Porting Applications in Rfusion VO

Enabling Grids for E-sciencE

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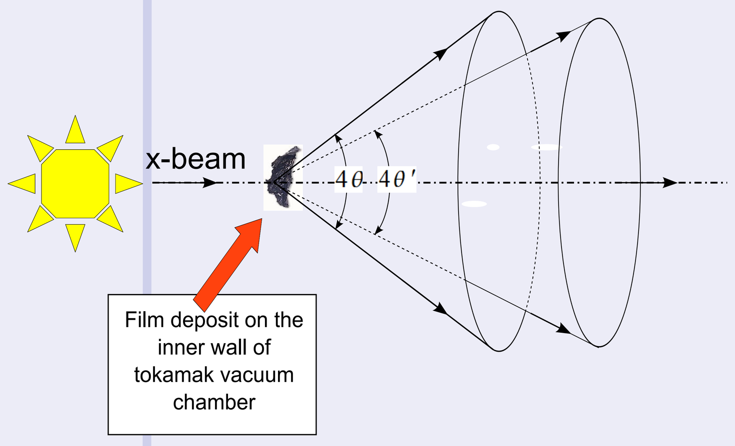
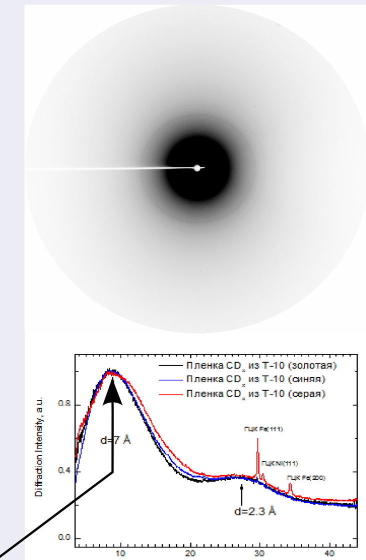
Modeling of X-ray Diffraction by Carbon Nanostructures and Interpretation of Diffractometry of the Films Deposited in Tokamak T-10

Experiment

Kurchatov Institute synchrotron radiation source





Angular distribution of X-ray diffraction

Svechnikov N.Yu., Stankevich V.G., …, Zubavichus Ya.V., et al. Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques, 2009, Vol. 3, No. 3, pp. 420-428.

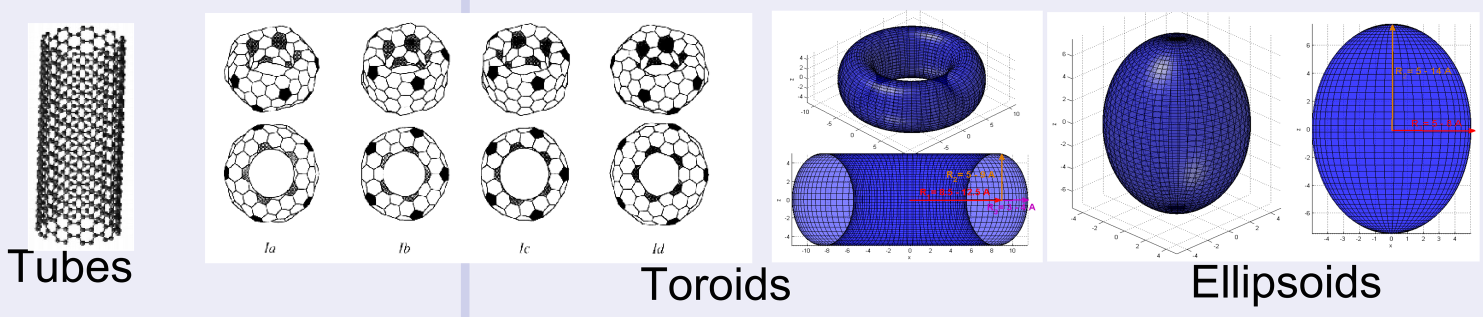
Smirnov V.P., ..., Stankevich V.G., et al. "The problems of nanostructures in controlled fusion." XIII National Conference on Crystal Growth, Institute of Crystallography RAS, Moscow, 2008 http://www.kiae.ru/nsi/nsi.htm

Goal: solving an inverse problem of reconstructing major parameters of carbon nanotubes and other nanostructures.

