Appendix 2

Summary of professional accomplishments

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SUMMARY OF PROFESSIONAL ACCOMPLISHMENTS

1. First and last name

   Bogdan Rosa

2. Possessed diplomas, degrees – with an indication of name, place and year of obtaining them and the title of the doctoral dissertation

   Doctor of physical sciences 2005, University of Warsaw, Institute of Geophysics

   Doctoral dissertation title: *Analysis of turbulence behind the shield of the ultrafast aircraft thermometer*

   PhD advisor: prof. dr hab. Tomasz Jan Szoplik

   Master in optical information processing 2000, Faculty of Physics, University of Warsaw, Institute of Geophysics, Section of Information Optics

   Master dissertation title: *Construction of a 3D terrain model based on hand-drawn topographical maps*

   Supervisor: prof. dr hab. Tomasz Jan Szoplik

3. Information on positions held, including employment in a scientific institutions

October 2000 – June 2005	Ph.D. study at Faculty of Physics, University of Warsaw, specialization geophysics
September 2005 – December 2005	Full-time assistant professor (*pol. adiunkt*) at Faculty of Physics, University of Warsaw, specialization geophysics
January 2006 – December 2008	Post-doc position at Department of Mechanical Engineering, University of Delaware, USA
January 2009 – December 2009	Professional researcher at Institute of Meteorology and Water Management, Poland
January 2010 - up to now	Full-time assistant professor (*pol. adiunkt*) at Institute of Meteorology and Water Management – National Research Institute, Poland

4. Academic achievements pursuant to Art. 16 Paragraph 2 of the Act of March14, 2003 on the Academic Degrees and the Academic Title as well as on the Degrees and the Title within the scope of Art. (Dziennik Ustaw – Official Journal of Laws No. 65, item 595, as amended):

The achievement pursuant to the abovementioned act is habilitation dissertation entitled "Dynamics of inertial particles in turbulent flows", IMGW Publishing Institute, IMGW Monograph Series, ISBN 978-83-64979-19-4, Warsaw 2016

Discussion of the research achievements

Turbulent flows and particle transport are very common phenomena in nature. The processes occur continuously, with different intensity and at different scales. In fact, the majority of flows in nature are turbulent. Particle transport by a turbulent fluid phase is also an important mechanism for many technological processes. They find numerous applications in industry and other fields related to the power engineering and motorization. Examples of these include: efficient combustion of pulverized coal in boilers, pneumatic transport in pipelines, combustion of the fuel in engines or spraying of fertilizers and plant protection products.

Particle transport in turbulent flows is also important in other areas such as environmental protection and environmental engineering. This applies to the problems related to dispersion of pollutants in the atmosphere and prediction of environmental disasters (risk evaluation by determining the maximum concentration of harmful substances in the atmosphere or water reservoirs). Turbulent transport is the main mechanism, which controls the cycling of organic matter in the oceans and transport of pollutants and sediments in water reservoirs. Detailed knowledge of turbulent transport is also beneficial for a number of meteorological applications. These include: modeling of sandstorms, volcanic ash transport and precipitation formation. Furthermore, the knowledge about turbulent transport and particle interaction may also have purely scientific applications. An example here is astrophysical application related to modeling the growth of particles in protoplanetary disks.

A thorough analysis of turbulent transport is an important research task, because it leads to better control of the above-mentioned processes, facilitates their optimization, contributes to development of new devices and helps to develop more accurate weather forecasts.

Studies on the dynamics of particles in turbulence require addressing a number of difficulties and limitations. The general description of the multiscale interaction of inertial particles with turbulent flow is a challenging task due to inherent nonlinearities, inhomogeneities and coupling over extended length and time scales. Motion of particles of non-zero inertia in the turbulent flow results in their distribution in space (grouping), collision frequency, and settling velocity (the later is present only if gravity is considered). In addition, turbulence affects the strength of aerodynamic (hydrodynamic) interaction between the individual particles and between the particle clusters [1]. Due to practical importance, these processes have been extensively investigated in many scientific studies. Nevertheless, complete quantitative understanding of the mechanisms is still insufficient.

Experimental studies of multiphase flows are usually difficult, because these processes span a wide range of spatial and temporal scales. Furthermore, the measuring devices have technical limitations and do not allow to simultaneously measure the 3D particle position and velocity. When it comes to cloud processes, the additional difficulty is to perform measurements directly in clouds. Remote measurements with the sensing radars usually do not yield desired accuracy.

Exact solutions that can be found in the literature are valid only for a very simplified cases, for example trajectories of particles in a two-dimensional steady flow [2] or the interaction of particles with axially symmetrical eddies [3]. Generalization of these idealized analytical solutions for the case of three-dimensional time-dependent homogeneous and isotropic turbulence may lead to erroneous conclusions.

In recent years direct numerical simulations (DNS) have become an important tool for modeling multiphase flows. In the simulations turbulent flow is modeled using Eulerian approach i.e. by solving the incompressible Navier-Stokes equations on a regular 3D grid [4]. Modeling of particle motion is carried out in the Lagrange approach. The algorithm tracks the trajectory of the individual particles. Turbulent flow is forced using special numerical algorithm, which parameterizes the fluid flow at large scales. The energy transfer from large to small scales (the energy cascade) is governed by the Navier-Stokes equations and described by the Kolmogorov theory [4].

My work was focused mainly on modeling of cloud microphysical processes. In recent years an increasing number of studies have been initiated to quantify the effects of air turbulence on the growth of cloud droplets during warm rain initiation. A thorough study of this mechanism is important, because it helps to fully understand this complex process. Warm rain processes account for about 31% of the total rainfall and 72% of the total rain area in tropics [5]. Due to the relative rarity of ice forming nuclei, this process is active in most climate zones in all seasons.

