Consejo de la Division de Ciencias Naturales e Ingeniería
Universidad Autónoma Metropolitana Unidad Cuajimalpa
Cuajimalpa de Morelos 05348, Ciudad de México, Mexico

Potsdam, 23th September 2022

Sabbatical leave final report

Dear Members of DCNI Board,

Please find herewith the final sabbatical report of Dr. Guillermo Chacón Acosta corresponding to the period from January to September 2022.

According to the program, research was conducted on diffusion in confined media and anomalous diffusion in the dynamics of complex systems and its relation to the geometrical characteristics of the boundaries. Activities during this period fall into two main categories, those carried out in the Theoretical Physics group of the Institute of Physics and Astronomy of the University of Potsdam and additional activities previously included in the work planning, including the follow-up of established collaborations and student advisory.

Activities at the Institute of Physics and Astronomy of the University of Potsdam

- During the entire visit, we actively participated in the seminars of Prof. Dr. Ralf Metzler's Theoretical Physics group, which are held mainly on Fridays and in which students, researchers of the institute, guest researchers, and visitors present their work.

- On January 28th, the talk "**Geometric description of diffusion in narrow environments**" was presented at the group's seminar.

- On July 22th, the talk "**Effective 1D heterogeneous diffusion in narrow channels**" was presented at the group's seminar.

- Discussions have been made with some researchers from where some specific topics have emerged, as listed below:

    - Effects of boundary geometry on transport in a porous system modeled by heterogeneous diffusivity. Discussions have been held mainly with Prof. Dr. Ralf Metzler and Ph.D. student Timo Dörries. The effective diffusivities for some particular cases of heterogeneous coefficients have been calculated. Ph.D. student T. Dörries write a Brownian simulation code, and we start the comparison of the simulated results with the analytical expressions obtained.

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- Study of alternative boundary conditions for diffusion in narrow channels. In this direction, discussions were held with Prof. Dr. Aleksei Chechkin and Dr. Inti Pineda of UAM-A. We obtained the appropriate boundary conditions for the diffusion equation for various gas-wall interactions, specifically in the case of the so-called diffuse reflection, either ealstic or inelastic. With a first-order perturbation analysis, we obtain an effective 1D diffusion equation similar to the so-called Fick-Jacobs equation but with an extra term accounting for the effects of the different types of boundary.

- With Dr. T. Sandev from the University of Potsdam, the Macedonian Academy of Sciences and Arts, and Dr. F. Sevilla of IF-UNAM, a model for the 2D diffusion of non-interacting active particles that considers an arbitrary distribution of the scattering angles in the direction of motion is studied. In this case, the time operator in the corresponding generalized Fokker-Planck equation is replaced by a fractional operator in the Caputo sense. The second and fourth-order moments and certain exact expressions have been obtained.

- From discussions with Prof. Dr. R. Metzler and Dr. T. Sandev, we proposed a model for a Levy process within a channel by the use of a Riesz-Feller fractional derivative. We calculate the corresponding projected equation equivalent to the Fick-Jacobs equation for this case. We are on the way to calculating the related moments and higher-order corrections.

- Generalization of Fick-Jacobs equation when the dynamics occur in a comb-like structure inside a narrow channel, and stochastic resetting is allowed. This topic has been discussed mainly with Dr. T. Sandev and Dr. E. Kaminski Lenzi. The generalized Fick-Jacobs equation was obtained together with one solution for the case of a linear channel. Other solutions are still to be found for different initial conditions and channel shapes.

- With Dr. I. Petrevska and T. Sandev, we study the interplay between the so-called comb model and the geometric properties that arise in channel confinement. An in-depth analysis will be done.

- Possible heterogeneities in the medium require considering memory terms in channel diffusion, which can be modeled with fractional derivatives. With Ph.D. student Q. Wei we discussed the possible use of different fractional derivatives to address the problem. We plan to compare the solutions with these operators and the non-fractional case to study the coupling between the geometry and the fractional index. Some specific cases will be studied.

The above are the main topics that were addressed during the visit; however, there were discussions on other issues with Prof. Dr. Metzler, Dr. A. Chechkin, Dr. T. Sandev, Dr. I. Petrevska, Dr. S. Thapa, Dr. A. Cherstvy, Dr. W. Wang, Dr. Y. Liang, Dr. K. Goswami, Dr. P. Meyer, and Ph.D. students T. Dörries, Q. Wei, C. Di Bello, and E. Kalz.

Activities at the University of Barcelona

- During June and the first week of September, a visit was made to the Condensed Matter Physics Group of Prof. Dr. Miguel Rubí at the University of Barcelona. Several discussions were held with Dr. Miguel Rubí, and students A. Arango, J. Torrenegra, and Dr. D. Reguera.

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- We worked on deriving a position- and time-dependent diffusion coefficient from the boundary fluctuations using our geometric method. Positive results were obtained, and a manuscript is being prepared for publication.

- We started a discussion with Dr. Rubí and the Ph.D. students on the influence of diffusive flux on the confining boundaries, and significant progress was made. This topic will continue to be explored, and a publication is expected to be published shortly.

- These were the advances during the visit; however, we also had some exciting discussions with Dr. D Reguera, Dr. P. Margaretti, and Ph.D. students A. Arango and J. Torrenegra.

Additional activities

- Presentations

  - The talk entitled "**Las aventuras del señor Tompkins en planilandia**" was presented at the popular science "Jornada de Divulgación científica y tecnológica" event, held online by BUAP on February 9, 2022.

