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# High accuracy compact difference schemes for differential equations in mathematical sciences

## Prof. Murli M. Gupta

Our work on high order compact difference schemes was initiated about 35 years ago when we first presented new 4th and 6th order discretizations for convection-diffusion equations in 2-dimensions. This work is now routinely applied to complex fluid flow problems, and has also been developed for 3-dimensional differential equations. In our quest to apply these ideas to the biharmonic equation, we discovered that it is beneficial to carry the unknowns and their derivatives as computational parameters. This allowed us to propose the streamfunction-velocity formulations for the Navier-Stokes equations.

In this presentation, I would describe the historical developments of the high order compact difference schemes and their evolution into the powerful computational techniques that are now available to solve fluid flow problems of important physical interest. Some theoretical analysis on stability and convergence of these schemes will be presented. I would also present ideas for future works.

# Nonlinear stability of Rayleigh-Benard convective flows

Prof. Pradeep G. Siddheshwar

Weakly nonlinear and local nonlinear stability analyses shall be discussed leading to various versions of the Lorenz and Ginzburg-Landau equations. Need for additional modes in the Lorenz model and the importance of the cubic-quintic Ginzburg-Landau equation shall be dwelt upon. The importance and distinct possibility of making such an analyses with realistic boundary conditions and for specific liquids shall be highlighted. Dynamical situations giving rise to nonautonomous systems and ways of handling them shall also be presented. In addition to primary, secondary instabilities shall also be dealt with.

# Ψ-v computation of flow past sharp edges in uniform and accelerated flow

Prof. Jiten C. Kalita

We present two compact finite difference schemes on nonuniform Cartesian grids without transformation for the Biharmonic form of the Navier-Stokes equation: one for the steady [1] and the other, for the unsteady state. Employing the later one, we then carry out numerical investigations of the unsteady wake for flow past sharp edges in uniform and accelerated flow. As test cases, we have chosen the flow past a flat plate and a wall mounted wedge for a wide range of Reynolds numbers. For the flat plate in uniform flow, numerical results are presented for the steady state regime up to Reynolds number Re=20 and unsteady flow executing vortex shedding up to Re=100. For the accelerated case, we present results for Re=400. For the wedge, we have specifically chosen the famous Pullin and Perry [3] experiment as our model problem where flow is simulated for Re=6873 with wedge angle 60° for a much longer duration than the actual lab experiment. All the typical

three-fold structure of the starting vortex observed by Lian and Huang [4] was confirmed by our simulation. In all the cases, our results compare very well with established numerical and experimental results.

Reference

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## Nonlinear thermohaline convection

## Prof. Yadagiri Rameshwar

Linear and weakly nonlinear properties of thermohaline convection at the onset are investigated for the stress-free boundary conditions using perturbation analysis. Linear stability analysis is studied by plotting graphs for different values of physical parameters relevant to the ground water and oceanic water. The nonlinear governing equations describing the motion, temperature and concentration are expanded in the sequence of non-homogeneous linear equations, which depend on the solutions of the linear stability problem. The dependence of heat transfer rate on thermal Rayleigh number, solutal Rayleigh number, Lewis number and thermal Prandtl number is extensively examined up to sixth order using an expansion of R as proposed by Kuo [1]. The results of flow field and heat transfer characteristics are depicted in the form of streamlines and isotherms (hot regions), respectively. To trace the path of convective heat transport, the concept of heat function has been employed. This methodology explains the comprehensive interpretation of energy distribution in terms of heatlines.

## Reference

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## A hyperbolic-elliptic splitting method for barotropic fluid equations with inertiatype regularization

Prof. Keh-Ming Shyue

Our goal in this talk is to describe a fractional-step approach based on the hyperbolicelliptic operator splitting for an efficient numerical approximation of barotropic fluid equations with inertia type regularization. In the algorithm, we will consider examples arising from both the theory of water wave (the Serre-Green-Naghdi equations) and the theory of bubbly fluids (the Iordanski-Kogarko-Wijngaarden equations). Sample numerical results will be present to validate the proposed method.

