KNOWLEDGE INCUBATION FOR TEQIP, IIT KANPUR

TEQIP Workshop on Rarefied & Microscale Gases and Viscoelastic Fluids: A Unified Framework

February 23-March 2, 2017

Non-equilibrium flows, such as rarefied flows through micro/nano-channels and around vehicles operating at high altitudes, are now widely studied flows because of their applications in many areas of engineering including MEMS devices. Considering the ongoing focus of research/industries on micro/nano scale technologies, it is important to have a graduate level course such as “Rarefied and Microscale Fluid Flows”. Such a course would not only prepare graduate students for working on state-of-the-art research problems, but also would train them to suit to the changing job requirements in the market. Therefore, TEQIP course on Rarefied & Microscale Gases and Viscoelastic Fluids: a Unified Framework was organized with the aim of disseminating the knowledge in this interesting subject. The audience included faculty members/post-graduate students from NITs/Engineering Colleges, young engineers from R&D labs. The experts chosen to deliver the lectures were academicians, and not only working in the said area, but are also teaching the same at their Institutes. The course was conducted through lectures, case studies and assignments.

TOPICS DISCUSSED

- History of Rarefied & Microscale Gasdynamics (RMG)
- Introduction to (Physical & Mathematical) Fluid Dynamics and CFD
- Uniqueness of Mesoscale Modeling of RMG and Various Methods
- Continuum Breakdown and the Need for Molecular Description of Fluid Flows
- Molecular Dynamics Simulations: An Introductory Address
- Gas Kinetic Theory and Boltzmann Equation
- Method of Moment, 2nd Law of Thermodynamics, Cumulant Expansion and Balanced Closure
- 2nd-Order NCCR, NCCR-Burgers and Method of Iteration
- Non-equilibrium Gas Flows and The Boltzmann Transport Equation
- Introduction to the DSMC Method
- RMG-External Flows (Compressible Shock Wave and Incompressible Flow over a Sphere)
- Role of Surface Radiation in Micro-heat Exchanger
- Δp in Incompressible Laminar Micro-Convective Flow with Variable Properties of Compressible Fluid (air)
- Reactive Cross-Section Database for Air Chemistry for use in DSMC
- RMG-Internal Flows (Langmuir & Maxwell Slip/Jump, Poiseuille Flow)
- Modeling of Some Interesting Non-equilibrium Flow Problems by the DSMC Method
- Multi-physics Modeling in the Particle based Computational Framework
- Analytical Solutions of Force-Driven Poiseuille Flow and Knudsen Layer and Thermal Effects
- Second-Order Boltzmann-Based Non-Navier Non-Fourier Constitutive Laws and Their Validation via MD
- Lattice Boltzmann Method (LBM) Framework for Modeling of Low-speed Microscale Flows
- Mesoscale Modeling of Polyatomic Gas and NCCR in Phase Portraits
- Multi-dimensional Extension of NCCR via Decomposition
- Search for Higher-Order Continuum Transport Equations
- 2-D, 3-D Mixed DG Method for 2nd-Order Model and Parallelization
- Continuum Mechanics, Constitutive Modeling of Viscoelastic Fluids, and HWNP
- Unified Framework: Boltzmann-Based 2nd-Order Model for Viscoelastic Fluids, and Challenging Topics in RMG

SPEAKERS

- **Professor Rho Shin Myong**
  Department of Aerospace & Software Engineering, Gyeongsang National University, South Korea
- **Professor Shripad P. Mahulikar**
  Department of Aerospace Engineering, IIT Bombay
- **Professor Amit Agrawal**
  Department of Mechanical Engineering, IIT Bombay
- **Professor Upendra V. Bhandarkar**
  Department of Mechanical Engineering, IIT Bombay
- **Professor Sarith P. Sathian**
  Department of Applied Mechanics, IIT Madras
- **Professor Rakesh K. Mathpal** (Course Coordinator)
  Department of Aerospace Engineering, IIT Kanpur

Workshop Organizer

Rakesh K. Mathpal
Assistant Professor
Department of Aerospace Engineering
IIT Kanpur
Webpage: http://home.iitk.ac.in/~rkm/

PARTICIPATING INSTITUTES

Institute	Number of Participants
Government Engineering College, Ajmer	2
MMMUT, Gorakhpur	2
HBTU	1
Sardar Vallabhbhai National Institute of Technology, Surat	1
IIT Bombay	1
Total	**7**

