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

Workshop on scientific computing 2022

May 26 - 29, 2022. Děčín, Czech Rep. + Online

Conference Information

The scientific colloquium of CTU organized by the departments of Software Engineering and Mathematics, FNSPE CTU in Prague 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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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-2022`
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. SGS20/184/OHK4/3T/14, 2020–22.

List of Participants

The list of all participants in alphabetical order.

Name	University / Institute	
Monika Balázsová	FNSPE CTU in Prague	
Michal Beneš	FNSPE CTU in Prague	
Jan Bureš	FNSPE CTU in Prague	Student
Michaela Diasová	FNSPE CTU in Prague	Student
Pavel Eichler	FNSPE CTU in Prague	Student
Radek Fučík	FNSPE CTU in Prague	
Vladimír Fuka	Faculty of Mathematics and Physics, Charles University	
Radek Galabov	FNSPE CTU in Prague, IKEM Prague	Student
František Gašpar	FNSPE CTU in Prague	Student
Jooyoung Hahn	Slovak University of Technology	Invited
Tomáš Halada	FME CTU in Prague	Student
Robert F. Holub	Clarkson University, Potsdam, New York, U.S.A	
Dominik Horák	FNSPE CTU in Prague	Student
Lenka Horvátová	FNSPE CTU in Prague	Student
Pavel Hron	Siemens Industry Software	Invited
Ladislav Kalvoda	FNSPE CTU in Prague	
Jakub Klinkovský	FNSPE CTU in Prague	Student
Miroslav Kolář	FNSPE CTU in Prague	
Jan Kovář	FNSPE CTU in Prague	Student
Bořivoj Kronowetter	FNSPE CTU in Prague	Student
Jaromir Kukal	FNSPE CTU in Prague	
Jiří Mikyška	FNSPE CTU in Prague	
Jiří Minarčík	FNSPE CTU in Prague	Student
Hirofumi Notsu	Kanazawa University	
Tomáš Oberhuber	FNSPE CTU in Prague	
Seol Ah PARK	Slovak University of Technology in Bratislava	
Petr Pauš	FNSPE CTU in Prague	
Julius Fergy Rabago	Institute of Science and Engineering, Kanazawa University	
Jelena Radović	Faculty of Mathematics and Physics, Charles University	Student
Md Mamunur Rasid	Kanazawa University	Student
Koya Sakakibara	Okayama University of Science	
Yusaku Shimoji	Meiji University	Student

Aaron Schick	FNSPE CTU in Prague	Student
John Sebastian Simon	Kanazawa University	Student
Jakub Solovský	FNSPE CTU in Prague	Student
Pavel Strachota	FNSPE CTU in Prague	
Robert Straka	AGH University of Science and Fiction	Invited
Jan Šembera	Technical University of Liberec	
Daniel Ševčovič	Comenius University Bratislava	
Kateřina Škardová	FNSPE CTU in Prague	Student
Jan Thiele	FNSPE CTU in Prague	Student
Jaroslav Tintěra	IKEM Prague	Invited
Quang Van Tran	FNSPE CTU in Prague	
Cyril Izuchukwu Udeani	Comenius University in Bratislava	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 (the main building of CTU at Pohraniční street, 1288/1):
Thursday: from 13:00 to 13:50
Friday: from 8:30 to 9:00 (and 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 = max 15 min talk + 5 min for discussion.

