**SYLLABUS VT21, version 3**

# MJ2424 Computational Methods in Energy Technology[1]

**Course Leader and Examiner: Prof. Andrew Martin, Department of Energy Technology**

**Teachers: Dr. Mauricio Gutierrez, MSc Arijit Roy, MSc Carlos Tavera, Dr. Wujun Wang**

*NOTE ON COVID-19*

The severity of the pandemic with accompanying public health recommendations has placed restrictions on our physical interaction. This course has been judged to be a good candidate for digital teaching, therefore all activities will be held in this format. Please contact the examiner if you have any special needs or if there are questions.

## Introduction

The purpose of this course is to provide a solid background on numerical methods relevant to fluid flow and heat transfer in energy applications. With this background, participants will have adequate insight in implementing models in commercial computational fluid dynamics (CFD) codes and in interpreting the results. The following topics are covered in the course:

1. Storing of large numbers in computers (single and double precision)
2. Numerical solutions to differential equations
3. Error analysis in numerical methods (rounding, truncation etc)
4. Main equations for heat transfer in solid materials
5. Divergence theorem
6. Equations for compressible flow: conservation of mass, linear momentum and energy
7. Finite difference method for 1D and 2D heat transfer
8. Euler's solution method for transient heat transfer
9. Stability curves for explicit time marching solutions
10. Higher order time discretisation (Predictor-Corrector Scheme and Runge-Kutta method)
11. Crank-Nicolson method (implicit time marching)
12. Mesh generation
13. Advection equation and upwind schemes
14. Lax-Wendroff scheme
15. Introduction to solutions for inviscid flow
16. Introduction to Navier-Stokes equations and turbulence

[1] Also valid for MJ2444 Theory and Practice of Computational Methods in Energy Technology with differences indicated herein.

**Intended Learning Outcomes (ILO's)**

After completing the course with a passing grade the student should be able to:

| | |
|---|---|
| ILO1 | Describe numerical methods for treating partial differential equations, derive specific expressions for programming, and analyze sources of error |
| ILO2 | Define governing equations for relevant physical processes and construct representative numerical simulations |
| ILO3 | Conduct numerical simulations with commercial computational fluid dynamics software and analyze results in terms of validity and accuracy, including comparisons to real processes |
| ILO4 | (MJ2444 only) Account for current developments in computational fluid dynamics methods and software, contrasting selected approaches in analysis |

**Target Group and Prerequisites**

MJ2424 is recommended for students in the SEE Program (TSUEM), while MJ2444 is offered for those planning to join this program.

Prerequisites: coursework in heat transfer, fluid mechanics, and thermodynamics. Programming experience is assumed.

**Activities**

- Lectures
  - Traditional teacher-led lectures, examples, and problem solving held mostly during Period 3, with emphasis on subject material presented in textbook. All activities offered via Zoom which each session recorded.
- Home assignments (INLA and INLB, 0.5 hp each)
  - Two assignments to be solved individually. Details including submission instructions available in Canvas.
  - <u>All programming must be performed in Matlab.</u>
  - Dedicated question and answer (Q&A) session for each home assignment
  - Each graded P/F
- Examination (TEN1, 3.0 hp)
  - New for VT21: take-home exam with emphasis on topics included in home assignments. See below and appendix for more information.
  - Graded A-E.
- CFD lab (LAB1, 2.0 hp)
  - Group project consisting of numerical modeling with commercial software, with teacher support provided during Period 4.
  - Oral presentation mandatory for all students.
  - Lab report to be submitted by group, graded P/F.
  - MJ2444 only: literature survey, 1.5 hp

**Support for Students with Disabilities**

*English* Students with special needs who have obtained a recommendation from KTH FUNKA for examination support are entitled to the following:

- Support linked to codes R (i.e. accommodations concerning room, duration, and physical surroundings) is granted without examiner approval required.
- In accordance with KTH regulations, a request for support linked to code P (pedagogical accommodation) is to be submitted by the student to the examiner, who needs to actively approve or reject the request.

