Centre Específic de Recerca de
Mètodes Numèrics en Ciències Aplicades i Enginyeria

2010 ANNUAL REPORT
MISSION STATEMENT

The Laboratori de Càlcul Numèric (LaCàN) is a research group of the Universitat Politècnica of Catalunya (UPC) created in 1995. In 2009 the UPC promoted it to a “Centre Específic de Recerca” (unitat acadèmica) because of its scientific productivity and its interdepartamental and intercampus extension. LaCàN is a research group internationally recognized and the Catalan Government has awarded its maximum research recognition continuously since its first call.

CER-LaCàN is a young and dynamic research group: it is composed by a total of 14 tenured professors (9 of them below 40 years old), several post-doc researchers, 21 PhD students. It is also a highly international group with: 11 foreign PhD students, 6 faculty obtained their PhD degree in US, British or Italian universities.

The group is diverse in terms of the basic training of its members (engineers, mathematicians, physicists), the research topics and funding sources (industrial projects, cutting-edge research projects, international consortia). However, group members have a powerful common denominator in research and teaching: mathematical modeling, numerical methods, and interest in their applicability.

RESEARCH GOALS

CER-LaCàN mission is to be a reference research unit with scientific and socio-economic impact, with technology transfer to industry and consolidated training in the field of mathematical modeling and numerical simulation in applied sciences and engineering. More specifically, it is important to note that currently, researchers in LaCàN produce quality research, publish in high impact international journals, and consistently receive recognition in the form of awards, invited lectures and editorial boards, as well as citations of their work. Moreover, the level of internationalization is high. However, to be reinforce these aspects, we have identified three major challenges that will benefit from the recruit of a young highly productive researcher with experience in international project:

• Scientific research production must be increases to compete with the top most research groups in the area. This handicaps: young faculty, inefficient allocation of micro-management tasks, and strong teaching load; can be overcome by full time researcher leading its active group.

• Some of the research under development is incremental in well-established lines. While it is important to consolidate it, it is also crucial to invest resources in creating new lines that put the center at the forefront of research in their field

• It is everyday more difficult to attract top-level talent to cover eligible for PhD scholarships or competitive grants. Bringing new internationally recognized people could improve our visibility.

Continuously and consistently proposing innovative ideas at the frontier of knowledge is the best approach to have a strong impact, attract talent, and achieve high productivity (i.e. to be leaders in our field). Therefore, we promote and support original initiatives that explore new potential lines, despite their risk if they open new horizons.
PERSONNEL

Director
Full Professor
ANTONIO HUERTA

Deputy director
Full Professor
PEDRO DÍEZ

Faculty
Associate Professor
IRENE ARIAS
Associate Professor
MARINO ARROYO
Lecturer
MARCO DISCACCIATI
Associate Professor
ROSA ESTELA
Associate Professor
SONIA FERNANDEZ-MENDEZ
Associate Professor
ADELINE DE MONTLAUR
Associate Professor
JOSÉ MUÑOZ
Associate Professor
NÚRIA PARÉS
Associate Professor
AGUSTÍ PÉREZ-FOGUET
Lecturer
JORDI POBLET
Full Professor
ANTONIO RODRÍGUEZ-FERRAN
Associate Professor
JOSEP SARRATE
Lecturer
YONGXING SHEN
Lecturer
SERGIO ZLOTNIK
Postdoctoral Researcher

CARLOS BRAGA
SUSANTA GHOSH
XEVI ROCA

PhD students

AMIR ABDOLLAHI
ALEKSANDAR ANGELOSKI
EVA CASONI
CRISTINA DIAZ
ABEL GARALLO
GIORGIO GIORGIANI
SAQIB HAMEED
BEHROOZ HASHEMIAN
OMID JAVADZADEH
DANIEL MILLAN
DAVID MODESTO
CHRISTIAN PECO
ALBA PROS
MOHAMMAD RAHIMI
ADRIAN ROSOLEN
ELOI RUIZ
ESTHER SALA
LINDAURA STEFFENS
ELENA TAMAYO
FRANCESC VERDUGO
KUAN ZHANG

