Departments of Software Engineering and Mathematics
FNSPE CTU in Prague, Czech Republic

Student workshop on scientific computing 2024

May 30 - June 2, 2024. Děčín

Conference Information

The international scientific colloquium is organized by the Faculty of Nuclear Sciences and Physical Engineering of the Czech Technical University in Prague on annual basis. It is devoted to the meeting of students and young applied mathematicians dealing with numerical solution of partial differential equations, mathematical modelling, numerical simulation of problems in technology, environment, biology and computer science.

Organizers

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Conference office

I. Kukalová, Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague

Organizing committee

R. Fučík, K. Horaisová, P. Pauš, T. Oberhuber, J. Mikyška, P. Strachota, P. Eichler

Additional information

URL: `http://mmg.fjfi.cvut.cz/wsc2024`
Venue: Faculty of Nuclear Sciences and Physical Engineering,
Pohraniční 1288/1, 405 02 Děčín
and MS Teams online

Acknowledgement

This workshop was supported by the Grant Agency of the Czech Technical University in Prague, grant No. SVK 26/24/14.

List of Participants

The list of all participants in alphabetical order.

Name	University / Institute	
Michal Beneš	FNSPE CTU in Prague	
Arkadiusz Czader	AGH	Student
Pavel Eichler	FNSPE CTU in Prague	
Petr Filip	FNSPE CTU in Prague	Student
Radek Fučík	FNSPE CTU in Prague	
František Gašpar	FNSPE CTU in Prague	Student
František Hájek	Institute of Physics, Czech Academy of Sciences	Invited
Tomáš Halada	FME CTU in Prague	Student
Kateřina Horaisová	FNSPE CTU in Prague	
Dominik Horák	FNSPE CTU in Prague	Student
Lenka Horvátová	FNSPE CTU in Prague	Student
Kryštof Jakůbek	FNSPE CTU in Prague	Student
Vladimír Jarý	FNSPE CTU in Prague, CERN	
Jakub Klinkovský	FNSPE CTU in Prague	
Miroslav Kolář	FNSPE CTU in Prague	
Jaromír Kukal	FNSPE CTU in Prague	
Dana Majerová	FNSPE CTU in Prague	
Ondřej Marek	FNSPE CTU in Prague	Student
Jiří Mikyška	FNSPE CTU in Prague	
Maneesh Narayanan	FNSPE CTU in Prague	Student
Tomáš Oberhuber	FNSPE CTU in Prague	
Petr Pauš	FNSPE CTU in Prague	
Matěj Pokorný	FNSPE CTU in Prague	Student
Neda Bagheri Renani	Comenius University	Student
Aaron Schick	FNSPE CTU in Prague	Student
Richard Schlösinger	FNSPE CTU in Prague	Student, Poster
Jakub Solovský	FNSPE CTU in Prague / RERI	
Martin Srnec	J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences	Invited
Pavel Strachota	FNSPE CTU in Prague	
Robert Straka	AGH - USF	Invited
Daniel Ševčovič	Comenius University	

Adam Štampach	FNSPE CTU in Prague	Student
Jan Thiele	FNSPE CTU in Prague	Student, Poster
Dalibor Trampota	FNSPE CTU in Prague	Student
Quang Van Tran	FNSPE CTU in Prague	
Cyril Izuchukwu Udeani	Comenius University in Bratislava	
Nichita Vatamaniuc	FNSPE CTU in Prague	Student
František Voldřich	FNSPE CTU in Prague	Student
Filip Voženílek	FNSPE CTU in Prague	Student
Aleš Wodecki	FEL CTU in Prague	Invited
Serhii Yaskovets	TU Dresden, Max Planck Institute of Molecular Cell Biology and Genetics	Invited

Scientific Programme

Conference venue:

The conference venue: **the main building of CTU at Pohraniční street, 1288/1**
or
Online: MS Teams

Registration for local participants:

Registration for local participants takes place at the conference venue:
Thursday: from 13:00 to 14:00
+ during coffee breaks between the sessions

Invited talks

Invited oral presentation duration is 30 min = 25 min talk + 5 min for discussion.

Regular talks

Oral presentation duration is 20 min = 15 min talk + 5 min for discussion.

