THE INSTITUTE PURSUES ITS MISSION THROUGH A VARIETY OF PROGRAMMES

THE ERWIN SCHRODINGER INTERNATIONAL INSTITUTE FOR MATHEMATICS AND PHYSICS (ESI), founded in 1993 and part of the University of Vienna since 2011, is dedicated to the advancement of scholarly research in all areas of mathematics and physics and, in particular, to the promotion of exchange between these disciplines.

THEMATIC PROGRAMMES offer the opportunity for a large number of scientists at all career stages to come together for discussions, brainstorming, seminars and collaboration. They typically last between 4 and 12 weeks, and are structured to cover several topical focus areas connected by a main theme. A programme may also include shorter workshop-like periods.

WORKSHOPS with a duration of up to two weeks focus on a specific scientific topic in mathematics or physics with an emphasis on communication and seminar style presentations.

THE JUNIOR RESEARCH FELLOWSHIP PROGRAMME supports external or local graduate students and recent postdocs to work on a project of their own.

THE SENIOR RESEARCH FELLOWSHIP PROGRAMME aims at attracting internationally renowned scientists to Vienna for visits to the ESI for up to several months. Senior Research Fellows contribute to the scientific training of graduate students and postdocs of Vienna’s research institutions by teaching a course and by giving scientific seminars.

THE ESI FREQUENTLY HOSTS GRADUATE SCHOOLS organized by research groups at the University of Vienna on topics in mathematics or physics aimed at local as well as external PhD students.

THE RESEARCH IN TEAMS PROGRAMME offers support for research teams to carry out collaborative work on specific projects at the ESI in Vienna for periods of one to four months.

DETAILED INFORMATION about all ESI programmes and the respective application procedures and deadlines are available on the ESI website www.esi.ac.at
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Preface

Message from the Director

Just like for the entire world, the year 2020 has been a very challenging one for the Erwin Schrödinger Institute. While the year began like many others with a workshop and a school as well as several Junior and Senior Research Fellows visiting the Institute, everything changed in March when the COVID-19 pandemic took the world by surprise. Following the safety measures and travel restrictions put in place by health authorities worldwide, the ESI was completely shut from mid-March to the end of July 2020 and several thematic programmes and workshop had to be postponed, severely disrupting the programme of the ESI for 2020 and beyond. In the summer of 2020 the situation improved to a degree that allowed certain activities to be resumed. The thematic programme Higher Structures and Field Theory took place in August in hybrid mode with some participants at the ESI and others following online and, fortunately, we were also able to carry out the Award Ceremony for the first ESI Medal, awarded to Anton Alekseev (the only downer was that the awardee could participate only remotely). However, the break from the pandemic was short-lived and immediately after the ESI Medal Ceremony the ESI was shut down again for the rest of the year. With the exception of a few Junior Research Fellows and several visitors in our Research in Teams Programme, the ESI remains essentially closed at the time of writing, but we hope that some activities will be possible on-site later in the summer.

The success of a visitors oriented institute like the ESI depends on the dedicated work of many individuals, particularly in difficult situations. I would like to emphasize that all the ESI staff has reacted very quickly and has adapted to the changed circumstances working very efficiently from their home offices. Constantly rescheduling events, cancelling and rebooking accommodations and revising safety protocols was certainly a frustrating experience for the ESI staff, but with great teamwork they managed the situation very well. While at the beginning of the pandemic most organizers chose to postpone their activities, later they were increasingly interested in online options. In fact, in early 2021 the ESI adopted a strategy, developed by the ESI Kollegium in consultation with the ESI Scientific Advisory Board, which specifies that activities that are not held online are cancelled rather than postponed. This policy has prompted some difficult decisions, but it is necessary in order to prevent the ESI programme from clogging up far in the feature and to leave some space for new activities. I would like to thank all the organizers who have shown great patience and understanding in this difficult situation. The present yearly report, a little thinner than usual, gives an overview of the ESI activities that took place either in person or online and includes a documentation of their outcomes and achievements as well as a list of all visitors. Also included in the report is a list the activities that could not take place in 2020, but will hopefully happen at some time in the future.

Despite all the problems the pandemic has caused for the ESI, it also taught us some valuable lessons. Online meetings, and particularly hybrid activities, not only require appropriate digital
communication tools, but also demand a different approach in designing the programmes. A major effort is needed to enable informal online communication, which is particularly challenging for meetings that aim at bringing together people who are not already part of tightly knit community. While we know from social networks that digital communication works (not without its problems, though), many of us have realized, sitting in front of their computers during countless online meetings, how precious physical proximity is for developing new ideas together. It will be a challenge for the future to find the right balance between online and physical meetings, but it is clear that the way we communicate in science will be different after the pandemic. Returning to the *status quo ante* is not really an option, particularly in the light of the current climate crisis, and at the ESI we will try to contribute to innovative solutions. We hope that in the course of 2021 we will be able to resume in-person activities, complemented with online and hybrid elements, and we look forward to welcome many old and new visitors at the ESI soon.

Christoph Dellago  
Director of the ESI  
August 2021

**The Institute and its Mission**

The Erwin Schrödinger International Institute for Mathematics and Physics (ESI), founded in 1993 and part of the University of Vienna since 2011, is committed to the promotion of scholarly research in mathematics and physics, with an emphasis on the interface between them.

It is the Institute’s foremost objective to advance scientific knowledge in all areas of mathematics and physics and to create an environment where scientists can exchange ideas and fruitful collaborations can unfold. The Institute provides a place for focused collaborative research and interweaves leading international scholars, both in mathematics and physics, with the local scientific community. In particular, the research and the interactions that take place at the Institute are meant to have a lasting impact on those who pursue their scientific education in Vienna.

In the following, we will give a brief overview of the institutional structure of the ESI and the various programmatic pillars of its scientific activities. Thematic programmes form their core, supplemented by workshops, graduate schools and lecture courses given by Senior Research Fellows at the ESI. All activities include strong educational components. Guided by strict scientific criteria and supported by an international Scientific Advisory Board (SAB), the various actual components of the scientific activities of the ESI are chosen on a competitive basis.

The Institute currently pursues its mission in several ways:

(a) primarily, by running four to six *thematic programmes* each year, selected about two years in advance on the basis of the advice of the international ESI Scientific Advisory Board;

(b) by organizing additional *workshops* which focus on topical recent developments;

(c) by a programme of *Senior Research Fellows* (SRF), who give lecture courses at the ESI for graduate students and post-docs;

(d) by setting up *summer/winter schools* for graduate students and postdocs;
(e) by a programme of Junior Research Fellows (JRF), which supports graduate students or recent postdocs to work on a project of their own that is either connected to a research direction carried out at the University of Vienna or to an ESI thematic programme;

(f) by a programme of Research in Teams (RiT), which offers groups of two to four Erwin Schrödinger Institute Scholars the opportunity to work at the Institute for periods of one to four months;

(g) by inviting individual scientists who collaborate with members of the local scientific community.

**Scientific Activities in 2020**

**Thematic Programmes**

In 2020, the following thematic programme took place at the ESI:

– **Higher Structure and Field Theory**  
  August 3 – September 25, 2020  
  (org.: Anton Alekseev (U Genève), Stefan Fredenhagen (U Vienna), Nicolai Reshetikhin (UC, Berkeley), Thomas Strobl (U Lyon), Chenchang Zhu (U Göttingen))

The following thematic programmes, scheduled for 2020, could not take place due to the spread of the COVID-19 pandemic. All these programmes were postponed to the year 2022.

– **Chromatin Modeling: Integrating Mathematics, Physics, and Computation for Advances in Biology and Medicine**  
  March 2 – 27, 2020  
  (org.: Christos Likos (U Vienna), Tamar Schlick (NYU, New York))

– **Computational Uncertainty Quantification: Mathematical Foundations, Methodology & Data**  
  May 4 – June 26, 2020  
  (org.: Clemens Heitzinger (TU Vienna), Fabio Nobile (EPFL Lausanne), Robert Scheichl (U Heidelberg), Christoph Schwab (ETH Zürich), Sara van de Geer (ETH Zürich), Karen Willcox (U of Texas, Austin))

– **Large Deviations, Extremes and Anomalous Transport in Non-equilibrium Systems**  
  October 16 – November 13, 2020  
  (org.: Christoph Dellago (U Vienna), Satya Majumdar (U Paris Sud, Orsay), David Mukamel (Weizmann Institute, Rehovot), Harald Posch (U Vienna), Gregory Schehr (U Paris Sud, Orsay))

– **Mathematical Methods for the Study of Self-organization in the Biological Sciences**  
  November 14 – December 9, 2020  
  (org.: Pierre Degond (Imperial College, London), Marie Doumic (Sorbonne U, Paris), Anna Kicheva (ISTA, Klosterneuburg), Sara Merino-Aceituno (U Vienna), Christian Schmeiser (U Vienna))

A detailed account of the thematic programme that has taken place is given in subsequent sections of this report.
Workshops

In addition to this thematic programme, only one workshop and one graduate school took place on-site at the ESI in 2020, complemented by visits of several individual scholars who collaborated with scientists of the University of Vienna and the local community. In addition, some organizers agreed to organize pure online workshops in a reduced form to share their current scientific work with each other and to stay in touch. Here is a list of these activities:

- **Mathematical Aspects of Geophysical Flows**  
  January 20 – 24, 2020  
  (org.: Adrian Constantin (U Vienna), George Haller (ETH Zürich))

- **VDSP-ESI Winter School on Machine Learning in Physics**  
  February 10 – 20, 2020  
  (org.: Markus Arndt (U Vienna), Christoph Dellago (U Vienna), Viktoria Erben (U Vienna), Christiane Losert-Valiente Kroon (U Vienna), Massimiliano Procura (U Vienna))

- **Online-Workshop: Multilevel and multifidelity sampling methods in UQ for PDEs**  
  May 4 – 5, and May 13, 2020  
  (org.: Kody Law (U Manchester), Fabio Nobile (EPFL Lausanne), Robert Scheichl (U Heidelberg), Karen Willcox (U of Texas, Austin))

- **Online-Workshop: Higher Structures Emerging from Renormalisation**  
  October 12 – 16, 2020  
  (org.: Pierre Clavier (U of Potsdam), Kurusch Ebrahimi-Fard (NTNU, Trondheim), Peter K. Friz (TU Berlin) Harald Grosse (U Vienna), Dominique Manchon (U of Auvergne), Sylvie Paycha (U of Potsdam))

- **Online-Workshop: Mathematical Methods for the Study of Self-organization in the Biological Sciences**  
  December 10 – 11, 2020  
  (org.: Pierre Degond (Imperial College, London), Marie Doumic (Sorbonne U, Paris), Anna Kicheva (ISTA, Klosterneuburg), Sara Merino-Aceituno (U Vienna), Christian Schmeiser (U Vienna))

The following workshops, scheduled for 2020, could not take place due to the spread of the COVID-19 pandemic. All these activities were postponed to the year 2021 or 2022.

- **Interdisciplinary Challenges in Nonequilibrium Physics**  
  March 30 – April 3, 2020  
  (org.: Demian Levis (U Barcelona), Emanuele Locatelli (U Vienna), Jan Smrek (U Vienna), Francesco Turci (U Bristol))

- **Topology, Disorder, and Hydrodynamics in Non-equilibrium Quantum Matter**  
  April 20 – 24, 2020  
  (org.: Jörg Schmiedmayer (TU Vienna), Maksym Serbyn (ISTA, Klosterneuburg), Romain Vasseur (U Massachusetts, Amherst))

- **Non-regular Spacetime Geometry**  
  Juni 15 – 19, 2020  
  (org.: Piotr T. Chrusciel (U Vienna), Michael Kunzinger (U Vienna), Ettore Minguzzi (U Florence), Roland Steinbauer (U Vienna))
– **Memory Effects in Dynamical Processes: Theory and Computational Implementation**
  Juni 29 – 1 July, 2020
  (org.: Christoph Dellago (U Vienna), Anja Kuhnhold (U of Freiburg), Hugues Meyer (U of Luxembourg), Tanja Schilling (U of Freiburg))

– **International Mathematical Olympiad Training 2020**
  July 5 – 11, 2020
  (org.: Lukas Andritsch (U Vienna), Michael Eichmair (U Vienna))

– **Set-Theory**
  July 6 – 10, 2020
  (org.: Jörg Brendle (Kobe U), Vera Fischer (U Vienna), Sy David Friedman (U Vienna), Benjamin Miller (U Vienna))

– **Arithmetic Statistics and Local-Global Principles**
  July 20 – 24, 2020
  (org.: Tim Browning (ISTA, Klosterneuburg), Daniel Loughran (U Bath), Rachel Newton (U of Reading))

– **Spectral Theory of Differential Operators in Quantum Theory**
  September 7 – 11, 2020
  (org.: Jussi Behrndt (TU Graz), Fritz Gesztesy (Baylor U, Waco), Ari Laptev (Imperial College, London), Christiane Tretter (U Bern))

**Senior Research Fellows**

As in previous years, within the Senior Research Fellows programme, the ESI offered a lecture course on an advanced graduate level.

In the winter term 2019/2020 Shahar Mendelson (Australian National U, Canberra) gave a course on Geometric Aspects of Statistical Learning Theory. The lecture course of Piotr Bizó (Jagiellonian University, Kraków) on Dynamics in Spatially Confined Hamiltonian Systems scheduled for the summer term 2020 had to be cancelled as a consequence of the COVID-19 pandemic.

**Research in Teams**

Established in 2012, the Research in Teams Programme provides the opportunity for research teams of a few people to work at the Institute in order to concentrate on new collaborative research in mathematics and physics. The interaction between the team members is a central component of this programme. The following research teams worked at the ESI in 2020:

– Philipp Haslinger (TU Vienna), Francesco Intravaia (Humboldt University Berlin), Dennis Rätzel (Humbolt University Berlin), Matthias Sonnleitner (U Innsbruck), Blackbody Radiation induced inertial Effects and collective Phenomena - Theoretical Basis and Experimental Feasibility, February 25 – March 1, June 2 – 8, November 18 – 22, 2019. The planned stays for the year 2020 had to be postponed to 2021. This year a progress report on the previous visits is delivered.

– Yacin Ameur (Lund U), Naomi Feldheim (Bar Ilan U), Antti Haimi (Acoustics Research Institute, Vienna), Günther Koliander (Acoustics Research Institute, Vienna), José Luis
Romero (U of Vienna), *Time-Frequency Analysis of Random Point Processes*, January 9 – 18, 2020. The further stays scheduled for April 9 - 18, 2020 and July 13 - 18, 2020 had to be postponed to the year 2021. As a consequence the report on this project will be part of the Annual Report 2021.


– Robert Kurinczuk (Imperial College London), Nadir Matringe (U of Poitiers), Alberto Minguez (U of Vienna), Vincent Sécherre (Versailles U), *L-modular Langlands Quotient Theorem and Applications*, September 12 – 27, 2020. The further stays scheduled for 2020 had to be postponed to the year 2021. As a consequence the report on this project will be part of the Annual Report 2021.

