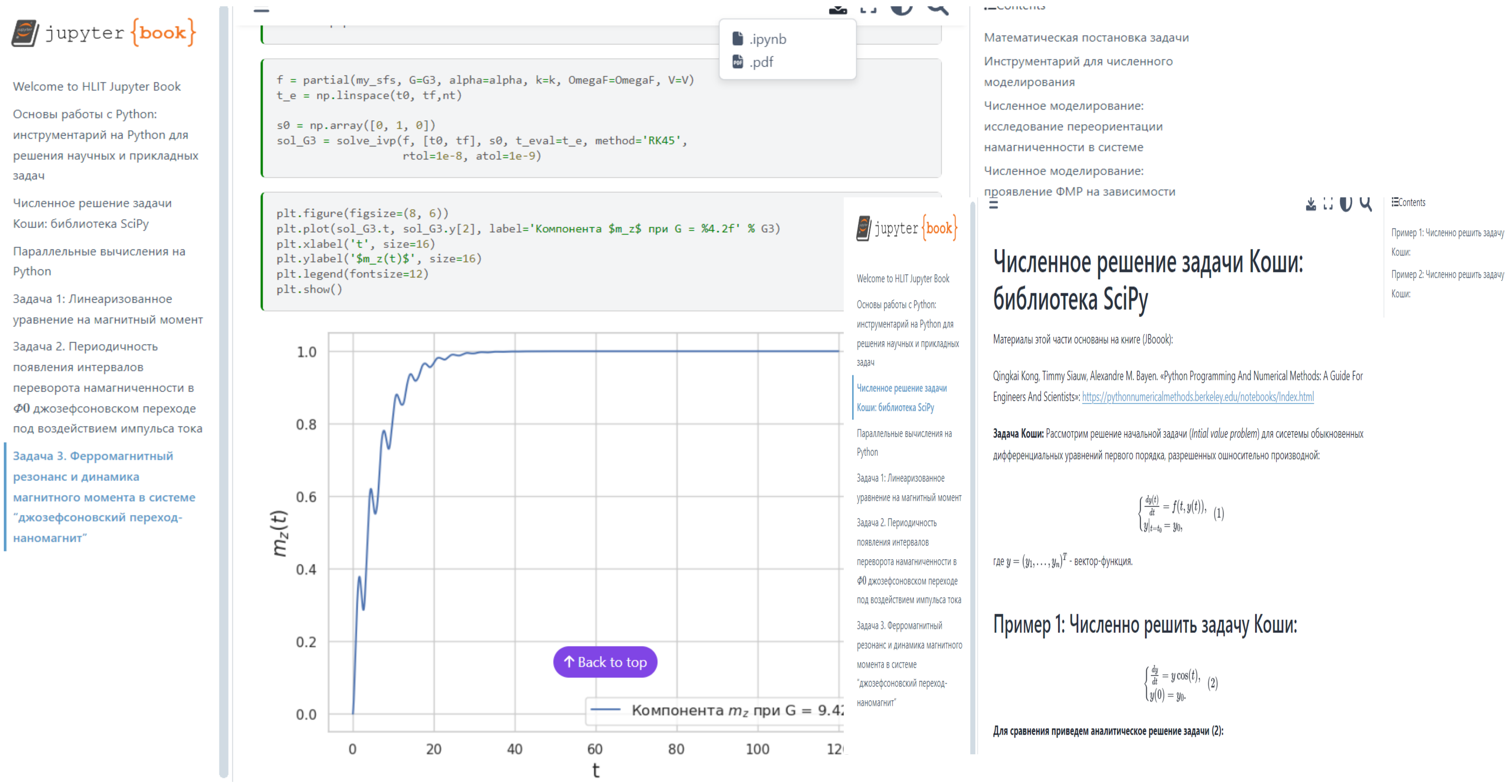
SciPy is an open-source software for mathematics, science, and engineering.