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

Assumption: Carbon nanotubes (randomly dispersed in the film or somehow assembled in some structures) may be responsible for the observed peak.

Carbon nanostructures under consideration



Tubes Toroids Ellipsoids

The local best fits of distribution of carbon nanostructures

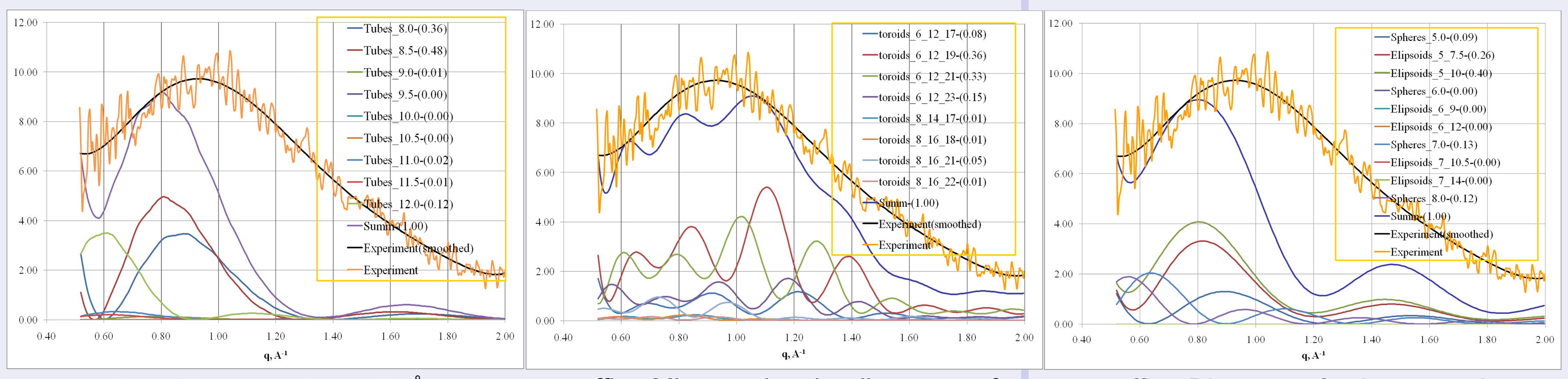
An inverse problem of reconstructing the distribution of carbon nanostructures over a fixed set of structural patterns is formulated as a search for the closest approach from the bottom to the observed curve $S_{exp}(q)$, not exceeding it everywhere. The non-unique solutions give the local best fitting, namely, a local minimum, in functional space, of (integrated over q) difference of the curves. Here we give partial solution in a limited interval of q:

$$q = \left|\vec{k}_s - \vec{k}_i\right| = \frac{4\pi}{\lambda}\sin(\theta)$$

- modulus of scattering wave vector; θ - scattering angle; λ - diagnostic x-ray wavelength.