*svenska* För studenter med funktionsvariationer som har utlåtande från KTHs FUNKA-enhet om rekommenderade stödinsatser vid examination gäller följande i denna kurs:

- Alla stödinsatser under kod R (d.v.s. anpassningar som rör rum, tid och fysisk omständighet) beviljas utan särskilt beslut av examinator
- Stödinsatser under kod P (pedagogisk anpassning) ska aktivt beviljas eller avslås av examinatorn efter kontakt tagen av studenten i enlighet med KTHs regler.

Please contact the course leader if there are any questions.

**Assessment**

The first two ILO's are mapped to each of the 16 topics covered in the course, which in turn are assessed according to the prevailing grading scale: P/F for the home assignments, and A-E for TEN1. For the home assignments, the minimum thresholds or achieved learning outcomes, ALO's, for receiving a passing score correspond to Grade E in the table below. For TEN1 the full grading scale is applied to each of the problems.

*ILO1* *Describe numerical methods for treating partial differential equations, derive specific expressions for programming, and analyze sources of error*

*ILO2* *Define governing equations for relevant physical processes and construct representative numerical simulations*

| | **Grade E** | **Grade C** | **Grade A** |
|---|---|---|---|
| **ALO1** | List some of the characteristics of relevant numerical methods for the modeling of physical processes. | Analyze the characteristics of relevant numerical methods for the modeling of physical processes. | Criterion for Grade C including the ability to use more than one analysis method and /or handle more complex cases. |
| **ALO2** | Provide a rudimentary description of governing equations, set up a numerical solution procedure. | Provide rigorous definition of govering equations, identify and quantify applicable numerical methods. | Criterion for Grade C including the ability to use more than one analysis method and /or handle more complex cases. |

ILO3 and ILO4 (MJ2444 only) are assessed via LAB1.

The level of difficulty for each of the home assignments is the reference for assessing the minimum level of achievement for the respective topic. Successful completion of a particular home assignment will thus greatly facilitate demonstrating Grade E for this topic on the exam. Topics and problem solving covered through lectures are indicative of the level of achievement for higher grades.

TEN1 features six problems and includes material representing the 16 topics of this course. As stated above, each problem is graded F (fail), E, C, or A according to the ALO table, with points assigned as follows:

| | |
|---|---|
| Grade F | <10 points |
| Grade E | 10 points |
| Grade C | 11-17 points |
| Grade A | 18-20 points |

The overall exam grade is determined as follows:

| | |
|---|---|
| Grade F | three or more problems at Grade F, irrespective of overall score [v. 3] |
| Grade Fx | no more than two problems at Grade F, irrespective of overall score [v. 3] |
| Grade E | 60-66 points, with all problems at Grade E or higher (valid for all subsequent grades) |
| Grade D | 67-79 points |
| Grade C | 80-93 points |
| Grade B | 94-105 points |
| Grade A | 106-120 points |

The final course grade is equivalent to the grade for TEN1, provided that home assignments and CFD lab report are passed.

**Re-exams**

TEN1 is offered as a re-exam. It is possible to take a re-exam in order to make an attempt towards raising the final grade.

**Project work**

Students will be divided into groups of three or four persons for handling the CFD lab. Students within a group work collectively on model set-up, execution, and assimilation, while individual efforts are required for analyzing the influence of key variables. More information to be provided in Canvas.

**Late assignments**

Late assignments will be graded after final grades are posted.

**Schedule**

Zoom links have been included below (all participants must log in with kth.se credentials).