Ускорение многопараметрических расчетов

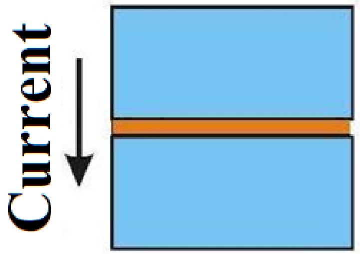
Joblib is a set of tools to provide lightweight pipelining in Python

Numba is an open source JIT compiler that translates a subset of Python and NumPy code into fast machine code.

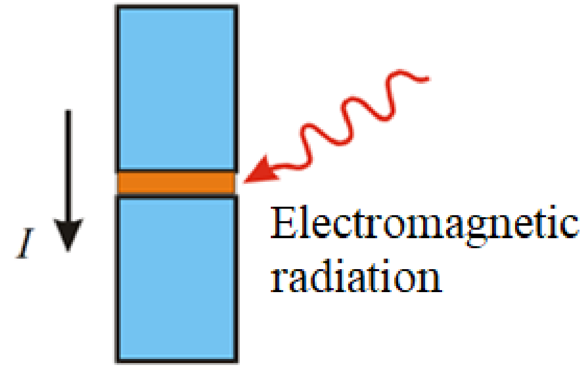
Various possibilities of Jupyter Book



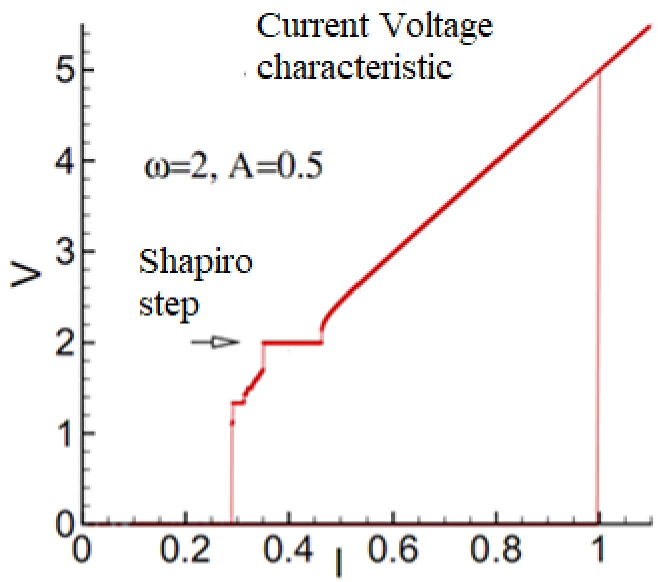
Influence of external radiation on the dynamics of the Josephson junction



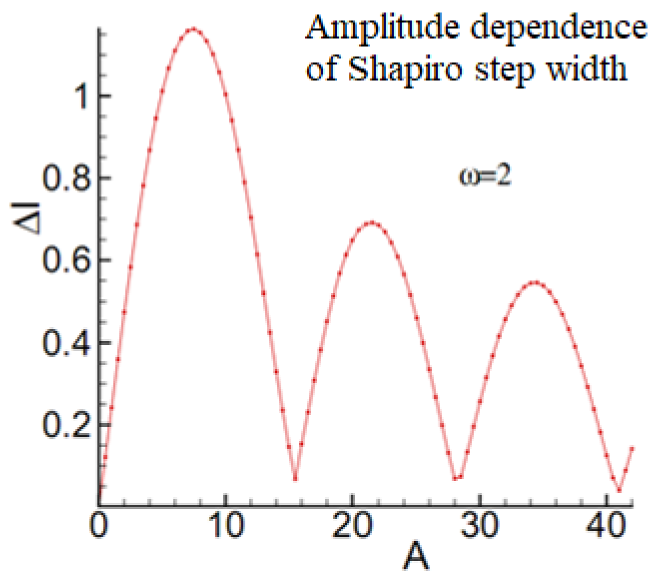
The coupling of two superconducting layers through a thin non-superconducting barrier forms a Josephson junction.



Under the influence of external radiation, provided that the Josephson frequency is a multiple of the radiation frequency (**$n\,\omega_J = k\,\omega$**), a constant voltage step appears on the current-voltage characteristic of the Josephson junction. This step is called the Shapiro step.