May 26

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

Chairman: Michal Beneš

14:10 – 14:40 **Pavel Hron**: The Mortar Finite Element Method in Industrial Applications
14:40 – 15:10 **Robert Straka**: Lattice on fire – Lattice Boltzmann Method for non-isothermal reactive flows
15:10 – 15:30 **Radek Fučík**: Equivalent partial differential equation of the lattice Boltzmann method
15:30 – 15:50 **Tomáš Halada**: SPH method for free surface flow in discharge object

15:50 – 16:10 *Coffee + tea + snacks*

Chairman: Radek Fučík

16:10 – 16:30 **Jan Šembera**: Formulation of reaction terms for reactive transport problems
16:30 – 16:50 **Jakub Klinkovský**: Modeling vapor transport in air using LBM and MHFEM

16:50 – 17:10 **Pavel Eichler**: Lattice Boltzmann method and Boundary conditions
17:10 – 17:30 **Jakub Solovský**: Investigation of brine leakage from a deep aquifer

18:00 – 19:30 *Friendly football game at nearby Mariánská louka (weather permitting). Group departure around 17:55 from the Castle grange.*

May 27

07:30 – 09:00 *Breakfast*

Chairman: Petr Pauš

09:00 – 09:20 **Md Mamunur Rasid**: A Lagrange–Galerkin Scheme of second order in time for the shallow water equations with a transmission boundary condition
09:20 – 09:40 **Vladimír Fuka**: LES and DNS of flow and scal dispersion in a street canyon
09:40 – 10:00 **Koya Sakakibara**: Analysis of the well-conditioned method of fundamental solutions for the Laplace equation
10:00 – 10:20 **Yusaku Shimoji**: Numerical computation for 2-phase viscous fluids Hele-Shaw flow with sink/source by the method of fundamental solutions
10:20 – 10:40 *Coffee + tea + snacks*

Chairman: Monika Balázsová

10:40 – 11:10 **Jooyoung Hahn**: What is a proper boundary condition to solve eikonal equation on a non-convex domain?
11:10 – 11:20 *technical break due to technical breakdown (microsoft-made)*
11:20 – 11:40 **Jelena Radović**: High resolution modeling with LES models
11:40 – 12:00 **Julius Fergy Rabago**: On a numerical shape optimization approach to the exterior Bernoulli problem via the coupled complex boundary method
12:00 – 12:20 **John Sebastian Simon**: A lifting theorem for the Dirichlet-data for the Navier-Stokes equations with open boundary condition
12:20 – 14:30 *Lunch break*

Chairman: Jakub Klinkovský

14:30 – 15:00 **Jaroslav Tintěra**: Quantitative cardio MR examination and new imaging options
15:00 – 15:20 **Kateřina Škardová**: Application of Neural Networks and Mathematical Models for T1 Relaxation Time Estimation
15:20 – 15:40 **Radek Galabov**: In vitro experiments and computational simulations of blood flow
15:40 – 16:00 **Jan Kovář**: Mathematical modeling of myocardial perfusion using lattice Boltzmann method
16:00 – 16:10 *group photo*

16:10 – 16:30 *Coffee + tea + snacks*

Chairman: Pavel Eichler (+ Tomáš Ober

16:30 – 16:50 **Jan Bureš**: On stress integration method for lattice Boltzmann method in 2D

16:50 – 17:10 **Lenka Horvátová**: Mathematical modeling of transport and transfer of contrast agent in myocardial perfusion problems

17:10 – 17:30 **Dominik Horák**: Mathematical modeling of flow around obstacles using the lattice Boltzmann method

Chairman: Tomáš Oberhuber

17:30 – 17:40 *Information about Saturday's hiking excursion*

17:40 – 18:00 **Seol Ah PARK**: Cell tracking based on image segmentation in 2D+ and 3D+time microscopy data

18:00 – 18:20 **Cyril Izuchukwu Udeani**: Maximal monotone operator technique for solving Hamilton-Jacobi-Bellman equation arising from optimal portfolio selection problem

18:45 – 19:45 *Football - group departure at 18:40 from the grange*

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: Kateřina Škardová

09:00 – 09:20 **Tomáš Oberhuber**: Optimization with PDEs and connection to machine learning

09:20 – 09:40 **Monika Balázsová**: Adjoint method for PDEs

09:40 – 10:00 **Michaela Diasová**: Iterated Function Systems, Their Invariant Sets and Measure

