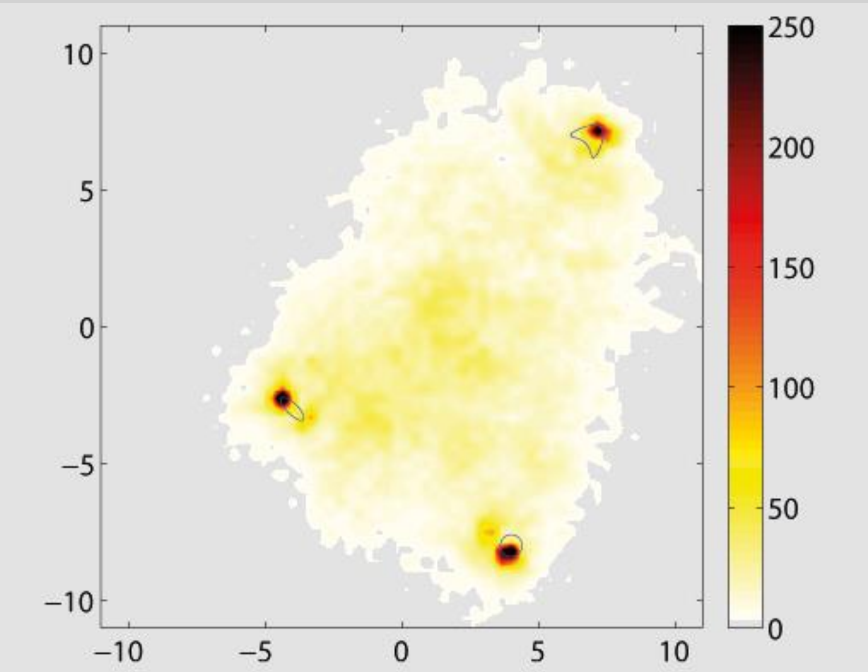
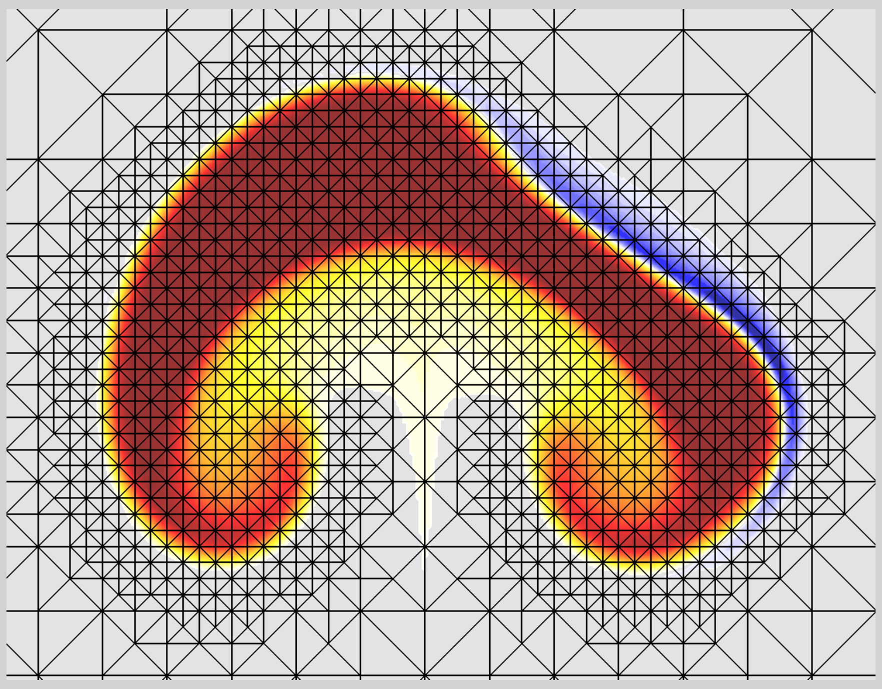
Oberseminar Numerik

