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

Workshop on scientific computing 2023

May 25 - 28, 2023. Děčín, Czech Rep. + Online

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

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Organizing committee

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

Additional information

URL: `http://mmg.fjfi.cvut.cz/wsc-2023`
Venue: Faculty of Nuclear Sciences and Physical Engineering,
Pohraniční 1288/1, 405 02 Děčín
and MS Teams online

Acknowledgement

This event is supported by the project of the Student Grant Agency of the Czech Technical University in Prague No. SVK 44/23/F4

List of Participants

The list of all participants in alphabetical order.

Name	University / Institute	
Michal Beneš	FNSPE, CTU in Prague	
Štěpán Bezděk	FNSPE, CTU in Prague	Student
Michal Bohatý	FNSPE, CTU in Prague	Student
Jan Bureš	FNSPE, CTU in Prague	Student
Arkadiusz Czader	AGH University of Science and Technology	Student
Nikola Drnková	FNSPE, CTU in Prague	Student
Jaroslav Drobný	FNSPE, CTU in Prague	Student
Pavel Eichler	FNSPE, CTU in Prague	Student
Roman Fencl	FNSPE, CTU in Prague	Student
Kryštof Filip	FNSPE, CTU in Prague	Student
Radek Fučík	FNSPE, CTU in Prague	
František Gašpar	FNSPE, CTU in Prague	Student
Jiří Hájek	FNSPE, CTU in Prague	Student
Tomáš Halada	FME, CTU in Prague	Student
Zuzana Hodboďová	FNSPE, CTU in Prague	Student
Robert F. Holub	Clarkson University, Potsdam	
Dominik Horák	FNSPE, CTU in Prague	Student
Lenka Horvátová	FNSPE, CTU in Prague	Student
Pavel Hron	Siemens Industry Software	
Radek Hřebík	FNSPE, CTU in Prague	Student
Vladimír Jarý	FNSPE, CTU in Prague	
Martin Jex	FNSPE, CTU in Prague	Student
Martin Jochec	FNSPE, CTU in Prague	Student
Jakub Klinkovský	FNSPE, CTU in Prague	Student
Miroslav Kolář	CTU in Prague	
Jan Kovář	FNSPE, CTU in Prague	Student
Bořivoj Kronowetter	FNSPE, CTU in Prague	Student
Jaromír Kukal	FNSPE, CTU in Prague	
Alexander Kuzmin	FNSPE, CTU in Prague	Student
Dana Majerová	FNSPE, CTU in Prague	
Jiří Mikyška	FNSPE, CTU in Prague	
Jiří Minarčík	FNSPE, CTU in Prague	Student

Maneesh Narayanan	FNSPE, CTU in Prague	Student
Radek Novotný	FNSPE, CTU in Prague	Student
Sebastian Nývlt	FNSPE, CTU in Prague	Student
Tomáš Oberhuber	FNSPE, CTU in Prague	
Jan Oršl	FNSPE, CTU in Prague	Student
Jan Palán	FNSPE, CTU in Prague	Student
Petr Pauš	FNSPE, CTU in Prague	
Vilém Pejpek	FNSPE, CTU in Prague	Student
Tomáš Princ	FCE, CTU in Prague	Student
Martin Procházka	FNSPE, CTU in Prague	Student
Jan Sequens	FNSPE, CTU in Prague	Student
Aaron Schick	FNSPE, CTU in Prague	Student
Richard Schlösinger	FNSPE, CTU in Prague	Student
Jakub Solovský	FNSPE, CTU in Prague / RERI	
Pavel Strachota	FNSPE, CTU in Prague	
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Jan Šembera	TUL	
Daniel Ševčovič	Comenius University Bratislava	
Jakub Šístek	Institute of Mathematics of the Czech Academy of Sciences	
Kateřina Škardová	FNSPE, CTU in Prague	
Adam Štampach	FNSPE, CTU in Prague	Student
Jan Thiele	CTU FNSPE	Student, Poster
Jaroslav Tintěra	IKEM, Prague	
Dalibor Trampota	FNSPE, CTU in Prague	Student
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Jana Zavadilová	FNSPE, CTU in Prague	Student
Martin Zemko	FNSPE, CTU in Prague	Student
Dominik Žurek	FNSPE, CTU in Prague	Student

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 13:50
+ 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 15 min = max 13 min talk + 2 min for discussion.

