

MIMS/CMMA Czech-Japanese Seminar in Applied Mathematics

September 5-8, 2013 Meiji University, Nakano Campus

Invited speakers: Yoshihisa Morita (Ryukoku University, Japan) Daniel Sevcovic (Comenius University, Slovakia)

Speakers:

Kensuke Aihara (Tokyo University of Science, Japan) Michal Benes (Czech Technical University in Prague, Czech Republic) Peter Frolkovic (Slovak University of Technology, Slovakia) Akiko Fukuda (Tokyo University of Science, Japan) Daisuke Furihata (Osaka University, Japan) Tereza Jindrova (Czech Technical University in Prague, Czech Republic) Masato Kimura (Kanazawa University, Japan) Vladimir Klement (Czech Technical University in Prague, Czech Republic) Petr Knobloch (Charles University, Czech Republic) Miroslav Kolar (Czech Technical University in Prague, Czech Republic) Pavol Kutik (Slovak University of Technology, Slovakia) Radek Maca (Czech Technical University in Prague, Czech Republic) Takayasu Matsuo (The University of Tokyo, Japan) Jiri Mikyska (Czech Technical University in Prague, Czech Republic) Karol Mikula (Slovak University of Technology, Slovakia) Hideki Murakawa (Kyushu University, Japan) Yoshiaki Muroya (Waseda University, Japan) Katsuhisa Ozaki (Shibaura Institute of Technology, Japan) Ondrej Polivka (Czech Technical University in Prague, Czech Republic) Pedro Polvora (Technical University of Liston, Portugal) Robert Spir (Slovak University of Technology in Bratislava, Slovakia) Robert Straka (AGH University of Science and Technology, Poland) Karel Svadlenka (Kanazawa University, Japan) Takeshi Takaishi (Hiroshima Kokusai Gakuin University, Japan) Tohru Tsujikawa (University of Miyazaki, Japan)

Poster session:

Masakazu Akiyama (Hokkaido University, Japan) Koichi Anada (Waseda University Senior High School, Jap h Republic) Michal Benes (Czech Technical University in Prague, Cze Tomoyuki Idogawa (Shibaura Institute of Technology, Japa **h)** Tetsuya Ishiwata (Shibaura Institute of Technology, Japan) ech Republic) Tereza Jindrova (Czech Technical University in Prague, C Vladimir Klement (Czech Technical University in Prague, **Czech Republic**) Yasuaki Kobayashi (Hokkaido University, Japan) ch Republic) Miroslav Kolar (Czech Technical University in Prague, Cz Radek Maca (Czech Technical University in Prague, Cze **Republic**) Rhudaina Z. Mohammad (Kanazawa University, Japan) Harunori Monobe (Meiji Institute for Advanced Study of Mathematical Sciences, Japan). Takayuki Narumi (Kwansei Gakuin University, Japan) Kei Nishi (Hokkaido University, Japan) Ondrej Polivka (Czech Technical University in Prague, Czech Republic) Takiko Sasaki (The University of Tokyo, Japan) Hirotoshi Sato (Kwansei Gakuin University, Japan) Nur Shofianah (Kanazawa University, Japan) <u>Slovakia</u>) Robert Spir (Slovak University of Technology in Bratislava , Poland) Robert Straka (AGH University of Science and Technolog Kenta Uemichi (Kwansei Gakuin University, Japan)

Organizers: Tetsuya Ishiwata, Toshi Ogawa, Takashi Sakamoto and Shigetoshi Yaszaki The organizations on Japanese side are Department of Mathematical Sciences, College of Systems Engineering, Shibaura Institute of Technology, Department of Mathematical Sciences Based on Modeling and Analysis, School of Interdisciplinary Mathematical Sciences, Meiji Univer Department of Mathematics, School of Science and Technology, Meiji University, and the organization on Czech side is • Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague. The seminar is partially supported by

- Grant-in-Aid for Scientific Research (C) No.28540150 (Shigetoshi Yaz
 Meiji University Headquarters of International Collaboration; and
- Meiji Institute for Advanced Study of Mathematical Sciences (MIMS), the Center for Mathematical Modeling and Applications (CMMA), Meiji Un

<u>次</u>

Czech

apan

Se For further information -http://www.isc.meiji.ac.jp/~cjs/cjs2013/

Czech-Japanese Seminar in Applied Mathematics 2013

Sep. 5 (Thu)		Sep. 6 (Fri)		
		9:50-10:15	Tohru Tsujikawa	
			Global solution branches of some	
		10:15-10:40	Robert Straka	
			Computational model of	
		10:40-10:50	Break	
		10:50-11:10	Robert Spir	
			Tracking of cells in Zebrafish	
		11:10-11:30	Radek Maca	
			Segmentation of 3D MRI images by \ldots	
		11:30-13:00	Lunch	
13:00-13:10	Opening	13:00-13:25	Akiko Fukuda	
13:10-13:35	Peter Frolkovic		Conserved quantities of the integrable	
	Semi-implicit finite volume level	13:25-13:50	Yoshiaki Muroya	
13:35-14:00	Karel Svadlenka		Global stability of Lotka-Volterra	
	Numerical computation of		systems with infinite delays and	
	with nonlocal constraints	13:50-14:00	Break	
14:00-14:25	Karol Mikula	14:00-14:20	Tereza Jindrova	
	Surface evolution with		Computation of two-phase equilibrium \ldots	
14:25-14:45	Break	14:20-14:40	Pedro Polvora	
14:45-15:10	Kensuke Aihara		Optimal value of a firm investing in	
	Solving sparse linear systems	14:40-14:50	Break	
15:10-15:35	Katsuhisa Ozaki	14:50-15:10	Ondrej Polivka	
	Accurate algorithms for matrix		Compositional modeling of two-phase	
15:35-15:50	Break	15:10-15:35	Jiri Mikyska	
15:50-16:40	Daniel Sevcovic (Plenary talk (1))		Modeling diffusion in multicomponent	
	On nonlocal geometric flows and	15:35-15:45	Break	
17:30-19:30	Welcome reception	15:45-17:15	Poster session (1)	
	(Restaurance at the 1st floor)	18:30-20:30	Conference dinner	
			(The 14th floor, SUNPLAZA)	
			Meeting point: 18:00, Entrance	

The 6th floor (classroom and presentation space), Nakano Campus

Sep. 7 (Sat)		Sep. 8 (Sun)		
9:50-10:15	Masato Kimura	9:50-10:15	Takayasu Matsuo	
	Continuous and discrete crack		A discontinuous Galerkin method	
10:15-10:40	Takeshi Takaishi	10:15-10:40	Pavol Kutik	
	Complicated propagation of cracks in		A stabilized finite volume numerical	
10:40-10:50	Break	10:40-10:50	Break	
10:50-11:10	Miroslav Kolar	10:50-11:15	Daisuke Furihata	
	Mathematical model and numerical		An iteration method for the numerical	
11:10-11:30	Vladimir Klement	11:15-11:40	Michal Benes	
	GPU multigrid solver for		Numerical simulation of flow in	
11:30-13:00	Lunch	11:40-11:50	Closing and Poster award ceremony	
13:00-14:30	Poster session (2)			
14:30-14:50	Break			
14:50-15:40	Yoshihisa Morita (Plenary talk (2))			
	Spectral comparison and gradient-like			
15:40-16:00	Break			
16:00-16:25	Norbert Pozar		Departure to	
	A viscosity approach to total			
16:25-16:50	Petr Knobloch			
	A nonlinear local projection finite			
16:50-17:15	Hideki Murakawa			
	Convergence rates of discrete-time			

${\bf SUNPLAZA}$ (in front of Nakano Station):



List of posters (in alphabetical order)

Sep. 6 (Fri), 15:45-17:15 Poster session (1)

- 1. Masakazu Akiyama (Hokkaido University, Japan) A mathematical model of planar cell polarity
- 2. Koichi Anada (Waseda University Senior high school, Japan) Some features for blow-up solutions of a nonlinear parabolic equations
- 3. Michal Benes (Czech Technical University in Prague, Czech Republic)
 - (1) Interaction of dynamically evolving dislocations