The width of the Shapiro step depends on the amplitude and frequency of the radiation.



Dynamical equations for describing of the Josephson junction under the influence of radiation

$$\frac{dV}{dt} = I - \beta V - \sin\varphi + A\sin(u)$$
$$\frac{d\varphi}{dt} = V$$
$$\frac{du}{dt} = \omega$$

Initial condition $t=0, V=0, \varphi=0, u=0$

Tasks

a) Calculation of the current-voltage characteristic of a Josephson junction under the influence of external radiation.
b) Calculation of the amplitude dependence of the width of the Shapiro step

HLIT Jupyter book

Welcome to HLIT Jupyter Book

Python-инструментарий для моделирования динамики джозефсоновского перехода под воздействием внешнего излучения

Вычисляем ВАХ

Задаем значения параметров для вычисления ВАХ

Отметим, что при вычислении необходимо согласовать все временных характеристики с периодом внешнего излучения во избежании накоплении ошибок при усреднении. Для этого нужно вычислить период внешнего излучения $T = 2\pi/\omega$. Из построенных выше графиков видно, что решения стабилизируется после $T_{\min} = 60$ (для $\omega = 2$), это соответствует примерно $T_{\min} = 20T$ (начало интервала для усреднения). Для вычисления ВАХ если выберем временной интервал $T_{\max} = 250$ это будет соответствовать примерно $T_{\max} = 80T$ (максимальное значение времени) и, соответственно, шаг по времени $\Delta t = T/50$.

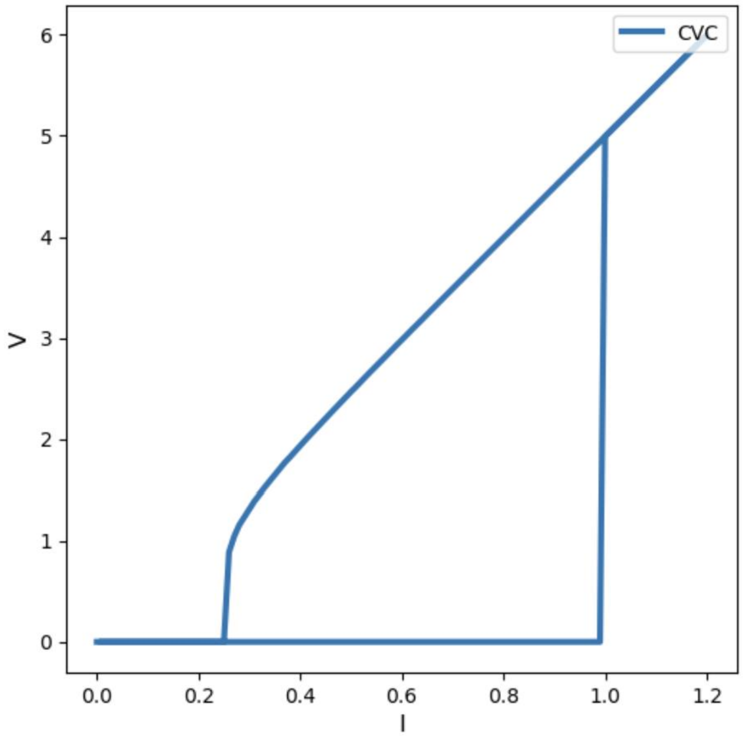
```
T = 2 * np.pi/omega  # Период внешнего излучение
Tmin = 20 * T  # Начало интервала для интегрирования для усреднения
Tmax = 80 * T  # Максимальное значение времени
deltat = T/50  # шаг по времени
ntmin = int(Tmin/deltat)
nt = int(Tmax/deltat)

deltaIext = 0.01
Iext = 0.0
a = 1.0
Iext_max = 1.2
A = 0.5
Vplot = []
Iplot = []
s0 = np.array([0, 0, 0])
```

Введем параметр `Ilimit` ограничивающий интервал изменеия по току для избежания зацикливания