Thursday, May 25

Chairman: Pavel Strachota

14:00 – 14:30	**Jakub Šístek**: A scalable multilevel domain decomposition solver for immersed boundary finite element method
14:30 – 14:45	**Tomáš Halada**: Numerical aspects of Smoothed Particle Hydrodynamics Method in hydraulic applications
14:45 – 15:00	**Jan Valášek**: Dynamic mode decomposition and its application to the flutter analysis
15:00 – 15:15	**Pavel Eichler**: Non-Newtonian Blood Flow in Aortic Phantom: An Experimental and Computational Study
15:15 – 15:45	*Coffee + tea + snacks*

Chairman: Jakub Klinkovský

15:45 – 16:00	**Martin Zemko**: High-throughput readout and filtering systems for the AMBER experiment

16:00 – 16:15 **Quang Van Tran**: Bankruptcy prediction by a combined approach of LDA and ANN with robust whitening
16:15 – 16:30 **Vladimír Jarý**: Recent updates in development of the Data Acquisition System of the AMBER experiment
16:30 – 16:45 **Jakub Solovský**: Numerical Optimization of Neumann Boundary Condition for thermal lens construction
17:15 – 19:00 *Football game at nearby Mariánská louka (weather permitting). Tentative group departure at 17:15 from the Castle grange.*

Friday, May 26

07:30 – 09:00 *Breakfast*

Chairman: Pavel Eichler
09:00 – 09:15 **Robert Straka**: Lattice Boltzmann Method and reacting flows
09:15 – 09:30 **Arkadiusz Czader**: Simulation of airflow in an air quality measurement chamber
09:30 – 09:45 **Dominik Horák**: Numerical model of non-isothermal flow around obstacles based on the lattice Boltzmann method
09:45 – 10:00 **Bořivoj Kronowetter**: Optimization methods based on lattice Boltzmann method
10:00 – 10:15 **Maneesh Narayanan**: Visualization of curvature flow of smooth parametrized closed curves.
10:15 – 10:45 *Coffee + tea + snacks*

Chairman: Petr Pauš
10:45 – 11:00 **Cyril Izuchukwu Udeani**: Physics-informed DeepONets for HJB equation arising from portfolio management
11:00 – 11:15 **Tomáš Oberhuber**: TNL: Numerical library for modern parallel architectures
11:15 – 11:30 **Dominik Žurek**: Dynamics of Signal Propagation in Excitable Media
11:30 – 11:45 **Jakub Klinkovský**: Overview of parallel and asynchronous computing in Python

11:45 – 12:00 *Group photo!*

12:00 – 14:00 *Lunch break*

Chairman: Radek Fučík
14:00 – 14:30 **Jaroslav Tintěra**: New methods in MRI data reconstruction: Deep learning and Artificial inteligence
14:30 – 15:00 **Lucie Súkupová**: The overview of image reconstructions in Computed Tomography
15:00 – 15:15 **Jan Bureš**: Optimal shape design of walls of blood flow mathematical model focusing on the total cavopulmonary connection
15:15 – 15:35 *Coffee + tea + snacks*

Chairman: Dana Majerová

15:35 – 15:45 *Information about Saturday's hiking excursion*
15:45 – 16:00 **Jan Kovář**: An Overview of 4D Flow Reconstruction using the Adjoint Method
16:00 – 16:15 **Lenka Horvátová**: Mathematical modeling of contrast agent transport in vascular bed with transfer to surrounding tissue in myocardial perfusion problems
16:15 – 16:30 **Kryštof Filip**: Comparison of Pre-Trained CNN in Image Classification
16:30 – 16:45 **Jaromír Kukal**: Numeric Formulas for Fractional Laplacian and Fractional Gradient

17:00 – 18:30 *Football game at nearby Mariánská louka (weather permitting).*

19:00 – 22:00 *Conference social event at the conference venue*

Saturday, May 27

WARNING: During the weekend, the entry to the main building is possible only through the main door through the reception.
07:30 – 09:00 *Breakfast*

Chairman: Robert Straka
09:00 – 09:15 **Pavel Hron**: Parallel performance of STAR-CCM+
09:15 – 09:30 **Tomáš Princ**: Pore-network modeling of air entrapment in randomized pore medium
09:30 – 09:45 **Michal Bohatý**: Numerical solution of the adjoint equation for the phase-field model
09:45 – 10:15 *Coffee + tea + snacks*

Chairman: Michal Beneš
10:15 – 10:30 **Kateřina Škardová**: Effect of spatial and temporal resolution on the accuracy of motion tracking using 2D and 3D cine cardiac magnetic resonance imaging data
10:30 – 10:45 **Sebastian Nývlt**: Brief Introdiction to VR-1 Reactor Technology and Reactor Kinetics
10:45 – 11:00 **Pavel Strachota**: Numerically Efficient Determination of Kinetic Parameters of the VR-1 Nuclear Reactor based on Experimental Data and ODE-Constrained Optimization
11:00 – 12:15 *Lunch break*

12:15 – 16:30 *Hiking Excursion*

16:30 – 17:30 *Panel discussions*

17:30 – 19:00 *Football game at nearby Mariánská louka (weather permitting).*

Sunday, May 28

WARNING: During the weekend, the entry to the main building is possible only through the main door through the reception.

