Załącznik 2 do wniosku o wszczęcie postępowania habilitacyjnego - ENG

Author's Summary
of Professional Accomplishments

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1. Curriculum vitae.

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EDUCATION

1996 M.Sc. Atmospheric Physics, Physics Department, University of Warsaw.
Master's Thesis: "Numerical model of atmospheric airflow over topography. Izerskie Mountains". Adviser: Dr Szymon P. Malinowski

2001 Ph.D. Atmospheric Physics, Physics Department, University of Warsaw.
Doctoral Thesis: "The influence of internal gravity waves on the lower atmosphere". Adviser: Dr hab. Szymon P. Malinowski

PROFESSIONAL RECORD

2013-current Team Leader, of the COSMO Numerical Weather Forecasting Division, Institute of Meteorology and Water Management – National Research Institute, Warszawa, Poland
2012-2013 Project Scientist, NCAR, CISL/IMAGE, Boulder, CO, USA.
2008-2011 Researcher: Science and Technology in Atmospheric Research (STAR), Boulder, USA.
2005-2012 Project Scientist, NCAR, Research Application Laboratory (RAL), Boulder, CO, USA.
2004-2005 Postdoctoral Fellowship: IBM, Biomolecular Dynamics and Scalable Modeling Research Division at Thomas J. Watson Research Center, Yorktown Heights, NY, USA.
2001-2004 Postdoctoral Fellowship: Los Alamos National Laboratory, Los Alamos, NM, USA. Joint Postdoctoral Position in the Institute for Geophysics and Planetary Physics (IGPP) and Earth and Space Sciences Division (EES-2).
2001 Project Scientist, Institute of Geophysics, University of Warsaw, Poland

SHORT TIME SCIENTIFIC VISITS

2011 Noveltis, Toulouse, France. Collaboration with Dr Jean-Francois Vinuesa.
2010 Institute of Meteorology and Water Management (IMGW), Warsaw, Poland.
2005 Argonne National Laboratory, Argonne, IL, USA
2000, 2001, 2005 National Center for Atmospheric Research, Boulder, Co, USA. DOE/CHAMMP program on "Forward-In-Time Differencing for Shallow Fluid Flows on the Sphere". Collaboration with Dr Piotr Smolarkiewicz.
2000 ECMWF, Reading, England. Development of parallel version of the model in spherical geometry on Fujitsu Vpp700. Collaboration with Dr Piotr Smolarkiewicz.
1999 DLR (Institut fur Physik der Atmosphre), Oberpfaffenhofen, Germany. "DLR Wake Vortex (Wirbelschleppe) Project". Collaboration with Dr Andreas Dornbrack.
1999 Physics Department of UMIST, Manchester, England. Computations of moist airflows over Snowdon Mountain. Collaboration with Dr Anthony Dore.
1997-1998 NCAR, Mesoscale and Microscale Meteorology (MMM) Division, Boulder, Co, USA; DOE/CHAMMP "Forward-In-Time Differencing for Shallow Fluid Flows on the Sphere"

2. Academic and research career.

2.1 Employment history prior to the PhD awarding.

I started my professional career by completing **Master's degree** in atmospheric physics in 1996 at the **Atmospheric Physics Division** of the **Institute of Geophysics**, **Department of Physics**, **University** of **Warsaw (IGF-UW)**. My **Master's thesis** "Numerical model of atmospheric airflow over topography; Izerskie Mountains" was based on numerical studies of moist and dry orographic flows past idealized hills and the real orography of Izerskie Mountains using the geophysical model EULAG (ang. *EULerian-LAGrangian*). This model is based on the anelastic approximation of the Navier-Stokes equations. Results from my thesis were presented at two workshops: "Climatological Aspects of Environment Protection in Mountain Areas" in Karpacz (1995) and the "International Summer School of Meteorology, Eta - model" in Krivaja (Jugoslavia, 1996). During my graduate studies I have participated also in several geophysical field experiments: TTZ (Teisseyre-Tornquist Zone) seismic profile measurements of the crustal Trans-European zone (1993) [F1]; LIDAR measurement of the ozone vertical distribution over Kamieńczyk Valley (Karpacz, 1996) [F2]; and an airborne moto-glider measurements with ultrafast resistance thermometer (Kętrzyn, 1996) [F3].

In 1996 I began my **Ph.D studies** at IGF-UW. My Master's research represented an original contribution to atmospheric community and was internationally recognized. This resulted in an invitation to **National Center for Atmospheric Research** (NCAR, Boulder, USA) as a visiting scientist to work under the auspices of the Department of Energy (DOE) program: "Forward-In-Time Differencing for Shallow Fluid Flows on the Sphere", led by Dr Piotr Smolarkiewicz. The visit resulted in two journal publications on breaking gravity waves at the stratospheric altitudes [A1, A2]). Later on, I was participating in several international projects: in 1999 I was invited to the Institut Für Physik Der Atmosphere (DLR, Germany) by Dr. Andreas Dörnbrack to work on massive parallel computations of turbulent flows; and in 1999 to the Department of Physics at the University of Manchester Institute of Science and Technology (UMIST, Manchaser, UK) by Dr. Anthony Dore to investigate moist air flow over the Snowdon Mountains. In 2000 I was invited to the European Center for Medium Range Weather Forecasting (ECMWF, Reading, UK) collaborating with Dr Smolarkiewicz.

In April 2001**,** I completed my Ph.D with thesis devoted to study the excitation of internal gravity waves by convective eddies within atmospheric boundary layer (ABL), the interaction between waves, eddies, and cumulus convection in the lower troposphere, including waves trapped within the inversion layer at the top of ABL [N1]. The resonant mechanisms and mode selection define classes of the vortical flows such as cloud streets, cellular convection and convective thermals. These complex interactions were investigated by means of numerical simulation and linear theory, and results were presented at the General Assembly of EGU in Nice, France [K1] and ICCP conference in Reno, USA [K2].

During my **Ph.D studies** I was also involved in several internal projects. In collaboration with Dr Szymon Malinowski, I have prepared setup for the numerical experiments to validate small-scale cloud/clear-air mixing in the laboratory chamber. For this purpose, I have ported EULAG to computers at the Interdisciplinary Computer Modeling Center (ICM) at University of Warsaw; implemented Advanced Visualization System (AVS), Matlab and Vis5D software for postprocessing and visualization. In collaboration with ICM and Warsaw University of Technology I was involved in the Precision Weather Forecasting System for Multimodal Transport (PRESTO) project - focused on providing atmospheric conditions for pilots of small VFR-flights, leisure and commercial aviation, and balloons. Under PRESTO, I have performed simulations of the shallow moist convection driven by the time-dependent environmental conditions from weather forecasting Unified Model (UM-PL) run operationally at ICM [N2].

2.2 Employment history after the awarding of PhD.

2.2.1 Research assistant at IGF-UW (01–06 / 2001)

While completing my PhD, from January till June 2001 I was employed as a research assistant at the IGF-UW continuing collaboration with Dr Szymon Malinowski, and Dr Hanna Pawłowska in the project dedicated to numerical studies of the stratocumulus convection and its comparison with available field data sets. In this short period I have prepared first setup of the idealized stratocumulus convection. This model configuration was further polished and advanced by the IGF-UW team and successfully implemented in numerous projects.

2.2.2 Postdoctoral research at LANL (07/2001 - 08/2004)

After six months of completing my Ph.D, I have been awarded a **postdoctoral fellowship** at the **Los Alamos National Laboratory** (LANL, New Mexico, USA) between July 2001 and August 2004. During my postdoctoral appointment I was involved in a number of projects.