Administrative staff

PURI VILLARES
DAVID ORTIN
IMMA RIUS
**PhD THESES**

**Assessment of the dispersion error and goal-oriented adaptivity for wave propagation problems**

Lindaura Maria Steffens
Facultat de Matemàtiques i Estadística
Universitat Politècnica de Catalunya
14 July, 2010

**Key challenges in the governance of rural water supply: lessons learnt from Tanzania**

Alejandro Jiménez Fernández de Palencia
ETSE de Camins, Canals i Ports de Barcelona
Universitat Politècnica de Catalunya
Premio extraordinario de doctorado UPC
17 May, 2010
MANAGEMENT & GOVERNANCE

MANAGEMENT COMMITTEE

Antonio Huerta
Pedro Díez
Irene Arias
Marino Arroyo
Sonia Fernández Mendez
Adeline de Montlaur
José Muñoz
Agustí Pérez-Foguet
Antonio Rodríguez Ferran
Josep Sarrate
Puri Villares

Director
Deputy Director
Research Coordinator
SEED Coordinator
Recruiting Coordinator
ICT Coordinator
Head of Administration
RESEARCH

PUBLICATIONS

A flux-free a posteriori error estimator for the incompressible Stokes problem using a mixed FE formulation
Larsson, F; Díez, P and Huerta, A.

A multiplicative Schwarz method with active subdomains for transient convection-diffusion problems
Sandoval, M.L. and Rodríguez-Ferran, A.

A new least-squares approximation of affine mappings for sweep algorithms
Roca, X., Sarrate, J and Huerta, A.

Accurate recovery-based upper error bounds for the extended finite element framework
Ródenas, J.J.; González-Estrada, O.A.; Diez, P. and Fuenmayor, F.J.

An automatic and general least-squares projection procedure for sweep meshing
Roca, X. and Sarrate, J.

An error estimator for separated representations of highly multidimensional models
Ammar A; Chinesta F; Díez, P and Huerta, A

Assembling sparse matrices in MATLAB
Zlotnik, S. and Díez, P.

Bipenalty method for time domain computational dynamics
Askes, H.; Caramés-Saddler, M and Rodríguez-Ferran, A.

Building the role of local government authorities towards the achievement of the human right to water in rural Tanzania
Jiménez, A. and Pérez-Foguet, A.
Natural Resources Forum, Vol. 34, Issue 2, pp. 93-105, 2010
Challenges for water governance in rural water supply: lessons learnt from Tanzania
Jiménez, A. and Pérez-Foguet, A.

Controls on subduction reorganization in the Hellenic margin, eastern Mediterranean
Capitanio, F.; Zlotnik, S. and Faccena, C.
Geophysical Research Letters, Vol. 37, pp. 1-5, 2010

Discontinuous Galerkin methods for the Navier-Stokes equations using solenoidal approximations
Montlaur, A.; Fernandez-Mendez, S.; Peraire, J. and Huerta, A.

Diverse corrugation pattern in radially shrinking carbon nanotubes
Shima, H.; Sato, M.; Iiboshi K.; Ghosh S. and Arroyo M.

Error assessment and mesh adaptivity for regularized continuous failure models
Pannachet, T; Diez, P; Askes, H and Sluys, L. J.

Error Estimation and Quality Control
Diez, P.; Parés, N. and Huerta, A.

Generation of structured hexahedral meshes in volumes with holes
Ruiz-Gironés, E. and Sarrate, J.

Generation of structured meshes in multiply connected surfaces using submapping
Ruiz-Gironés, E. and Sarrate, J.

Improved method to calculate a Water Poverty Index at local scale
Giné, R. and Pérez-Foguet, A.

Local dual contributions: Representing dual surfaces for block meshing
Roca, X. and Sarrate, J.
Modeling, with a unified level-set representation, of the expansion of a hollow in the ground under different physical phenomena
Cottereau, R; Diez, P and Huerta, A

Numerical analysis of the Navier-Stokes/Darcy coupling.
Badea, L.; Discacciati, M. and Quarteroni, A.

On the optimum support size in meshfree methods: a variational adaptivity approach with maximum entropy approximants
Rosolen, A.; Millán, D. and Arroyo, M.