07:30 – 09:00 *Breakfast*

Chairman: Tomáš Oberhuber

09:00 – 09:15 **Michal Beneš**: Pore-scale Model of Soil Freezing

09:15 – 09:30 **Radek Hřebík**: Imperfect Classifier Using Hidden Classes

09:30 – 09:45 **Jan Palán**: Phase field models in materials science and their numerical solution

09:45 – 10:00 **Miroslav Kolář**: Image segmentation techniques by means of evolving curves

10:15 – 10:45 *Coffee + tea + snacks*

Chairman: Miroslav Kolář

10:45 – 11:00 **Petr Pauš**: Numerical simulation of dislocation multiple cross-slip

11:00 – 11:15 **František Gašpar**: Oscilations of Absolute Moments of Fractal Diffusion Simulations

11:15 – 11:30 **Jiří Minarčík**: Trajectory Surfaces of Framed Curvature Flow

11:30 – 11:45 **Adam Štampach**: Aplication of fuzzy management to analysis financial state of firms

11:45 – 12:00 **Aaron Schick**: Geometric image processing by the Allen-Cahn equation

List of Abstracts

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

Pore-scale Model of Soil Freezing

Michal Beneš, Alexandr Žák and Tissa H. Illangasekare Sunday, May 28, 09:00 – 09:15
FNSPE, CTU in Prague, FNSPE, CTU in Prague and Colorado School of Mines, Golden, USA

We present results of the finite-element simulation of ice nucleation and growth in pores of a saturated porous medium. The ice volume expansion leads to structural changes. The ice phase is captured by the phase-field method including anisotropy. We discuss computational results and future steps in the model development.

Numerical solution of the adjoint equation for the phase-field model

Michal Bohatý Saturday, May 27, 09:30 – 09:45
FNSPE, CTU in Prague

This contribution is concerned with the optimization problem of controlling crystal growth by manipulating temperature at the edges of the crystallization region. Our approach is based on solving the adjoint equation, which enables efficient computation of gradient of the objective function. To describe phase transitions, we utilize the phase-field model consisting of partial differential equations. During the optimization process, those equations are solved numerically using the finite difference method. The main result of this work is a computational study in which we try to gain more insight into the problem of controlling crystallization using boundary conditions.

Optimal shape design of walls of blood flow mathematical model focusing on the total cavopulmonary connection

Jan Bureš Friday, May 26, 15:00 – 15:15
FNSPE, CTU in Prague

This work deals with the optimization of shape of walls and with flow modelling of incompressible Newtonian fluid with a focus on modelling of blood flow in blood vessels. An optimization framework is presented and implemented, which can then be used to solve optimization problems involving fluid flow around rigid objects in 2D. The lattice Boltzmann method is used as the numerical solver and is briefly described. The theoretical section then describes the mathematical optimization methods used in this work. Interpolation boundary conditions, which are described and later used, are prescribed on the boundary of the objects. Thanks to the interpolation boundary conditions, the actual shape of the boundary of the objects is taken into account. Furthermore, the package used to automatically generate geometries used in the numerical simulations, which was implemented for the purpose of this work, is described. The next part demonstrates and analyses the application

of the optimization framework on a series of test problems. Finally, the results of the optimization problem of a simplified 2D total cavopulmonary connection model are presented, which are in agreement with the available literature. Thus, the application of the optimization framework can be considered successful.

Simulation of airflow in an air quality measurement chamber

Arkadiusz Czader Friday, May 26, 09:15 – 09:30
AGH University of Science and Technology

With the development of industry and technology, there is a growing need to study the quality of the air we breathe, which is a more complicated task than one might think. Measurement devices can behave very differently on different operating conditions. The quality of measurement can be affected by temperature, pressure, air humidity, level of measured parameter, air speed and air flow character.

The project involved the simulation of airflow in a measurement chamber used to measure concentration of PM2.5 particulate matter. For this purpose, a program implementing the Lattice Boltzmann Method on the D3Q27 lattice and cumulant based kernel was written.

Analysis of the results shows two vortices inside the chamber. This information can be used to design the geometry of new chamber versions which get rid of these vortices. It might lead to improved chamber measurement quality.

Non-Newtonian Blood Flow in Aortic Phantom: An Experimental and Computational Study

Pavel Eichler, Radek Galabov, Radek Fučík, Kateřina Škardová, Tomáš Oberhuber, Jaroslav Tintěra, Radomír Chabiniok Thursday, May 25, 15:00 – 15:15
FNSPE, CTU in Prague, IKEM, Prague; Department of Pediatrics, Division of Pediatric Cardiology, UT Southwestern Medical Center, 5323 Harry Hines Blvd., Dallas, TX 75390, USA

This study investigates the need for non-Newtonian models to accurately represent blood flow in large vessels. A specially-designed phantom of the aorta is used in conjunction with phase-contrast magnetic resonance imaging (PC-MRI) and lattice Boltzmann method (LBM) computational fluid dynamics (CFD) simulations to compare the results of non-Newtonian and Newtonian fluid models. The experiments are conducted using three types of acrylic plates to represent varying degrees of aortic stenosis, and two constant flow rates. The PC-MRI flow measurements are assessed for accuracy, and it is found that they underestimate flow due to turbulence. The results show that, for the studied conditions, Newtonian models produce comparable results to non-Newtonian models, which suggests that they may be a more cost-effective alternative.