## Magnetohydrodynamic modeling of thermal plasma flow and its application to directcurrent plasma torch

Prof. Shiu-Wu Chau

Direct-current plasma torch is a widely adopted thermal plasma device applied to various industrial applications, where high-temperature plasma jets are produced due to the substantial interaction between neutral working gases and arc columns. The applied electric arc principally works as the main energy provider to accelerate the plasma flow along with elevating its temperature to obtain the required processing abilities. A steady magnetohydrodynamic model is proposed in this paper to describe the thermal plasma flow of a direct-current plasma torch, where the continuity, momentum and energy equations incorporated with a turbulence model are considered to depict the dependence among the flow velocity, working pressure and gas temperature of the plasma jet subjected to an applied electric accompanied by a self-induced magnetic field. The azimuthal velocity accompanied by a self-induced magnetic field. The

## component is also considered in the proposed model for capturing the significant rotational motion of plasma flow as a consequence of tangential inflow design. The thermal plasma is assumed electrically neutral, optically thin and in local thermal equilibrium. The

time-averaged solution is employed because of a mean operation engineering focus. For reactive thermal plasmas, the transport equations of charged particles described by a driftdiffusion approximation as well as the transport equations of the neutral species are modeled following the chemical and plasma kinetics among different plasma components. The energy balance equation of electron is furthermore introduced when the non-thermal equilibrium plasma is considered. The governing equations are segregated solved on a Cartesian grid via a finite volume discretization, where a linear parallelization is achieved through the MPI library. The proposed numerical scheme is implemented in an in-house code PTCAX. Several applications of the direct-current plasma torch are discussed in this paper to disclose the complex physics of thermal plasma flow interacting with a directcurrent arc.

Keywords: magnetohydrodynamic modeling, thermal plasma, direct-current, plasma torch.

## **Two-dimensional continuum simulation of dense granular flows using the regularized μ(I) rheology** Prof. Fu-Ling Yang

Predicting dense granular flow dynamics has been a challenging task for researchers and engineers as the material exhibits the characteristic behavior of viscoplastic fluids that it flows only in regions where local stress magnitude exceeds a yielding threshold. After set into motion, shear-thinning rheology is observed in granular flows and a so-called local  $\mu(I)$ rheology law has been proposed from fitting among data from particle-based simulations and experimental measurements. The nonlinear dependence of local  $\mu(I)$  on flow velocity and its singular behavior near flow cessation makes analytic solution nearly impossible while posing challenges to numerical simulation.

Here, we present how we handle the singularity in the local  $\mu(I)$  relation by the regularization method to develop a dense granular flow solver with the Pressure-Implicit-Splitting-Operator (PISO) method and the finite volume method. Furthermore, we extend the solver to incorporate non-local momentum transport due to enduring grain friction with a second regularization. The local and the non-local flow solver are applied to two generic flow problems (simple shear flows and surface inclined flows) to examine the effect of non-local momentum transport on bulk dynamics.

## Optimal design of airfoil using direct-forcing immersed boundary modeling

Prof. Ming-Jyh Chern

Wind energy is an important renewable energy source. A wind turbine is commonly used to covert flow energy to electrical energy. In the present study, the blade design of the wind turbine using computational fluid dynamics (CFD) coupled with genetic algorithm (GA) is discussed. The blade shape is the most significant effective factor in the wind energy conversion. Hence, an optimal method for the cross-section of blade is established to get the better efficiency for producing the higher lift and lower drag to drive the wind turbine. According to the literature, the Genetic Algorithm (GA) is known to be the robust method in the optimal design area. The real-coded Genetic algorithm is considered since it is able to solve the defect of binary code. That is, the chromosomes

length is too long to code. While the PARSEC parameterization method is used to represent the shape of airfoil through the eleven parameters as the control variables. Furthermore, a direct-forcing immersed boundary (DFIB) method is employed for simulations of interaction of rotating blades in a flow field at a moderate low Reynolds number. Numerical results reveal that the shape of airfoil can be optimized and the proposed DFIB model coupled with GA successfully simulates the moving blade in flow field for obtaining the high performance.