Thursday, May 30

13:00 – 14:00 *Registration of participants*

14:00 – 14:10 *Opening ceremony by Michal Beneš*

Chairman: Petr Pauš

14:10 – 14:40 **František Hájek**: Numerical solutions of practical problems in semiconductor research

14:40 – 15:00 **Pavel Eichler**: Quantum qubit state and Schrödinger equation

15:00 – 15:20 **Maneesh Narayanan**: Computational Studies of Space Curve Dynamics

15:20 – 15:40 *Coffee + tea + snacks*

Chairman: Miroslav Kolář

15:40 – 16:00 **Miroslav Kolář**: Diffusion and transport mechanism on moving space curves

16:00 – 16:20 **Lenka Horvátová**: Mathematical modeling of contrast agent transport in vascular bed with transfer to surrounding tissue in myocardial perfusion problems in 3D

16:20 – 16:40 **Jakub Solovský**: Numerical optimization of Neumann boundary condition for thermal lens construction

16:40 – 17:00 **Dominik Horák**: Mathematical modeling of non-isothermal turbulent flow around obstacles using the lattice Boltzmann method

17:30 – 19:00 *Football game at nearby Mariánská louka (weather permitting). Tentative group departure at 17:25 from the Castle grange.*

Friday, May 31

08:00 – 09:00 *Breakfast at the venue*

Chairman: Pavel Eichler

09:00 – 09:20 **František Gašpar**: Fractal Diffusion Modelling Using Constraint Convolution Schema

09:20 – 09:40 **Pavel Strachota**: DEM Simulations of Settling of Spherical Particles using a Soft Contact Model and Adaptive Time Stepping

09:40 – 10:00 **Ondřej Marek**: Mathematical modelling of compressible two-dimensional fluid flow using lattice Boltzmann method

10:00 – 10:20 **Jakub Klinkovský**: Modern data formats for visualization: Adiós, VTK?

10:20 – 10:40 *Coffee + tea + snacks*

Chairman: Tomáš Oberhuber

10:40 – 11:00 **Daniel Ševčovič**: Multidimensional linear and nonlinear partial integro-differential equation in Bessel potential spaces

11:00 – 11:20 **Vladimír Jarý**: Development of the Triggerless Data Acquisition System for the AMBER experiment

11:20 – 11:50 **Serhii Yaskovets**: OpenFPM: scalable open-source C++ framework for particle and particle-mesh codes on parallel computers.

11:50 – 12:00 *Group photo*

12:00 – 14:00 *Lunch break*

Chairman: Radek Fučík

14:00 – 14:30 **Martin Srnec**: Non-traditional concepts in chemical reactivity

14:30 – 14:50 **Robert Straka**: Bloody LBM: bypass grafts simulation tool

14:50 – 15:10 **Jaromír Kukal**: Anomalous Diffusion Coefficient via Simple Particle Hopping Analysis

15:10 – 15:30 *Coffee + tea + snacks*

Chairman: Jiří Mikyška

15:30 – 16:00 **Aleš Wodecki**: Globally convergent optimization methods: polynomial optimization and beyond

16:00 – 16:20 **František Voldřich**: On Board Telemetry Anomaly Detection using Machine Learning

16:20 – 16:40 **Tomáš Halada**: TNL-SPH: A way to implement particle methods

16:40 – 16:50 *Hiking excursion information*

18:00 – 21:00 *Conference social event + + at the conference venue (+ poster session)*

Saturday, June 1

08:00 – 09:00 *Breakfast at the venue*

Chairman: Jakub Klinkovský

09:00 – 09:20 **Neda Bagheri Renani**: A Comparison Study of ADI and ADE Methods of the Black-Scholes equation on option pricing models

09:20 – 09:40 **Arkadiusz Czader**: Air chamber shape optimization using lattice Boltzmann method

09:40 – 10:00 **Petr Filip**: Curve Dynamics in Plane and Space and Its Applications

10:00 – 10:20 *Coffee + tea + snacks*

Chairman: Pavel Strachota

10:20 – 10:40 **Matěj Pokorný**: Local and Global Image Texture Invariants

10:40 – 11:00 **Aaron Schick**: Image processing by diffusive PDEs and Sobolev gradients

11:00 – 11:20 **Adam Štampach**: Analysis of materials structure by image processing methods based on machine learning

11:20 – 11:30 *update on hiking excursion*

11:30 – 14:00 *Lunch break*

14:00 – 18:00 *Hiking Excursion - Original plans cancelled due to weather and slippery conditions. Alternative plan: Děčín Zoo map. Departure from the venue at 14:00, trip leader Dana Majerová!*

Sunday, June 2

08:00 – 09:00 *Breakfast at the venue*

Chairman: Dana Majerová

09:00 – 09:20 **Quang Van Tran**: Unconditional and conditional heavy-tailed distributions for returns of cryptocurrencies

09:20 – 09:40 **Nichita Vatamaniuc**: Machine Learning for Musculoskeletal Disorders Classification