Comparison of Pre-Trained CNN in Image Classification

Kryštof Filip, Dana Majerová
FNSPE, CTU in Prague

Friday, May 26, 16:15 – 16:30

¡/p¿¡p¿In recent years, convolutional neural networks have become increasingly popular in various fields, and pre-trained models have shown promising results in image classification tasks. This contribution compares the performance of four pre-trained convolutional neural networks (Googlenet, Alexnet, Squeezenet, and Resnet-50) in distinguishing between different car species. Thousands of images were obtained from various sources using different web scraping techniques, including Google images, Bing images, Pinterest, second-hand and advertising sites. Our empirical results show that certain pre-trained models outperform others in this specific classification task. This presentation will provide complete results and further details on the methodology. ¡p¿¡/p¿

Equivalent Partial Differential Equations for LBM and LBMAT: Open Problems

Radek Fučík
FNSPE, CTU in Prague

A general method for the derivation of equivalent finite difference equations (EFDEs) and subsequent equivalent partial differential equations (EPDEs) presented for a general matrix lattice Boltzmann method (LBM). The method can be used for both the advection diffusion equations and Navier-Stokes equations in all dimensions. In principle, the EFDEs are derived using a recurrence formula. A computational algorithm is proposed for generating sequences of matrices and vectors that are used to obtain EFDEs coefficients. The resulting EFDEs and EPDEs are derived for selected velocity models and include the single relaxation time, multiple relaxation time, and cascaded LBM collision operators. The algorithm for the derivation of EFDEs and EPDEs is implemented in C++ using the GiNaC library for symbolic algebraic computations. Its iplementation is available under the terms and conditions of the GNU general public license (GPL). The talk will summarize open problems for EPDEs for LBM with source terms.

Oscilations of Absolute Moments of Fractal Diffusion Simulations

František Gašpar, Jaromír Kukal
FNSPE, CTU in Prague

Sunday, May 28, 11:00 – 11:15

This contribution addresses the discrepancy between analytical studies and published simulations regarding the presence of oscillations in fractal diffusion. By summarizing findings from multiple self-similar sets simulations, this contribution discusses oscillations in estimated absolute moments. The importance of incorporating oscillations into the dimension estimation procedure is emphasized, and a simple parametric form for the absolute moment model is proposed based on observed oscillatory behaviour.

Numerical aspects of Smoothed Particle Hydrodynamics Method in hydraulic applications

Tomáš Halada, Luděk Beneš
FME, CTU in Prague

Thursday, May 25, 14:30 – 14:45

SPH is a mesh-free particle Lagrangian method that can successfully solve problems that are difficult or even impossible to handle with a conventional mesh-based method. We use a weakly compressible formulation of the SPH method (WCSPH) for free-surface flow and discuss some of its numerical aspects. Two hydraulic application are presented, free-surface flow in open channels with a complex geometry and simulation of mechanical mixing. These applications are used to highlight some numerical issues of the method, that need to be addressed and which are not clear from the standard, widely used benchmarks. Problems with negative pressure, pressure oscillations and numerical viscosity are discussed. Emphasis is placed on the additional stabilizing diffusive terms, realization of viscous terms, artificial viscosity and its relation to physical viscosity. Moreover, some additional improvement based on regularization techniques (PST) are mentioned, which eventually leads to a modern and promising Quasi-Lagrangian and Arbitrary Lagrangian-Eulerian schemes. Recent results from both of these applications are presented and analyzed in terms of the numerical aspects of the weakly compressible SPH method, and some improvements are suggested based on this analysis.

Numerical model of non-isothermal flow around obstacles based on the lattice Boltzmann method

Dominik Horák
FNSPE, CTU in Prague

Friday, May 26, 09:30 – 09:45

The work deals with the mathematical modeling of non-isothermal flow of incompressible Newtonian fluids. The aim of the work is to implement and describe heat transfer in a 3D numerical model. In the theoretical part, the mathematical model of non-isothermal flow of Newtonian fluids is presented together with a basic description of the cooling circuit of a student formula car. 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

Lenka Horvátová
FNSPE, CTU in Prague

Friday, May 26, 16:00 – 16:15

This work 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 using the finite volume method, and in the extravascular medium using the finite difference method.

Parallel performance of STAR-CCM+

Pavel Hron
Siemens Industry Software

Saturday, May 27, 09:00 – 09:15

One of the key requirements of commercial Computational Fluid Dynamics (CFD) based simulation software is great parallel scalability. The parallel performance of STAR-CCM+ is evaluated on several industrial test cases for both, modern CPU and GPU architectures. The computational times on high-end hardware can be reduced from weeks to hours.

Imperfect Classifier Using Hidden Classes

Radek Hřebík
FNSPE, CTU in Prague

Sunday, May 28, 09:15 – 09:30

The presented imperfect classifier builds on using results of various learning methods, whether in the form of supervised or unsupervised learning. The results form so-called hidden classes. The number of these hidden classes is higher compared to the original output classes. The classifier stands on the optimal unioning of these hidden classes. The first two layers of the proposed classifier are for optional linear and or non-linear transformations. After this optional transformation, the set of imperfect classifiers is followed by hidden and final classification. The aim of the new classifier is to achieve the highest critical sensitivity.

