DEVELOPMENT OF SIMULATION FRAMEWORKS TO SUPPORT BIOGEOCHEMICAL MODEL APPLICATION

THESIS OF PhD DISSERTATION

Roland Hollós

Doctoral Program of Environmental Earth Sciences,
Doctoral School of Environmental Sciences
Eötvös Loránd University

Director:
Dr. Tamás Turányi, DSc

ELTE
EÖTVÖS LORÁND
TUDOMÁNYEGYETEM

Supervisors:
Dr. Zoltán Barcza, associate professor
Dr. Nándor Fodor, senior research fellow

Budapest, 2024

1. Introduction and objectives

Terrestrial ecosystems are crucial components of the global climate system and also provide essential ecosystem services. However, our understanding of the underlying processes of the soil-vegetation system is inadequate to address global challenges such as the increasing need for food and raw material. Furthermore, since the soil-vegetation system is closely linked to the underlying climate system, further investigation is needed to address the interplay of the terrestrial ecosystems and the greenhouse gas budget of the atmosphere.

Modeling provides a well-established method to better understand the functioning of the soil-vegetation system. Process-based models are constructed by the combination of empirical evidence and mathematical formulations. At present, a large number of models are available that are widely used in the scientific literature (Canadell, 2021). However, due to the development of these models the research community faces several new challenges. State-of-the-art models are extremely complex, have extensive data requirements, and use many parameters that are difficult to estimate. This hinders their usability and applicability for real world systems. Due to the economic and political implications of the current models, there is a great need to simplify their use. This will enable users to carry out informative simulations with little background knowledge of modeling and informatics.

The objective of my doctoral research was to develop frameworks that support the application of an advanced biogeochemical model called Biome-BGCMuSo, in complex simulation cases. As part of the work, I also developed a novel parameter estimation procedure, which is unprecedented according to my knowledge. The new method is suitable for optimizing process-oriented models using machine learning. I also aimed to develop and apply an easy-to-use graphical decision support system to investigate the future prospects of crop production in Hungary.

2. Materials end methods

My research was built upon the Biome-BGCMuSo biogeochemical model. As part of my research, I have been involved in the development of the model and have contributed to the dissemination of the latest model version (Hidy et al., 2021; 2022). The source of the meteorological data was the so-called FORESEE database (Kern et al., 2024), to which I also contributed. I used the DOSoReMI database (Pásztor et al., 2020; Fodor et al., 2021) to satisfy the soil data requirements of the model. Maize yield data from Long Term Field Experiments (LTFE) performed at Martonvásár were used as observational evidence for the model.

One of the main focuses of my work was to optimize (or in other words to calibrate) the Biome-BGCMuSo to make the model simulations more realistic. The goal of model optimization is to reduce the uncertainty of the model parameters and thus the simulations results. For complex models this is typically done using a Monte Carlo-based approach, which traditionally optimizes the model (minimizes modeling error) while ignoring other quality measures. To address current problems of these approaches (e.g. getting good results from wrong reasons, or equifinality), I have developed a new method (Hollós et al., 2022). This method combines traditional statistical methods with the practice of trial-and-error model fitting and uses machine learning to narrow down the parameter space by applying quality criteria to the derived results. The mathematical background of the new method is described in detail in the dissertation.

I have created two open-source software packages (called RBBGCMuso and AgroMo) in R to support the Biome-BGCMuSo model application. They provide higher-level functionality, user and programming interfaces, generic functions to address common modeling problems, and model-data fusion for low-data situations. Both packages and their documentation are available on GitHub.

3. Results: theses of dissertation

The results of my doctoral research can be summarized in the following thesis points.

