Enabling Grids for E-sciencE

Porting fusion applications for Russian Data Intensive Grid

Nikolay MARUSOV, Vlad NEVEROV,

Konstantin DYABILIN

RRC "Kurchatov Institute",

Moscow Engineering Physics Institute

EGEE 4th User Forum/OGF25 & OGF-Europe's 2nd International Event

2-6 March 2009, Catania, Sicily, Italy

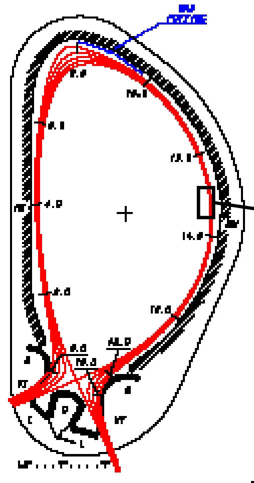
www.eu-egee.org

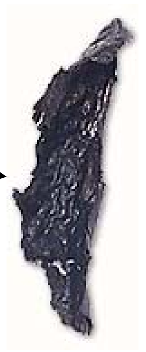
Information Society

Application 1

X-ray diffraction by carbon nanotubes

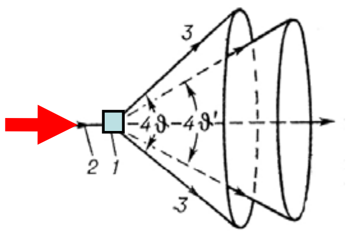
Experiment



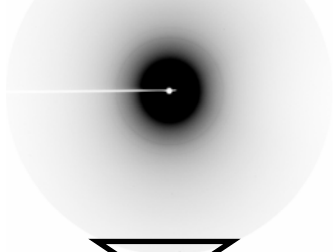


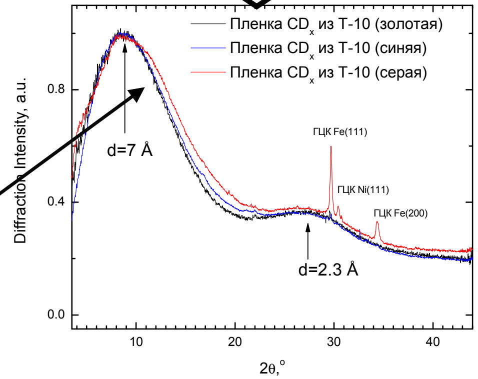
Film deposit on the inner wall of tokamak vacuum chamber

Wavelength 1 Å



Angular distribution of X-ray diffraction at Kurchatov Institute synchrotron radiation source





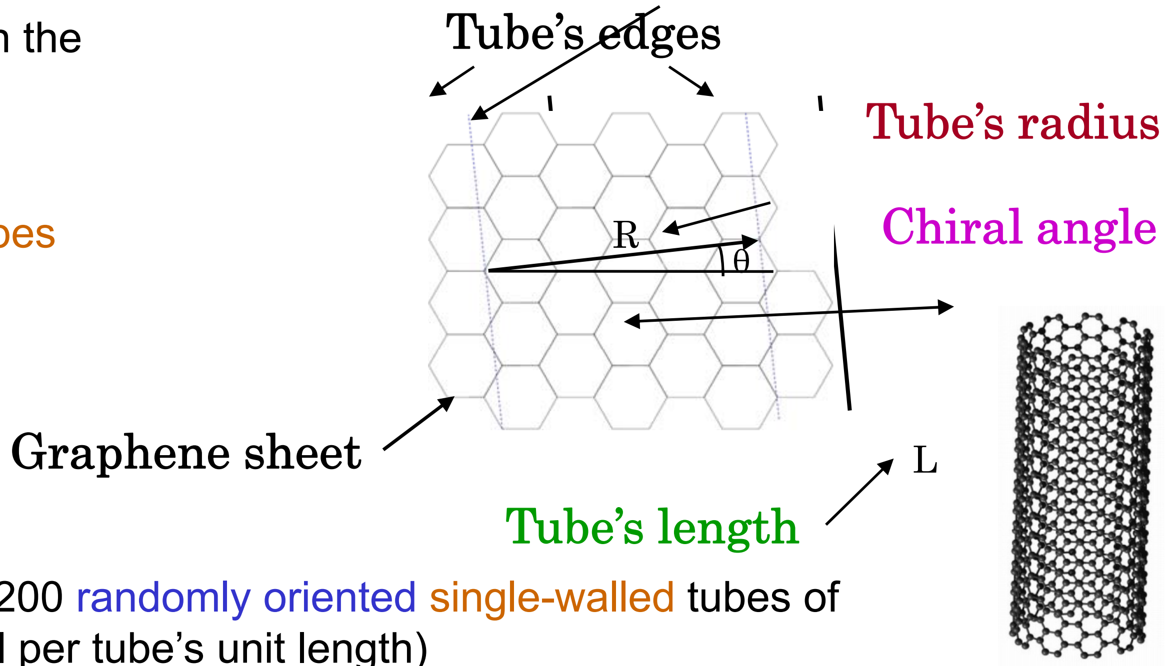
Motivation:
Observed peak cannot be explained as caused by graphite (too wide peak) or fullerenes (too high peak as compared with that from carbon hexagon)

