Computational Geosciences

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Course Summary

With the advancement of modern computing technology, computation has become one of the most important research tools in many fields, including geosciences. In this course, we will explore commonly used computational methods, namely, finite-difference method, pseudo-spectral method, finite-element method, and spectral-element method applied to problems in geosciences. Specifically, we will solve wave propagation, tsunami problem, steady-state, and unsteady-state heat diffusion equations. We will start from 1D examples and gradually expand to 2D and 3D examples. All examples will be supplemented by programming exercises. We will provide program templates for most exercises in Matlab or C, or FORTRAN. Students are welcome to use any language of their choice. At the end of the course, students will be able to design and solve their own problems in computational geosciences. Additionally, students will be able to make informed decision on using geoscientific software rather than simply using them as black boxes.

This course is intended for senior undergraduate and graduate students with both science and/or engineering backgrounds.

Prerequisites

- Basic knowledge of differential/integral calculus.
- Basic experience with any programming languages: Matlab/Mathematica, Python, Fortran, and C/C++.

Course Outline

1. Continuum Mechanics: Governing Equations
   - Conservation of mass
   - Conservation of linear momentum
   - Linearised version of conservation laws
   - Constitutive law
   - Second-order wave equation
   - Pressure wave equation
   - Assignment 0: Index notation
1. **Finite Difference Method: 1D Wave equation**
   - First- and Second-order Finite Difference Method
   - Boundary conditions
   - Assignment 1: 1D Wave Equation [Matlab]

2. **Finite Difference Method: Tsunami**
   - Tsunamis
   - Shallow water wave equations
   - 2D Finite Difference Method
   - Fourth-order Finite Difference Method
   - Assignment 2: 2D Wave Equation: Tsunami [C]

3. **Finite Difference Method: Heat Equation**
   - Conservation of energy
   - Heat equation
   - Explicit and implicit methods
   - Crank-Nicolson scheme
   - Assignment 3: 1D Heat Equation [Matlab]

4. **Finite Difference Method: Stability and Accuracy**
   - Stability analysis (implicit versus explicit schemes, velocity stress, central differences)
   - Resolution of numerical grid
   - Grid dispersion and anisotropy

5. **Pseudo Spectral Method**
   - Fourier transform, differentiation in frequency domain
   - Accuracy, periodic boundary conditions, higher dimensions, Gibbs phenomenon
   - Comments on basis functions (Chebychev, non-periodic, spherical harmonics)
   - Assignment 4: 1D Wave Equation [Matlab]

6. **Finite Element Method**
   - Weak form
   - Finite element method
   - Shape functions
   - Local and Global formulations
• Assembling global matrix and vector
• Assignment 5: 1D steady-state Heat-diffusion Equation [Matlab]
• Assignment 6: 1D unsteady sate Heat-diffusion equation [Matlab]

7. Spectral Element Method

• Higher order Lagrange polynomials
• Gauss-Lobatto-Legendre quadrature
• Mass matrix
• Spectral element method
• Assignment 7: 1D heat-diffusion equation using Spectra-element method [Matlab]
• Assignment 8: 1D wave propagation using Spectral-element method [Matlab]

8. Spectral Element Method: 2D

• 2D spectral-element method
• Assignment 9: 2D wave propagation using Spectral-element method [FORTRAN]

9. SPECFEM2D/SPECFEM3D

• Demonstration of SPECFEM2D/SPECFEM3D
• Demonstration of external meshing
• Final Project: Students will design and solve their own problems that can be solved using any of the numerical methods. Students will get access to The Centre for Advanced Computing (CAC) cluster if necessary.

Grading

• Assignments: 70%
• Final project: 30%

Course Materials

• Any slides or lecture notes will be posted at the end of each class.
• All programs templates will be posted at the end of each Assignment class.
• All solutions will be posted after the deadline of each Assignment.

Further references

Class notes and slides will be sufficient for the class. However, students are encouraged to refer to any of the following references for specific interest.
W. Michael Lai, David Rubin, and Erhard Krempl: Introduction to Continuum Mechanics

John H. Heinbockel: Introduction To Tensor Calculus And Continuum Mechanics

George E. Mase: Theory and Problems of Continuum Mechanics, Schaum's Outline Series

John H. Heinbockel: Introduction to Tensor Calculus and Continuum Mechanics

Seth Stein and Michael Wysession: An Introduction to Seismology: Earthquakes and Earth Structure

H. Igel: Computational Seismology: A Practical Introduction


Jan S. Hesthaven, Sigal Gottlieb, and David Gottlieb: Spectral Methods for Time-Dependent Problems

Lloyd N. Trefethen: Spectral Methods in MATLAB

T. Gerya: Introduction to Numerical Geodynamic Modelling

J. N. Reddy: An Introduction to the Finite Element Method

I. M. Smith and D. V. Griffiths: Programming the Finite Element Method

C. Pozrikidis: Introduction to Finite and Spectral Element Methods Using MATLAB