Research unit MUSAM
Multi-scale Analysis of Materials

Annual Report – 2015
## Contents

1 Mission of the research unit ........................................ 1

2 The team ........................................................................ 1

3 Research activities .......................................................... 3

4 Educational activities ......................................................... 3

5 Guest scholars and seminars ............................................. 4

6 Outreach activities ............................................................ 5
   6.1 Special sessions and workshops .................................... 8
   6.2 Invited seminars and lectures ..................................... 9

7 Funding and technology transfer ......................................... 10
   7.1 Funding ..................................................................... 10
   7.2 Technology transfer .................................................. 11

8 Scientific results ............................................................... 12
   8.1 Peer-reviewed journal publications ............................. 17
   8.2 Peer-reviewed conference publications ...................... 19

9 Future perspectives ........................................................... 19
Preface

This report provides an overview of the activities carried out by the research unit MUSAM (Multi-scale Analysis of Materials) in 2015, along with a summary of the main results achieved and an outlook on future directions of research.

MUSAM has been founded in November 2013 within the area of Computer Science and Applications of the IMT School for Advanced Studies Lucca to contribute to the research on complex technological systems by promoting the highest as possible scientific excellence in mathematical modelling, numerical analysis and experimental methods.

So far, the research activities have been partially supported by the project ERC Starting Grant CA2PVM Multi-field and multi-scale Computational Approach to design and durability of Photovoltaic Modules by the European Research Council which allowed the recruitment of four post-doctoral fellows and three visiting professors in 2015, to further strengthen the research group towards the accomplishment of the aims of the ERC project. Additional resources have been provided by the Italian Ministry of Education, University and Research to the FIRB Future in Research Project Structural Mechanics Models for Renewable Energy Applications, supporting the activities of collaborators enrolled at Politecnico di Torino. Last but not least, the school support to one Assistant Professorship and one new PhD scholarship in 2015 is gratefully acknowledged.

The scientific results achieved during 2015 have been remarkable, with publications in top journals of mechanics, physics, and energy. Noteworthy is the ability of the unit to contribute to the attraction of PhD students and research scholars with international experience. The 160 Worldwide applications selecting MUSAM as the preferred research unit for the PhD Track in Computer Science and Systems Engineering are very promising and confirm the figures of 2014.

Finally, I would like to express my personal gratitude for their support to the former and present Directors of the School, Professor Alberto Bemporad and Professor Pietro Pietrini, to the Colleagues for constructive discussions, and to all the collaborators and visiting scholars that have contributed with their passion and commitment to the scientific results achieved in 2015.

With sincere greetings from the beautiful City of Lucca,

Prof. Dr. Ing. Marco Paggi
(Director of the research unit)
1 Mission of the research unit

MUSAM – Multi-scale Analysis of Materials – is a research unit of the IMT School for Advanced Studies Lucca belonging to the area of Computer Science and Applications. The research unit contributes to the research and educational programmes of the School by developing mathematical models, computational methods and experimental techniques for the characterization and prediction of nonlinear phenomena in physical systems characterized by multiple scales or in the presence of multiple fields.

The web-site of the research unit is:
http://musam.imtlucca.it

The web-site of the MUSAM-Lab is:
http://www.imtlucca.it/research/laboratories/musam-lab

2 The team

The research unit is composed of:

- Prof. Dr. Ing. Marco Paggi (Director) www.imtlucca.it/marco.paggi
- Dr. Ing. Andrea Bacigalupo, Assistant Professor
- Dr. Claudia Borri, Post-doctoral fellow responsible for the activities in the MUSAM-Lab
- Dr.-Ing. Pattabhi Budarapu, Post-doctoral fellow
- Dr. Ing. Mariacristina Gagliardi, Post-doctoral fellow
- Mr. Pietro Lenarda, PhD student (cycle XXIX)
- Ing. Valerio Carollo, PhD student (cycle XXX)
- Ing. Paolo Cinat, PhD student (cycle XXX)
- Ing. Vigneswaran Govindarajan, PhD student (cycle XXX)
- Ms. Rosaria Del Toro, PhD student (cycle XXXI)
Visiting scholars and professors from other institutions involved in the activities of the research unit:

- Prof. Dr. Ing. Davide Bigoni, Full Professor, Visiting Professor at IMT Lucca (University of Trento, Trento, Italy)
- Dr. Ing. Alessio Gizzi, Assistant Professor, Visiting Professor at IMT Lucca (Università Campus Bio-Medico di Roma, Rome, Italy)
- Dr. Ing. José Reinoso, Assistant Professor, Visiting Professor at IMT Lucca (University of Seville, Seville, Spain)
- Ing. Irene Berardone, PhD student at Politecnico di Torino (cycle XXVIII) and DAAD Visiting Scholar at the Institute for Solar Energy Research (Hamelin, Germany)
- Dr. Ing. Mauro Corrado, Assistant Professor, Visiting scholar at IMT Lucca (Politecnico di Torino, Torino, Italy; presently Marie Curie Fellow at the École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland)
- Ing. Andrea Infuso, PhD student at Politecnico di Torino (cycle XXVIII)
Ing. Saheed Olalekan Ojo, PhD student at Politecnico di Torino (cycle XXVIII)

