TUMOR SIMULATION BY USING SUPERMODELING - AN EXAMPLE OF A NEW CONCEPT OF DATA ASSIMILATION IN MODELING OF COMPLEX SYSTEMS

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ABSTRACT

We introduce a new concept of data assimilation in simulation of complex systems, such as tumor proliferation, by using supermodeling paradigm. We demonstrate that the integration of the supermodel with real data involves learning only a limited number of sub-model coupling coefficients instead of a lot of parameters of a single, usually complex and overfitted cancer model.

1   INTRODUCTION

Currently, the advanced tumor models are not suitable for direct employment in real-*life* cancer therapies due to their tremendous complexity on the one hand, and important model imperfections on the other. A huge number of model parameters does not enable data adaptation because of the problem of overfitting and their high spatio-temporal variability.
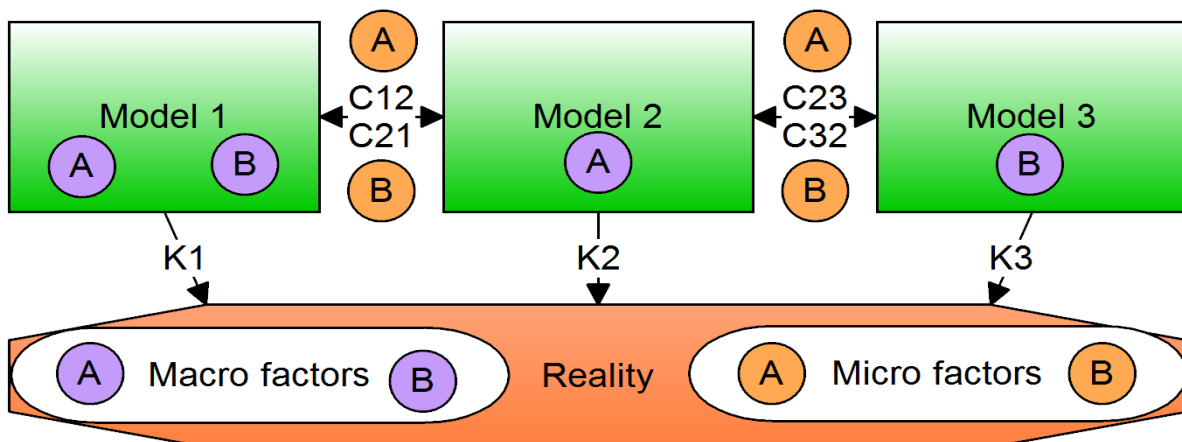

Figure 1: The scheme of supermodeling and data adaptation. The models are paired with each other by C_{ij} and with data by K_j learning weights. In data adaptation only a few C_{ij} and K_i parameters are learned. "A" and "B" represent factors of reality.

To decrease the number of learnable parameters we employ the supermodeling concept, which was used previously in climate modeling and weather forecast for improving quality of predictions (Shen et al. 2016). We demonstrate that it is possible to obtain reliable prognosis for tumor dynamics by creating its supermodel, which consists of several paired simple tumor models. The sub-models can represent incomplete and simplified models of a very complex tumor model, parameterized by different "guessed" and constant parameter sets. Instead of adapting these parameters to data, we propose to match (learn)

only a small number of coupling coefficients C_{ij}. The Figure 1 shows our concept. We assume that all fine-grained features and other unpredictable events accompanying tumor dynamics and not included in the sub-models are hidden in data. The formal mathematical framework plays the role of an additional knowledge, which defines more precisely the feature space topology for machine learning tools. Due to data adaptation learning schemes, all microscopic factors will be represented by the values of the non-zero coupling coefficients C_{ij}.

2   RESULTS

To define a proper cancer model (for a framework for supermodeling) we have developed a novel macroscopic one-phase computational model of melanoma tumor (Dzwinel, Kłusek and Vasilyev 2016). To make the model implementation efficient computationally, we implemented our code (classical FDM solver) in GPU speeding up its computational performance two orders of magnitude comparing to its serial version (Dzwinel et al. 2017). Having in mind that data adaptation process will require even more efficient numerical solvers, the isogeometric and wavelet collocation methods are under adaptation (Łoś et al. 2017). In (Dzwinel, Kłusek and Vasilyev 2016; Kłusek, Dzwinel and Dudek 2016) we demonstrate that the supermodel of melanoma cancer connected only by one dynamical variable, produces broader melanoma invasion scenarios than the single melanoma model. In (Dzwinel, Kłusek and Paszyński 2017) we present the concept of a prognostic system for anti-tumor therapy based on supermodeling. This learning scheme is exploited for teaching the cancer supermodel consisting of a simple zero-dimensional ODS based sub-models. Input data are generated by previously devised 3-D melanoma model (Dzwinel, Kłusek and Vasilyev 2016) and just this model is treated as the ground truth. We show that the supermodel predictions are better than these produced by a single sub-model while the quality of supermodel predictions strongly depends on the number of sub-models. At present, we are investigating the influence of the number of couplings between sub-models on the supermodel stability and quality.

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REFERENCES

Dzwinel, W., A. Kłusek, R. Wcisło, M. Panuszewska, and P. Topa. 2017. "Continuous and Discrete Models of Melanoma Progression Simulated in Multi-GPU Environment". PPAM 2017, LNCS.

Dzwinel, W., A. Klusek, and M. Paszynski. 2017. "A Concept of a Prognostic System for Personalized Anti-Tumor Therapy Based on Supermodeling". *Procedia of Computer Science* 108C:1832–1841.

Dzwinel, W., A. Kłusek, and O. V. Vasilyev. 2016. "Supermodeling in Simulation of Melanoma Progression". *Procedia Computer Science* 80:999-1010.

Kłusek, A., W. Dzwinel, and A. Z. Dudek. 2016. "Simulation of Tumor Necrosis in Primary Melanoma". In *Proceedings of 2016 Summer Computer Simulation Conference SCSC 2016* edited by W. Rango, and J. L. R. Martin, 55-62. Society for Modeling & Simulation International.

Łoś, M., M. Paszyński, A. Kłusek, and W Dzwinel. 2017. "Application of Fast Isogeometric L2 Projection Solver for Tumor Growth Simulations". *Computer Methods in Applied Mechanics and Engineering* 316:1257-1269.

Shen, M. L., N. Keenlyside, F. Selten, W. Wiegerinck, and G. S. Duane. 2016. "Dynamically Combining Climate Models to "Supermodel" the Tropical Pacific". *Geophysical Research Letters* 43(1): 359-366.