One of the most important mechanisms that affects the rate of warm rain formation is the atmospheric turbulence. The turbulent flow can enhance the rate of droplet collisions and thus speed up the development of precipitation. It should be noted, however, that turbulence is not the only mechanism that determines the rate of precipitation formation. Droplets less than 10 μm in radii grow efficiently through diffusion. The impact of turbulence on collision-coalescence of such small droplets is very limited because the droplets have low inertia and behave like fluid elements. Droplets larger than 60 μm in radius grow efficiently through gravitational collisions. This directly results from different settling velocities [6,7]. Moreover, the large drops can collect all small droplets that are on their way. The mechanism of gravitational collision-coalescence is efficient only for large droplets. Also in this case, the role of turbulence is rather limited. This is because the motion of such heavy droplets is determined mainly by gravitational acceleration. Therefore I have focused on modeling the collision–coalescence of cloud droplets in the size range from 10 to 60 μm in radius (so called the size gap problem).

The aim of my work was to quantify turbulent collision rate of inertial particles relevant to cloud droplets of radius from 10 to 60 μm, under physically realistic conditions. For turbulence modeling and particle tracking, I used direct numerical simulation (DNS). To set the numerical experiment, the characteristic scales of the turbulent flow should match the conditions in real clouds. One of those parameters is the Taylor microscale Reynolds number R_λ [8] defining the range of length scales represented in the flow. In DNS the largest scales are limited by the domain size while the smallest scales depend on grid spacing. Numerical complexity limits the DNS of turbulent collision to small Taylor microscale Reynolds number (R_λ~100), though in real clouds the value is a few orders of magnitude larger (R_λ~10^4). Achieving high Reynolds numbers in DNS is not feasible, but fortunately small flow structures are mainly responsible for droplets collision thus a truncated representation of turbulence is revealing.

Research tool

My research tool is an innovative DNS code that allows to integrate the Navier-Stokes equations using pseudo-spectral method. The code has been developed in collaboration with scientists from University of Delaware. Performed simulations show that the code has an excellent numerical performance. The implementation is designed to run on supercomputers with distributed memory. The strategy of parallelization is based on 2D domain decomposition. For data communication, the MPI (Message Passing Interface) library is used. Such a treatment allows the use of a larger number of processors, memory, and improved cache utilization, leading to a much better overall computational efficiency. As a result, the code enables performing high-resolution DNS of turbulent collisions so the simulation results can be used to address the question of Reynolds number dependence of pair and collision statistics. Moreover, larger domains (equivalently larger Reynolds number) make the simulations closer to the physical conditions in turbulent clouds.

Detailed tasks and research goals

1. *Examine the dependence of the structure and statistics of turbulent flow on the grid resolution.*

   This task can be formulated equivalently in terms of the physical parameters, namely, how the structure of the flow depends on the Reynolds number at fixed energy dissipation rate. Since the flow at large scale may be affected by the forcing method, the simulations have been performed using two different forcing schemes.

2. *Two-point statistics related to the spatial distribution of cloud droplets (radial distribution function - RDF) and their radial velocity relative (RRV).*

   I analyzed statistics in both kinematic and dynamic (dynamic collision kernel) formulation. Sensitivity of the above-mentioned statistics on the Reynolds number, particle inertia and forcing scheme has also been carefully examined.

3. *The role of gravity on the kinematic and dynamic collision statistics and collision rate.*

   Since the effect of gravity on these statistics depends on the particle inertia, simulations have been performed for different droplet sizes. Examination of this problem is particularly important for the monodisperse suspensions i.e. when all particles have the same inertia, size and the terminal velocity (settling velocity in stagnant air).

4. *Effects of the large scale forcing time scale on the simulated flow structures and statistics of forced turbulence.*

   The forcing time scale is typically made much smaller than the large-eddy turnover time but larger than the time step size (for integrating Navier–Stokes equations), in order to generate a desired energy dissipation rate. In general, different forcing time scales relative to the flow physical time scales could be used to represent different mechanisms of the energy input. For example, a short forcing time scale mimics random energy input, while a forcing time scale comparable to the flow integral time scale could be viewed as an energy transfer from larger scales that are not included in the simulation. In this sense, different choices of the forcing time are physically meaningful.

5. *Settling velocity of non-interacting small heavy particles, relevant to cloud droplets, in homogeneous isotropic turbulence.*

   The goal was to examine the role of several basic mechanisms that may increase or reduce the settling velocity. These include: preferential sweeping, drag nonlinearity, vortex trapping and loitering. To examine the role and importance of these mechanisms a number of DNS simulations were performed for an extended range of flow Taylor microscale Reynolds numbers (up to $R_\lambda = 500$) with varying particle terminal velocity (relative to the Kolmogorov velocity) and particle inertia, by changing the particle-to-fluid density ratio and energy dissipation rate. In order to examine the possible effects of the forcing mechanism, my simulations were carried out using two different forcing schemes.

6. *Development of an efficient numerical method to computing the aerodynamic interaction forces and torques between particles/droplets in the Stokes flow.*

   The proposed method combines different approaches, namely the FTS (Force-Torque-Stresslet) multipole expansion for the long-range interaction with lubrication expansion at short separation. The new approach allows to examine the effect of particle rotation on collision efficiency.