(2) Numerical simulation of anomalous transport in porous media described by fractional-advection dispersion equation

4. Kota Ikeda (Meiji University, Japan)

Collective motions of particles with diffusive interactions

- 5. Tomoyuki Idogawa (Shibaura Institute of Technology, Japan) Research on an expansion to the continuous version of morphological contour decomposition-reconstruction algorithm
- 6. Tetsuya Ishiwata (Shibaura Institute of Technology, Japan)
 - (1) Spiral-shaped solutions to crystalline motion with a rotating tip
 - (2) Structure-preserving finite difference scheme for Heisenberg equation and its application to a vortex filament motion
- 7. Tereza Jindrova (Czech Technical University in Prague, Czech Republic) General computation of phase equilibrium in multicomponent mixtures
- 8. Vladimir Klement (Czech technical University in Prague, Czech Republic) Algebraic multigrid for Navier-Stokes problems
- 9. Yasuaki Kobayashi (Hokkaido University, Japan) Mathematical modeling of epidermal homeostasis
- 10. Miroslav Kolar (Czech technical University in Prague, Czech Republic) Computational study of planar curve dynamics
- 11. Radek Maca (Czech Technical University in Prague, Czech Republic) CFD simulation of two phase flow in fluidized bed boiler geometry
- Rhudaina Z. Mohammad (Kanazawa University, Japan)
 Multiphase volume-preserving interface motions via localized signed distance vector scheme
- Harunori Monobe (Meiji Institute for Advanced Study of Mathematical Sciences, Japan)
 On a free boundary problem describing cell motility
- 14. Kei Nishi (Hokkaido University, Japan)Dynamics of two interfaces in a hybrid system with jump-type heterogeneity

- 15. Ondrej Polivka (Czech Technical University in Prague, Czech Republic) Numerical simulations of two-phase multicomponent compressible flow in porous media
- 16. Takiko Sasaki (The University of Tokyo, Japan)A second-order time-discretization scheme for a system of nonlinear Schrodinger equations
- 17. Nur Shofianah (Kanazawa University, Japan)Simulation of triple junction motion Ab0 with arbitrary surface tensions Ab0
- Robert Spir (Slovak University of Technology in Bratislava, Slovakia)
 Tracking of cells in Zebrafish embryogenesis by finding centered paths in 4D spatio-temporal structures
- 19. Robert Straka (AGH University of Science and Technology, Poland) Computational model of combustion in rock-melting cupola

Sep. 7 (Sat), 13:00-14:30 Poster session (2)

- 20. Takayuki Narumi (Kwansei Gakuin University, Japan) Three-dimensional pattern formation in a chemotaxis system with logistic source
- 21. Hirotoshi Sato (Kwansei Gakuin University, Japan) Kinematic equation for open curves with tangential velocities
- 22. Kenta Uemichi (Kwansei Gakuin University, Japan) A mathematical model for honeybee comb construction

Abstracts (Posters and Talks in random order)

Robert Straka (AGH University of Science and Technology, Poland)

P || T | Computational model of combustion in rock-melting cupola

Rock melting cupolas are special shaft furnaces used in mineral wool production. Their design is similar as of blast furnaces i.e. tube-like shape with tuyeres and siphon in the bottom, feeding and exhaust pipe in the top. The furnace is fed by mixture of stone and coke and during combustion of coke the stone is melted in very high temperature to produce lava which is used to make mineral wool. Due to high temperatures inside the furnace and rapid oxygen consumption, gasification of coke naturally occurs. Gasification is source of unwanted CO emmision and energy losses. We develop a mathematical model of coke combustion and rock melting in cupola in order to inspect the influence of secondary air tuyeres. The model provide valuable insight in operation of rock-melting cupolas and is able to predict important parameters as lava temperature, flue gas concentrations and temperature and heat losses to the water jacket. The validation of the model will be also presented.

Keywords: multiphase reacting flow, coke combustion, rock melting, mineral wool production

Takiko Sasaki (The university of Tokyo, Japan)

P A second-order time-discretization scheme for a system of nonlinear Schrödinger equations

We propose a new time discretization scheme for a system of nonlinear Schrödinger equations which is a model of the interaction of a non-relativistic particles with different masses. Our scheme is composed of two (complexvalued) linear systems at each time step, and the solution is shown to converge at a second order rate. We report numerical example to confirm the theoretical results. Our idea can be applied to a large class of nlinear PDEs.

Keywords: finite difference method, nonlinear Schrödinger equation

Takayasu Matsuo (The University of Tokyo, Japan)

T A discontinuous Galerkin method based on variational structures

We consider partial differential equations with certain variational structures, which have invariants or dissipation properties in relation to the structure. We propose a unified approach for constructing discontinuous Galerkin schemes based on the variational structure, so that the invariants or dissipation properties are kept in the resulting schemes.

This is a joint work with Yuto Miyatake and Yoshifumi Aimoto.

Pavol Kutik (Slovak University of Technology, Slovakia)

T A Stabilized Finite Volume Numerical Scheme for Solving the Partial Di erential Equation in the Heston Model

The article is aimed to provide a stable numerical scheme, based on the finite volume method discretization, for solving the partial di erential equation arising in the Heston model. In order to build a scheme which does not violate the discrete minimum-maximum principle a diamondcell approximation of the gradient is used and a splitting into an inflow/implicit and an outflow/explicit part is applied. By the use of appropriate weights, a suciently large set of the outflow fluxes are transferred to the corresponding inflow fluxes of the neighbouring nite volumes. We illustrate the stability and accuracy of the scheme on two numerical experiments, the former one with a European binary option and the latter one with a European call option.

Keywords: Finite volume method, Heston model, Stabilized scheme

Petr Knobloch (Charles University, Czech Republic)

T A nonlinear local projection finite element method for convection-diffusion-reaction equations

This contribution is devoted to the numerical solution of convection-diffusion-reaction equations by means of the finite element method (FEM). It is well known that the standard Galerkin discretization is inappropriate if convection dominates diffusion since the approximate solution is usually globally polluted by large spurious oscillations. The usual way of treating dominating convection consists in adding extra terms to the Galerkin formulation, aimed at enhancing the stability of the approximate solution. Among such stabilized FEMs, the local projection stabilization (LPS) method has received some attention over the last decade. Originally proposed for the Stokes problem and extended to the Oseen equations, the LPS method has also been used recently to treat convection-diffusion equations.

We introduce an extension of the LPS FEM and analyze it both in the steady-state and transient settings. In addition to the standard LPS method, a nonlinear crosswind diffusion term is introduced, which accounts for the reduction of spurious oscillations. The time-dependent equation is discretized in time with an implicit one-step theta-scheme. We prove the existence of a solution and, depending on the choice of the stabilization parameter, also its uniqueness. To our best knowledge, this is the first nonlinear discretization for convection-diffusion-reaction equations for which both existence and uniqueness of a solution can be shown. Moreover, we derive error estimates which are supported by numerical studies. These studies demonstrate also a reduction of the spurious oscillations.

Keywords: finite element method; local projection stabilization; crosswind diffusion; convection-diffusionreaction equation; well posedness; time dependent problem; stability; error estimates

Katsuhisa Ozaki (Shibaura Institute of Technology, Japan)

T Accurate Algorithms for Matrix Multiplication with Error-Free Splitting

Recently, we proposed accurate algorithms for matrix multiplication. First, the matrix multiplication is transformed into an unevaluated sum of several floating-point matrices. Next, we evaluate the sum of floating-point matrices by accurate summation algorithms. The algorithm is fast in many cases, compared to component-wise accurate dot product algorithms. We introduce recent progress of our accurate algorithms for matrix multiplication: improvement of error-free spitting, application to interval arithmetic, reduction of working space and so forth as long as time allows.

Kei Nishi (Hokkaido University, Japan)

P Dynamics of two interfaces in a hybrid system with jump-type heterogeneity

We study the behavior of a localized moving pattern arising in an activator-inhibitor-type reaction-diffusion system with heterogeneity. It is well known that front solutions typically appear in bistable systems. When the nonlinearity of the system is slightly perturbed from the odd symmetry, such front solutions are glued together to form a spatially localized pulse (front-back pulse). The front-back pulse exhibits not just traveling but also oscillatory motions via the Hopf bifurcations depending the parameters. The global behaviors of such pulse solutions have already been studied numerically and analytically.