Keywords: immersed boundary method, air foil, ray-casting algorithm, genetic algorithm.

## Application of smoothed particle hydrodynamics (SPH) for modeling open channel and overland flows

## Prof. Kao-Hua Chang

In hydraulics, open channel and overland flows are the common flow characteristics in rivers and floodplains, respectively. The scale of a real-world case involving either a river or a floodplain is usually large. Thus, a shallow water model, in which the shallow water equations (SWEs) solved using a numerical method, is developed to conduct numerical prediction. A Lagrangian meshless and particle method called smoothed particle hydrodynamics (SPH) is introduced. It has three attractive features for solving the SWEs: (1) complex boundary geometries, such as watershed outlines, can be flexibly constructed without mesh limitations in simulations; (2) there are no nonlinear convective terms in the SWEs, i.e., the propagation of dynamic waves is simulated without numerical dispersive errors associated with the discretization of the nonlinear

convective terms; and (3) wet/dry bed transitions are described without special treatment. In this study, we propose one- and two-dimensional well-balanced and positivitypreserving SPH-SWE models to improve the traditional SPH-SWE models. The first property to preserve the motionless steady state solution for non-flat bottom topography is satisfied by solving the continuity equation describing the water surface level. As to the second property, an additional condition derived from temporal discretization to determine the time step size forces the water depth to be positive. Two study cases including a one-dimensional Chicago area waterways system and a twodimensional partial dam-break flow are adopted. The proposed models are validated by comparison with the measured data, and their performance are also addressed when applied to practical hydraulic problems.

Keywords: smoothed particle hydrodynamics, shallow water equations, well-balanced, positive-preserving.

## Large bubble entrapment due to a falling drop on a liquid surface

Prof. Gautam Biswas

When a drop of a liquid falls through air to impact on the liquid-air interface of a liquid pool, depending on the size and velocity of the drop, it may become partially or completely coalesced in the liquid, or splash. The transition between complete coalescence and splashing proceeds via a number of intermediate steps, such as thick and thin jet formation and air-bubble entrapment and vortex-ring formation. The impact of the drop on the interface can produce a crater in the liquid pool. The crater produced by the drop impact, expands radially and closes at the top to entrap a large bubble. The large bubble entrapment takes place if the prolate shaped drop impacts onto a liquid pool. Researchers have classified different forms of the bubble entrapment scenario on a velocity versus drop-diameter map (V-D map). On the traditional classification map, the large bubble entrapment zone occupies a small region. Wang et al. [1] experimentally observed large bubble entrapment outside heretofore reported small region of the 16

traditional V-D map. This new finding raised two questions in the mind of the researchers. The first question is, "How does the large bubble entrapment take place?", and second question is, "What is the exact boundary of large bubble entrapment regime on the V-D map?". Thoroval et al. [2] reported that the entrapment of large bubble is a vortex driven phenomena. The vortex deforms the interface and produces an elongated roll jet, which then collapses on the central axis to entrap the large bubble. However, the exact boundary of large bubble entrapment regime on the V-D map is still unexplored. In this work we have attempted to find out the exact regime of large bubble entrapment on the V-D map. Within the given range of aspect ratio variation of the impacting drop, we have been able to draw a conclusion about the boundary of large bubble entrapment regime.

The entrapment of large bubble is always accompanied by a high speed inward jet which is commonly known as Worthington jet and an outward jet. The inward jet and the outward jet start to emerge as the liquid tongue merges at the top of the crater to entrap the bubble. The inward liquid jet moves downward and penetrates the bubble. [1]. A.-B. Wang, C.-C. Kuan, and P.-H. Tsai, "Do we understand the bubble formation by a single drop impacting upon liquid surface?" Physics of Fluids 25, 101702 (2013)

[2]. M.-J. Thoraval, Y. Li, and S. T. Thoroddsen, "Vortex-ring-induced large bubble entrainment during drop impact," Phys. Rev. E 93, 033128 (2016)

## **Bubble Dynamics for some applications of Boiling**

Prof. Gautam Biswas

The bubble formation sites in film boiling are the nodes of instability occurring at the liquidvapor interface. We perform simulations to capture periodic cycles of bubble release from the nodes and antinodes.