10:00 – 17:00 *Hiking Excursion*

17:00 – 18:00 *Panel discussions*

18:00 – 19:00 *Friendly football game at nearby Mariánská louka (weather permitting).*

19:30 – 22:00 *Conference dinner at Fabrika restaurant at 19:30!*

May 29

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: Miroslav Kolář

09:00 – 09:20 **Michal Beneš**: Modeling Experiments in Freezing and Thawing of Porous Media

09:20 – 09:40 **Quang Van Tran**: Renyi Entropy Derived Distribution for Returns of Financial Assets

09:40 – 10:00 **Daniel Ševčovič**: Construction of Fermat-Torricelli points by means of semi-definite optimization methods

10:00 – 10:20 **Pavel Strachota**: Numerically Efficient Optimization of Kinetic Parameters of the VR-1 Experimental Nuclear Reactor

10:20 – 10:40 *Coffee + tea + snacks*

Chairman: Pavel Strachota

10:40 – 11:00 **Jiří Mikyška**: An alternative model of multicomponent diffusion based on a combination of the Maxwell-Stefan theory and continuum mechanics

11:00 – 11:20 **František Gašpar**: Properties of Diffusion over Sparse Grids

11:20 – 11:40 **Jan Thiele**: Forecasting cryptocurrency price dynamics using reinforcement learning

11:40 – 12:00 **Jiří Minarčík**: Discrete Torsion

12:00 – 12:20 **Jaromir Kukal**: Fast Evaluation of Modified Renyi Entropy for Fractal Analysis

List of Abstracts

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

Adjoint method for PDEs

Monika Balázsová
FNSPE CTU in Prague
May 28, 09:20 – 09:40

In a numerical optimization problem the adjoint method allows us to compute the gradient of a functional or operator in an effective and cheap way. In this contribution we demonstrate the adjoint method on the optimization problem for heat equation with a Dirichlet boundary control and show some possible applications and numerical results.

Modeling Experiments in Freezing and Thawing of Porous Media

Michal Beneš, Michal Sněhota, Martina Sobotková
FNSPE CTU in Prague, Faculty of Civil Engineering, CTU in Prague
May 29, 09:00 – 09:20

In the contribution, we discuss the modeling of freezing and thawing in a fully saturated porous medium at the experimental laboratory scale. The phase transition leaves the grains intact but involved in the heat transfer and mechanical interaction due to the difference in specific volumes of the liquid and solid phase. The model based on conservation laws of mass, energy and momentum is used for simulation of particular laboratory experiments.

Iterated Function Systems, Their Invariant Sets and Measure

Michaela Diasová
FNSPE CTU in Prague
May 28, 09:40 – 10:00

This contribution deals with iterated function systems (IFS), its invariant sets and the chaos game algorithm, which is used to display them. In order to analyze these sets some properties of the inductive, Hausdorff, similarity and box-counting dimension are shown. Subsequently, the changes inside invariant sets caused by recurrent IFS are studied. The aproximation of the box-counting dimension for some of these sets is introduced.

Lattice Boltzmann method and Boundary conditions

Pavel Eichler
FNSPE CTU in Prague, FNSPE CTU in Prague
May 26, 16:50 – 17:10

Classical problems for the incompressible fluid flow simulations are given in the macroscopic description, i.e., using the initial and boundary conditions for the fluid velocity and pressure. In the

case of the mesoscopic simulations, the macroscopic conditions must be transferred to the mesoscopic description. The commonly used way is based on the setting of the discrete density function to its equilibrium part. This method neglects the non-equilibrium part and is correct only for cases with constant pressure and velocity in space and time.
In this contribution, the other commonly used approximations of the boundary conditions are discussed and analyzed on the 3D periodic fluid flow between parallel plates. Finally, the newly derived momentum boundary conditions for the D3Q27 are introduced and tested. These boundary conditions present a more accurate alternative to the other mesoscopic boundary conditions.

Equivalent partial differential equation of the lattice Boltzmann method

Radek Fučík
FNSPE CTU in Prague
May 26, 15:10 – 15:30

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).