Discussion of research findings

Task 1

A number of DNS simulations of homogeneous and isotropic turbulence have been performed using the newly developed pseudo-spectral code (parallel implementation based on 2D domain decomposition). The grid size (resolution) varied from 32^3 up to 1024^3 and the turbulence was forced using two different algorithms i.e. deterministic [9] and stochastic [10]. The parameter setup and realized statistics at the statistically stationary stage of the simulated flows are published in the habilitation dissertation. A comparison of the obtained statistics leads to the conclusions, that for a given grid resolution, the deterministic forcing yields a larger R_λ. The highest Reynolds number $R_\lambda = 500$ is obtained using the deterministic forcing scheme and mesh with 1024^3 nodes.

In order to verify whether the simulated turbulent flows are indeed homogeneous and isotropic, the 1D energy spectra is compared against experimental data of grid-generated turbulence from two different wind tunnel experiments. I chose the 1D energy spectrum for comparison because this quantity can be directly measured in the wind tunnel. Moreover, the 1D energy spectrum can be more accurately computed than for example the 3D. The results show that in the inertial and dissipation subranges, the experimental spectra agree very well with energy spectra from the numerical simulations. Moreover, there is no significant difference between simulations performed with different forcing methods.

Task 2

Here I analyzed the possible consequences of using different flow forcing methods on two-point droplet statistics, such as radial distribution function and radial relative velocity. The motivation to investigate this problem were certain differences in the results of previous research, such as [11]. I employed two different forcing schemes i.e. deterministic and stochastic to test the sensitivity of the simulation results on the large-scale driving mechanism.

The often-used working assumption in DNS of the turbulent collision of cloud droplets is that the relative motion of droplets, is governed primarily by small-scale eddies of turbulence which are adequately resolved in DNS. This assumption is usually justified if considered droplets are much smaller than Kolmogorov length scale ($a << \eta$) and if their inertia is low (Stokes number $St \sim 1$ or less). On the other hand, this assumption may be questionable for larger droplets in low Reynolds number DNS turbulence as larger droplets could respond to a range of flow scales. My study confirmed that, in general, the results using the two forcing schemes are quantitatively similar, with the deterministic forcing yielding a slightly larger RDF. The collision kernel is up to 20% larger for the largest droplets (a = 60 μm) considered in my study and 15% for droplets with radii a = 50 μm – it should be noted that part of this difference is due to the larger flow Reynolds number associated with the deterministic forcing. The difference is negligible for droplets of radii a < 30 μm.

The second aspect of this task concerns the effect of flow Reynolds number or equivalently the range of flow scales represented in DNS on the collision statistics. My high-resolution simulations (performed at meshes up to 1024^3) provided a range of flow Reynolds number R_λ, making it possible to study the dependence of droplet pair statistics on R_λ. I have shown that the Reynolds number dependence due to droplet interaction with large-scale fluid motion is of secondary importance. The interaction will eventually saturate, leading to R_λ-independent results at some large R_λ. It has been shown by both DNS results and by theoretical arguments that the saturation happens at a smaller R_λ for smaller droplets.

Task 3

Since most previous studies of the turbulent collision of inertial particles concerned non-sedimenting particles (i.e. gravity was not considered), I have specifically addressed the role of gravity on collision statistics, by simultaneously simulating collision statistics with and without gravity. I have shown that the collision statistics is not affected by gravity when $a < a_c$. For larger droplets, gravity alters the particle-eddy interaction time and significantly reduces the RRV. The critical droplet radius is found to be around 30 μm for the RRV, and around 20 μm for the RDF. This critical a_c size is expected to increase with the flow dissipation rate. I have proposed a concept of gravity-independent interaction versus gravity-modulated interaction to address the secondary effect of large-scale motion. The effect of gravity on the RDF is rather complex: gravity reduces the RDF for intermediate-sized droplets but enhances the RDF for larger droplets. This could be a combined result of reduced interaction time due to gravity and inertia-induced preferential sweeping [8].

In addition, I have also studied the scaling exponents of both RDF and RRV. For non-sedimenting particles, my results of scaling exponents are in excellent agreement with published results from other studies. I found that gravity modifies the RDF scaling exponents for both intermediate-sized and large particles, in a manner very similar to the effect of gravity on the RDF at contact. Gravity is shown to cause the scaling exponents, to level off for large droplets, in contrast with diminishing exponents for non-sedimenting particles. The results together suggest that the effect of gravity on the scaling exponents for cloud droplets needs to be parameterized in the future.

Task 4

Using direct numerical simulations, I have examined the effects of the forcing time scale (t_f) on the characteristics of the forced turbulent flows. The numerical simulations were performed employing the well-known random forcing method developed by Eswaran and Pope [10]. The main focus was on the relationship between the forcing time scales and the vortical structures of turbulent flows. A number of statistics characterizing the turbulent flow, such as R_λ, integral length scale, flatness, and skewness, have been computed and analyzed. Also, effects of the forcing time scale on the kinematic collision statistics of inertial particles have been investigated. The results provide insight into simulations of forced turbulence and its applications.

The DNS data confirm that the energy spectra of the simulated flows computed with different forcing time scales and at different grid resolutions are in excellent agreement with experimental data, i.e., the energy spectra of grid generated turbulence in wind tunnel. The probability density functions for the normalized vorticity obtained with different forcing time scales differ only in the tails. It can be assumed that these differences result mainly from different flow Reynolds numbers. The size of vortical structures at small scales increases with increasing t_f.

The energy dissipation rate obtained in the numerical simulations agrees well with the analytical formula of Eswaran and Pope [10]. Energy dissipation rate remains constant for any $t_f < \tau_K$ or $t_f < 0.1Te$, where Te is eddy turnover time. Similar conclusions can be drawn for the other flow statistics. Taylor microscale flow Reynolds number, integral length scale, skewness, and flatness do not change if $t_f < \tau_K$. For large forcing time scales, the skewness and flatness show a strong dependence on the t_f, which could be a result of very low flow Reynolds numbers.