In collaboration with Dr Len Margolin (LANL) and Dr Piotr Smolarkiewicz (NCAR), I investigated an Implicit Large Eddy Simulations (ILES) for turbulent high Reynolds number flows [B1], a pioneering work described in more detail later in section 3.2. In collaboration with Dr Balu Nadiga I was working on parallel solvers for the elliptic Poisson equations [N3]. The major accomplishment of this postdoc appointment was work with Dr John Reisner and his fellow colleagues on enhancing numerical methods for hydrodynamic model HIGRAD, solving fully implicit Navier-Stokes equations by employing robust and accurate Jacobian-Free Newton-Krylov (JFNK) methods [B2]. This model was utilized for the studies of extreme atmospheric phenomena such as hurricanes [B3]. A version of HIGRAD combined with chemical model FIRETEC, was designed for predicting the development of wildfires.

While working at LANL, I was also involved in project on implementing parallel adaptive mesh refinement (AMR) package PARAMESH for HIGRAD, aiming at developing new Martian General Circulation Model (MGCM). The goal for this development was to employ a fully implicit solver with the capability to selectively zoom into regions on Mars with high spatial resolution, to address questions of e.g. how much water vapor is transported upwards by the global scale hurricane into the outer space; or how does the gas composition over the polar regions change with the freeze of considerable amounts of gaseous carbon dioxide. I left LANL while this project was still continuing, to a new postdoctoral position at the IBM.

2.2.3 Postdoctoral research at IBM (08/2004 - 09/2005)

After finishing the postdoctoral position at LANL I was hired in 2004 as a **research scientist** at the **IBMs T.J. Watson Research Center**, Yorktown Heights, NY, USA. There has long been a worldwide competition to create the most powerful and fastest supercomputer. In 1993, the "Top 500" project (www.top500.org) started as a way to track the trends and show which computing system is at the top of the list. In 2004, IBM (the world's largest information technology company), forged ahead to be number one on the Top500 list and created new supercomputer named BlueGene which utilized 64,000 energy efficient computing cores. The IBM was conducting several scientific projects in order to demonstrate feasibility and performance of this system. My responsibilities as an expert in High Performance Computing (HPC) and atmospheric sciences included participation in the development of a new dynamical core for climate models: High Order Multi-Scale Modeling Environment (HOMME) a joint project between NCAR and Colorado University (CU). I tuned the HOMME code algorithms on BlueGene system, and evaluated its accuracy, efficiency, and scalability [B4].

2.2.4 Research scientist at NCAR (09/2005 - 08/2013)

Between 2005-2012 I was employed as a **Project Scientist** at the **Research Applications Laboratory (RAL)** division of **NCAR**, the **National Security Applications Program** (NSAP), and also part time employed at **Science and Technology in Atmospheric Research** (STAR) Institute in Boulder, USA. In the summer of 2012 I have changed my appointment within NCAR moving out from RAL to the **Computational & Information Systems Laboratory (CISL)** and **Institute for Mathematics Applied to Geophysics (IMAGE)**.

Since coming to NCAR, I was involved in NSAP's applications and base science projects, founded by the government organizations: *Federal Aviation Application* (FAA), *Department of Energy* (DOE), *Department of Defense* (DOD), and *Defense Treat Reduction Agency* (DTRA). For the purpose of urban modeling, hazardous pollutant *transport*, and trace gas *dispersion* (T&D) I was enhancing *Immersed Boundary Methods* (IMB) within EULAG model. The significant part of my activities was devoted to solving basic science problems and their verification, e.g. structure of the *planetary boundary layer* (PBL), complex geometry urban modeling, aircraft generated wake vortices, thermally driven topographical circulations and cloud processes and formation of rainfall. For example, in the DTRA6.1 program I was aiming at sensitivity of convective planetary boundary-layer (PBL) structure to properties of heterogeneous land surfaces and clouds [K3], and on novel techniques of incorporating turbulent boundary conditions in convective flows [K4]. Most of these activities will be presented in section 3 and 4 which describes **significant accomplishments**.

Part of my time spent at RAL was dedicated to conducting independent verification of several operational numerical weather prediction installations of the *Weather Research and Forecasting* (WRF) model, e.g. operational installations over Saudi Arabia, [N4], Wyoming [N5], and evaluation of an Airdat project incorporating commercial aircraft measurements (TAMDAR) into the WRF's *Real Time Four-Dimensional Data Assimilation* (RTFDDA) system [B5]. In the latest year of my NCAR appointment, in the CISL/IMAGE group I was involved in the *National Science Foundation* (NSF) collaborative project: "A multiscale unified simulation environment for geo-scientific applications" devoted to development of an EULAG model version on the unstructured meshes, its parallelization and validation.

2.2.5 Team leader for operational NWP at IMGW-PIB (09/2013 -)

In September of 2013 I returned to Poland, wher I was offered a position at the Institute for **Meteorology and Water Management – National Research Institute** (IMGW-PIB) as the head of the **Department of the COSMO Numerical Weather Prediction** (NWP), currently being a part of the **National Centre for Meteorological Protection** (CMOK). I am responsible for the design, maintenance and operations of the NWP system based on COSMO model, cross-disciplinary models (e.g. nowcasting, hydrology, water wave and dispersion of the pollutions) and related systems as data assimilation, visualization and verification. A part of my current duties is to provide support in research and operations activities to the hydro-meteorological weather services. I also provide assistance in the development of funding proposals (e.g. NCBiR, NCN), contribute to the internal program planning and weather forecast product distributions among internal and external (academic or commercial) users.

Since January 2014 I am the member of the COSMO Steering Committee (STC) as the official representative of IMGW-PIB, participating in the planning and management for each consortium activities. I was selected as the Chairman of COSMO STC for years 2017-2018. In addition to the official duties, I'm collaborating with internal and external scientist in conducting the base science research [B6, K7], model applications [K5, K6, K8, N7], and development of model numeric on the contemporary computing architectures [N6].

2.3 Bibliography for chapter 2.

Scientific publications in journals contained in JRC database, before PhD:

A1 Prusa, J.M., P.K. Smolarkiewicz, and A.A. Wyszogrodzki, 1999: Massively parallel computations on gravity wave turbulence in the Earth's atmosphere. *SIAM News*, **32**, 10-13.

A2 Prusa, J.M., P.K. Smolarkiewicz, and A.A. Wyszogrodzki, 2001: Simulations of gravity wave induced turbulence using 512 PE CRAY T3E. *Int. J. Appl. Math. Comp. Sci.*, **11**, No. 4, 101-115.

Scientific publications in journals contained in JRC database, after PhD:

B1 Margolin, L.G., P.K. Smolarkiewicz, and A.A. Wyszogrodzki, 2002: Implicit turbulence modeling for high Reynolds number flows. *J. Fluid Eng.*, **124**, No. 4, 862-867.

B2 Reisner, J., A. Wyszogrodzki, V. Mousseau, and D. Knoll, 2003: An efficient physics-based preconditioner for the fully implicit solution of small-scale thermally driven atmospheric flows. *J. Computat. Phys*., **189**, 30-44.

B3 Reisner, J., V. Mousseau, A. Wyszogrodzki, and D. Knoll, 2005: An Implicitly balanced hurricane model with physics-based preconditioning. *Mon. Wea. Rev.*, **133**, No 4, 1003-1022.

B4 Bhanot G., J.M. Dennis, J. Edwards, W. Grabowski, M. Gupta, K. Jordan, R.D. Loft, J. Sexton, A. St-Cyr, S.J. Thomas, H.M. Tufo, T. Voran, R. Walkup, and A.A. Wyszogrodzki, 2008: Early Experiences with the 360TF IBM BlueGene/L Platform. *Int.J. of Computational Methods*, **5**, 237-253.