The following Research in Teams Projects that were accepted for 2020 had to be postponed to the years 2022 due to worldwide travel restrictions in the year 2020.


**Junior Research Fellows**

In the year 2020 the following Junior Research Fellows visited the ESI to work on their research projects:


– Lorenzo Del Re (Georgetown U), *Dimensional Crossover of Layered Strongly Correlated Ultracold Fermi Gases*, January 1 – 31, 2021. The last month of his stay planned for September 2020 had to be postponed to 2021.


Aliaksandr Hancharuk and Alexander Evetts had to postpone the second part of their Fellowships to 2022. Their reports on their stays in 2020 are progress reports. The following Junior Fellows had to postpone their stays to 2021 or 2022 due to COVID-19.


**Other activities**

The COVID-19 pandemic also made it impossible to host any events of the Vienna Doctoral School, nor to hold an Erwin Schrödinger Lecture or an Erwin Schrödinger Colloquium.
**The Institute’s Management**

**Kollegium**

The ESI is governed at the organizational and scientific level by a board (Kollegium) of six scholars, all faculty members of the University of Vienna. Their term of office is three years. The members of this board are appointed by the President (Rektor) of the University after consultations with the Deans of the Faculties of Physics and Mathematics. In the period January 1 - December 31, 2020, the Kollegium consisted of A. Constantin (Mathematics), C. Dellago (Physics), M. Eichmair (Mathematics), S. Fredenhagen (Physics), A. Hoang (Physics), I. Perugia (Mathematics). All members of the Kollegium act as professors at the University.

At the operational level, the ESI is managed by the director supported by two deputy directors. This team of directors is proposed by the Kollegium and appointed by the Rector of the University. Currently, the ESI is managed by Christoph Dellago (Director), Stefan Fredenhagen (Deputy Director), who became deputy director on January 1, 2020, and Ilaria Perugia (Deputy Director).

**Scientific Advisory Board**

The scientific activities of the ESI are supervised by the Scientific Advisory Board (SAB), composed of leading scientists. The SAB also reflects the international ties which are essential for the ESI. In 2020, the SAB consisted of: Douglas N. Arnold (U Minnesota), Alberto Bressan (Penn State U), Mirjam Cvetic (U of Pennsylvania, Philadelphia) [chair], Sandra Di Rocco (KTH, Stockholm), Domenico Giulini (U Hannover), Gerhard Huisken (U Tübingen), Stefano Ruffo (SISSA, Trieste), and Martin Zirnbauer (U Cologne).

Douglas N. Arnold (U Minnesota) and Sandra Di Rocco (KTH, Stockholm) joined the Board on January 1, 2020, as new members.

**Administration**

Theresa Kalchhauser left the administration by the end of the year 2020. We would like to thank her for her valuable work for the ESI and her support of the administrativ team. Especially, we would like to thank her for her contribution to the success of the Erwin Schrödinger Lecture and the ESI Medal Award Ceremony 2020 by providing a festive athmosphere by playing the violine together with her musician colleagues. The administration team continued its work with customary efficiency for our visitors, research fellows and board. Through the COVID-19 pandemic it was forced to work from home office during the larger part of the year. With great support from our IT specialist Sascha Biberhofer, the team members nevertheless managed to handle the difficult circumstances of this year very efficiently.

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Christoph Dellago

ESI Director

August 4, 2021
The ESI in 2020: facts and figures

Management and Administration:

Director: Christoph Dellago
Kollegium: Christoph Dellago (Director), Stefan Fredenhagen (Deputy Director), Ilaria Perugia (Deputy Director), Adrian Constantin, Michael Eichmair, André H. Hoang
Administration: Isabella Janger, Theresa Kalchhauser, Maria Marouschek, Beatrix Wolf (Head)
Computing and networking support: Sascha Biberhofer, Thomas Leitner
Video recording and publishing: Sophie Kurzmann

International Scientific Advisory Board in 2020:

Douglas N. Arnold (U Minnesota) Domenico Giulini (U Hannover)
Alberto Bressan (Penn State U) Gerhard Huisken (U Tübingen)
Sandra Di Rocco (KTH, Stockholm) Stefano Ruffo (SISSA, Trieste)
Miriam Cvetic (U Pennsylvania, Philadelphia) [chair] Martin Zirnbauer (U Cologne)

Budget and visitors:  In 2020 the support of ESI received from the University of Vienna amounted to €790 000 plus extra budget of EUR 100 000 to increase the visibility of the Institute. In addition, the ESI obtained a total of €16 535 in third party funds from external sources for the support of the various activities.

The total amount spent in 2020 on scientific activities was €107 237, while the expenditures for administration (mainly salaries) and infrastructure (mainly rent) amounted to €471 435.

The total number of scientists visiting the Erwin Schrödinger Institute in 2020 on-site was 176, see pages 63 – 66 Gender ratio: male: 126 (72 %), female: 25 (14 %), non-binary: 2 (1 %), unspecified 23 (13 %). Moreover, 260 registered people participated online in various activities of the ESI.

ESI research documentation: Starting from January 2013, the ESI research output is tracked using the published articles and the arXiv database. The ESI website provides web links to these arXiv preprints and to the local ESI preprints collected until December 2013. It also contains the bibliographical data of the already published articles. Moreover, publications which appeared in 2020 but are related to past ESI activities, starting from 2011, have been tracked as well in order to provide a long-term evidence of the ESI research outcome success.

The total number of preprints and publications contributed to the ESI research documentation database in 2020 is 54 [related to the activities in 2020: 28, related to the activities in previous years: 26], see pages 58 – 61 for details.

Since the summer of 2019, lectures given at the ESI are routinely recorded and the videos are published on the ESI Youtube-Channel. In total 126 videos were recorded in 2020 amounting to about 107 hours of video material. These videos have been accessed more than 36 000 times.
in 2020 alone. Currently, the number of views is growing quickly indicating the strong interest for recorded ESI lectures in the community.
Scientific Reports

Main Research Programmes

Higher Structure and Field Theory

Organizers: Anton Alekseev (U Genève), Stefan Fredenhagen (U Vienna), Nicolai Reshetikhin (UC, Berkeley), Thomas Strobl (U Lyon), Chenchang Zhu (U Göttingen)

Dates: August 2 – September 25, 2020

Budget: ESI € 11 600

Report on the thematic programme

The programme has been devoted to the fruitful interaction between the theory of higher structures and mathematical approaches to field theory. This interaction goes in both directions. On the one hand, field theory constantly inspires new developments in almost all fields of mathematics. And higher structures including the modern homotopy theory and supergeometry are among the first recipients of these ideas. There is also a renewed interest in mathematical approaches to field theory including algebraic perturbative quantum field theory, factorization homology etc.

On the other hand, many tools of the higher structure theory naturally enter the language of quantum field theory. Among the examples are $A_m$ and $L_m$ stuctures, Batalin-Vilkovisky structures (first discovered in physics, they made their home in mathematics, and are now back on the physics arena) and many others. An impressive recent development is the use of higher structures in the classification of states of matter.

The programme brought together specialists in higher structures and classical and quantum field theory to create more interaction on these exciting topics. Among the highlights of the programme were a focus week on the use of higher structures for a classification of states of, what is called, topological matter (during week 1), a workshop on higher structures (week 3), a focus week on the interaction between quantum field theory and higher structures (week 5), and a focus week on supergeometry and gauge theory (week 7). Among the programme events there were mini-courses on perturbative algebraic quantum field theory, BV-methods, factorization algebras, and supergeometry.

Activities

Due to the pandemic, the first three weeks were turned into purely online events, the remaining five took place in a hybrid fashion.
Our programme was made of 8 weeks:

- Week 1 (August 3 - 7, 2020) Focus week on Topological Matter — online
- Week 2 (August 10 - 14, 2020) Mini-course on The Poisson sigma model and integrable systems (N. Reshetikhin) - online
- Week 3 (August 17 - 21, 2020) Workshop on Higher Structures - online
- Week 4 (August 24 - 28, 2020) Mini-course on Advances in Algebraic Quantum Field Theory (K. Fredenhagen)
- Week 5 (August 31 - September 4, 2020) Focus week on Higher Structures in Quantum field theory, Mini-course on Higher structures in algebraic quantum field theory (A. Schenkel)
- Week 6 (September 7 - 11, 2020) Mini-course on Courant algebroids, generalized Ricci flow, and T-duality (P. Severa)
- Week 7 (September 14 - 18, 2020) Focus week on Supergeometry and Gauge Theory, Mini-course on Geometry of Q-manifolds and Gauge Theories (A. Kotov)
- Week 8 (September 21 - 25, 2020) collaborations and ESI Medal Award Ceremony

Focus week on Topological Matter

Topological orders relate condensed matter physics (2016 there was a Nobel Prize distributed for this) and higher categorical theory and field theory. Many things come into play.

We invited Dirac Medal and Buckley Condensed Matter Prize winner Xiao-Gang Wen from MIT, together with Anton Kapustin from CalTech, to give two series of mini-course on this exciting intersection area.

Many young mathematicians, such as David Reuter, from representation theory, Claudia Schenimbauer from field theory, together with young physicists, Zheng-Cheng Gu, Tian Lan, all had a chance to communicate and exchange ideas. Some talks casted very intense discussion lasting for hours. Mathematical physicists, such as Christoph Schweigert, Jürgen Fuchs, intersected well with operator theorists such as Yasuyuki Kawahigashi.

We also organised individual online-discussion rooms for each speaker (some of them joined their discussion rooms together). That provides virtual space and time for discussion. We would say, even though it was not happening with physical contact, people still managed to interact well.

Moreover some online-effect, such as an enlarged audience, is also a strength of such a format.

Workshop on Higher Structures

Higher Structures is a vast topic which unifies modern approaches to homotopy theory and quantization and their links to quantum field theory. The workshop on Higher Structures naturally fits in a long series of events which took place over the last ten years.

The workshop took place on-line with three 45 minutes long talks per day and with simultaneous breakout sessions for the three speakers which took place after the talks. This format proved to be very useful: relatively short talks allowed the speakers to introduce a topic and to
state the main results, and one hour long breakout sessions gave a natural discussion platform for the audience (which was otherwise lacking because of the on-line format).

The workshop featured talks by some of the leading figures in the field such as K. Fukaya, E. Getzler and B. Tsygan. The topics covered in the workshop included higher analogues of the Goldman theory (F. Naef and N. Rozenblyum), new developments in the Batalin-Vilkovisky (BV) and AKSZ theories (T. Schedler, C. Scheimbauer and P. Severa), applications of operads (T. Willwacher and N. Wahl), 2-vector spaces and 2-algebroids (M. Jotz-Lean and K. Waldorf) and quantization of moduli spaces (A. Brochier and X. Xu). It was very useful that each of these topics was covered in at least two talks, and it was briefly discussed in several other talks as well.

One should also mention a very interesting talk of A. Henriques on unitary fusion categories which was the most original in terms of on-line presentation: the speaker was filming a board to which he was attaching carefully prepared pieces of paper which contained different parts of the material.

Despite the on-line format, the workshop led to intense interactions between the participants, 40 and 60, depending on the talk, in the spirit of usual ESI events.

**Hybrid part**

Due to the COVID-19 pandemic, travelling was highly restricted during the programme. Weeks 4 to 8 were organized in a hybrid setup: online participants and participants present in the ESI lecture hall followed the talks together. Talks were given both by speakers at ESI (60 minutes slots) as well as by online participants whose talks (45 minutes) were projected on the screen in the ESI lecture hall. While during weeks 4 and 8 only very few researchers participated on site, during the intermediary weeks 5, 6, and 7 there was a normal participation (15-20 people in the lecture hall) with lively discussions at ESI. The mini-courses were held online with the exception of the course by P. Severa.

**Specific information on the thematic programme**

The special situation forbidding many scientists to participate in person evidently had many disadvantages, but also led to some benefits: One could put some emphasis on younger people and last minute additions to the programme, in particular from nearby countries. For example, Cornelia Vizman (Timisoara, Romania) arrived in the last week of the programme, so as to proceed with a joint paper written in collaboration with Leonid Ryvkin (Göttingen University); this fruitful interaction was made possible by the additional flexibility.

In general, many young researchers participated in the programme, contributed talks, and profited from talks and mini-courses of the experts. The relatively low number of participants at ESI allowed for more talks by younger participants. For example, Jan Pulman, PhD student from Geneva, gave two excellent blackboard talks on moduli spaces of flat connections as quasi-BV manifolds and on the quantization of Poisson-Hopf algebras which stimulated interesting discussions.

**Outcomes and achievements**

The programme brought together mathematicians and theoretical physicists, experienced researchers as well as young scientists. Mini courses on different topics fostered an exchange
between the disciplines, and the talks on different aspects of the fields initiated many discussions. The discussions in breakout rooms in the online part and the discussions happening on-site at ESI have led to interesting new developments as is evident from the list of preprints that have been published in the context of the programme. We mention here selected additional outcomes:

- The focus week on topological matter raised a lot of interest and attention. The mini-course by Xiao-Gang Wen was attended by more than 200 people, and the trans-cast in China of his lecture attracted around 2000 people attending online. Topological orders has recent emergent interaction with higher categorical theory, field theory. Many things come into play. One of our mini-course speaker, Xiao-Gang Wen is a Dirac Medal and Buckley Condensed Matter Prize winner. There were more than 200 people attending online (and the trans-cast in China of Xiao-Gang’s lecture, attracted around 2000 people attending online).

- The Higher Structures workshop continued a series of conferences devoted to this rapidly growing topic. Despite the on-line format, there were interesting exchanges between participants during dedicated breakout sessions organized after the talks.

- The ESI meeting brought together scientists around V. Salnikov for a (also hybrid) meeting on the CNRS project GraNum that explores the possibilities of using contemporary achievements in graded geometry and higher structures in the context of mechanics.

- The excellent mini-course by A. Schenkel illuminated the relation of algebraic quantum field theory and higher structures. It was accessible for a wide audience and prepared the ground for further discussions among field theorists and mathematicians.

