

Challenges and Prospects for Numerical Techniques in Atmospheric Modeling

J. Li , Y. Li, J. Steppeler, A. Laurian, F. Fang, and D. Knapp

Mathematics of the Weather 2022

What: Scientists in atmospheric science and high-performance computing gathered to discuss the new numerical techniques and algorithms that could be/have been applied in atmospheric modeling, research, and new discoveries in model development. A special theme in the workshop is the application of deep learning methods in data assimilation, numerical weather, and climate prediction.

When: 4–6 October 2022

Where: Bad Orb, Germany

KEYWORDS: Data assimilation; Numerical analysis/modeling; Adaptive models; Neural networks; Numerical weather prediction/forecasting; Deep learning

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Corresponding author: J. Li, ljx2311@mail.iap.ac.cn

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AFFILIATIONS: J. Li—International Center for Climate and Environment Sciences, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, China; Y. Li—State Key Laboratory of Numerical Modeling for Atmospheric Sciences and Geophysical Fluid Dynamics, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, China; **Steppeler**—Climate Service Center Germany (GERICS), Helmholtz-Zentrum Hereon, Hamburg, Germany; **Laurian**—Meteorologisches Institut, Ludwig-Maximilians-Universität, Munich, Germany; **Fang**—Applied Modelling and Computation Group, Department of Earth Science and Engineering, Imperial College London, London, United Kingdom; **Knapp**—Deutsches Zentrum für Luft- und Raumfahrt (DLR), Cologne, Germany

The Mathematics of the Weather (MOW) workshops have been held under different names since 1999. Early conferences were organized by the Short-Range Numerical Weather Prediction project team and were called “SRNWP” (<http://srnwp.met.hu>). These workshops addressed the numerical aspects of atmospheric models. The participants were invited to report on preliminary and ongoing work. This year, the MOW workshop was held in hybrid form in Bad Orb, Germany, from 4 to 6 October 2022 (<https://www.wavestoweather.de/meetings/mow2022>). Thirty-five participants presented and discussed recent developments in machine learning, data assimilation, numerical modeling of the atmosphere, as well as in regional climate modeling. Online participants from China, Russia, Ukraine, and the United States presented their work and took part in the discussions. The contents of this workshop are summarized in Table 1.

Applications of artificial intelligence in the atmosphere

Artificial intelligence (AI) models are trained to learn the physical processes from observations and replace existing subgrid models and physical parameterizations in numerical weather prediction (NWP) (Chantry et al. 2021). There is a controversy over the future for purely AI—whether AI models can replace existing NWP physical models. AI techniques have been leveraged to improve the accuracy and efficiency of NWP due to the expansion of computing capabilities. AI developers are seeking a substitute for numerical prediction from short range to climate scale. In this session, the lectures of Dale Durran (Univ. of Washington, United States), Fangxin Fang (ICL, United Kingdom), Jannik Wilhelm (KIT, Germany), and Jinxi Li (IAP, CAS, China) presented atmospheric forecasts using AI.

Dale Durran reported that a hybrid deep learning weather prediction (DLWP) model learning dynamics and physical parameterizations simultaneously made a breakthrough for climate-scale forecasting. Such a combination will be the optimal way by which physical modeling results can provide dynamic understanding from the governing equations, while data-driven modeling results may find some patterns which are not expected from physical modeling. Such forecasts have a remarkable predictive quality while the simulation time is reduced by orders of magnitude. Fangxin Fang presented a hybrid adversarial network model for real-time ozone forecasting. The results showed that the hybrid adversarial network model was able to capture the spatial and temporal evolution patterns of ozone concentrations during the predictive period of 2018 and 2019 in China. Jannik Wilhelm introduced a systematic testbed for basic research and explored machine learning techniques along an NWP process chain. A long short-term memory (LSTM) tetrahedral mesh generator was

Table 1. Sessions of MOW2022.