B5 Wyszogrodzki A.A., Y. Liu, G. Roux, Y. Zhang, P. Childs, N. Jacobs., and T. T. Warner, 2013: Analysis of the surface temperature and wind forecast errors of the NCAR-AirDat operational CONUS 4km RTFDDA forecasting system. *Meteorol. Atmos. Phys*., **122** (3), 125-143.

B6 Wyszogrodzki A.A., and L.L Lobocki, 2016: Towards the Parameterization of the Atmospheric Surface Layer over Inclined Terrain for Use in Non-Hydrostatic Models: Reference Tests. *Met. Zeit*., in review.

Other publications: journals not in the JCR database, reports and monographs

N1 Wyszogrodzki, A. A., 2001: "The influence of internal gravity waves on convection and clouds in the lower atmosphere". Ph.D dissertation, University of Warsaw, Institute of Geophysics, 99 pp.

N2 Wyszogrodzki, A.A., 2002: Numerical simulations of the evolution of a three-dimensional convection field. Research works based on the ICM's UMPL Numerical Weather Prediction System. Warsaw University Print, 35-52.

N3 Wyszogrodzki, A.A. 2003: Parallel iterative methods for solving 2D Poisson equation in a barotropic model. LA-UR-03-4463, 25 pp.

N4 Wyszogrodzki A. 2008: MM5 based RTFDDA system over Arabian Peninsula. "Kingdom of Saudi Arabia Assessment of Rainfall Augmentation" (KSAARA) project. NCAR internal report, 30pp.

N5 Wyszogrodzki A. 2008: Evaluation of the RT-FDDA system for the Wyoming Weather Modification Pilot Project (WWMPP). NCAR internal report ,25pp.

N6 Rosa B., L. Szustak, A. Wyszogrodzki, K. Rojek, D. Wójcik and R. Wyrzykowski, 2015: Adaptation of Multidimensional Positive Definite Advection Transport Algorithm to modern high-performance computing platforms, *International Journal of Modeling and Optimization,* 5 (3), 171-176.

N7. Duniec G., W. Interewicz, A. Mazur, and A. Wyszogrodzki, 2016: Operational Setup of the COSMO-based, Time-lagged Ensemble Prediction System at the IMWM - NRI. MHWM, 00057-2016-01, accepted.

Selected conference presentations and conference published articles

K1 Wyszogrodzki, A.A., 2000: The influence of internal gravity waves on convection and clouds in the lower atmosphere. Proceedings of European Geophysical Society, XXV General Assembly, 24-29 April 2000, Nice, France.

K2 Wyszogrodzki, A.A., 2000: The influence of internal gravity waves on convection and clouds in the lower atmosphere. Proceedings 13th International Conference on Clouds and Precipitation 14-18 August 2000, Reno, Nevada, USA.

K3 Hacker, J., and A. Wyszogrodzki, 2006: The Relationship between PBL Winds and Scale-Dependent Uncertainty in Land-Surface Heterogeneity. Eos Trans. AGU, 87(52), Suppl., Abstract A32D-06. Fall Meeting, 11-15 December, 2006, San Francisco, California, USA.

K4 Wyszogrodzki, A.A., J.P. Hacker, J.C. Weil, 2008: Turbulent lateral boundary conditions for LES of heterogeneous boundary layers. *Chemical and Biological Defense: Physical Science and Technology Conference*, 17-21 November 2008, 3 pp, New Orleans, LA, USA.

K5 Linkowska, J. A. Mazur, A. Wyszogrodzki, "Verification of COSMO model over Poland", EGU General Assembly 2014, 27April - 2 May, 2014, Vienna, Austria.

K6 Korycki, M. L. Łobocki, A.A Wyszogrodzki, "Application of EULAG to the simulation of flow through the urban structure in Warsaw", 4th International EULAG Workshop, October 20th-24th, 2014, Mainz, Germany.

K7. Wyszogrodzki A.A., and L. Łobocki "Surface-layer flux-gradient relationships over inclined terrain: implementation in EULAG", 4th International EULAG Workshop, October 20th-24th, 2014, Mainz, Germany.

K8 Starosta K., and A. Wyszogrodzki, "Analiza wiatru w Warszawie pod kątem wykorzystania energii wiatru w przestrzeni miejskiej", V Ogólnopolska Konferencja, "Klimat i bioklimat miast", 21–23 września 2015 r. Łódź, Polska.

External publications describing field experiments in which I was participating

F1 Grad M., Janik T., Yliniemi J., Guterch A., Luosto U., Tiira T., Komminaho K., Oeroda P., Höing K., Makris J. And Lund C.-E., 1999: Crustal structure of the Mid-Polish Trough beneath the Teisseyre-Tornquist Zone seismic profile. Tectonophysics, **314**, 145–160.

F2 Zwoździak A., J., Zwoździak A., Sówka I., Ernst K., Stacewicz T., Szymański A., Chudzyński S., Czyżewski A., Skubiszak W., Stelmaszczyk K, 2001: Some results on the ozone vertical distribution in atmospheric boundary layer from LIDAR and surface measurements over the Kamienczyk Valley, Poland, Atmos. Research **58**, 55-70.

F3 Haman, K. E. and Malinowski, S. P., 1996: Temperature measurements in clouds on a centimeter scale – Preliminary results, *Atmos. Res*., **41**, 161–175.

3. Achievement justifying the application for habilitation.

As an achievement defined by Art. 16, § 2 Act of on Academic Degrees and Academic Title and on Degrees and Title in Arts14 March 2003, I am indicating a series of 14 related publications (C1-C14), under the common title:

"Development of a numerical solver of Navier-Stokes equations in an anelastic approximation and its application to multiscale geophysical flows".

C1 Smolarkiewicz, P.K., L.G. Margolin and A.A. Wyszogrodzki, 2001: A class of nonhydrostatic global models. *J Atmos. Sci.*, **58** (4), 349-364.

C2 Margolin, L.G., P.K. Smolarkiewicz, and A.A. Wyszogrodzki, 2006: Dissipation in implicit turbulence models: A computational study. ASME *J. Appl. Mechanics,* **73** (3), 469-473.

C3 Schmidli J., B. J. Billings, R. Burton, F. K. Chow, S. F. J. De Wekker, J. D. Doyle, V. Grubisic, T. R. Holt, Q. Jiang, K. A. Lundquist, A. N. Ross, L. C. Savage, P. Sheridan, S. Vosper, C. D. Whiteman, A.A. Wyszogrodzki, G. Zaengl, and S. Zhong, 2011. Intercomparison of mesoscale model simulations of the daytime valley wind system. *Mon. Wea. Rev*., **139**, 1389–1409.

C4 Wyszogrodzki A.A., Grabowski W.W., and L-P. Wang, 2011: Activation of cloud droplets in bin-microphysics simulation of shallow convection. *Acta Geophys*., **59**, 1168-1183.

C5 Wyszogrodzki A.A., M. Shiguang, and F. Chen, 2012: Evaluation of the coupling between mesoscale-WRF and LES-EULAG models for simulation fine-scale urban dispersion. *Atmos. Research*, **118**, 324-345.

C6 Smolarkiewicz, P.K., J. Szmelter and A.A Wyszogrodzki, 2013: An unstructured-mesh atmospheric model for nonhydrostatic dynamic, *J. Comput. Phys*., **254**, 184–199.

C7 Smolarkiewicz, P.K., L.G. Margolin and A.A. Wyszogrodzki, 2007: Implicit large-eddy simulation in meteorology: from boundary layers to climate. *J. Fluid Eng*. **129** (12), 1533-1539.

C8 Prusa, J.M., P.K. Smolarkiewicz, and A.A. Wyszogrodzki, 2008: EULAG, a computational model for multiscale flows. *Computers and Fluids*, **37**, 1193–1207.