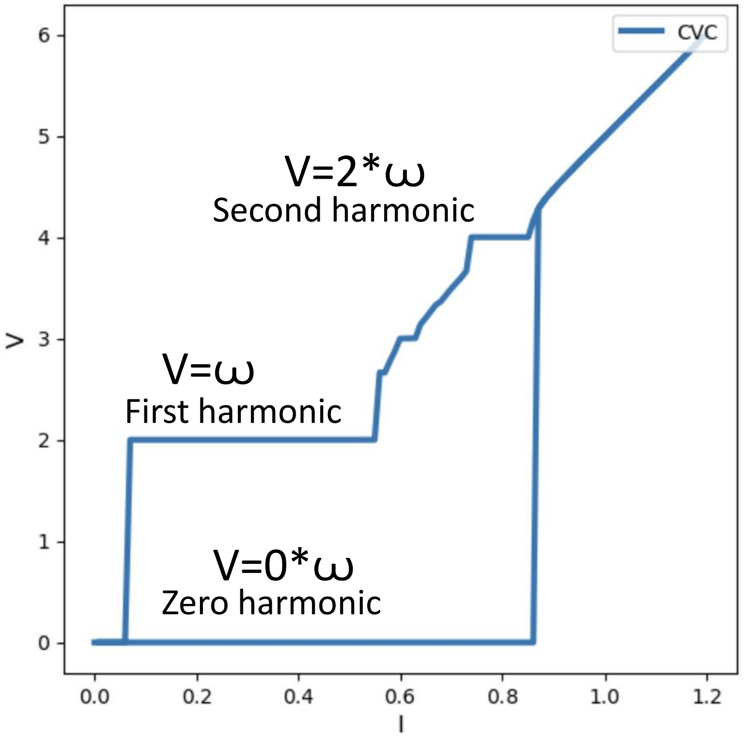
http://studhub.jinr.ru:8080/jjbook/intro.html

Realization of numerical calculations

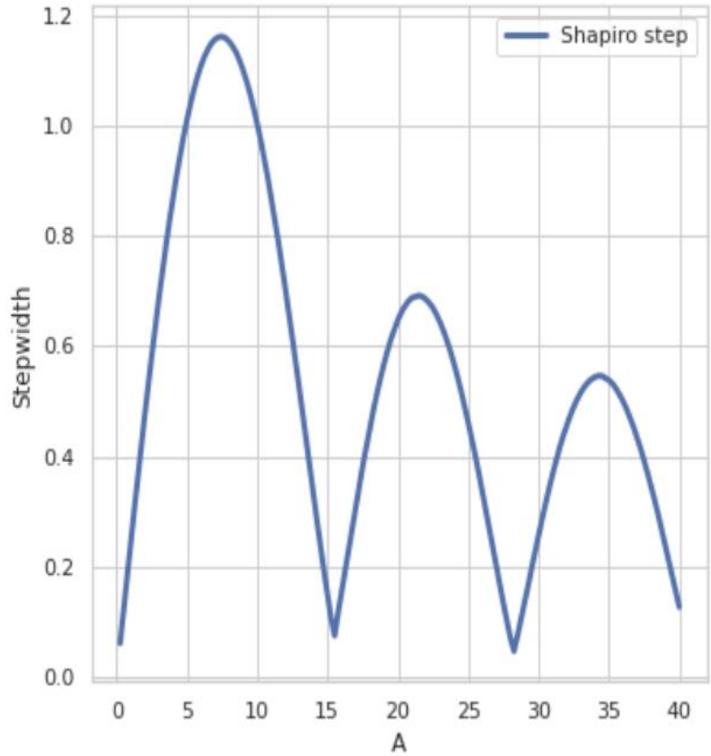
Calculated current-voltage characteristics at ω=2 and amplitude values: A=0, A=3