Speaker, affiliation, country (if not Germany)	Session	Content	
J. Steppeler (GERICS)	Welcome	Opening	
T. Janjic-Pfander (KUEI)		A note concerning climate activists	
D. Durran (Univ. of Washington, United States)	Artificial intelligence in the atmosphere	DLWP model	
F. Fang (ICL, United Kingdom)		AI and DA for pollution modeling	
J. Li (IAP, CAS, China)		LSTM and Multigrid HFM	
J. Wilhelm (KIT)		A new Testbed	
T. Janjic-Pfander		Data assimilation	
T. Kawabata (JMA, Japan)	Data assimilation	W2W, DA	
Y. Ruckstuhl (Ludwig-Maximilians-Univ.)		Storm-scale particle filter	
C. Snyder (NCAR, United States)		Uncertainty representation	
		EnKF	
M. Baldauf (DWD)	Numerical approaches for the atmospheric models	ICON DG solver	
A. Gassmann (TRR 181 "Energy transfers in Atmosphere and Ocean")		Upgrade of TRISK	
D. Knapp (DLR)		Adaptive mesh refinement	
O. Knoth (Leibniz-Institut für Troposphärenforschung)		CG/DG dynamical core	
F. Mesinger (SASA, Serbia)		Cut-cell ETA model	
V. Shashkin (Marchuk INM, RAS, Russia)		Grid imprinting on Cube Sphere	
J. Steppeler		Local-Galerkin	
J. Szmelter (Loughborough Univ., United Kingdom)		Unstructured mesh based on non-oscillatory forward-in-time model	
J. Rosemeier (Univ. of Exeter, United Kingdom)		Parallel computing architecture	
J. Dorrington (KIT)		New insights for the atmospheric modeling and dynamics	Interaction of stochasticity
D. Jacob (GERICS)			Remarks of climate modeling in Hessia and request of a new model generation for local climate
R. Klein (Freie Univ. Berlin)			Diabatic layer
J. Klemp (NCAR, United States)	Vertical coordinate		
S. I. Mahó (Univ. Hamburg)	Mixed Rossby-gravity waves		
V. Neduhai (Univ. Hamburg)	Tropical divergence decomposition		
V. Shpyg (UHMI, Ukraine)	Heavy precipitation modeling		
W. Skamarock (NCAR, United States)	Vertical resolution and filters		
C. Teichmann (GERICS)	GERICS climate modeling overview		
E. Huckert	Special topics		Programming for collaboration
Y. Li (IAP, CAS, China)			Mars GCM in China
X. Wu (ICL, United Kingdom)			Urban canopy model

proposed by Jinxi Li to optimize the mesh adaptivity criterion for the targeted prognostic variables, reducing the computational cost and expanding the mesh generator to dynamically adaptive mesh. Jinxi Li also proposed the AI-based high fidelity model (HFM) for solving differentiation equations that underpin the ocean and atmosphere circulations, as well as its linkage with new AI-based (data-driven) surrogate models. This new approach to solve differential equations uses predefined neural network weights, which effectively re-implements traditional numerical methods, with no training, to find the solution of the equations.

Data assimilation

Data assimilation (DA) aims to incorporate the incomplete, heterogeneous, and scattered observational data into numerical models. DA employs a variety of mathematical methods from optimization, numerical analysis, and statistics to achieve this goal. This session was composed of four presentations.

Tijana Janjic-Pfander (KUEI, Germany) reviewed the Kalman filter and ensemble Kalman filter (EnKF) and pointed out three problems to be solved in EnKF: 1) covariance localization for small ensemble size, 2) specification on model and observation errors, and 3) optimization on equations for non-Gaussian problems. Chris Snyder (NCAR, United States) investigated the sampling error in EnKF for small ensembles, high-dimensional states, and observations. He proposed canonical coordinates to diagonalize the Kalman filter update and to detect the catastrophically too small posterior covariance. In a next step, the significance of the localization was further stressed for sampling error reduction in practical approximation. Regarded as an extension of the stochastic EnKF, Janjic-Pfander proposed a QPEns algorithm by imposing additional physical constraints on the atmospheric states when updating the ensemble members. The formalism is able to consider nonlinear relationships and non-Gaussian moments, which optimizes the selection of the equations for non-Gaussian problems.

To reduce the computational cost to represent forecast error distribution in ensembles, Yvonne Ruckstuhl (Ludwig-Maximilians-Univ., Germany) treated the uncertainty representation in DA with stochastic Galerkin method where the stochastic variables are approximated with a Hermite polynomial expansion. Two sets of experiments were conducted to show that the stochastic variable representation is able to reduce sample numbers by four orders of magnitude compared to Monte Carlo cloud forecasts. The root-mean-square errors in EnKF were reduced.

A particle filter for storm-scale data analysis was presented by Takuya Kawabata (JMA, Japan). He investigated the non-Gaussian probability density functions in convection initiation and development by observing system simulation experiments.

Numerical approaches for the atmospheric models

The session on numerical methods for atmospheric models consisted of nine presentations, addressing 1) the discrete algorithms that are currently used for scientific research/operational weather service, 2) the generation of new dynamical cores and the model improvements, and 3) challenges for atmospheric modeling.