In this study, we consider the traveling pulse dynamics in the jump- type heterogeneous media, in which one constant parameter value jumps up (or down) to another constant value at one point in space. By numerical simulation, it is found that five different behaviors occur through the collision between the pulse and the heterogeneity. Especially, we focus on the sliding motion of an oscillating pulse observed in some parameter regime.

To clarify the mechanism for this behavior, the system is first reduced to a singular limit system, which we call a hybrid system. For hybrid system, the equation for the activator in the original PDEs is replaced by two ODEs for the motion of the interfaces, which are coupled with a PDE for the inhibitor field. It is numerically confirmed that this reduced hybrid system reproduces the pulse dynamics for the original PDEs qualitatively very well.

By applying the center manifold theory near Hopf bifurcation point, the hybrid system is further reduced to finite dimensional ODEs to analyze the sliding motion. The hybrid system facilitates the calculation needed for the reduction. The details will be shown in the poster session.

Keywords: Dynamical System, Reaction-Diffusion Equations, Center Manifold Reduction

Kensuke Aihara (Tokyo University of Science, Japan)

T Solving sparse linear systems with an enhanced implementation of IDRstab

The IDRstab method is often more effective than the conventional Krylov subspace methods for solving large nonsymmetric linear systems. In this talk, we propose an alternative implementation of IDRstab to improve the accuracy of the approximate solutions. Our variant also reduces the computational costs by saving the number of vector updates. Numerical experiments show that our variant is more effective than the original IDRstab for sparse linear systems.

Keywords: linear systems, Krylov subspace method, Induced Dimension Reduction, IDRstab method

Akiko Fukuda (Tokyo University of Science, Japan)

T Conserved quantities of the integrable discrete hungry Lotka-Volterra system

In this talk, we derive new conserved quantities of the integrable discrete hungry Lotka-Volterra system, which has an application to computing eigenvalues of banded matrices, from the characteristic polynomial of the matrices. Conserved quantities of the integrable discrete hungry Toda equation and the box and ball system with M kinds of balls are also presented.

Keywords: Conserved quantities Discrete hungry Lotka-Volterra system Discrete hungry Toda equation Box and ball system

Takeshi Takaishi (Hiroshima Kokusai Gakuin University, Japan)

T Complicated propagation of cracks in a 3 dimensional phase-field model

Complicated phenomenon of crack propagation in 3 dimensional material is studied. Usefulness of the phase field model for 3 dimensional crack growth that Kimura and the author introduce from Francfort-Marigo's energy is verified.

Keywords: Numerical simulation, phase-field, mathematical modeling

Karol Mikula (Slovak University of Technology, Slovakia)

T Surface evolution with tangential redistribution

Authors: Karol Mikula, Mariana Remesikova, Peter Sarkoci and Daniel Sevcovic

We propose several techniques for tangential redistribution of points on evolving surfaces. This is an important issue in numerical approximation of any evolution model, since the quality of the mesh has a significant impact on the result of the computation. We explain the volume-oriented and length-oriented tangential redistribution methods in a general setting of an *m*-dimensional manifold evolving in an *n*-dimensional manifold. After, we apply the proposed techniques to the particular case of mean curvature evolution of surfaces in \mathbb{R}^3 . We explain the numerical approximation of the model and present several experiments illustrating the performance of the redistribution techniques.

Radek Maca (Czech Technical University in Prague, Czech Republic)

P CFD simulation of two phase flow in fluidized bed boiler geometry

This contribution presents the CFD simulation of two phase flow in fluidized bed boiler geometry. The CFD simulation is performed using a free, open source CFD software package OpenFOAM. OpenFOAM provides a wide range of features to solve complex fluid flows. Computations were performed both for 2D and 3D geometry. Partially, 1D model is discussed.

Acknowledgement: Advanced Control and Optimization of Biofuel Co-Firing in Energy Production, project No. TA01020871 of the Technological Agency of the Czech Republic

Keywords: fluidized bed, two phase flow, OpenFOAM

T Segmentation of 3D MRI Images by Degeneare Diffusion Method

The contribution presents a 3D (2D+time) segmentation of the real cardiac MRI data using the level set formulation of the geodesic active contour model and its semi-implicit complementary volume discretization. In particular, the application is focused on the segmentation of the heart ventricles from the cine MRI data. The algorithm is compared to the Allen-Cahn approach, software package SEGMENT and to manually segmented data.

Acknowledgement: Advanced Supercomputing Methods for Implementation of Mathematical Models, project of the Student Grant Agency of the Czech Technical University in Prague No. SGS11/161/OHK4/3T/14

Keywords: image processing, image segmentation, level set, MRI

Masato Kimura (Kanazawa University, Japan)

Continuous and discrete crack propagation models with energy gradient property Keywords: crack propagation, gradient flow

Takayuki Narumi (Kwansei Gakuin University, Japan)

P Three-Dimensional Pattern Formation in a Chemotaxis System with Logistic Source

We study three-dimensional pattern formation in a chemotaxis-diffusion-growth system. In one- and twodimensional domains we have found various nonuniform spatial patterns; however, we still do not know much about pattern formations in three-dimensional domains. In our poster presentation, we will review two-dimensional pattern formations near bifurcation points, and discuss some sufficient conditions for stability of piled-hexagonal patterns in three-dimensional rectangular parallelepiped.

Keywords: chemotaxis, pattern formation, three-dimensional pattern, bifurcation, numerical calculation

Kenta Uemichi (Kwansei Gakuin University, Japan)

P A Mathematical Model for Honeybee Comb Construction

Honeycombs consist of several combs, of which structure is made of the hexagonal two sides. The hexagonal structure has fascinated lots of people, but the mechanism of the emergence has not been unraveled yet. We have examined the behavior of European honeybees at the first stage of comb construction. From the result, we propose a mathematical model for honeybee comb construction.

Keywords: pattern formation, insect, honeybee, taxis

Tohru Tsujikawa (University of Miyazaki, Japan)

T Global solution branches of some shadow system

We consider the stationary problem of a reaction-diffusion-advection system. In order to find clues for the global structure of non-constant solutions of the system, we introduce a shadow system in the limiting case that the advectoin coefficients tends to infinity. Our methods to solve it are based on the bifurcation, singular perturbation, a level set analysis.

Keywords: bifurcation, stationary solution, reaction-diffusion system

Hirotoshi Sato (Kwansei Gakuin University, Japan)

P Kinematic Equation for Open Curves with Tangential Velocities

The kinematic equation was proposed by Brazhnik, Davydov, Mikhailov and Zykov for analyzing the spiral wave motion in an excitable medium. In their paper, they pointed out that if the wave sprouts up or retracts from its free end(s), there is a need to reset the arc-length variable at each time in the equation. In our study, we will refine this ambiguity in the mathematical model of kinematic equation.

Keywords: kinematic equation, pattern formation, spiral wave, BZ reaction

Robert Spir (Slovak University of Technology, Slovakia)

P T Tracking of cells in zebrafish embryogenesis by finding centered paths in 4D spatio-temporal structures Authors: Karol Mikula and Robert Spir

The paper presents numerical algorithms leading to automatic cell tracking and reconstruction of the cell lineage tree during the first hours of animal embryogenesis. We present results obtained for large-scale 3D+time confocal microscopy image sequences of early stages of Zebrafish embryo development. Our approach consists of three basic steps - the image filtering, the cell centers detection and cell trajectories extraction yielding the lineage tree reconstruction. In all three steps we use nonlinear partial differential equations. For the filtering the geodesic mean curvature flow in level set formulation is used, for the cell center detection the motion of level sets by a constant speed regularized by mean curvature flow is used and the solution of the eikonal equation is essential for the cell trajectories extraction. The core of our new tracking method is an original approach to cell trajectories extraction based on finding a centered paths inside the spatio-temporal tubular structures representing cell movement and divisions. The paths are found by using a properly designed distance functions from cell centers detected in every time step and by a backtracking in steepest descent direction of a potential field built from these distance functions. We also present efficient and naturally parallelizable discretizations of the aforementioned nonlinear PDEs and discuss properties and results of our new tracking method.

