



**Międzynarodowa Środowiskowa Szkoła Doktorska
przy Centrum Studiów Polarnych
w Uniwersytecie Śląskim w Katowicach**

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No. of PhD project: IEDS/2023/IM/02

Title of PhD project: *Computational mathematics for quantum mechanics*

The leading unit: Institute of Mathematics, Polish Academy of Sciences (IM PAN), Warsaw

Requirements:

1. Finished studies in mathematics or similar (computer sciences, physics). Knowledge of numerical analysis, approximation theory, ODEs and PDEs, functional analysis, programming skills.
2. Knowledge of the issues: approximation, interpolation, ODEs, PDEs, Fourier transform, programming (preferably matlab, julia or python).
3. Knowledge of English language.
4. Being ready for constant developing skills and broadening knowledge.

Tasks description:

1. Numerical and analytical analysis of differential equations undergoing highly oscillatory phenomena.
2. Searching for, reading, learning and analysis of research articles corresponding to the subject of studies.
3. Research travels (in order to collaborate) to places: University of Cambridge, UK, Sorbonne University, France, University of Manchester, UK, University of Bath, UK, University of Singapore, Singapore.
4. Theoretical research and programming (ex matlab, python or julia).
5. Preparing research articles and presentations.
6. Regular collaboration and reporting on research progress.

Abstract:

The significance of differential equations, as a leading tool in mathematically describing phenomena of our everyday lives requires neither further elaboration nor explanation. Differential equations are the dominant instrument in formulating mathematical models in science and engineering and, increasingly, in other areas of scholarship: they are truly the main language of applied mathematics. Once a differential system has been formulated and analysed, typically there is an imperative to find its solution. Very few differential equations have known explicit solutions and in practice we must resort to computation. However, stepping from rigorous formulation and analysis of differential equations to their computation does not mean that we are somehow abandoning mathematics. Once



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discretised, differential equations are still mathematical objects (arguably, even more complicated mathematical objects!) and need be analysed with the full arsenal of mathematical tools.

Computational differential equations featuring highly oscillatory phenomena are one of the largest and most rapidly evolving area of numerical mathematics, of critical importance to applications. The variety, importance and sheer dynamism of advances in DEs explains the rapid pace and wide scope of development of numerical tools dedicated to various specific problems in the rich area of differential equations.

Together with the candidate, we will choose a specific research direction depending on the candidate's preferences and skills. We will pay special attention to the numerical approximation of solutions on the entire real plane, and not, as it has been done so far, on finite sections requiring the imposition of artificial periodic or zero boundary conditions. Another topic of great demand is the problem of multi-frequency solutions, where resonances that are dangerous from the computational point of view occur. A difficult topic of numerical analysis of equations is the approximation of the behaviour of several (or several thousand!) particles in three-dimensional space - today it seems that Kohn-Sham functional density theory is the only promising (however very difficult) direction. In the field of supervisor's interest is also the theory of quantum control, where we design the optimal operation of lasers (on a system) in order to obtain the desired solutions of differential equations. Analytical developments of asymptotic solutions to problem equations with highly oscillatory input term are an interesting and still requiring attention area of research. Computational methodologies that preserve total energy and / or mass of solutions to problems like Schroedinger, Dirac, Klein-Gordon, Pauli (various types: in electric, electromagnetic fields, linear or non-linear) are a widely studied but still inexhaustible area of research.

Other information:

The work will be carried out under supervision of: dr hab. Karolina Kropielnickia, prof. IM PAN, kkropielnicka@impan.pl, Institute of Mathematics of the Polish Academy of Sciences, branch in Sopot.

Secretary of the IEDS Recruitment Committee: +48 32 3689 380, e-mail: polarknow@us.edu.pl

Information on the IEDS admissions: https://www.mssd.us.edu.pl/en/admission_2023_2024-reg/