Assumption: carbon nanotubes (randomly dispersed in the film or somehow assembled in some structures) may be responsible for the observed peak.
Goal: solving an inverse problem of reconstructing major parameters of carbon nanotubes and other nanostructures.

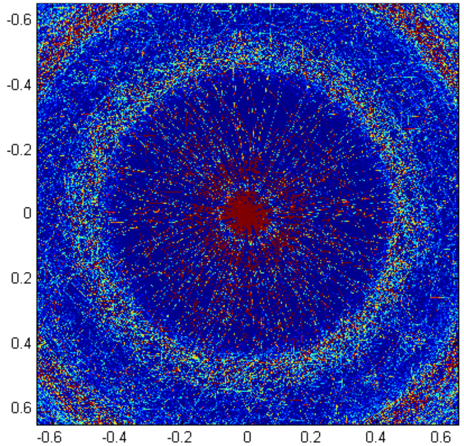
Modeling

Parameters that have an effect on the diffraction pattern:

- Tube's spatial orientation
- Number of walls in multiwall tubes
- Tube's radius
- Chiral angle
- Tube's length

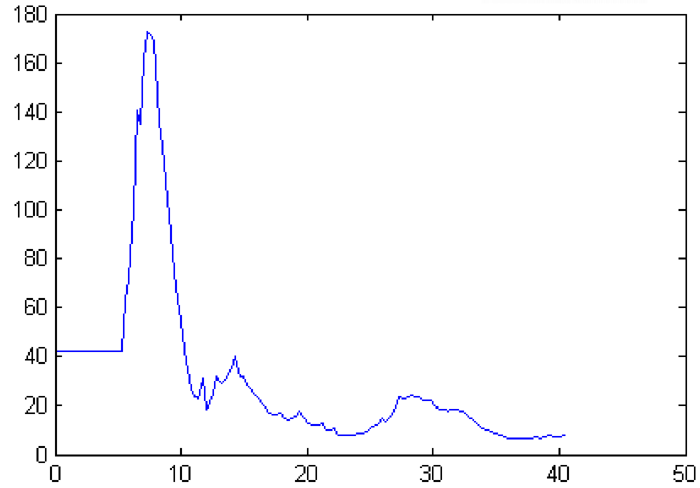


Simulated diffraction pattern from 200 randomly oriented single-walled tubes of infinite length (i.e. diffraction signal per tube's unit length)

