NATIONAL TSING HUA UNIVERSITY

DEPARTMENT OF POWER MECHANICAL ENGINEERING 2014 Fall Semester

Course No.: 10310 PME 510200

Course Title: Multiscale Transport (多尺度傳輸)

(Fluid, Molecule and Quantum Particle Flows)

Hours/Week: T6 T7 T8

Classroom: エー館 R 209

Teacher: Prof. Che-Wun Hong (洪哲文教授)

Contents:

(1) Introduction to Multi-scale Transport

- 1.1 Development of Multi-scale Transport in Physics
- 1.2 Classical Physics and Modern Physics
- 1.3 Macroscopic and Microscopic Models
- 1.4 Micro Flow Examples
- 1.5 Macro Flow Development
- 1.6 Kinetic and Transport Properties of Fluids
- 1.7 General Boundary Conditions

(2) Macro Flow Models (The Navier-Stokes Equation)

- 2.1 Fundamental Equations
- 2.2 Conservation of Mass (Continuity Equations)
- 2.3 Conservation of Momentum (Navier-Stoke Equations)
- 2.4 Conservation of Energy (1st Law of Thermodynamics)
- 2.5 Summary of the Basic Equations
- 2.6 Examples of Boundary Conditions
- 2.7 Orthogonal Coordinate System
- 2.8 Mathematical Characters of the Basic Equations
- 2.9 Dimensional Analysis and Dynamic Similarity
- 2.10 Summary of the Basic Equations in CFD
- 2.11 Control Volume Formulations
- 2.12 Integral Form of the Generic Conservation Equation

(3) Analytical Solutions of the Continuum Flow

- 3.1 Classification of Solutions
- 3.2 Couette Flows
- 3.3 Poiseuille Flow through Ducts
- 3.4 The Circular Pipe: Hagen-Poiseuille Flow

- 3.5 Combined Couette-Poiseuille Flow between Plates
- 3.6 Noncircular Ducts
- 3.7 Temperature Distribution in Fully Developed Duct Flow
- 3.8 Thermal Entrance: The Graetz Problem
- 3.9 Creeping Flow (Low Reynolds Number Flow)

(4) Numerical Solutions of the N-S Equations (CFD)

- 4.1 Differential Form of the N-S Equations
- 4.2 Integral Form of the N-S Equations
- 4.3 Mathematical Characters of the Basic Equations
- 4.4 Finite Difference Methods for Elliptic Problems
- 4.5 Finite Difference Methods for Parabolic Problems
- 4.6 Finite Difference Methods for Hyperbolic Problems
- 4.7 Finite Difference Methods for CFD
- 4.8 Finite Volume Methods for CFD
- 4.9 Finite Element Methods for CFD

(5) Micro Flow Models (The Boltzmann Equation)

- 5.1 Basic Equations for Micro Flows
- 5.2 Rarefied Gas Flows
- 5.3 Basic Kinetic Theory
- 5.4 The Boltzmann Equation
- 5.5 The Moment of the Boltzmann Equation
- 5.6 Conservation Equations
- 5.7 Exact Solution to the Boltzmann Equation
- 5.8 Micro Flows and Macro Flows

(6) Numerical Solutions of the Lattice Boltzmann Model (LBM)

- 6.1 From the Boltzmann Equation to the Lattice Boltzmann Equation
- 6.2 BGK Lattice Boltzmann Model in 3D and 2D
- 6.3 Entropy and Equilibrium Distribution
- 6.4 Flow Chart of the BGK LBM Algorithm
- 6.5 Boundary Conditions
- 6.6 More Boundary Conditions

(7) Nano Flows (Molecular Dynamics and Monte Carlo)

- 7.1 Macro, Micro, and Nano Scales
- 7.2 Intermolecular Potential Models
- 7.3 Periodical Boundary Condition
- 7.4 Initialization
- 7.5 Equilibration
- 7.6 Fluid and Solid Mechanics

- 7.7 Radial Distribution Function
- 7.8 General Monte Carlo Methods
- (8) Quantum Flows (The Schrödinger Equation)
 - 8.1 Development of Quantum Mechanics
 - 8.2 The Born Interpretation
 - 8.3 Classical Wave Equations
 - 8.4 The 1-D Simple Harmonic Oscillator
 - 8.5 Wavefunction for a Free Particle
 - 8.6 Wavefunctions in the Presence of Potential Forces
 - 8.7 Numerical Method for the Schrödinger Equation
 - 8.8 The Particle in a Box
 - 8.9 The Finite Square Well
 - 8.10 The Square Potential Barrier
 - 8.11 Electron, Photon and Phonon Statistics
 - 8.12 Unified Quantum Fluid Dynamics and Quantum LBM
- (9) Computational Quantum Mechanics (CQM) ← depends on time left

Lecture Notes: Supplement notes provided by PDF before each lecture

- **References:** (1) "Viscous Fluid Flow" F.M. White, 3rd Ed., McGraw-Hill, 2006 (N-S Eq.)
 - (2) "Computational Methods for Fluid Dynamics", J.H. Ferziger, M. Peric, Springer, 2002. (CFD)
 - (3) "Molecular Gas Dynamics and the Direct Simulation of Gas Flows", G.A. Bird, Clarendon Press, 1994. (DSMC+MD)
 - (4) "Lattice-Gas Cellular Automata and Lattice Boltzmann Models- An Introduction", D. A. Wolf-Gladrow, Springer, 2005 (LBM)
 - (5) "Modern Physics", 3rd Ed., R.A. Serway, C.J. Moses, C.A. Moyer, Thomson, 2005 (Schrodinger Eq.)

Grades: Exercises (20%)

Midterm Exam (40%), close book Final Report and Presentation (40%)