1. I contributed to the optimization and sensitivity analysis of Biome-BGCMuSo with fundamental methodological developments. One of these is the support of more advanced Monte Carlo based simulations of process-based models. It is based on a mathematical method not yet widely used for process-based modelling, called Hit and Run (Chen & Schmeiser 1996), and provides a solution for sampling parameters that are highly interdependent, such as many parameters of Biome-BGCMuSo. The other method allowed asynchronous parallelization of the Biome-BGCMuSo model, which reduced the computational time of Monte Carlo simulations by orders of magnitude. This made it feasible to execute the model hundreds of thousands or even millions of times on personal computers within realistic time frames.
2. I created and disseminated the RBBGCMuso software to the research community, which integrates the difficult-to-use Biome-BGCMuSo model into the R programming environment and provides access to high-level modeling features using only a few R commands. The software package is open source and available on GitHub together with its documentation (Hollós et al., 2023). The package has already been used in international publications (Ren et al., 2022).
3. I developed and published the so-called CIRM ("Conditional Interval Reduction Method") method (Hollós et al., 2022), which offers a new solution for the optimization of process-oriented models in various disciplines. The CIRM method is unique in a sense that it combines traditional, probabilistic inverse methods with expert knowledge that cannot be considered as measurement data. This feature ensures that the optimization results are realistic.
4. I have successfully applied the CIRM method in a so-called “low data” situation (i.e. when only few or poor-quality measurement data is available). The LTFE

data observed at Martonvásár were used as the basis for the simulation. The conventional method of model optimization did not allow reducing the parameter intervals in a meaningful way. In contrast, the use of CIRM resulted in an average interval reduction of 44%, while the uncertainty of the simulations was reduced by 42.3%. In addition, 95.5% of the runs in the reduced intervals were realistic, compared to 7% for the conventional method.

5. As a major contributor, I developed AgroMo, a decision support software package with a graphical user interface that allows the execution of point and spatial simulations and is also suitable for CIRM-based optimization of Biome-BGCMuSo and the creation of different farming scenarios. AgroMo is based on the RBBGCMuso software and allows the user to exploit the potential of the model without any programming knowledge. AgroMo is an open source software package that has also been published on GitHub and documentation has been produced.
6. I carried out a climate change related impact assessment using the AgroMo software focusing on national scale maize production simulation. For the experiment, the meteorological data were provided by two scenarios (RCP4.5 and RCP8.5) of the FORESEE database, while the soil data were provided by DoSoReMi. I assumed that management practices remain the same, which means that I investigated the combined effect of future weather and increasing atmospheric CO_2 concentration. The results show an average maize yield change of -1% (-1.17 t/ha; RCP4.5) and -13% (-1.01 t/ha; RCP8.5) in Hungary by the mid-century and -10% (-0.77 t/ha; RCP4.5) and -28% (-2.20 t/ha; RCP8.5) change by the turn of the century, respectively, compared to the reference period 2001-2020. Unlike previous studies, the RCP8.5 scenario is more favorable for the near future than the RCP4.5 scenario.

Publications related to the PhD Dissertation

Peer reviewed articles

Kern, A., Dobor, L., **Hollós, R.**, Marjanović, H., Torma, C.Z., Kis, A., Fodor, N., Barcza, Z., 2024. Seamlessly combined historical and projected daily meteorological datasets for impact studies in Central Europe: The FORESEE v4.0 and the FORESEE-HUN v1.0. Climate Services 33, 100443. doi:10.1016/j.cliser.2023.100443

Kalmár, T., Kristóf, E., **Hollós, R.**, Pieczka, I.,Pongrácz, R., 2023. Quantifying uncertainties related to observational datasets used as reference for regional climate model evaluation over complex topography — a case study for the wettest year 2010 in the Carpathian region. Theoretical and Applied Climatology 153, 807–828. doi:10.1007/s00704-023-04491-4

Bellocchi, G., Barcza, Z., **Hollós, R.**, Acutis, M., Bottyán, E., Doro, L., Hidy, D., Lellei-Kovács, E., Ma, S., Minet, J., Pacskó, V., Perego, A., Ruget, F., Seddaiu, G., Wu, L., Sándor, R., 2023. Sensitivity of simulated soil water content, evapotranspiration, gross primary production and biomass to climate change factors in Euro-Mediterranean grasslands. Agricultural and Forest Meteorology 343, 109778. doi:10.1016/j.agrformet.2023.109778

