the nanostructures is based on finite elements method.The proposed models can be used in standard applications of the finite element software packages or molecular dynamics packages in order to study the elastic properties of graphene and diamond-like structures.

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10:40–Function Hall C

Matching boundary conditions for lattice dynamics

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We develop a new class of accurate and efficient absorbing boundary conditions, named as matching boundary conditions (MBC's), which are used to suppress spurious reflections at artificial boundaries for molecular dynamics simulations of crystalline solids. For one dimensional chains, MBC's render the form of a linear combination of displacement and velocity at atoms near the boundary, with the coefficients determined by matching the dispersion relation of the lattice vibrations. For multiple dimensional lattices, we construct multi-directional MBC's via operator multiplications, which considerably improve the absorption in all directions. Furthermore, MBC's for diatomic chains are proposed, which can treat both the acoustic and optical phonons simultaneously. The effectiveness of MBC's for spurious reflection suppression is verified by reflection coefficient analysis and numerical studies. MBC's are compact and local in both space and time, therefore applicable to nonlinear lattices. The design and implementation are straightforward.

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11:00–Function Hall C

Molecular model of skeletal muscle contraction

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It was generally regarded that changing the filament load would lead to the proportional change of the force on individual working motors during skeletal muscle shortening. However, recent experiment has convincingly demonstrated that individual myosin motors maintain a force of about 6 pN during a working stroke at a wide range of shortening velocities. To understand how such force "homeostasis" can be so precisely regulated in an apparently chaotic system, here we develop a mechanics model stringent down to the molecular level, which reveals that the unique force-stretch relation of myosin motor and the stochastic behavior of actin-myosin binding cooperatively cause the average number of working motors to increase in linear proportion to the filament load, so that the force on each working motor is regulated at 6 pN, in agreement with experiment.

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FM04: Compressible flow
13:49–14:40, Thursday, 23 August
Takeshi Sugimoto, Japan, Chair
Hong Yan, China, Chair
Room: Function Hall C

13:49–Function Hall C

Aerothermal optimization of hypersonic vehicle leading edge based on genetic algorithm

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This work is concerned with the design of a leading edge for hypersonic vehicles used to minimize the peak heat flux of the leading edge. The leading edge is parameterized by using B-spline curve method. The hypersonic flow field and the heat flux distribution around the leading edge is evaluated by computational fluid dynamics. Genetic algorithm is used to obtain a novel leading edge shape that greatly reduces the peak heat flux of the leading edge. The aerothermal design of a 2D leading edge with the thickness of 5 mm was carried out in the design condition Mach 6.5 and no flight attack angle. The peak heat flux reduced about 20% compared to the circular leading edge, and the optimization result is also effective with the attack angle less than 15°. Besides, the result is confirmed by different Mach number, wall temperature, altitude and thickness of the leading edge.

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13:52–Function Hall C

Development of the $\gamma - Re_{\theta_t}$ transition model for high speed flows

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The objective of the paper is to further the understanding of the transition to turbulence mechanism at high speeds. The main focus is on the transition happens in high-speed flow that caused by back pressure and separation. The $\gamma - Re_{\theta_t}$ transition model suggested by Langtry and Menter is used as the baseline model. Regarding the modification and development, a shock correction and a modification of the separation function were proposed. In particular, the shock correction is used to damp the artificially rapid increase of turbulent kinetic energy when shock waves exist. The modification of the separation fuction is to implement the effect of pressure gradients into the modeling of transition process in a separation bubble. Numerical simulation of a double ramp case showed that the modified model predicts the transition process as well as the size of the separation bubble correctly.

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