Local best fitting of observed angular distribution $S_{exp}(q)$

Nanotubes of equal length — Toroids — Spheres and ellipsoids



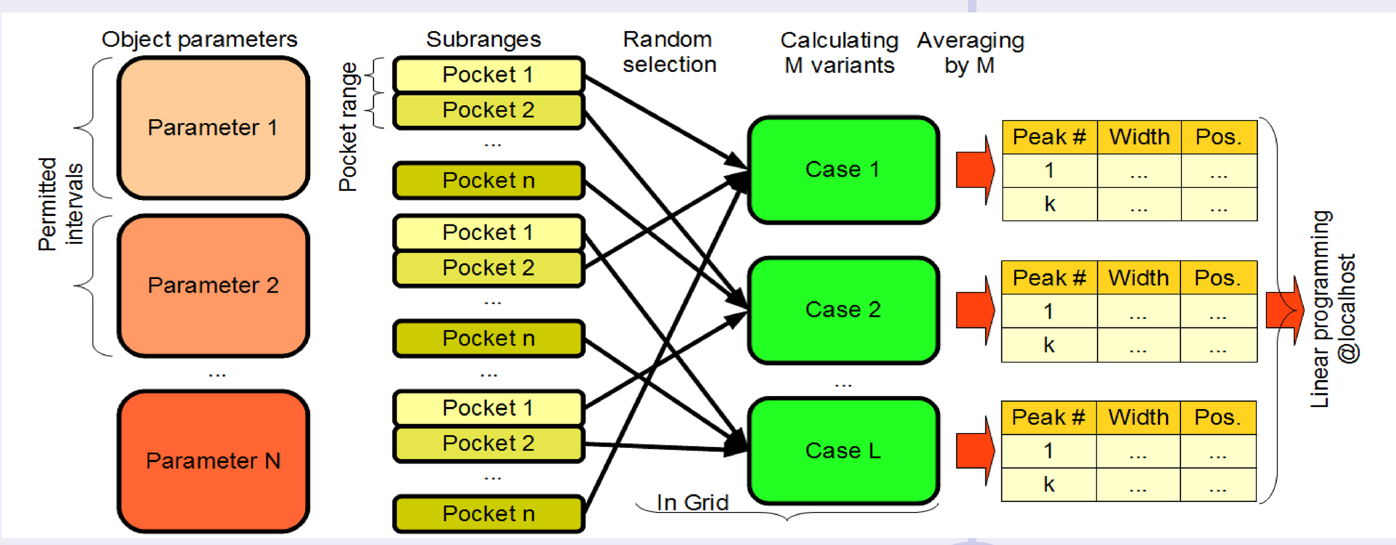
suffix - Diameter of tube, in Å

suffix - Minor and major diameters of elliptic cross-section, and major diameter of toroid, in Å

suffix - Diameter of spheres, and minor and major diameters of ellipsoids, in Å

The probability of elementary scatterer (carbon atom) belonging to this structure is indicated in brackets.

Algorithm



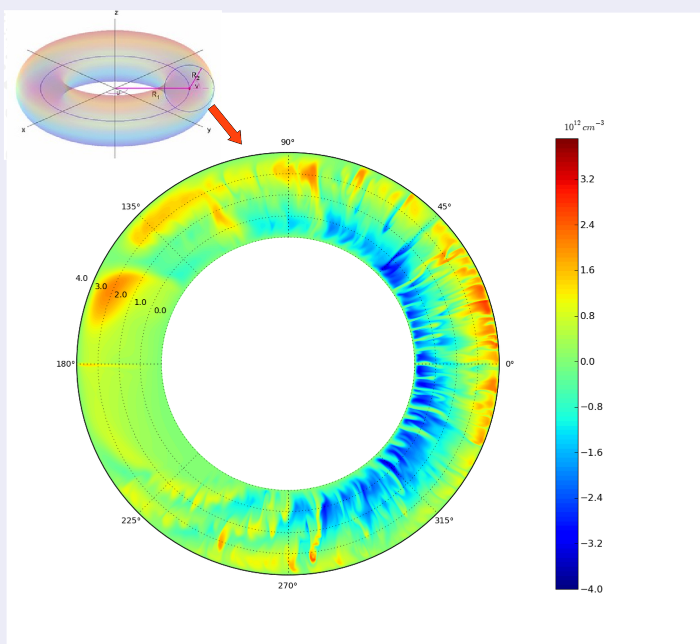
Conclusions

1. Suboptimal interpretation of experimental results has been found.
2. Optimisation time using Grid has been reduced by 34 times as compared with quad-core PC.