Recent updates in development of the Data Acquisition System of the AMBER experiment

Vladimír Jarý, Bc. Jan Vondruška. Ing. Martin Zemko Thursday, May 25, 16:15 – 16:30
FNSPE, CTU in Prague

Modern experiments in high energy physics strongly depend on effient data acquistion (DAQ) systems. In this contribution, we will focus on the DAQ system of the AMBER experiment at CERN laboratory in Geneva, Switzerland. We briefly introduce overall hardware architecture of the system, then we will present the software part that is used mainly for run control, configuration, and monitoring.
Often, it is necessary to access the system remotely. However, as the main parts of the software are desktop applications with Qt-based graphical user interface, the remote access requires fast and stable network connection. We analyse the possibility to replace selected configuration tools with web applications. We also propose to develop library of functions to implement a common command line library that would cover the most important aspects of the control and monitoring functionality. The combination of both approaches would greatly reduce requirements on the connection and would simplify the remote work.
We discuss the current state of the implementation of the proposed applications. We summarize the contribution by giving outlook into the future development.

Highly Efficient Phase Split Calculations in 2, 3, and 4 Phases through Combination of Stability, Minimization, and Newton Methods

Martin Jex, Jiří Mikyška, Abbas Firoozabadi
FNSPE, CTU in Prague, Chemical and Environmental Engineering,Yale University

Successful large-scale compositional reservoir simulation requires robust and efficient phase equilibrium calculations. In recent years a large number of papers have been published on the topic of three-phase vapor-liquid-aqueous (VLA) equilibria which frequently appear in hydrocarbon reservoirs. The presence of the aqueous phase increases the probability of equilibrium calculations to have issues. One may experience convergence problems or even not being able to distinguish a fourth phase altogether. This is generally due to the lack of good initial guesses, which is usually solved by proposing supplementary inital guesses which are designed to deal with a particular mixture. The commonly used approach is to perfrom a stability test before the equilibrium calculation, which determines whether it is needed to add an additional phase. Another benefit of this approach is that the result from the stability testing provides a good initial guess for the phase equilibrium calculation. In this contribution we present a robust algorithm which can deal with up to four phase equilibrium calculation. We demonstrate the algorithm and its robustness and efficiency in several examples from literature.

Overview of parallel and asynchronous computing in Python

Jakub Klinkovský Friday, May 26, 11:30 – 11:45
FNSPE, CTU in Prague

In recent years, Python has been consistently ranked as one of the most popular programming languages in the world. It is a general and high-level language that is used in many fields, including graphical interfaces, web applications, and data science. In this talk, we review its capabilities for for parallel and asynchronous computing, including coroutines with async and await syntax that was introduced in Python 3.5.

Image segmentation techniques by means of evolving curves

Miroslav Kolář Sunday, May 28, 09:45 – 10:00
CTU in Prague

In this talk we focus on the problem of image segmentation by means of the flow of smooth parametrized curves. Particular reason for the choice of direct description of moving segmentation curve is simplistic descritption and easiness to recover geometrical information of the segmented object. The motivation is in the medical imaging, nd more precisely, in retrieving the geometrical information of tumor slices.

An Overview of 4D Flow Reconstruction using the Adjoint Method

Jan Kovář, Pavel Eichler, Kateřina Škardová Friday, May 26, 15:45 – 16:00
FNSPE, CTU in Prague, FNSPE CTU in Prague

TBA

Optimization methods based on lattice Boltzmann method

Bořivoj Kronowetter Friday, May 26, 09:45 – 10:00
FNSPE, CTU in Prague

The aim of this work is to derive a method for the reconstruction of blood flow according to
data obtained from magnetic resonance imaging. As a first step, a simplified problem is solved, in which
the blood flow is simulated using the lattice Boltzmann method and the data from this simulation are
saved. We then try to reconstruct the control parameters from the stored data using the adjoint method.
Several optimization problems are going to be introduced. The acceleration caused by the external force field and the inlet velocity profile were chosen as the control parameters in these problems. Both the discrete adjoint approach and the continuous adjoint approach are going to be presented. In the last part, numerical results of these approaches are compared.

Numeric Formulas for Fractional Laplacian and Fractional Gradient

Jaromír Kukal, Michal Beneš Friday, May 26, 16:30 – 16:45
FNSPE, CTU in Prague

New difference schemes for fractional Laplacian and fractional gradient wil be presented for 1 < alpha < 2. They are develped for regular meshes (linear, tetragonal, cubic, hexagonal, dodecahedral) and have maximum possible approximation order 4 - alpha in all grid cases and any function from C4 class. The approximation error has been verified numerically. The hexagonal and dodecahedral meshes are recommended for radially symmetric solutions.