LES and DNS of flow and scal dispersion in a street canyon

Vladimír Fuka, Štěpán Nosek, Jelena Radović
Faculty of Mathematics and Physics, Charles University, Institute of Thermomechanics CAS, Department of Atmospheric Physics MFF UK
May 27, 09:20 – 09:40

In previous large eddy simulations (LES) and wind-tunnel measurements of several street-network configurations it was found that one particular configuration of building shapes poses a particular challenge to the numerical model and even the mean flow in the street canyon differs considerably between the measurement and the simulation.
To be able to conduct simulation for the analysis of the role of the coherent structures for the street canyon ventilation we need to be able to simulate this flow confidently. Therefore, a series of simulations that test the sensitivity of the LES simulations to various setup parameters were performed. Additionally, also direct numerical simulations were performed in a small domain with a reduced Reynolds number (while remaining fully turbulent). The parameters tested are the size of the domain - in particular when interested about persistent large scale structures and convergence of the flow towards a homogeneous mean, the subgrid model, the order of the finite difference

approximation and lateral boundary conditions.

In vitro experiments and computational simulations of blood flow

Radek Galabov, Jan Rydlo, Jaroslav Tintěra May 27, 15:20 – 15:40
FNSPE CTU in Prague, IKEM Prague, Institute for Clinical and Experimental Medicine, Prague

Computational models of flow dynamics have a potential to enhance medical decision-making. The accuracy of flow models depends on a number of conditions such as fluid properties, vessel anatomy, vessel wall properties and flow regime. These properties can be controlled in physical models of blood flow. In this talk, such a physical model of the abdominal aorta is presented together with a pumping system providing pulsatile flow. Flow through the system can be measured by a magnetic resonance imaging scanner (MRI). This system and MRI-obtained data will be used later to adjust a lattice Boltzmann method-based computational model of blood flow through aorta.

Properties of Diffusion over Sparse Grids

František Gašpar, Jaromír Kukal May 29, 11:00 – 11:20
FNSPE CTU in Prague, Department of Software Engineering, FNSPE, Czech Technical University in Prague

The contribution presents the statistical properties of the diffusion process over fractal sets represented as sparse grids. The summary of differences between regular grid diffusion and sparse grid diffusion is presented together with an overview of dimension estimation methods. The main focus is given to less than one dimensional sets which allow for analytical study of return probability. Properties of sparse grid diffusion are demonstrated using data from simulations and improved dimension estimation method is shown.

What is a proper boundary condition to solve eikonal equation on a non-convex domain?

Jooyoung Hahn May 27, 10:40 – 11:10
Slovak University of Technology

In this talk, boundary conditions to solve the eikonal equation are discussed in the case of non-convex computational domains. One of the proper conditions has been known as the Soner (or no-inflow) boundary condition written by an inequality. Considering an application to industrial problems, domains in three-dimensional space are discretized by polyhedral cells and a cell-centered finite volume method is used to solve the eikonal equation. We briefly check how the mentioned inequality boundary condition can be straightforwardly implemented in the finite volume method. If time permits, I would like to share a short working experience in a company as an applied mathematician. It is my personal story of how I could survive by working with others from the other world.

SPH method for free surface flow in discharge object

Tomáš Halada, Luděk Beneš, Jiří Fürst May 26, 15:30 – 15:50
FME CTU in Prague

Smoothed particle hydrodynamics, a meshfree particle method based on Lagrangian description is used for simulation of free surface flow in 3D complex geometries of discharge objects of turbine and pump stations. Possibilities and benefits of the method are demonstrated as well as drawbacks mostly related to boundary condition are shown. Arising problems are not connected with particular case but these are general topics of research in SPH method. Motivated by that, we focus on comparasement of some realization of boundary conditions. Moreover, modern SPH formulation based on partially Lagrangian partially Eulerian description and approximate Riemann solvers (R-ALE-SPH) with new proposed scheme is presented as possible improvement of the method.