Hollós, R., Fodor, N., Merganičová, K., Hidy, D., Árendás, T., Grünwald, T., Barcza, Z., 2022. Conditional interval reduction method: A possible new direction for the optimization of process based models. Environmental Modelling and Software 158, 105556. doi:10.1016/j.envsoft.2022.105556

Kern, A., Barcza, Z., **Hollós, R**., Birinyi, E., Marjanović, H., 2022. Critical Climate Periods Explain a Large Fraction of the Observed Variability in Vegetation State. Remote Sensing 14, 5621. doi:10.3390/rs14215621

Haszpra, L., Barcza, Z., Ferenczi, Z., **Hollós, R.**, Kern, A., Kljun, N., 2022. Real-world wintertime CO, N_2O, and CO_2 emissions of a central European village. Atmospheric Measurement Techniques 15, 5019–5031. doi:10.5194/amt-15-5019-2022

Hidy, D., Barcza, Z., **Hollós, R.**, Dobor, L., Ács, T., Zacháry, D., Filep, T., Pásztor, L., Incze, D., Dencső, M., 2022. Soil-related developments of the Biome-BGCMuSo v6.2 terrestrial ecosystem model. Geoscientific Model Development 15, 2157–2181. doi: 10.5194/gmd-15-2157-2022

Gelybó, Gy., Barcza, Z., Dencső, M., Potyó, I., Kása, I., Horel, Á., Pokovai, K., Birkás, M., Kern, A., **Hollós, R.**, Tóth, E., 2022. Effect of tillage and crop type on soil respiration in a long-term field experiment on chernozem soil under temperate climate. Soil and Tillage Research 216, 105239. doi:10.1016/j.still.2021.105239

Fodor, N., Pásztor, L., Szabó, B., Laborczi, A., Pokovai, K., Hidy, D., **Hollós, R**., Kristóf, E., Kis, A., Dobor, L., Kern, A., Grünwald, T., Barcza, Z., 2021. Input database related uncertainty of Biome-BGCMuSo agro-environmental model outputs. International Journal of Digital Earth 14, 1582–1601. doi:10.1080/17538947.2021.1953161

Dávid, R.Á., Barcza, Z., Kern, A., Kristóf, E., **Hollós, R.**, Kis, A., Lukac, M., Fodor, N., 2021. Sensitivity of Spring Phenology Simulations to the Selection of Model Structure and Driving Meteorological Data. Atmosphere 12, 963. doi:10.3390/atmos12080963

Pokovai, K., **Hollós, R.**, Vidnyánszky-Bottyán, E., Kis, A., Marton, T., Pongrácz, R., Pásztor, L., Hidy, D., Barcza, Z., Fodor, N., 2020. Estimation of agro-ecosystem services using biogeochemical models. Időjárás/Quarterly Journal of the Hungarian Meteorological Service 124, 209–225.

Presentations/posters related to the topic of the dissertation at international and national conferences

Kern, A., Dobor, L., **Hollós, R.**, Marjanović, H., Torma, C., Kis, A., Fodor, N., Barcza, Z., 2022. Climate data for 1951–2100 for scientific, societal and policy purposes in Central Europe: the FORESEE database, in: Book of Abstracts: Natural Resources, Green Technology and Sustainable Development. p. 32.

Merganicova, K., Dobor, L., **Hollós, R**., Merganič, J., Barcza, Z., Kurjak, D., Novák, J., Sitková, Z., Fleischer, P., Marjanovic, H., Hidy, D., Střelcová, K., and Hlásny, T., 2021. Can we reach a sensible balance between generality of model parameters and accuracy of simulations?, EGU General Assembly 2021, online, 19–30 Apr 2021, EGU21-10889, doi:10.5194/egusphere-egu21-10889

Fodor, N., Pásztor, L., Tóth, B., Barcza, Z., Hidy, D., **Hollós, R.**, Kristóf, E., Kern, A., Kis, A., 2020. Database Sensitivity of the Biome-BGCMAg Biogeochemical Model, in: Book of Abstracts: Second International Crop Modelling Symposium. pp. 544–545.

