# NATIONAL TSING HUA UNIVERSITY DEPARTMENT OF POWER MECHANICAL ENGINEERING 2013 Fall Semester

Course No.:	PME 510200
Course Title:	Multiscale Transport (多尺度傳輸)
	(Fluid, Molecule and Quantum Flows)
Hours/Week:	T6 T7 T8
<b>Classroom:</b>	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)

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) 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

Lecture Notes: Supplement notes provided by PDF before each lecture

### References: (1) "Viscous Fluid Flow"

F.M. White, 3<sup>rd</sup> 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", 3<sup>rd</sup> Ed., R.A. Serway, C.J. Moses, C.A. Moyer, Thomson, 2005 (Schrodinger Eq)
- (6) "Simulating the Physical World: Hierarchical Modeling from Quantum Mechanics to Fluid Dynamics", 4<sup>th</sup> Ed., H.J.C. Berendsen, Cambridge Univ. Press, 2007
- Grades: Exercises (20%) Midterm Exam (40%), close book Final Report and Presentation (40%)