### List of talks

**Online Focus Week on “Topological Orders and Higher Structures”, August 2 – 7, 2020**

- **Xiao-Gang Wen (MIT, Boston)**
  - Topological order and higher category – a physical point of view, I - III (Introductory talk)

- **Davide Gaiotto (PITP, Waterloo)**
  - Topological aspects of QFT

- **Anton Kapustin (Caltech, Pasadena)**
  - Geometry and topology of gapped lattice systems, I - III (Introductory talk)

- **Zheng-Cheng Gu (Chinese U, Hong Kong)**
  - Construction and classification of symmetry

- **Meng Cheng (Yale U, New Haven)**
  - Fractonic topological phases: coupled layers and beyond

- **Juven Wang (Princeton U)**
  - Ultra Unification

- **and Q&A Zheyan Wan (Tsinghua U, Beijing)**

- **Clement Delcamp (MPI, Garching)**
  - Excitations in strict 2-group higher gauge models of topological phases

- **Alex Bullivant (U of Leeds)**
  - A tube algebra prospective on the higher quantum double

- **Yasu Kawahigashi (U of Tokyo)**
  - Topological order, tensor networks and subfactors

- **Jürgen Fuchs (Karlstad U)**
  - PEPS and bicategories

- **Christoph Schweigert (U Hamburg)**
  - Bulk fields in conformal field theory

- **David Reutter (Oxford U)**
  - On fusion 2-categories

- **Yin Tian (Tsinghua U)**
  - The Drinfeld center of monoidal 2-categories in 3+1D

- **Claudia Scheimbauer (TU Munich)**
  - Dijkgraaf-Witten Theory

- **Higher Morita categories**
Theo Johnson-Fryd (Dalhousie U)  Algebraic definition of topological order  
Tian Lan (U Waterloo)  Higher symmetry enriched topological phases

“Mini-course Week” in Week 2, August 10 – 14, 2020

Nicolai Reshetikhin (UC, Berkeley)  The Poisson sigma model and integrable systems, I - III

The talks were recorded beforehand and could be watched online by all participants during the week. At the end of the week a discussion session on the topic was hold online via zoom.

Online Workshop on “Higher Structures”, August 17 – 21, 2020

Ezra Getzler (Northwestern U, Evanston)  Gluing local gauge conditions in BV quantum field theory  
Kenji Fukaya (Stony Brook U)  Equivariant Lagrangian Floer theory  
Thomas Willwacher (ETH Zurich)  Automorphisms of rationalizations of the little n-disks operads  
Nathalie Wahl (U Copenhagen)  Infinity operads: an example  
Nick Rozenblyum (U Chicago)  Hamiltonian flows in Calabi-Yau categories  
Florian Naef (MIT, Boston)  The string coproduct/cobracket  
Xiaomeng Xu (ETH Zurich)  Stokes phenomenon and Knizhnik–Zamolodchikov equations  
Travis Schedler (Imperial College, London)  Tate–Hochschild cohomology of hypersurfaces and singularity categories

Andre Henriques (U of Oxford)  Representation theory for unitary fusion categories  
Madeleine Jotz-Lean (U Göttingen)  On LA-Courant algebroids and Poisson Lie 2-algebroids  
Claudia Scheimbauer (TU Munich)  The AKSZ construction as a fully extended topological field theory  
Adrian Brochier (U Paris-Diderot)  Topological field theories, quantum character varieties and the Riemann–Hilbert correspondence  
Konrad Waldorf (U Greifswald)  2-vector bundles, with applications to spin geometry and twisted K-theory  
Pavol Severa (U Genève)  Dualities and boundary conditions  
Boris Tsygan (Northwestern U)  Traces and higher structures

“Mini-course Week” in Week 4, August 24 – 28, 2020

Klaus Fredenhagen (U Hamburg)  Advances in Algebraic Quantum Field Theory I: Framework of AQFT - ONLINE  
Klaus Fredenhagen (U Hamburg)  Advances in Algebraic Quantum Field Theory II: Perturbative approach towards AQFT - ONLINE  
Klaus Fredenhagen (U Hamburg)  Advances in Algebraic Quantum Field Theory III: Perspectives and open problems - ONLINE  
Nils Carqueville (U Vienna)  Topological quantum field theory with defects  
Jan Pulmann (U Genève)  Moduli spaces of flat connections as quasi-BV manifolds  
Damjan Pistalo (U Zadar)  Some topics in derived geometry motivated by the BV formalism

Alexander Schenkel (U of Nottingham)  Higher structures in algebraic quantum field theory I - III - ONLINE  
Albin Grataloup (U Montpellier)  Shifted Symplectic Geometry and Derived Critical Loci  
Jan Pulmann (U Genève)  Quantization of Poisson-Hopf algebras  
Jae-Suk Park (Postech)  Fundamental group of quantum field theory - ONLINE  
Viet Dang Nguyen (U Lyon)  Dynamical zeta functions and topology - ONLINE  
Rinat Kashaev (U Genève)  On the spectral problem of a three term difference operator - ONLINE
Christoph Schweigert (U Hamburg)  
Topological field theories with boundaries - some constructions and some applications - ONLINE

Eli Hawkins (U of York)  
Deformations in Algebraic Quantum Field Theory - ONLINE

“Mini-course Week” in Week 6, September 7 – 11, 2020

Pavol Severa (U Genève)  
Courant algebroids, generalized Ricci flow, and T-duality I - III

Sergei Merkulov (U of Luxembourg)  
On the classification of Kontsevich formality maps - ONLINE

Mikhail Vasiliev (Lebedev Inst., Moscow)  
Higher-Spin Gauge Theory and Locality - ONLINE

Noriaki Ikeda (Ritsumeikan U, Kusatsu)  
BV and BFV for the H-twisted Poisson sigma model - ONLINE

Kasia Rejzner (U of York)  
Asymptotic fields in QFT from the point of view of BV-BFV formalism - ONLINE

Eugene Skvortsov (MPI, Potsdam-Golm)  
New integrable models from (non-commutative) deformation quantization

Miquel Cueca (U Göttingen)  
Dimensional reduction for Manin triples

Robert A. Iseppi (U Aarhus)  
The BV formalism in the framework of noncommutative geometry: the case of finite spectral triples

Branislav Jurco (Charles, Prague)  
Quantum homotopy algebras and the homological perturbation lemma

“Mini-course Week” in Week 7, September 14 – 18, 2020

Alexei Kotov (U Hradec Kralove)  
Geometry of Q-manifolds and Gauge Theories I - III - ONLINE

Henning Samtleben (ENS Lyon)  
Exceptional field theory and exotic supergravity

Fridrich Valach (Imperial College, London)  
Equivariant Poisson-Lie T-duality and supergravity

Olaf Hohm (HU Berlin)  
Duality Hierarchy

Maxim Grigoriev (Lebedev Inst., Moscow)  
Presymplectic AKSZ orm of Einstein gravity - ONLINE

Pietro Grassi (U of Eastern Piedmont)  
Supergeometry and Applications - ONLINE

Rafal R. Suszek (U Warzawa)  
The higher supergeometry of the super-o-model

Athanasios Chatzistavrakidis (RBI, Zagreb)  
Graded geometry for mixed-symmetry tensor gauge theories and duality

Camille Laurent-Gengoux (U Lorraine)  
Q-manifolds, singular foliations, and singular leaves.

Talks in Week 8, September 21 – 25, 2020

Leonid Ryvkin (U Duisburg)  
Multisymplectic (co-)momentum geometry

Chencang Zhu (U Göttingen)  
Higher Structures and Embedding tensors - ONLINE

Marc Henneaux (UL Brussels)  
The antifield-BRST approach to (gauge) field theories: an overview - ONLINE

Alejandro Cabrera (UF Rio de Janeiro)  
Semiclassical quantization of Poisson structures: local symplectic groupoids, generating functions and the Poisson sigma models - ONLINE

Publications and preprints contributed


List of participants


Invited scientists that participated online

Workshops organized independently of the main programmes

Mathematical Aspects of Geophysical Flows

Organizers: Adrian Constantin (U Vienna), George Haller (ETH Zürich)

Dates: January 20 – 24, 2020

Budget: ESI € 9 767, other sources € 5 000.

Report on the workshop

Activities

The workshop did focus on mathematical studies of geophysical flows, covering topics in oceanography and in atmospheric sciences. The emphasis was placed on the interpretation of geophysical coherent structures in geometric dynamical systems terms and on qualitative studies. A successful interaction between researchers in mathematics, physics and engineering took place during the workshop. We are very pleased that the topics that were presented and discussed ranged from the very applied to the very theoretical: we had discussions of field data, modelling aspects, numerical studies, and analytical results. Most of the participants gave talks: 50 min long for established researchers and 30 min long for postdoctoral researchers and for (two) PhD-students near the completion of their theses.

Specific information on the workshop

Rather than crowding the week with talks, we opted for a balance between talks and discussions. Based on our impressions and on the gathered feedback, several discussions were perceived as very useful.

Outcomes and achievements

Several scientific collaborations were started during this workshop. For example, a group from the University of Vienna started a joint research endeavour on the topic of wind-induced ocean currents flows with researchers at the Hebrew University of Jerusalem and with researchers at St. Andrews University (UK). Also, the existing scientific collaboration on topics related to geophysical fluid flows, between the University of Vienna and ETH Zürich, were strengthened. Furthermore, useful contacts were established between people at the University of Vienna with expertise in theoretical aspects and experimentalists from Budapest.
List of talks

**Workshop, January 20 – 24, 2020**

Robin S. Johnson (U of Newcastle) On the use of the thin-shell approximation for modelling atmospheric flows

George Haller (ETH Zürich) Material barriers to active transport

David Dritschel (U St. Andrews) Two-dimensional models of a rotating shallow fluid layer

Anatoly Abrashkin (HSE, Nishny Novgorod) Large Oceanic Gyres: Lagrangian Description

Miklos Vincze (ELTE Budapest) Climate impact of the Drake Passage opening: lessons from a minimalistic laboratory experiment

Joe LaCasce (U Oslo) Topographic effects on large scale ocean flows

Francisco J. Beron-Vera (U of Miami) Inertial ocean dynamics

Rossen I. Ivanov (Dublin Inst. of Tech.) Equatorial wave - current interactions

Thomas Bartsch (U Giessen) Periodic solutions of the point vortex Hamiltonian system in domains

Nikolas Aksamit (ETH Zürich) Machine-Learning Mesoscale and Submesoscale Surface Dynamics from Lagrangian Ocean Drifter Trajectories

Stergios Katsanoulis (ETH Zürich) Vortex boundaries as barriers to diffusive vorticity transport in two-dimensional flows

Adrian Constantin (U Vienna) Frictional effects in wind-driven ocean currents

Branko Grisogono (U Zagreb) On meso- and micro-scale atmospheric flows

Maria Olascoaga (U Miami) Observed Inertial Ocean Dynamics

Imre M. Janosi (ELTE Budapest) Single super-vortex as a proxy for geostrophic ocean surface flow fields

Takashi Sakajo (U Kyoto) Vortex dynamics on the sphere

Sandor Balazs (Budapest U of Tech.) Topographic effects on the vorticity equilibrium in shallow-fluid formalism

Daniel Karrasch (TU München) Lagrangian perspectives on advection-diffusion transport in the low-diffusivity limit

Nathan Paldor (Hebrew U) A lagrangian view of evaporation from the ocean

Tamas Tel (ELTE Budapest) On the theory of parallel climate realizations

Publications and preprints contributed


Several preprints are currently in the submission stage.

Invited scientists

Anatoly Abrashkin, Nikolas Aksamit, Thomas Bartsch, Biswajit Basu, Francisco J. Beron-Vera, Adrian Constantin, David Dritschel, Branko Grisogono, George Haller, Susanna Haziot, Delia Ionescu-Kruse, Rossen I. Ivanov, Imre I. Janosi, Robin S. Johnson, Daniel Karrasch, Stergios Katsanoulis, Vikas Krish-
namurthy, Joe LaCasce, Tony Lyons, Calin Martin, Maria Olascoaga, Nathan Paldor, Ronald Quirchmayr, Takashi Sakajo, Balazs Sandor, Raphael Stuhlmeier, Tamas Tel, Miklos Vincze.

**VDSP-ESI Winter School on Machine Learning in Physics**

**Organizers:** Markus Arndt (U Vienna), Christoph Dellago (U Vienna), Christiane Losert-Valiente Kroon (U Vienna), Massimiliano Procura (U Vienna)

**Dates:** February 10 – 20, 2020

**Budget:** The Winter School "Machine Learning in Physics" was organised jointly and financed in parts by the Vienna Doctoral School in Physics (VDSP) and the Erwin Schrödinger International Institute for Mathematics and Physics (ESI). It was co-financed by the Vienna Doctoral Program on Complex Quantum Systems (CoQuS) and the Doctoral College Particles and Interactions (DKPI).

ESI: € 11 600  
VDSP: € 9 000  
CoQuS: € 1 100  
DKPI: € 400

**Report on the School**

Machine learning, which encompasses a broad range of powerful analysis and modeling tools, is increasingly used in many branches of physics and is changing the way in which research is performed. These novel tools and methodologies inspire research to explore new fundamental questions and technological challenges such as the development of new materials, the design of quantum experiments or the tracking of particles produced in accelerators. But the significance of machine learning goes far beyond its application in science and it is key for future innovations and economic growth, as reflected in the Digital Europe Program of the EU. Due to the growing importance of machine learning in physics and related disciplines, students are strongly interested to learn about these new approaches, but machine learning is not (yet) part of standard physics curricula. The goal of this school was to fill in this gap and provide the participants with an introduction to machine learning methods and their application in various areas of physics (materials science, particle physics and quantum science) represented at the Faculty of Physics of the University of Vienna.

**Activities**

The aim of the VDS-P ESI Winter School on Machine Learning in Physics was to highlight the possibilities for new routes to discovery in several fields of data-driven research complementing standard physics curricula, which focus on modelling based on the fundamental equations of physics and do not yet reflect new data-based paradigms.

The activities were tailored to Master and PhD students of physics, chemistry and materials science as well as early postdocs to provide them with a better understanding of fundamental concepts and practical applications of machine learning as well as skills to develop and apply this technique to concrete research tasks.
During the ten days of the winter school, leading scientists in machine learning gave eight introductory lectures (three hours each morning) on the topic of their expertise spanning the mathematical foundations of machine learning, machine learning in materials science, quantum science and technology and high-energy physics. The international experts provided an overview of the general methodology of machine learning, their importance for the simulation of data and development of new algorithms, the exploration of more exotic hardware, discoveries of new strategies to replace or speed-up existing programmes and of applications of various machine learning tools to achieve more effective and insightful analyses.

The morning lectures were complemented by eight hands-on class activities (three hours each afternoon) which were additionally supervised by tutors of the research groups of the keynote speakers – see .

On the first evening the participants of the school had the opportunity to informally network with the guest scientists and foster interactions between all participants at a welcome dinner.

**Specific information on the school**

The school was structured in four modules. Apart from the compulsory attendance of the introductory module on the first two days and the case study day concluding the first week, participants had to choose at least one of the topical modules.

*Module 1: Introduction to Machine Learning; Mon, 10 Feb, & Tue, 11 Feb 2020*

The elementary lectures of this module explored the relation between the theoretical and methodological basis and the implementation of machine learning in cutting-edge research in physics. Moreover, this introductory module included a discussion of how statistical physics concepts can be used to understand methods in machine learning.

*Module 2: “Material Science”; Wed, 12 Feb, & Thu, 13 Feb 2020*

This module of the Winter School focused on applications of machine learning in the domain of atomistic materials simulations. The lectures covered the construction of appropriate descriptors for atomic structures and discussed several methods (neural networks, Gaussian process regression, support vector machines) to predict total energies and forces based on the descriptors underlined by specific examples to illustrate the capabilities of the methods.