Stability and convergence proofs for a discontinuous-Galerkin-based extended finite element method for fracture mechanics
Shen, Y. and Lew, A.

Stress-dependent morphogenesis: continuum mechanics and truss systems
Muñoz, J; Conte, V and Miodownik, M
Biomechanics and Modeling in Mechanobiology, Vol. 9, Issue 4, pp. 451-467, 2010

Strict error bounds for linear and nonlinear solid mechanics problems using a patch-based flux-free method
Cottereau, R., Chamoin, L. and Diez, P.
Mécanique & Industries, Vol. 11 Number 3-4, pp. 249-254, 2010

SUPG-based stabilization using a separated representations approach
González, D.; Debeugny, L.; Cueto, E.; Chinesta, F.; Diez, P. and Huerta, A.

The block Gauss-Seidel method in sound transmission problems
Poblet-Puig, J. and Rodríguez-Ferran, A

XFEM+: una modificación de XFEM para mejorar la precisión de los flujos locales en problemas de difusión con conductividades muy distintas
Cordero, F. and Díez, P.
# Research Seminars

<table>
<thead>
<tr>
<th>DATE</th>
<th>PRESENTER</th>
<th>TITLE</th>
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<tbody>
<tr>
<td>30 JAN</td>
<td>Liu, Zhanli, Department of engineering mechanics, Tsinghua University, China</td>
<td>X-FEM modeling of polyurea-based composites.</td>
</tr>
<tr>
<td>1 FEB</td>
<td>Zhuo Zhuang, Applied Mechanics Lab., School of Aerospace, Tsinghua University, China</td>
<td>Computation model on dislocation-based crystal plasticity at sub-micron scale.</td>
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<tr>
<td>4 MAR</td>
<td>Serguei Iakovlev, Dalhousie University</td>
<td>Computationally efficient pre-design analysis of fluid-interacting structures using classical methods of mathematical physics.</td>
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<tr>
<td>2 APR</td>
<td>Giorgio Giorgiani, LaCaN, UPC- BarcelonaTech</td>
<td>Adaptive hybrid discontinuous methods for fluid and wave problems.</td>
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<tr>
<td>3 MAY</td>
<td>Amir Abdollahi, UPC LaCaN</td>
<td>Effect of flexoelectricity on the electromechanical response of nano cantilever beams.</td>
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<tr>
<td>8 MAY</td>
<td>Kaushik Bhattacharya, CalTech</td>
<td>Cyclic deformation and the interplay between phase transformation and plasticity in shape-memory alloys.</td>
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<tr>
<td>22 MAY</td>
<td>Jorge Alcalá, UPC-BarcelonaTech</td>
<td>The interpretation of indentation experiments through multiscale material modeling.</td>
</tr>
<tr>
<td>31 MAY</td>
<td>Xavier Sanchez-Vila, UPC-BarcelonaTech</td>
<td>Modeling multicomponent reactive transport with particle tracking and smoothing techniques.</td>
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<tr>
<td>20 JUN</td>
<td>Shi-hai Li, Institute of Mechanics, Chinese Academy of Sciences</td>
<td>Continuum-discontinuum element method.</td>
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<td>Date</td>
<td>Name</td>
<td>Institution / Organization</td>
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<td>13 SEP</td>
<td>M.B. Liu</td>
<td>Institute of Mechanics, Chinese Academy of Sciences</td>
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<tr>
<td>11 OCT</td>
<td>Martin Michael Müller</td>
<td>Equipe BioPhysStat, Université de Lorraine, Metz</td>
</tr>
<tr>
<td>30 OCT</td>
<td>Rubén Sevilla</td>
<td>Civil and Computational Engineering Centre, College of Engineering, Swansea University</td>
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MEETINGS, EVENTS, WEBSITE & PRESENCE IN MEDIA

9th Workshop on Numerical Methods in Applied Science and Engineering
Workshop
by: LaCàN
DATE: 18 - 19 January, 2010
LOCATION: "Vilars Rurals", Cardona

High Performance Computing for Computational Mechanics
Course
by: A. Coutinho and M. Storti (COPPE/Universidade Federal do Rio e Janeiro)
DATE: February 8 to 18, 2010
LOCATION: Room A1 103, Campus Nord UPC

Fluid-structure interaction in fast transient dynamics
Course
by: Folco Casadei (Joing Research Center, Ispra, Italy)
DATE: May 31 - June 4, 2010
LOCATION: See the course schedule
The Laboratori de Càlcul Numeric offers high-quality computational facilities to fulfill its research and educational mission.

