Can the artificial neural network be applied to estimate the atmospheric contaminant transport?

A. Wawrzynczak, M. Berendt-Marchel

Release of hazardous materials in chemical industries is a significant threat to surrounding areas especially in the urban terrain. To face this thread there are proposed a frameworks capable to estimate the contamination source parameters like localization and release rate based on the substance concentrations recorded by the sensors network. In such systems the parameters of the given dispersion model are sampled to fit the model output to the registrations. Application of such approach in the urbanized terrain requires the use of the of the complicated and computationally expensive dispersion models taking into account the complicated wind field. As a result the localization systems requires to much time to be applied in the real toxin threat situation, when the reaction time is the most crucial.
We examine the possibility of training an artificial neural network (ANN) so that it could effectively simulate the atmospheric toxin transport. The use of a fast neural network in place of costly computational dispersion models in systems localizing the source of contamination might significantly improve their efficiency (speed). In this paper, we present results of training the ANN with the use of dataset covering the contamination source term parameters and point output concentrations generated by the The Quick Urban & Industrial Complex (QUIC) Dispersion Modeling System. We test various ANN structures, i.e., numbers of ANN layers, neurons, and activation functions to achieve the ANN capable of estimating the contaminant concentration. The performed tests confirm that trained ANN has the potential to replace the dispersion model in the contaminant source localization systems, however its efficiency requires the carefully generated training data.

Computational Strategies for Two-Dimensional Wigner Monte Carlo

Josef Weinbub and Mihail Nedjalkov

Among the available solution techniques to solve the quantum Wigner equation, the Wigner Monte Carlo method based on a signed particle approach is a particularly attractive way: It allows for acceptable runtimes for two-dimensional simulations and paves the way for future three-dimensional simulations; multi-dimensional simulations are particularly important for simulating nanoelectronic devices which operate in presence of electromagnetic fields and are controlled by intricate three-dimensional boundary geometries. However, critical computational challenges remain: The primary challenge lies in the fact that the essential annihilation algorithm requires the entire Wigner state to be stored; the thus necessary storage size is proportional to

the dimensionality and resolution of the phase space. This quickly results in exorbitant memory requirements which easily exceed the limited memory of a single compute node. A spatial domain decomposition approach has been introduced for the one- and two-dimensional Wigner Monte Carlo method to (1) distribute the memory load among the compute nodes and (2) significantly reduce simulation runtimes via parallelization. The approach uses distributed-memory parallelization via the message passing interface on top of the stochastic simulation kernel. The software is made available via the ViennaWD software package. The fundamental parallelization layer and other computational aspects of solving two-dimensional problems for nanoelectronics will be discussed.

The financial support by the Austrian Federal Ministry for Digital and Economic Affairs and the National Foundation for Research, Technology and Development is gratefully acknowledged.

Immunogenicity Prediction of Bacterial Proteins by Machine Learning Algorithms

Nevena Zaharieva, Irini Doytchinova and Ivan Dimitrov

Immunogenicity is the ability of an antigen or epitope to provoke an immune response in the host. Modeling and prediction of the immunogenicity of proteins of different origin is the first step in the process of vaccine design and development.
Ten years ago the VaxiJen server for immunogenicity prediction of proteins of bacterial, viral, tumor and fungus origin (http://www.ddg-pharmfac.net/vaxijen/VaxiJen) was developed in our Lab. Since then, Vaxijen has proven to be a reliable tool for antigen recognition and it has been widely used. The models implemented in VaxiJen were derived by partial least square (PLS) discriminant analysis on sets of immunogenic and non-immunogenic proteins.
Recently, the set of bacterial immunogens was updated and now it contains 317 proteins from 47 species (http://www.ddg-pharmfac.net/vaxijen/VaxiJen/database.fasta). A mirror set of non-immunogenic proteins from the same species was collected. The protein sequences were described by E-descriptors and transformed into uniform vectors by auto- and cross-covariance. The datasets were analyzed by several machine learning algorithms: PLS discriminant analysis, logistic regression, random forest, k-nearest neighbors, support vector machines and neural networks. The predictive ability of the derived models was assessed by sensitivity, specificity, accuracy, positive predictive value, receiver operating characteristics curves (ROC-statistics) and Matthews coefficient.