The transition in interfacial instability behavior occurs with increase in superheat, the bubble release being periodic both in space and time. Discrete bubble growth occurs at a smaller superheat whereas vapor columns form at the higher superheat values.

Application of electric field results in shorter bubble separation distances, faster growth of the instability, and higher bubble release frequency. Increasing the electric-field intensity shows an increase in the space averaged Nusselt number, thus indicating the role of electric field in the enhancement of heat transfer.

The change in dynamics of bubble growth due to increasing superheat at a high intensity of electric field is also studied. The effect of increasing intensity of electric field on the heat transfer rate at different superheats is determined. The boiling characteristics are found to be influenced significantly only above a minimum critical intensity of the electric field.

A threshold intensity of applied electric field is required to achieve a significant effect in bubble morphology and heat transfer rate. In the reduced gravity condition, the electrohydrodynamic forces are the dominant reasons for the instability at the interface. Hence, the electric field can be utilized to acquire the same heat transfer rate during boiling as in the earth's condition. The vapor generation rate can also be controlled.

## Autophoretic motion of an isotropic particle

Prof. Te-Sheng Lin

We study the spontaneous autophoretic motion of an isotropic particle by considering the dynamics of a two-dimensional circular shaped particle immersed in the Stokes flow. The particle is assumed to be chemically patterned uniformly and its surface either emits or absorbs surrounding solute particles. The solute concentration is governed by the advection-diffusion equation that is solved numerically by ultraspherical-Fourier spectral method. It is found that the particle exhibits symmetry-breaking behavior as well as chaotic-like motions.

# Flame-front instabilities and acceleration in outward propagation

Prof. Kuo-Long Pan

Flame propagation has revealed profound fluid-dynamic characteristics and significance in myriads of practical problems such as industrial furnaces, aircraft/rocket combustors, internal combustion (IC) engines, and gas turbines. The motions of flames are dominant in the performance of combustion specifically concerned by the efficiency, energy transformation and pollutant release. Comprehension and predictability paving the way for optimum design of the devices, however, are often frustrated by the inherent complexity owing to the interplays of fluid dynamics, heat and mass transfer, and chemical reactions. In an effective approach, the sophisticated structure is decomposed into a minimum set of elemental units of significance while isolating the others not in focus. Specifically, we have computationally investigated the propagation of a premixed flame under the influence of external flow such as turbulence and clarified the roles of inherent flame-front instability that appears as a hydrodynamic type and external flow,

forcing in terms of vortices, as reported in [1]. This work succeeded our previous studies that identified the role of Darrieus-Landau (D-L) instability in wrinkling the flame fronts and achieved a preliminary insight to the pattern formation in the evolution of nonlinear flame motion [2,3]. The clarification for the key mechanisms would help establishment of an effective turbulent flame model which is in such an imminent need for engineering design of efficient burners with low emission of pollutants. In addition, our study on the outward expansion of a cylindrical flame [4], which simulates the propagation of a spherical flame surface after ignition, investigates self-acceleration caused by the selfsimilar structure that leads to a universal behavior for various compositions and test conditions. This issue is closely related to many reacting flow processes such as combustion and knocks in IC engines, and formations of explosion waves in mines and supernova (in which thermonuclear flames exhibit rapid reactions in an analogous form as that presented in combustion). The contribution is particularly emphasized on the elucidation of the diversity of the key growth exponent as well as the corresponding fractal dimension that had been debated in the literature. Furthermore, we have unequivocally demonstrated that it is the coupling of environmental noises and the hydrodynamic instability to cause the flame acceleration and self similarity [5]. In

addition, recognizing the growing significance of gravity in a larger dimension such as supernova and strongly buoyant flow on earth associated with slowly moving flames, we have studied the roles of hydrodynamic instability and body forces which present various patterns in different regimes of propagation velocity, as summarized in [6,7]. In particular, an initially slow flame is first accelerated by wrinkling via the D-L instability and further distorted by the ensuing Rayleigh-Taylor (R-T) instability when the expansion scale grows to such a level that the gravitational field becomes dominant. The studies shed more light on the mechanisms underlying the formation of explosion waves which is critical to the utilization of hydrogen energy and fire prevention.