Hidy, D., Fodor, N., **Hollós, R.,** Barcza, Z., 2020. Building a modelling framework to simulate ecosystem processes under changing climate: the long road from Biome-BGC to Biome-BGCMAg, in: EGU General Assembly Conference 2020. p. 21688.

Kis, A., Barcza, Z., Hidy, D., Hollós, R., Kristóf, E., Kern, A., Fodor, N., 2020. Bias correction of regional climate model results for crop simulations: hidden pitfalls and possible solutions, in: Book of Abstracts: Second International Crop Modelling Symposium. p. 410.

Kern, A., Dobor, L., Horváth, F., **Hollós, R.**, Márta, G., Barcza, Z., 2019. FORESEE: egy publikus meteorológiai adatbázis a Kárpát-medence tágabb térségére, in: Az Elmélet És a Gyakorlat Találkozása a Térinformatikában X.: Theory Meets Practice in GIS. pp. 131–138.

Sándor, R., Fodor, N., **Hollós, R**., Martin, R., Piseddu, F., Bellocchi, G., 2019. Expanding the potential applications of dynamic agro-ecosystem models in support of the sustainable development of agricultural production, in: 2. Francia-Magyar Tudományos Kutatói Fórum. Budapest, Magyarország 2019-09-27 — 2019-09-27

Fodor, N., Barcza, Z., Hidy, D., **Hollós, R.**, Dobor, L., Kis, A., Ádámné Pokovai, K., Gell, G., Pásztor, L., Takács, T.M., Cseresnyés, I., Nagy, Z., Salma, I., Bartholy, J., 2019. AgroMo - Interdiszciplináris Kísérleti Platform és Modellezési Keretrendszer, AgroMo konferencia, Martonvásár, Hungary 2019-04-18 2019-04-18

Hidy, D., Fodor, N., Hollós, R., Dobor, L., Ádámné Pokovai, K., Barcza, Z., 2019. A biogeokémiai modellek szerepe az éghajlatváltozás kutatásában, AgroMo konferencia, Martonvásár, Hungary 2019-04-18.

Hollós, R.**,** Fodor, N., Kis, A., Kristóf, E., Hidy, D., Ádámné Pokovai, K., Dobor, L., Barcza, Z., 2019. Biome-BGCMuSo felhasználóbarát keretrendszerének alkalmazási lehetőségei a klímaváltozás vonatkozásában. AgroMo konferencia, Martonvásár, Hungary 2019-04-18.

Sándor, R., Bellocchi, G., Bottyán, E.A.M., Doro, L., Hidy, D., **Hollós, R.**, Minet, J., Lelleiné Kovács, E., Ma, S., Perego, A., Ruget, F., Sanna, M., Seddaiu, G.W.L., Barcza, Z., 2019. Sensitivity analyses of simulated biomass yield and carbon-fluxes from Euro-Mediterranean grasslands, in: 3rd Agriculture and Climate Change Conference, Budapest, Magyarország 2019.03.24. - 2019.03.26

Hollós, R.**,** Fodor, N., Hidy, D., Marton, T., Bottyán, E., Barcza, Z., 2018. Mezőgazdasági célú Integrált Modellrendszer megvalósítása, in: Aktuális Környezeti Problémák Az Időjárás És Az Éghajlat Összefüggésében. pp. 69–75. doi:10.31852/EMF.30.2018.069.075

Other publications

Hollós, R., Fodor, N., Hidy, D., Marton, T., Bottyán, E., Barcza, Z. 2018. Mezőgazdasági célú Integrált Modellrendszer megvalósítása. In. Aktuális környezeti problémák az időjárás és az éghajlat összefüggésében, Budapest: ELTE TTK Meteorológiai Tanszék, Egyetemi Meteorológiai Füzetek doi: /10.31852/EMF.30.2018.069.075

Hidy, D., Barcza, Z., **Hollós, R.,** Thornton, P., Running, S.W. és Fodor, N., 2021. User's Guide for Biome-BGC MuSo. 6.2. http://nimbus.elte.hu/bbgc/files/Manual_BBGC_MuSo_v6.2.pdf.