Keywords: 4D spatio-temporal tracking, cell tracking

Masakazu Akiyama (Hokkaido University, Japan)

P A Mathematical Model of Planar Cell Polarity

In considering the morphogenesis of tissue of multicellular organisms, the orientation of the cell placement is very important. For example, in the inner ear of a person, a function hear the sound is produced by cells called hair cell arranged in a particular direction. The phenomenon caused by individual cells, such as having an asymmetric spatial pattern are called PCP (Planar cell polarity). Not only in hair cells but also in the various organisms and tissue, PCP is seen as a universal phenomenon. Hence many researchers have been study about PCP phenomena. Since easy to control experimental environment and abundance of generic information, There are a lot of study of PCP in Drosophila (Fly). For instance, there is small hair on the wing of Drosophila, the hair has same orientations. This is also function of PCP. Protein that includes the seven-pass transmembrane receptor Frizzled (Fz), the four-pass transmembrane protein Strabismus (Stbm), the golgi-kinase Four-jointed (Fj) and atypical cadherin Dachsous (Ds) in the cell is critical for PCP to work. In Drosophila, PCP molecules such as Ds and F_j may function as global directional cues orienting cellular asymmetry, which is manifested as polarized localization of the PCP core proteins such as Fz. However, the relationship between Ds/Fj gradient slopes and Fz asymmetry in the eye is opposite to that in the wing, thereby causing controversy about how these two systems are connected. In this study, we show our mathematical model which is constructed from only 3 term. Mathematical model is very simple, various aspect of PCP are shown using numerical simulations. To construct model, we proposed the key concept of GLOBAL and LOCAL rules. In the poster, we also show about the relationship these rules and proteins in the cell.

Keywords: Cell Polarity, Mathematical Model, Numerical Simulation

Daisuke Furihata (Osaka University, Japan)

T An iteration method for the numerical solution of the discrete variational derivative schemes

The discrete variational derivative method (DVDM) is a structure-preserving numerical method for partial differential equations.

The obtained schemes inherit the conservation property or dissipation one.

If the original equation is nonlinear, the normal DVDM schemes are nonlinear.

This nonlinearity means that we should pay much computational cost to obtain numerical solutions.

There exists a linear-decomposition technique to consist linear DVDM schemes, but this technique is applicable to only low order polynomial equations.

We consider a new generalized decomposition technique and to use the obtained extended scheme as a predictor of the iteration solver for the original DVDM scheme.

Keywords: discrete variational derivative method, structure preserving, iteration method, predictor

Yasuaki Kobayashi (Hokkaido University, Japan)

P Mathematical modeling of epidermal homeostasis

We present a mathematical model of the epidermis, consisting of keratinocyte dynamics including cell division and hard-core repulsive interactions, and the calcium dynamics based on the one-pool model. We show that experimentally observed calcium localization phenomena under the stratum corneum, which is considered to be important for the epidermal homeostasis, can be reproduced by our model. We further introduce an evaluation function that quantifies the stability of the epidermis and investigate what is responsible for a stable epidermal structure.

Keywords: partial differential equation, dynamical system, reaction-diffusion systems

Yoshiaki Muroya (Waseda University, Japan)

T Global stability of Lotka-Volterra systems with infinite delays and feedback controls

In this talk, to multiple species Lotka-Volterra systems with infinite delays and feedback controls, applying Lyapunov functional techniques, we establish sufficient conditions of the global stability for the unique saturated equilibrium. The feedback controls can be eliminated from the Lyapunov functional, whereas feedback controls have influence on boundedness conditions for the positive density of saturated equilibrium and change the position of a unique saturated equilibrium, and for the saturated equilibrium on the boundary of R^n_+ , we obtain new sharper criteria on stability conditions. Moreover, we extend this to a model with patch structure and obtain the similar result to multi-group SIR epidemic model with patch structure.

Keywords: Lotka-Volterra system, feedback control, saturated equilibrium, global stability, infinite delay MSC: 34K20, 34K25, 92D30

Tomoyuki Idogawa (Shibaura Institute of Technology, Japan)

P Research on an Expansion to the Continuous Version of Morphological Contour Decomposition-Reconstruction Algorithm

We had proposed an algorithm to decompose and reconstruct binary images by using morphological contours. In this algorithm, images were treated as binary discrete ones, namely, were regarded as subsets of Z^2 . In this research, we will try to expand the algorithm to binary but continuous settings (subsets of R^2) and consider the meanings of our "2 contours" in the Euclidean space R^2 .

Keywords: mathematical morphology, image decomposition-reconstruction, continuous setting

Hideki Murakawa (Kyushu University, Japan)

T Convergence rates of discrete-time schemes to approximate nonlinear cross-diffusion systems

This talk is concerned with nonlinear and linear discrete-time algorithms for cross-diffusion systems. The nonlinear scheme corresponds to backward differences in time. The linear algorithm is a very easy to implement scheme we proposed. The main purpose of this talk is to derive convergence rates of the discrete-time schemes. We obtain the same orders for both the nonlinear and the linear schemes. Moreover, these orders are optimal. We also establish uniqueness and regularity results of weak solutions of the cross-diffusion systems.

Keywords: cross-diffusion systems, discrete-time schemes, optimal error estimates, uniqueness

Tetsuya Ishiwata (Shibaura Institute of Technology, Japan)

- P Spiral-shaped solutions to crystalline motion with a rotating tip
- P Structure-preserving finite difference scheme for Heisenberg equation and its application to a vortex filament motion

Harunori Monobe (Meiji University, Japan)

P On a free boundary problem describing cell motility

Norbert Pozar (Kanazawa University, Japan)

T A viscosity approach to total variation flows of non-divergence type

Kota Ikeda (Meiji University, Japan)

P Collective motions of particles with diffusive interactions

Peter Frolkovic (Slovak University of Technology, Slovakia)

T Semi-implicit finite volume level set methods

In this talk we introduce new semi-implicit finite volume discretization method for the numerical solutions of level set advection equation to capture moving interfaces. The method is based on the implicit in time treatment of fluxes at inflow boundaries and the explicit in time treatment of outflow boundaries. The resulting algebraic systems of equations can be solved efficiently using Gauss-Seidel iterative method in four (2d) or nine (3d) directions. Several numerical examples will illustrate the advantages of this method. Some applications like wildland fire spreading or mobing groundwater table will be briefly discussed. This talk is based on the joint work with Karol Mikula and Jozef Urban.

Keywords: advection equation, level set method, finite volume method, semi-implicit method

Koichi Anada (Waseda University Senior High School, Japan)

P Some Features for Blow-up Solutions of a Nonlinear Parabolic Equations

In previous studies we have shown some conjectures for behavior of blow-up solutions to a nonlinear parabolic equations. They are very important features to investigate behavior of solutions near their blow-up time. The purpose of our talk/poster is to prove one of them that we call "weak eventual monotonicity".

Keywords: parabolic equations, blow-up solutions, eventual monotonicity

Daniel Sevcovic (Comenius University, Slovakia)

Plenary T On nonlocal geometric flows and minimization of isoperimetric ratio in relative geometries

We analyze a gradient flow of closed planar curves minimizing the soperimetric ratio in the relative Finsler geometry. For such a flow the normal velocity is a function of the anisotropic curvature and it also depends on the total interfacial energy and enclosed area of the curve. The governing system of equation consists of nonlinear parabolic equations with nonlocal terms. In contrast to the gradient flow for the isoperimetric ratio, we show there exist initial curves for which the enclosed area is decreasing with respect to time. We also derive a mixed anisoperimetric inequality for the product of total interfacial energies corresponding to different anisotropy functions. Finally, we present several computational examples illustrating theoretical results. This is a joint work with Shigetoshi Yazaki.

References

[1] D. Sevcovic and S.Yazaki: On a gradient flow of plane curves minimizing the anisoperimetric ratio, IAENG International Journal of Applied Mathematics 43(3) (2013), 160-171.

[2] D. Sevcovic and S.Yazaki: Computational and qualitative aspects of motion of plane curves with a curvature adjusted tangential velocity, Mathematical Methods in the Applied Sciences, 35(15) (2012), 1784-1798.