*Module 3: “Quantum Science”; Mon, 17 Feb, & Tue, 18 Feb 2020*

In recent years researchers have been exploring potential benefits of the interplay between machine learning approaches and systems that are described by quantum mechanics. Based on the theoretical background covered in the keynote lectures the participants of this module built their own physics-inspired reinforcement learning (RL) environment featuring simulations of a few ions manipulated by laser pulses. Furthermore, the application of neural-networks based "reinforcement learning" to quantum physics was examined, where a computer develops from scratch useful sequences of quantum operations e.g. showing how a network-based "agent" can discover complete quantum-error-correction strategies, protecting a collection of qubits against noise.

*Module 4: “Particle Physics”; Wed, 19 Feb, & Thu, 20 Feb 2020*

In the field of particle physics recent progress has resulted in the use of machine learning techniques to reconstruct and analyse data from the CMS detector at the Large Hadron Collider at CERN, to improve measurements of the Higgs boson properties and to optimise searches for New Physics. This module illustrated applications in the context of optimal readout of the
hardware of the experiments and in analysis of the physics data as well as the speed-up of quantum field theory calculations.

The first week of the school concluded with a public event, the case study day, where everyone interested in the topic of machine learning in the natural sciences was invited to attend. Plenary talks on “Learning Science from Data” saw four distinguished speakers from academia and the private sector providing their perspective on applying machine learning methods in science and technology beyond physics. Representatives of Artificial Intelligence Start-Ups gave insights into the mission of their companies in flash talks and in personal conversations at the AI Start-Up World Café. Taking inspiration from an introduction to a philosophical perspective all plenary speakers of the day engaged with the audience in a joint panel discussion.

Outcomes and achievements

Graduate students and early stage researchers from local and international research institutions were invited to join the Winter School to facilitate exchange among the participants on an international level. The Winter School received 143 applications from 19 countries which was far beyond the capacity of the event. In order to enable intensive interactions between students and speakers, 74 participants were selected by the organizing committee based on their science career development and their academic achievements. Due to the great interest in the talks also from the local research community, the organizing committee decided to open the morning lectures to all. At the keynote talks, the school welcomed an audience of around 120 participants.

The morning lectures were given by sixteen renowned researchers at the forefront of the new developments, allowing the participants to gain a broader view of the possibilities of applications of machine learning in physics and enabling them to explore the potential of machine learning tools for use in their own field of expertise. The overview of the central concepts of machine learning, their significance for specific research areas and discussions on recent progress in physics facilitated by machine learning were complemented dedicated programming hands-on tutorials where the participants applied and practiced the material covered in the morning sessions. The tutorials were facilitated by nine tutors, senior members of the research groups or collaborators of the keynote speakers. The lecture notes and scripts were made available on a dedicated, password protected cloud.

List of talks

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Cameron Buckner (U of Houston) Is model transparency good or bad for scientific applications of deep learning?
Hans Briegel (U of Innsbruck) Machine learning in Quantum Science, I - II
Florian Marquardt (MPI Erlangen) Machine learning in Quantum Science, III - IV
Wolfgang Waltenberger (HEPHY, Vienna) Machine learning in Particle Physics, I - II
Gregor Kasieczka (U of Hamburg) Machine learning in Particle Physics, III - IV

Invited scientists

Online-Workshop: Multilevel and multifidelity sampling methods in UQ for PDEs

Organizers: Kody Law (U Manchester), Fabio Nobile (EPFL Lausanne), Robert Scheichl (U Heidelberg), Karen Willcox (U of Texas, Austin)

Dates: May 4 – 5 and May 13, 2020

Budget: No budget was used since the workshop was held online.

Report on the workshop
This workshop covered multilevel and multifidelity sampling methods in uncertainty quantification for PDEs, with a particular focus on moving beyond forward propagation of uncertainty. The workshop originally formed part of a Thematic Programme (TP) on “Computational Uncertainty Quantification: Mathematical Foundations, Methodology & Data” (Main Organizer: Christoph Schwab, ETH Zürich) that was supposed to take place at the Erwin Schrödinger Institute May 4 – June 26, 2020, covering a much wider spectrum of problems and methodologies related to this topic. Due to the COVID-19 pandemic the TP had to be postponed and will take place May 2 – June 24, 2022.

Since all speakers had already been confirmed and since the research themes of the programme are expected to remain highly topical also in two years time, the TP will essentially run with
the same workshop structure as originally planned in 2020, including an opening workshop on “Multilevel and multifidelity sampling methods in UQ for PDEs”. However, as a precursor for this event in 2022, we proposed to the Director of ESI to run a reduced version of the opening workshop online on May 4 and 5, 2020, with the aim to advertise the future programme and to initiate a 2-year collaborative research effort on this very active, specialist subtopic in Computational UQ. This proposal was enthusiastically supported by the Director of ESI and by the entire ESI team. Overall this proved to be a great success and the format of the online workshop offered sufficient interaction to achieve the goals and to initiate the collaboration.

Numerical Uncertainty Quantification (UQ for short) is an emerging research area in engineering and in the sciences, drawing expertise from applied mathematics, scientific computing and high-dimensional, computational statistics. In particular, the mathematical foundations and underpinnings of novel computational strategies for the efficient numerical approximation of PDEs with uncertain inputs, as well as the analysis of statistical methodologies for high-dimensional statistical data resulting from such PDE simulations are at the center of current research, both in the context of forward and inverse problems. Upon placing probability measures on input parameter spaces, randomized (sampling) approximations can be employed to sample from the parametric solution manifolds. The thematic programme will have a broader focus, considering also other algorithmic techniques, such as adaptive collocation and Galerkin methods, model order reduction, reduced basis methods, low-rank approximations in tensor formats, compressed sensing, or kernel and machine learning based approximations.

A powerful and attractive way for uncertainty propagation and for Bayesian inference in random and parametric PDEs are multilevel sampling approaches, such as multilevel Monte Carlo, multilevel quasi-Monte Carlo, multilevel stochastic collocation, to name but a few. These methods exploit the natural hierarchies of numerical approximations (mesh size, polynomial degree, truncations of expansions, regularisations, model order reduction) to efficiently tackle the arising high- or infinite-dimensional quadrature problems. Their efficiency is based on variance reduction through a systematic use of control variates and importance sampling (in the stochastic setting) and of the sparse grid recombination idea (in the deterministic setting). The variance reduction is intrinsically tied to a priori and a posteriori error control in the numerical approximations, which in turn has spawned a resurgence in fundamental research in the mathematical and numerical analysis of PDEs with spatiotemporally heterogeneous data.

A related body of work has focused on combining models of varying fidelity (such as 1D and 3D models, reduced-order models, differing physical assumptions, data-fit surrogate models, and look-up tables of experimental results) in multifidelity uncertainty quantification methods. These methods similarly use control variate formulations (the multifidelity Monte Carlo method) and importance sampling. This multifidelity setting differs from the multilevel setting above because the different models do not need to form a fixed hierarchy. The relationships among the models are typically unknown a priori and are learned adaptively as the computation advances.

All these methodologies have most notably been developed in the context of forward propagation of uncertainty, or quadrature with respect to a known (prior) distribution, but they have also been extended to inverse problems and intractable (posterior) distributions that arise when incorporating data in a Bayesian inference framework, and to in optimization under uncertainty.
Activities

This online workshop took place right at the start of the COVID-19 pandemic with little experience about online workshops and an unclear picture of people’s availability or interest to take part in an interactive research workshop online. In addition, the range of timezones where the field of international participants were located added a further difficulty with respect to the scheduling of the workshop. Therefore, we concentrated the workshop in two 5-hour-blocks on May 4-5, 2020, reducing the workshop programme to eight live presentations and one recorded talk, complemented with breakout room discussions and feedback sessions on each day. These 5-hour blocks were timed between 14:00 and 19:00 CEST to allow (reasonable) participation for participants from Central Asia all the way through to the American West Coast (even including a talk by an Australian participant at the start of the session on one of the days).

The theme of the first day centered around the question of how model hierarchies and models of differing fidelity can be adaptively constructed and then used in combination for efficient uncertainty quantification in a multilevel or multi-fidelity setting. The talks on the second day and the pre-recorded talk expanded this theme in the direction of multilevel quasi-Monte Carlo methods, multi-index variants and the inverse Bayesian setting, as well as to nested expectations.

The talks were followed on each day by breakout room discussions, lead by individual breakout room session chairs, where the participants discussed in smaller subgroups the talks of the day – also with reference to their own research – with a view of identifying interesting research avenues and possible common collaboration topics. The speakers had been instructed to include open-ended research questions in their presentations. The participants were randomly assigned to the groups (about 10-12 participants per group and 5 groups) and the numbers of participants that actually participated in the subgroups varied between 4 and 10 people. Each group collected their ideas in a shared Google document and, following the breakout room discussions, one representative from each group then presented the ideas to the plenum.

Many interesting ideas were generated. Those were collected together in one large, joint document by the organizers following the meeting and arranged according to common, possible collaboration themes. Workshop participants were then asked to put their names down against themes they were interested in and wanted to be involved with. In a short follow-up event one week after the workshop, on May 13, these collaborative themes and groups were consolidated and speakers for each team were chosen. Since then the activities of the collaborative groups have happened independently, lead by the speakers and driven on by the participants themselves.

Specific information on the workshop

In inviting the participants for this workshop, a lot of attention had been put at finding a good balance between assembling the leading researchers in the field of multilevel and multifidelity uncertainty quantification methods and also offering the possibility for young researchers to participate and to interact and collaborate directly with the former. We were truly impressed by the extremely positive feedback from both groups, but especially from the leading researchers – almost all of the invited people accepted the invitation and participated actively! – offering a unique opportunity for the young researchers. About 50 people actively participated in the workshop; of those more than half were PhD students and postdocs.

The original plan had been to offer 8-10 of those junior researchers also the opportunity to
present their research. This was not possible due to the reduced programme, but it will now form a central part of the planned 2022 multilevel workshop during the postponed thematic programme, with the prospect to actually have presentations on the outcomes of the collaborative efforts spawned by this online event.

The feedback from junior researchers was extremely positive, with a very large number of them individually thanking us for the stimulating event.

**Outcomes and achievements**

Some of the main collaborative themes that were established through the workshop, to be pursued in the coming two years until the 2022 Thematic Programme (together with the researchers that indicated an interest to be involved; speaker underlined):

A. **Adaptivity within multilevel & -fidelity methods (adaptive mesh refinement, adaptive surrogates, adaptive choice of samples):** Scheichl (Heidelberg), Barth (Stuttgart), Chaudhuri (MIT), Croci (Oxford), Cui (Monash), Dodwell (Exeter & Turing Institute), Farcas (UT Austin), Feischl (TU Vienna), Ganesh (EPFL), Garbuno (Caltech), Haji-Ali (Heriot-Watt), Jakeman (Sandia Lab), Nobile (EPFL), Papaioannou (TU Munich), Peherstorfer (Courant), Qian (MIT), Willcox (UT Austin), Zech (Heidelberg)

B. **Multilevel & -fidelity methods for chaotic systems and models that are difficult to couple pathwise:** Haji-Ali (Heriot-Watt), Barth (Stuttgart), Croci (Oxford), Ganesh (EPFL), Garbuno (Caltech), Giles (Oxford), Lang (Chalmers), Latz (Cambridge), Law (Manchester), Nobile (EPFL), Qian (MIT), Teckentrup (Edinburgh), Willcox (UT Austin)

C. **Multi-index versus Multi-Fidelity Monte Carlo (relationship, differences, theory):** Law (Manchester), Haji-Ali (Heriot-Watt), Jakeman (Sandia Lab)

D. **Estimating covariances or other more difficult nonlinear QoIs (incl. rare events):** Peherstorfer (Courant), Chaudhuri (MIT), Dodwell (Exeter & Turing), Kirchner (TU Delft), Lang (Chalmers), Papaioannou (TU Munich), Qian (MIT)

E. **Extending multilevel methods to theoretical physics applications (MCMC, nested simulation, importance weighting):** Madrigal (EPFL), Cui (Monash), Scheichl (Heidelberg)

F. **Multilevel Bayesian inference (analysis of coupling, posterior concentration, comparison of approaches):** Farcas (UT Austin), Latz (Cambridge), Cui (Monash), Dodwell (Exeter & Turing), Garbuno (Caltech), Jakeman (Sandia Lab), Law (Manchester), Madrigal (EPFL), Papaioannou (TU Munich), Peherstorfer (Courant), Qian (MIT), Scheichl (Heidelberg), Teckentrup (Edinburgh)

G. **Open source software, software integration and definition of benchmark problems:** Nobile (EPFL), Croci (Oxford), Cui (Monash), Dodwell (Exeter & Turing), Giles (Oxford), Haji-Ali (Heriot-Watt), Jakeman (Sandia Lab), Law (Manchester), Seelinger (Heidelberg), Teckentrup (Edinburgh)

H. **Multilevel & -fidelity methods for learning tasks with different-sized data sets:** Haji-Ali (Heriot-Watt), Cui (Monash), Dodwell (Exeter & Turing), Feischl (TU Munich), Jakeman (Sandia Lab), Latz (Cambridge), Law (Manchester), Madrigal (EPFL), Teckentrup (Edinburgh), Ullmann (TU Munich)
List of talks

Josef Dick (UNSW, Sidney) - Multi-Index Monte Carlo methods for PDEs with random coefficients
Raul Tempone (RWTH Aachen) - Forward and Inverse Problems with Multilevel Monte Carlo
Benjamin Peherstorfer (CIMS, New York) - Context-aware learning of surrogate models for multifidelity computations
Alex Gorodetsky (U of Michigan, Ann Arbor) - Sampling algorithms for generalized model ensembles in multifidelity uncertainty quantification
Elisabeth Ullmann (TU Munich) - On Multilevel Best Linear Unbiased Estimators
Tiangang Cui (Monash U, Melbourne) - Advanced Multi-Level Sampling Methods for Large-Scale Bayesian Inverse Problems
Matti Vihola (JYU) - Unbiased estimators and multilevel Monte Carlo
Abdul-Lateef Haji-Ali (Heriot-Watt U, Edinburgh) - Sub-sampling and other considerations for efficient risk estimation in large portfolios
Dirk Nuyens (KU Leuven) - Quasi-Monte Carlo sampling in multilevel, multiindex and multivariate-decomposition methods

Publications and preprints contributed

None so far, but expected as a consequence of the collaborative effort for the 2022 multilevel workshop as part of the thematic programme.

Invited scientists


ESI Medal Award Ceremony 2020

Organizer: Christoph Dellago, ESI Director (U Vienna)

Dates: September 24, 2020

ESI Medal

The *Medal of the Erwin Schrödinger Institute for Mathematics and Physics*, in short ESI-Medal, has been created to recognize outstanding achievements in any area of mathematics or physics, including contributions at the interface of the two fields.