On one hand a computer room equipped with a 14 workstations is available for researchers and students. On the other hand, a cluster for high-performance computing is also available for LaCàN members. This year we have acquired a cluster dedicated to distributed memory and composed by a master node (Dell PE R610) and eight computation nodes (Dell PE C6100). All nodes are connected using an Infiniband network. To increase the storage capabilities of the cluster we have also acquired a new disk array (EqualLogic) of 16Tby. In addition we have renewed a router and a switch in order to increase the bandwidth of the network connection.
LaCàN is involved in the coordination of educational and training programs. In particular, professors from LaCàN are responsible of the coordination of prestigious program awarded with the Erasmus Mundus distinction by the European Commission:

- The **Master of Science in Computational Mechanics** started in the academic year 2007-2008 (http://www.cimne.com/cm-master/) coordinated by UPC and having as partners: University of Swansea, l'École Centrale de Nantes and University of Stuttgart.

We also participate in several UPC masters such as

- Master in Aerospace Science and Technology
- Master Ingeniería Matemática/Matemática Aplicada (Msc of Mathematical Engineering/Applied Mathematics)
- Master Ingeniería Civil (master in Civil Engineering)
- Master Ingeniería Ambiental (master in Environmental Engineering)
FINANCIAL REPORT

2010 Income

<table>
<thead>
<tr>
<th>Project Description</th>
<th>Funding Source</th>
<th>TOTAL FUNDING</th>
<th>FUNDING 2010</th>
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<td>Modelos numéricos predictors para la gestión medioambiental</td>
<td>MICINN</td>
<td>92 617,62€</td>
<td>30 872,54€</td>
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<td>Modelización numérica de estructuras e infraestructuras: diseño, durabilidad y estados límite</td>
<td>MICINN</td>
<td>185 130,00€</td>
<td>61 710,00€</td>
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<tr>
<td>Modelización y simulación multiscale para el diseño virtual en micro y nano tecnología y sistema bio-inspirados</td>
<td>MICINN</td>
<td>119 669,00€</td>
<td>39 889,66€</td>
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<tr>
<td>Modelización numérica de flujos, sólidos y estructuras para aplicaciones industriales</td>
<td>MICINN</td>
<td>210 935,02€</td>
<td>70 3100,07€</td>
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<td>Marie Curie Initial Training Network in Advanced Techniques in Computational Mechanics - ATCOME Predictive models and simulations in nano- and biomolecular mechanics: A multiscale approach(PREDMODSIM)</td>
<td>Marie Curie FP7, ERC ST.G, ICREA Academia, GenCat</td>
<td>506 694,35€, 1 462 198,00€, 100 000,00€, 48 880,00€</td>
<td>126 673,58€, 292 439,60€, 25 000,00€, 9 776,00€</td>
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<td>ICREA 2009 SGR 00875 – Métodes numèrics en ciències aplicades i enginyeria</td>
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<td>Analisis numéricas KIT ANFOR</td>
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<td><strong>TOTAL</strong></td>
<td><strong>673 672,45€</strong></td>
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Income

<table>
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<th>Funding Source</th>
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<tr>
<td>Competitive Grants EU</td>
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<td>Competitive Grants ES</td>
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<td>Competitive Grants CAT</td>
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</tr>
<tr>
<td>Private Research Funding</td>
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<tr>
<td><strong>Total Income</strong></td>
<td><strong>673 672,45€</strong></td>
</tr>
</tbody>
</table>
ENQUIRIES AND FURTHER INFORMATION

Prof. Antonio Huerta
Director
Prof. Pedro Diez
Deputy Director

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