ML/DL/HPC Ecosystem of the HybriLIT Heterogeneous Platform (MLIT JINR): New Opportunities for Applied Research

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The 6th International Workshop on Deep Learning in Computational Physics (DLCP-2022)
Dubna, JINR, 6-8 July 2022

DATA SCIENCE
IT SCHOOL

Educational program on the MICC

JINR MLIT

Training courses, master classes and lectures

LIT staff and leading scientists from JINR and its Member States

Leading manufacturers of modern computing architectures and software

Parallel programming technologies

OpenMP
MPI
OpenCL
NVIDIA CUDA

Tools for debugging and profiling of parallel applications

Intel Cluster Studio

Work with applied software packages

COMSOL MULTIPHYSICS
ROOT Data Analysis Framework
MATLAB
Wolfram Mathematica
GEANT4
Maple

Frameworks and tools for ML/DL tasks

jupyterhub
TensorFlow
scikit learn
NumPy

Ecosystem for ML/DL/HPC tasks

Development component

VM with JupyterHub
https://jhub.jinr.ru

jupyterhub

VM:
CPU: 24 Cores
RAM: 32 GB

Keras
TensorFlow
learn
NumPy
pandas

Computation component

Servers with
NVIDIA
Volta & Intel Xeon Gold
https://jhub2.jinr.ru

Dell Volta specs:
GPU: 4x Nvidia Volta V100-SXM2 NVLink 32Gb HBM2
CPU: 2x Intel(R) Xeon(R) Gold 6148 CPU @ 2.40GHz 20 Cores/40 Threads
RAM: 512 GB DDR4 2666MHz
SSD: 2*240 GB

HPClab component

VM with
JupyterHub and SLURM
https://jlabhpc.jinr.ru/

jupyterhub

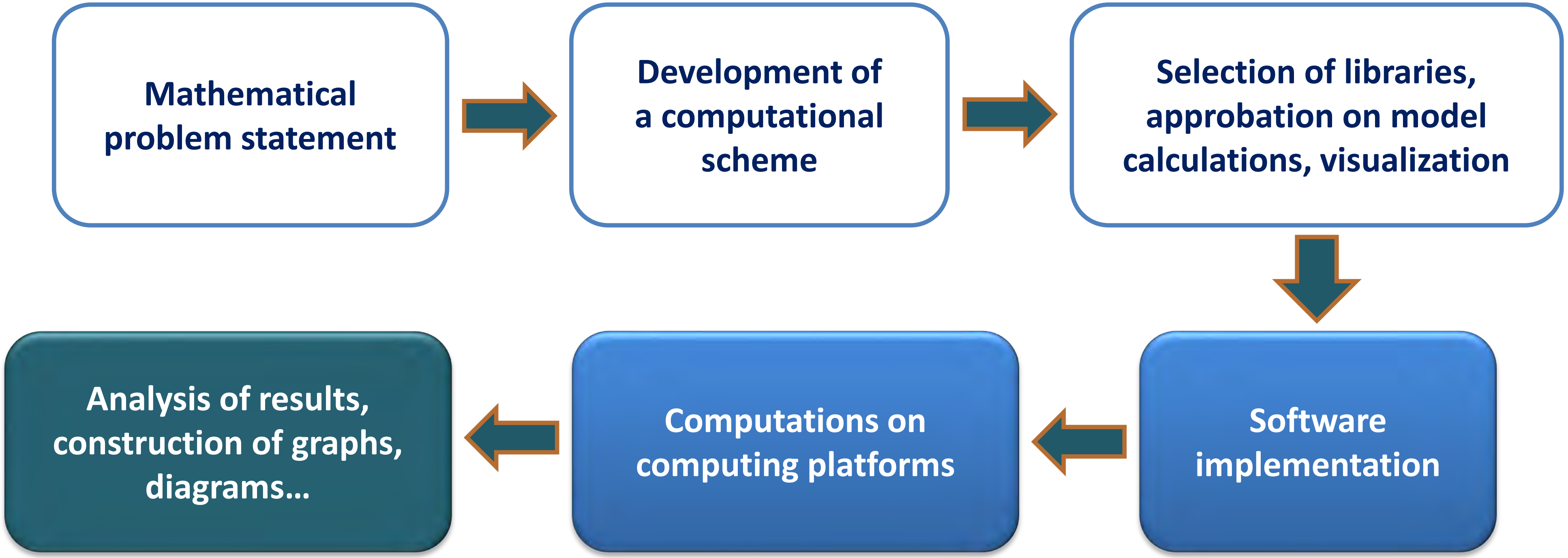
VM:
CPU: 24 Cores
RAM: 64 GB

Keras
TensorFlow
learn
NumPy
pandas

High **P**erformance **C**omputing

Relevance of the work

Numerical research process



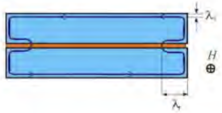
The creation of a toolkit that allows one to carry out computations, to visualize the results within a single application, and perform the most resource-intensive calculations in parallel is an urgent task.
The *Jupyter Notebook* environment provides this capability.