[3] D. Sevcovic and S.Yazaki: Evolution of plane curves with a curvature adjusted tangential velocity, Japan J. Indust. Appl. Math., 28(3) (2011), 413-442.

Spectral comparison and gradient-like property for some reaction-diffusion systems

Yoshihisa Morita

Department of Applied Mathematics and Informatics Ryukoku University Seta Otsu 520-0803, Japan morita@rins.ryukoku.ac.jp

ABSTRACT

We are dealing with the FitzHugh-Nagumo equations $u_t = d\Delta u + f(u) - v$, $v_t = \Delta v - \gamma v + u$, and the equations $u_t = d\Delta u - g(u+v) + v$, $v_t = \Delta v + g(u+v) - v$ which have a conservation property, in a bounded domain with the Neumann boundary condition. Those systems with appropriate nonlinearities share the common feature such that the Turing instability takes places, namely a stable constant solution loses its stability in the presence of the diffusion terms. Moreover, the stationary equations of each system can be reduced to a scalar elliptic equation with a nonlocal term, whose solution is given by a critical point of an energy functional.

Our aim is to show the gradient-like dynamics of the semiflow generated by the solutions of each system and the coincidence of the dimension of the unstable manifold of any equilibrium solution and the Morse index of the corresponding critical point of the energy functional. The former result is proved by the presence of the Lyapunov function while the latter is done by the spectral comparison method. These results are based on the recent joint works with Chao-Nien Chen and Shuichi Jimbo.

Key words: Reaction-diffusion system, spectral comparison, Lyapunov function, FitzHugh-Nagumo equations, conservation property.

Michal Beneš Czech Technical University in Prague, Czech Republic michal.benes@fjfi.cvut.cz

Pavel Strachota Czech Technical University in Prague, Czech Republic pavel.strachota@fjfi.cvut.cz

Tomáš Oberhuber Czech Technical University in Prague, Czech Republic tomas.oberhuber@fjfi.cvut.cz

Radek Máca Czech Technical University in Prague, Czech Republic radek.maca@fjfi.cvut.cz

Radek Fučík Czech Technical University in Prague, Czech Republic radek.fucik@fjfi.cvut.cz

Keywords: Two-phase flow; conservation laws; finite-volume method; fluidized bed.

Oral presentation. In the contribution, we present the mathematical model of two-phase flow in fluidized-bed combustors. The model consists of conservation laws for mass, momentum and energy of both phases. The fluidized bed is formed due to the interaction with gravity. The model reflects the bed formation and behaviour. The one-dimensional model describes the integral behaviour of corresponding quantities in the horizontal cross-section of the combustor volume whereas the multidimensional model can provide more detailed information. Numerical solution is obtained by means of the finite-volume method in space and by a higher-order time solver. The model is discussed with respect of the bed formation, reaction to the control parameters and the energy transfer. A series of computational results is presented to demonstrate the model capabilities.

Acknowledgement. The research is supported by the Technological Agency of the Czech Republic through the project No. TA102871.

References

- Beneš M., Oberhuber T., Strachota P., Straka R. and Havlena V.: Mathematical modelling of combustion and biofuel co-firing in industrial steam generators, RIMS Kokyuroku Bessatsu B35 (2012), 141–157.
- [2] Hoang Dieu H., Mach J.: Fluidized Bed Design and Applications. Functional Design Specification MMG 1-12, Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, 2012
- [3] Máca R. and Strachota P.: Solid Gas Flow One-dimensional Numerical Simulation. Functional Design Specification MMG 2-12, Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, 2012

17

Interaction of Dynamically Evolving Dislocations

Michal Beneš Czech Technical University in Prague, Czech Republic michal.benes@fjfi.cvut.cz Petr Pauš Czech Technical University in Prague, Czech Republic petr.paus@fjfi.cvut.cz Jan Kratochvíl Czech Technical University in Prague, Czech Republic kratochvil@fsv.cvut.cz

Keywords: Mean curvature flow; degenerate diffusion; flowing finite-volume method; defects in materials.

Poster. The contribution describes the mathematical model of the glide dislocation motion, interaction with other objects such as dipolar dislocation loops or precipitates, and the topological changes - generation of glide dislocations from the Frank-Read source or annihilation. The model represents the glide dislocations as parametrically described curves moving in the glide planes. The motion law considers the normal velocity given by the line tension and by the forces of external origin as well as the mutual interaction with other objects. The law is reformulated into the parametric form. The redistribution along the tangential direction is incorporated which allows to stabilize the dislocation discretization in the long term simulations using the numerical algorithm based on the flowing finite volume method. The model is generalized to handle the topological changes of the dislocations or during the annihilation by cross slip. As the computational complexity increases with the number of interacting objects considered, the simulation model is designed by advanced computational studies of various dislocation and object configurations including the interaction of glide dislocations with obstacles, encounters in the band channels, sweeping of dipolar loops by glide dislocations, loop clustering and dislocation cross slip annihilation.

Acknowledgement. The research is supported by the project No. P108/12/1463 of the Grant Agency of the Czech Republic.

- Beneš M., Kratochvíl J., Křišťan J., Minárik V. and Pauš P.: A parametric simulation method for discrete dislocation dynamics, European Phys. J. ST 177 (2009) 177–192.
- [2] Minárik V., Beneš M., Kratochvíl J.: Simulation of dynamical interaction between dislocations and dipolar loops, J. Appl. Phys. 107, 1 (2010).
- [3] Pauš P., Beneš M., Kratochvíl J.: Simulation of dislocation annihilation by cross-slip, Acta Physica Polonica A, 122, No. 3 (2012) 509–511.

Numerical simulation of anomalous transport in porous media described by fractional-advection dispersion equation

Michal Beneš Czech Technical University in Prague, Czech Republic michal.benes@fjfi.cvut.cz

> Tissa H. Illangasekare Colorado School of Mines, Golden, U.S.A. tissa@mines.edu

> Dave Dean Colorado School of Mines, Golden, U.S.A. deandw@mail.com

Keywords: FADE; anomalous transport; Levy flights; porous media.

Poster. In the contribution, we present computational studies of the fractional-advection dispersion equation containing the fractional-derivative multidirectional diffusion term which can be responsible for anomalous transport effects. Known justification of this model relies on the relation with the Levy stochastic processes. The solution of the model exhibits anisotropic features and variety of interesting phenomena not observed in the Brownian diffusion. Numerical solution of the transport equation leads to the linear systems of equations with full matrices which slows down the solution process. We couple the transport equation to the single-phase saturated flow in a heterogeneous medium and study the anomalous contaminant transport in it.

Acknowledgement. The research was supported by the project of Czech Ministry of Education, Youth and Sports Kontakt ME10009, and by the project No. SGS11/161/OHK4/3T/14 of the Student Grant Agency of the Czech Technical University in Prague.

- D.A. Benson, S.W. Wheatcraft, and M.M. Meerschaert, Application of a Fractional Advection-Dispersion Equation, Water Resources Reasearch, 36, no. 6 (2000), 1403–1412.
- [2] D.A. Benson, S.W. Wheatcraft, and M.M. Meerschaert, The Fractional-Order Governing Equation of Lévy Motion, Water Resources Reasearch, 36, no. 6 (2000), 1413–1423.
- [3] R.F. Holub, M. Beneš, and Honeyman, B.D., Interfacial Phenomena in Fluid Dynamics: Linking Atomistic and Macroscopic Properties: Can They Explain the Transport Anomalies? in Beneš, M., Mikyška, J. and Oberhuber, T., editors, Proceedings of the Czech Japanese Seminar in Applied Mathematics. Prague: Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, 2005. ISBN 80-01-03181-0, pages 57-62.