The ESI-Medal is awarded annually, for the first time this year. Emphasis is generally given to recent achievements not older than ten years. There is no age limitation for the recipient and ordinarily the ESI-Medal is awarded to one person only.
The recipient of the ESI-Medal receives a medal, a certificate and a monetary award of € 4 000.

Nominations for the ESI-Medal can be made by organizers of ESI Thematic Programmes taking place in the year following the nomination deadline, former members of the Scientific Advisory Board of the ESI, former recipients of the ESI-Medal, former Directors of the ESI and the President of the ESI Association. The recipient is selected by the Scientific Advisory Board of the ESI.

**Winner of the ESI Medal 2020**

The winner of the the *Medal of the Erwin Schrödinger Institute for Mathematics and Physics* for the year 2020 is Anton Alekseev from the University of Geneva.

Prof. Alekseev has been honoured for his recent outstanding contributions to mathematics, in particular for the discovery of the link between the Grothendieck-Teichmüller group and the long-standing Kashiwara-Vergne problem in Lie theory, for the program of tropicalization of Poisson structures, and for the proof of the Goldman-Turaev formality in 2-dimensional topology. His work unites brilliant intuition, deep knowledge, and remarkable technical skills.

**Award Ceremony**

The award ceremony took place on September 24, 2020 at the ESI Boltzmann Lecture Hall. While some people attended the ceremony on-site, others (including the awardee) participated online.

**Agenda of the Ceremony**

- Christoph Dellago  Welcome
- Thomas Strobl  Laudatio
- Christoph Dellago  Award of the ESI Medal
- Anton Alekseev  Award Lecture
- Christoph Dellago  Closing

**Online Workshop: Higher Structures Emerging from Renormalisation**

**Organizers:** Pierre Clavier (U Mulhouse), Kurusch Ebrahimi-Fard (NTNU, Trondheim), Peter K. Friz (TU Berlin), Harald Grosse (U Vienna), Dominique Manchon (U of Auvergne), Sylvie Paycha (U Potsdam)

**Dates:** October 12 – 16, 2020

**Budget:** No budget was needed since the workshop was held online.

**Report on the workshop:**

The international research workshop aimed at offering a place to create new as well as enhance already existing interactions between different aspects of renormalisation in mathematics and
physics. It brought together mathematicians and physicists from diverse communities, ranging from category theory to stochastic partial differential equations with talks by Y. Bruned (U Edinburgh), A. Chandra (Imperial College London), B. de Tiliere (U Paris Dauphine), K. Fredenhagen (U Hamburg), D. Kreimer (Humboldt U, Berlin), A. Kupiainen (U Helsinki), C. Malvenuto (U La Sapienza Rome), L. Schneps (CNRS, U Paris), K. Reizner (U York), B. Vallette (U Paris Nord) and R. Wulkenhaar (U Münster) among many other speakers.

A research school with some four introductory 4hrs mini-courses by I. Chevyrev (U Edinburgh), F. Patras (CNRS, U Nice), K. Rejzner (U York) and L. Zambotti (U Paris) was postponed to 2021.

Activities

Each day consisted of three talks in the morning and three to four in the afternoon complemented with a panel discussion on What is renormalisation? What next? on Wednesday evening with the panelists G. Dunne, B. Vallette, K. Rejzner, V. Rivasseau and L. Zambotti.

We complemented the online format of the workshop with a Zulip chat, where participants could share questions, ideas, comments and references, during the whole week. It was organised by Pierre Clavier (U Mulhouse) and involved PhD students (Diego Caudillo (NTNU), Emanuele Verri (U Greifswald), Ludwig Rahm (NTNU), Adrián Celestino (NTNU)) and Post-Docs (Cécile Mammaz (U Lille), Lisa Glaser (U Nijmegen)) who ensured a lively Zulip chat.

Specific information on the workshop

There was a number of young researchers from various fields of research who could benefit both from presenting their results to a broad and rather receptive audience and from learning about other topics from the other talks. We had explicitly asked the speakers to make a special pedagogical effort keeping in mind that the audience was very mixed with a number of non-experts.

Here is the list of young researchers who delivered a talk:

- Alexander Schmeding
- Antoine Hocquet
- Carlo Bellingeri
- Enrico Russo
- Joscha Diehl
- Nicolas Gilliers
- Yannic Vargas

Outcomes and achievements

We were somehow worried about going online yet were rather positively suprised by the outcome. The informal atmosphere of the workshop, probably induced by its pronounced interdisciplinary was propitious for participants to ask questions.

Also, the Zulip chat very much contributed to creating a lively atmosphere with numerous informal interactions among the participants.
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Publications and preprints contributed

We are considering the publication of part of the contributions in a volume of proceedings.

Invited scientists


Online Workshop: Mathematical Methods for the Study of Self-organization in the Biological Sciences

Organizers: Pierre Degond (Imperial College, London), Marie Doumic (Sorbonne U, Paris), Anna Kicheva (IST Austria), Sara Merino-Aceituno (U Vienna), Christian Schmeiser (U Vienna)

Dates: December 10 – 11, 2020

Budget: No budget was needed since the workshop was held online.

Report on the workshop

Activities

The actual thematic programme “Mathematical Methods for the Study of Self-Organization in the Biological Sciences” has been postponed to November 14th - December 9th, 2022 due to the spread of the Covid-19 infection. We held this workshop to keep the event alive.

Scientific description: Self-organization is pervasive in biology as living organisms are by essence systems that have self-assembled and self-organized in the course of their development. Self-organization refers to the ability of systems made of a large number of independent agents interacting through rather simple and local rules to generate large scale spatio-temporal coherent structures with typical dimensions orders of magnitude larger than those associated with
each individual agent. Examples of self-organisation are natural network formation (like capillaries and leaf venation), collective dynamics (like flocking, herding and pedestrian dynamics), opinion dynamics, landscape formation, tissue and organ formation...

**Aim of the workshop/programme:** The programme brings together mathematicians and biologists to provide a broad overview of the various self-organization mechanisms that prevail at the various scales and the mathematical models by which they can be described or even explained.

In particular, the workshop consisted on a series of online talks pairing-up a mathematician/theoretician and a biologist/experimentalist that work together. Each one gives approximately half an hour talk to present their joint work. Titles and abstracts can be found at: [https://www.univie.ac.at/projektservice-mathematik/e/index.php?event=MathSelfBio2020](https://www.univie.ac.at/projektservice-mathematik/e/index.php?event=MathSelfBio2020)

**Specific information on the workshop**

Many young participants (PhD students and post-docs) registered for this event (around 50).

Local participants included:

**University of Vienna**

- Angeles, Gervy Marie
- Kanzler, Laura
- Kholmatov, Shokhrukh
- Mussnig-Wytrzens, Claudia
- Plunder, Steffen
- Ravi Sundar Jose Geetha, Aarathy
- Schwanhaeusser, Axel
- Völkli, Isabella

**TU Vienna:**

- Ponomarev, Dmitry
- Wöhrer, Tobias

**Max Perutz-Laboratories:**

- Bragulat Teixidor, Helena
- Buecker, Christa
- Garcia Baucells, Júlia
- Jayaram, Swathi
- Kuchler, Karl
- Lombardo, Salvo Danilo
Outcomes and achievements

It is too early to see the outcomes of the meeting. However, some of the speakers mentioned that it was very helpful for them to prepare the talk as they needed to discuss with their collaborator (since they needed to coordinate their joint talks). It seems that these discussions were very helpful.

List of talks

Pairs of talks are listed below. The talks were recorded and wherever access was granted, talks will be posted in the ESI YouTube Channel. In general, biologists talked first and then the mathematicians.

• Laurent Blanchoin (University of Grenoble and University Paris Diderot, France)/ Angelika Manhart (U College London, UK):
  Experimental and modelling study of the dynamic steady state of actin networks.

• Human Rezaei (INRIA Paris, France)/ Mathieu Mezache (INRAe, France):
  Coexistence of multiple prion conformation leads to a catalytical conformational exchange
  Modeling of the oscillating polymerization/demopolymerization process of Prions

• Osvaldo Chara (Sysbio Group, Argentina)/ Diane Peurichard (INRIA Paris, France):
  Spatiotemporal distribution of cell proliferation rules the regenerative response in axolotl spinal cord
  A 2D hybrid agent-based/continuum model for the regeneration of axolotl spinal cord

• Gantas Perez-Mockus (Francis Crick Institute, UK)/ Sophie Hecht (INRIA Paris, France):
  Mechanical constraints to cell cycle progression in a pseudostratified epithelium

• Wei-Feng Xue (University of Kent, UK)/ Magali Tournus (École Centrale Marseille, France):
  Experimental analysis of the division of amyloid fibrils
  How to recover the fragmentation rate and kernel characterizing a size-structured population undergoing fragmentation?

• Eric Theveneau (U Paul Sabatier, France)/ Marina A. Ferreira (U of Helsinki, Finland):
  Challenging epithelial stability
  Modelling a packed cell tissue

Titles and Abstracts

Experimental and modelling study of the dynamic steady state of actin networks. (Angelika Manhart and Laurent Blanchoin)

The dynamic assembly and turnover of actin networks in cells control shape changes, migration and organelle function, as well as communication with extracellular substrates or neighbors. The intracellular actin cytoskeleton forms such complex intricate networks in cells that it is difficult to identify the principles of their dynamic self-organization. We have developed reconstituted systems in vitro as simplified models for the study of the cytoskeleton. We use a high-resolution surface structuration assay combined with mathematical modelling to describe the length dependence of a dynamic reconstituted actin network. We found that the length of the network is controlled by its porosity and the ADF/cofilin-actin ratio. Based on our mathematical model, we could explain how the steady state length of branched actin network emerges from the complex interplay between its biochemical, structural and mechanical properties.
Coexistence of multiple prion conformation leads to a catalytical conformational exchange (Human Rezaei)

The prion pathology is based on autonomous structural information propagation towards single or multiple protein conformational changes. Since this last decade the prion concept referring to the transmission of structural information has been extended to several regulation systems and pathologies including Alzheimer and Parkinson’s diseases. The unified theory in Prion replication implies structural information transference (SIT) from the prion to a non-prion conformer through a mechanism also called improperly, with regards to biophysical considerations “seeding” phenomenon. Recently we reported that prion replication is intrinsically source of structural diversification. The coexistence of multiple of prion assemblies with different structural and replication propensity questions how they are maintained within the same media and how they escape to best replicator selection. The analysis of the quaternary structure dynamic of prion assemblies by light scattering, and differential scanning calorimetry revealed the existence of an exchange process within the structurally diverse prion assemblies. This exchange process has for consequence the apparition of dumped-oscillation. Data assimilation and kinetical modelling conduced us to propose a kinetical scheme in which structurally diverse prion assemblies catalytically exchange material. According to this kinetic scheme a catalytical depolymerization competes with a catalytic conformational change.

Modeling of the oscillating polymerization/depolymerization process of Prions (Mathieu Mezache)

The process of protein aggregation and fragmentation is linked to the contraction and development of a broad class of incurable neurodegenerative diseases: amyloid diseases. More especially, oscillatory kinetic phenomena are identified during the experiments on Prions diseases. We introduce a kinetic model capable of generating oscillations. The model is a variant of the polymerization/depolymerization system and considers two monomer species: a pathological monomer that polymerizes and a monomer healthy that depolymerizes. Unlike seminal models, the depolymerization is catalytic and non-linear and a phenomenon of exchange operates between the two species of monomers and polymers. The model couples a Lotka-Volterra system for monomers to a system of growth/fragmentation: Becker-Döring in the discrete size case, Lifshitz-Slyozov in the continuous case.

Spatiotemporal distribution of cell proliferation rules the regenerative response in axolotl spinal cord (Osvaldo Chara)

Axolotls can fully regenerate spinal cord after amputation, but the underlying mechanisms are still unclear. We previously found that tail amputation triggers the reactivation of a developmental-like program in spinal cord ependymal cells (Rodrigo Albors et al., 2015. eLife. 4:e10230). We also determined a high-proliferation zone that expands and moves posteriorly over time and demonstrated that cell cycle acceleration, due to shortening of G1 and S cell cycle phases, is the major driver of regenerative growth (Rost et al., 2016. eLife. 5:e20357). What organizes cell proliferation in space and time remains unknown. In this talk, we present some results obtained from a very simple 1-dimensional stochastic mathematical model, assuming a signal initiated at the amputation plane that propagates over the spinal cord tissue with constant velocity, recruiting the ependymal cells. We also assumed that the coordinates along the cell cycle of the recruited cells are irreversibly transformed, depending on the cell cycle phase in which the cells are. Finally, we will see that the spatiotemporal distribution of cells in G1/G0 and S/G2 predicted from the model are in qualitative agreement with the experimental data gathered in a FUCCI axolotl, a transgenic axolotl that reports cell cycle status fluorescently in vivo.

A 2D hybrid agent-based/continuum model for the regeneration of axolotl spinal cord (Diane Peurichard)

Based on the simple 1D model that was shown in the previous talk, we aim to extend the model in 2D to provide a more realistic model for axolotl spinal cord regeneration. To that aim, in this talk we introduce a 2D hybrid agent-based/continuum model coupling cell dynamics, cell proliferation and injury signalling chemical flow during tissue repair. Tissue cells are modelled as non-overlapping 2D spheres which divide randomly with space-dependent proliferation rates. We suppose that cell proliferation rates depend on the local concentration of injury signalling chemicals, continuously produced at the boundary of the tissue after injury/amputation. These chemicals diffuse in the tissue and degrade at a given rate, accelerating the division of tissue cells which are in contact. We show that this simple model is able
to reproduce the tissue outgrowth measured experimentally in axolotl, and we numerically analyze the influence of the chemical signal parameters on the tissue outgrowth dynamics. The model suggests that the proliferative response in axolotl spinal cord regeneration could be mainly controlled by a chemical signal spreading in the tissue after injury, and provides new insights on the signal dynamics that may be responsible for successful spinal cord regeneration.

**Mechanical constraints to cell cycle progression in a pseudostratified epithelium** (Gantas Perez-Mockus & Sophie Hecht)
Mechanical feedback has been proposed to constraint growth in developing epithelia. So far, much of the attention has been focused on the role of adherens junctions as mechanical sensors. Here we consider the possible role of mechanical influences that operate throughout the epithelial volume. This is particularly relevant in pseudostratified epithelia, where nuclei must migrate to the apical surface in order to proceed through mitosis. We explore how the mechanical constraints imposed by nuclear crowding and space confinement affect interkinetic nuclear migration and hence cell cycle progression. We first catalogue the 3D position, crowding index and cell cycle position for thousands of nuclei in fixed wing imaginal discs at different developmental stages. We use these data to devise an individual-based model that treats nuclei as deformable objects constrained by their cell membrane and the presence of other nuclei. In this model, the duration of G1 and S phase are imposed whereas the duration of the G2 phase is a read-out of the model. Our simulations recapitulate the increased crowding and number of nuclear layers observed in fixed tissues, and show how increase crowding impedes apical-ward movement, forcing nuclei more time in G2 before they can reach the apical surface for mitosis. The simulations also predicts that an active downward movement in G1 is required to reproduce the apical/basal distribution of nuclei in this phase, a prediction that we validate experimentally. Finally, we explore the necessity of a basal signal required for S phase entry, to account for the observed reduction of the G1 phase duration. Thus, while the crowding increases only the nuclei that are able to migrate to the basal region and back to the apical surface would be able to complete the cell cycle. Our two-gate model of cell cycle progression could account for the progressive slowing down of growth and the finite thickness of pseudostratified epithelia.