Developed services

saas.jinr.ru

- Long Josephson junctions stack simulation
- Superconductor-Ferromagnetic-Superconductor Josephson junction simulation
- Annular Array of JJs average
- Long Josephson junction coupled with the ferromagnetic thin film
- Stack of short JJ with LC shunting
- Stack of short JJ

$$\begin{cases} \frac{\partial \varphi}{\partial t} = V, \\ \frac{\partial V}{\partial t} = \frac{\partial^2 \varphi}{\partial x^2} - \sin\varphi - \beta V + I. \end{cases}$$



$$\varphi(x,t)|_{t=0} = 0, \quad \left.\frac{\partial \varphi(x,t)}{\partial t}\right|_{t=0} = 0.$$

граничные условия

$$\left.\frac{\partial \varphi(x,t)}{\partial x}\right|_{x=0} = H_{ext}, \quad \left.\frac{\partial \varphi(x,t)}{\partial x}\right|_{x=L} = H_{ext}$$

Manual

JINR cloud SaaS

This work is supported by the Russian Science Foundation under grant #18-71-10095

JINR CLOUD SERVICE
for scientific and engineering computations

Sign in via JINR Single Sign-On

Demo

This work is supported by the Russian Science Foundation under grant #18-71-10095

Job parameters

Physical parameters

B_c: 25
G: 0.1
r: 0.1
α: 0.1
ω_p: 0.5

Parameters of external radiation ☐

Calculational parameters

T_{max}: 1000
T_i: 100
Δt: 0.005
I_0: 0.01
I_{max}: 1.5
I_{min}: 0
I_{break}: 0
I_{noise}: 0
I_{more1}: 0.1
I_{more2}: 0.9
ΔI_0: 0.005
ΔI_i: 0.0005

Resources

- JINR cloud
- HybriLIT cluster

Number of VMs: 10/20 — 1
CPU per VM: 15/22 — 1
RAM per VM (GB): 27/41 — 1

../		
Idisp.dat	02-Apr-2021 11:04	32K
Iq.dat	02-Apr-2021 11:04	32K
Is.dat	02-Apr-2021 11:04	32K
Is_w_down.dat	02-Apr-2021 11:04	32K
Is_w_up.dat	02-Apr-2021 11:03	0
Isum.dat	02-Apr-2021 11:04	32K
Voltage.dat	02-Apr-2021 11:04	32K
initial_cond.dat	02-Apr-2021 11:05	184K
m_Tf.dat	02-Apr-2021 11:05	48K
m_max_w_down.dat	02-Apr-2021 11:05	75K
m_max_w_up.dat	02-Apr-2021 11:03	8192
mx_max_I_down.dat	02-Apr-2021 11:05	52K
mx_max_I_up.dat	02-Apr-2021 11:03	8192
my_max_I_down.dat	02-Apr-2021 11:05	52K
my_max_I_up.dat	02-Apr-2021 11:03	8192
mz_max_I_down.dat	02-Apr-2021 11:05	50K
mz_max_I_up.dat	02-Apr-2021 11:03	8192
sfsjj.836337.err	02-Apr-2021 11:02	99
sfsjj.836337.log	02-Apr-2021 11:05	1594
sfsjj.836337.out	02-Apr-2021 11:05	36K

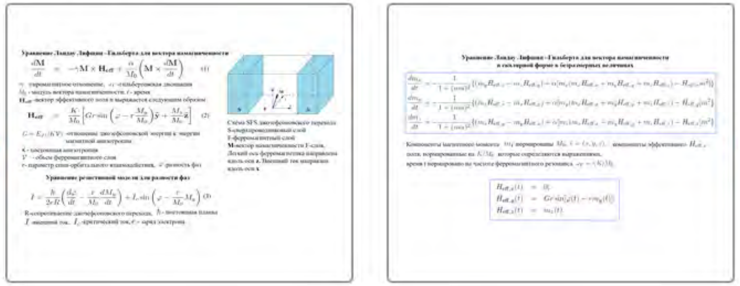
Developed services

sconduct.jinr.ru

Главная | Демо модели | Публикации | Войти

Расчет временной динамики сверхпроводник/ферромагнит/сверхпроводник

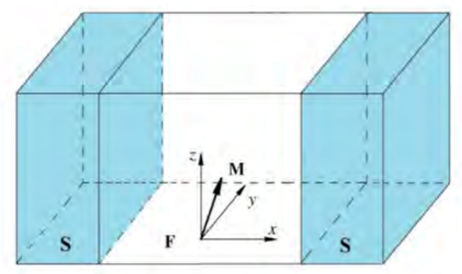
Справочные материалы



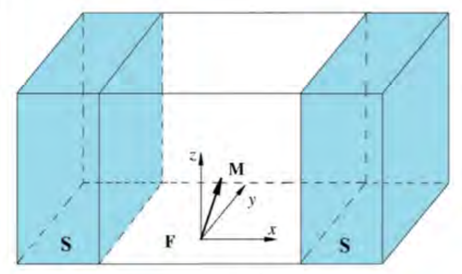
Параметры модели

α	0.1
G	8
r	0.1
ω	1
As	1.5
dt	6

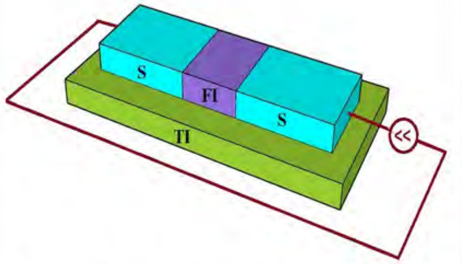
Примеры реализованных алгоритмов:



Временная зависимость



Параметрическая зависимость



Зависимость переворота магнитного момента от dt и As

Выбранный файл: my_time.dat

0.000000	0.000000000000000
0.010000	0.000000000000000
0.020000	0.000000000000000
0.030000	0.000000000000000
0.040000	0.000000000000000
0.050000	0.000000000000000
0.060000	0.000000000000000
0.070000	0.000000000000000
0.080000	0.000000000000000
0.090000	0.000000000000000
0.100000	0.000000000000000
0.110000	0.000000000000000
0.120000	0.000000000000000
0.130000	0.000000000000000
0.140000	0.000000000000000
0.150000	0.000000000000000
0.160000	0.000000000000000
0.170000	0.000000000000000
0.180000	0.000000000000000
0.190000	0.000000000000000
0.200000	0.000000000000000
0.210000	0.000000000000000
0.220000	0.000000000000000
0.230000	0.000000000000000
0.240000	0.000000000000000
0.250000	0.000000000000000
0.260000	0.000000000000000
0.270000	0.000000000000000
0.280000	0.000000000000000
0.290000	0.000000000000000
0.300000	0.000000000000000
0.310000	0.000000000000000
0.320000	0.000000000000000
0.330000	0.000000000000000
0.340000	0.000000000000000
0.350000	0.000000000000000
0.360000	0.000000000000000
0.370000	0.000000000000000

Полученные файлы:

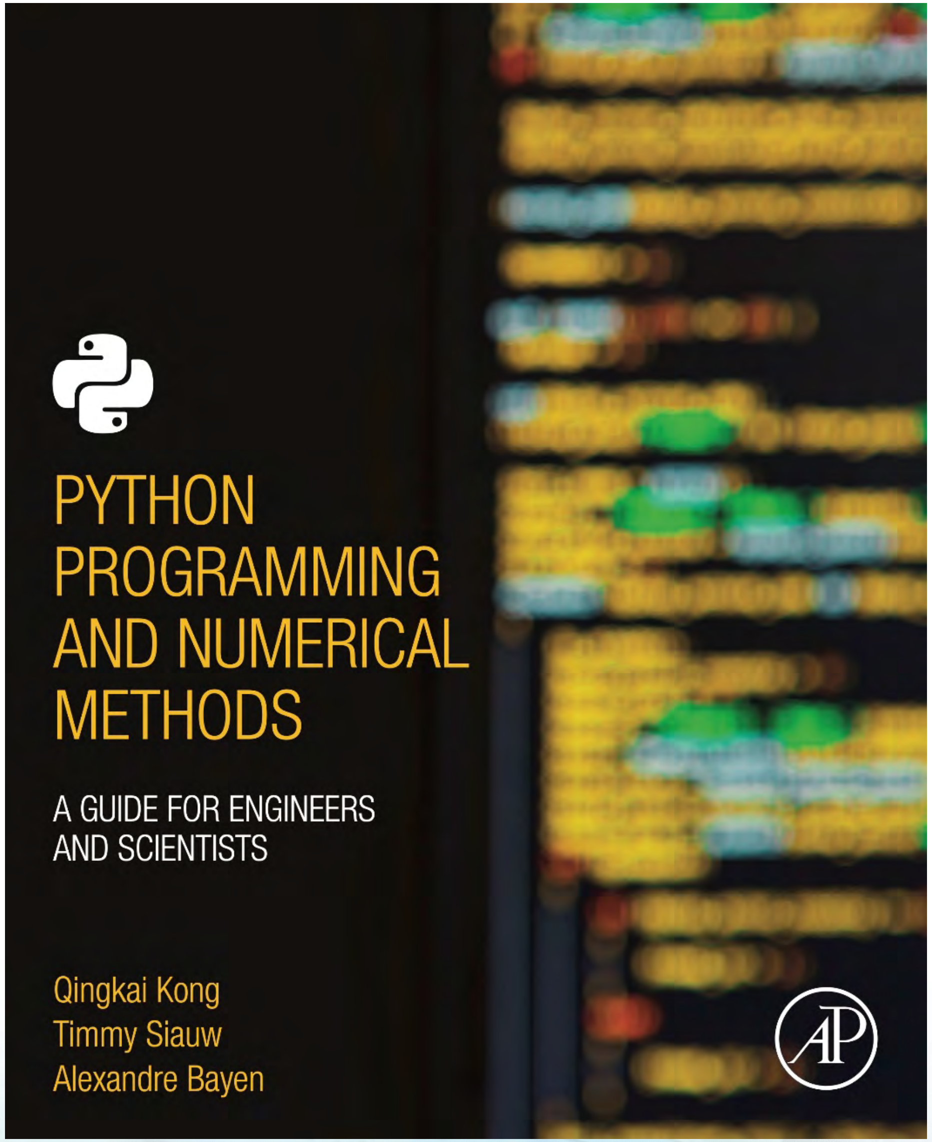
mz_time.dat | mx_time.dat | my_mx.dat | mz_mx.dat | my_time.dat | mz_my.dat

