Mathematical Aspects of Population Dynamics and Polymers.

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Target category: Existing and Emerging Excellence

Keywords: phase transition, protein, propagation front, random process

Executive summary

Both topics in the title belong to interface of biology, social sciences, chemistry, and mathematics. The present group focuses on mathematical modeling for analysis of different phenomena across a variety of spatial scales: from the microscopic scales in microbiology to macroscopic scales in demography.

I. Population dynamics is a branch of mathematics describing the evolution of sets of spices (particles). In applications, the word particle can refer to a specific gene, a microbe, a plant, an animal, a representative of a human race, etc. The first models in population dynamics appeared at the end of the 19-th century (Galton-Watson) in the study of the extinction of noble family names. In 1930s, several groups in UK and Russia studied models for the propagation of new genes and the spread of infections using the famous KPP equation.

Modern, more realistic, models are much more complicated. They include features such as variable birth and death rates of particles, immigration of particles, their migration, the interaction between particles when, for instance, the mortality rate depends on the local density of the population (competition effects), the appearance of different types of particles (as in Covid-19 mutations), etc. There are models where particles can move only slowly and models (heavy-tailed) where particles can jump by large distances. One of the most important directions of research in the area is the existence of states that are homogeneous in space and time as well as their stability with respect to local and random perturbations of the environment. Another direction concerns the study of the propagation of the population (ecological waves). It is also important to describe the intermittency phenomenon (i.e., a highly non-uniform structure of the population with heavily populated clusters inside of the front of propagation).

II. Fast progress in modern biotechnology requires new theoretical and experimental results on polymers, particularly in the study of phase transitions (with respect to temperature, concentration, pressure, etc.) and in the study of diffusion processes in liquid solutions. Proteins, as well as closely related chains of DNA and RNA, are the most important components of the cell. There are at least 10^5 different proteins in humans, all of them are linear polymers composed from elementary blocks, monomers. Typically, each chain contains up to several thousand monomers. Since the chain is long, one can use the machinery developed for large systems (thermodynamics, statistical physics) to study its properties. The proteins are biologically active in the globular form, when the chain is folded into a compact ball. The destruction of a globule (unfolding) is one of the most important biological phase transitions. The simplest example of this transition can be observed in the process of boiling eggs. There are different mathematical models of this phase transition from folded to unfolded states. They have different complexity and different level of approximation to the reality. Their study is still far from being complete.

Other questions concern the diffusion of proteins inside the cells and through membranes (intercell diffusion). In particular, it was shown by the present group that the diffusion processes in polymer solutions differs from the classical diffusion. While the diffusion coefficient grows linearly with temperature in the classical setting (the famous Einstein-Smoluchowski theory for rigid spherical particles), it decreases near the critical temperature for proteins.

Evidence of Strength and Excellence

Prof. S. Molchanov and Prof. B. Vainberg are prominent scientists who are well known by scientists across a variety of disciplines:

1) Wikipedia has articles devoted to each of them.

2) After receiving the PhD degrees, they both received the highest scientific degree, Doctor of Science, which exists in several European Countries (France, Germany, Russia). Their Doctor of Science degrees were issued by the Moscow State University in 80s. They were Professors of Moscow State University and came to UNCC in 1995 and 1992, respectively.

3) S. Molchanov is a fellow of American Mathematical Society.

4) The area of research of this group is very wide: mathematical physics, partial differential equations, random processes, and their applications: scattering theory, oceanography, quantum graphs, homogenization, localization, intermittency, fractals, population dynamics, etc.

5) S. Molchanov is an author of 4 monographs and more than 250 papers in mathematical journals.

B.Vainberg is an author of 3 monographs, a chapter in another monograph, and around 180 papers.

The vast majority of their papers are published in leading mathematical journals, such as Annals of Probability, Communications in Mathematical Physics, Journal of Functional Analysis, Journal of Spectral Theory, etc. They published 35 joint papers.

6) The list of their coauthors includes very prominent mathematicians from the USA and abroad such as M. Aizenman (Princeton), R. Carmona (Princeton), M. Cranston (UC, Irvine), G. Derfel (Israel), A. Grigoryan (Germany), W. Kirsh (Germany), A. Klein (UC, Irvine), A. Komech (Austria), V. Konotop (Portugal), L. Koralov (UMD), P. Kuchment (Texas A&M Univ.), V. Maz'ya (Sweden), S. Menozzi (France), R. Novikov (France), L. Pastur (Ukraine), B. Simon (Caltech).

7) Throughout the period 1996-2020 (except one year), S. Molchanov and B. Vainberg had joint NSF grants. The last two are:

"Asymptotic and Spectral Analysis of Applied Non-self-adjoint Problems", 2014-2017, and

"Applied Spectral Analysis in Population Dynamics, Biophysics, and Physical Chemistry", 2017-2020.