Trajectory Surfaces of Framed Curvature Flow

Jiří Minarčík, Michal Beneš Sunday, May 28, 11:15 – 11:30
FNSPE, CTU in Prague, FNSPE, CTU in Prague

The framed curvature flow is a generalization of the curve shortening flow and the vortex filament equation, where the magnitude of the velocity vector is determined by the curvature, and its direction is given by an associated time-dependent moving frame. The flow can be defined in such a way that it sweeps out trajectory surfaces of constant mean or Gaussian curvature.

Visualization of curvature flow of smooth parametrized closed curves.

Maneesh Narayanan, Michal Beneš Friday, May 26, 10:00 – 10:15
FNSPE, CTU in Prague

This work consists of the motion of the closed curve given by the motion law $V = K_\Gamma + F$ (1). We used discretization techniques to solve (1) for various smooth parametrized closed curves. We studied the effects of K_Γ and F on the evolution of different types of smooth closed curves using MATLAB. Our aim of this work is to apply those techniques to physical science problems.

Brief Introdiction to VR-1 Reactor Technology and Reactor Kinetics

Sebastian Nývlt, Pavel Strachota, Aleš Wodecki Saturday, May 27, 10:30 – 10:45
FNSPE, CTU in Prague

This presentation should provide the mainly mathematical audience with the physical background for the previous presentation "Numerically Efficient Determination of Kinetic Parameters of the VR-1 Nuclear Reactor based on Experimental Data and ODE-Constrained Optimization" by Dr. Pavel Strachota. This short presentation will provide the audience with a summary of the key information from reactor physics of zero-power research reactors. The main goal is to summarize the theory of reactor kinetics and all possible approaches to determining the kinetic parameters of a research reactor. The presentation also briefly introduces the VR-1 reactor operated by the Dept. of Nuclear

Reactors of FNSPE CTU in Prague where the results of this research might be implemented once the work is done and the approach is defended against the national regulatory body.

TNL: Numerical library for modern parallel architectures

Tomáš Oberhuber, Jakub Klinkovský, Radek Fučík Friday, May 26, 11:00 – 11:15
FNSPE, CTU in Prague, FNSPE, CTU in Prague

TNL (www.tnl-project.org) is a collection of building blocks that facilitate the development of efficient numerical solvers and HPC algorithms. It is implemented in C++ using modern programming paradigms in order to provide a flexible and user-friendly interface similar to, for example, the C++ Standard Template Library. TNL provides native support for modern hardware architectures such as multicore CPUs, GPUs, and distributed systems, which can be managed via a unified interface. In our presentation, we will demonstrate the main features of the library together with efficiency of the implemented algorithms and data structures including sparse matrices and unstructured numerical meshes.

Phase field models in materials science and their numerical solution

Jan Palán Sunday, May 28, 09:30 – 09:45
FNSPE, CTU in Prague

This thesis deals with the simulation of crystal growth during solidification of a pure supercooled substance using the phase field method, which describes the phase interface as a smooth transition layer between the liquid and solid state. Firstly, the mathematical model is presented. The anisotropic model for pure substance in the three-dimensional case is based on Finsler geometry. Furthermore, the work summarizes the phase field approaches to modeling binary alloy soldification. The main objective is the numerical solution of the phase field models on unstructured meshes. Due to the easy adaptation to an unstructured mesh, the finite volume method is used to discretize models. The implementation of the program in C++ is based on the GTMesh library. Finally, numerical simulations are performed especially to compare the phase field model behavior on an unstructured mesh and on a structured one.

Numerical simulation of dislocation multiple cross-slip

Petr Pauš Sunday, May 28, 10:45 – 11:00
FNSPE, CTU in Prague

Our contribution deals with the phenomenon in material science called multiple cross-slip of dislocations in slip planes. The numerical model is based on a mean curvature flow equation with additional forcing terms included. The curve motion in 3D space is treated using our tilting method, i.e., mapping of a 3D situation onto a single plane where the curve motion is computed. The physical forces acting on a dislocation curve are evaluated in the 3D setting.

Pore-network modeling of air entrapment in randomized pore medium

Tomáš Princ, Michal Sněhota Saturday, May 27, 09:15 – 09:30
FCE, CTU in Prague, FCE, CTU in Prague

The research deals with pore-network (PN) modeling and its use for the simulation of flow in the pore medium. This model allows the simulation of water flow on the pore scale, thanks to which it is possible to relatively accurately capture the process of air entrapment. Furthermore, a solution for two-phase flow is used, which makes it possible to determine the relative hydraulic conductivity values dependent on the air saturation.

Geometric image processing by the Allen-Cahn equation

Aaron Schick Sunday, May 28, 11:45 – 12:00
FNSPE, CTU in Prague

This work examines the use of PDEs for image processing, specifically the Allen-Cahn equation and its modification on rectangular domains. Differential law of motion of curves according to its curvature is introduced and we discuss its connection to the solution of the Allen-Cahn equation. We present a segmentation model based on this observation and apply it to test cardiac MRI data.

Numerical Optimization of Neumann Boundary Condition for thermal lens construction

Jakub Solovský, Aleš Wodecki, Monika Balázsová, Kateřina Škardová, Tomáš Oberhuber Thursday, May 25, 16:30 – 16:45
FNSPE, CTU in Prague / RERI, FNSPE, CTU in Prague

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.
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.