Выбранный файл: **my_time.dat**

Просмотреть файл | Построить график

Python Numerical Methods

pythonnumericalmethods.berkeley.edu



jupyter {book}

jupyter

Keras

matplotlib

pandas

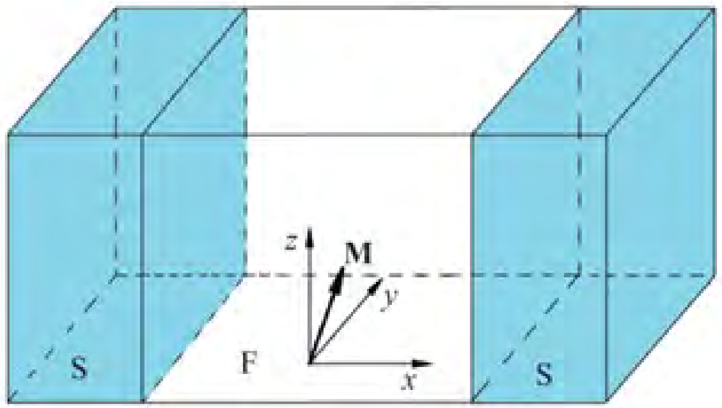
NumPy

seaborn

Joblib

Example 1. Problem to study the dynamics of magnetization in a Phi-0 Josephson Junction (SFS structure)

Collaboration with Ilhom Rahmonov (Bogoliubov Laboratory of Theoretical Physics, JINR)



The dynamics of the magnetic moment M of the system under consideration is described by the Landau-Lifshitz-Gilbert equation:

$$\frac{dm_x}{dt} = -\frac{1}{1+M^2\alpha^2}\{m_y H_z - m_z H_y + \alpha[m_x(M,H) - H_x]\},$$
$$\frac{dm_y}{dt} = -\frac{1}{1+M^2\alpha^2}\{m_z H_x - m_x H_z + \alpha[m_y(M,H) - H_y]\}$$
$$\frac{dm_z}{dt} = -\frac{1}{1+M^2\alpha^2}\{m_x H_y - m_y H_x + \alpha[m_z(M,H) - H_z]\},$$

$M = [m_x, m_y, m_z]$ are the magnetic moment components; the effective field components $H = [H_x, H_y, H_z]$ depend on the Josephson phase difference ϕ and are defined as follows:

$$H_x(t) = 0,$$
$$H_y = Gr\sin(\phi(t) - tm_y(t)),$$
$$H_z(t) = m_z(t).$$

The equation for the Josephson phase difference $\phi(t)$ is determined from the equation for the electric current I flowing through the Josephson junction, measured in units of the critical current I_c:

$$\frac{d\phi}{dt} = -\frac{1}{w}\left(\sin(\phi - rm_y) + r\frac{dm_y}{dt}\right) + \frac{1}{w}I,$$

Model parameters:
G – ratio of the Josephson energy to the magnetic anisotropy energy;
r – spin-orbit interaction constant;
α – Hilbert dissipation parameter;
in this study $w = 1$.

Example 1. Python implementation

Calculations for different values of parameters

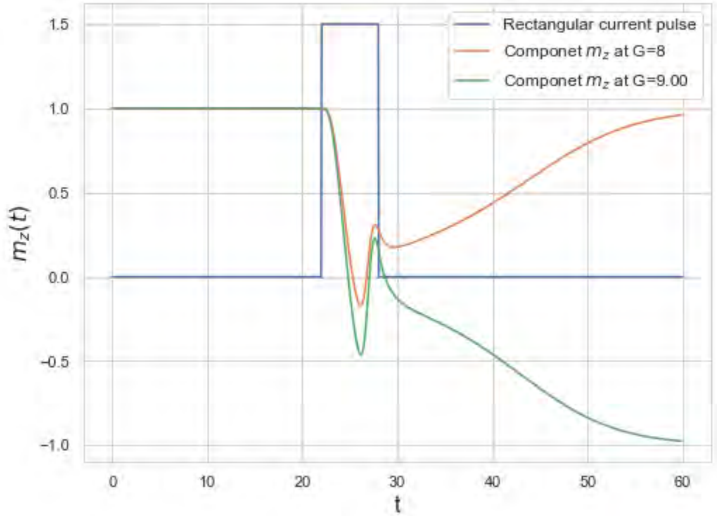
To analyze the possibility of reversing the magnetic moment of the ϕ_0-Josephson junction at different values of the parameters, we will carry out calculations for G=8.9.

```
from scipy.integrate import solve_ivp
from functools import partial
```

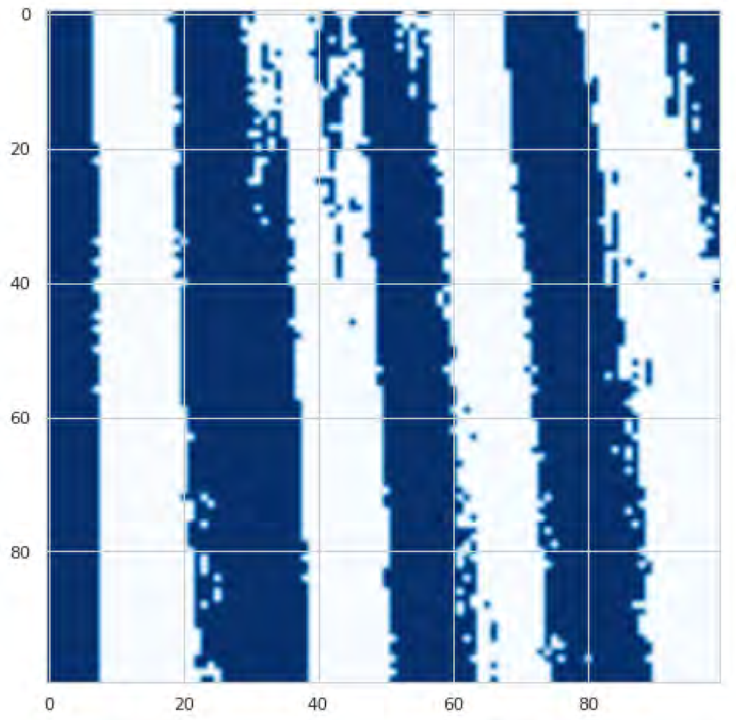
```
G=9
f = partial(my_sfs,  G=G, r=r, alpha=alpha, \
                As=As, t_s=t_s, delta_t=delta_t)
#t_e = np.arange(0, 25, 0.0001)
t_e=np.linspace(0,60,1000)

s0 = np.array([0, 0, 1, 0])
sol_2=solve_ivp(f,[0,60],s0, t_eval=t_e) # method = 'Radau'
```