09:40 – 10:00 **Cyril Izuchukwu Udeani**: Learning the Solution operator of HJB equation using deep learning

10:00 – 10:20 **Filip Voženílek**: Overview: Qualitative Theory of Ordinary Differential Equations

10:20 – 10:40 *Coffee + tea + snacks*

Chairman: Kateřina Horaisová

10:40 – 11:00 **Dalibor Trampota**: Computer graphics using WebGL and voxel engine

11:00 – 11:20 **Richard Schlösinger**: Inclinations of the orbital planes of recaptured, previously perpendicularly ejected planets

11:20 – 11:40 **Kryštof Jakůbek**: Efficient numerical solution to the two dimensional Stefan problem

11:40 – 11:50 *Closing ceremony*

List of Abstracts

The list of abstracts of all talks and posters in alphabetical order.

Air chamber shape optimization using lattice Boltzmann method

Arkadiusz Czader
AGH

Saturday, June 1, 09:20 – 09:40

The project focuses on optimizing the shape of a 2D air chamber using velocity field obtained from LBM simulations. The goal is to develop a code that finds the optimal chamber shape regarding equal velocity distribution. Due to the large computational domain, finding the optimal shape for most optimization functions is time-consuming. To address this, several methods for identifying potentially profitable changes were implemented. The code allows simple change of optimized functions and optimization constraints.

Artificial Neural Networks for a nonlinear System of Mosquito Epidemic Model through Levenberg Marqduardt Computing Technique

Dr Tahir Nawaz Cheema
Pakistan Model Higher Secondary School for girls Saroke Cheema Wazirabad

The present novel study was directed to analyse the transmission dynamics of Mosquitos in human population. The system of ordinary differential equations and a real dataset were studied with the help of Artificial Neural Networks Levenberg Marqduardt Back Propagation.A dynamic system will be used to determine the solution with different aspects of the physical compatibility of the default values to be examined and developed from time to time. The testing, performance and validation process are exploited.Numerical experiments are performed for very fast phrases and the prolonged evolution of a stable state for individual parameters, which are rarely proved in the counterpart of the integer order.System control is validated by assessing accuracy obtained by mean square error,

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evolution of a stable state for individual parameters, which are rarely proved in the counterpart of the integer order.System control is validated by assessing accuracy obtained by mean square error,

Quantum qubit state and Schrödinger equation

Pavel Eichler
FNSPE CTU in Prague

Thursday, May 30, 14:40 – 15:00

This contribution introduces you to the basics of quantum computing problematics. In this context, one of the currently investigated problems is the preparation of the initial state of quantum qubit and accurate operation with its states. Instead of amazing new results, open questions will be discussed and our plans for the future will be presented. Finally, you can look forward to LBM in a quantum context as well.

Curve Dynamics in Plane and Space and Its Applications

Petr Filip
FNSPE CTU in Prague

Saturday, June 1, 09:40 – 10:00

This contribution will discuss theoretical and computational behavior of curves moving by curvature in the normal direction in plane and space. The motion will be solved numerically using the parametric approach and finite difference method. The natural and asymptotically uniform redistribution of points along the curve will be compared in various examples of solution in the plane and in generalized form in space.

Radek Fučík
FNSPE CTU in Prague

Fractal Diffusion Modelling Using Constraint Convolution Schema

František Gašpar, Jaromír Kukal
FNSPE CTU in Prague, FNSPE CTU in Prague

Friday, May 31, 09:00 – 09:20

A novel constrained convolution schema (CCS) is introduced as a robust alternative to Monte Carlo simulations for diffusive processes over fractal sets. Unlike stochastic methods, CCS is a deterministic numerical algorithm tailored for grid-based set models, including random sets, ensuring reproducibility and computational efficiency. CCS is designed to yield the complete distribution of diffusion processes within a specified timeframe, offering comprehensive insights into the dynamics of diffusion phenomena. This contribution not only outlines the theoretical framework of CCS but

also provides illustrative examples demonstrating its applicability across a diverse range of fractal sets. Through its deterministic nature and versatility, CCS emerges as a valuable tool for exploring diffusion phenomena in complex systems with enhanced precision and computational tractability.