**Experimental analysis of the division of amyloid fibrils** (Wei-Feng Xue)
The division of amyloid protein fibrils is required for the propagation of the amyloid state, and is an important contributor to their stability, pathogenicity and normal function. Here, I will present our experimental work on resolving amyloid division and biological impact of their size distributions. By applying new theoretical results emerging from collaboration with mathematicians (detailed by Magali Tournus), these experiments to profile the dynamical stability towards breakage for different amyloid types using AFM imaging reveal particular differences in the division properties of disease- and non-disease related amyloid. Here, the disease associated amyloid formed from alpha-synuclein show lowered intrinsic stability towards breakage and increased likelihood of shedding smaller particles compared with non-disease related amyloid models. Our results enable the comparison of protein filaments’ intrinsic dynamic stabilities, which are key to unravelling their toxic and infectious potentials.

**How to recover the fragmentation rate and kernel characterizing a size-structured population undergoing fragmentation?** (Magali Tournus)
We address the question of estimating the fragmentation parameters – i.e. the division rate $B(x)$ and the fragmentation kernel $k(y,x)$– from measurements of the size distribution $f(t,.)$ at various times. This is a natural question for any application where the sizes of the particles are measured experimentally whereas the fragmentation rates are unknown. The application that drives our work is the study of mechanical properties of amyloid fibrils that undergo fragmentation (are the mechanical properties related to toxicity?) and will be detailed by Wei-Feng Xue. In this talk, I will explain why the inverse problem is well posed under reasonable assumptions, and I will focus on how we can recover the fragmentation rate and kernel.

**Challenging epithelial stability** (Eric Theveneau)
Epithelia are a special type of cell arrangement in which cells are tightly attached to one another. During embryo development cells can aggregate as epithelia and disperse as a mesenchyme, a collection of motile and loosely connected cells. This occurs multiple times to form the organs. These processes of dispersion and aggregation known as epithelial-mesenchymal and mesenchymal-epithelial transitions (EMT, MET) are extremely complex. They involve qualitative and quantitative changes in cell-cell and
cell-matrix adhesion, cell polarity and remodeling of extracellular matrix. The paths leading to EMT have been thoroughly studied experimentally. One striking observation is that there is a wide diversity of strategies to toggle between epithelial and mesenchymal phenotypes even within a given cell population. The impact of this cell heterogeneity on the dynamic of the process is not understood. We do not know whether cells with different strategies compete or cooperate. We do not know whether a given path to EMT affects the migratory behavior of cells once they have left an epithelium. Answering these questions is important if we want to better understand the driving forces of morphogenesis during embryo development. But also, if we want to better understand how EMT might affect a tissue when it occurs as part of a disease. Indeed, in carcinoma (cancer of epithelial tissues), EMT leads to dispersion of cells and promotes stemness, migration and eventually secondary metastasis. In the lab, we use the neural tube of the chicken embryo as model of a growing epithelia that produces mesenchymal cells by EMT during embryo development. In my presentation, I will present the main principles of EMT, the experimental model, the questions we would like to address, the techniques and strategies that can be used and more importantly what currently cannot be done that led us to develop a computational strategy to substantiate our experimental work.

Modelling a packed cell tissue (Marina A. Ferreira)
In pseudostratified epithelial tissues, cells are tightly packed with almost no intercellular space. The force each cell exerts on its neighbours plays an important role in the dynamics and shape of the tissue. However the precise effect of these contact forces is not well understood, nor easily studied in the lab. To study this system, we propose a modelling framework consisting of a geometric representation of a cell which interacts with other cells through springs and non-overlapping constraints, aiming at minimizing a potential energy. Mathematically, this can be formulated as a nonconvex constrained minimization problem with a time-dependent minimizing function. Our numerical implementation consists on a time-stepping scheme involving the damped Arrow-Hurwicz algorithm for nonconvex problems. The model is validated against in vivo data taken from the chick neuroepithelium. In silico experiments show how interkinetic nuclear movements influence cell distribution and shape of the tissue over time. Our results also suggest that apicobasal elongation is not completely explained by the mechanics of the tissue, but rather requires a specific elongation programme.

Publications and preprints contributed
This is too early to say. Online events are less prone to create new collaborations as there is no real possibility for interactions. This is why the actual thematic programme in 2022 is fundamental as it will allow people to really meet and discuss.

Invited scientists
The event was based on registration, since it was online. The list of registered participants can be found at: [https://www.univie.ac.at/projektservice-mathematik/e/index.php?event=MathSelfBio2020&page=participants](https://www.univie.ac.at/projektservice-mathematik/e/index.php?event=MathSelfBio2020&page=participants).

We decided to make the event based on registration because right now people are not so free (they are overloaded with commitments; in Covid times teaching duties take more time and are more tiring and people cannot stop their teaching duties during online workshops). A total of 100 people registered for the event and we had always around 33 people participating in each of the talks.

Pedro Aceves Sanchez, Marina Amado Ferreira, Gerry Marie Angeles, Stefan Badelt, Thibault Bertrand, Helena Bragulat Teixidor, Christa Buecker, Valeria Caliaro, José A. Carrillo, Louis-Pierre Chaintron, Jean Clairambault, Grégoire Clarte, Clara Conrad-Billroth, Jake Cornwall Scoones, Cathy Danesin, Julia Delacour, Antoine Diez, Raluca Eftimie, Christian Esparza, Nandha Kumar Ettikkan, Alexander
Research in Teams

Research in Teams Project 1/2019: Blackbody Radiation Induced Inertial Effects and Collective Phenomena - Theoretical Basis and Experimental Feasibility

Collaborators: Philipp Haslinger (TU Vienna), Francesco Intravaia (HU Berlin), Dennis Rätz (HU Berlin), Matthias Sonnleitner (U Innsbruck)

Dates: February 25 – March 1, 2019, June 2 – 8, 2019, November 18 – 22, 2019

Budget: ESI € 14 400 (for the whole project)

Report on the project

Scientific Background

Blackbody radiation is omnipresent. It is emitted by objects at finite temperature with an outward energy-momentum flow, which exerts an outward radiation pressure. For example, in a radiation field at room temperature, a caesium atom would scatter less than one thermal photon every $10^8$ years on average. Thus, it is generally assumed that any scattering force exerted on atoms by such radiation is negligible. In 2013, Sonnleitner et al. theoretically predicted that particles should also interact coherently with the thermal electromagnetic field due to their polarizability [2]. This can lead to a surprisingly strong force that is attractive in contrast to radiation pressure. This prediction has sparked a hot debate in the related scientific community.

The quantum mechanical phase of massive particles enables us to sense accelerations and potential energy differences with unprecedented accuracy using matter-wave interferometry. Atoms provide nearly perfect test-particle properties as they can be selected isotopically pure, cooled down to nano-Kelvin temperatures, and have well understood and easily tunable magnetic and electric properties. Atom interferometric methods have been used to measure local gravity, gravitational gradients, the gravitational constant, and the fine-structure constant. Furthermore, atom interferometry has been employed to test the universality of free fall and to search for dark energy. Due to recent experimental improvements in the Müller group at UC Berkeley, Philipp Haslinger and coworkers reached the needed sensitivity to search for the theoretically predicted attractive blackbody radiation force using an optical cavity enhanced atom interferometer. The observed force [1] agrees perfectly with the theoretical predictions of Sonnleitner et al. [2].

Blackbody radiation also induces a thermal friction force on neutral particles, which is related to the Einstein-Hopf drag on harmonic oscillators in thermal baths. The thermal friction force exists independently of any gradient of the radiation field. In analogy to the velocity-independent case, inhomogeneities in the radiation in space modify the frictional force, in particular when the atom moves near macroscopic objects.

Most of the effects described above apply to individual atoms interacting with external (thermal) radiation. However, a dense ensemble of atoms will react to external radiation in unison and this gives way to collective effects. For atoms or (sub-)micron-sized scatterers inter-particle effects such as optical binding have been studied mostly using coherent laser beams. Recently, in addition to van der Waals/Casimir-Polder forces, artificial dispersion forces generated by random fields have become a focus of growing interest. In general, the low polarizability of individual atoms makes it difficult to measure collective motional effects without a cavity or
other setups. One therefore usually expects that intense fields are required to generate measurable effects such as self-organization or deformation of a trapped atomic cloud. However, the improvements achieved in the experimental techniques involving atom-interferometry and the present ability of creating and controlling very dense clouds, can be used to measure light induced dipole-dipole interactions with a high degree of precision and accuracy also in weak radiation fields.

**Project aims and scope**

The focus of this project is to derive the results of Haslinger et al. [1] with the elaborate and highly accurate quantum field theoretical methods of the Casimir-Polder force community represented by Francesco Intravaia in this collaboration. The comparison to the results of Sonnleitner et al. [2] is expected to lead to a common theoretical basis for the description of the effect and consequently to the resolution of present disagreements. Furthermore, an advantage of the methods used by the Casimir-Polder force community is that the material properties of the sources of thermal radiation are taken into account from first principles and do not need, as it is done presently, to be introduced by hand later. Also, retardation and distance dependence are treated explicitly in that framework. Therefore, the significance of the increased accuracy can be evaluated by comparison to the geometrical approach of Sonnleitner et al. [2].

Since the attractive blackbody radiation force dominates for a large temperature range over both gravity and radiation pressure, it may significantly affect the ultimate accuracy of atom interferometric metrology (as it already does for optical clocks), and it may have implications for astrophysical scenarios. Therefore, a high accuracy of theoretical predictions is desirable, which could be supplied by the theoretical framework that is being developed during this project. Based on the insights from the theoretical work, further experiments to investigate the attractive blackbody radiation force are being considered.

Another goal of this project is to evaluate the feasibility of an experimental detection of (thermal) frictional forces using interferometric methods. We are estimating the strength of the frictional force for different experimental configurations and the feasibility of its measurement as well as its relative size compared to other interactions present in the system. During this project, we are developing new experimental proposals to measure the predicted thermal friction and a possible accelerating thermal force due to the dynamical Stark shift.

We are also developing the theoretical and experimental tools to investigate inter-atomic forces induced by blackbody radiation using atom-interferometry.

**Outcomes and achievements**

Due to the Covid-19 pandemic, this project was not continued as planned in 2020 and did not finish yet. Therefore, only intermediate results can be reported here.

The theoretical description of the effect described in [2] and experimentally measured in [1] is being developed mostly by Francesco Intravaia and his student Daniel Reiche. Results are likely to be presented and discussed during the RIT meetings in 2021.

During the first RIT meetings, estimates where made of the size of the effects of friction forces on moving cold atoms in vacuum or a thermal field. Discussions between the theoreticians and the experimentalist Philipp Haslinger showed that their detection is challenging. Further considerations will also involve nano-particles instead of atoms and elaborate geometries and material properties to enhance the effects significantly. This is planned for the upcoming meet-
Philipp Haslinger, Matthias Sonnleitner and Dennis Rätzel are participating in a project in collaboration with Jörg Schmiedmayer at the Atominstitut, TU Wien, to test for black-body-radiation-induced collective effects in cold atomic clouds. The experimental setup is capable of producing very dense and ultra-cold atomic samples (Rb-BEC), and it is highly sensitive to measure potential energy differences between the separated atomic wave functions. It is a perfect testbed to sense for blackbody-radiation induced interactions. During this RIT project, Matthias Sonnleitner derived a full theoretical description for the experiments and predicted an attractive force between the atoms that should be visible in the experiments. This effort was supported by Matthias Sonnleitner regularly reporting and discussing his results at the RIT meetings with the three collaborators. At the moment, the experiment is performed, data is taken and analyzed.

Discussions during the first meetings also involved the project "Quantum Klystron" by Philipp Haslinger and Dennis Rätzel which was reported on in a preprint published on the arXiv-server [3].

**Publications and preprints contributed**


**References**


**Research in Teams Project 1/2020: Higher-order Corrections to Parton Branching at Amplitude Level**

**Collaborators:** Jeffrey Forshaw (U of Manchester), Jack Holguin (U of Manchester), Maximilian Löschner (KIT, Karlsruhe), Simon Plätzer (U Vienna), Emma Simpson Dore (KIT, Karlsruhe)

**Dates:** January 13 - February 14, 2020

**Budget:** ESI € 8 000

**Report on the project**

**Scientific Background**

Precise quantum field theory calculations need to re-arrange the perturbative series to include logarithmically enhanced terms to all perturbative orders. For gauge theories like the strong interactions described by Quantum Chromodynamics (QCD), this re-summation can be carried...
out thanks to universal properties of infrared divergences. These divergences occur in the limits of low-energy or (quasi-)collinear emission of additional partons, the fundamental quarks and gluons, and cancel against universal singularities from loop corrections, leading to a logarithmic enhancement in infrared sensitive observables which probe final state jets of hadrons emerging from parton radiation.

Effective field theories such as Soft-Collinear Effective Theory (SCET) [1] can be used for resummation, or a direct analysis of scattering cross sections in QCD [2] can be employed. Here, coherence properties of QCD radiation allows to formulate the resummation programme for global observables by using probabilistic parton branching algorithms. In this case, quantum mechanical interference between different scattering amplitudes can be absorbed into ordering subsequent emissions in collinearity, or opening angle, in the large-$N$ limit of infinitely many QCD charges. These algorithms have also been the main design rationale behind the more flexible Monte Carlo (MC) simulations, which predict jet properties from cascades of partons. The parton branching algorithms to date lack a systematic expansion, even if some subleading effects can be incorporated approximately. For the more general and realistic non-global observables, the large-$N$, leading logarithmic case can still be solved with probabilistic dipole branching, but subleading-$N$ contributions, which become parametrically as important as the subleading logarithmic corrections, enforces all interferences to be considered. These effects hence set the level of complexity to obtain more precise resummation algorithms, and a new generation of MC simulations.

An analysis of QCD amplitudes themselves [3], as well as effective field theory considerations [4] reveal the relevance of evolution equations of a density-operator type object which simultaneously contains the amplitude and its conjugate. Within this framework, parton radiation and loop corrections will act as operators in the space of $SU(N)$ tensor structures, usually referred to as colour space, thus replacing the probabilistic paradigm with parton branching at the amplitude level, from which differential cross sections are only obtained by tracing the density operator at the end of its evolution.