C9 Piotrowski, Z.P., P.K. Smolarkiewicz, S.P. Malinowski, A.A. Wyszogrodzki: 2009: On numerical realizability of thermal convection. *J. Computat. Phys*., **228**, 6268-6290.

C10 VanZanten, M.C., B.B. Stevens, L. Nuijens, A.P. Siebesma, A. Ackerman, F. Burnet, A. Cheng, F. Couvreux, H. Jiang, M. Khairoutdinov, Y. Kogan, D.C. Lewellen, D. Mechem, K. Nakamura, A. Noda, B. J. Shipway, J. Slawinska, S. Wang, A. Wyszogrodzki, 2011: Controls on precipitation and cloudiness in simulations of trade-wind cumulus as observed during RICO. *J. Adv. Model. Earth Syst*., **3**, M06001.

C11 Chen, F., H. Kusaka, R. Bornstein, J. Ching, C.S.B. Grimmond, S. Grossman-Clarke, T. Loridan, K. W. Manning, A. Martilli, S. Miao, D. Sailor, F. P. Salamanca, H. Taha,, M. Tewari, X. Wang, A.A. Wyszogrodzki, C. Zhang,, 2011: Developing the integrated WRF/urban modeling system and its applications to urban environmental problems. *Int. J. of Climatology*, **31**, 273-288.

C12 Piotrowski, Z.P., A.A. Wyszogrodzki, and P.K. Smolarkiewicz: 2011: Towards petascale simulation of atmospheric circulations with soundproof equations. Acta Geophys., **59**, 1294-1311.

C13 Wyszogrodzki A.A., Grabowski W.W., and L-P. Wang, and O. Ayala, 2013: Turbulent collision-coalescence in maritime shallow convection.. Atmos. Chem. Phys., **13** (16), 8471-8487

C14 Korycki, M., L.L. Łobocki, and A.A Wyszogrodzki, 2016: Application of EULAG to the simulation of flow through the urban structure in Warsaw, *Environmental Fluid Mechanics*, **16** (6), 1143–1171.

3.1 The content and scientific background of the research.

Comprehension of atmospheric dynamics and physics with their multiscale interactions comes from the observations and numerical experiments with models. Because of the enormous range of spatial and temporal scales in geophysical flows, explicit integrations of generic compressible equations with existing computational resources are prohibitively expensive for the majority of applications. In order to account for a broad range of scales, one has to invoke analytic or numerical approximations that allow for a relatively large time-step integrations of the governing equations. In effect, meteorological models encompass a variety of approximate systems of fluid equations (e.g., hydrostatic, elastic, anelastic, Boussinesq) and engender many split-explicit or semi-implicit methods for their integration. However, for the best efficiency and accuracy, particular methods and algorithms applied in the research are tailored to the spatial and temporal scales of the investigated phenomena. This is resulting in development of dedicated models of various complexity, e.g. *global circulation* (GCM), mesoscale *numerical weather prediction* (NWP), *cloud-resolving* (CRM), *large-eddy simulation* (LES), and *direct numerical simulation* (DNS).

A major accomplishment of my research was contribution to the development of computational methods for solving Navier-Stokes equations in the anelastic approximation within the framework of EULAG model and their application to research problems in a broad range of physical scales from micro O(10^{-2} m) to planetary (10^4 m). In particular, methods these are based on an accurate non-oscillatory forward-in-time (NFT) algorithms formulated on structured refined grids or unstructured meshes constructed for an efficient work on the most advanced contemporary computing architectures.

3.2 Advancing numerical methods in the anelastic EULAG model.

During my research career, I have been involved in the development of several advanced numerical modeling systems built on the subset form of Navier-Stokes equations, including global dynamical core (HOMME), numerical weather prediction (WRF, COSMO), and multiscale atmospheric research (HIGRAD, EULAG) models. However, my most significant achievement was a contribution to the development of a nonhydrostatic, Eulerian/ semi-Lagrangian model EULAG – a versatile numerical laboratory used for studies of physical processes in a broad range of spatial and temporal scales. Historically, while being developed by Dr Smolarkiewicz in the early 90's, EULAG originated as a model to test advanced numerical methods for integrating atmospheric and oceanic fluid equations. Later, the model evolved into a wide-purpose research tool for a broad range of fluid dynamics problems.

The general solution of the Navier-Stokes equations often contains modes of quickly propagating gravitational or acoustic waves, so the explicit methods integrating these equations are computationally very expensive. The anelastic approximation of EULAG designed to filter acoustic waves is a variant of generalized Boussinesq approximation, where the effects of density changes on the mass balance and inertia are neglected in the equations of mass continuity and momentum, but they are still accounted by the buoyancy forces. This leads to an implicit problem requiring solution of a linear elliptic Poisson equation for given boundary conditions. In EULAG, this is accomplished with a class of *Conjugate Gradient* (CG)/*Conjugate Residual* (CR) methods in the Krylov subspace. The accuracy of the implemented scheme is controlled within an iterative process by the assumed residual error. In application to problems with variable number of degrees of freedom (i.e. multi-physics processes as well as the size and structure of the computational grid, as the microscale Cartesian flows or global flows in the spherical coordinates), the efficiency of the algorithm is guaranteed by the application of the *Alternate Direction Implicit* (ADI) preconditioner. The successful multiscale nature of the anelastic approximation adopted in the EULAG results from its rigorous mathematical formulation and dissipative properties of NFT time stepping algorithms. More details of model algorithms and numerical properties are available in the presented list of publications. In this section I will elaborate on these developments in which I was involved while conducting my own research.

I have started my journey with EULAG by completing master's degree in atmospheric physics at the IGF-UW in 1996. A significant contribution to the atmospheric community from my master's degree was to port EULAG to the local computing systems at existing IGF/ICM facilities, its application to common geophysical problems (e.g. atmospheric convection, shallow cumulus clouds development, orographical flows), and to prepare documentation which could be used by a broader scientific community. My master's thesis was widely recognized, which resulted in the scientific visit at NCAR between 1997-1998. My primary assignment during that visit was to advance development of the massively parallel message-passing version of the EULAG numerical code using *Message Passing Interface* (MPI) libraries. Further, in collaboration with Dr Piotr Smolarkiewicz and Dr Joseph Prusa (TeraFlux), I have extended small-to mesoscale non-hydrostatic model EULAG to a rotating sphere, thereby creating unique high-performance semi-implicit anelastic global model (EULAS) that overcome traditional geophysical simplifications of hydrostaticity, gentle terrain slopes, or weak rotation. Using a benchmark "dynamical core" experiments on a sphere (i.e. idealized orographic flows with baroclinic instability and thermally forced Held-Suarez climates), we have evaluated relative accuracy and efficiency of different variants of the model: hydrostatic, nonhydrostatic, implicit, explicit, semi-Lagrangian, Eulerian, elastic, incompressible, and anelastic [C1]. This work also demonstrated that nonhydrostatic global models derived from small-scale atmospheric code adequately capture a broad range of planetary flows, adding relatively minor overhead due to the nonhydrostatic formulation. The efficiency and versatility of this approach was further shown with idealized planetary flows with an arbitrary diameter and angular speed of rotation [N8].

The key factors through which hydrodynamic equations can be effectively used for multiscale flows are the numerical properties of the time-stepping algorithms. While working at LANL and NCAR I was advancing anelastic methods in accordance to the nature of projects in which I was involved. One topic of my research was related to improve the performance of an elliptic solver. The elliptic problems in atmospheric applications are difficult to solve and require robust and universally effective schemes which provide judicious compromise between accuracy of the numerical solution and computational expense. The effective method applied in EULAG is a preconditioned nonsymmetric *conjugate-residual* (CR) iterative algorithm. Part of the scheme is an artful preconditioner able to dramatically accelerate solver convergence. In collaboration with Dr Smolarkiewicz I have developed new parallel preconditioner based on one-dimensional spectral transforms [N8], which is a viable alternative to the previously developed linear relaxation ADI method for a specific applications (e.g. orographic flows, small scale turbulence).