Numerical solutions of practical problems in semiconductor research

František Hájek, Filip Dominec
Institute of Physics, Czech Academy of Sciences, Institute of Physics, Czech Academy of Sciences

Thursday, May 30, 14:10 – 14:40

Semiconductor research produce large amount of data which need further processing by numerical methods. Once evaluated, these large datasets can serve also as a potential input for machine learning processes aiming to speed up the development of desired semiconductor devices. In this talk, I would like to provide an overview of topics involving numerical modelling which have been dealt with in the past years at Department of Semiconductors, Institute of Physics, CAS. The research has been focused on development of nitride-based scintillators for fast-timing application. Outcomes of the experimental characterization of these devices often need a numerical processing like image recognition, image overlay methods or filtering and fitting of spectral maps. Approaches to these tasks will be introduced.
Machine learning algorithms were also used to design device with optimal performance and the results will be shown.

TNL-SPH: A way to implement particle methods

Tomáš Halada, Tomáš Oberhuber, Jakub Klinkovský
FME CTU in Prague, FNSPE CTU in Prague

Friday, May 31, 16:20 – 16:40

Particle methods for solution of partial differential equations are an effective tool for a number of problems where the mesh based methods are difficult to employ. This includes for example free surface flows or problem with moving boundaries. We present a parallel GPU implementation of structures for particle computations, a general particle solver and implementation of SPH method and mesh-free finite difference methods for fluid dynamics problems. The tools are implemented as a submodule of the TNL library: TNL-SPH. Implementation of particle methods brings a number of challenges related to a neighbor search procedures or domain decomposition. We present our solution to these problems along with a tool for easy implementation of numerical schemes of particle methods or particle methods in general.

Mathematical modeling of non-isothermal turbulent flow around obstacles using the lattice Boltzmann method

Dominik Horák
FNSPE CTU in Prague

Thursday, May 30, 16:40 – 17:00

The work deals with the mathematical modeling of non-isothermal turbulent flow of incompressible Newtonian fluids. The aim of the work is to implement and test heat transfer and investigate usage of coupled LBM-LBM scheme for solving Navier-Stokes equations and advection-diffusion equation. In the theoretical part, the mathematical model of non-isothermal flow of Newtonian fluids is presented together with the description of turbulent flow. In the second part, the reader is introduced to the lattice Boltzmann method (LBM), and the last part discusses the results of the application of LBM with implemented heat transfer to the mathematical model. The implementation of heat transfer was successful, and the method produces satisfactory results.

Mathematical modeling of contrast agent transport in vascular bed with transfer to surrounding tissue in myocardial perfusion problems in 3D

Lenka Horvátová
FNSPE CTU in Prague

Thursday, May 30, 16:00 – 16:20

This research project deals with mathematical modeling of problems arising during myocardial perfusion using the contrast agent. The description of the transport and transfer of the contrast agent from vascular bed to extravascular medium is divided into two tasks. First, the velocity in the vascular system is computed based on pressures. Then, a contrast agent with a given concentration is injected into the vascular system. The transfer of the contrast agent from the vascular system to the extravascular system is modeled using convolution with the Dirac delta function. In the second step, the concentration in both media is calculated. For this mathematical model, we consider an incompressible Newtonian fluid that is not subject to any external forces. The extravascular environment is considered to be porous and rigid. The main goal of this project is to solve the problem of transport and transfer of contrast agent in the vascular system of healthy and unhealthy myocardium using the finite volume method, and in the extravascular medium using the finite difference method.

Grafické webové rozhraní pro nastavení systému pro sběr dat pro experiment AMBER

Jozef Hrdý
FNSPE CTU in Prague

This work focused on the development of an existing web application containing the identification of application shortcomings in the frontend and backend, analysis of possible solutions and final practical implementation. Use of frontend framework, responsive interface layout and appearance modernization. Overall code maintenance and MVC architecture implementation.

Efficient numerical solution to the two dimensional Stefan problem

Kryštof Jakůbek
FNSPE CTU in Prague

Sunday, June 2, 11:20 – 11:40

We introduce the Allen-Cahn equation, describing phase transition in undercooled media, as a method for solving the Stefan problem. Finite difference discretization in two dimensions is performed and the resulting problem is formulated as an explicit and semi-implicit numerical scheme. Subsequently, we investigate errors caused by the operator splitting technique and propose two potential corrections. Finally, we discuss the CUDA implementation and explain several optimized parallel algorithms employed.

Development of the Triggerless Data Acquisition System for the AMBER experiment

Vladimír Jarý, Martin Zemko, Jan Vondruška, Jozef Hrdý
FNSPE CTU in Prague, CERN, FNSPE CTU in Prague, CERN

Friday, May 31, 11:00 – 11:20

Nowadays, the modern experiments in the particle physics heavily rely on the efficient data acquisition systems (DAQ). In this contribution we will focus on the DAQ of the AMBER experiment at CERN laboratory. At first, we will briefly introduce the scientific program of the experiment. Then we will describe the traditional architecture of the DAQ systems that strongly depend on the trigger subsystem that selects potential event candidates in high rate, distributed network environment almost in real time. We will analyze disadvantages of such systems which will lead us to proposal of the triggerless DAQ in which the filtering logic is moved to the higher levels (the high level trigger HLT). This allows development of more sophisticated filtering algorithms that in turn select more appropriate event candidates. We will discuss the design and current status of the implementation of this system in the context of the AMBER experiment.