General computation of phase equilibrium in multicomponent mixtures

Tereza Jindrová Czech Technical University in Prague, Czech Republic jindrter@fjfi.cvut.cz Jiří Mikyška Czech Technical University in Prague, Czech Republic jiri.mikyska@fjfi.cvut.cz

Mathematical models of phase stability and phase equilibrium computation of multicomponent fluids play an important role in large-scale compositional hydrocarbon reservoir simulations, in interpretation of laboratory experiments which are performed to understand the behaviour of chemical species in hydrocarbon reservoirs, or in multiphase-flow simulations in porous media. Dealing with phase stability and phase equilibrium at constant volume, temperature and moles (the so-called VT-stability and VTflash), we have recently developed a new algorithm for the constant-volume two-phase split calculation (see [1]) based on the direct minimization of the total Helmholtz free energy of the mixture with respect to the mole- and volume-balance constraints. In the contribution, we focus on a general strategy for Nphase equilibrium computation at constant volume, temperature and moles, where $N \in \mathbb{N}$ is the number of phases (see [2]). The problem is formulated using the Helmholtz free energy and two equations of state: the Peng-Robinson equation of state and the Cubic-Plus-Association equation of state. Finally, we present several numerical examples of two-phase and three-phase equilibrium calculations showing the performance of the general algorithm on multicomponent mixtures of different complexity.

Key words

phase equilibrium, constant-volume flash, VT-flash, constant-volume stability, VT-stability, Helmholtz free energy minimization.

- T. Jindrová and J. Mikyška: Fast and Robust Algorithm for Calculation of Two-Phase Equilibria at Given Volume, Temperature, and Moles, Fluid Phase Equilibria (2013) 353, 101–114.
- [2] T. Jindrová: Computational Methods in Thermodynamics of Multicomponent Mixtures, master degree thesis Czech Technical University in Prague (2013).

Computation of two-phase equilibrium in multicomponent mixtures

Tereza Jindrová Czech Technical University in Prague, Czech Republic jindrter@fjfi.cvut.cz Jiří Mikyška Czech Technical University in Prague, Czech Republic jiri.mikyska@fjfi.cvut.cz

The contribution is focused on the investigation of two-phase equilibrium at constant volume, temperature and moles (the so-called VT-flash) in a multicomponent mixture. The problem is formulated using the Helmholtz free energy and two equations of state: the Peng-Robinson equation of state and the Cubic-Plus-Association equation of state. Recently, we have developed a new algorithm for the constant-volume phase-split calculation (see [1]) based on the direct minimization of the total Helmholtz free energy of the mixture with respect to the mole- and volume-balance constraints. The algorithm uses the Newton-Raphson minimization method with line-search and modified Cholesky decomposition of the Hessian matrix to produce a sequence of states with decreasing values of the total Helmholtz free energy. To initialize the algorithm, an initial guess is constructed using the results of stability testing at constant volume, temperature and moles (see [2]). The performance and efficiency of the algorithm are shown on several examples of two-phase equilibrium calculations. In the end, we discuss reasons supporting the fact that the VT-approach seems more natural than the classical formulation at constant pressure, temperature and moles (PT-flash), especially when using pressure-explit equations of state.

Key words

two-phase equilibrium, constant-volume flash, VT-flash, Helmholtz free energy minimization, Newton-Raphson method, modified Cholesky factorization.

- T. Jindrová and J. Mikyška: Fast and Robust Algorithm for Calculation of Two-Phase Equilibria at Given Volume, Temperature, and Moles, Fluid Phase Equilibria (2013) 353, 101–114.
- [2] A. Firoozabadi and J. Mikyška: Investigation of Mixture Stability at Given Volume, Temperature, and Number of Moles, Fluid Phase Equilibria (2012) 321, 1–9.

Algebraic multigrid for Navier-Stokes Problems

Petr Bauer Czech Technical University in Prague, Czech Republic bauerpet@kmlinux.fjfi.cvut.cz Vladimír Klement Czech Technical University in Prague, Czech Republic wlada@post.cz Tomáš Oberhuber Czech Technical University in Prague, Czech Republic tomas.oberhuber@fjfi.cvut.cz Vítězslav Žabka Czech Technical University in Prague, Czech Republic zabkav@gmail.com

Algebraic multigrid is an advanced method for solving systems of equations arising from various numerical problems. On this poster we will describe this method and its implementation (based on [1]) for the simulation of heat equation. We will also point out main differences compared to geometric multigrid, compare the speed of both methods and present modifications needed to implement algebraic multigrid on GPU.

Keywords: Algebraic multigrid, GPU.

- [1] D. Göddeke: Dissertation thesis: Fast and Accurate Finite-Element Multigrid Solvers for PDE Simulations on GPU Clusters, Technischen Universität Dortmund, 2010
- [2] Nils Klimanis: Generic Programming and Algebraic Multigrid, VDM Verlag Dr. Mueller e.K., 2008

GPU multigrid solver for Navier-Stokes problems

Petr Bauer Czech Technical University in Prague, Czech Republic bauerpet@kmlinux.fjfi.cvut.cz Vladimír Klement Czech Technical University in Prague, Czech Republic wlada@post.cz Tomáš Oberhuber Czech Technical University in Prague, Czech Republic tomas.oberhuber@fjfi.cvut.cz Vítězslav Žabka Czech Technical University in Prague, Czech Republic zabkav@gmail.com

In this contribution we present implementation of geometric multigrid solver on GPU. This method will be used to solve problem of air flow simulation in atmospheric boundary layer [4], which is governed by the Navier-Stokes equations for incompressible flow. The problem is discretized by finite elements method [3] with the Crouzeix-Raviart elements [2]. We will describe basic aspects of GPU programming. Based on them we will present modified multigrid algorithm from [1] and obtained speed-up.

Keywords: Multigrid, GPU, Navier-Stokes flow.

- [1] V. V. Shaidurov: Multigrid Methods for Finite Elements. Kluwer Academic Publishers, Dordrecht, 1995.
- [2] M. Crouzeix, P. A. Raviart: Conforming and nonconforming finite element methods for solving the stationary Stokes equations I, Rev. Franc. Automat. Inform. Rech. Operat, 1973
- [3] F. Brezzi and M. Fortin: Mixed and hybrid finite-element methods, Springer Verlag, NewYork, 1991
- [4] P. Bauer: Dissertation thesis: Mathematical modelling of pollution transport in urban canopy, CTU-FNSPE, 2011
- [5] V. Klement: Master's thesis: Implementation of the sparse matrix solvers on the GPU, CTU-FNSPE, 2008

Computational Study of Planar Curve Dynamics

Miroslav Kolář, Michal Beneš Czech Technical University in Prague, Czech Republic kolarmir@fjfi.cvut.cz, michal.benes@fjfi.cvut.cz

Keywords: Planar curve, mean curvature flow, parametric approach, level set method.

The contribution deals with the numerical solution of curve evolution in plane. The smooth curves are described by means of the parametric approach [3] and the level set formulation [1]. Their evolution is given by the equation for the mean curvature flow, which reads as

$$v = -k + F,$$

where v is the normal velocity, k is the mean curvature, and F is the spatially dependent force term bringing nonlinearities to the motion. Parametrized equations for the mean curvature flow are numerically solved by means of semi-implicit finite differences method and flowing finite volumes method [2]. We improve the behaviour and the stability of the numerical algorithm by adding the tangential redistribution of curve discretization nodes. The level set equation is solved by means of the method of lines, and arisen system of ODEs is integrated via the Runge-Kutta-Merson method with adaptive time step. Numerical results contain the computational study of both open and closed curves, parametric study of the redistribution algorithm, and numerical tests of area and length conservation. The comparison of parametric and level set approach is presented.

Acknowledgement. The authors were partly supported by the project "Advanced Supercomputing Methods for Implementation of Mathematical Models", project of the Student Grant Agency of the Czech Technical University in Prague No. SGS11/161/OHK4/3T/14 of the Grant Agency of the Czech Republic.

- K. Deckelnick and G. Dziuk: Numerical Approximation of mean Curvature Flow of Graphs and Level Sets, Mathematical Aspects of Evolving Interfaces (2003), 53–87
- [2] M. Beneš, M. Kimura, P. Pauš, D. Ševčovič, T. Tsujikawa and S. Yazaki: Application of a Curvature Adjusted Method in Image Segmentation, Bulletin of the Institute of Mathematics, Academia Sinica (New Series) (2003) No. 4, 509–523. 437–453.
- [3] D. Ševčovič and S. Yazaki: Evolution of plane curves with a curvature adjusted tangential velocity. Japan J. Industrial and Applied Mathematics (2011) 28, 413–442.