My major accomplishment, however, was the pioneering work on dissipative properties of the *Multidimensional Positive Defined Advection Transport Algorithm* (MPDATA). In general, NFT approximations such as MPDATA improve the physical realizability of simulations by preserving monotonicity of the solution, ensuring positiveness of the scalar fields, and warranting nonlinear stability. For the problems of decaying turbulence in a triply periodic cubic box [B1], MPDATA was shown to possess the ability to represent dissipative effects of turbulence in high Reynolds number flows without the need for any explicit subgrid scale (SGS) parameterizations, which is known as the *Implicit Large Eddy Simulation* (ILES). Our results confirmed earlier insights from simulations of convective boundary layers with and without subgrid models, that implicit turbulence property of MPDATA is not overly dissipative but adaptive to the flow [C2]. This is a key factor in preserving model stability and accuracy across a broad range of temporal and spatial scales of geophysical flows.

Beside model numerics, most of my research was focused on enhancing parameterizations of physical processes, such as the one acting in the atmospheric surface layer (SL) or the model subgrid scale turbulence. In particular I have extended the full model generalized coordinate transformations within the SGS scheme which later on allowed for a realistic experiments, with the formulation of model vertical coordinates to be consistent with the state of art mesoscale weather prediction models. I have adopted SL parameterization based on the one-dimensional force restore scheme which accounts for orographical effects and computes land surface thermal balance, along with the use of a classical Monin-Obukhov similarity theory. This development was summarized in the model intercomparison study for simulation of the three-dimensional daytime thermally induced wind valley system [C3].

Another two broad areas of my activity were a major topic of my base research and will be described in more details in the chapter 4. This includes the work on the parameterization of cloud microphysics [C4], and the development of *Immersed Boundary Methods* (IMB) for transport and dispersion (T&D) problems in the urban environment [C5]. In the last year of my NCAR appointment, I was involved in the NSF project, entitled "*A multiscale unified simulation environment for geo-scientific applications*" devoted to the development of an edge-based version of EULAG on unstructured meshes, which integrates nonhydrostatic anelastic equations suitable for simulation of small-to-mesoscale atmospheric flows [C6].

3.3 Model verification and applicability to multiscale geophysical flows.

Taking advantage of the unique numerical properties of EULAG, I have applied anelastic methods to many physical problems overlapping a broad range of spatial and temporal scales, from the canonical decaying turbulence in a triply-periodic box, to the development of convective planetary boundary layers and breaking of the gravity waves in the Earth's atmosphere, to the dynamics of global Earth circulations and the planetary scale weather. These model applications are summarized in a series of publications which evaluates the performance of model numeric [C1, C7, C8]. In particular, the problem of decaying micro-scale turbulence reported earlier in [B1, C2], focuses on the convective derivatives of the momentum equation assuming homogeneity of thermodynamics and lack of the near-wall effects. Such properties are the base for studies of small-scale mixing within clouds and the cloud-clear air interfacial interactions investigated by the IGF-UW team members. On the other hand, global simulations of the orographic flows and Held-Suarez climates [C1] show usability of the nonhydrostatic dynamics. Traditional numerical models employ hydrostatic primitive equations – a truncated form of Navier-Stokes equations with simplified Coriolis forces and neglected vertical accelerations. Our results proved that at the higher resolution allowed by computational resources, nonhydrostatic effects become noticeable, increasing accuracy of the numerical solutions while entailing negligible computational overhead.

In most cases, I have employed the *Large-Eddy Simulation* (LES) approach, understood as a numerical integration of a filtered Navier-Stokes' equations, where all scales of motion larger than scale of the grid interval are resolved explicitly, but the effects of finer (unresolved) scales are modeled, based on universal properties of fully developed turbulence. However, the ILES option was important for obviating the need of evaluating viscous stresses - a formidable task in generalized curvilinear frameworks. The Earth's climate contains additionally many physical processes extending beyond fluid dynamics, which can be further studied using hybrid LES/ILES approach. This practicality was evaluated by assessing role of the anisotropic viscosity in the development of convective structures in the atmospheric boundary layer [C9]. Our results were sensitive to the viscosity, either incorporated a priori by explicit subgrid-scale turbulence models or effectively realized in computational models. In particular, anisotropic viscosity can lead to the development of spurious regular convective structures that mimic naturally realizable Rayleigh–Benard cells, however unphysical for the specified external parameter range. Details of how the viscosity is introduced play secondary role: similar structures can develop for prescribed viscosities, explicit SGS turbulence models, ad-hoc numerical filters, or implicit dissipation of numerical schemes. This implies a need for careful selection of algorithms suitable for convection resolving simulations.

A significant effort was put on a rigorous evaluation of the numerical algorithms and physical parameterizations. The numerical advancements in the unstructured version of the model were evaluated with canonical simulations of the convective planetary boundary layer (PBL) and stably stratified orographic flows [C6], with results compared to equivalent solutions generated with established structured-grid models and field observations. A preliminary evaluation of the unstructured version of model for the urban layer flows was done in comparison with respective IMB methods [K10]. The structured version of the EULAG was used in several model inter-comparison projects; for example, the surface layer parameterizations were evaluated in studies of PBL structure determined by thermally driven circulations, such as wind valley flows [C3]. Nine nonhydrostatic mesoscale models participating in this intercomparison used the same initial and lateral boundary conditions, while applying distinct parameterizations of turbulence, radiation, and land surface processes. This evaluation proved that parameterizations of the surface–layer-atmosphere interactions and SGS turbulence developed in EULAG provides competitive results to these developed in current state of the art NWP models. There was also a significant effort put on verification of the transport and dispersion (T&D) of nonreactive contaminants in the urban environment [C5] - by coupling EULAG to the WRF NWP system [C11]. The evaluation of transport and dispersion modeling and urban canopy flows was conducted over an extended period of time and is described in chapters 4.1 and 4.2. Model microphysics was evaluated in the study of trade-wind shallow cumulus precipitation [C10] and is further described in section 4.3.

As an example of challenging applications, I will mention two distinct subjects. In a FAA project I was investigating wake vortices generated by commercial aircrafts at the en route - upper troposphere/lower stratosphere (UTLS) altitudes, at which aircrafts spend most of their flight time. Both ILES and the explicit turbulence parameterizations were successfully applied to simulate highly energetic coherent vortex structures, which are shed from the wing tips and persist downstream for a significant distance and time. I have evaluated the characteristics of such wake vortices in the function of atmospheric stability, wind shear, and the background turbulence intensity. Promising results from this project were presented at the 3rd EULAG workshop [K9], however the project was cancelled by FAA due to financial problems. More recently the IMB method is used to investigate stratified flows around an isolated, complex-shaped tall building represented by the Palace of Culture and Science (PKiN) in Warsaw [C14]. This study focuses on the identification of the dominant flow structures in the building wake for high and low Froude number regimes. Presented analysis reveal interesting flow organizations as a stationary disturbances akin to mountain gravity waves and multiple pairs of symmetric vortices associated with these waves. This work was conducted in cooperation with the Faculty of Environmental Engineering of the Warsaw University of Technology.

3.4 Aspects of the high performance computing.

One of the most significant factors in the successful implementation of the numerical algorithms to the multi scale physical problems is the model performance and portability over the accessible parallel computing systems. Since my Ph.D studies, I was actively involved in the work on parallelization of model algorithm and high performance computing which led to increase model's portability and efficiency. During my first scientific visit at NCAR in 1997 I have developed the MPI version of the EULAG code, and ported it on different computer architectures, as e.g., a 512 processor Cray system at NERSC, USA, and a long list of other parallel, vector and serial platforms [A1, A2].