We conclude the contribution with presentation of plans of future upgrades of the system that include several opportunities for students of Bachelor's and Master's degree courses at out faculty.

Modern data formats for visualization: Adiós, VTK?

Jakub Klinkovský
FNSPE CTU in Prague

Friday, May 31, 10:00 – 10:20

Scientific visualization in our research group is mostly based on the traditional VTK file formats. However, these formats are not flexible and cause bottlenecks in high-performance applications operating on large datasets. In this talk, we summarize our progress towards using the ADIOS2 library, a unified, MPI-based and streaming-oriented high-performance I/O framework, for managing data output in the TNL-LBM project.

Diffusion and transport mechanism on moving space curves

Miroslav Kolář
FNSPE CTU in Prague

Thursday, May 30, 15:40 – 16:00

We discuss the motion of closed non-intersecting space curves driven by curvature in binormal and normal directions coupled with advection-diffusion equation for a scalar quantity defined on a curve. We formulate the general motion law in space in binormal and normal directions by curvature and mention some known analytical properties. The finite-volume scheme allows us to solve both the advection-diffusion problem defined on the curve as well as the motion of the curve itself. The numerical scheme is stabilized by the tangential velocity redistributing discretization nodes. We demonstrate the behavior of the solution on several computational studies combining the motion in normal and binormal velocity with the evolution of the scalar quantity.

Anomalous Diffusion Coefficient via Simple Particle Hopping Analysis

Jaromír Kukal, Michal Beneš
FNSPE CTU in Prague, FNSPE CTU in Prague

Friday, May 31, 14:50 – 15:10

One-dimensional partice hopping with constrained variance is a well known model of Brownian motion and therefore the traditional particle diffusion. Model analysis is possible using the Central Limit Theorem (CLT) which produces Einstein formula. Another strategies of heavy tile hopping with discrete Pareto distribution can be studied by the Generalized CLT (GCLT).
Doing the same using only Fourier transform and l'Hospital rule without CLT or GCLT is the main subject of presentation.

Mathematical modelling of compressible two-dimensional fluid flow using lattice Boltzmann method

Ondřej Marek
FNSPE CTU in Prague, FNSPE CTU in Prague

Friday, May 31, 09:40 – 10:00

This contribution discusses the application of lattice Boltzmann method (LBM) on compressible fluid flow in two dimensions. First, a brief introduction to fluid dynamics and weakly compressible LBM is given. Subsequently, possible extensions of LBM to compressible fluid flow are covered with focus on entropic LBM models for which an analytical single-speed model D2Q9 is derived and Newton method for model D2Q49 is formulated. Finally, both models are verified on the problem of Poiseuille flow in 2D and demostrated on fluid flow in a channel with an obstacle.

Computational Studies of Space Curve Dynamics

Maneesh Narayanan, Michal benes
FNSPE CTU in Prague, Czech Technical University

Thursday, May 30, 15:00 – 15:20

This paper presents a computational investigation into the dynamics of space curves, utilizing parametric method and flowing finite volume techniques. The parametric approach is employed to solve the equations governing the curves,

$$\partial_t X = \alpha T + \beta N + \gamma B + F, \qquad X(0) = X_0 \tag{4.1}$$

with a focus on discretization. The evolution equation is then solved using the method of lines. To mitigate instability issues inherent in the computation process, both natural redistribution and uniform redistribution techniques are implemented.
Furthermore, the study introduces a special force term to examine its effect on curve dynamics. By integrating this term into the computational framework, we explore its impact on the behaviour and shape evolution of space curves. Through these computational methodologies and techniques, this research contributes to a deeper understanding of space curve dynamics, offering insights into their behaviour under various conditions and the influence of external forces.

