Scientific report of Václav Štěpán for STSM COST-STSM-P9-03012
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The group of Dr. Werner Friedland at GSF focuses its research activities on theoretical modeling of biological effects of ionizing radiation in cell using stochastic model PARTRAC. PARTRAC is a biophysical Monte-Carlo modeling code for evaluating radiation induced DNA damage in the whole human cell nucleus. It is built as a modular system. The most important parts are the particle track generator, genome model structure generator, chemistry module and modules for damage evaluation. The spherical chromosome domain (SCD) model from Kirchhoff-Institut fűr Physik (KIP) can be used for the description of high-order nucleus organization.

During the STSM at GSF Václav Štěpán participated on further development and testing of the PARTRAC modules:

- The electron thermalization code in the PARTRAC particle track generator was recently updated by penetration depth data from Meesungnoen *et al.*, Radiat. Res. 158, 657 (2002). During the STSM the penetration depths for electrons in the 10-100 eV energy region were checked to verify whether an adjustment is necessary. Good agreement with the above cited article was found.
- The PARTRAC code has been ported to the 32-CPU 64-bit GSF cluster. Tests to find and isolate issues resulting from the transition to a 64-bit cluster environment were carried out and the issues were dealt with. Software tools have been written to enable an effective parallelization of the computations.
- The computing power gained from transition to the cluster was used to test and enhance the pair-wise exchange chromosome aberrations model developed during previous STSM of Václav Štěpán (3/04-30/04/2006). Selected results for an ensemble of 200 fibroblast nucleus prototypes were presented by Dr. Werner Friedland at Modelling Radiation Damage Workshop, 3rd-7th December 2007 at the European Centre of Atomic and Molecular Computations in Lyon, France.
- The possibility to use the PARTRAC software suite for providing supplemental data to the experiments carried out by the group of Peter O'Neill was studied. Probabilities of occurrence of specific simple DNA damage clusters in a given relative distance of the elementary damages participating in the cluster were computed. Clusters comprised of a single strand break and a modified base and of two single strand breaks were studied. The results were found in agreement with published data (Štěpán, Davídková, Radiat. Prot. Dosim. 122, 113 (2006)).

During the STSM the PARTRAC code was adapted to the parallel computing cluster environment, the chromosome aberrations model was extended, specific DNA damage clusters were studied and multiple minor enhancements were introduced in the code.

The parallelization of the computations was the key to effectively work with large sets of spherical chromosome domain nuclei prototypes and thus to fully exploit the properties of the SCD nucleus model and further develop the model of chromosome aberrations.

Realized STSMs of Vaclav Stepan in GSF established solid bases for future cooperation between the NPI and GSF.