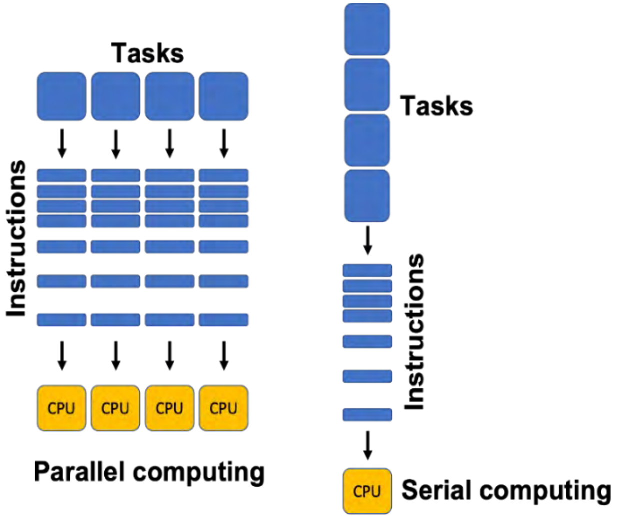
```
plt.figure(figsize = (8, 6))
plt.plot(t_e,y_I,  label= 'Rectangular current pulse')
plt.plot(sol_1.t, sol_1.y[2], label= 'Componet $m_z $ at G=8' )
plt.plot(sol_2.t, sol_2.y[2], label= 'Componet $m_z $ at G=%4.2f' %G)
plt.xlabel('t', size=16)
plt.ylabel('$m_z(t)$', size=16)
plt.legend(fontsize=12)
plt.show()
```




```
#plt.figure(figsize = (8, 6))
fig, ax1 = plt.subplots(figsize=(8, 8))
# mask out the negative and positve values, respectively
#Zpos = np.ma.masked_less(alpG[:,:,0], 0)
Z1 = Zc.reshape(N, N)
plt.imshow(Z1, interpolation='bilinear', cmap='Blues')
#plt.contourf(X, Y, Zc, 100)
#fig.colorbar(Zc, ax=ax1)
plt.show()
```



Example 1. Parallel implementation with Python



Define a function called by each process

```python
from joblib import Parallel, delayed
import numpy as np
```

```python
def funk_parall(k):
    i=k%N
    j=k//N
    mz_sol=0
    G=G0+delta_G*i
    alpha=alpha0+delta_alpha*j
    f = partial(my_sfs, G=G, r=r, alpha=alpha, \
                As=As, t_s=t_s, delta_t=delta_t)
    t_e=np.linspace(0,60,1000)
    s0 = np.array([0, 0, 1, 0])
    sol_i=solve_ivp(f,[0,60],s0, t_eval=t_e) # method = 'Radau'
    if sol_i.y[2][999] < 0:
        mz_sol= -1
        # alpGxy[i+j*N,2] =- 1
    return mz_sol
```

Serial mode calculation

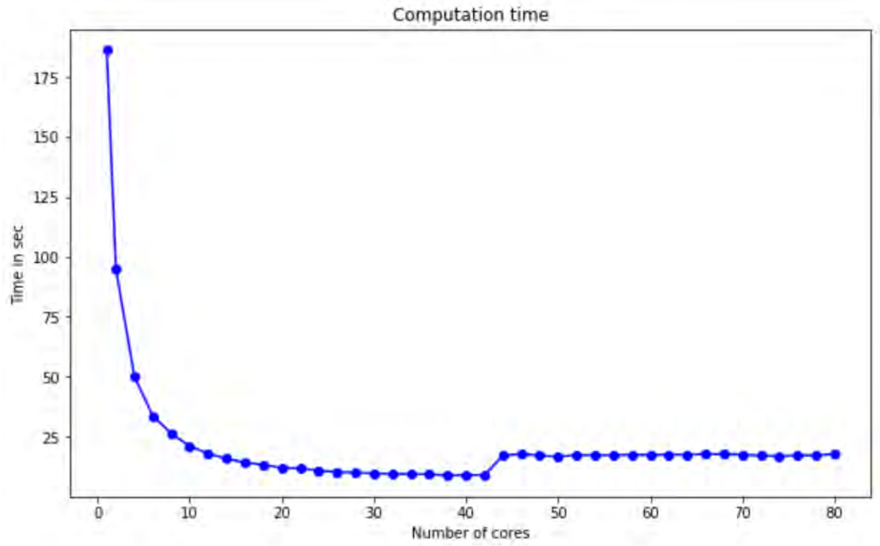
```python
t0 = time.time()
rez= Parallel(n_jobs=1)\
    (delayed(funk_parall)(k) for k in range(N*N) )
t1 = time.time()
print(f'Execution time {t1 - t0} s')
```