The Mortar Finite Element Method in Industrial Applications

Pavel Hron May 26, 14:10 – 14:40
Siemens Industry Software

The Mortar Finite Element Method allows the coupling of arbitrary nonconforming interface meshes. We exploit this capability and apply it to real 3D engineering applications in solid energy and solid mechanics. Advantageous properties of the devised algorithms comprise superior robustness as compared with the traditional node-to-segment approach, the absence of any unphysical user-defined parameters (e.g. penalty or Nitsche methods) and the possibility to condense the discrete Lagrange multipliers from the global system of equations.

Modeling vapor transport in air using LBM and MHFEM

Jakub Klinkovský, Andrew C. Trautz, Radek Fučík, Tissa H. Illangasekare May 26, 16:30 – 16:50
FNSPE CTU in Prague, USACE ERDC in Vicksburg, FNSPE CTU in Prague, CSM in Golden

We present an efficient computational approach for simulating component transport within single-phase free flow in the boundary layer over porous media. A numerical model based on this approach is validated using experimental data generated in a climate-controlled wind tunnel coupled with a 7.3 m long soil test bed. The developed modeling approach is based on a combination of the lattice Boltzmann method (LBM) for simulating the fluid flow and the mixed-hybrid finite element method (MHFEM) for solving constituent transport. Both those methods individually, as well as when coupled, are implemented entirely on a GPU accelerator in order to utilize its computational power and avoid the hardware limitations caused by slow communication between the GPU and CPU over the PCI-E bus. We describe the mathematical details behind the computational method, focusing primarily on the coupling mechanisms. The performance of the solver is demonstrated on a modern high-performance computing system. Flow and transport simulation results are validated and compared herein with experimental velocity and relative humidity measurements made above

a flat partially saturated soil layer exposed to steady air flow. Model robustness and flexibility is demonstrated by introducing rectangular bluff-bodies to the flow in several different experimental scenarios.

Fast Evaluation of Modified Renyi Entropy for Fractal Analysis

Jaromir Kukal, Martin Dlask May 29, 12:00 – 12:20
FNSPE CTU in Prague, FNSPE CTU in Prague

A fractal dimension is a non-integer characteristic that measures the space filling of an arbitrary set. The conventional grid based methods usually provide a biased estimation of the fractal dimension, and therefore it is necessary to develop more complex methods for its estimation. A new characteristic based on the Parzen estimate formula is presented here as the modified Renyi entropy. A novel approach that employs the log-linear dependence of a modified Renyi entropy is used together with very fast implementation of epsilon search in k-d tree.

An alternative model of multicomponent diffusion based on a combination of the Maxwell-Stefan theory and continuum mechanics

Jiří Mikyška May 29, 10:40 – 11:00
FNSPE CTU in Prague

TBA

Optimization with PDEs and connection to machine learning

Tomáš Oberhuber May 28, 09:00 – 09:20
FNSPE CTU in Prague

In the presentation, we will show how to solve optimization problems with ordinary and partial differential equations by solving adjoint differential equations. We will show similarities with residual neural networks, convolution neural networks, and the backpropagation algorithm. We will point out difficulties arising from solving the optimization problems with partial differential equations.

Cell tracking based on image segmentation in 2D+ and 3D+time microscopy data

Seol Ah PARK, Tamara Sipka, Zuzana Kriva, George Lutfalla, Mai Nguyen-Chi, Karol Mikula May 27, 17:40 – 18:00
Slovak University of Technology in Bratislava, LPHI, CNRS, Univ. Montpellier, Montpellier, France

We introduce the new cell tracking algorithm for time-lapse images. By using the segmented images, the time-relaxed Eikonal equation is solved inside every segmented cell to find the approximate cell

centers. Next, the approximate cell centers form trajectories when the segmented cells overlap each other in the temporal direction. Finally, these firstly formed trajectories are connected by computing a tangent allowing us to estimate the direction of movement of the cells. The results of trajectories obtained from the proposed cell tracking method are presented visually and quantitatively.