In order to make the model attractive for adaptation in a wide range of academic/industrial environments, I have proved the model performance on different leading (at that time) TeraScale supercomputing architectures (e.g. IBM BlueGene/L/W, Cray T3E/XD) and demonstrated perfect scalability up to O(10^4) computing cores. Results of such activities were accumulated in the paper of [C11], which also contains examples of an anelastic atmospheric flows in the range of scales from micro to planetary.

Later on, with the advent of PetaScale computing architectures, the EULAG model has been rewritten with a new three-dimensional domain decomposition (3P) for increase its scalability and performance [C12]. In this project I was collaborating with Dr Zbigniew Piotrowski who became a new postdoctoral student at NCAR in 2009. The 3P model formulation was also applied to several idealistic microphysical problems and a real test case of shallow non-precipitating convection based on BOMEX (Barbados Oceanographic and Meteorological Experiment) observations [C13], showing good scalability up to O(10^5-10^6) computing cores. In a more recent NCN project a new version of EULAG was developed, being able to use contemporary computing architectures as the Graphic Processing Units (GPU) and Many Integrated Cores (MIC), with initial results published in [N6]. Currently, I'm serving as a coordinator of the component within the Horizon 2020 project ESCAPE (entitled "*Energy-efficient Scalable Algorithms for Weather Prediction at Exascale*") dedicated to the development of scalable and efficient methods for integrating of the Navier-Stokes equations.

3.5 Model maintenance, popularization and tutoring.

As the EULAG model was advancing and became much more popular in atmospheric community at the international level, I was leading activities related to model tutoring and its external distribution among the new users. I have created and I still serve as the administrator of the official EULAG model web page available at www.mmm.ucar.edu/eulag/. I'm providing tutoring service to new model users, and to a large number of students (e.g. from IGF-UW, Warsaw University of Technology, University of Arizona, University of Munich, University of Montreal) while they are conducting their MSc and PhD theses by using the EULAG model.

I was also a member of the organizing committee of first three international EULAG User Workshops which took place in Kolberbrau (Germany), Sopot (Poland) and Loughborough (UK). That activities included preparation of workshop sessions and tutorials for new users, creating and maintaining workshops web pages, and publishing post conference materials. After the second workshop the selected presentations were published in the special issue of Acta Geophysica, dedicated to problems of the pseudo-incompressible geophysical flows, where I served as a guest editor, selecting reviewers and accepting final publications.

3.6 Additional bibliography of the significant research achievement.

Other publications: journals not in the JCR database,

N8 Smolarkiewicz, P. K., C. Temperton, S. J. Thomas, and A. A. Wyszogrodzki, 2004. Spectral preconditioners for nonhydrostatic atmospheric models: Extreme applications. Proceedings of The ECMWF Seminar Series on *Recent developments in numerical methods for atmospheric and ocean modelling*, pp. 203—220, 6-10 September 2004, Reading, UK,.

N9 Wyszogrodzki, A.A. Z.P. Piotrowski, and W.W. Grabowski, 2012: Parallel implementation and scalability of cloud resolving EULAG model. PPAM 2011, *Lec. Not. Comp. Sci*., 7204, 252-261.

Conference presentations

K9 Wyszogrodzki A.A., P.K. Smolarkiewicz and R. Sharman, 2012: En route wake vortex dynamics; a computational study. 3rd International EULAG Workshop on Eulerian/Lagrangian methods for fluids. 25-28 June, 2012, Loughborough UK

K10. Wyszogrodzki A.A., P.K. Smolarkiewicz, and J. Szmelter, 2013: An application of the continuous feedback forcing immersed boundary and edge-based unstructured mesh models to the atmospheric flow problems. Joint EUROMECH / ERCOFTAC Colloquium 549, “Immersed Boundary Methods: Current Status and Future Research Directions”, Leiden, The Netherlands, 17-19 June 2013

4. Related scientific achievements.

4.1 Modeling transport and dispersion for homeland security applications.

During my stay at NCAR, my primary assignment was on homeland security projects, founded by the government agencies, such as the Federal Aviation Administration (FAA), the Defense Treat Reduction Agency (DTRA), the Department of Defense (DOD) and the Department of Energy (DOE). For these projects I was also employed at Science and Technology in Atmospheric Research (STAR) Institute in Boulder. The key role in these tasks were T&D capabilities of EULAG to simulate passive gas tracers and small scale dynamics in realistic conditions (e.g. boundary layer flows in a complex terrain and in an urban environment). Such capabilities are a powerful tool for assessing consequences of industrial emissions, accidental releases of hazardous materials, or dissemination of chemical, biological and radiological (CBR) warfare agents [K11, K12].

In these projects, I have coupled EULAG model with the Lagrange Particle Dispersion Model (LPDM) developed by Dr Weil (NCAR) and applied this modeling system to several DOD projects dedicated to improve CBR source characterization: Sensor Data Fusion (SDF), Virtual Threat Response Emulation Testbed (VTHREAT) [K13, K14]. VTHREAT supplement field datasets by represent wider range of possible environments with synthetic meteorological conditions, and to operate in restricted or inaccessible areas. It emulate entire process involved in detecting, characterizing, and responding to CBR treat in real rural or urban settings under realistic meteorological conditions [K15]. For the practical use in the CBR agent evaluation and contamination avoidance systems I have validated VTHREAT using several field experiments including classified trials (e.g. DTRA-DPG, FFT-07), open source field data sets (Prairie Grass, CONDORS) as well as wind tunnel data [K16]. In the same project, in order to utilize meteorological conditions generated by mesoscale weather prediction models (e.g. WRF/MM5) and on the site measurements within transient boundary layers, I have implemented the high resolution nudging technique to assimilate variable in time and space atmospheric conditions. I have also extended the passive tracer algorithm to include buoyancy effects for the purpose of modeling dense/buoyant gas emissions. Most of the results from such projects were presented at the topical conferences as some examples were listed above, however due to sensitive nature of these projects, only the limited number of journal articles were published [C15].

4.2 Enhancing immersed boundary methods for urban layer flows.

Another aspect of my work at RAL was on enhancing and utilizing *Immersed Boundary Methods* (IMB) to study boundary layer flows, hazardous pollutant transport and dispersion in high resolution urban environments [K17]. The IMB method commonly used in computational fluid dynamics (CFD), allows the building structures to be explicitly resolved. The algorithm implemented in the EULAG adds fictitious body forces into the equations of motion, to effectively impose no-slip/impervious boundary conditions at building walls. Method this was initially applied to the Pentagon Shield project and validated with the wind tunnel data. I have utilized the IMB method for the assessment of building-induced errors from rooftop mounted anemometer observations [K18]. These measurements are critical for defining wind field on the neighborhood and city scales, and must be sufficiently accurate for assimilation into mesoscale NWP models, or as the direct input to simulate atmospheric T&D. A sensitivity to use corrected roof-top winds was investigated for the Washington D.C. area, using combined EULAG/SCIPUFF T&D models driven by the WRF generated wind conditions. Later on I have coupled EULAG with MM5 based Global Climatology Analysis Tool (GCAT) to track hazardous gas traces in the urban atmosphere. GCAT climatology was downscaled and applied by EULAG to provide street-level transport of airborne contaminants in Oklahoma City downtown [K19].