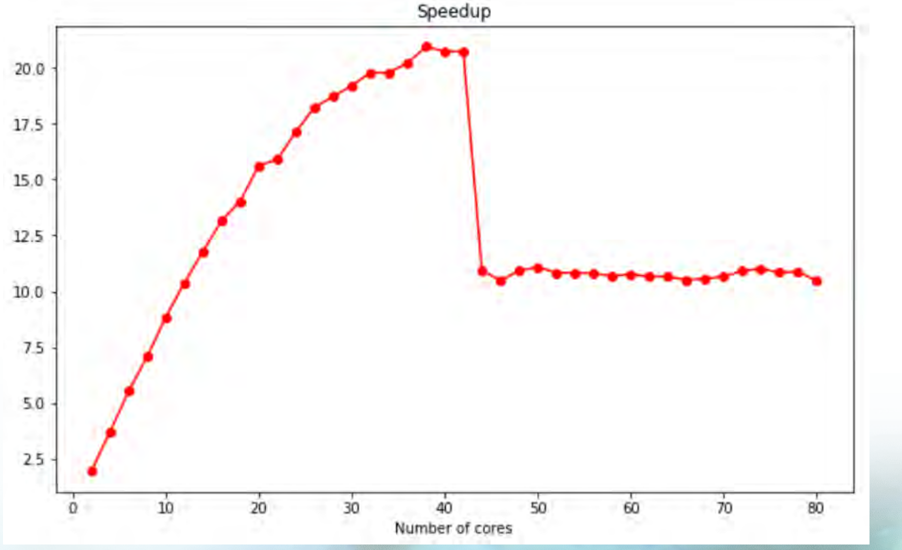
```
Execution time 159.9254457950592 s
```

Computing in Parallel Mode

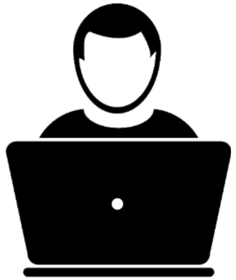
```python
t0 = time.time()
rez= Parallel(n_jobs=6)\
    (delayed(funk_parall)(k) for k in range(N*N) )
t1 = time.time()
print(f'Execution time {t1 - t0} s')
```

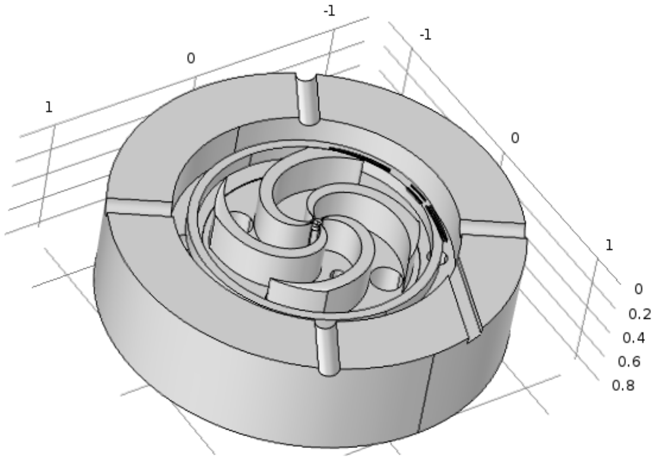
```
Execution time 34.51503801345825 s
```