Almut Gassmann (TRR 181 “Energy Transfers in Atmosphere and Ocean,” Germany) presented a new usage of vorticities in the TRiSK energy conserving scheme on geodesic C-grids to solve the problematic Hollingsworth instability (Thuburn et al. 2009; Ringler et al. 2010). Based on the conservative transport schemes of Skamarock and Gassmann (2011), a third-order momentum advection operator can be introduced instead of the second-order part in the flux operator. She reported that the problems requiring TRiSK to solve are not present when using Galerkin approaches. However, Galerkin schemes can show boundary-related noise with an inappropriate treatment. Joanna Szmelter (Loughborough Univ., United Kingdom) discussed the progress of specialized preconditioners (the Richardson, Jacobi, and multigrid type of advanced preconditioning) on unstructured meshes for the nonsymmetric Krylov-subspace solver. To exploit the potential of modern computing architectures, Juliane Rosemeier (Univ. of Exeter, United Kingdom) presented a new coarse propagator using parareal methods (a parallel-in-time approach) to mitigate oscillatory stiffness through a filter function with averaging window and validated a significant parallel speedup over standard parareal methods. Vladimir Shashkin (Marchuk INM, RAS, Russia) proposed an approach called Summation-by-Parts Finite Differences to achieve a stable high-order spatial

approximation with mass and total energy conservations. This method is mainly applied to the differential operator approximation satisfying a discrete analog of integration by parts analytic property and can be used for block-structured logically-rectangular curvilinear grid. David Knapp (DLR, Germany) reported on a new model for grid refinement. The model extends the tree-based space-filling-curve approach to all types of elements needed for fully hybrid meshes in 3D. The refinement is based on the red-refinement and results in a quadtree (two-dimensional elements) or octree (three-dimensional elements). Some participants remarked that hanging nodes can occur, which is challenging for finite volumes methods. They use their approach for DG methods, where such difficulties can be circumvented.

Oswald Knoth (Leibniz-Institut für Troposphärenforschung, Germany) reported on a new continuous Galerkin (CG)/discontinuous Galerkin (DG) dynamical core for NWP using the programming language Julia. Michael Baldauf (DWD, Germany) promulgated a new DG solver as a possible alternative dynamical core for the ICON model with the support of the project BRIDGE. Fedor Mesinger (SASA, Serbia) reported on lessons learnt from the cut-cell model ETA. Mathematical errors of early versions discovered by Gallus and Klemp (2000) were removed, and he concluded that coordinate systems intersecting topography are able to perform better than terrain-following systems. Mesinger presented results with the new model version that were improved compared to the ECMWF scores for some cases.

Jürgen Steppeler (GERICS, Germany) highlighted the remarkable fact that the increase of the order of approximation and the corresponding increase of accuracy in numerical schemes lead to better predictions with toy models, but did not result in increased forecast scores in real-life models over the past two decades. Challenges for the mathematical implementation that can lead to errors were discussed. For example, Galerkin methods using low-order basis functions need special attention if a high-order approximation is to be achieved by super-convergence.

New insights for the atmospheric modeling and dynamics

A number of lectures dealt with the results of forecasts and dynamics of the weather and climate. To inspire the common interests, the general public was invited to attend this section.

Three lectures talk about the regional climate modeling. Claas Teichmann (GERICS, Germany) introduced the regional climate model REMO with its performance on regional climate simulations for the globe. In the context of global warming, he further emphasized the importance of using large eddy simulation model PALM for urban applications (including thermal comfort and cold air analysis, wind comfort and risks and pollutant dispersion). This is relevant for serving the urbanization process. Daniela Jacob (director of GERICS, Germany) challenged the audiences by requesting a new local climate model, in particular suited to accurately localize precipitation forecasts on small scales. Vitalii Shpyg (UHMI, Ukraine) presented heavy precipitation modeling in the Dniester River basin using the WRF Model.

Two lectures dealt with climate bifurcation. Jürgen Steppeler considered the chaos model of Lorenz, which gives an analytic form of the attractor. This attractor shows climate bifurcation for people living in a rectangular cave. For people living in such a cave, the attractor is given by the Lorenz model of scientific chaos. At a given location, dry and moist periods follow in an unpredictable way. Joshua Dorrington (KIT, Germany) presented results on climate bifurcation and the stochastic influence on bifurcation for Atlantic blocking. This work was coauthored by Tim Palmer (Jesus College, Univ. of Oxford, United Kingdom). The discussion focused on practical aspects of this work. The audience was interested in prospects of seasonal forecasts in the Atlantic area by forecasting blocking.

Two lectures focus on the vertical aspect of a model design. Joe Klemp (NCAR, United States) modified the MPAS model to allow for a constant pressure upper boundary (variable height upper boundary remains a material surface), which is suitable for the deep

atmosphere. The viability of the work was confirmed by an idealized diurnal heating test case. William Skamarock (NCAR, United States) reported on numerical experiments using the MPAS model with different vertical resolutions. He found that horizontal and vertical resolutions need to be considered jointly to allow for the convergence of atmospheric kinetic energy and to avoid spurious structures and noisy fields.