CVC without radiation

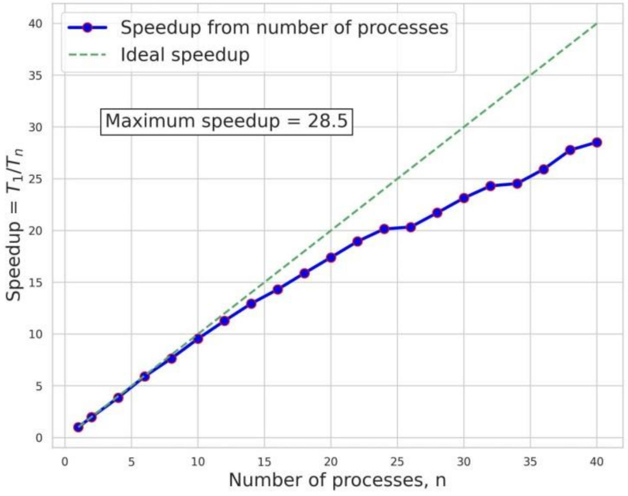


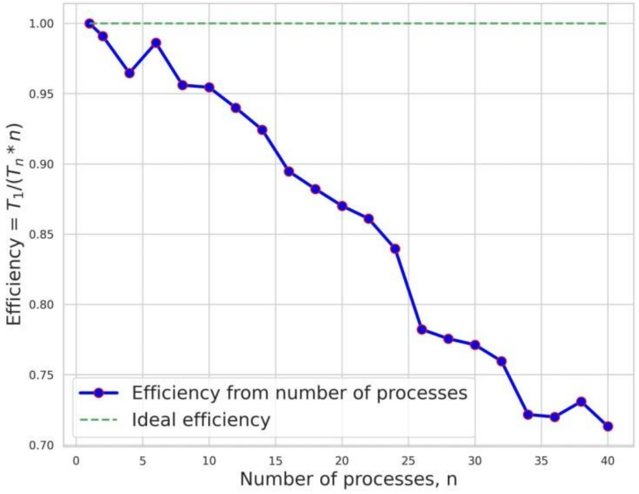
CVC with radiation at ω=2 and A=3



Amplitude dependence of Shapiro step

Acceleration of calculations



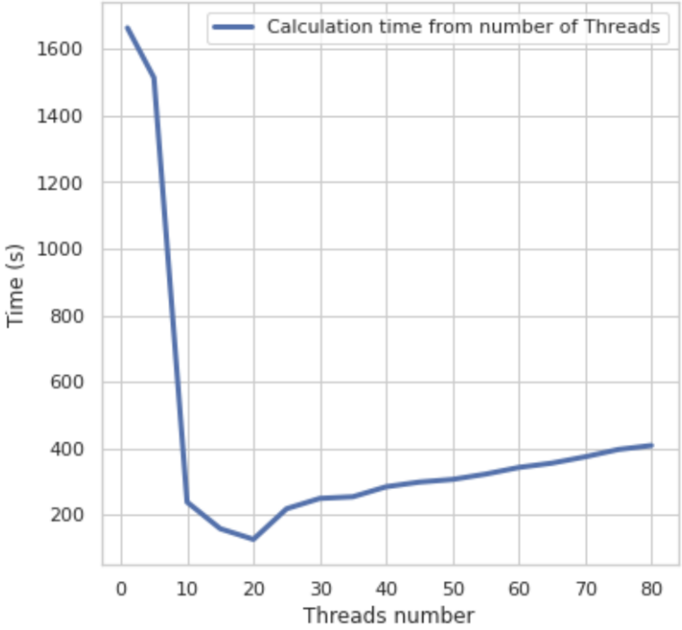


For 160 values of amplitude with stepsize ΔA = 0.25 the duration of the calculation in serial mode was 29 hours. Parallel calculations were carried out using the **Joblib** library. An acceleration of about 28.5 times was obtained when using 40 threads and the calculation time was reduced to 1 hour.

Numba results

Calculations were carried out for the same values as on the previous result, i.e. for 160 amplitude values with a stepsize of ΔA = 0.25 and calculation duration in serial mode was 5 min.

In parallel mode using 20 threads, the calculation time was 26 seconds. Acceleration of calculations - 11 times. Also, if we compare calculation times using Numba, a 70 time acceleration was achieved



Thank you for your attention

Toolkit based on Python libraries and Jupyter ecosystems for solution scientific and applied problems