

NATIONAL TSING HUA UNIVERSITY
DEPARTMENT OF POWER MECHANICAL ENGINEERING
2011 Fall Semester

Course No.: PME 510200
Course Title: **Multiscale Transport (多尺度傳輸)**
(Fluid, Molecule and Electron Flows)
Hours/Week: T3 T4 R4
Classroom: 工一館 R 209
Teacher: Prof. Che-Wun Hong (洪哲文教授)

Objective: This course covers the classical physics and modern physics developed from 19th to 21st centuries. The contents introduce the multiscale transport phenomena of fluid particles (continuum), molecules (non-continuum), electrons and photons (particle-wave duality). Mathematical models of each scale of flow models are derived and their exact solutions as well as numerical solutions will be explained. This is a general course for senior undergraduates, postgraduates from every background, including thermofluids, solid mechanics, optoelectronics, MEMS/NEMS groups.

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-Stokes 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)
 - 3.10 Lubrication Theory
- (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)

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) Introduction to Quantum Mechanics (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 Particle Statistics

8.12 Quantum Fluid Dynamics and Quantum LBM

(9) Computational Quantum Mechanics (CQM)

9.1 Introduction

9.2 3-D Schrödinger Equation

9.3 Exact Solutions and Molecular Orbitals

9.4 The Periodic Table

9.5 General Poly-electronic Systems

9.6 The Energy of a General Poly-electronic System

9.7 The Hartree-Fock and Roothaan-Hall Equations

9.8 Ab Initio Method

9.9 Semi-empirical Methods

9.10 Density Functional Theory (DFT)

9.11 Multiscale Transport Examples

Lecture Notes: Supplement notes provided by PDF before each lecture

- References:**
- (1) “Viscous Fluid Flow”
F.M. White, 3rd Ed., McGraw-Hill, 2006
 - (2) “Molecular Gas Dynamics and the Direct Simulation of Gas Flows”, G.A. Bird, Clarendon Press, 1994.
 - (3) “Lattice-Gas Cellular Automata and Lattice Boltzmann Models- An Introduction”, D. A. Wolf-Gladrow, Springer, 2005
 - (4) “Modern Physics”, 3rd Ed., R.A. Serway, C.J. Moses, C.A. Moyer, Thomson, 2005
 - (5) “Simulating the Physical World: Hierarchical Modeling from Quantum Mechanics to Fluid Dynamics”, 4th Ed., H.J.C. Berendsen, Cambridge Univ. Press, 2007

Grades: Exercises (20%),
Midterm Exam (40%), close book
Final Exam (40%), open book