Reference

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## Lattice Boltzmann simulations of turbulent flows Prof. Chao-An Lin

Lattice Boltzmann method has achieved considerable success in simulating hydrodynamic problems and the significant advantages of the LBM are explicit, easy to implement, and natural to parallelize. Despite the above merits, there are several issues commonly addressed to improve the lattice Boltzmann method predicting capability, such as the simulation of turbulent flows. With the use of graphic processing unit, LBM can perform large scale turbulence simulations. There test cases will be used to demonstrate this capability, i.e. turbulent channel flows with and without periodic hills and turbulent duct flows.

## A nonlinear elimination preconditioner for fully coupled space-time solution algorithm for hyperbolic PDEs Prof. Feng-Nan Hwang

As the computing power of the latest parallel computer systems increases dramatically, the fully coupled space-time solution algorithms for the time-dependent PDEs obtain their popularity recently for temporal domain parallelism. In this space-time algorithm, we solve the resulting large, space, nonlinear systems in an all-at-once manner. A robust and efficient nonlinear solver plays an essential role as a critical kernel of the whole solution algorithm. In this talk, we introduce some nonlinear preconditioned Newton algorithm for the space-time formulation of Burgers' equation with shock presented. In that case, the history of the nonlinear residual norm for the classical Newton method suffers from a long stagnation period due to strong local nonlinearity. To overcome the difficulties, we apply an adaptive nonlinear elimination preconditioning technique to enhance the robustness of the inexact Newton method, in the sense that the number of inexact Newton iterations required to converge is almost independent of both of the time-step and the mesh sizes.

## A direct-forcing immersed boundary projection method for simulating fluid-solid interaction problems

Prof. Suh-Yuh Yang

We introduce a simple direct-forcing immersed boundary projection method for simulating the dynamics of fluid-solid interaction problems, in which the immersed rigid solid object can be stationary or moving in the fluid. The main idea of this direct forcing approach is that we first consider the solid object as a portion of the fluid and then introduce a virtual force, which is distributed only in the whole solid object region, appended to the momentum equations to make the region acts exactly as if it were a solid rigid body immersed in the fluid. After introducing the momentum forcing, we employ a second-order in time Choi-Moin projection scheme over a staggered Cartesian grid to discretize the resultant system on the entire domain including the portion occupied by the

solid body. The most advantageous feature of this approach is that the time-discrete virtual force can be explicitly determined in the projection solution process such that the internal velocity boundary condition at the immersed solid boundary is satisfied. This direct forcing approach can also be applied to study the heat transfer phenomena in fluid-solid interaction problems if we additionally introduce a virtual heat source to the energy transport equation. Numerical experiments are performed to illustrate the simplicity and efficient performance of the proposed direct-forcing method. We find that our numerical results are in very good agreement with the previous works in the literature.

## Numerical simulation of the unstable Boycott effect in incline water columns

## Prof. Yi-Ju Chou

We present three-dimensional simulations of sedimentation of suspended solids in inclined vessels using an Eulerian-Lagrangian model developed specifically for the study of solid-liquid mixtures. The simulation results reveal the three-dimensional vortical flow structures that follow the occurrence of flow instability and induce strong mixing between the particle-laden and clear-fluid layers. The vortices and turbulence result in significant resuspension from the particle-laden layer and weaken the convective effect that enhances sedimentation. We show that for the present flow condition and particle size, particle inertia plays an important role in particle resuspension. Analysis of the release of potential energy is presented to examine the sedimentation efficiency under different flow conditions. The analysis for cases with different particle sizes shows that the faster settling associated with larger particles stabilizes the flow by reducing the interfacial shear while settling. From simulation results using various angles of inclination, we can find the optimal angle of inclination to achieve the greatest efficiency in settling enhancement. Finally, critical modeling aspects, including the importance of different forcing terms and two- or three-dimensional considerations, are discussed. 30

