

cfaed Colloquium

DATE: 27 September 2019

TIME: 5:15 pm

LOCATION: TU Dresden, Barkhausen-Bau (BAR), Heinz-Schönfeld-
Hörsaal BAR I90, Georg-Schumann-Str. 13, 01187 Dresden

SPEAKER: **Dr. Dmitry Ryndyk**

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TITLE: ***"On the Way to Quantitative Nanoscale Modeling
(TraNaS OpenSuite)"***



Abstract:

Theoretical and computational modeling of real systems requires multiscale and multiphysics approach linking atomistic ab initio description, quantum transport methods and 3D continuous methods for classical electric fields (also stress, thermal flow, etc.). For atomistic modeling, the semi-empirical, ab initio, Density Functional Theory (DFT) and hybrid methods are used. The Density Functional Tight-Binding (DFTB) approach is especially effective for large (devices, bio) systems, being orders of magnitude faster than full DFT approach with similar accuracy. Atomic and molecular scale systems are naturally described by discrete-level models, based, for example, on atomic orbitals or molecular orbitals. Starting from discrete-level representations we arrive at matrix Green functions, being the main theoretical tool at the nanoscale, convenient for numerical implementation. We develop our own open source DFTB+XT package as a core of the TraNaS OpenSuite – Integrated open software suite for nanoscale modeling. We also develop the extended version of the CP2K package, called CP2K+XT. The idea of TraNaS OpenSuite for nanoscale modeling is to combine our home quantum transport code TraNaS with several top-level open source projects with free licenses, which append each other to give together full set of tools for nanoscale modeling. All parts of the suite are modified and integrated at the library level. The packages are synchronized with the state-of-the-art versions of mother packages using git technology.

The other significant peculiarity of nanoscale systems is the enhanced role of interactions. Both electron-electron and electron-vibron interactions may be strong and the Landauer approach for coherent transport can not be used anymore. Fortunately, Nonequilibrium Green Function (NGF) methods are able to treat the many-body problems. We are working on effective parallel methods to solve the complicated equations of the many-body theory within the DFTB+XT package.

For real device geometries, the influence of external systems (electrodes, gates, STM tip) should be taken into account. In many cases, one can use the classical Finite Element Method (FEM) to model the electric potentials produced by the charges in the classical part, as well as electric and mechanic state of the classical part. We work on integration with FEM methods using the ElmerSolver code.

TraNaS OpenSuite code is adopted for use at the HPC clusters and uses fast mathematical libraries. Python scripting is suggested for complex computational tasks. We are working on GUI for input/output preparation and analysis. First applications include transport with dephasing and simulation of STM imagies and spectroscopy. The suite is supplied by the Guide, Manual, Tutorial, Tests, Examples.

The site of TraNaS OpenSuite is: trans.org/opensuite

TraNaS OpenSuite is open project hosted at GitHub: github.com/trans-open