On a numerical shape optimization approach to the exterior Bernoulli problem via the coupled complex boundary method

Julius Fergy Rabago May 27, 11:40 – 12:00
Institute of Science and Engineering, Kanazawa University

We propose a shape optimization formulation of the exterior Bernoulli problem using the the so-called coupled complex boundary method.
The idea of this approach is to transform the overdetermined problem to a complex boundary value problem with a complex Robin boundary condition coupling the Dirichlet and Neumann boundary conditions on the free boundary. Then, we optimize the cost function constructed by the imaginary part of the solution in the whole domain in order to identify the free boundary. To numerically solve the minimization problem, we compute the shape gradient of the cost functional and apply iterative algorithm based on a Sobolev gradient scheme via finite element method. We illustrate the feasibility of the method through several numerical examples, both in two and three spatial dimensions.

High resolution modeling with LES models

Jelena Radović, First part – TURBAN project: Michal Belda1, Jaroslav Resler2, Pavel Krč2, Martin Bureš2, Kryštof Eben2, Jan Geletič2; Second part - "The Role of coherent structures' dynamics on scalar transport and dispersion in the urban canopy layer" project: Vladimír Fuka1, Štěpán Nosek 3 May 27, 11:20 – 11:40
Faculty of Mathematics and Physics, Charles University, 1 - Department of Atmospheric Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic; 2 - Institute of Computer Science of the Czech Academy of Sciences, Prague, Czech Republic ;3 - Institute of Thermomechanics AS CR, v.v.i., Dolejškova 1402/5, Prague 8 182 00, Czech Republic

This work is a combination of two different studies conducted within two independent projects in which the high-resolution Large Eddy Simulations (LES) were performed by using two different numerical models: The Parallelized Large-Eddy Simulation Model (PALM) and the OpenFOAM model.
In the course of the first study in which the PALM model was used, three LES simulations were performed using three different sets of initial and boundary conditions obtained from the mesoscale numerical model called WRF. The simulations were performed on an 8 x 8 km domain in 10 m resolution which is capturing a real city area in the southeast part of Prague. In order to obtain preliminary conclusions, a comparison of the WRF model and PALM model outputs against observations obtained from the University of Wyoming (UW) was performed as well. The ultimate goal

of this still ongoing study is to develop a mechanism for determining the best possible initial and boundary conditions for the initialization of the PALM model, perform a series of different simulations on a real urban environment and validate the accuracy of the model for given conditions. This study is a part of an international project called the Turbulent-resolving urban modeling of air quality and thermal comfort (TURBAN).
The high-resolution LES simulations in the second study were performed on a 3D urban array by the model OpenFOAM with the goal of capturing the turbulent flow in the street canyons of the mentioned urban array. The configuration and the setup of these simulations are built upon the results previously published by Nosek et al., 2018, BAE 138; Kluková et al., 2021, JWEIA 208. The final objective of this study is to determine and investigate to what extent the coherent structures' dynamics influence the scalar transport and dispersion in the urban canopy layer. The outputs of the OpenFOAM model simulations will be compared to the data obtained during the wind tunnel experiment. This research experiment is a part of the GAČR funded project named "The Role of coherent structures' dynamics on scalar transport and dispersion in the urban canopy layer".

A Lagrange–Galerkin Scheme of second order in time for the shallow water equations with a transmission boundary condition

Md Mamunur Rasid, Hirofumi Notsu, Masato Kimura, Erny Rahayu Wijayanti and Md Masum Murshed
Kanazawa University
May 27, 09:00 – 09:20

This study presents a Lagrange-Galerkin(LG) scheme of second order in time for the shallow water equations (SWEs) with a transmission boundary condition. Firstly, we confirm the experimental order of convergence of the scheme. Secondly, we apply the scheme to a practical case, i.e., a complex domain with a transmission boundary condition. Finally, based on the numerical experiments, we summarize the advantages of our scheme, second-order accuracy in time, mass conservation, and no significant reflection from the transmission boundaries.