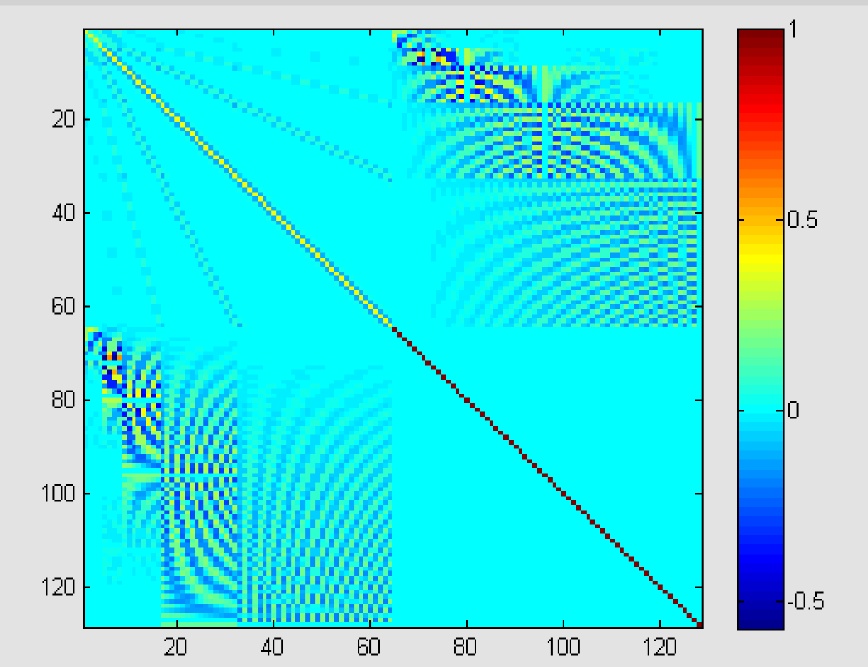


Herr Prof. Dr. Illia Horenko (Universität Lugano, Schweiz)

31.05.16
10:15 Uhr
Hilbertraum (05-432)
Staudingerweg 9, 55128 Mainz



„On numerical modelling and HPC-inference of unresolved scale effects in realistic multiscale systems “



Abstract:
Modeling and simulation of unresolved scale effects is an important problem in many areas dealing with multiscale processes and systems, e.g. in fluid mechanics (subgrid-scale mo-delling and Large Eddy Simulations), in geosciences (subgridscale "physics" parametrisation in weather and climate models), in biophysics (thermostate models, meso-scopic MD force field parametrisations) and in economics (latent factor models in economics and finance). Standard approach to subgridscale-modeling is based on the i.i.d. assumptions (indepen-dence and identity of distribution) for the unre-solved scale effects, that - through application of appropriate central limit theorems from probability theory - leads to formulation of stochastic subgridscale (SGS) models in a form of stationary/homo-genous parametric processes like Gauss, Poisson, etc. However, in a very generic setting of Markov chain models of dynamical systems one can demonstrate that the violation of indepen-dence assumptions leads to the intrinsic nonstationarity/nonhomogeneity of the resulting models - practically meaning that the underlying model parameters become infinite dimensional objects (i.e., functions in time and space) - and not anymore finite-dimensional numbers and vectors as it is the case for the standard SGS models based on independence assumption [1]. This leads to funda-mental problems with applicability of standard SGS approaches from machine learning and statistics (like artificial neuronal networks, support vector machines, generalised linear models etc.) in such multiscale situations [1].

Nonparametric (i.e., not being a priori confined to some parametric stochastic model family like Gauss, Poisson, etc.) and nostationary/nonhomogenous approach to SGS modeling and inference will be presented [2,3]. It is based on the variational formulation of the parameter inference problem - allowing to deploy already existent efficient tools from the numerics of Partial Differential Equations (like adaptive Finite Element Methods) in context of data analysis and statistics. Since very many model classes can be used to describe the same data, a ques-tion of model discrimination arises: i.e., which of the many possible models provides in some sense "optimal" description of the given data. It will be demonstrated how this problem can be solved in the same context of nonparametric and nonstationary variational framework by formulating the "optimality" principle by means of information theory concepts like entropy and information criteria - and once again deploying the efficient tools from PDE numerics and convex constrained optimisation. Aspects related to high performance computing (HPC), scalability on emerging supercomputing facilities based on graphical processing units (GPUs) will be discussed and some examples from fluid mechanics, weather/climate research and biomolecular dynamics will be presented.

[1] J. de Wiljes, L. Putzig and I. Horenko: "Discrete non-homogenous and non-stationary logistic and Markov regression models for spatio-temporal data with unresolved external influences„; Communications in Applied Mathematics and Computational Science, 9, No. 1, 1–46 (2014)
[2] I. Horenko: "Finite Element Approach to Clustering of Multidimensional Time Series„; SIAM J. Sci. Comp. 32 (1), pp. 62-83 (2010)
[3] Ph. Metzner, L. Putzig and I. Horenko: "Analysis of persistent non-stationary time series and applications„; Communications in Applied Mathematics and Computational Science, 7(2), 175–229, (2012)

Hierzu sind alle herzlich eingeladen.

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