Mathematical Model and Numerical Simulation of Dislocation Dynamics

Miroslav Kolář, Michal Beneš

Czech Technical University in Prague, Czech Republic kolarmir@fjfi.cvut.cz, michal.benes@fjfi.cvut.cz

Keywords: Dislocation, mean curvature flow, parametrization, redistribution, PSB channel.

This contribution deals with the numerical simulation of dislocation dynamics. In the field of solid state physics, the term dislocation describes some irregularity in crystal structure of material (see [1,2]). The presence of dislocations considerably affects many of material properties. The dislocation itself can be modelled as a line defect in crystalline lattice causing the disturbance of the regularity of the crystallographic arrangement of atoms.

From the mathematical point of view, the dislocations are defined as smooth closed or open planar curves which evolve in time. The motion itself is only two-dimensional and is driven by the equation for the mean curvature flow, which reads as Bv = -Tk + F, where v is the normal velocity, k is the mean curvature, and F is the spatially and time dependent external force term acting on the dislocation curve in normal direction. The force F is caused by various stress fields. The coefficient B denotes drag coefficient, and T is the line tension, which is the force causing straightening of dislocation curve.

In this contribution, we describe the evolving curves by parametric (also called direct or Lagrangian) approach, where the family of planar curves is described by a two-dimensional smooth spatially and time-dependent vector function X = X(u,t) called parametrization. This model is solved by means of semi-implicit finite differences method and flowing finite volumes method. However, this aproach exhibits unintended behaviour, since during the time evolution, the grid points can accumulate somewhere, and then can be sparse somewhere else. One way to overcome this problem is to add the tangential velocity to the dislocation motion law, which moves the grid points along the curve (see [3]). Since the tangential terms do not affect the shape of the curve, we can achieve better numerical stability, especially in long-term computation.

The presented numerical results contains the motion of dislocation curves in the so called PSB (persistent slip band) channel, which is a pattern consisting of areas with very high and very low dislocation density.

Acknowledgement. The authors were partly supported by the project "Two scales discrete-continuum approach to dislocation dynamics", project No. P108/12/1463 of the Grant Agency of the Czech Republic.

- P. Pauš, M. Beneš, J. Kratochvíl: Simulation of dislocation annihilation by cross-slip, Acta Physica Polonica A, 122, No. 3 (2012) 509–5011
- [2] V. Minárik, M. Beneš, J. Kratochvíl: Simulation of Dynamical Interaction between Dislocations and Dipolar Loops, Journal of Applied Physics 107, 061802 (2010)

[3] M. Beneš, J. kratochvíl, J. Křišt'an, V. Minárik and P. Pauš: A parametric simulation method for discrete dislocation dynamics, European Physical Journal ST, Special Topics 177 (2009) 177–192

Modeling diffusion in multicomponent mixtures in porous media: overview of available theories, their limitations, and introduction of a generalized Maxwell-Stefan-Darcy approach

Jiří Mikyška

Czech Technical University in Prague, Czech Republic jiri.mikyska@fjfi.cvut.cz Abbas Firoozabadi Reservoir Engineering Research Institute, Palo Alto, CA

Diffusion of components in a multicomponent mixture flowing through a porous medium is an important transport process that needs to be taken into account when simulating problems of gas injection into reservoirs [1]. These models find applications in enhanced oil recovery or CO_2 geological sequestration. In the contribution we discuss available diffusion theories including Fick's law and its generalization, and the Maxwell-Stefan approach to mass transfer [2]. We will show several limitations of these models related to modeling of the molecular diffusion in porous media. Although some of these limitations have been described in the literature, it seems that many authors in the porous medium community are not aware of them. Identifying these limitations leads us to the proposition of a new generalized Maxwell-Stefan-Darcy model describing transport of several chemical species in the porous medium. We will discuss the basic assumptions and formulation of this model. At the end, we will present some desirable features of the new model and indicate some future extensions of this approach.

Keywords

diffusion, multicomponent mixture, Fick's law, Maxwell-Stefan model, Darcy's law, compositional model

- H. Hoteit, and A. Firoozabadi: Numerical modeling of diffusion in fractured media for gas-injection and recycling schemes, SPE Journal (June, 2009) 323–337.
- [2] R. Krishna, and J. A. Wesselingh: The Maxwell-Stefan Approach to Mass Transfer, Chem. Eng. Sci (1997) 52 861–911.

Compositional Modeling of Two-Phase Multicomponent Compressible Flow in Porous Media

Ondřej Polívka

Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Czech Republic ondrej.polivka@fjfi.cvut.cz

Jiří Mikyška

Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Czech Republic jiri.mikyska@fjfi.cvut.cz

Keywords

Two-Phase Compressible Multicomponent Flow, Mixed-Hybrid Finite Element Method, Finite Volume Method, Newton-Raphson Method, Phase-by-Phase Upwinding, Constant-Volume Phase Splitting.

Abstract

In the contribution, we present the numerical model of two-phase compressible multicomponent flow in porous media. The mathematical model is formulated by means of partial differential equations representing the conservation laws, extended Darcy's laws, and by means of the conditions of local thermodynamic equilibrium in a form of algebraic relations describing the pressure and the distribution of components between the phases. Appropriate initial and boundary conditions are prescribed.

The formulated problem is solved numerically using the Mixed-Hybrid Finite Element Method [1, 2] for Darcy's law discretization, and the Finite Volume Method [3] for the component transport equations discretization. To discretize the component fluxes across the boundaries of the elements a special upwind technique is used. The time discretization is carried out by the backward Euler method [3]. The resulting system of nonlinear algebraic equations is solved by the Newton-Raphson iterative method. The derived numerical scheme ensures the local mass balance and correct treatment of the phase fluxes between elements in a way that no phase identification and decisions on the corresponding phases is necessary.

- [1] F. Brezzi, M. Fortin. Mixed and Hybrid Finite Element Methods. Springer-Verlag, New York Inc. (1991).
- [2] G. Chavent, J. E. Roberts. A unified physical presentation of mixed, mixed-hybrid finite elements and standard finite difference approximations for the determination of velocities in waterflow problems. Advances in Water Resources, 14(6) (1991), pp. 329–348.
- [3] R. J. Leveque. *Finite Volume Methods for Hyperbolic Problems*. Cambridge University Press, Cambridge (2002).

Numerical Simulations of Two-Phase Multicomponent Compressible Flow in Porous Media

Ondřej Polívka

Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Czech Republic ondrej.polivka@fjfi.cvut.cz

Jiří Mikyška

Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Czech Republic jiri.mikyska@fjfi.cvut.cz

Keywords

Two-Phase Compressible Multicomponent Flow, Enhanced Oil Recovery, CO₂ Sequestration, Mixed-Hybrid Finite Element Method, Finite Volume Method, Newton-Raphson Method.

Abstract

On the poster, we show a few numerical simulations of two-phase compressible multicomponent flow in porous media which occurs in many engineering problems like enhanced oil recovery or CO_2 sequestration. We simulate injection of different gases into horizontal and vertical reservoirs filled with different species and two-phase flow of the mixture.

Equations describing this kind of flow consist of the conservation laws, extended Darcy's laws, and means of the conditions of local thermodynamic equilibrium. Our numerical solution of the problem is based on a combination of the Mixed-Hybrid Finite Element Method [1, 2] for Darcy's law discretization, and the Finite Volume Method [3] for the component transport equations discretization. The system of equations is linearized by the Newton-Raphson iterative method.

- [1] F. Brezzi, M. Fortin. Mixed and Hybrid Finite Element Methods. Springer-Verlag, New York Inc. (1991).
- [2] G. Chavent, J. E. Roberts. A unified physical presentation of mixed, mixed-hybrid finite elements and standard finite difference approximations for the determination of velocities in waterflow problems. Advances in Water Resources, 14(6) (1991), pp. 329–348.
- [3] R. J. Leveque. *Finite Volume Methods for Hyperbolic Problems*. Cambridge University Press, Cambridge (2002).