Analysis of the well-conditioned method of fundamental solutions for the Laplace equation

Koya Sakakibara
Okayama University of Science
May 27, 09:40 – 10:00

The method of total solution (MFS for short) is a mesh-free numerical solution method for potential problems, and under certain conditions, the error decays exponentially for the number of approximation points. On the other hand, the condition number of the coefficient matrix of the collocation equation increases exponentially, and efforts have been made to overcome this ill-conditioning. In this talk, we consider the MFS-QR method proposed by Antunes (2018), which uses QR decomposition to replace the basis functions and prove that the error decays exponentially despite the condition number being O(1).

Numerical computation for 2-phase viscous fluids Hele-Shaw flow with sink/source by the method of fundamental solutions

Yusaku Shimoji, Shigetoshi Yazaki
Meiji University, Meiji University

May 27, 10:00 – 10:20

The boundary between two viscous fluids is known to destabilize depending on the situation, producing a finger-like pattern, which is called the Saffman-Taylor instability. We were able to simulate the Saffman-Taylor instability in a Hele-Shaw cell by using the method of fundamental solutions (MFS for short). MFS is a mesh-free numerical solution method for mainly potential problems. Here, we present the implementation of MFS for 2-phase viscous fluids Hele-Shaw flow with sink/source and its numerical results.

A lifting theorem for the Dirichlet-data for the Navier-Stokes equations with open boundary condition

John Sebastian Simon, Hirofumi Notsu
Kanazawa University, Kanazawa University

May 27, 12:00 – 12:20

We shall present a Navier-Stokes equation coupled with a general class of nonlinear Robin-type boundary condition. The lifting theorem allows a prescription of a non-homogeneous Dirichlet condition on a portion of the boundary that excludes where the open boundary condition is prescribed. We present the existence of weak solutions, and end by illustrating particular forms of the boundary condition and show their differences numerically.

Investigation of brine leakage from a deep aquifer

Jakub Solovský
FNSPE CTU in Prague

May 26, 17:10 – 17:30

Damage to the caprock and potential leakage of brine from a deep aquifer is one of the risks during CO2 sequestration.
To reduce the complexity of the numerical solutions the fractures are considered one-dimensional objects whereas the rest of the domain is considered two-dimensional.
In this work, we assume that the flow is described by Darcy's law both in porous media and fractures. We present the mathematical model of single-phase flow and transport in porous media and its coupling between 1D and 2D computational domains.
The numerical solution is based on the mixed-hybrid finite element method with fully implicit time discretization.
The capabilities of the model are demonstrated in scenarios arising from the laboratory experiments mimicking the brine leakage from a deep aquifer.

Numerically Efficient Optimization of Kinetic Parameters of the VR-1 Experimental Nuclear Reactor

Pavel Strachota, Sebastian Nývlt, Jan Rataj, Aleš Wodecki May 29, 10:00 – 10:20
FNSPE CTU in Prague, FNSPE CTU in Prague, Department of Nuclear Reactors

We present a work in progress 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 in small-scale reactors where the spatial distribution of fuel and other components in the reactor core can be neglected. We solve the ODE-constrained minimization problem to determinine 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 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. The results of both approaches in terms of accuracy, robustness and computational costs are compared.

Lattice on fire – Lattice Boltzmann Method for non-isothermal reactive flows

Robert Straka May 26, 14:40 – 15:10
AGH University of Science and Fiction

A Lattice Boltzmann Method (LBM) is able to - more or less - efficiently solve Navier-Stokes equations (NSE) together with Advection-Diffusion-Reaction equations (ADRE) for passive scalars. Simplified models of combustion could be easily solved by the LBM, especially when one could neglect radiation, temperature dependence of material properties, and other stuff related to non-ideal gases. Such idealized models of the combustion are good starting point playground, that could be followed by further refinement and enhancement towards more complex and accurate ones. The application of the LBM in problems related to combustion will be presented, the premixed combustion of a propane-air mixture and the combustion of a solid fuel.