In a series of simulations, I investigated the effects of forcing time scale on the kinematic collision statistics. The RDF does not reveal significant differences if $t_f / \tau_K < 600$. As expected, these differences are greater for heavier particles. Interestingly, for very large forcing scales $t_f / \tau_K \approx 600$, the differences in the RDF become important. It should be emphasized that the magnitude of these differences depends much on the domain size and thus on R_λ.

Results of the kinematic collision statistics (RDF and relative velocity) obtained with stochastic forcing scheme have been compared to the analogous statistics computed with deterministic forcing. Simulations performed with different forcing methods produce the same kinematic statistics for small inertia particles ($St < 0.5$). The only exception are simulations performed with the very long forcing time scale ($t_f / \tau_K \approx 600$). The effect of the forcing method becomes more evident for the particles with larger inertia and especially in the RDF. For larger particles ($a > 25$ μm), the RDF computed with deterministic scheme is about 15% greater. Radial relative velocity is less sensitive to the forcing mechanism. Simulations at the 128^3 resolution show that the difference in the radial relative velocity, computed with different forcing methods, becomes smaller as t_f decreases. For simulations at higher resolution (256^3), the statistics of RRV are in the quantitative agreement. The results show that the RDF and radial relative velocity may depend on the forcing time scale if it becomes large. This dependence, however, can be largely explained in terms of the altered flow Reynolds number and the changing range of flow length scales present in the turbulent flow. The conclusion of my work is that both flow statistics and particle kinematic statistics are not sensitive to the forcing time scales if the scales are smaller than τ_K. To avoid the undesirable dependency on t_f, I suggest to set the forcing time scales as $dt < t_f < \tau_K$.

Finally, conditional statistics have been obtained. I analyzed two-point statistics conditioned on the local enstrophy and the energy dissipation rate. It has been found that the regions of higher collision rate are well correlated with the regions of lower vorticity. Regions of higher concentration of pairs at contact are highly correlated with the region of high energy dissipation rate. The normalized conditional statistics computed with different forcing time scales appear to be very similar, but they depend nonlinearly on the particle size, local flow vorticity, and dissipation rate.

Task 5

Using direct numerical simulations, I have examined the different mechanisms and factors affecting the average settling velocity of inertial particles in a turbulent flow. The main focus was on water droplets of 10–60 μm in radius suspended in air. It has been shown that the difference between the particle settling velocity and their terminal velocity is approximately a linear function of square root of energy dissipation rate. Simulations with the Stokes drag and various density ratios show that the average settling velocity is consistently larger or equal to the terminal velocity. Additionally, I have shown that the maximum increase in the settling velocity highly depends on the turbulence intensity or the energy dissipation rate at fixed R_λ and kinematic viscosity.

The next goal of my work was to quantify the effects of the Taylor microscale Reynolds number on the settling rate of cloud droplets. Obtained DNS results are consistent with observations of [12] and show that at a fixed energy dissipation rate and a low Taylor microscale Reynolds number ($R_\lambda < 100$) the maximum level of increase scales with R_λ and hence rms fluctuation velocity (u'). On the other hand, for larger R_λ the increase in settling velocity saturates and this saturation is observed only for low-inertia particles ($a < 30$ μm).

The DNS results were used to develop an empirical parameterization that relates the settling velocity to three nondimensional parameters, namely, the Stokes number, the particle Froude number (Fr) and R_λ. The accuracy of the new parameterization has been verified by comparing against DNS data. For a wide range of the nondimensional parameters, I obtained quantitative agreement between the DNS results and the parameterization. Only for large R_λ and $1 < Fr < 20$ the parameterization yields a rather qualitative agreement.

In order to examine the possible effects of the forcing mechanism, my simulations were carried out using two different forcing schemes. Results obtained using both stochastic and deterministic forcing method show a similar trend, although there is a significant difference in magnitude of the settling velocity for a given particle radius and R_λ. At a given grid resolution, particles settle faster in the flow forced by the deterministic scheme. This is partially caused by the different values of R_λ.

Additionally, I have examined the role of the gravitational acceleration. It has been shown that a larger gravity magnitude pushes the settling velocity of high-inertia particles (St > 0.2) to quickly converge to their terminal velocity. For low-inertia particles (St < 0.0504), however, I observed a small increase in the settling velocity when gravity is increased from $1g$ to $2g$.

Another important issue explored in my study is the non-linear drag and its effect on particle settling rate. In the considered range of Stokes number, the difference in the settling velocity due to different drag forces is very small and is independent of the energy dissipation rate. My results are in qualitative agreement with the results of Wang and Maxey [8]. The study confirmed that the non-linear drag slightly reduces the net increase in the settling velocity.

Finally, to turn off the preferential sweeping mechanism, I performed simulations in which the horizontal motion of particles is blocked. Turning the preferential sweeping off causes the average settling velocity to be lower than the terminal velocity. This implies that the dynamics of particle-eddy interaction in the horizontal plane plays a central role in influencing the particle velocity in the vertical direction.

Task 6

Another objective of my research was to develop a numerical model to represent the aerodynamic interactions of cloud droplets. Such a model should be computationally efficient to be used in simulations with a large number of droplets. In literature there are only few studies, in which analytical formulas defining the forces/torques acting on two interacting spheres (for small Reynolds number) are derived. Usually, the solutions are represented in a form of infinite series expansions and can be applied only to a certain types of motion. For example, Maude [13] developed analytical representation for forces acting on two spheres moving along a straight line passing through the centers of these spheres. The key problem with employing these solutions in computer programs is the difficulty of implementing recursive relations – needed for computing subsequent terms of the expansions.