Numerically Efficient Determination of Kinetic Parameters of the VR-1 Nuclear Reactor based on Experimental Data and ODE-Constrained Optimization

Pavel Strachota, Sebastian Nývlt, Jan Rataj, Aleš Wodecki Saturday, May 27, 10:45 – 11:00
FNSPE, CTU in Prague

We follow up on the work presented at WS2022 aimed at determining the correct contributions of different classes of delayed neutrons to the kinetics of the VR-1 experimental nuclear reactor. The facility is installed at the Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague. We consider the system of equations of point kinetics, which is a system of linear ODE with source terms. This model can be used provided that the spatial distribution of reaction parameters inside the nuclear reactor core evolves slowly with respect to the reaction dynamics. We solve the ODE-constrained minimization problem to determine the correct values of the model parameters based on experimental measurement of reactor power output response to the changes in reactivity. The difference between the results of the simulations and the experiments is minimized by several gradient descent techniques. For the computation of the gradient, we employ both the direct method (sensitivity analysis) and the adjoint method based on solving the adjoint equation for Lagrange multipliers. We demonstrate the advantages of the adjoint approach, discuss the influence of ODE solver accuracy, properties of the individual gradient descent variants, and the structure of the local minima of the cost functional.

Lattice Boltzmann Method and reacting flows

Robert Straka Friday, May 26, 09:00 – 09:15
AGH University of Science and Technology

Combustion problems are usually described by a set of Navier-Stokes equations (NSE) together with Advection-Diffusion-Reaction equations (ADRE) for scalar quantities. We use a Lattice Boltzmann Method (LBM) to solve a system of equations related to simplified models of combustion i.e. we neglect radiation, temperature dependence of material properties, and assume ideal gases. Examples of solid state fuel combustion will be presented.

The overview of image reconstructions in Computed Tomography

Lucie Súkupová Friday, May 26, 14:30 – 15:00
IKEM, Prague

Computed Tomography (CT) is an imaging technique that uses X-ray radiation to generate axial slices of patients from acquired data. Acquired data are in the form of attenuation profiles in the sinogram space that can be filtered (here or in the frequency space), and then backprojected to the image space. One of major developments in reconstructions was use of iterative reconstructions (IR) of different types, firstly hybrid IR, later model-based IR that uses forward and backforward projections. Unfortunately, IR changes the texture of noise that negatively affects image appearance. These days, use of artificial intelligence is beneficial because it keeps the noise texture unchanged, but the magnitude can be decreased.

A scalable multilevel domain decomposition solver for immersed boundary finite element method

Jakub Šístek Thursday, May 25, 14:00 – 14:30
Institute of Mathematics of the Czech Academy of Sciences

Immersed boundary finite element method (FEM) presents an attractive approach to simulations avoiding the generation of large body-fitted meshes. This can be tedious and challenging for complex geometries as well as for very fine meshes distributed over a parallel computer and adaptively refined during a computation. However, the price to pay are more complicated formulations for the weak enforcement of Dirichlet boundary conditions, poor conditioning of stiffness matrices, and nonstandard numerical integration at the vicinity of the boundary. We develop multilevel balancing domain decomposition by constraints (BDDC) method tailored to the solution of the linear systems arising in the context of immersed boundary FEM with parallel adaptive grid refinement. A crucial challenge is presented by fragmenting of subdomains, which has two sources: i) the partitioning strategy based on a space-filling curve, and ii) extraction of the elements contributing to the stiffness matrix.

We present these concepts, the challenges, our implementation, and numerical results for the Poisson problem on complex geometries from engineering. This is joint work with Fehmi Cirak, Eky Febrianto, Matija Kecman, and Pavel Kůs.

Effect of spatial and temporal resolution on the accuracy of motion tracking using 2D and 3D cine cardiac magnetic resonance imaging data

Kateřina Škardová, Tarique Hussain, Martin Genet, Radomír Chabiniok Saturday, May 27, 10:15 – 10:30
FNSPE, CTU in Prague

This contribution explores how the spatial and temporal resolution of cardiac MRI cine images can affect the accuracy of the extracted left ventricle motion. Using a previously validated finite-element-based image registration method, the study was conducted on three subjects, for which both standard 2D cine stack (SA) and 3D cine MRI series imaging were acquired. Additionally, artificial SA-like cine image series were created from the 3D cine images to further augment the dataset. The study evaluated image series with various combinations of spatial and temporal resolution for each subject. Results indicated a strong correlation between slice thickness and the accuracy of extracted longitudinal displacement.

Aplication of fuzzy management to analysis financial state of firms

Adam Štampach, doc. Ing. Quang Van Tran, Ph.D.
FNSPE, CTU in Prague

Sunday, May 28, 11:30 – 11:45

Thesis examines the possibility of applying fuzzy management in financial analysis, specifically the prediction of corporate bankruptcy according to selected financial indicators. This task was implemented by converting Altman's bankruptcy model into a fuzzy form, and subsequently its use was verified using a data file of approximately 10 500 companies. The prediction results of the proposed fuzzy model were compared with the results obtained by other selected bankruptcy models on a data set of approximately 5 500 companies.