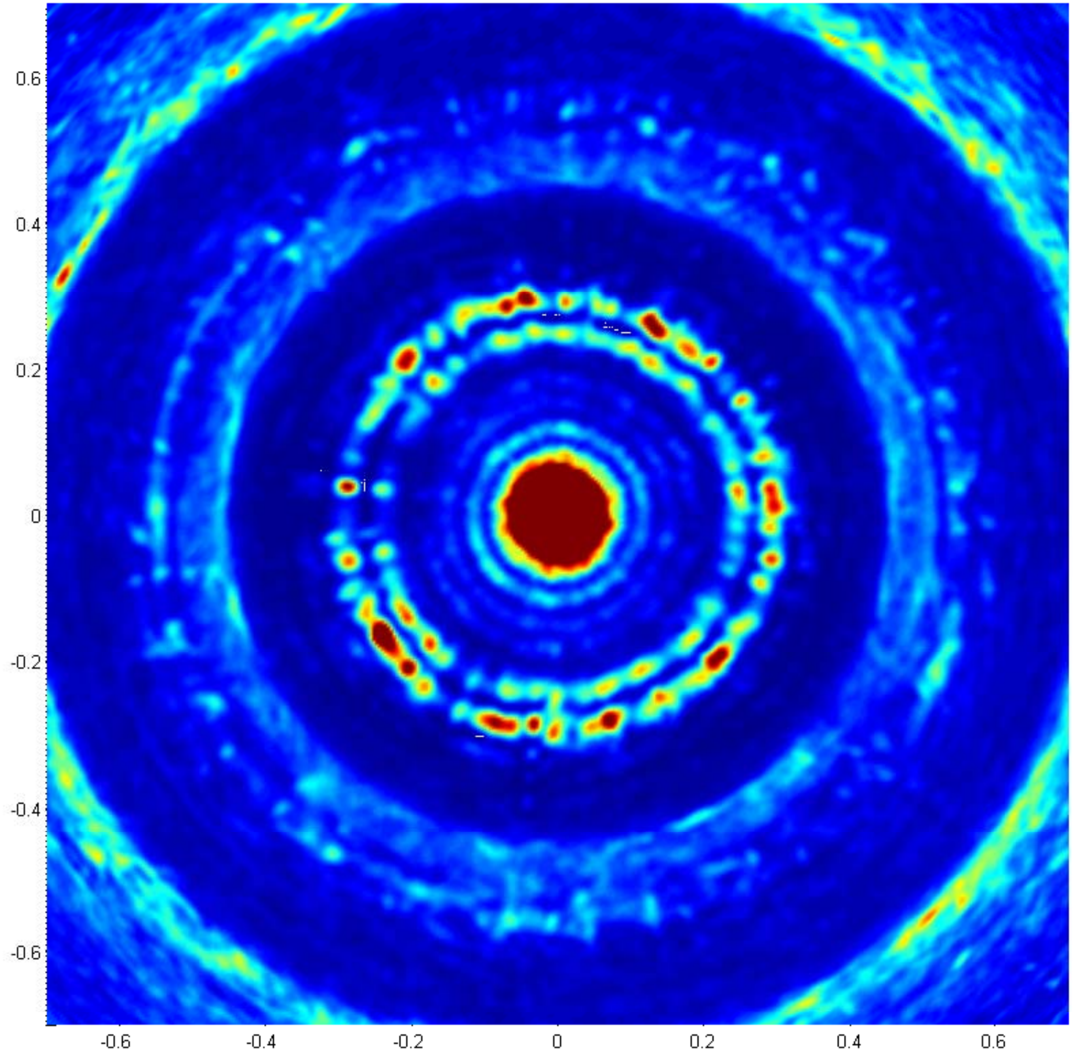


Radius: from 3.5 Å to 4.9 Å
Chiral angle: from 0^0 to 30^0

Intensity as a function of scattering angle

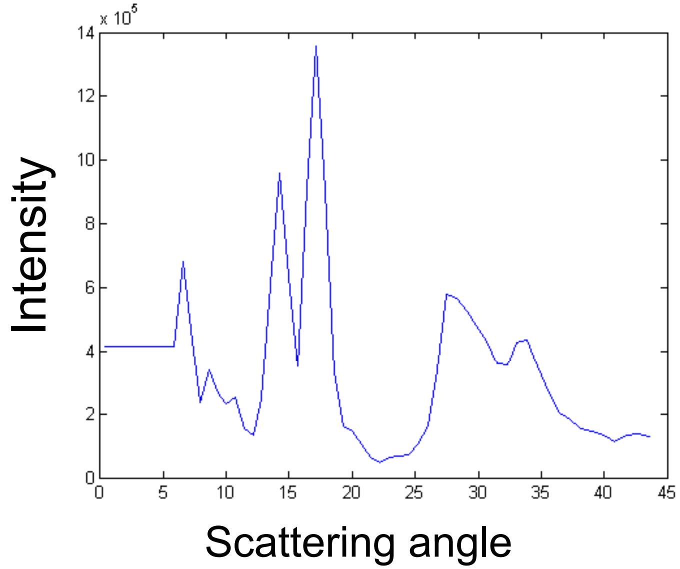


Simulated angular distribution of X-ray diffraction

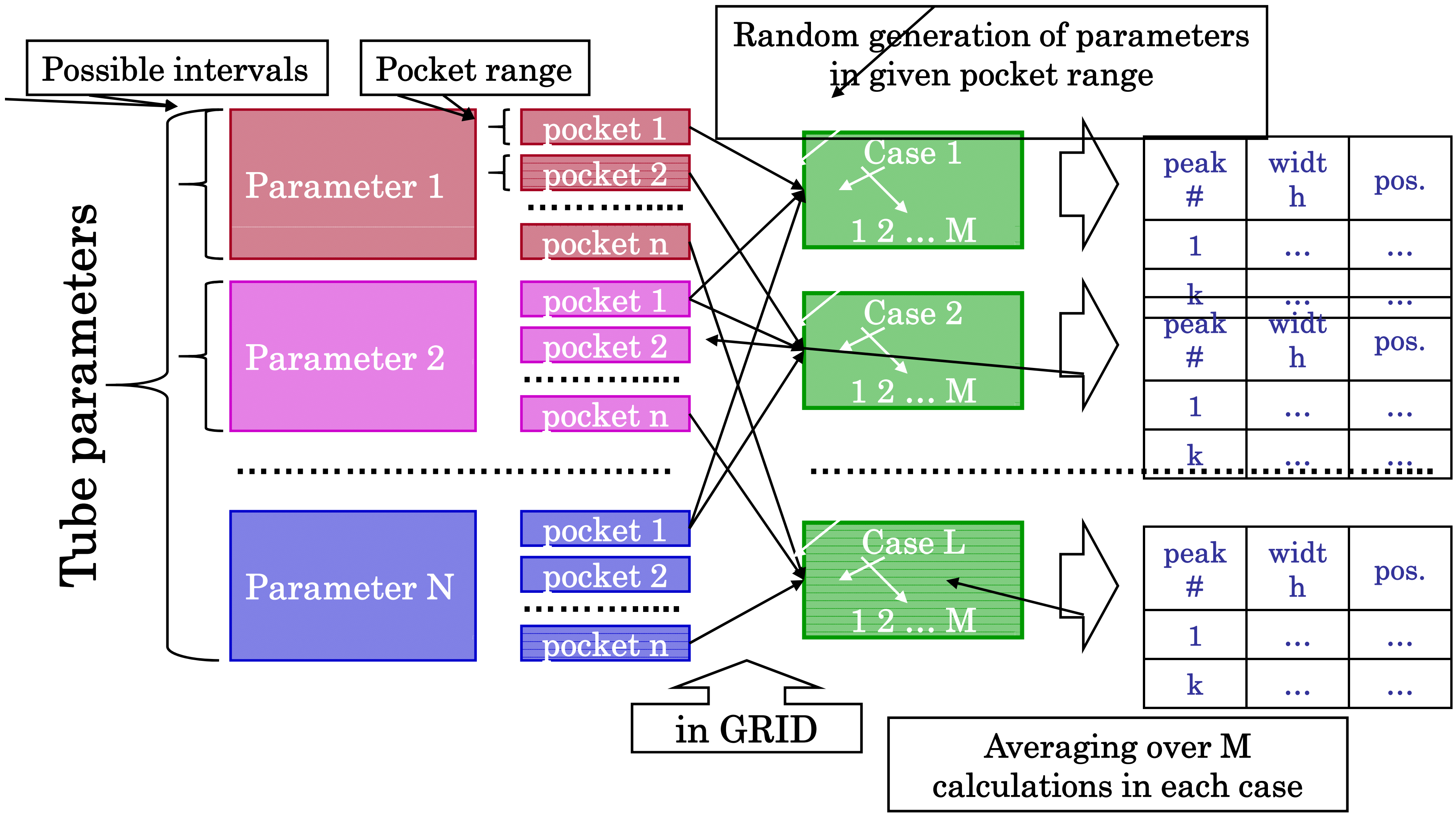


Simulated diffraction pattern from 100 randomly oriented multi-walled tubes of finite length

Inner shell radius: 3.5 Å
Outer shell radius: 10.3 – 13.7Å
Chiral angle: from 0^0 to 30^0



Algorithm


Possible intervals
Pocket range
Random generation of parameters in given pocket range
Tube parameters
Parameter 1
Parameter 2
Parameter N
pocket 1
pocket 2
pocket n
pocket 1
pocket 2
pocket n
pocket 1
pocket 2
pocket n
Case 1
1 2 … M
Case 2
1 2 … M
Case L
1 2 … M
peak #
width
pos.
1
k
in GRID
Averaging over M calculations in each case

Conclusion 1

Obtained results

- comparison of computed data with available experimental data
- estimation of relative composition of carbon nanotubes, graphene flakes, and fullerenes in the analyzed films
- validation of main assumption: dominance of carbon nanotubes over other nanostructures in the analyzed films