My method is numerically efficient and allows to evaluate the aerodynamic interactions acting on two droplets settling in viscous air under gravity. This method combines three different approaches for computing the interacting forces and torques. The choice of the specific approach depends on the instantaneous distance between the droplets. For the long-range interaction a multipole expansion known as the Force–Torque–Stresslet (FTS) [14] formulation is applied. It should be noted that most previous applications of the FTS formulation have been adapted to equal-size particles. The new method addresses the more general problem of unequal-size particles/droplets. The short-range interactions are treated by a few leading order terms from the explicit bi-spherical expansion [16]. Finally, for the intermediate range where no simple method is available, a third-order polynomial fitting is proposed to bridge the treatments for long-range and short-range interactions. The locations of the matching points are found by minimizing the difference between the exact force representation and this integrated approach. After optimizing the precise form of the polynomial fitting and matching locations, the force representation is found to be highly accurate when compared with the exact solution for Stokes flows.

A characteristic feature of the new method is a decomposition of the entire problem (of 3D motion) into six simple configurations. Such decomposition greatly simplifies force and torque computation and is justified because the Stokes flow equation is linear. The new method can be applied to compute the interactions of all rigid spherical particles in a Stokes flow.

Using this new method, I have computed collision efficiencies of cloud droplets settling with different velocities in a stagnant air. The collision efficiency depends sensitively on the droplet size and can change by several orders of magnitude. To compute the collision efficiency, a simultaneous consideration of droplet inertia and rapidly changing lubrication force is required. In general this is a multi-scale problem that couples the droplet inertial effect to local aerodynamic lubrication force and attractive coalescing force. Previously no efficient method was available for accurate determination of the collision efficiency.

The new integrated model enables to compute collision efficiency with high accuracy. The resulting collision efficiencies are in excellent agreement with those based on the exact Stokes flow solution developed by Jeffrey and Onishi [16], with a relative error of typically 2% or less for most cases. The largest relative error does not exceed 18% (note that 18% is not significant since the collision efficiency itself can vary by several orders of magnitude). This is achieved at a small fraction of the computational time needed for the exact treatment. The level of accuracy represents a significant improvement over for example the improved superposition method [15] that was used in the HDNS approach [1].

An important achievement of this project was also computing of the collision efficiency based on the exact [16] force/torque representations. The results have been tabulated and published in the habilitation dissertation for future benchmarking. Careful comparisons of the new results with the classical results of Davis and Sartor [18] and Hocking and Jonas [17] have been performed. The comparison leads to the conclusion that some small but finite corrections to these results are needed. In several cases, I have been able to extend the range of the collision efficiency data to the regime where the radii ratio of the droplets tends to zero and the collision efficiency is very low. In this range computation is more expensive.

Performed simulations show that the droplet rotation tends to reduce the collision efficiency, particularly for small droplets of similar size. Davis and Sartor [18] commented very briefly on the effect of droplet rotation on collision efficiency. They compared their own results with rotation with the earlier results of Hocking [19] without rotation, but that comparison was incomplete due to the very limited range of the radii ratio studied in Hocking [19] and other erroneous treatments in Hocking [19]. I presented a more complete comparison of results with and without rotation to illustrate the level of errors that would incur if the rotational degrees of freedom were omitted in the calculation. For larger droplets ($a > 30$ μm), the effect of rotation is only of secondary importance.

In order to simplify the time integration, most previous calculations of collision efficiency used a finite gap to model the effect of very short-range molecular attractive interaction such as the van der Waals force that eventually led to coalescence. I performed additional series of simulations considering the van der Waals force explicitly. For droplets of either similar or very difference sizes, I found that a precise treatment of the coalescence force such as van der Waals interaction force is necessary. Namely, the simplified finite-gap model could lead to significant errors in collision efficiency for small cloud droplets. As a result of larger collision efficiency values, the effect of droplet rotation appears to be less important when the van der Waals force is considered, than in the finite-gap model.

The new model of aerodynamic interactions has been recently incorporated into the DNS code, suitable for modeling dynamics of many particles in homogeneous isotropic turbulence. Details of the implementation and preliminary DNS results have been published in [20]. In these simulations, aerodynamics forces acting on the droplets were computed using a hybrid method, which is a combination of the new algorithm (integrated model) and binary-based superposition method (BiSM) [21]. BiSM is based on an assumption, that interactions via three or more particles are negligible. Such approximation is valid only for dilute concentrations and small size particles. With a good approximation such conditions are typical for cloud processes. For completeness it should be added that the code for modeling homogeneous and isotropic turbulence employs the finite difference integration scheme [21]. The main conclusions of this study can be briefly summarized as follows: i) lubrication forces reduce the collision rate of low inertia droplets (7.5 μm) by about 20%, ii) the effect of the lubrication forces on the collision rate of larger droplets is weaker, and iii) for 30 μm droplets (in radius) the reduction is only a few percent.

Summary

My research was focused on numerical modeling of the cloud microphysical processes. In particular, I analyzed different mechanisms that affect the rate of warm rain formation. Warm rains accounts for more than 30% of the total rainfall on the globe and can occur in most climate zones. Therefore, quantification of this process is of great importance for the development of accurate parameterization for numerical weather predictions models. The time required for the formation of the warm rain depends on the growth of cloud droplets. The growth of the droplets of radius from 10 to 60 μm depends mainly on collision and coalescence, while the rate of collisions depends on characteristic features of turbulence. The developed numerical tools and analysis greatly increase our knowledge on these processes.