Three lectures emphasize atmospheric dynamics. By decomposition of the tropical divergence into Rossby and non-Rossby components, Valentino Neduhai (Univ. Hamburg) found that the synoptic- and planetary-scale Kelvin waves made a significant contribution to the tropical divergence field. Sándor István Mahó (Univ. Hamburg) reported on the nonlinear interactions for the excitation of mixed Rossby-gravity waves on the sphere using the TIGAR model. Rupert Klein (Freie Univ. Berlin) introduced a new approach for quasigeostrophic diabatic layer and outlooked the future use of this new theory for climate dynamics.

Special topics

Three talks were devoted to this special session with the aim to share research experiences on the start of development of a Mars general circulation model (GCM), the progress of scale-selected urban canopy parameterization, and an idea for establishing a platform to collaborate among scientists.

Yiyuan Li (IAP, CAS, China) reported on her project to simulate the atmosphere of Mars. She reviewed the basic characteristics of the Mars' GCM and introduced the roadmap of the project as well as the recent requests during China's Mars mission Tianwen-1 and Tianwen-3. She also conceived potential future developments on exploiting more numerical methods to solve the dynamical core (e.g., discretization methods, horizontal grids, vertical coordinates/grids) and implementing sensor data assimilation methods for the model initialization.

Xiaofei Wu (ICL, United Kingdom) developed a resolution-variable building-resolving urban canopy scheme by implementing tree and land surface processes to keep the energy balance of ground surface for city-scale modeling. This urban canopy package is designed to fit the unstructured tetrahedral adaptive mesh and used for urban microclimate and air quantity simulations considering a rapid urbanization statistically significant increases in the intensity and frequency of urban extreme rainfall events.

Edgar Huckert presented a software package aiming at easily sharing results among scientists at different locations (huckert.com). Now, it had been applied to the research on Galerkin and cut-cell methods. He is committed to provide a collaboration server with uniform compilers, shared documentation/recipes (offered via WEB), open libraries, and WEB interface for more complex applications (CGI Programs, see the Lorenz attractor). With this server, several scientists/groups can reuse the same infrastructure, which is crucial, e.g., in the context of COVID-19 outbreak.

Highlights and possible conclusions of this workshop are as follows:

- 1) With the rapid development of computing technology in recent decades, many operational centers and meteorological administrations are devoted to develop high-resolution and highly scalable weather and climate models. Numerical algorithms with high accuracy and strong scalability, high-resolution computational mesh, and scale-selective physical parameterizations (even the building-resolving packages) must be designed to fit with the exaFLOP supercomputers. This new model generation should address the question of lower boundary conditions and problems arising from lack of a homogeneous order of approximation.
- 2) Given the rise of deep learning techniques, many centers and universities aim to develop NWP-AI hybrid models for computing acceleration and representing some nonlinear

physical processes. DLWP (taking observations as input and generating end-user forecast products directly, see Dale Durrán's contribution) has the potential to revolutionize weather forecasting. The development of DLWP, or even deep learning Earth system models, is a challenge to the conventional numerical models and we are looking forward to more theoretical and technical surprises.

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Appendix: Abbreviations

BRIDGE	Basic Research for ICON with DG Extension
CAS	Chinese Academy of Sciences, China
DLR	Deutsches Zentrum für Luft- und Raumfahrt, Germany
DWD	Deutscher Wetterdienst (German Weather Service), Germany
ECMWF	European Centre for Medium-Range Weather Forecasts, United Kingdom
GERICS	Climate Service Center Germany
IAP	Institute of Atmospheric Physics, CAS, China
ICL	Imperial College London, United Kingdom
ICON	Icosahedral Nonhydrostatic model, Germany
INM	Institute of Numerical Mathematics, Russia
JMA	Japan Meteorological Agency, Japan
KIT	Karlsruher Institut für Technologie, Germany
KUEI	Katholische Univ. Eichstätt-Ingolstadt, Germany
NCAR	National Center for Atmospheric Research, United States
RAS	Russian Academy of Sciences, Russian
SASA	Serbian Academy of Sciences and Arts, Serbia
TIGAR	Transient Inertia-Gravity And Rossby
TRiSK	Thuburn–Ringler–Skamarock–Klemp
UHMI	Ukrainian Hydro-Meteorological Institute, Ukraine
W2W	Waves to Weather, Collaborative Research Center 165, Germany; https://www.wavestoweather.de
WRF	Weather Research and Forecasting Model, United States

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