**Project aims and scope**

The project builds on the expertise on soft gluon evolution, colour space, and parton branching algorithms see e.g. [5, 6, 7, 8], which has been pioneering the formulation of parton branching at the amplitude level [9]. It has a clear objective to include higher order corrections and to provide the computational methods and a numerical program for dedicated re-summation calculations and as basis for a new generation of MC simulations.

The aims of the project were to consolidate and combine the various research directions on the topic in which the team members have been involved. The main objective of the project was the work on extending the parton branching algorithm to the next order in resummed perturbation theory, on which significant progress has been made both regarding virtual corrections as well as real corrections. The project further focused on using the parton branching evolution equations to analyze and possibly improve existing algorithms from the point of view of branching at the amplitude level.

All of the analytic aspects went hand-in-hand with algorithmic and methodological questions arising from implementing the new evolution equations in a Monte Carlo code. A further goal of the research in teams stay was to get the different team members in closer contact and to have a vital exchange in between the different sub-projects.
Outcomes and achievements

During the stay at the ESI, several core aspects of the proposed work have been addressed and results have been published or publications are in preparation: with the collaborators Forshaw and Holguin, Plätzer has published work on the accuracy of existing parton branching algorithms, and possible incremental improvements thereof [10]. A pitfall in work by a competing group has also been identified [11] during the stay at the ESI.

Plätzer and Forshaw extensively worked on the numerical methods and implementation, work which ultimately broke a gridlock to obtain stable numerical results from parton branching at the amplitude level which have been published on the arXiv in summer and has been accepted by Physical Review Letters [12].

Together with the collaborators Löschner and Simpson Dore further significant steps have been undertaken to formulate a comprehensive framework of analysing the factorization properties of QCD amplitudes in singular limits, exposing close links to Soft-Collinear Effective Theory (SCET), and related work on subleading-power corrections. A considerable publication is nearing submission to the arXiv. This is one of the key steps to formulate the parton branching algorithm at the next order in perturbation theory.

A second key step has been addressed by Plätzer with Master student Ruffa, resulting in a manuscript [13] (submitted to the Journal of High Energy Physics) which covers the colour structures and kinematic dependence of soft gluon virtual corrections at the two loop order, such that now all ingredients are readily available for an implementation, which has been the main focus of the proposed programme.

Publications and preprints contributed


References


Senior Research Fellows Programme

To stimulate the interaction with the local scientific community the ESI offers regular lecture courses on an advanced graduate level. These courses are taught by Senior Research Fellows of the ESI whose stays in Vienna are financed by the Austrian Ministry of Education, Science and Culture and the U of Vienna. In exceptional cases this programme also includes long-term research stays of small groups or individual distinguished researchers. These lecture courses are highly appreciated by Vienna’s students and researchers.

This year’s programme was focused on the following Lecture Course:

Lecture Courses, Winter Term 2019/20:

Shahar Mendelson (Australian National U, Canberra):
Geometric Aspects of Statistical Learning Theory
Lecture Course 250108 VO: January 7 – 22, 2020
Tuesday and Wednesday: 13:15 - 14:45

Shahar Mendelson: Geometric Aspects of Statistical Learning Theory

Course

Statistical learning theory plays a central role in modern data science. The main aim of the course was to describe the solution to what was, arguably, the key question in the area since the late 60s.

To describe the problem, let $F$ be a class of functions defined on a probability space $(\Omega, \mu)$, set $X$ to be distributed according to $\mu$ and consider a random variable $Y$. The goal is to find some function that is almost as close to $Y$ as the best approximation to $Y$ in $F$ (for a reasonable notion of approximation, e.g., the $L_2$ sense).

Unlike questions in approximation theory, here one has access to rather limited information: $X$ and $Y$ are not known, and instead, one is given an independent sample $(X_i, Y_i)_{i=1}^N$, selected according to the joint distribution $(X, Y)$. The sample is used to produce a (data-dependent) function $\hat{f}$, which is the learner’s “guess” of a good approximating function, and the procedure $(X_i, Y_i)_{i=1}^N \rightarrow \hat{f}$ is called a learning procedure. A learning procedure performs with accuracy $\epsilon$ and confidence $1 - \delta$ if, with that probability w.r.t $(X_i, Y_i)_{i=1}^N$, $\hat{f}$ is “$\epsilon$-close” to the best possible choice in the class $F$.

Obviously, high accuracy and high confidence are conflicting features. The question is to find the optimal tradeoff between accuracy and confidence: given a class $F$, a distribution $(X, Y)$, and a sample size $N$, identify the tradeoff between the wanted accuracy $\epsilon$ and the confidence $1 - \delta$ with which that accuracy can be achieved. And, for a satisfactory solution one has to identify a suitable choice of procedure $\hat{f}$ that attains the optimal tradeoff.

During the course the following aspects of the question have been covered:

- Introduction: why is learning possible at all, and what estimates can one hope for?
- The excess risk functional and the random processes it leads to.
- Complexity measures of classes of functions. Chaining methods for Bernoulli and gaussian processes; combinatorial dimension and metric entropy.
• The small-ball method and (some of) its applications.
• Median-of-means tournaments and the solution of the problem for convex classes.

Research

During my stay I have started what I hope will be a long and fruitful collaboration with Prof. Philipp Grohs and with Dr. Daniel Bartl.

One project with Dr. Bartl that is close to completion deals with the analysis of stochastic optimization problems. Specifically, we show that the small-ball method can be used to improve significantly on the state-of-the-art performance bounds in natural convex stochastic optimization problems.

Roughly put, in such problems the goal is to solve \( \min_{x \in X} f(x) \) where \( f(x) = \mathbb{E}[F(x, \xi)] \); \( x \) belongs to some (convex) parameter space \( X \); and \( \xi \) is a random variable/vector. However, one does not have access to the function \( f \). Instead, the information given are \( F(\cdot, \xi_i), i = 1, \ldots, N \), where \( (\xi_i)_{i=1}^N \) are independent copies of \( \xi \).

The standard solution for such problems is to minimize \( \sum_{i=1}^N F(\cdot, \xi_i) \). The idea behind this approach is that empirical means are good approximations of true means, and in particular a minimizer of the empirical functional should not be “to far” from the minimizer of \( \mathbb{E}[F(x, \xi)] \).

Unfortunately, except in very special situations, that approach is true only in the limit \( N \to \infty \). It is rather misleading when dealing with a finite sample size—which happens to be the case in real-world problems.

We introduce a new procedure that yields almost optimal quantitative estimates for every sample size \( N \). It does so under rather minimal assumptions on \( \xi \), and in particular even in heavy-tailed scenarios.

Lecture Notes

The lecture notes for the course are available online. See the ESI website of the course: https://www.esi.ac.at/events/e32/

Publications and preprints contributed

Junior Research Fellows Programme

Erfan Esmaeili Fakhabi: Soft Charges in Anti de Sitter Space

Erfan Esmaeili Fakhabi (IPM, Tehran): January 1 – April 30, 2020:

Report

A subsystem in a gauge theory is well-defined, only if boundary conditions on gauge variables on the boundary are properly imposed. In a canonical analysis, gauge transformations which preserve boundary condition have well-defined Hamiltonians, so they are symmetries of the theory. This group of asymptotic symmetries has been of physical interest before and after the advent of holography. My research at ESI mainly consisted of two parallel projects with the central concept of asymptotic symmetry group described below.

Soft charges on Anti-de Sitter space

In asymptotically flat spacetimes, scattering processes in massless gauge theories involve very low momentum exchange and emission of very low energy (soft) gauge bosons. The relation between the soft radiation and asymptotic symmetry group has been established [1]. In Anti-de Sitter spacetime, however, there is not a notion of soft radiation, while we have introduced infinite dimensional asymptotic symmetry group for Maxwell theory [2]. For $p$-form theories we followed [3] by decomposing the fields in representations of rotation group. The propagating degrees of freedom in a $p$-form abelian gauge theory with gauge field $A_{\mu_1\cdots\mu_p}$ are two sets of differential forms on $(d-2)$-sphere: a $p$-form $\Psi_{i_1\cdots i_p}$ and a $(p-1)$-form $\Phi_{i_2\cdots i_p}$. We have shown that the soft charge for large gauge transformations on anti de Sitter boundary are given by

$$Q_{\lambda} = \oint \sqrt{q} \lambda_{i_2\cdots i_p} \Phi^{i_2\cdots i_p}$$

(1)

where $\lambda$ is the gauge parameter and $q_{ij}$ the metric on unit sphere. However, this quantity is not conserved. We have to add surface terms to (1) to obtain the infinite set of conserved quantities corresponding to $(p-1)$-form parameters $\lambda_{i_2\cdots i_p}$. Another conundrum is the absence of exact charges in global coordinates, as compared to hyperbolic coordinates (see [4]). We have yet no clue how to implement exact charges in anti-de Sitter $p$-form theories.

We exhibited the consistent set of $p$-form boundary conditions for general dimensions. In particular spacetime dimensions, there are two sets of boundary conditions for any $p$, as is known for scalar fields [5].

Higher spin theory on two-dimensional Minkowski spacetime

Higher spin theory, as the extension of gravity to higher rank massless gauge bosons is known to exist in three and higher dimensions [6]. The two dimensional theory is however poorly understood, and the studies are limited to anti-de Sitter background [7].

In this project, we began to define a higher spin theory on flat space by considering a two dimensional $BF$-theory. We identified a ten dimensional algebra in two spacetime dimensions for the spin-3 gravity which contains the Maxwell algebra and can be obtained by truncation of the spin-3 gravity in three dimensions.
A tentative set of boundary conditions have been prescribed and the allowed transformations correctly imply a spin-3 field. The role of higher spin fields will be made more clear after the 2nd order formalism of the theory is written down.

A feature of the $SL(N)$ theory on two dimensional flat space is the existence of $N - 1$ central charges, demanded by the existence of a well-defined Killing form.

The on-shell action of the theory has been computed by quadratic and cubic Casimir operators of the algebra. The physical significance of the fields appearing in the gauge field is still unclear.

References


Publications and preprints contributed

H. Afshar, E. Esmaeili, D. Grumiller, Spin-3 gravity on two dimensional flat space, ongoing project.

E. Esmaeili, V. Hosseinzadeh, M.M. Sheikh-Jabbari, p-form soft charges on anti-de Sitter background, ongoing project.

Lorenzo Del Re (Georgetown U): Dimensional Crossover of Layered Strongly Correlated Ultracold Fermi Gases

Lorenzo Del Re (Georgetown U): September 1 – 30, 2019, December 1, 2019 – January 31, 2020:

Report

The original aim of the project was to investigate how properties of strongly correlated electrons systems change as a function of a parameter that allows to continuously interpolate from a three dimensional to a two dimensional system. Such a parameter could be the difference between the in plane hopping $t_\parallel$ from the inter-planes hopping $t_\perp$ in the three-dimensional Hubbard model. The study of such a system has been partially undertaken in Ref.[1], where the authors solved the model using a static mean-field approach, and our original idea was to include quantum
fluctuations using the Dynamical Vertex Approximation (DGA)[2], that falls into the category of the diagrammatic expansions[3] of Dynamical Mean Field Theory (DMFT)[4].

However, in order to provide with a satisfactory description of the dimensional crossover from 3D to 2D, one should let the system to spontaneously break symmetries such as the SU(2) spin symmetry in the repulsive case and the U(1) symmetry of pseudo-spins in the attractive case [5]. In fact, we expect that such a dimensional crossover would induce a phase transition fixing the temperature and varying $t_{\perp} - t_{\parallel}$.

Therefore, as a first step we decided to focus on the case of repulsive interactions and we have generalized the DGA formalism to treat magnetically ordered phases. To this aim, we started by concisely illustrating the many-electron formalism for performing ladder resummations of Feynman diagrams in systems with broken SU(2)-symmetry, associated to ferromagnetic or antiferromagnetic (AF) order. In particular, we found very useful to introduce the following change of basis in the space of four-point correlation functions:

$$c_{ab}(x_1, x_2, x_3, x_4) = T(a) c_{ab} c_{gd}(x_1, x_2, x_3, x_4) T(b),$$

where $T(a)$ are observable representation matrices, and their indices $a, b$ represent fermions spin-orbital degrees of freedom. We then analyzed the algorithmic simplifications introduced by taking the local approximation of the two-particle irreducible vertex functions in the Bethe-Salpeter equations, which defines the ladder implementation of DGA for magnetic systems. In particular, we found a block diagonal form of the Bethe Salpeter equation in the case of antiferromagnetism in the spin-longitudinal channel that reads:

$$\bar{F}_{kk'} = \frac{1}{(\beta V)^2} \sum_{k_1, k_2} \bar{\Gamma}_{k, k', \pm} \bar{\mathcal{G}}_{k_1 k_2, \pm} \bar{\mathcal{F}}_{k_2 k', \pm},$$

where $\mathcal{F}$ is the full scattering amplitude, $\Gamma$ the irreducible vertex function. The $\pm$ indices correspond to the representation sub-spaces that are even/odd with respect to the symmetry operation $t_x \sigma_x$. As a last step, we have derived the expression for the ladder DGA self-energy in the ferro- anti-ferromagnetically ordered phases of the Hubbard model and illustrate the emerging physics by means of approximated calculations based on a mean-field input. In particular, in the AF case, we found that the self energy of electrons reads:

$$\sigma^\pm_k (\nu \to 0) \propto -\text{sign} (\Omega^\pm_k) \ln \left( \frac{1}{|\Omega^\pm_k|} \right) - i \nu \frac{1}{|\Omega^\pm_k|}.$$  \hspace{1cm} (1)

In the case of particle-doping $\Omega^+$ vanishes at the Fermi surface, therefore leading to a divergence of the self-energy $\sigma^+$. However, we were able to show that the conduction electrons are dressed by $\sigma^-$. The latter does not diverge because of the finite gap between the two bands, hence giving a rigorous argument for the stability of metallic phases in doped AF in two dimensions [6].