Use of 3D printing for MRI phantom construction

Jan Thiele
CTU FNSPE

TBA

New methods in MRI data reconstruction: Deep learning and Artificial inteligence

Jaroslav Tintěra
IKEM, Prague

Friday, May 26, 14:00 – 14:30

Recently, new software to reconstruct highly accelerated data from under-sampled acquisition has appeared commercially available. This SW utilizes several modern mathematical methods to effectively denoise acquired data and also to increase sharpness of reconstructed magnetic resonance images (MRI). It includes tailored noise analysis (spatially selective noise mask), deep learning and also artificial intelligence methods based on large data sets training. We will present first experience with this new technology and also we want to show both the clear benefit from using it but also potential risk of artifacts coming with reconstruction techniques.

Bankruptcy prediction by a combined approach of LDA and ANN with robust whitening

Quang Van Tran
FNSPE, CTU in Prague

Thursday, May 25, 16:00 – 16:15

We propose a new approach prediction of firm's bankruptcy in which the neural network is combined with linear discriminant analysis. We also try to improve LDA algorithm with the introduction of the robust covariance matrix. We verify the applicability of our approaches on a relatively large-scale dataset of Polish firms in manufacturing sector in period 2000–2013. The results of our analysis show that this approach can correctly classify all cases of non-bankrupted firms (in-sample and out-of-sample) and the rate of correct prediction of bankrupted firms is over eighty percent for the given dataset.

Physics-informed DeepONets for HJB equation arising from portfolio management

Cyril Izuchukwu Udeani, Daniel Sevcovic Friday, May 26, 10:45 – 11:00
Comenius University in Bratislava, Comenius University in Bratislava

Several differential equations from many scientific and engineering fields for modeling physical phenomena are analytically intractable, especially in high-dimensional space. Traditional numerical methods, including neural network approaches, have been extensively used to approximate solutions of such differential equations. Although some machine learning approaches, such as physics-informed neural networks, are faster than the conventional numerical methods; however, a slight change in the underlying parameters governing the differential equation could result in the retraining of the model. Therefore, in this study, we employ the physics-informed DeepONet (PI-DeepONet) to approximate the solution operator of a fully nonlinear partial differential equation arising from finance. PI-DeepONet incorporates known physics into the neural network, which consists of a deep neural network that learns the solution of the PDE and an operator network that enforces the PDE at each iteration. 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 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 PI-DeepONet.

Dynamic mode decomposition and its application to the flutter analysis

Jan Valášek Thursday, May 25, 14:45 – 15:00
Institute of Mathematics, CAS

In this talk the dynamic mode decomposition (DMD) method will be introduced. It is a data-driven and model-free method which decomposes a given set of signals to DMD modes and associated DMD eigenvalues. Thus it offers a very interesting alternative to the proper orthogonal decomposition (POD) and similar methods usually used for the low-rank representation of the high-dimensional data. The advantage of DMD is better physical interpretation of the decomposition as the DMD modes have monofrequency content and the complex DMD eigenvalues provide the frequency as well as the growth/decay rate of particular mode. Moreover the DMD has solid theoretical underpinnings given by the Koopman operator. The disadvantage of DMD is a relative ambiguity of DMD mode selection which are not sorted as in the case POD decomposition. Finally an application example of the DMD analysis to the numerical simulation of flutter vibrations is presented.

High-throughput readout and filtering systems for the AMBER experiment

Martin Zemko
FNSPE, CTU in Prague

Thursday, May 25, 15:45 – 16:00

Traditional triggered data acquisition systems provide limited capabilities of acquisition modes, usually relying on perfectly synchronized detectors. This contribution describes a novel triggerless approach removing low-level trigger logic and detector dead times. We developed such a streaming acquisition system for the AMBER experiment at CERN. It is based on high-speed data handling FPGA modules and advanced software processing on conventional x86 processors. The triggerless mode provides enough time for complex data filtering and online track reconstruction. Moreover, the readout system utilizes a custom data protocol optimized for the needs of the streaming system. The filtering procedure takes place in a distributed server farm playing the role of the high-level filter. For this purpose, we implemented a high-performance filtering framework providing high-throughput, parallel algorithms and load balancing to cope with excessive data rates. Furthermore, this work also describes the filtering pipeline and the generator chain simulating the readout system and producing artificial data for system validation.

Dynamics of Signal Propagation in Excitable Media

Dominik Žurek
FNSPE, CTU in Prague

Friday, May 26, 11:15 – 11:30

The contribution is devoted to mathematical modelling of signal propagation in excitable media by the FitzHugh–Nagumo model. This model weakly formulated, analyzed and numerically solved in 1D and 2D. It is also converted to curvilinear coordinates along a closed curve simulating the myocard crossection. Numerical solution is obtained by the finite-difference method and method of lines and verified by evaluating the experimental order of convergence.