Local and Global Image Texture Invariants

Matěj Pokorný
FNSPE CTU in Prague

Saturday, June 1, 10:20 – 10:40

Texture-based analysis of two- and three-dimensional images is a field of immense importance, which keeps rising every year, especially because of the need for fast and reliable analysis of biomedical imaging data. The Fourier transform-based approaches are useful, when we want to compute rotationally invariant image features. We introduce a fast method of producing local translationally-rotationally-mirroring (TRM) invariant local image features through the frequency domain convolution of orthonormal Zernike polynomials with two- or three-dimensional images. In a direct continuation, we also define the global statistical characteristics that will act as textural image features and input data for various image classifiers.
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A Comparison Study of ADI and ADE Methods of the Black-Scholes equation on option pricing models

Neda Bagheri Renani
Comenius University

Saturday, June 1, 09:00 – 09:20

This study examines the pricing of options in marketing, focusing on two assets with risk and one asset without risk. The Black-Scholes model and European options applicable at the due date are utilized for this investigation. To determine the appropriate price for the European option, it is necessary to solve an equation with partial derivatives involving two spatial variables. Finite differences are employed for these equations. For one-dimensional equations, finite differences typically result in a three-diagonal set that can be solved with calculation costs O(n), where n is the number of discrete points. However, in this case, as the problems are two-dimensional, the

Alternating Direction Implicit (ADI) and Alternating Direction Explicit (ADE) methods are used to reduce calculation costs. These methods offer advantages at the discrete points level and demonstrate acceptable stability. Despite their equal ease of calculation, evaluating these methods in option pricing reveals that the ADI method is sensitive to discontinuity or non-derivability, which is a common property of income functions.

Image processing by diffusive PDEs and Sobolev gradients

Aaron Schick
FNSPE CTU in Prague
Saturday, June 1, 10:40 – 11:00

This work examines the use of diffusive PDEs for image processing, specifically the Allen-Cahn equation and its modification on rectangular domains. Namely, a segmentation model is presented, and we show its application to test cardiac MRI data. Additionally, the Sobolev gradient method is introduced in the context of the calculus of variations, and its properties are demonstrated in the numerical results.

Inclinations of the orbital planes of recaptured, previously perpendicularly ejected planets

Richard Schlösinger
FNSPE CTU in Prague
Sunday, June 2, 11:00 – 11:20

This work focuses on finding the conditions resulting in a celestial body, previously ejected perpendicularly to the galactic accretion disc from a solar system, being recaptured into an orbit, tilted 60 degrees to the accretion disc. Using simulations based on the laws of classical physics, if such recapture is proven possible, the work may provide one more way of explaining excessive inclinations of planetary systems to the galactic plane and the origin of planets orbiting greatly inclined to their system's plane of reference, like, for example, WASP 79b with its near-polar orbit around WASP 79.

Numerical optimization of Neumann boundary condition for thermal lens construction

Jakub Solovský, Aleš Wodecki, Monika Balázsová, Kateřina Škardová, Tomáš Oberhuber
FNSPE CTU in Prague / RERI
Thursday, May 30, 16:20 – 16:40

The refractive index of thermo-optic materials changes significantly with temperature. This property allows for a layer of material with a certain temperature profile to act as a lens with desired optical properties. The goal is to find the heat fluxes through the domain boundary that result in the given temperature profile at the given time while considering heat losses into the surrounding material.

We solve the PDE-constrained optimization problem using the gradient descent method. For the computation of the objective function gradient, we employ the approach based on solving the adjoint equation for Lagrange multipliers. Both the primary and adjoint problems are solved by the Mixed-Hybrid Finite Element Method with fully implicit discretization in time.
We demonstrate that the temperature profiles given by Zernike polynomials on a circular domain can be obtained.

Non-traditional concepts in chemical reactivity

Martin Srnec, Zuzanna Wojdyla, Jan Kovář, Radek Fučík Friday, May 31, 14:00 – 14:30
J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague

I will briefly introduce computational chemistry, a field that provides a unique perspective on the properties and reactivity of molecules. In my talk, I will then introduce some of our concepts and theoretical frameworks that aim to understand the physicochemical factors that determine the rate and selectivity of chemical reactions and enable reliable predictions.

DEM Simulations of Settling of Spherical Particles using a Soft Contact Model and Adaptive Time Stepping

Pavel Strachota Friday, May 31, 09:20 – 09:40
FNSPE CTU in Prague

We present a simple and flexible Discrete Element Method (DEM) model for simulating the dynamics of spherical particle systems. The aim is to utilize commonly available ODE integrators that are usually inappropriate for DEM, in particular the Runge-Kutta-Merson and Dormand-Prince solvers with adaptive time stepping. This is achieved by using a novel soft contact model with repulsive and frictional forces smoothly varying in time, which allows the time step adaptivity algorithms to work properly. The model parameters are calibrated so that a realistic random close packing can be obtained from simulations of particle settling at the bottom of a container. A reference minimal implementation in MATLAB and a complete implementation in C with OpenMP parallelization are introduced and their computational performance is assessed.