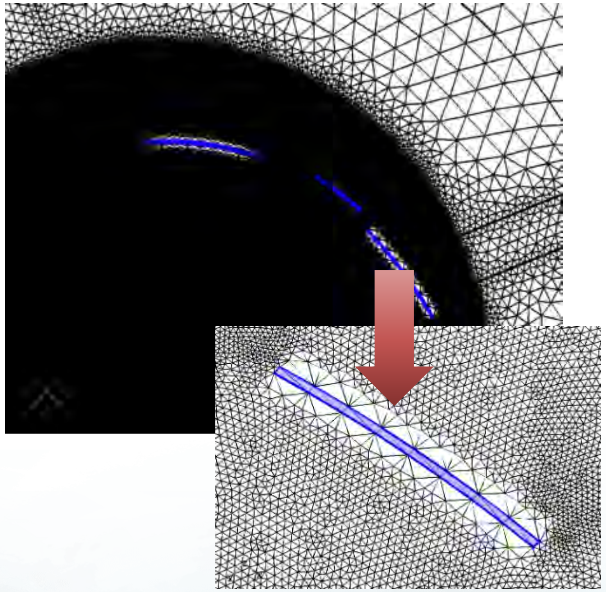


HLIT-VDI – Virtual desktops system

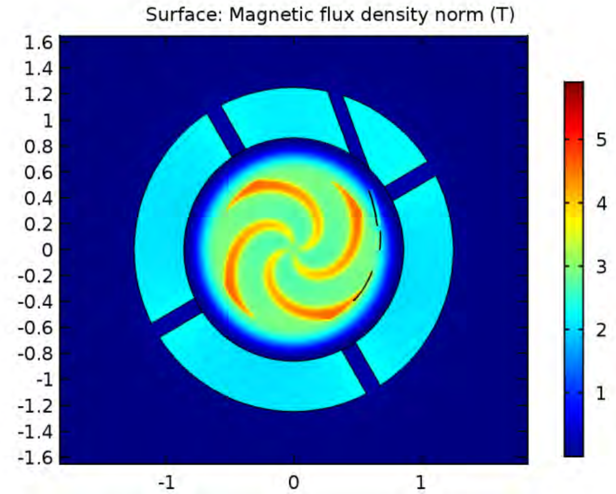




Superconducting magnet SC200 designed for medical application



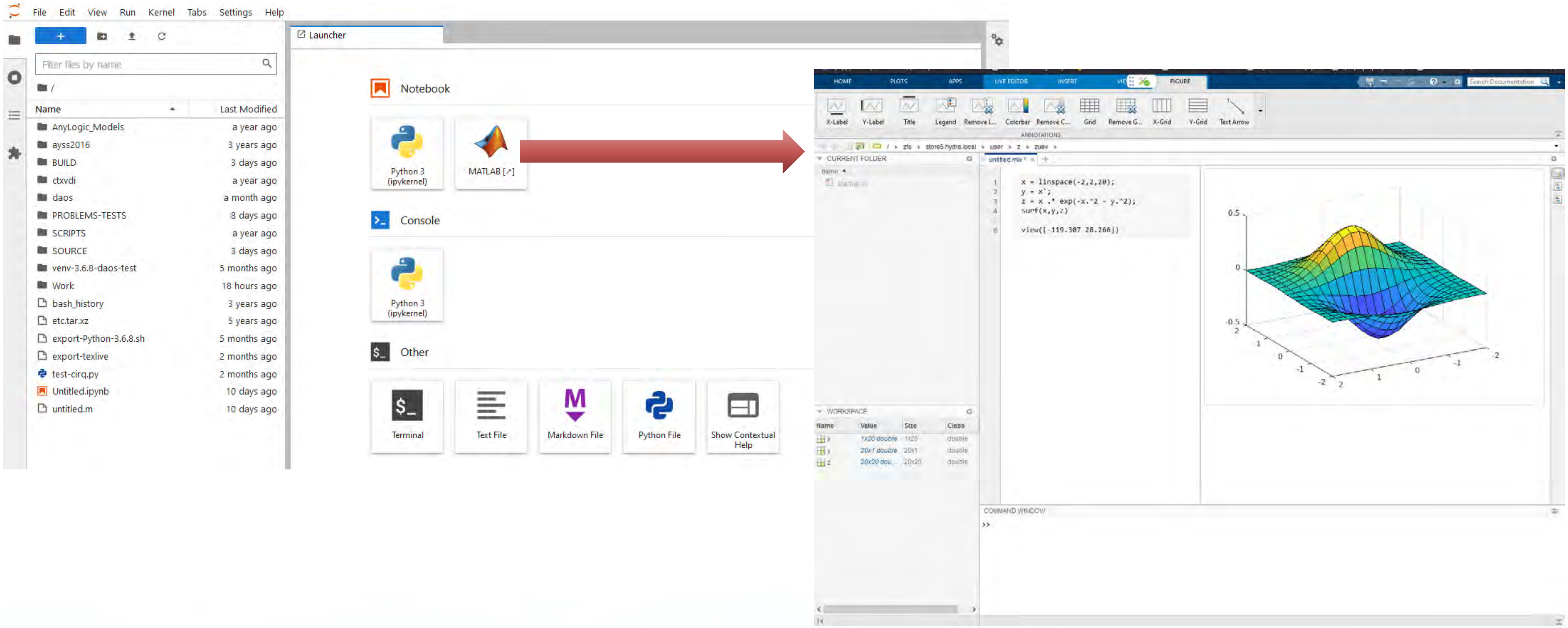
Computational mesh



Magnetic field distribution at median plane of the magnet

Example 2. MATLAB Integration for Jupyter *

https://jhub2.jinr.ru