Optimal Value of a Firm Investing in Exogenous Technology

Pedro Pólvora

September 2013 Tokyo,Japan

Abstract

We study the optimal value for a Firm whose value is function of an exogenous technology level. At any point in time the Firm can invest in a new technology, incurring in an immediate cost and in return it will become able to use that technology yielding profit through a given profit flow function. The technology is modelled by a discrete stochastic process with a time-dependent arrival rate. We study the optimal stopping time that will correspond to the point in time when the firm will invest. We use a dynamic programming approach, finding the Hamilton-Jacobi-Bellman equation whose solution gives us the optimal value of the firm. We particularise for two cases, one with a constant arrival rate and the other with a time-dependent and non-monotonic arrival.

Multiphase Volume-preserving Interface Motions via Localized Signed Distance Vector Scheme

Rhudaina Z. Mohammad¹ and Karel Svadlenka²

¹Graduate School of Natural Science and Technology, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192 rhudaina@polaris.s.kanazawa-u.ac.jp

> ²Institute of Science and Engineering, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192 kareru@staff.kanazawa-u.ac.jp

Abstract

We develop a signed distance vector approach for approximating volume-preserving mean curvature motions of interfaces separating multiple phases – a variant of the MBO (Merriman-Bence-Osher) thresholding dynamics. We use vector-type discrete Morse flow and adopt a variational method, which allows us to easily treat volume constraint via penalization without having to change the threshold value. Moreover, the method is designed to allow subgrid accuracy on uniform grids without adaptive refinement; thereby, alleviating the well-known MBO time and grid restrictions.

Keywords: multiphase flow, signed distance vector, mean curvature motion, volume preservation, constrained variational method, MBO thresholding

1

Simulation of Triple Junction Motion with Arbitrary Surface Tensions

¹Nur Shofianah, ²Rhudaina Z. Mohammad and ³Karel Svadlenka

¹Graduate School of Natural Science and Technology, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192 viena_shofianah@yahoo.com
²Graduate School of Natural Science and Technology, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192 rhudaina@polaris.s.kanazawa-u.ac.jp
³Institute of Science and Engineering, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192 vience and Engineering, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192 kareru@staff.kanazawa-u.ac.jp

Abstract

We aim at simulating triple junction motion that is given by the gradient flow of surface energy with arbitrary surface tensions of the individual interfaces. The fundamental method is the diffusion-based BMO algorithm in vector-valued formulation. We modify the original BMO method, so that it can accommodate motions for any triple of given surface tensions. The main idea of the modification is to change the coefficients in the underlying diffusion system and the reference vectors, which correspond to the position of wells in the phase-field method. Analysis and numerical results of this generalized BMO algorithm are presented.

Keywords: triple junction motion, gradient flow of surface energy, surface tension, vector-valued thresholding.

Numerical computation of motion of interface networks with nonlocal constraints

Karel Svadlenka¹, Rhudaina Z. Mohammad², Nur Shofianah²

¹Institute of Science and Engineering, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192 kareru@staff.kanazawa-u.ac.jp

²Graduate School of Natural Science and Technology, Kanazawa University Kakuma-machi, Kanazawa, Japan 920-1192

Abstract

Numerical approximation of gradient flow of surface energy for networks of interfaces including junctions is considered. Moreover, the volume of each region surrounded by the interfaces is to be preserved. The main tool is the thresholding algorithm due to Merriman, Bence and Osher, which is reformulated in a vector-valued fashion and suitably modified. Analysis of interface velocity and junction stability under this new algorithm will be presented. The treatment of arbitrary surface tensions will also be mentioned.

Keywords: curvature-dependent interface motion, nonlocal constraints, triple junction stability, thresholding method

Talk

	Surname	Name	Japanese expression	Institution	Talk	Poster
1	Abe	Kuniyoshi	阿部邦美	Gifu Shotoku University	-	-
2	Aihara	Kensuke	相原研輔	Tokyo University of Science	Х	-
3	Akiyama	Masakazu	秋山正和	Hokkaido University	-	Х
4	Anada	Koichi	穴田浩一	Waseda University Senior High school	-	Х
5	Benes	Michal	ミハル・ベネシュ	Czech Technical University in Prague	X	X
6	Chalupecky	Vladimir	ヴラディミール・ハルペツキー	Fujitsu	-	-
7	Frolkovic	Peter	ペテル・フロルコヴィッチ	Slovak University of Technology	Х	-
8		Akiko	福田亜希子	Tokyo University of Science	X	-
9		Daisuke	降旗大介	Osaka University	X	-
10		Tomoyuki	井戸川知之	Shibaura Institute of Technology	-	X
11		Kota	池田幸太	Meiji University	-	X
12		Emiko	石渡恵美子	Tokyo University of Science	-	-
13		Tetsuya	石渡哲哉	Sibaura Institute of Technology	-	x
14		Takahiro	伊藤貴大	Kanazawa University		^
14			げ藤貝へ テレザ・インドロバー	-	x	x
		Tereza		Czech Technical University in Prague	-	-
16		Yohei	鹿島洋平	University of Tokyo		-
17		Masato	木村正人	Kanazawa University	X	-
18		Vladimir	ヴラディミール・クレメント	Czech Technical University in Prague	Х	X
19		Petr	ペトル・クノブロフ	Charles University	Х	-
20		Yasuaki	小林康明	Hokkaido University	-	X
21	Kolar	Mirosla∨	ミロスラフ・コラージュ	Czech Technical University in Prague	Х	X
22	Kutik	Pavol	パボル・クチーク	Slovak University of Technology	Х	-
23	Maca	Radek	ラデック・マーツァ	Czech Technical University in Prague	Х	Х
24	Matsuo	Takayasu	松尾宇泰	The University of Tokyo	Х	-
25	Mikyska	Jiri	イジー・ミキシュカ	Czech Technical University in Prague	Х	-
26	Mikula	Karol	カロル・ミクラ	Slovak University of Technology	Х	-
27	Mohammad	Rhudaina Z.	ルダイナ・ムハンマド	Kanazawa University	-	Х
28		Harunori	物部治徳	Meiji Institute for Advanced Study of Mathematical Sciences	-	X
29		Yoshihisa	森田善久	Ryukoku University	x	-
30		Hideki	村川秀樹	Kyushu University	X	-
31		Yoshiaki	室谷義昭	Waseda University	X	-
32		Masaharu	長山雅晴	Hokkaido University	-	-
33		Masaaki	中村正彰	Nihon University		_
34		Takayuki	鳴海孝之		_	x
				Kwansei Gakuin University	_	-
35		Kei	西慧	Hokkaido University	-	X
36		Yasumasa	西浦廉政	Tohoku University	-	-
37	<u> </u>	Toshiyuki	小川知之	Meiji University	-	-
38		Seiro	小俣正朗	Kanazawa University	-	-
39		Katsuhisa	尾崎克久	Shibaura Institute of Technology	Х	-
40		Ondrej	オンドレィ・ポリーフカ	Czech Technical University in Prague	Х	X
41	Polvora	Pedro	ペドロ・パルヴォラ	Technical University of Lisbon	Х	-
42	Pozar	Norbert	ノルベルト・ポジャール	Kanazawa University	Х	-
43	Sakamoto	Takashi	坂元孝志	Meiji University	-	-
44	Sasaki	Takiko	佐々木多希子	The University of Tokyo	-	Х
45	Sato	Hirotoshi	佐藤宏俊	Kwansei Gakuin University	-	X
46	Sevcovic	Daniel	ダニエル・シェフチョヴィッチ	Comenius University	Х	-
47	Shofianah	Nur	ショフィアナ・ヌル	Kanazawa University	-	X
48		Robert	ロベルト・シュピール	Slovak University of Technology in Bratislava	Х	x
49		Robert	ロベルト・ストラッカ	AGH University of Science and Technology	X	X
50		Karel	カレル・シュヴァドレンカ	Kanazawa University	X	-
51		Takeshi	高石武史	Hiroshima Kokusai Gakuin University	x	-
52		Takeshi Tohru	局石武史 辻川亨	University of Miyazaki	X	-
52 53	-				-	- X
		Kenta	上道賢太	Kwansei Gakuin University	-	-
54	Yazaki	Shigetoshi	矢崎成俊	Meiji University	-	