Bloody LBM: bypass grafts simulation tool

Robert Straka Friday, May 31, 14:30 – 14:50
AGH - USF

The assessment of volumetric blood flow in bypass grafts stands as a pivotal parameter indicative of the overall success of surgical intervention. In cases where blood flux diminishes significantly, the efficacy of the bypass may be compromised, potentially leading to failure. We present a novel bypass graft simulation tool (currently under development :). This tool comprises three integral

components: segmentation of X-ray coronary angiography, bypass graft planning, and simulation of blood flow, alongside an anastomosis optimization module. Our presentation deals primarily with the blood flow modeling aspect, which is performed by the Lattice Boltzmann Method. We conduct simulations on three scenarios involving the left coronary artery – healthy, stenosed and stenosed with a bypass – and verify our findings with those obtained from the SimVascular - a specialized software for medical image data segmentation and patient specific blood flow simulation and analysis.

Multidimensional linear and nonlinear partial integro-differential equation in Bessel potential spaces

Daniel Ševčovič, Cyril Udeani
Comenius University, Comenius University

Friday, May 31, 10:40 – 11:00

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In this talk we analyze solutions of a non-local nonlinear partial integro-differential equation (PIDE) in multidimensional spaces. Such class of PIDE often arises in financial modeling. We employ the theory of abstract semilinear parabolic equations in order to prove existence and uniqueness of solutions in the scale of Bessel potential spaces. We consider a wide class of Levy measures satisfying suitable growth conditions near the origin and infinity. The novelty consists in the generalization of already known results in the one space dimension to the multidimensional case. We consider Black-Scholes models for option pricing on underlying assets following a Levy stochastic process with jumps. As an application to option pricing in the one-dimensional space, we consider a general shift function arising from nonlinear option pricing models taking into account a large trader stock-trading strategy. We prove existence and uniqueness of a solution to the nonlinear PIDE in which the shift function may depend on a prescribed large investor stock-trading strategy function.

Analysis of materials structure by image processing methods based on machine learning

Adam Štampach, Pavel Strachota
FNSPE CTU in Prague, FNSPE CTU in Prague, Departments of Mathematics

Saturday, June 1, 11:00 – 11:20

This work focuses on the segmentation of microscopic images of cross-sections of zirconium fuel cladding of a nuclear reactor, on which high temperature experiments were conducted. These experiments result into changes in the internal structure of the zirconium. A thresholding method was used to segment the metal and oxide classes. A neural network was used to segment the alpha and beta classes. The training data set was created by a combination of specialized algorithms and manual interventions. To ensure the correct functioning of the model, appropriate data preprocessing algorithms were implemented, consisting of geometric transformation, brightness normalization and image subdivision into blocks. Three neural network models were trained and compared on the

created data set. After obtaining the resulting feature map, the quantitative characteristics of the examined sample were calculated, such as the minimum, maximum and average height of the oxide layer. The result of segmentation are documents containing these characteristics and a visual map of the segmented areas of the image.

Use of 3D printing for MRI phantom construction

Jan Thiele
FNSPE CTU in Prague

Magnetic Resonance Imaging (MRI) phantoms are crucial for calibrating, testing, and validating MRI systems and mathematical models. Traditional methods for constructing phantoms are time-consuming and inflexible. 3D printing provides a new way to create customizable and modular MRI phantoms efficiently. Our research focuses on designing and creating a modular MRI phantom frame and assessing the suitability of various 3D printing materials for building these phantoms.

Computer graphics using WebGL and voxel engine

Dalibor Trampota
FNSPE CTU in Prague

Sunday, June 2, 10:40 – 11:00

This work focuses on computer graphics, more precisely on the web using WebGL. The main goal is to explore the possibilities of WebGL and the Three.js library and create a voxel game similar to Minecraft.

Unconditional and conditional heavy-tailed distributions for returns of cryptocurrencies

Quang Van Tran
FNSPE CTU in Prague

Sunday, June 2, 09:00 – 09:20

We investigate which distribution is most appropriate for modeling returns of cryptocurrencies. We study distribution of both unconditional returns and conditional returns. Four well-known heavy-tailed distributions Generalized Normal, Student t-, Normal Inverse Gausian, Alpha stable and two recently suggested distributions and four GARCH models plain GARCH, range GARCH, TGARCH and EGARCH are studied. The results estimated for Bitcoin, Binance Coin, Ethereum, Solana and Ripple are unambiguous. For each cryptocurrency, the most appropriate distribution is the generalized normal distribution. This conclusion holds not only for returns, but also for conditional returns (residuals from a conditional mean model in the presence of heteroscedasticity), and for all considered volatility models. The most suitable GARCH model is the EGARCH model, and the range GARCH model performs very well in some cases.

