PX921-7.5 Micro & Nano Flows across Scales & Phases

21/22

Department
    Physics
Level
    Taught Postgraduate Level
Module leader
    Nicholas Hine
Credit value
    7.5
Assessment
    60% coursework, 40% exam
Study location
    University of Warwick main campus, Coventry

Description

Introductory description

N/A.

[Module web page](#)

Module aims

Provide students with techniques to model small-scale flows, which necessitate the inclusion of complex interfacial dynamics and the adoption of theories that go beyond the Navier-Stokes-Fourier paradigm. Introduce students to multiscale modelling methods that connect microscopic physics to engineering-scale system properties.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

The module will cover two of the topics listed below, which will differ from year to year.

Topic 1: Interfacial phenomena
a. formulation of surface tension driven flows

i. dynamic BC, kinematic BC, Young's law
b. exemplars
i. statics (capillary rise, Young-Laplace equation)
ii. dynamics (stability of jets/films, cavitation of bubbles, thin films)
iii. wetting (moving contact line paradox, dynamic contact angles)
c. additional nanoscale physics
i. slip conditions (underlying physics, models,
ii. disjoining pressures (for film breakup)
iii. thermal fluctuations (in stability problems)
Topic 2: Kinetic theory for gas microflows
d. Grad's method
e. Chapman-Enskog expansions
f. NSF derivation and models that go beyond (e.g. G13)
Topic 3: Molecular dynamics for liquid nanoflows
g. non-equilibrium Molecular Dynamics (algorithms, thermostats, controllers)
h. nano-channel flows
i. carbon nanotube membranes
j. open-source codes (mdFoam+, LAMMPS)
Topic 4: Multiscale fluid dynamics
k. domain decomposition
l. the Heterogeneous Multiscale Method (HMM)
m. time-step multi-scaling
n. applications in micro/nano-scale internal flows
o. machine learning and surrogate micro-model generation.

Learning outcomes

By the end of the module, students should be able to:

- Understand the limitations of classical fluid dynamics.
- Recognise circumstances in which additional microscale physics is required.
- Be confident in formulating models that go beyond NSF.
- Be able to solve computationally the formulated models.

Indicative reading list

Topic 1: Capillarity & Wetting Phenomena: Drops, Bubbles, Pearls & Waves, by deGennes et al
Topic 2: Macroscopic Transport Equations for Rarefied Gas Flows, by Struchtrup
Topic 3: Computer Simulation of Liquids (2nd Edition). M. P. Allen & D. J. Tildesley, Clarendon Press
Topic 4:
W. E, B. Engquist, X. Li, W. Ren, E. Vanden-Eijnden, Heterogeneous multiscale methods: a review, Commun. Comput. Phys. 2 (2007) 367–450.
K.M. Mohamed, A.A. Mohamad, A review of the development of hybrid atomistic-continuum methods for dense fluids, Microfluid. Nanofluid. 8 (2010) 283–302.

Subject specific skills

Understand the limitations of classical fluid dynamics;
Recognise circumstances in which additional microscale physics is required;
Be confident in formulating models that go beyond NSF.
Be able to solve computationally the formulated models.

Transferable skills

Programming, modelling, data analysis

Study

Study time

Type	Required
Lectures	6 sessions of 2 hours (75%)
Practical classes	2 sessions of 2 hours (25%)
Total	16 hours

Private study description

Reading etc

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group D

	Weighting	Study time
Computational Project (1 of 2)	30%	10 hours
Based on topic 1.		
Computational Project (2 of 2)	30%	10 hours
Based on topic 2.		
Viva Voce examination	40%	5 hours
30 Mins. On the core material.		

Feedback on assessment

-\tWritten annotations to submitted computational notebooks\r\n-\tVerbal discussion during viva voce exam\r\n-\tWritten summary of viva performance

[Past exam papers for PX921](#)

Availability

Courses

This module is Core optional for:

- Year 1 of TPXA-F344 Postgraduate Taught Modelling of Heterogeneous Systems

This module is Core option list A for:

- Year 2 of TPXA-F345 Postgraduate Taught Modelling of Heterogeneous Systems (PGDip)