## **An equilibrium tendentious car-following model** Prof. Yao-Hsin Hwang

The present study aims at developing a microscopically equilibrium tendentious carfollowing model based upon a macroscopically continuous traffic flow model, which is designed to fulfill some practical requirements in traffic experiences. Simple finitedifference tactics are employed to obtain the equivalently discretized form to ensure equilibrium condition. Using the stability analysis and practical model practicing, it is shown that the resulting car-following will predict an equilibrium tendentious characteristic inherent in the original continuous model. Numerical calculations also provide reasonable results to highlight the feasibility of present model for further modification as well as simulating more complicated traffic phenomenon.

## Scientific computing for solving computational aeroacoustics problems

Prof. Yogesh G. Bhumkar

In this talk, application of a physical dispersion relation preserving (DRP) scheme will be discussed in detail for solving computational aeroacoustics problems, accurately. A newly developed optimized five stage Runge-Kutta time integration scheme (been based on the low storage formulation), provides accurate solutions at a considerably higher time step as compared to other widely used multistage time integration schemes in the literature. Developed scheme has the ability to add numerical diffusion as and when required in an adaptive manner. Solutions of the model problems involving propagation, reflection and diffraction of sound have been obtained to demonstrate the accuracy of the developed scheme and its applicability to solve complex problems. Solutions for sound emission due to turbulent fluctuations in the rocket exhaust during launch operation will be reported. Further simulation results for generation of Aeolian tones due to flow past bluff bodies will be discussed in detail.

## Coupled chemotaxis fluid model with dynamic free surface

Dr. Filip Ivancic

Suspension of an oxytactic bacteria (e.g. the species Bacillus subtilis) placed in a container with its upper surface open to the atmosphere results in the formation of complex bioconvection patterns. The bacteria consume the oxygen diluted in the water, thereby causing the decrease of oxygen concentration everywhere except on the free surface. Through the free surface, which is in direct contact with the air, oxygen diffuses into the water. Slightly denser than water, the oxytactic bacteria are able to swim towards the higher concentration of oxygen (i.e. upwards) and they concentrate in a thin layer bellow the free surface. This causes the change of the suspension density and Rayleigh–Taylor type instabilities to occur. The chemotaxis phenomenon has been successfully modeled within continuum mechanics approach under certain simplifications. The set of (nonlinearly) coupled equations describing the process involves the Boussinesq approximation

of the Navier–Stokes equations governing the fluid motion and two convection–diffusion type equations governing the bacteria and oxygen concentrations. One of the simplifications that might significantly influence numerical simulations is the boundary condition for fluid equation on the free surface. This condition ensures that the vertical component of the velocity is zero, thus keeping the position of free surface fixed. This assumption significantly simplifies numerical procedure since the non-linearly coupled system can then be solved on stationary grid. However, allowing the motion of the free surface and completing the system with appropriate boundary conditions on contact line (liquid-solid-gas interface), a more realistic model is derived and new insights on nonlinear dynamics of the chemotaxis phenomenon are obtained. Our aims are to upgrade the currently available model into a more realistic one in both two and three dimensions, to propose a numerical procedure to deal with the new system (now posed on time-depended domain) and, finally, to show the difference between this new model and the previous simplified one.

Keywords: chemotaxis–convection–diffusion, bioconvection, time–dependent domain, moving grid, Arbitrary Lagrangian–Eulerian framework, surface tension, dynamic contact line.

