250970 - DESDOMCOM - Domain Descomposition and Large Scale Scientific Computing

Coordinating unit: 250 - ETSECCPB - Barcelona School of Civil Engineering
Teaching unit: 751 - ECA - Department of Civil and Environmental Engineering
Academic year: 2015
Degree: MASTER'S DEGREE IN NUMERICAL METHODS IN ENGINEERING (Syllabus 2012). (Teaching unit Compulsory)
ERASMUS MUNDUS MASTER'S DEGREE IN COMPUTATIONAL MECHANICS (Syllabus 2013). (Teaching unit Optional)
ECTS credits: 5

Teaching languages: English

Teaching staff
Coordinator: SANTIAGO IGNACIO BADIA RODRIGUEZ
Others: SANTIAGO IGNACIO BADIA RODRIGUEZ, ALBERTO FRANCISCO MARTIN HUERTAS

Degree competences to which the subject contributes

Specific:
8378. Practical numerical modeling skills. Ability to acquire knowledge on advanced numerical modeling applied to different areas of engineering such as: civil or environmental engineering or mechanical and aerospace engineering or bioengineering or Nanoengineering and naval and marine engineering, etc..
8379. Knowledge of the state of the art in numerical algorithms. Ability to catch up on the latest technologies for solving numerical problems in engineering and applied sciences.
8380. Materials modeling skills. Ability to acquire knowledge on modern physical models of the science of materials (advanced constitutive models) in solid and fluid mechanics.
8382. Experience in numerical simulations. Acquisition of fluency in modern numerical simulation tools and their application to multidisciplinary problems engineering and applied sciences.
8383. Interpretation of numerical models. Understanding the applicability and limitations of the various computational techniques.
8384. Experience in programming calculation methods. Ability to acquire training in the development and use of existing computational programs as well as pre and post-processors, knowledge of programming languages ??and of standard calculation libraries.

Teaching methodology

The course consists of 0,5 hours per week of classroom activity (large size group) and 1 hour weekly with half the students (medium size group).

The 0,5 hours in the large size groups are devoted to theoretical lectures, in which the teacher presents the basic concepts and topics of the subject, shows examples and solves exercises.

The 1 hour in the medium size groups is devoted to solving practical problems with greater interaction with the students. The objective of these practical exercises is to consolidate the general and specific learning objectives.

The rest of weekly hours devoted to laboratory practice.

Support material in the form of a detailed teaching plan is provided using the virtual campus ATENEA: content, program of learning and assessment activities conducted and literature.
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Learning objectives of the subject

This course provides the student with different efficient numerical tools for the solution of the large linear systems that result from the discretization of partial differential equations on large-scale distributed memory machines (supercomputers). We will primarily focus on Krylov subspace iterative methods and domain decomposition preconditioners. Further, the student is introduced to parallel computing, multi-threaded programming (OpenMP), and message-passing programming (MPI).

* To understand the benefits and limitations of sparse direct and iterative solvers
* To understand the importance of preconditioners, and their impact in computational performance of solvers
* To understand how to define/implement preconditioners that efficiently exploit concurrency (supercomputers)
* To understand the different types of scalability and the main features that an algorithm must enjoy in order to be scalable
* To understand domain decomposition algorithms, their properties, and limitations
* To be familiar with multi-threaded programming (OpenMP) and message-passing programming (MPI)
* To be able to implement OpenMP/MPI parallel solvers based on domain decomposition preconditioners and Krylov subspace iterative solvers

* PRELIMINARIES -- FINITE ELEMENT DISCRETIZATION
* PRELIMINARIES -- INTRODUCTION TO NUMERICAL LINEAR ALGEBRA
* DOMAIN DECOMPOSITION ALGORITHMS
* BALANCING DOMAIN DECOMPOSITION ALGORITHMS
* HIGH PERFORMANCE COMPUTING

REFERENCES

Domain Decomposition Algorithms
A. Toselli and O. Widlund. Springer, 2005

Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations
B. Smith, P. Bjorstad, and W. Gropp. Cambridge University Press, 2004

Finite Elements and Fast Iterative Solvers

Iterative Methods for Sparse Linear Systems
Y. Saad. SIAM books, 2006

Numerical Solution of Partial Differential Equations by the Finite Element Method.
C. Johnson. Dover, 2009

The Sourcebook of Parallel Computing
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Introduction to High-Performance Scientific Computing

Scientific Parallel Computing

Numerical Linear Algebra on High-Performance Computers

This course provides the student with different numerical tools for solving large linear elements that result from the discretization of partial differential equations on distributed memory machines on a large scale (super computers). We will focus primarily on Krylov subspace iterative methods and domain decomposition preconditioners. Students also will come first parallel computing, multi-threaded programming (OpenMP) and message-passing programming (MPI).