WORKSHOP SCHEDULE

Day -1

9:30am- 10:45am	Introduction of the Course and History of Rarefied & Microscale Gasdynamics (RMG) ***Prof. Rho S. Myong***
10:45am- 11:00am	**Tea Break**
11:00am- 12:15pm	Introduction to (Physical & Mathematical) Fluid Dynamics and CFD ***Prof. Rho S. Myong***
12:15pm- 2:00pm	**Lunch Break**
2:00pm-3:00pm	Uniqueness of Mesoscale Modeling of RMG and Various Methods ***Prof. Rho S. Myong***
3:00pm- 3:15pm	**Tea Break**
3:15pm-4:15pm	Continuum Breakdown and the Need for Molecular Description of Fluid Flows ***Prof. Rakesh K. Mathpal***
4:15pm-5:15pm	Molecular Dynamics Simulations: An Introductory Address ***Prof. Sarith Sathian***

Day -2

9:30am- 10:45am	Gas Kinetic Theory and Boltzmann Equation ***Prof. Rho S. Myong***
10:45am- 11:00am	**Tea Break**
11:00am- 12:15pm	Method of Moment, 2nd Law of Thermodynamics, Cumulant Expansion, and Balanced Closure ***Prof. Rho S. Myong***
12:15pm- 2:00pm	**Lunch Break**
2:00pm-3:00pm	2nd-Order NCCR, NCCR-Burgers, and Method of Iteration ***Prof. Rho S. Myong***
3:00pm- 3:15pm	**Tea Break**
3:15pm-4:15pm	Non-equilibrium Gas Flows and The Boltzmann Transport Equation ***Prof. Rho S. Myong***
4:15pm-5:15pm	Introduction to the DSMC Method ***Prof. Rakesh K. Mathpal***

Day -3

9:30am- 10:45am	RMG-External Flows (Compressible Shock Wave and Incompressible Flow over a Sphere) ***Prof. Rho S. Myong***
10:45am- 11:00am	**Tea Break**
11:00am- 12:15pm	Role of Surface Radiation in Micro-heat Exchanger ***Prof. Shripad P. Mahulikar***
12:15pm- 2:00pm	**Lunch Break**
2:00pm-3:00pm	Δp in Incompressible Laminar Micro-Convective Flow with Variable Properties of Compressible Fluid (air) ***Prof. Shripad P. Mahulikar***
3:00pm- 3:15pm	**Tea Break**
3:15pm-4:15pm	Reactive Cross-Section Database for Air Chemistry for use in DSMC: Part 1 ***Prof. Upendra V. Bhandarkar***
4:15pm-5:15pm	Reactive Cross-Section Database for Air Chemistry for use in DSMC: Part 2 ***Prof. Upendra V. Bhandarkar***

Day -4

9:30am- 10:45am	Computational lab session-01 at the New Core lab
10:45am- 11:00am	**Tea Break**
11:00am- 12:15pm	Computational lab session-02 at the New Core lab
12:15pm- 2:00pm	**Lunch Break**
2:00pm-3:00pm	RMG-Internal Flows (Langmuir & Maxwell Slip/Jump, Poiseuille Flow) ***Prof. Rho S. Myong***

3:00pm- 3:15pm	**Tea Break**
3:15pm-4:15pm	Modeling of Some Interesting Non-equilibrium Flow Problems by the DSMC Method ***Prof. Rakesh K. Mathpal***
4:15pm-5:15pm	Multi-physics Modeling in the Particle based Computational Framework ***Prof. Rakesh K. Mathpal***

Day -5

9:30am- 10:45am	Computational lab session-03 at the New Core lab
10:45am- 11:00am	**Tea Break**
11:00am- 12:15pm	Computational lab session-04 at the New Core lab
12:15pm- 2:00pm	**Lunch Break**
2:00pm-3:00pm	Analytical Solutions of Force-Driven Poiseuille Flow and Knudsen Layer and Thermal Effects ***Prof. Rho S. Myong***
3:00pm- 3:15pm	**Tea Break**
3:15pm-4:15pm	Second-Order Boltzmann-Based Non-Navier Non-Fourier Constitutive Laws and Their Validation via MD ***Prof. Rho S. Myong***
4:15pm-5:15pm	Lattice Boltzmann Method (LBM) Framework for Modeling of Low-speed Microscale Flows ***Prof. Rakesh K. Mathpal***

Day -6

9:30am- 10:45am	Computational lab session-05 at the New Core lab
10:45am- 11:00am	**Tea Break**
11:00am- 12:15pm	Computational lab session-06 at the New Core lab.
12:15pm- 2:00pm	**Lunch Break**
2:00pm-3:00pm	Mesoscale Modeling of Polyatomic Gas and NCCR in Phase Portraits ***Prof. Rho S. Myong***
3:00pm- 3:15pm	**Tea Break**
3:15pm-4:15pm	Multi-dimensional Extension of NCCR via Decomposition ***Prof. Rho S. Myong***
4:15pm-5:15pm	Search for Higher-Order Continuum Transport Equations ***Prof. Amit Agrawal***