For the purpose of realistic simulations within urban areas (e.g. Oklahoma City and Washington DC) I have coupled EULAG model to the WRF system [K20]. This effort was inspired from the fact that, at the urban scales, information on the meteorological conditions (related to e.g. heat island effects, thermally driven scale circulations, convergence zones) is incomplete and inconsistent due to limited and irregular network of meteorological stations located often away of the area of interest [C16]. Thus, an important aspect is to provide an appropriate meteorological information from high resolution NWP systems aware of diverse urban effects. WRF model uses an urban parameterization that handles information from land use characteristics, surface emission sources, high-resolution data assimilation systems, or fine-scale atmospheric analysis and uses it with either a simple bulk parameterization, or with a more complex urban-canopy model (UCM) [C8]. I have validated the coupling approach with the Oklahoma City URBAN 2003 experiment results, where the WRF-generated meso-scale conditions (i.e. wind, temperature, and turbulence fields) were downscaled and used to supply initial and boundary conditions of the T&D simulations at 3-6 meter grid spacing, improving accuracy of the urban scale transport and dispersion of a passive tracer [C5].

Yet another project related to this topic used analogy to theoretical formulation for the microscopic flows in porous media, relating porosity (topological and geometrical morphology) of the real building structures to the flow estimates of permeability and tortuosity. The flows through street-level building structures of the Oklahoma City, were analyzed in statistical terms of random porous media, seeking relations between the momentum flux and the macroscopic pressure gradient; i.e., a high-Reynolds-number analogy of Darcy's law. I have evaluated utility of this analogy for parameterizing urban effects in mesoscale weather predictions [K21].

The most recent work with the IMB method investigates before mentioned stratified flows around a complex-shaped building of the Palace of Culture and Science (PKiN) in Warsaw [C14]. This is a subject of a recent PhD thesis, where I serve as a co-advisor.

4.3 Investigation of shallow cumulus convection and formation of precipitation.

Due to limited computational resources, micro- and macroscopic properties of clouds and precipitation can be taken into account only by appropriate parameterizations, which mimic our understanding of the real physics. My first steps in the cloud modeling began during my PhD studies (see section 2) when I performed simulations of the shallow cumulus convection, prepared preliminary setup for the stratiform cloud simulations and microscale simulations mimicking experiments in the cloud chamber. Later on, during my work at the NCAR, special attention in my research was put to the convective and trade wind boundary layers topped with tropical and subtropical clouds such as stratocumulus and trade-wind cumulus - systems playing significant role in the Earth climate with their radiative properties and effects on large scale precipitation. My long term interest in these topics was a part of a large collaborative effort with the international group of scientists from NCAR (Prof. Wojciech Grabowski), University of Warsaw (Prof. Szymon Malinowski and Prof. Hanna Pawłowska), and University of Delaware (Dr. Lian-Ping Wang with collaborators). As a result of this collaborative research, three types of microphysics parameterization were successively implemented into the EULAG model:

- **bulk** - warm (ice free) clouds are at water saturation, cannot exist in the under-saturated conditions, non-precipitating volumes are diluted by entrainment of environmental air.
- **double moment** warm-rain - allows for secondary activation of cloud droplets above cloud base influencing mean microphysics and optical characteristics of the cloud field.
- **warm-rain bin microphysics -** represents the whole spectrum of cloud droplets and accounts for the effects of turbulence in the development of precipitation through the warm-rain (collision/coalescence) processes. A part of this parameterization - **collision kernels** - apply the theoretical model of the turbulent droplet collisions, verified by Direct Numerical Simulation (DNS) of the droplet-laden turbulent flows.

In the publications concerning “bulk” [C10, C17] and double moment schemes [C18, C19, C21], my role was focused mainly on providing supervisory and technical support to the visiting scientists and students completing their PhD theses (Dr. Joanna Sławińska, Dr. Dorota Jarecka, Dr. Marcin Kurowski, mgr Marta Kopeć), by setting up the numerical experiments, checking and verifying the model results, and by final preparation and editing of the manuscripts. In the later stage I have played the leading role for implementing and evaluating the bin microphysics parametrization in the process of shallow cumulus field development and the initiation of precipitation [C4, C12, C13]. Activities these are summarized in the next subchapters.

a) Numerical experiments with single moment bulk approach

For the LES of a shallow non-precipitating convection based on the BOMEX observations [C17], I have set up fine scale experiments on NCARs IBM BG/L supercomputer (“*frost*”), using 8000 computing cores. This project was investigating convective–radiative quasi-equilibrium mimicking the mean Earth conditions, with emphasis on the indirect aerosol effects. Cloud microphysical properties are to a large extent determined by the cloud condensation nuclei (CCN), cloud-base updraft strength, and transformation resulting from entrainment and mixing: dilution, homogeneity of the cloud-environment mixing or entrainment-related activation. Two limits of the concentration of cloud droplets were considered: low (“*pristine*”), and high (“*polluted*”). From estimates of spatial variability of an effective radius r_e (ratio between the third and the second moment of the cloud droplets size distribution) we have found that bulk model misses to some degree microphysical transformations associated with cloud-environment mixing and entrainment processes. These transformations combined with additional nucleation of cloud droplets above the cloud base due to increasing updraft strength or entrainment are important factors and contribute to observed variability.

Prior to the application of a more advanced parameterization, the performance of "*bulk*" microphysics was tested with 11 state-of-the-art cloud models and field observations in the *Rain in Cumulus over Ocean* (RICO) inter-comparison study of precipitating trade wind cumulus [C10]. Simulations do show differences between model's results in the representation of the cloud microphysical structure and surface precipitation rates. However, the ensemble average of the simulation results plausibly reproduces many features of the observed clouds, including the vertical structure of cloud fraction, profiles of cloud and rain water; therefore, the computed statistics qualify bulk parameterization as suitable for real-case applications.

b) **Effects of double moment warm-rain microphysics**

Following the outcomes of [C17] a more sophisticated double-moment warm-rain microphysics was applied to the EULAG model, which is able to predict number of cloud droplets and mixing ratios, which allows for various scenarios of microphysical transformations due to turbulent entrainment and mixing. The changes of supersaturation within shallow ice-free clouds and the in-cloud nucleation enhancement in the process of drizzle/rain formation was investigated in [C18]. In this work we have predicted the homogeneity of SGS turbulent mixing between cloud and its environment, which affects the mean droplet size associated with evaporation of cloud water due to entrainment. In our results, mixing homogeneity increases with height, because of higher turbulence intensity and larger droplet sizes aloft. This brings to the attention the higher importance of turbulent mixing, which can be significantly changed by homogeneity due to spatial variability of the intensity of turbulence and the mean droplet radius.

In the paper [C19] we have utilized RICO case again to validate double-moment scheme for two aerosol environments (pristine and polluted) and two contrasting SGS mixing scenarios (homogeneous and extremely inhomogeneous). In contrast to the bulk results, the cloud field gradually deepened and a sharp temperature and moisture inversions developed in the lower troposphere. Pristine and polluted environments featured different cloud droplet concentrations and large differences in rainfall rates. However, the macroscopic cloud characteristics appeared similar regardless of aerosol type or SGS mixing homogeneity. The double-moment scheme was finally used to reproduce macroscopic and microphysical properties of clouds observed during the EUCAARI-IMPACT aircraft field campaign over North-Sea [C21]. Simulated mixing was on average quite inhomogeneous, with well-defined mean across entire depth of the cloud field, but with local variations especially near the base and the top of the cloud field. The model simulated adequately cloud structure: stratocumulus-over-cumulus formations..

c) **Extension to warm-rain bin microphysics**

As a step beyond the bulk approach, we have implemented warm-rain bin microphysics including the turbulent kernel, which provides significant challenge from the computational point of view, requiring to develop efficient algorithms capable of using the contemporary PetaScale computing architectures [C12, N9]. This objective was a part of a collaborative project with the Delaware University (prof Lian-Ping Wang and Dr. Orlano Ayala [N10]). This project was dedicated to resolve multiscale coupling between cloud dynamics and microphysics spanning spatial scales from meter to hundreds of meters, and to provide a quantitative assessment of the effect of cloud turbulence on rain development in shallow ice-free convective clouds. Initially, the newly implemented bin microphysics was applied to a shallow non-precipitating convection parametrization based on BOMEX observations, to investigate effects of the secondary activation of cloud droplets above the cloud base. In an earlier study with double-moment scheme [C19], in-cloud activation had significant implications on mean microphysical and optical characteristics of the cloud field. By contrasting simulations with, and without in-cloud activation, we showed [C4] that the lack of in-cloud activation produces quantitatively less intense decrease of the concentration of cloud droplets with height.