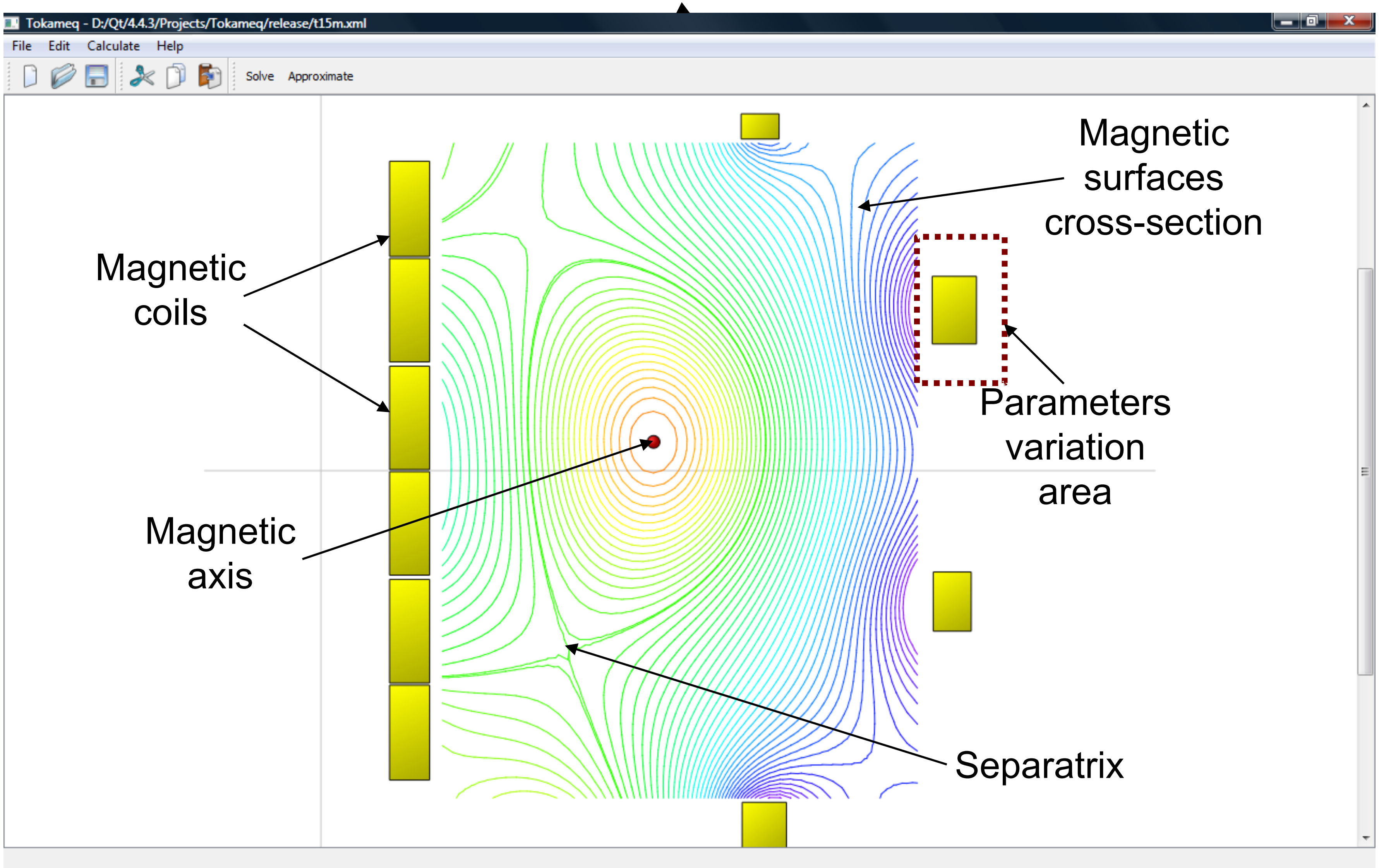
Expected results

- automatic processing (statistical analysis) of computed data for random distributions of main variables
- comparison of computed data with experimental data (angular distribution of x-ray diffraction signal)
- formulating an algorithm for reconstructing major parameters of main nanostructures under search (e.g., relative composition of carbon nanotubes, graphene flakes, and fullerenes, etc.) from experimental data