Although the simulations and analysis concern mainly the cloud microphysical processes, the conclusions are general and can be used as a reference to quantify other processes/flows. Obviously, those processes should be characterized by the same set of parameters such as Reynolds number and particle inertia (Stokes number).

Literature

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5. Significant scientific and research achievements on studying dynamics of particles in turbulent flows.

a) Development of MPI implementation for DNS, based on 1D domain decomposition.

My first tool for modeling multiphase flows was a pseudo-spectral code, fully parallelized with OpenMP (Open Multi-Processing) directives. This code can be run on computers with shared or distributed memory but only on a single node. This restricts the grid resolution typically below 256^3. Results from DNS performed using the OpenMP implementation were published in a series of peer-review articles [A13-A17] in journals listed on ISI.

To perform simulation of turbulence on 512^3 grid or larger, different method of parallelization has to be applied. Therefore, in 2010, I completed a new DNS code which can be run on supercomputers with distributed memory and is not limited to a single node. The code is fully parallelized in MPI and the strategy of parallelization is based on one-dimensional domain decomposition. The computational domain is divided into thin slabs in one direction and number of slabs corresponds to number of processors/cores used.

The pseudo-spectral method involves three-dimensional Fast Fourier transform (FFT), which requires global (i.e., whole-domain) data access or global data communication. This difficulty was overcome by splitting the full 3D (three dimensional) FFT into a series of 2D FFTs, parallel matrix transposition and then 1D FFTs. The transposition step reorganizes data to facilitate 2D and 1D FFTs within each process.

The newly developed MPI code can be run on computers with distributed memory and as such can take full advantage of available computational resources. This implementation was a significant step forward in modeling multiphase flows. It enabled utilization of a larger number of processors, large memory size and improved cache utilization, leading to a higher overall computational efficiency. The MPI code performs better than an earlier OpenMP code.

Description of the new implementation, results from scalability tests, and preliminary DNS results have been published in articles [B4] and [B6].

b) A spurious evolution of turbulence originated from round-off error in pseudo-spectral simulation

While testing of the new MPI implementation (based on 1D domain decomposition) for pseudo-spectral DNS, I encountered an unusual and hard-to-detect problem resulting from round-off error. This problem appeared after a long time of numerical integration of the Navier-Stokes equations. It turned out that if the effect of machine round-off on the divergence-free condition is not carefully controlled, the problem can develop slowly (over about 50 large-eddy turnover times) and eventually leads to an unphysical flow field. This artifact is not easily noticeable due to its very long development time, making it hard to detect. The artifact does not affect the dynamics of the turbulent flow until about 50 large-eddy turnover times and does not lead to numerical instability. Instead it produces a numerically realizable but unphysical flow field for incompressible fluid.

To understand the mechanism of the spurious turbulence evolution, I performed number of DNS using large computing resources. All simulations have been performed using the new MPI implementation adapted to computers with distributed memory [B6]. The problem is broadly discussed in [A12]. Moreover, we offered several remedies to correct the problem.

c) Effects of gravity on the acceleration and pair statistics of inertial particles in homogeneous isotropic turbulence

My other research project concerns the examination of the effect of gravity on the acceleration and pair statistics of inertial particles, relevant to cloud droplets, in homogeneous isotropic turbulence. Together with scientists from the University of Delaware we have obtained a range of original results. For particles/droplets with radius from 10 to 60 μm, we found that the gravity plays an important role, namely: (a) a peak value of particle acceleration variance appears in both the horizontal and vertical directions at a particle Stokes number of about 1.2, at which the particle horizontal acceleration clearly exceeds the fluid-element acceleration; (b) gravity constantly disrupts quasi-equilibrium of a droplet's response to local turbulent motion and amplifies extreme acceleration events both in the vertical and horizontal directions and thus effectively reduces the inertial filtering mechanism. These innovative results and analysis have been published in [A4]

In [A4], we also discuss the effects of gravity on droplet's radial relative velocity (RRV). First, we decomposed RRV into three parts: (1) differential sedimentation, (2) local flow shear, and (3) particle differential acceleration. Then we evaluated and compared their separate contributions. For monodisperse particles, we found that the presence of gravity does not have a significant effect on the shear term. On the other hand, gravity suppresses the probability distribution function tails of the differential acceleration term due to a lower particle-eddy interaction time in presence of gravity. For bidisperse cases, we found that gravity can decrease the shear term slightly by dispersing particles into vortices where fluid shear is relatively low. The differential acceleration term was found to be positively correlated with the gravity term, and this correlation is stronger when the difference in colliding particle radii becomes smaller.

We also developed a theory to explain the effects of gravity and turbulence on the horizontal and vertical acceleration variances of inertial particles. The theory is consistent with the DNS results for particles at small Stokes numbers.

d) DNS simulations and experiments in wind tunnel

In 2009, I started collaboration with a group of scientists headed by professor Alberto Aliseda at the University of Washington. This group investigates multiphase flows using advanced experimental techniques. They conduct different experiments and measurements in grid-generated wind tunnel turbulence. The aim of this cooperation was to compare my DNS results with those obtained experimentally in their wind tunnel. The first stage of this joint project was to set the same parameters of turbulent flow in both wind tunnel and DNS. By adjusting the size of the domain, viscosity and forcing parameters, I obtained similar (averaged) flow statistics as those measured in the wind tunnel. The second stage was to compare the intensity of particle clustering. The available measurement methods for detecting the spatial distribution of the droplets/particles have significant limitations. Typically the measurements allow to compute only one-dimensional radial distribution function (RDF 1D). Currently, there are no methods available for fast and precise measuring both particle locations and velocities in three-dimensional space. To compare the measured 1D RDF with the DNS results, I prepared a special computer program that allows to compute 1D RDF under similar condition.