Formulation of reaction terms for reactive transport problems

Jan Šembera May 26, 16:10 – 16:30
Technical University of Liberec

In reaction problem modelling appear many difficulties. One of them is even its correct mathematical formulation. Some remarks and a derivation of one specific example problem mathematical formulation will be presented.

Construction of Fermat-Torricelli points by means of semi-definite optimization methods

Daniel Ševčovič
Comenius University Bratislava

May 29, 09:40 – 10:00

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In this talk we construct Fermat-Torricelli points by means of semi-definite optimization techniques and methods. Fermat-Torricelli point is a minimizer of distances from a given set of points in the Euclidean space. We show how the Fermat-Torricelli point can be constructed by means of semi-definition programming technique. Various examples will be presented in this talk.

Application of Neural Networks and Mathematical Models for T1 Relaxation Time Estimation

Kateřina Škardová
FNSPE CTU in Prague

May 27, 15:00 – 15:20

¡/p¿¡p¿In this contribution, we discuss how mathematical models and machine learning methods can be combined in parameter estimation framework. We propose a two-stage method: in the first stage, we combine machine learning and mathematical model in order to obtain a fast first parameter estimation; in the second stage, the estimation is refined by numerical optimization. The proposed method is applied to the problem of estimating the relaxation time T1 from a series of images obtained by the standard Modified Look-Locker Inversion (MOLLI) restoration technique. We present the results of the proposed method applied to phantom and in vivo data and demonstrate some advantages of such a combined approach.

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Quantitative cardio MR examination and new imaging options

Jaroslav Tintěra, Dana Kautznerová
IKEM Prague, ZRIR, IKEM, Praha

May 27, 14:30 – 15:00

The issue of quantitative cardio MR examinations is discussed within the currently used methods. The lecture also serves as an introduction to the mapping of relaxation times and the clinical use of a quantitative approach to MR images. There are also some new techniques that increase the effectiveness of examinations, especially for severe patients.

Renyi Entropy Derived Distribution for Returns of Financial Assets

Quang Van Tran
FNSPE CTU in Prague

May 29, 09:20 – 09:40

We derive a new distribution using Renyi entropy principle with maximum entropy method under the absolute moment constraints. The new distribution has four parameters: two shape parameters and the remaining two are location and scale parameters. The density of this distribution is smooth and twice differentiable which allows its parameters to be estimated by maximum likelihood estimation method. This distribution can capture the heavy tail property of returns of financial assets and we use it to model returns of various financial assets and compare its ability to model this property with other heavy tail distributions often used for this purpose.

Maximal monotone operator technique for solving Hamilton-Jacobi-Bellman equation arising from optimal portfolio selection problem

Cyril Izuchukwu Udeani, Daniel Sevcovic
Comenius University in Bratislava

May 27, 18:00 – 18:20

This study investigates a fully nonlinear evolutionary Hamilton-Jacobi-Bellman (HJB) parabolic equation using the monotone operator technique. We consider the HJB equation arising from portfolio optimization selection, where the goal of an investor is to maximize the conditional expected value of the terminal utility of the portfolio. The fully nonlinear HJB equation is transformed into a quasilinear parabolic equation using the so-called Riccati transformation method. The transformed parabolic equation can be viewed as the porous media type of equation with the source term. Under some assumptions, we obtain that the diffusion function to the quasilinear parabolic equation is globally Lipschitz continuous, which is a crucial requirement for solving the Cauchy problem. We employ Banach's fixed point theorem to obtain the existence and uniqueness of a solution to the general form of the transformed parabolic equation in a suitable Sobolev space in an abstract setting. Some financial applications of the proposed result are presented in one-dimensional space.