Application 2

Optimization of tokamak magnetic system

Magnetic equlibrium



Tokamak poloidal cross-section

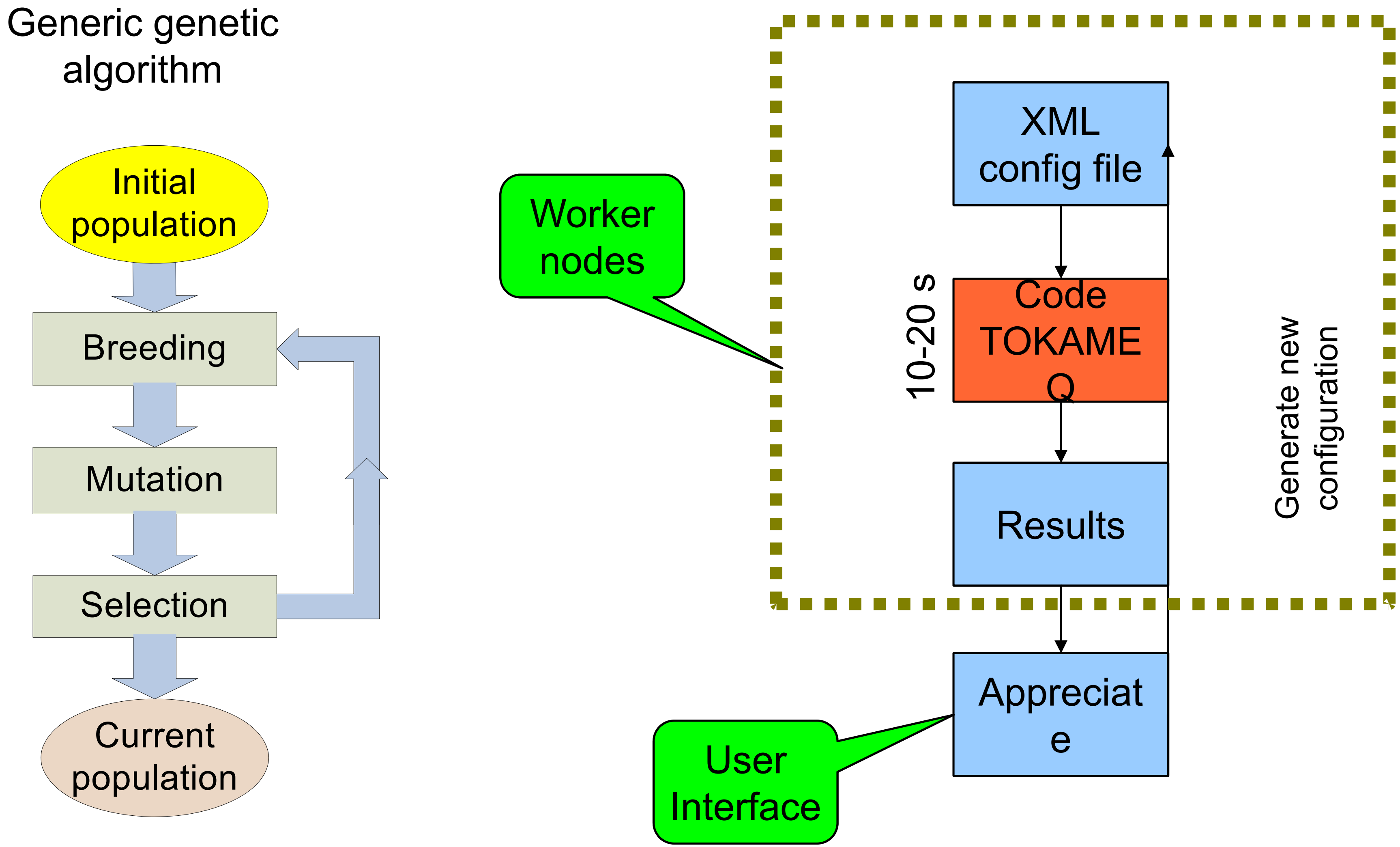
Goals

Code TOKAMEQ solves the inverse problem of magnetic equlibrium, i.e. for given magnetic configuration it finds the currents in the coils.

We want:

- Provide a tool for automatic search of the suboptimal subset of magnetic configuration for stationary regime, namely
- Decrease total coils current
- Decrease current density in coils
- Reduce the amount of copper needed for the coils