Learning the Solution operator of HJB equation using deep learning

Cyril Izuchukwu Udeani, Daniel Sevcovic
Comenius University in Bratislava

Sunday, June 2, 09:40 – 10:00

This study focuses on approximating the solution operator of a fully nonlinear partial differential equation arising from finance using machine learning techniques. We consider a fully nonlinear Hamilton–Jacobi–Bellman (HJB) equation arising from the stochastic optimization problem, where the goal of an investor is to maximize the conditional expected value of the terminal utility of a portfolio. The value function of the nonlinear HJB equation describes the optimal portfolio selection strategy. The fully nonlinear HJB equation is first transformed into a quasilinear parabolic equation using the Ricatti transform. Then, the solution of the transformed quasilinear equation is approximated using deep learning. Our qualitative analysis shows that the solution operator of the associated HJB equation can effectively be learned using a deep learning approach.

Machine Learning for Musculoskeletal Disorders Classification

Nichita Vatamaniuc
FNSPE CTU in Prague

Sunday, June 2, 09:20 – 09:40

This contribution focuses on processing and classification of data gained from motion sensors applied to the human body which suffers from neurological disease that leads to musculoskeletal system disorders. The signal generated by human movement is then transformed into the frequency spectrum and used to get the power spectral features. The power spectral features are classified into two classes depending on whether the patient is healthy. The classification step is performed by different classification algorithms with performance comparison.

On Board Telemetry Anomaly Detection using Machine Learning

František Voldřich, O. Luschykov, O. Harwot
FNSPE CTU in Prague, Huld s.r.o.

Friday, May 31, 16:00 – 16:20

Anomaly detection has numerous applications across various fields, including the space industry. A spacecraft must continuously monitor the health of its subsystems to detect non-nominal situations, but transmitting all telemetry data to ground for analysis is not feasible due to limited transmission capacity and potential delays. Therefore, autonomous fault and anomaly detection is essential for timely response to unexpected events and ensuring the mission's success. The conventional approach in Space Operations involves using Out-of-Limits (OOL) alarms for anomaly detection. which may prove unsufficient in identifying and responding to complex anomalies or unforseen novelties within the range of nominal values. This talk proposes a Machine Learning approach for anomaly/novelty detection embedded into the radiation-tolerant LEON 3 processor for the HERA mission.

Overview: Qualitative Theory of Ordinary Differential Equations

Filip Voženílek
FNSPE CTU in Prague
Sunday, June 2, 10:00 – 10:20

The qualitative theory of differential equations investigates the behaviour of solutions without the need for explicit solution methods. We give an overview of some qualitative theory of periodic solutions and behaviour of solutions in proximity of fixed points. The concepts will be illustrated on instructive examples.

Globally convergent optimization methods: polynomial optimization and beyond

Aleš Wodecki
FEL CTU in Prague
Friday, May 31, 15:30 – 16:00

In certain applications, classical gradient based methods often fail to find local minima due to the cost functional or feasible sets being non-convex. There exist techniques, which may be applied in such circumstances with associated numerical treatments that lead to computational results. The benefits of such methods, as well as the challenges, are briefly outlined and discussed. In particular, we focus on introducing polynomial optimization as a robust method used to arrive at global minima, whose applications range from optimization over graphs to PDE constrained optimization.

OpenFPM: scalable open-source C++ framework for particle and particle-mesh codes on parallel computers.

Serhii Yaskovets
TU Dresden, Max Planck Institute of Molecular Cell Biology and Genetics
Friday, May 31, 11:20 – 11:50

Scalable and efficient numerical simulations continue to gain importance, as computation is firmly established as the third pillar of discovery, alongside theory and experiment. OpenFPM is an open-source C++ framework that provides transparent and scalable infrastructure for shared-memory and distributed-memory implementations of particles-only and hybrid particle-mesh simulations of both discrete and continuous models. The infrastructure is complemented with frequently used numerical routines, as well as interfaces to state-of-the-art third-party numerical libraries. We present the architecture and design of OpenFPM, general overview of the underlying abstractions, and benchmark results in applications ranging from Smoothed-Particle Hydrodynamics (SPH) to Molecular Dynamics (MD), Discrete Element Methods (DEM), Vortex Methods, stencil codes (finite differences), and high-dimensional Monte Carlo sampling (CMA-ES).