The effect of cloud turbulence accounted as the enhancement of raindrops collection kernel (parameterization derived by prof Wang [N10] from the high resolution DNS) was compared with results from standard gravitational collection kernel [C13]. Simulations for a range of cloud condensation nuclei (CCN) concentrations show that the microphysical enhancement leads to an earlier formation of drizzle through faster autoconversion of cloud water, especially in simulations with high CCN. For low-CCN, dynamical enhancement (due to turbulent collection kernel) leads to a more efficient removal of condensed water from cloudy volumes, and to increase of buoyancy - enabling clouds to reach higher levels, and to a significant increase of the surface rain accumulation. An open questions required additional investigation was assessment of the impact of dynamical enhancement of cloud-scale processes on macroscopic cloud field characteristics that increases the amount of drizzle/rain fall.

4.4 Bibliography for related achievements in chapter 4

Scientific publications in journals contained in JRC database

C15 Platt N., D. DeRiggi, S. Warner, P. Bieringer, G. Bieberbach, A. Wyszogrodzki and J. Weil, 2012: Method for comparison of large eddy simulation generated wind fluctuations with short-range observations. *Int. J. of Environment and Pollution*., **48**, 22-30.

C16 Tewari M., H. Kusaka, F. Chen, W.J. Coirier, S. Kim, A.A. Wyszogrodzki, T.T. Warner, 2010: Impact of Coupling a microscale computational fluid dynamics model with a mesoscale model on Urban Scale Contaminant Transport & Dispersion. *Atmosph. Rresearch*, **96**, 656-664. ISSN 0169-8095.

C17 Slawinska, J., W. W. Grabowski, H. Pawlowska, and A. A. Wyszogrodzki, 2008: Optical properties of shallow convective clouds diagnosed from a bulk-microphysics LES. *J. Climate*, **21**, 1639-1647

C18 Jarecka, D., Grabowski, W. W., Pawlowska, H., and A.A Wyszogrodzki, 2011: Modeling of subgrid-scale cloud-clear air turbulent mixing in large-eddy simulation of cloud fields, *Journal of Physics: Conference Series,* **318**, 9pp, 072010

C19 Grabowski W.W., J. Slawinska, H. Pawlowska, and A.A. Wyszogrodzki, 2011: Macroscopic impacts of cloud and precipitation processes in shallow convection. *Acta Geophys*., **59**, 1184-1204.

C20 Malinowski, S.P., A.A. Wyszogrodzki, and M.Z. Ziemiański, 2011: Modeling atmospheric circulations with sound-proof equations – preface to the topical issue, *Acta Geophys*., **59**, 1073-1075.

C21 Jarecka D., H. Pawlowska, W.W. Grabowski. A.A. Wyszogrodzki, 2013: Modeling microphysical effects of entrainment in clouds observed during EUCAARI-IMPACT field campaign. *Atmos. Chem. Phys*., **13** (16), 8489-8503.

Other publications: journals not in the JCR database, reports and monographs

N10 Wang L-P., O. Ayala, H. Parishani, W.W. Grabowski, A.A Wyszogrodzki, Z. Piotrowski, G.R Gao, C. Kambhamettu, X. Li, L.Rossi, D. Orozco and C. Torres, 2011: Towards an integrated multiscale simulation of turbulent clouds on PetaScale computers. *J. Phys.: Conf. Ser*., 318, 072021.

Conference presentations and conference published articles

K11 Wyszogrodzki A., F. Vendenberghe & T. Warner, The use of coupled mesoscale and les models for calculating urban climatologies of street level and boundary layer winds with risk assessment

implications. 10th Annual George Mason University *Conference on Atmospheric Transport and Dispersion Modeling*. August 1-3, 2006, George Mason University Fairfax, Virginia, USA.

K12 Warner T., Swerdlin S., Wyszogrodzki A. and Fandenberghe F., A climate analysis tool for assessing the vulnerability of a region to a variety of disasters. *Conference on Dynamics and Disasters*, October 5-7, 2006, Athens, Greece.

K13 Bieberbach G., S. Swerdlin, P. Bieringer, R. Cabell, F. Vandenberghe, A. Wyszogrodzki, R-S. Sheu. Application of advanced numerical weather prediction techniques for improving CBR source characterization within a flexible simulation and evaluation development environment. *CBIS*, Austin, TX, January 8-12, 2007

K14 Bieringer P.E., J. Weil, J. Hurst, G. Bieberbach, A. Wyszogrodzki, R. Sheu & M. Raines, 2008: A framework for developing synthetic chemical and biological agent release data sets for use in virtual test and evaluation. *Chemical and Biological Defense: Physical Science and Technology Conference*, 17-21 November 2008, 3 pp, New Orleans, LA, USA.

K15 Bieberbach G., P. E. Bieringer, A. A. Wyszogrodzki, J. Weil, R. Cabell, and J. Hurst, 2010: Virtual Chemical and Biological (CB) Agent Data Set Generation to support the Evaluation of CB Contamination Avoidance Systems. *The Fifth International Symposium on Computational Wind Engineering*, May 23-27, 2010, Chapel Hill, NC, USA.

K16 Wyszogrodzki A..A., J. Weil, G. Bieberbach, P.E. Bieringer, N. Platt, and L.H. Jones, 2010: Evaluation of large eddy numerical simulations with observations from fusing sensor information from observing networks (FUSION) Field Trial 2007 (FFT-07). *16th Conference on Air Pollution Meteorology, AMS 90th Annual Meeting*, January 17-21, 2010, Atlanta, Georgia, USA.

K17 Wyszogrodzki A., P. Smolarkiewicz, R. Sharman & J. Szmelter, 2006: Large-eddy simulations of urban boundary layers. 10th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling. August 1-3, 2006, George Mason University Fairfax, Virginia, USA.

K18 Wyszogrodzki, A., Y. Liu, R.S. Sheu, R. Sharman & T. Warner , 2006: Assessment and removal of rooftop anemometer observation errors for use in mesoscale NWP and T&D applications. 10th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling. August 1-3, 2006, George Mason University Fairfax, Virginia, USA.

K19 Warner T., S. Swerdlin, A. Wyszogrodzki and F. Vandenberghe. Multi-scale urban weather analyses, forecasts and climatology. 6th Conf. Urban Climate, June 12-16. 2006, Göteborg, Sweden.

K20 Wyszogrodzki, A.A., F. Chen, S. G. Miao, and J. Michalakes, 2009: Two-way coupling approach between WRF NWP and EULAG LES models for urban area transport and dispersion modeling. Eighth Symposium on the Urban Environment, 10-15 January 2009, Phoenix Arizona, USA.

K21 Wyszogrodzki, A.A., P.K. Smolarkiewicz, 2010: Large-eddy simulation of urban flows: a porous-media analogy. Proceedings of *3rd Joint US-European Fluids Engineering Summer Meeting*, August 1-5, 2010, Montreal, Canada. paper no. FEDSM-ICNMM2010-30157.

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