Calculation scheme



Conclusion 2

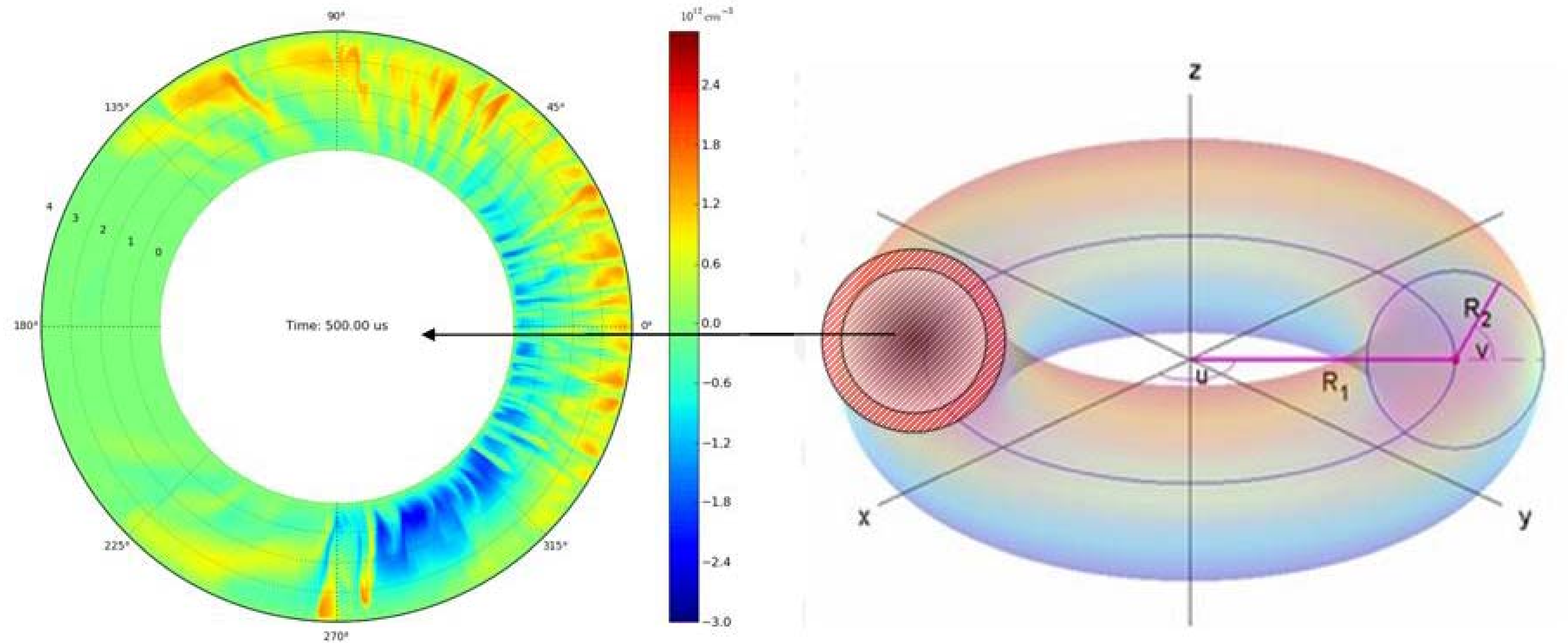
- Code TOKAMEQ is ported to Linux
- The set of scpits has been developed to realize the Grid-enabled genetic algorithm
- User-friendly viewer & editor of magnetic configuration has been developed

- The problem of calculation divergence for some configuration sets must be solved

Application 3

Simulation of the tokamak edge plasma turbulence

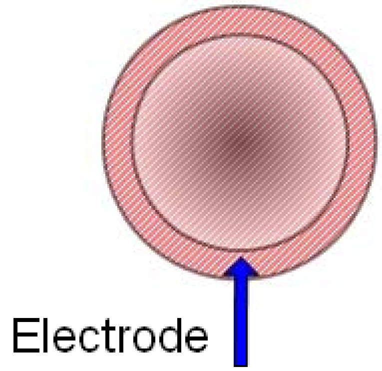
Introduction



turbulence, is widely believed to be responsible for the anomalous particle and energy losses in fusion devices.

Goal

- How to suppress the edge turbulence? Create the poloidal flow?
- We need to fit the parameters of the model to ensure the best likeness to experiment.
- Find phenomenological boundary conditions.
- Practical: find potential at the electrode and its radial position.



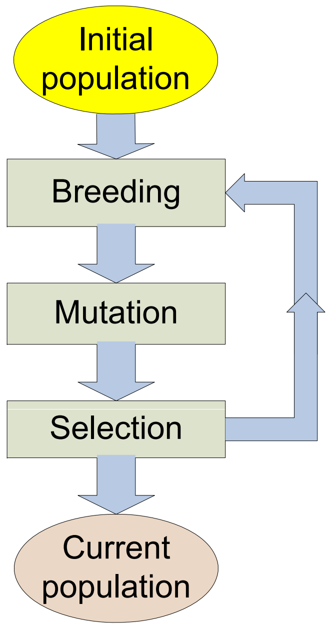
Fitting algorithm

There are 2 experimentally measured values:

- Level of fluctuations $\langle n_{\sim}^{2} \rangle$
- Correlation between density and potential

There are several intrinsic model parameters:

- Adiabaticity parameter
- Poloidal velocity profile
- Plasma pressure profile



- Use genetic algorithm
- Get Pareto-optimal set of variants

Conclusion 3

- The modeling was carried out for a set of model parameters in the Grid.
- The Grid advantages allows to perform the simulations with substantial saving of simulation costs.
- Grid enables time economy during visualization.

Thank you !