# Higher order compact scheme for time deforming domains

Prof. Shuvam Sen

In this work we report development of fourth order compact scheme for incompressible Navier-Stokes (N-S) equations in time varying domain. Sen [J. Comput. Phys. 251 (2013) 251–271] put forward an implicit compact finite difference scheme for unsteady twodimensional convection-diffusion equation. It is now further extended to simulate fluid flow problems on deformable surface using curvilinear moving grids. The formulation has been tested in conjunction with modern numerical grid deformations techniques such as inverse distance weighting (IDW) interpolation. Adequate emphasis is provided to approximate grid matrices up to the desired level of accuracy and freestream preserving property has been numerically examined. To the best of our knowledge this is the first higher order compact method that can directly tackle non-conservative form of N-S

equation in single and multi-block time dependent complex regions. The proposed methodology has been validated by computing analytical solution of flow decayed by viscosity problem. It is then applied to lid driven cavity problem before finally testing the scheme for vortex formation in case of a circular cylinder oscillating in cross flow. The results obtained are in good agreement with computational and experimental results available in literature, thereby establishing efficiency and accuracy of the proposed algorithm.

## Viscous fingering in radial displacement of immiscible reactive fluids: Effects of produced surfactants

## Prof. Ching-Yao Chen

Numerical simulations are performed on an immiscible reactive interface where a less viscous fluid is injected to displace a more viscous fluid. Surfactants are produced on the viscous unstable instable interface to complicate the fingering instability. A highly accurate phase-field method is applied in the present study. Effects of various dimensionless control parameters are evaluated systematically, such as the Damkohler number, the Atwood number and inject number, which represent the reaction rate, injection strength and viscous contrast, respectively. Because of the formation of fountain flow within the finger, the produced surfactants tend to accumulate on the sides of fingers, and result in more vigorous side-branching instability. In particular conditions of intermediate Damkohler number and inject number, the interfacial tension appears apparent variation along the interface because of significant accumulation of surfactants of the sides of fingers. Non-monotonic trend of the prominence of fingering instability, observed in the experiments, are also qualitatively reproduced by numerical simulations as shown in the figure. 37

# Stability analysis of a three-dimensional chemotaxis system

Dr. Symphony Chakraborty

Complex bioconvection patterns have been studied previously only for a flat free-surface of a suspension of chemotaxis bacteria in a chamber (shallow/deep). We have performed linear and weakly nonlinear stability analyses using a perturbation technique for a threedimensional chemotaxis-diffusion-convection system in a shallow chamber with deformed free-surface. The influence of aggregation of chemotactic cells on the deformed free-surface of a shallow chamber is studied analytically. The aim of our research is to investigate the nature of the instability in the chemotaxis-diffusionconvection system. We performed a detailed linear stability analysis of a steady-state cell and oxygen concentration distribution. The system becomes dominated by nonlinear convection terms beyond a critical Rayleigh number [Ra]\_τ which also depends on the critical wavenumber k as well as the other parameters. We have investigated that how the

critical Rayleigh number in this system varies with three different sets of parameters. A weakly nonlinear analysis is carried out as well to determine the relative stability of the pattern formation at the onset of instability. A reactance between rolls, squares, hexagons and mixed modes pattern is investigated in detail. Further research should link the weakly nonlinear analysis with the bifurcation analysis.

## Immersed boundary-Lattice Boltzmann method for flow inside an ion channel

Dr. Kumar Saurabh

In the study of ion-channel flow, continuum model; based on Poisson and Nernst-Planck equations (PNP), has been widely used. Although, the applicability of continuum approach for ion channel flow has been debated, it has been shown, repeatedly, to capture the properties of ion-channel fairly accurately. In addition to that, several improvements have been made to standard PNP models in order to remediate its short comings. One such approach is the introduction of Lennard-Jones potential to account for the ion-ion interaction and steric effect. In order to descritize this system of equations for ion channels, finite difference and finite element are quite popular. These methodologies, while solving ion-channel flows, assumes simplification of channel geometry and application on a body confirming grid. One rarely used approach is Lattice boltzmann method (LBM). LBM has been shown to accurately capture the flow properties for the

same system of equation (PNP) inside a micro channel. This study focuses on the application of Lattice Boltzmann Method for solving ion- channel flow. The system is represented by Modified PNP equations. Kong's combining rules are used for the calculation od ionic interactions. Further, direct forcing based immersed boundary method has been used to accomodate for complex geometry.

Keywords: ion-channel flow, IB-LBM, steric effect