  - The talk entitled "**Efectos geométricos en la formación de patrones a través del mecanismo de Turing**", was presented online at the Applied Mathematics seminar of the UASLP on March 16, 2022.

  - The talk entitled "**Estrellas de bosones no relativistas como sistemas cuánticos de *N*-cuerpos**" was presented online at the Research seminar of the Universidad Iberoamericana on April 1st, 2022.

  - The talk entitled "**Estrellas de bosones no relativistas como sistemas cuánticos de *N*-cuerpos**" was presented online at the "XXX Reunion anual de la DGFM" held online by UNAM 7 and 8 of Arpil.

  - The talk entitled "**Long-range effects in the Fick-Jacobs equation for diffusion in narrow channels**" was presented on-site at the international conference "Non-Markovian Dynamics Far From Equilibrium" at the ICTP in Trieste, Italy, from 4 to May 6th.

  - Interview for the specialized film podcast, Fonokinesis, entitled "**Ciencia y Ficción**", about the influence of science in contemporary cinematography. Recorded in June during the visit to the University of Barcelona and published online on September 19th, 2022.

  - The talk entitled "**Efectos de largo alcance en la difusión en canales estrechos**" was presented online at the seminar of the Field Theory and Gravitation Deparment of the Instituto de Ciencas Nucleares UNAM on August 18th, 2022.

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- Participation in the International Workshop "Transport in Narrow Channels," held at the Institute d'Etudes Scientifiques de Cargèse, Cargèse, France, September 5th to 9th, with the Invited talk "**Diffusion-driven instability and pattern formation in narrow channels**."

- Presentation at the 14th Conference of the Society of Physicists of Macedonia - CSPM 2022, with the talk "**Pattern formation and diffusion-driven instability in narrow environments."** This event took place from 15-18 September 2022 in Ohrid, North Macedonia.

- Student advisory

  - The terminal project of the student *Gabriel Gutierrez* entitled "**Kinetic Models for the Distribution of Wealth,**" was directed and finished on September 20th.

  - The project of Ph.D. student *Alejandro León Ramírez* entitled "**Application of semi-analytical methods in biomathematics**" is being co-advised. The work, "**Application of the Kudryashov Method for Finding Exact Solutions of the Schamel-Kawahara Equation**", was accepted and published during this period. A separate document on semi-analytical methods applied to epidemiology was also sent for peer review. A manuscript is prepared to submit about the study of biharmonic diffusion in narrow channels. We reviewed and approved the document for the presentation of Alejandro's predoctoral exam, which he presented and passed. Currently, Alejandro is calculating semi-analytical solutions of the Chavy-Waddy equation for bacterial aggregation.

- Published and ongoing works in Mexico

  - The article entitled "**Pattern formation in a predator-prey system with a finite interaction range in a channel-like region using the Fick–Jacobs diffusion approach**" by M. Núñez-López and G. Chacón-Acosta was accepted and published in this period.

  - During this period, the manuscript entitled "**Nonrelativistic Boson stars as *N*-body quantum systems**" by E. Castellanos, G. Chacón-Acosta, and J. Mastache was accepted and published online in early May.

  - The paper "**Application of the Kudryashov Method for Finding Exact Solutions of the Schamel-Kawahara Equation**," written by A. León Ramírez, G. Chacón-Acosta, and O. González-Gaxiola, was accepted and published during this period.

  - The manuscript "**Can non-developers learn a simplified modeling notation quickly?**" by Cervantes, Gómez, and Chacón-Acosta was accepted and published within this period.

  - The manuscript "**Rach-Adomian-Meyers decomposition method applied to a SIR with nonlinear media and psychological effects**" by A. León Ramírez, G. Chacón-Acosta, and O. González-Gaxiola, was submitted for review to Rev. Mex. Fís.

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- The manuscript entitled "**Mechanics of pearling instability in toroidal lipid membranes**" by D. M. Valencia, G. Torres, and G. Chacón-Acosta was submitted for review to Eur Phys. J. E.

- The paper "**The Rayleigh-Brillouin Spectrum for Bidimensional Relativistic Fluids in the Relaxation Approximation**," by A. L. García-Perciante, A. R. Méndez and G. Chacón-Acosta, is being prepared to submit to the proceedings of the 32nd International Symposium on Rarefied Gas Dynamics, that took place last July in Seoul, Korea.

- The manuscript entitled "**Patterns in a fractional predator-prey system with finite interaction range**," by G. Chacón-Acosta and M. Núlez-López, is being prepared for the proceedings of the 5th Mexican Workshop on Fractional Calculus that will take place next October in Monterrey, Mexico.

- The paper entitled "**Geometrical factors influencing the macroscopic diffusion coefficient on curved surfaces**" by A. Ledesma, A. León-Velasco, G. Chacón-Acosta, and H. Juárez is being prepared for submission.

- The manuscript entitled "**Biharmonic Fick-Jacobs diffusion in narrow channels**" by A. León, G. Chacón-Acosta, and O. Gonzalez-Gaxiola is about to be submitted.

Continuous meetings were kept with Dr. Mayra Núñez, Dr. Diana León, Dr. Aldo Ledesma, Dr. Héctor Juárez, Dr. Francisco Sevilla, Dr. Ana Laura García, Dr. Alma Méndez, Dr. Oswaldo González, Dr. Héctor Hernández, to follow up on the joint projects previously started.

Sincerely,

Dr. Guillermo Chacón Acosta

Prof. Dr. Ralf Metzler

APPROVED

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