The Turbulence Simulation at the Tokamak Periphery

Introduction

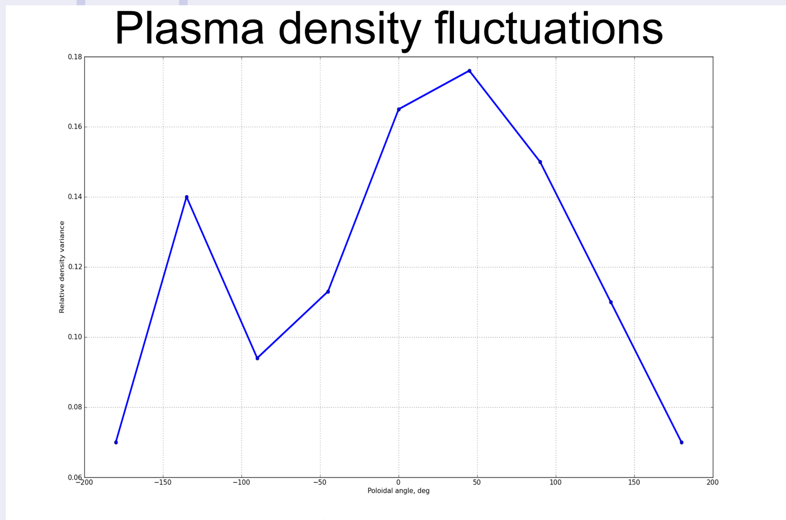
Basing on the Hasegawa-Wakatani approach, the 2-D numerical simulation of the tokamak's edge plasma turbulence was carried out. The computer code is compiled for the massive calculations in Grid.