Day -7

9:30am- 10:45am	2-D, 3-D Mixed DG Method for 2nd-Order Model and Parallelization ***Prof. Rho S. Myong***
10:45am- 11:00am	**Tea Break**
11:00am- 12:15pm	Continuum Mechanics, Constitutive Modeling of Viscoelastic Fluids, and HWNP ***Prof. Rho S. Myong***
12:15pm- 2:00pm	**Lunch Break**
2:00pm-3:00pm	Unified Framework: Boltzmann-Based 2nd-Order Model for Viscoelastic Fluids, and Challenging Topics in RMG ***Prof. Rho S. Myong***
3:00pm- 3:15pm	**Tea Break**
3:15pm-4:15pm	Course Examination
4:15pm-5:15pm	Certificate Distribution and Concluding Remarks

OUTCOME

- Through examples and discussions, the participants learned procedures of the subject in a simplistic manner.
- The hands-on sessions allowed participants to gain deeper insights into the subject.
- Participants developed an understanding/appreciation for the use of higher order continuum equations (extended hydrodynamics)/DSMC for studying flows of rarefied microscale gases and viscoelastic fluids.
- They learned procedures of the advanced subject of non-equilibrium fluid dynamics in a simplistic manner.
- Participants were introduced to state-of-the-art research going on in the world, and the opportunities/challenges that exist in this area.
- The participants and students explained their research problem to the Faculty members, and discussed the doubts and difficulties that they are currently facing with respect to the work.

Organizer's Report on Conduct of TEQIP Workshop

Title of the Course	Rarefied & Microscale Gases and Viscoelastic Fluids: A Unified
Period of Course	23-02-2017 to 02-03-2017
Course Coordinator	
Name	Rakesh K. Mathpal
Department	Aerospace Engineering, IIT Kanpur
Name and Affiliation of Invited Faculty	
Name and Affiliation	Prof. Shripad P. Mahulikar, AE, IIT Bombay
Name and Affiliation	Prof. Amit Agrawal, ME, IIT Bombay
Name and Affiliation	Prof. Upendra Bhandarkar, ME, IIT Bombay
Name and Affiliation	Prof. Sarith Sathian, Applied Mechanics, IIT Madras
Structure of the Course	
Duration of course	8 days
Participants of the Course	
Number of student participants	05
Number of participants from Industry/ Research Organizations	00
Number of Faculty participants	01
Total Number of participants	06

Details of the Workshop:

The workshop/short-term course was successfully conducted on a very important and contemporary subject in research and teaching at the graduate level, viz., Rarefied & Microscale Gases and Viscoelastic Fluids. The non-equilibrium flows, such as rarefied flows through micro/nano-channels and around vehicles operating at high altitudes, are now widely studied flows because of their applications in many areas of engineering including MEMS devices. The short-term TEQIP course on "**Rarefied & Microscale Gases and Viscoelastic Fluids: a Unified Framework**" from 23-02- 2017 to 02-03-2017 at IIT Kanpur was one such initiative in this direction, with the objective of disseminating the knowledge in this interesting subject. Considering the ongoing focus of research and industries on micro/nano scale technologies, it was a timely and appropriate course. Such a course would not only prepare the participants for working on state-of-the-art research problems, but also would train them to suit to the changing job requirements in the market.

In the length scales associated with rarefied and micoscale fluids, the underlying physics is not yet fully understood, and debate is going on whether the macroscopic laws of physics can simply be scaled down to such scales. Many a times, because of the small length scales associated with these flows, use of the Navier-Stokes equations becomes questionable. To handle these flows, it is possible to change the governing equations of flow from the Navier-Stokes to equations containing higher order terms in the constitutive relationship along with appropriate velocity slip and temperature jump models. Such equations fall under the general category of extended hydrodynamics. In this course, an attempt was made to cover the subjects of rarefied, microscale gases and viscoelastic fluids in one unified framework.

At the same time, the Boltzmann equation (kinetic theory) was also studied as part of the course. Since the analytical solution of the Boltzmann equation is not possible for most practical flow situations, approximate methods such as the Direct Simulation Monte-Carlo (DSMC) was discussed with the participants. The algorithm and procedures of the DSMC method were explained in detail.

The experts that were chosen to deliver the lectures are academicians, and not only working in the said area, but are also teaching the same at their Institutes. Therefore, having them here at one platform enabled the participants to generate interest and knowledge in this area by directly interacting with the experts. Through examples and discussions, an attempt was made to explain the procedures of the subject in a simplistic manner. The hands-on sessions (6 in number, 1:15 hours each) allowed them to gain deeper insights into the subject.

The invited Faculty also spent a lot of time with the participants and the graduate students of the host faculty. The participants and students explained their research problem to the Faculty members, and discussed the doubts and difficulties that they are currently facing with respect to the work. In total, it was a very useful interactive session for all of them.

All in all, it was a very productive course. With more of such courses in the future, it is strongly believed that induction of such an important course at the Graduate level can be realized.