In the course of my visiting period at the ESI, we could also address another fundamental problem that is deeply connected with the general theory of many electrons systems, and in particular with the algorithmic implementation of the DGA, i.e. the occurrence of several divergences of the irreducible vertex function [7]. This issue, which is also related to the multivaluedness of the Luttinger-Ward functional [8, 9] was hitherto understood only as a mere formal manifestation of the breakdown of the perturbation theory. We made a clear step forward in the fundamental theoretical understanding, as we we were able to unveil important physical implications of the vertex divergences in the charge channel, within a basic DMFT framework. In
particular, we could express the isothermal compressibility of the Hubbard model on a Bethe Lattice as:

$$\kappa = \sum_i \frac{w_i}{\lambda_i + \frac{1}{2} \beta \sigma^2},$$  \hspace{1cm} (2)

where $\lambda_i$ are the eigenvalues of the generalized charge susceptibility and $w_i$ are weights that depend on its eigenvectors. It is clear from the last formula that when $\lambda_i = -\frac{2}{\beta \sigma^2} < 0$, the compressibility can diverge leading to a phase separation. We have checked numerically that the lowest eigenvalue of the charge susceptibility reaches indeed this critical value at a critical value of $U$ for a fixed temperature [10]. Close enough to the phase transition Eq. (2) can be approximated to its first contribution $i = 0$ and reads:

$$\kappa = \chi_c(q = 0, \omega = 0) \sim \frac{\chi_{0}^{\text{eff}}}{1 + U_{\text{eff}} \chi_{0}^{\text{eff}}},$$

where $U_{\text{eff}} = \beta \sigma^2 / 2 w_0 < 0$ and $\chi_{0}^{\text{eff}} = \lambda_0 w_0 > 0$. Interestingly, the RPA-like formula that we found it is valid only for $q = 0$ and therefore, we found that a strong repulsion leads to an attractive one only in specific physical sectors.

Given the substantial progress that we have achieved in developing several missing pieces of the theory, we are confident that in the last month of the ESI-JRF we will make progress in the study of the dimensional crossover as well.

Eventually, during my staying at the ESI, I have also achieved important results in another research field that were reported in [11]. Hence, the "Erwin Schrödinger International Institute for Mathematics and Physics, University of Vienna" has been included as an additional affiliation also in this case.

References


Sebastian Falkner: Heterogeneous cavitation on graphitic surfaces in a Lennard-Jones fluid and water at negative pressures

Sebastian Falkner (Goethe University of Frankfurt): August 1 – November 30, 2020:

Report

During my stay at the Erwin Schrödinger International Institute I focused on the estimation of state-dependent diffusion constants and free energies for nucleation processes using Bayesian trajectory analysis. The process of nucleation is omnipresent in a broad range of active research areas such as cell biology, engineering and climate forecast. It is often described using the classical nucleation theory where a phase transition is assumed to occur by the formation and subsequent growth of a nucleus. The growth of the initial nucleus is first hindered by a free energy barrier. After passing the critical nucleus size at the top of the barrier, the transition to the new phase is favoured.

In previous studies, Kramers’ model of diffusive barrier crossing has been used to describe the stochastic nature of nucleation processes in combination with the classical nucleation theory [1,2]. In this model, the dynamics of a many-body system are described as a diffusive process on a one-dimensional reaction coordinate. The free energy along this coordinate and the position-dependent diffusion coefficient determine the behaviour of a system in Kramers’ model. Therefore, an accurate prediction of these two functions is crucial to describe barrier crossing in the framework of the classical nucleation theory.

While numerous methods to estimate free energies along a reaction coordinate were being developed, the calculation of state-dependent diffusion coefficients remained a challenging problem. Hummer [3] introduced a novel method to determine state-dependent diffusion coefficients from trajectories using a Bayesian approach. Here, a rate matrix is constructed describing the dynamics on a discretized periodic reaction coordinate. Hummer proposed an optimization
scheme based on the likelihood of observing a rate matrix given existing trajectory data. Based on the optimized rate matrix, free energies and state-dependent diffusion coefficients can be estimated. Innerbichler and coworkers applied the method to understand water cavitation at negative pressures. In the same study, they adjusted the method for absorbing boundary conditions with a non-periodic reaction coordinate.

A major drawback of the Bayesian analysis is the computational cost which scales cubically with the number of bins used to discretize the reaction coordinate. The main contribution to the overall cost can be traced to the evaluation of a matrix exponential in the optimization procedure.

During my stay, I established a Python-based library to efficiently estimate free energies and position-dependent diffusion coefficients from trajectories. The implementation of the quasi-Newton optimizer L-BFGS-B with an analytical log-likelihood gradient calculation resulted in a significant performance increase. After initial tests, the program was used to estimate diffusion coefficients and free energies for ice nucleation in an ongoing collaboration.

As my stay took place amid the COVID-19 pandemic, restrictions on contacts and travel complicated the organization of the stay. Nevertheless, the support coming from the ESI was exceptional and enabled research even in these difficult times. Therefore, I would like to thank the whole team at the ESI for their great work. Moreover, I would like to thank Prof. Dr. Christoph Dellago for our great discussions and his advice during my stay.

References


Aliaksandr Hancharuk: Higher Gauge Theories

Aliaksandr Hancharuk (U Lyon): August 24 – September 25, 2020:

Report

The project was dedicated to the study of the Lie algebroid Yang-Mills (LAYM) gauge theories. These can be understood as a generalization of Yang-Mills gauge theories, replacing the structural Lie algebra by a Lie algebroid E. The problem we addressed is a construction of B(F)V formulation of such theories.

During my stay at the ESI I studied different toy models inspired by the LAYM gauge theories and constructed BV and BFV formulations under simplifying assumptions. Namely, I considered two dimensional theory, which is the Poisson Sigma Model added with the non-Casimir hamiltonian as well as mechanical models grasping the essential symmetries of the LAYM theory. To perform the task one needs to consider Hamiltonian formulation of the theory and identify all the constraints. It turns out that the models in question have mixed (first and second
class) constraints and under the assumption of vanishing basic curvature $\xi^E$ of the Lie algebroid we employed the results of Fisch-Henneaux [3],[4] and immediately found the result. To solve the general problem, some further work is required.

I would like to thank Prof. Thomas Strobl for useful discussions during the Junior Research Fellowship. I also benefited from the ESI thematic programme on ”Higher Structures and Field Theory” held from August 3 to September 25, 2020.

References


Publications and preprints contributed

Currently in preparation

Alexander Evetts: Combinatorial group theory and formal languages

Alexander Evetts (Heriot-Watt University, Edinburgh): October 14 – December 18, 2020:

Report

My work during my stay at the ESI revolved around the following topics.

Sofic groups and the word problem

A finitely generated group $G$ is said to be sofic if for all $n > 0$, there is some number $k_n$, and a map $\phi: B_G(n) \to \text{Sym}(k_n)$ such that $\phi$ is almost a homomorphism, and uniformly injective, with respect to the normalised Hamming distance on the symmetric group $\text{Sym}(k_n)$. We think of this as approximating the group $G$ by finite groups. It is an important open question whether or not there exist non-sofic groups. A group is said to be locally embeddable into finite groups, or LEF, if for each finite subset $A$ of $G$, there exists an injective partial homomorphism (a.k.a. a local embedding) from $A$ to some finite group $H_A$. LEF groups are clearly sofic.

The co-language (or word problem) of a finitely generated group is the language of all words over the generators which represent the identity element. It is a standard fact that the co-language of a group is regular (i.e. accepted by a finite state automaton) if and only if the group is finite.
With this fact in mind, it is natural to conjecture that a group is sofic if its co-language can be approximated by regular languages, although it is not clear exactly what should be meant by an approximation to a language here. In work began with Goulnara Arzhantseva (University of Vienna), we investigated possible notions of what it means for a language to be approximated by regular languages. We noted that LEF groups can be characterised by a language-theoretic condition on their co-languages. Namely, a group $G$ is LEF precisely when there exists a sequence of regular co-languages which converges to the co-language of $G$ (with an appropriate definition of convergence of languages). We hope to generalise this notion in the direction of soficity by relaxing the definition of convergence of languages.

**Product set growth**

For a finitely generated group $G$, with finite subset $U$, let $U^n = \{u_1u_2\cdots u_n \mid u_i \in U\}$. The product set growth of $U$ in $G$ is the function $|U^n|$, which counts the number of group elements expressible with words of length $n$ in $U^*$. Establishing asymptotic properties of this function has been the subject of much recent work. For example, Delzant and Steenbock [3] recently proved that if $G$ is hyperbolic, there is a constant $\alpha > 0$ such that for each $U$ that is not contained in a virtually cyclic subgroup, we have

$$|U^n| \geq (\alpha|U|)^{\left\lceil \frac{n+1}{2} \right\rceil},$$

where the square brackets denote the integer part.

In discussion with Markus Steenbock (University of Vienna), we proposed studying the generating function, or Poincaré series, associated to $|U^n|$. That is, the formal power series

$$S_{G,U}(z) = \sum_{n=0}^{\infty} |U^n|z^n \in \mathbb{Z}[[z]].$$

This is analogous to the well-established study of the generating function associated with the word growth of a finitely generated group. In this latter case, it was proved by Cannon [1] that for a hyperbolic group, the series is always a rational function. We studied Cannon’s proof, which uses cone-types and regular languages, with the aim of using similar ideas to approach $S_{G,U}(z)$ for hyperbolic groups. In fact, this is a challenging question, even the cyclic group.

We proved that if $U \subset \mathbb{Z}$ is any subset consisting of two elements, then the series $S_{\mathbb{Z},U}(z)$ is a rational function.

**Equations in groups**

Let $G$ be a group and $V$ some finite set of variables. An equation over $G$ is an element $w$ of the free product $G \ast F_V$, where $F_V$ is the free group on $V$. A solution to such an equation is an assignment of group elements to variables so that the word $w$ evaluates to the identity. More formally, a solution is a homomorphism $\phi: G \ast F_V \to G$ which fixes every element of $G$ and satisfies $\phi(w) = 1_G$. Two questions are interesting: firstly, for a given group, is there an algorithm to decide whether or not an equation has a solution? This is known as the equation problem, of the diophantine problem. Secondly, can we describe the set of all solutions to a given equation (or system of equations) in some group?

In foundational work, Makanin [4] proved that the equation problem is decidable in free groups, and Razborov [5] described the corresponding sets of solutions. More recently, it has been shown that the solution sets to equations in free groups, virtually free groups, right-angled artin
groups, and hyperbolic groups can be represented as EDT0L languages over a finite generating set (a specific subclass of indexed languages). See, for example, Ciobanu-Diekert-Elder [2].

During my time at ESI, I was able to complete the bulk of joint work with Alex Levine (Heriot-Watt University, UK), proving that the solution sets to systems of equations in virtually abelian groups are EDT0L languages, and that these sets have rational growth series [6]. I also spent time progressing a project addressing the same issue in the class of soluble Baumslag-Solitar groups $BS(1,k)$. This is joint work with Graham Campbell, Andrew Duncan, Sarah Rees (all University of Newcastle, UK) and Derek Holt (University of Warwick, UK).

References


Publications and preprints contributed

Seminars and colloquia outside main programmes and workshops

196 seminar and colloquia talks have taken place at the ESI in 2020 including the following individual lecture series.

Simon Lentner (U Hamburg): Lecture Series on “Towards a derived Topological Field Theory” held online on the following dates: 2020 11 09, Part 1, 2020 11 12, Part 2, 2020 11 16, Part 3, 2020 11 19, Part 4. This Lecture Series was organized by Nils Charqueville of the Faculty of Physics of the University of Vienna.
ESI Research Documentation

ESI research in 2020: publications and arXiv preprints

THEMATIC PROGRAMMES

Higher Structures and Field Theory (AFZ)


R. R. Suszek, *The higher-algebraic skeleton of the superstring – a case study* [arXiv:2102.08202] [hep-th].


WORKSHOPS

Mathematical Aspects of Geophysical Flows (CH)


RESEARCH IN TEAMS (RIT)


SENIOR RESEARCH FELLOWS PROGRAMME (SRF)


JUNIOR RESEARCH FELLOWS PROGRAMME (JRF)


ESI research in previous years: additional publications and arXiv preprints

The following papers and publications complement the ESI publications already taken into account in the previous years. The following codes indicate the association of publications and preprints with specific ESI activities:

CBS = Geometry and Relativity, 2017
CFG = Higher Spins and Holography, 2019
CMF = Advances in Chemical Reaction Network, 2018
IS = Individual Scientists
JAF = Geometric Transport Equations in General Relativity, 2017
JRF = Junior Research Fellows
KTF = Polarons in the 21st Century, 2019
LCW = Quantum Simulation, 2019
PDG = Tractability of High Dimensional Problems and Discrepancy, 2017
PSH = Numerical Analysis of Complex PDE Models in the Sciences, 2018
RFZ = New Trends in the Variational Modeling and Simulation of Liquid Crystals, 2019
RIT = Research in Teams
SRF = Senior Research Fellow


G. Di Fratta, A. Fiorenza, V. Slastikov, On symmetry of energy minimizing harmonic-type maps on cylindrical surfaces. [CVGMT preprint 5038] RFZ.


List of all visitors in 2020

A total of 176 scientists visited the ESI in 2020.

The gender distribution is as follows:
- female: 25
- male: 126
- non-binary: 2
- unspecified: 23

Affiliation by country:
- AUS, Australia: 1
- AUT, Austria: 88
- BEL, Belgium: 3
- BLR, Belarus: 1
- BGR, Bulgaria: 1
- HRV, Croatia: 6
- CZE, Czech Republic: 3
- DNK, Denmark: 1
- FRA, France: 8
- DEU, Germany: 14
- HUN, Hungary: 4
- IND, India: 2
- IRN, Iran: 1
- IRL, Ireland: 3
- ISR, Israel: 1
- ITA, Italy: 2
- JPN, Japan: 2
- NLD, Netherlands: 2
- NOR, Norway: 1
- POL, Poland: 1
- ROU, Romania: 2
- RUS, Russian Federation: 1
- SVK, Slovakia: 2
- SVN, Slovenia: 1
- ESP, Spain: 1
- SWE, Sweden: 2
- CHE, Switzerland: 10
- GBR, United Kingdom of Great Britain and Northern Ireland: 8
- USA, United States of America: 5
The following codes indicate the association of visitors with specific ESI activities:

AFZ = Higher Structure and Field Theory
CH = Mathematical Aspects of Geophysical Flows
DAP = VDS-ESI Winter School: Machine Learning in Physics
IS = Individual Scientists
JRF = Junior Research Fellow
RIT = Research in Teams
SRF = Senior Research Fellows

Abbara Alia, ENS Paris; 2020-02-09 - 2020-02-12, DAP20
Abrashkin Anatoly, HSE, Nizhny Novgorod; 2020-01-18 - 2020-01-25, CH20
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Vyvlecka Michal, U Vienna; 2020-02-10 - 2020-02-18, DAP20
Waltenberger Wolfgang, HEPHY Vienna; 2020-02-19 - 2020-02-19, DAP20
Wautischer Gregor, U Vienna; 2020-02-10 - 2020-02-20, DAP20
Wen Jin, U Vienna; 2020-02-10 - 2020-02-20, DAP20
Westermayr Julia, U Vienna; 2020-02-10 - 2020-02-14, DAP20
Winkler Klemens, U Vienna; 2020-02-10 - 2020-02-20, DAP20
Wirsberger Peter, DeepMind, London; 2020-02-13 - 2020-02-15, DAP20
Wirtitsch Daniel, U Vienna; 2020-02-10 - 2020-02-20, DAP20
Zagler Georg, U Vienna; 2020-02-10 - 2020-02-14, DAP20
Zhang Tiantian, TU Vienna; 2020-02-10 - 2020-02-14, DAP20
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