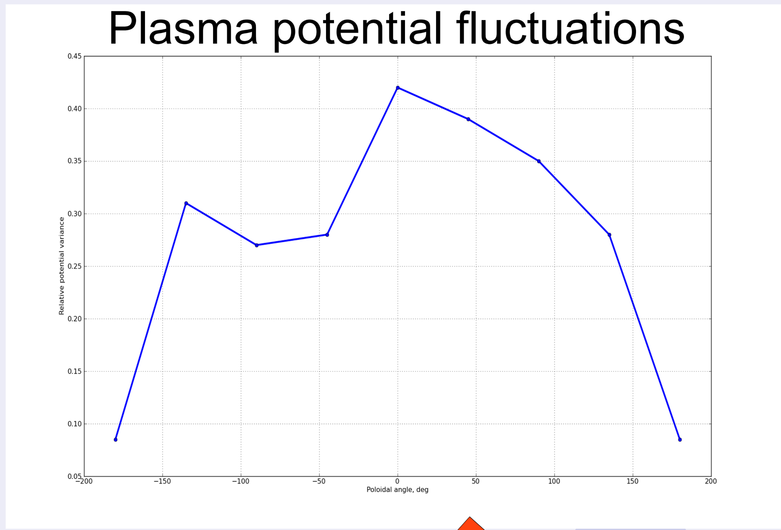
Tokamak's poloidal cross-section

The results of the modelling

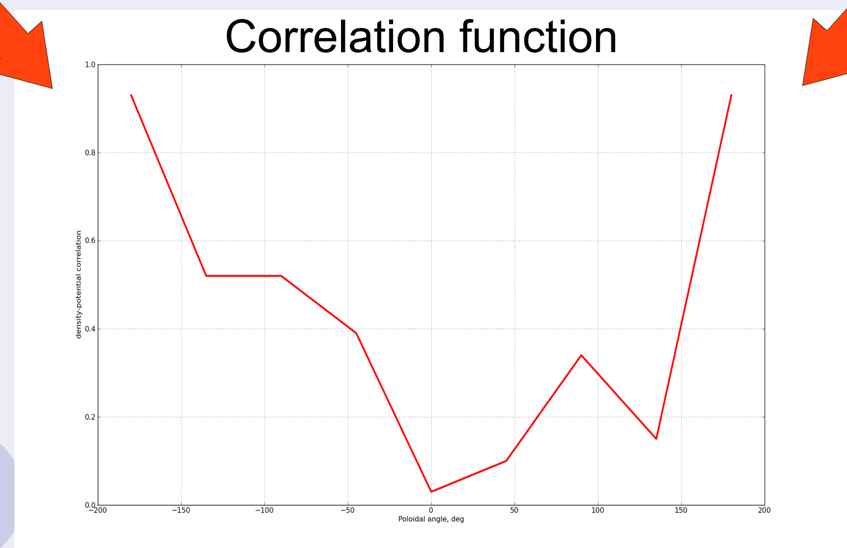
Plasma density fluctuations



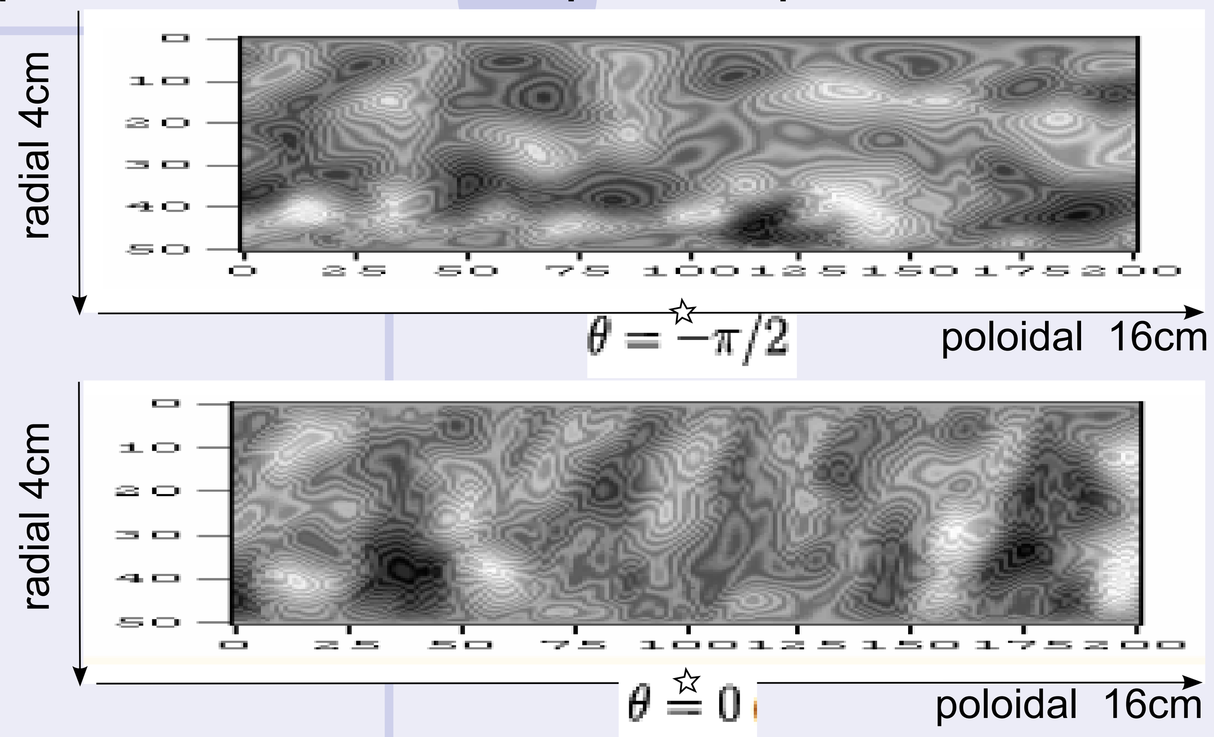
Plasma potential fluctuations



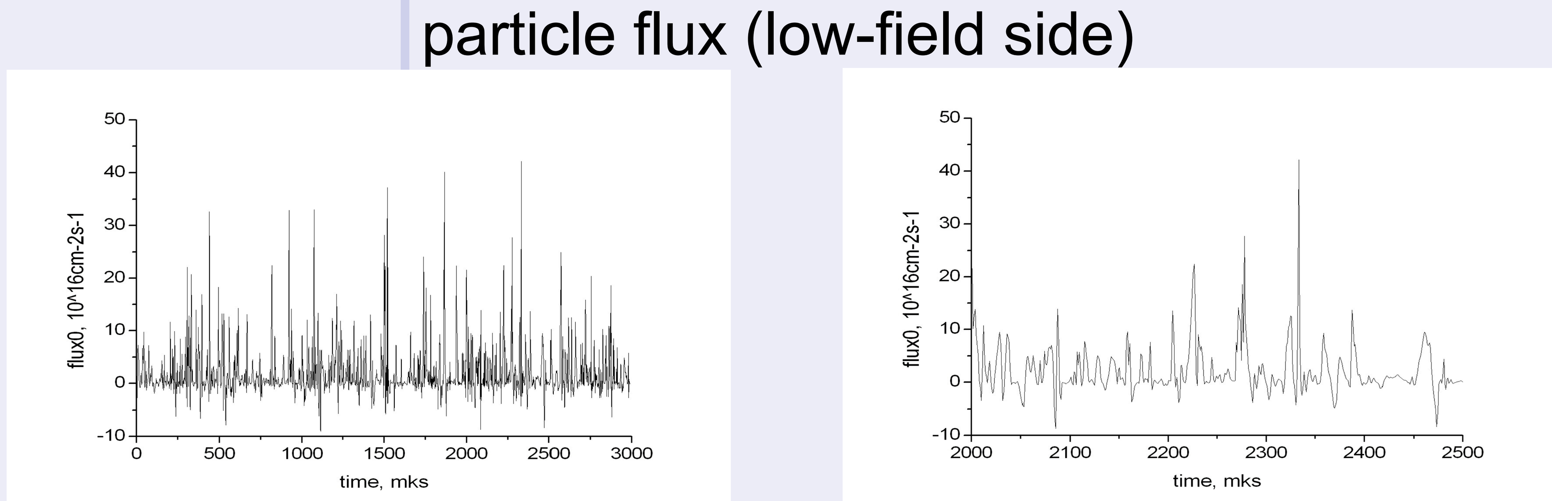
Correlation function



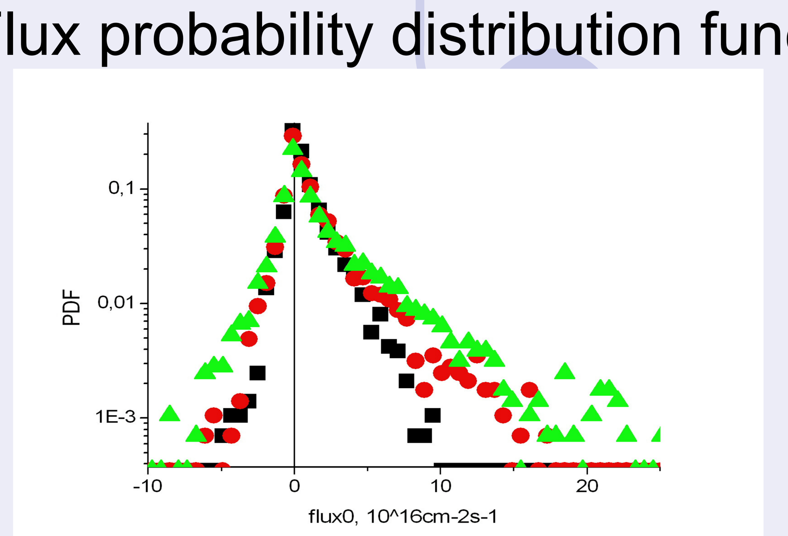
Space structure of the plasma potential fluctuations



Time behaviour of the radial fluctuations induced by particle flux (low-field side)



Flux probability distribution function



Conclusions

Using Grid the calculation time was reduced by a factor of about 5.

The EGEE project is building a Grid infrastructure for the scientific community. Grids are networks of computers spread across many sites but able to act together to provide a range of large scale facilities, from incredible processing power and mass storage to a platform for international collaboration.

www.eu-egee.org

e-infrastructure

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