- Understand the benefits and limitations of direct and iterative scattered solutores
- Understand importance of precondicionants and its impact on performance computational solutores
- Understand how to define / implement precondicionant efficiently exploiting concurrency (supercomputers)
- Understanding the different types of scalability and the main characteristics that an algorithm should have to
- Understand be scalable domain decomposition algorithms, their properties and limitations
- Be familiar with multi-threading programming (OpenMP) and message passing programming (MPI)
- Power solutores implement parallel OpenMP / MPI-based domain decomposition precondicionant and solutores iter

Study load

<table>
<thead>
<tr>
<th>Total learning time: 125h</th>
<th>Theory classes: 7h 30m 6.00%</th>
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<tbody>
<tr>
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<td>Practical classes: 15h 12.00%</td>
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<tr>
<td></td>
<td>Laboratory classes: 17h 30m 14.00%</td>
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<tr>
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<td>Guided activities: 5h 4.00%</td>
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<td>Self study: 80h 64.00%</td>
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### Content

#### Preliminaries

**Description:**

- 0.1 PDEs in strong form
- 0.2 PDEs in weak form
- 0.3 Galerkin discretization
- 0.4 Finite element spaces
- 1.1 Eigenvalues of a matrix
- 1.2 Condition number
- 1.3 Ill-conditioning
- 1.4 Conditioning of the mass matrix
- 1.5 Conditioning of the Laplacian matrix
- 1.6 Gaussian elimination
- 1.7 Richardson and Steepest Descent Method
- 1.8 Conjugate Gradient Method
- 1.9 Combining Preconditioners
- 1.10 Krylov methods for indefinite and nonsymmetric matrices

**Learning time:** 4h 48m  
Theory classes: 2h  
Self study: 2h 48m

#### Balancing Domain Decomposition Algorithms

**Description:**

- 2.1 Motivation of DDM
- 2.1.1 Overlapping approach
- 2.1.2 Nonoverlapping approach
- 2.2 Overlapping subdomain algorithms
- 2.2.1 Additive Schwarz algorithms
- 2.2.2 Multiplicative Schwarz algorithms
- 2.3 Nonoverlapping subdomain algorithms
- 2.3.1 Dirichlet-Neumann
- 2.3.2 Neumann-Neumann
- 2.3.3 The case of many subdomains
- 3.1 Coarse level algorithms
- 3.2 Balancing Neumann-Neumann
- 3.3 BDDC
- 3.4 Implementation aspects
- 3.5 Numerical experimentation
- 3.6 Further topics

**Learning time:** 50h 24m  
Theory classes: 6h  
Practical classes: 15h  
Self study: 29h 24m

#### Final Assignment

**Description:**

**Learning time:**

- Theory classes: 6h
- Practical classes: 15h
- Self study: 29h 24m
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**HIGH PERFORMANCE COMPUTING**

<table>
<thead>
<tr>
<th>Learning time: 40h 48m</th>
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<tr>
<td>Laboratory classes: 17h</td>
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<tr>
<td>Self study: 23h 48m</td>
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**Description:**
- 4.1 Parallel architectures (shared vs distributed memory)
- 4.2 Parallel efficiency
- 4.3 Programming paradigms (OpenMP vs MPI)
- 4.4 Data structures in numerical linear algebra
- 4.5 Domain decomposition via graph partitioning
- 4.6 Parallelization of an unpreconditioned linear system
- 4.7 Parallelization of one-level DD preconditioners
- 4.8 Introduction to the HPC assignment

**Qualification system**

The mark of the course is obtained from the ratings of continuous assessment and their corresponding laboratories and/or classroom computers.

Continuous assessment consist in several activities, both individually and in group, of additive and training characteristics, carried out during the year (both in and out of the classroom).

The teachings of the laboratory grade is the average in such activities.

The evaluation tests consist of a part with questions about concepts associated with the learning objectives of the course with regard to knowledge or understanding, and a part with a set of application exercises.

**Regulations for carrying out activities**

Failure to perform a laboratory or continuous assessment activity in the scheduled period will result in a mark of zero in that activity.

**Bibliography**

**Basic:**