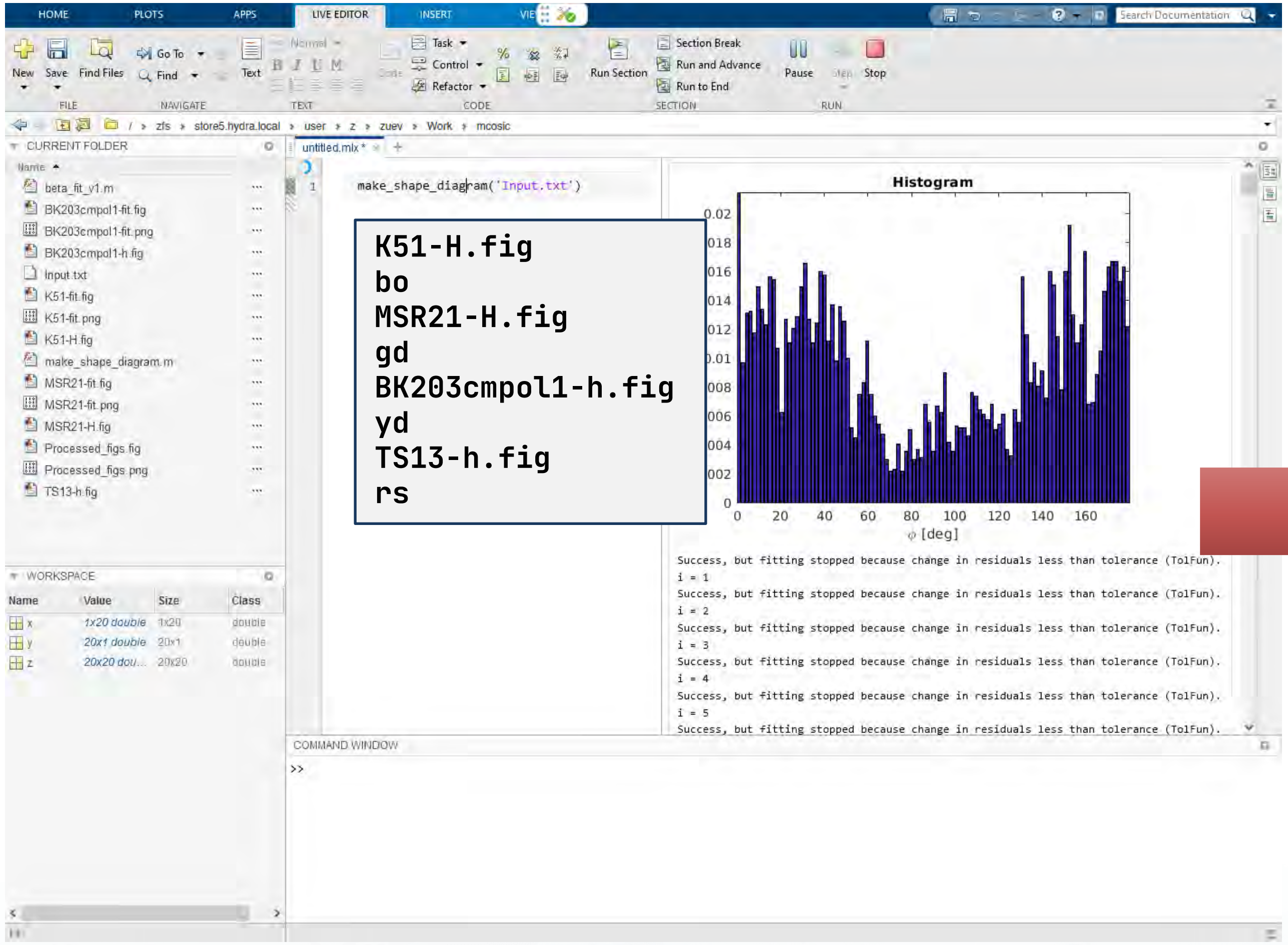


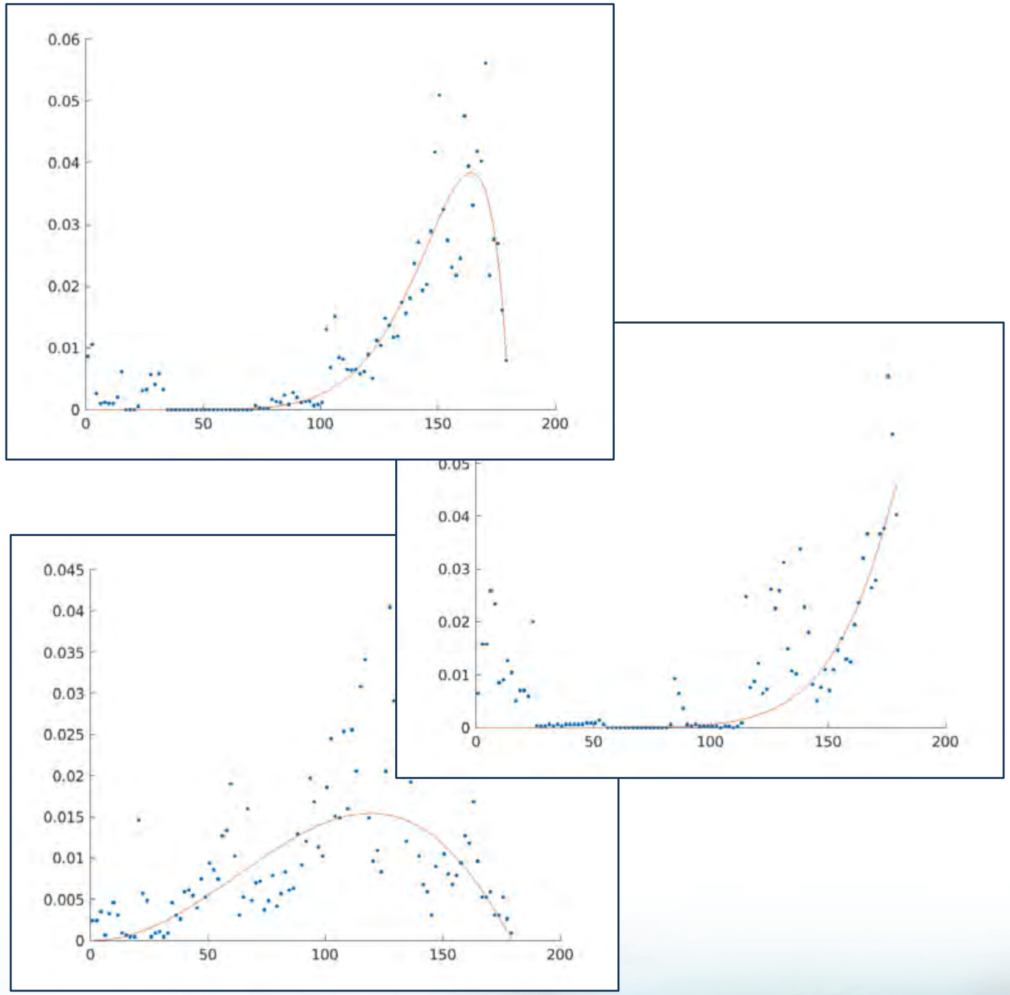
* https://www.mathworks.com/products/reference-architectures/jupyter.html

Example 2. MATLAB Integration for Jupyter

Collaboration with Marko Ćosić (Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia)

https://jhub2.jinr.ru





Thanks for your attention!

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