It has been shown that the DNS results are in good agreement with experimental data. The results of this project were published in the article [C8] and presented at several international scientific conferences [D35, D37, D39, D43, D54].

e) Investigation of the settling velocity of inertial particles in turbulent flows using Large Eddy Simulations (LES)

To study the gravitational settling of small inertial particles in turbulent flows, I also used an alternative (to DNS) approach, namely Large Eddy Simulations. The paper [C1] contains a detailed comparison of the results obtained using the standard DNS with the results computed using a priori LES and LES with a subgrid scale model, so called a posteriori LES. Simulations a priori LES are carried out as standard DNS but the fluid velocity is filtered before being used in the particle equation of motion. The filtering is applied to the high frequency and is performed using a standard spectral low-pass filter. To perform a posteriori LES, I employed a subgrid scale model, which is based on the concept of the spectral eddy viscosity. The conclusion resulting from this study is that the settling velocity of low inertia particles computed using LES is lower than the corresponding settling velocity obtained from DNS. With the increase of the particle inertia the LES results, both a priori and a posteriori converge to the DNS results. Moreover, in all performed simulations a reduction of average settling velocity (compared to the terminal velocity) has not been observed.

The results of this project has been presented at international scientific conference "8th International Conference on Multiphase Flow" [D5] and international scientific workshops [D4].

6. Other academic and research achievement

a) Development of the new dynamical core for numerical weather forecasting model COSMO

Since 2009, I am an employee of Institute of Meteorology and Water Management - National Research Institute (IMGW-PIB) and take part in a group project aimed at development of a new dynamical core for the regional numerical weather prediction model COSMO (Consortium for Small Scale Modeling). The COSMO model is the main tool used at IMGW-PIB for weather forecasting. The motivation to develop a new dynamical core for the COSMO framework stems from the fact that its current version does not conserve dynamical variables such as mass, momentum or energy. Conservation of these variables is important especially when the spatial resolution of computational grids approaches the 1 km scale. In addition, the original dynamical core of the COSMO model, which is based on the fully compressible Euler equations and 2nd order Runge-Kutta integration scheme has significant stability problems in modeling very high resolution flows over steep orography.

In view of these limitations, the consortium COSMO decided to work on a new dynamical core and launched a special priority project CDC (Conservative Dynamical Core). The project was focused on multiscale anelastic EULAG fluid solver (www.mmm.ucar.edu/eulag/ - Eulerian/semi-Lagrangian numerical model for fluids) as a candidate for future dynamical core of the consortium. The motivation of employing EULAG for weather forecasting was two fold: i) the model has considerable advantages concerning conservation properties, and ii) does not impose severe constraints on the maximal allowable steepness of the surface orography. In addition, EULAG features a high numerical robustness confirmed in number of benchmark tests.

In the first stage of the project, my efforts focused on preparation of a series of idealized and semi-realistic simulations. The goal of this work was to confirm suitability of EULAG for modeling processes characteristic for mesoscale weather forecasts. Results of these simulations have been published in 3 journal papers (listed in ISI) [A9, A10, A11]. In the second stage, our team worked on rewriting EULAG from FORTRAN 77 to the new standard Fortran 90. A concise summary of the results was published in article [B3]. The next step involved integration of the two models (i.e. EULAG and COSMO) and evaluation of the resulting one for idealized experiments. At the final stage, we developed a series of realistic simulations using the new hybrid model COSMO-EULAG. The results of these experiments have been published in the renowned journal Monthly Weather Review [A2].

Since September 2015 I am a leader of a follow-up priority project of the COSMO consortium aimed at operationalization of the COSMO-EULAG and named CELO. My goal is to coordinate the ongoing work of the IMGW-PIB team. The project CELO is carried out in collaboration with the COSMO consortium and involves integration of the latest version of the EULAG model with the COSMO framework. The new version of EULAG is based on the fully compressible Euler equations but has a general construction similar to its previous anelastic version.

In addition to the above-mentioned articles, realization of the projects resulted in number of conference lectures, presentations at meetings organized by the COSMO consortium and several conference papers.

b) Adaptation of multiscale fluid model EULAG to modern heterogeneous architectures

The aim of this project was to adapt the multiscale fluid solver EULAG to the new hybrid and heterogeneous supercomputers based on CPU (Central Processing Unit) and GPU (Graphics Processing Unit) architectures. The work was carried out in collaboration with scientists from Poznan Supercomputing and Networking Center and Czestochowa University of Technology. The main achievement of this collaboration is the development of effective methods and algorithms for two main modules of EULAG, namely the multidimensional positive definite advection transport algorithm, MPDATA, and the variational generalized conjugate residual elliptic pressure solver, GCR.

New C++ codes were developed based on a detailed analysis of the performance of the original algorithms. A number of innovatory solutions have been employed in the new codes, including stencil decomposition, block decomposition (with weighting analysis between computation and communication), reduction of intercache communication by partitioning of cores into independent teams, cache reusing and vectorization. The proposed methods allow to identify bottlenecks, which slow down the execution of successive tasks and reduce the parallel performance.

The correctness, accuracy and scalability of the new implementations have been tested in several benchmark experiments, such as: i) isotropic, homogeneous and decaying turbulence in periodic box, ii) flow on a sphere with non-periodic boundaries in the vertical and iii) advection of a scalar field around a diagonal axis in a cube.