References

Canadell, J.G., Monteiro, P.M.S., Costa, M.H., Cotrim da Cunha, L., Cox, P.M., Eliseev, A.V., Henson, S., Ishii, M., Jaccard, S., Koven, C., Lohila, A., Patra, P.K., Piao, S., Rogelj, J., Syampungani, S., Zaehle, S., Zickfeld, K., 2021. Global Carbon and other Biogeochemical Cycles and Feedbacks. Climate Change 2021: The Physical Science Basis. Contribution of

Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change. doi:10.1017/9781009157896.007

Chen, M.-H., Schmeiser, B.W., 1996. General Hit-and-Run Monte Carlo sampling for evaluating multidimensional integrals. Operations Research Letters 19, 161–169. doi:10.1016/0167-6377(96)00030-2

Fodor, N., Pásztor, L., Szabó, B., Laborczi, A., Pokovai, K., Hidy, D., **Hollós, R.**, Kristóf, E., Kis, A., Dobor, L., Kern, A., Grünwald, T., Barcza, Z., 2021. Input database related uncertainty of Biome-BGCMuSo agro-environmental model outputs. International Journal of Digital Earth 14, 1582–1601. doi:10.1080/17538947.2021.1953161

Hidy, D., Barcza, Z., **Hollós, R.,** Dobor, L., Ács, T., Zacháry, D., Filep, T., Pásztor, L., Incze, D., Dencső, M., Tóth, E., Merganicová, K., Thornton, P., Running, S., Fodor, N., 2022. Soil-related developments of the Biome-BGCMuSo v6.2 terrestrial ecosystem model. Geoscientific Model Development 15, 2157–2181. doi:10.5194/gmd-15-2157-2022

Hidy, D., Barcza, Z., **Hollós, R.,** Thornton, P., Running, S.W. és Fodor, N., 2021. User's Guide for Biome-BGC MuSo. 6.2. http://nimbus.elte.hu/bbgc/files/Manual_BBGC_MuSo_v6.2.pdf

Hollós, R., Kristóf, E., Fodor N., Hidy D., Horváth F., Barcza Z. 2023. RBBGCMuso: An R package to support the application of the Biome-BGCMuSo biogeochemical model [Computer software]. https://github.com/hollorol/RBBGCMuso

Hollós, R., Fodor, N., Merganičová, K., Hidy, D., Árendás, T., Grünwald, T., Barcza, Z., 2022. Conditional interval reduction method: A possible new direction for the optimization of process based models. Environmental Modelling & Software 158. doi:10.1016/j.envsoft.2022.105556

Kern, A., Dobor, L., **Hollós, R.**, Marjanović, H., Torma, C.Z., Kis, A., Fodor, N., Barcza, Z., 2024. Seamlessly combined historical and projected daily meteorological datasets for impact studies in Central Europe: The FORESEE v4.0 and the FORESEE-HUN v1.0. Climate Services 33, 100443. doi:10.1016/j.cliser.2023.100443

Pásztor, L., Laborczi, A., Takács, K., Illés, G., Szabó, J., Szatmári, G., 2020. Progress in the elaboration of GSM conform DSM products and their functional utilization in Hungary. Geoderma Regional 21, e00269. doi:10.1016/j.geodrs.2020.e00269

Ren, H., Zhang, L., Yan, M., Tian, X., Zheng, X., 2022. Sensitivity analysis of Biome-BGC-MuSo for gross and net primary productivity of typical forests in China. Forest Ecosystems 9, 100011. doi:10.1016/j.fecs.2022.100011