2016 CASTS MINI-WORKSHOP: MODELING, SIMULATION AND ANALYSIS OF BOUNDARY LAYERS

WORKSHOPS

CASTS
理論科學研究中心
Center for Advanced Study in Theoretical Sciences

2016. 5 . 12-13

Large eddy simulation of atmospheric boundary layer

Prof. Yu-Ting Wu

In this study, a large-eddy simulation framework is developed for simulating turbulent boundary layer flows. The framework involves solving the continuity equation, the momentum equation written in rotation form, and the scalar transport equation. The numerical scheme is based on a mixed pseudospectral finite-difference method, i.e., spatial derivatives are computed using pseudospectral representation in the horizontal directions and finite differences in the vertical direction. As a result, the lateral boundary conditions are periodic. The top boundary condition is a fixed stressfree lid. The bottom boundary condition consists of using similarity theory (Monin–Obukhov similarity) to calculate the instantaneous (filtered) surface shear stress as a function of the velocity field at the lowest vertical grid point. The code is fully dealiased using the 3/2 rule (Canuto et al. 1988) and time advancement is done using a secondorder accurate Adams–Bashforth scheme. The turbulent subgrid-scale stresses are parameterized with a tuning-free Lagrangian scale-dependent dynamic model.

The LES code is developed using Fortran 90 programming language together with the Message-Passing Interface (MPI) and Open Multi-Processing (OpenMP) for running on high-performance computing platforms. The parallel algorithm in the code is designed based on the following methods: (1) apply 1D domain decomposition with MPI parallelization along the vertical direction (z); (2) preserve pseudo-spectral (FFT) differencing using OpenMP parallel programing in x-y planes; and (3) maintain Boussinesq incompressible flow model. Both blocking and non-blocking communications have been used in the LES code. In particular, the latter allows the overlap of computation and communication, and greatly increases computation efficiency.

The developed LES framework has been widely used in previous studies associated with wind energy and atmospheric boundary layer. We will present a summary of recent efforts that we make LES a more reliable tool to study land-atmosphere interactions.

Boundary layer solutions of charge conserving Poisson-Boltzmann equations with variable dielectric coefficients

Prof. Chiun-Chang Lee

In this talk, some latest results for the asymptotic behavior of radial solutions of the charge conserving Poisson-Boltzmann (CCPB) equation over a bounded annular domain will be introduced. Under the Robin boundary conditions coming from the capacitance effect of the electric double layer, we establish the leading order term of the boundary layer solutions as the ratio of the Debye length to the length of the physical domain tends to zero. In particular, our results provide a theoretical point of view to see how the dielectric constant and ionic valences affect the potential difference in the electric double layer. This is a joint work with Tai-Chia Lin and Jhih-Hong Lyu.

新型原子力顯微鏡結合奈米探針工程術之應用

Prof. Feng-Sheng Kao

此次演講將分享本研究團隊如何利用新型原子力顯微鏡(Atom Force Microscope, AFM)，結合奈米探針工程技術，將表面特性分析技術往前推進一大步。新型態掃描模式的發明讓原子力顯微鏡的功能大幅提升，已經可以得到與形貌解析度相近的表面力學特性，如變形量、軟硬度、黏性等等。除了基本的物理力學特性外，在探針表面修飾不同的化學分子，讓材料分子的特徵被強化，在奈米尺度仍然可以區分出分子間作用力的差異，辨識材料的表面特性，即為分子辨識力顯微鏡(Molecular Recognition Force Microscope, MRFM)[1]。此項技術特別在材料的水中電性、親疏水性、表面能、抗汙能力...等等有相當出色的應用。本研究報告將以幾個材料研發過程與業界的案例，闡述新穎AFM的應用領域。

[1]. Barattin, R.; Voyer, N., Chemical modifications of AFM tips for the study of molecular recognition events. Chemical communications 2008, (13), 1513-32.

掃描探針顯微鏡技術及在過濾膜電性分析上的應用

Prof. Jen-You Chu

本次報告分兩個部分，第一個部分主要介紹掃描探針顯微技術原理及一般人所不知道的掃描探針顯微技術，並報告本團隊如何開發探針工程技術，將掃描探針顯微技術帶入一個全新的分析領域，及本團隊如何應用在軟物質的材料分析，產生突破性的發展。第二部分主要介紹工研院所開發的帶電過濾膜分析技術，所使用的高分子電解質(Polyelectrolyte, PolyE)材料應用在許多水處理濾膜的產品，其膜電位表現與膜性能之間的關係非常重要，本團隊開發新的膜電位分析方法，並研究以PolyE奈米纖維為基礎的逆滲透或奈濾膜的電性與特性之間的關係，通過使用掃描探針技術和跨膜電位分析的結果，結果證明其脫鹽效率是與表面電雙層(Electric Double Layer, EBL)和唐南排斥(Donnan Exclusion)效應有關聯性[1]

[1]. A.A. Hussain, S.K. Nataraj, M.E.E. Abashar , I.S. Al-Mutaz , T.M. Aminabhavi, J. of Membrane Science 310, 321–336, (2008).

Pseudospectral Poisson solver for Poisson-Nernst-Planck type equations: Green function approach

Prof. Chun-Hao Teng

In this talk we present a pseudospectral penalty approach for constructing Green-function-like solution operators for Poisson equations. The construction methodology is based on mimicking the analytic Green function approach for Poisson equations. Such a framework leads to a numerical solution expression which is an analogue of the classical Green function solution representation, and the constructed numerical solver can be used for simulating Poisson-Nernst-Planck type equations.

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Prof. Hung-Chi Kuo

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Stability of Boundary Layer Solutions of Poisson-Nernst-Planck Systems

Dr. Chia-Yu Hsieh

The Poisson-Nernst-Planck (PNP) system has been widely used to describe the ion transport of ionic solutions, and plays a crucial role in the study of many physical and biological problems. In order to see Debye layers, which occur in ionic liquids near electrodes and have many applications in the fields of chemical physics and biophysics, boundary layer solutions need to be investigated. If the Robin boundary condition is imposed for the electrostatic potential, the PNP system admits a boundary layer solution as a steady state. We study the stability of boundary layer solutions of PNP system. By transforming the perturbed problem into another parabolic system with a new and useful energy law, we prove that the H^{-1}-norm of the solution of the perturbed problem decays exponentially.