**Period 3**

| Date & Time | Activity | Instructor(s) |
|---|---|---|
| 18 Jan, 10:00-12:00 | Lecture 1: Course kick-off, Introduction to CFD | Andrew Martin |
| 22 Jan, 8:00-10:00 | Lecture 2: Storing large numbers, numerical solutions, error analysis; Matlab introduction | Andrew Martin, Arijit Roy |
| 26 Jan, 15:00-17:00 | Lecture 3: Heat conduction, divergence theorem, equations for compressible flow | Andrew Martin |
| 29 Jan, 10:00-12:00 | Lecture 4: Finite difference method for 1D/2D heat conduction, Euler's method for transient heat conduction | Andrew Martin |
| 4 Feb, 10:00-12:00 | Lecture 5: Stability curves, higher order time discretization | Andrew Martin |
| 5 Feb, 10:00-12:00 | Q&A Session, Home Assignment 1 | Arijit Roy, Carlos Tavera |
| 8 Feb, 13:00-15:00 | Lecture 6: Crank-Nicholson method, mesh generation | Andrew Martin |
| 11 Feb, 13:00-15:00 | Lecture 7: Advection equation and upwind schemes, Lax-Wendroff scheme | Andrew Martin |
| **16 Feb** | **Due date, Home Assignment 1** | -- |
| 17 Feb, 13:00-15:00 | Lecture 8: Review of Home Assignment 1 | Arijit Roy, Carlos Tavera |
| 19 Feb, 13:00-15:00 | Lecture 9: Introduction to solution of inviscid flow equations, Navier-Stokes equations | Andrew Martin |
| 23 Feb, 13:00-15:00 | Q&A Session, Home Assignment 2 | Arijit Roy, Carlos Tavera |
| 25 Feb, 13:00-15:00 | Lecture 10: Turbulence | Andrew Martin |
| 2 Mar, 13:00-15:00 | Lecture 11 Course wrap-up and exam preparation | Andrew Martin |
| **3 Mar** | **Due date, Home Assignment 2** | -- |
| 4 Mar, 15:00-17:00 | Lecture 12: Review of Home Assignment 2 | Arijit Roy, Carlos Tavera |
| **11 Mar, 14:00-18:00** | **TEN1 (Exam)** | -- |

**Period 4**

| Date & Time | Activity | Instructor(s) |
|---|---|---|
| 23 Mar, 13:00-15:00 | Lecture 13: Introduction to ICEM and Fluent | Wujun Wang |
| 25 Mar, 9:00-11:00 | Lecture 14: Introduction to ANSYS CFX | Mauricio Gutierrez |
| 1 Apr, 9:00-11:00 | Support session | Mauricio Gutierrez, Wujun Wang |
| 8 Apr, 9:00-11:00 | Support session | as above |
| 15 Apr, 9:00-11:00 | Support session | as above |
| 22 Apr, 9:00-11:00 | Support session | as above |
| 29 Apr, 9:00-11:00 | Support session | as above |
| 6 May, 9:00-11:00 | Support session | as above |
| 12 May, 9:00-11:00 | Support session | as above |
| 20 May, 9:00-11:00 | Oral presentations | |
| **24 May** | **Due date for project report** | |
| **3 Jun, 8:00-12:00** | **re-exam, TEN1 (Exam)** | |

**Learning Resources**

Jiyuan Tu, Guan-Heng Yeoh, and Chaoqun Liu, Computational Fluid Dynamics: A Practical Approach, 3rd ed., Butterworth-Heinemann (2018). [Available for download at KTH Library.]

S. D. Conte and Carl de Boor, Elementary Numerical Analysis: An Algorithmic Approach, SIAM (2018). [Available for download at KTH Library.]

## APPENDIX – TEN1

As stated previously, this year's exam is offered in a take-home format. A dedicated Canvas event will be accessible for all students who sign up for the exam. The exam paper with six problems will be distributed at the starting time of the exam, 14:00 CET on 2021-03-11. The exam is four hours and solutions, including Matlab codes, must be uploaded no later than 18:30 CET.

All course material including textbooks may be used along with material obtained through Internet searches. Required programming must be done in Matlab; students are highly encouraged to use own codes developed for the home assignments as a starting point.

**Help from persons enrolled in this course or outside the course is not permitted!**

The following measures are adopted to ensure that each submission is original:

- Input data or other specific attributes for each problem will be varied. In some cases the exact details of a particular problem will be unique, while in others certain variations may be implemented for groups of students.
- A check will be make on submissions, including codes, to see if there are any instances of obvious duplication.
- Finally, the examiner will follow up with an oral exam. This will be conducted in Zoom during the remaining days of the exam period, 12-19 March (details including sign-up to be announced in Canvas). During a maximum time of 15 minutes the examiner will ask each student to verify identification (passport, driver's license) and explain the reasoning behind solutions for specific problems, with uploaded solutions and Matlab codes used as a basis.

The examiner reserves the right to assign a failing grade if the student is unable to provide adequate clarification of the uploaded solutions or Matlab codes.