At the same time, they had additional grants. At the moment, S. Molchanov has a grant from Russian Science Foundation, 2016-2021, and a grant from Bielefeld University (Germany). B. Vainberg has the collaboration (travel) grant "Inverse problems and integrable equations" from the Simons Foundation, 2017-2022.

8) They are members of Editorial Boards of Mathematical journals:

S. Molchanov is a member of the Editorial Board of “Random Operators and Stochastic Equations”, “Journal of Spectral theory”, and “Mathematical and Theoretical Physics” (Russia).

B. Vainberg is a member of the Editorial Board of the journal “Applicable Analysis”.

9) Each year they participate in several international conferences as invited speakers.

10) Their former PhD students working in various universities in USA and abroad. In particular,

A. Agbor (York Technical College);
A. Alhakim (Amer. Univ. Beirut, Lebanon), professor;
L. Bogachev (Leeds Univ., UK), professor;
T. Cook (Univ. of NC), assistant professor;
Y. Feng (Ohio Univ.), assistant professor;
D. Han (Univ. of Kentucky), assistant professor;
J. Holt (Univ. of SC), associate professor;
O. Hrinev (Durham, UK), associate professor;
A. Malakhov (Univ. of Oklahoma), associate professor;
R. Puri (Wake Forest Univ.), instructor;
W. Shaban (UNCC), teaching professor;
L. Simon (Univ. of Budapest, Hungary), professor;
E. Yarovaya (Moscow State Univ.), professor;
L. Zheng (Univ. of Kentucky), assistant professor.

Our group lost one member 2 years ago: A. Gordon, a brilliant mathematician, author of a number of beautiful results in spectral theory and other areas of analysis, died in May 2019 after a long illness. Our group will be more successful if we have one more faculty in the area of mathematical physics.

Alignment with Regional and National Priorities.

The importance of studying polymers and proteins, in particular, has already been realized by scientific and executive entities. NIH put a significant emphasis on the basic structural biology research. Such institutes as NIHLBI, NIHGMS, NIAMS, NIEHS, NDDK, NIAID and NCI, all have their own structural biology units focusing on studying proteins. This study is also identified as one of the key areas in NIH-Wide strategic plan: "Because the private biopharmaceutical sector funds only a limited amount of basic research, NIH-supported research serves as the world leading source of fundamental knowledge…"

Models in population dynamics allow one to answer a wide variety of questions ranging from propagation of bacteria and viruses up to demography. The importance of these models can be proved by predictions of the propagation of the Covid-19 pandemic on news channels.

Mathematical studies in population dynamics and biology are mostly supported by NSF. Division of Mathematical Sciences (DMS) of NSF has several research programs (such as Analysis, Applied Mathematics, Mathematical Biology, Probability) that support mathematical studies on polymers and population dynamics. DMS also has Special Research Programs supporting these studies: Focused Research Groups in the Mathematical Sciences (FRGMS), Joint DMS/NIGMS Initiative to Support Research at the Interface of the Biology and Mathematical Sciences, Joint DMS/NLM Initiative on Generalizable Data Science Methods for Biomedical Research (DMS/NLM).

During the last eight years, the authors of this proposal were supported by NSF (DMS, Program of Applied Mathematics) exactly for the work on these topics.

As a part of applied mathematics, the area is supported by the Air Force Research Laboratory (AFOSR) and the Army Research Office (ARO). Society for Industrial and Applied Mathematics (SIAM) – the world's largest professional association devoted to applied mathematics – organizes special sections during its annual meetings dedicated to modeling and analysis of polymers and population dynamics.

There are many mathematical journals focused on applied research, and there are very specifically oriented journals among them such as Journal of Mathematical Population Studies. There are also very specifically oriented international conferences such as Conference on New Trends in Polymer Science: 17-19 May 2021, Turin, Italy https://polymers2021.sciforum.net/

The following email (Feb.13, 2021) from the Editorial Office of the journal Polymers is chosen to be put here only because it is the latest one among similar correspondence received by both members of the group
"Dear Dr. Vainberg,
Based on your contribution to the field of polymer science, we would like to cordially invite you to join the Reviewer Board of the open access journal Polymers (ISSN 2073-4360, IF 3.426,) http://mdpi.com/journal/polymers). …"

Supporting Documents.

Names	Titles	Expertise
Stanislav Molchanov	Full Professor	Mathematical physics, partial differential equations, random processes, and their applications: scattering theory, oceanography, quantum graphs, homogenization, localization, intermittency, fractals, population dynamics, etc.
Boris Vainberg	Full Professor	Mathematical physics, partial differential equations, scattering theory, asymptotic methods, inverse problems, free surface hydrodynamics, acoustic and electromagnetic waves, population dynamics and more.