

Course guide

250970 - DESDOMCOM - Domain Descomposition and Large Scale Scientific Computing

Last modified: 28/03/2024

Unit in charge: Barcelona School of Civil Engineering
Teaching unit: 751 - DECA - Department of Civil and Environmental Engineering.

Degree: MASTER'S DEGREE IN NUMERICAL METHODS IN ENGINEERING (Syllabus 2012). (Compulsory subject).
ERASMUS MUNDUS MASTER'S DEGREE IN COMPUTATIONAL MECHANICS (Syllabus 2013). (Optional subject).

Academic year: 2023 **ECTS Credits:** 5.0 **Languages:** English

LECTURER

Coordinating lecturer: RICCARDO ROSSI BERNECOLI

Others: POOYAN DADVAND, RICCARDO ROSSI BERNECOLI

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 1,5 hours per week of classroom activity (large size group) and 1.5 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.

Although most of the sessions will be given in the language indicated, sessions supported by other occasional guest experts may be held in other languages.

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

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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

H. Elman, D. Silvester, A. Wathen. Oxford Science Publications, 2006

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

J. Dongarra, I. Foster, G. C. Fox, W. Gropp, K. Kennedy, L. Torczon, A. White.
Morgan Kaufmann, 2003.

Introduction to High-Performance Scientific Computing

Victor Eijkhout, Edmond Chow, R. van de Geijn. lulu publications, 2011.

Scientific Parallel Computing

L. R. Scott, T. Clark, and B. Bagheri.
Princeton University Press, 2005.

Numerical Linear Algebra on High-Performance Computers

J. Dongarra, I. S. Duff, D. C. Sorensen, H. A. van der Vorst. SIAM books, 1998.

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 solvers * Understand importance of preconditioner and its impact on performance computational solvers * Understand how to define / implement preconditioner 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 solvers implement parallel OpenMP / MPI-based domain decomposition preconditioner and solu

STUDY LOAD

Type	Hours	Percentage
Hours large group	25,5	20.38
Hours small group	9,8	7.83
Hours medium group	9,8	7.83
Self study	80,0	63.95

Total learning time: 125.1 h

CONTENTS

PRELIMINARIES

Description:

Course Introduction

1.1 Matrix factorizations and inverses

1.2 QR & SVD

1.3 Eigenvalues of a matrix

1.4 Condition number

1.5 Ill-conditioning

1.6 Conditioning of the mass matrix

1.7 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

1.1 Penalty Method

1.2 Lagrange Multipliers

1.3 Multi Point Constraints

1.1 Conjugate Gradient

1.2 GMRES

1.3 Others

1.4 Matrix Free Methods

1.5 Newton-Krylov approaches

1.1 - Diagonal Preconditioning

1.2 - ILU type preconditioning

1.3 - AMG

Full-or-part-time: 33h 36m

Theory classes: 14h

Self study : 19h 36m

HIGH PERFORMANCE COMPUTING

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 Implementation of simple operations in MPI
- 4.6 HPC Assignments

Full-or-part-time: 38h 24m

Laboratory classes: 16h

Self study : 22h 24m

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
- FINAL ASSIGNMENT

Full-or-part-time: 36h

Theory classes: 9h

Practical classes: 6h

Self study : 21h

GRADING 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.



EXAMINATION RULES.

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:

- Toselli, A.; Widlund, O.B. Domain decomposition methods : algorithms and theory [on line]. Berlin, Heidelberg: Springer, 2005 [Consultation: 08/02/2021]. Available on: <http://dx.doi.org/10.1007/b137868>. ISBN 3540206965.
- Smith, B.; Bjorstad, P.; Gropp, W.D. Domain decomposition : parallel multilevel methods for elliptic partial differential equations. Cambridge: Cambridge University Press, 1996. ISBN 052149589X.
- Elman, H.C.; Silvester, D.J.; Wathen, A.J. Finite elements and fast iterative solvers : with applications in incompressible fluid dynamics. 2nd ed. Oxford: Oxford University Press, 2014. ISBN 9780199678808.