This work was supported by the Polish National Science Centre under grant no. UMO-2011/03/B/ST6/03500. My role as principal investigator (PI) was to coordinate research at IMGW-PIB.

Cooperation within the project consortium was fruitful and brought a number of publications. I am a co-author of three articles [A5, B1, B2] and several conference talks [D9, D18, D19, D22].

7. Quantitative record of scientific output

#	Specification	Before PhD	After PhD	Total
1	Monographs	0	1	1
2	Articles published in peer-reviewed journals indexed by ISI	1	17	18
3	Articles published in peer-reviewed journals not indexed by ISI	0	6	6
4	Conference papers	6	11	17
5	Cumulative impact factor	1.527	34.522	36.049
7	Presentation at international scientific conferences (not including meetings of the COSMO consortium)	2	69	71
8	Presentations at COSMO meetings	-	38	38
9	Technical reports	1	10	11
10	Presentations at national conferences / seminars	-	3	3
11	The total number of citations (Web of Science)	-	271	271
12	The total number of citations (Google Scholar)	-	442	442
13	H-index (Web of Science)	-	7	7
14	H-index (Google Scholar)	-	9	9

8. International activities and research cooperation

[1] The Netherlands, Amsterdam, Vrije Universiteit Amsterdam, Socrates / Erasmus scholarship at Research Institute of the Environment (IVM), (1.09. 2000 – 1.03. 2001)

[2] France, Toulouse, Meteo-France, working visit, (5/2005)

[3] USA, Colorado, Boulder, National Center for Atmospheric Research, a series of working visits and close cooperation with experts from the NCAR, (7-8/2006, 1/2007, 7-8/2007, 1/2008, 7-8/2008, 7-8/2009, 7-8/2009, 7-8/2010, 7-8/2011, 7-8/2012, 7-8/2013, 7-8/2014)

[4] Japan, Japan Agency for Marine-Earth Science and Technology (JAMSTEC), two working visits. This cooperation brought common publications and the computer code for modeling the dynamics of cloud droplets in turbulent flows. The code includes the full representation of aerodynamic interactions between droplets (5/2013, 5/2014).

[5] USA, Virginia, Norfolk, Old Dominion University, collaboration with doctor Orlando Ayala on article about settling velocity of cloud droplets in turbulent flows (8/2014).

[6] Collaboration with COSMO consortium (*Consortium for Small-scale Modeling*) 13.01.2009 – presently.

[7] Collaboration with doctor Hossein Parishani from Department of Earth System Science, University of California, Irvine, USA, 2014 – presently.

[8] Collaboration with professor Alberto Aliseda from University of Washington, Seattle, Washington, USA, 2010.

[9] Collaboration with doctor Marcin Kurowski from Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California – presently.

[10] Collaboration with professor Piotr Smolarkiewicz from European Centre For Medium-Range Weather Forecasts, Reading, UK– presently.

9. Post-doctoral and current research projects

[1] UMO-2011/03/B/ST6/03500 Grant from National Science Center. Project title: *Methods and algorithms for organization of computations in the class of anelastic numerical models for geophysical flows on modern computer architectures with realization in the EULAG model.* Bogdan Rosa was principal investigator at IMGW-PIB.

[2] AGS-1139743, ATM-0114100, ATM-0527140, ATM-0730766, OCI-0904534, CRI-0958512 and ATM-0731248 - National Science Foundation, USA (investigator).

[3] CISL-35751010, CISL-35751014 and CISL-35751015 Computing resources provided by National Center for Atmospheric Research (Boulder, USA) - Computational and Information Systems Laboratory (investigator).

[4] ATM-130019 Computing resources provided by Texas Advanced Computing Center, USA (investigator).

[5] G49-15 Computing resources provided by Interdisciplinary Centre for Mathematical and Computational Modeling (ICM), Poland (investigator).

[6] Project leader of the priority project "CELO". The project is carried out in cooperation with a consortium COSMO (presently)

10. Awards and Distinctions

[1] The first award for the best scientific poster at international conference „Parallel Processing and Applied Mathematics – PPAM". Poster title „A study on parallel performance of the EULAG F90/95 code", Toruń 2011.

[2] Diploma for the best scientific paper at international conference „International Conference on Engineering Mathematics and Physics". Article title „Porting Multiscale Fluid Model EULAG to Modern Heterogeneous Architectures", Hong Kong, 2014.

11. Reviewing national or international projects and publications in international journals

Reviews of articles submitted to international journals indexed in the JCR list *e.g. Fluid Dynamics Research* and *New Journal of Physics* and other *e.g. International Journal of Modeling and Optimization.*

12. Teaching experience

[1] Computer laboratory, M.Sc. course, University of Warsaw, Poland.

[2] Environmental Physics - B.Sc. course, University of Warsaw, Poland.

[3] Assistant teacher, *University of Delaware*, USA.

13. Membership in organizations and associations related to professional activity

[1] Member of American Physical Society

[2] Member of European Mechanics Society

[3] Member of American Meteorological Society

[4] Member of COST Action MP0806 "Particles in Turbulence"

14. **Co-organization of international conferences**

[1] 3rd International Conference on Engineering Mathematics and Physics, Hong Kong, PRCh, 14 – 15 June 2014.

[2] 4th International Conference on Engineering Mathematics and Physics, Kuala Lumpur, Malaysia, June 11-12 2015.

[3] European Conference on Design, Modeling and Optimization, Paris, France, 15 – 17 February 2017.

Bogdan Rosa

Warsaw, 27th March 2017

Bogdan Rosa