3 Research activities

Research activities undertaken in 2015 covered fundamental topics of mechanics of materials and structures, such as thermo-elastic stress analysis, fracture, fatigue, wave propagation in heterogeneous materials, homogenization techniques, and contact mechanics. Besides those topics, the unit promotes research in the field of computational materials science by combining computational methods proper of mechanics with advanced experimental techniques typical of materials science. This aim is pursued thanks to the experimental facilities of the MUSAM-Lab realized with the financial support of the European Research Council provided to the ERC Starting Grant project CA2PVM (GA no. 306622). In line with the ERC StG mission, fundamental research is carried out in the field of photovoltaics in order to understand the phenomenon of cracking in solar cells, design new solutions to limit its effect, and increase the overall durability and reliability of this renewable energy technology. Finally, a new collaboration with Dr. Alessio Gizzi on physical and mathematical modelling of biological objects interactions has been initiated in 2015 and will be exploited in 2016.

An interdisciplinary collaboration with the research unit DYSCO has been established in the field of performance of optimization algorithms applied to contact mechanics and metamaterials, as well as in techniques for model parameters identification applied to nonconvex nonlinear mechanical problems.

All the computational activities are performed in house by developing new routines for the finite element analysis programme FEAP (parallel version 8.3 and MATLAB interface to FEAP), the computational fluid dynamics software OpenFOAM, MATLAB routines for the boundary element method applied to contact mechanics, and LAMMPS for molecular dynamics simulations.

4 Educational activities

The research unit contributes since November 2014 to a PhD curriculum on Computational Mechanics whose peculiarity stems from the strong interdisciplinarity of the educational programme. Since November 2015 it collaborates with the research units SysMA, DISCO, PRIAn and NETWORKS on the PhD Track in Computer Science and Systems Engineering, focusing on modelling and simulation of cyber-physical systems.

The portfolio of courses delivered by the members of the research unit covers Numerical Methods for Partial Differential Equations, Micromechanics, Computational Contact and Fracture Mechanics, and Advanced Topics of Computational Mechanics. A long seminar on Management of Intellectual Property and Fund Raising is also offered to all the PhD students of the School. Seminars
on cutting-edge topics delivered by invited international experts complete the educational activities.

Finally, it is worth mentioning the course on *Computational Contact and Fracture Mechanics*, advertised on the web-page of the PhD School of the University of Pisa, attracted three PhD students from Pisa in the areas of Electronics and Aeronautical Engineering.

## 5 Guest scholars and seminars

During 2015, three visiting professorships have been funded within the ERC StG CA2PVM project to support the long stays by Prof. Dr. Ing. Davide Bigoni, Dr. Ing. José Reinoso and Dr. Ing. Alessio Gizzi. The research unit has also received short visits by Dr. Lorenzo Morini from the University of Trento, Prof. Elio Sacco from the University of Pisa, Dr.-Ing. Roman Pohrt from the Technical University of Berlin, and Ing. Francesca Fantoni from the University of Brescia.

A list of seminars organized by the research unit is provided below.

- A. Gizzi, Università Campus Bio-Medico di Roma. Theoretical and numerical modeling of nonlinear electromechanics with applications to biological active media (February 20, 2015).
- L. Morini, University of Trento. Analysis of interfacial crack problems using the weight functions technique (April 22, 2015).
- P. Cinat, IMT School for Advanced Studies Lucca. The HighTissue project (June 15, 2015).
- D. Bigoni, University of Trento. Folding and faulting of an elastic continuum (June 16, 2015).
- E. Sacco, University of Cassino. An interface damage model accounting for the confinement effect (September 18, 2015).
- F. Fantoni, University of Brescia. Crack growth as a standard dissipative system (October 26, 2015).
- L. Morini, University of Trento. Multiscale asymptotic homogenization analysis of thermo-diffusive composite materials (November 26, 2015).
6 Outreach activities

The research unit participates to the activities of the IEA-PVPS (International Energy Agency – Photovoltaic Power Systems Programme) Committee of Task 13 on Performance and Reliability of Photovoltaic Systems in the period 2015-2017, see http://www.iea-pvps.org. The Task 13 aims at publishing reports on field data degradation of PV modules and on critical examination of crack detection methods, along with guidelines for improved financial plans accounting for maintenance costs. These reports are conceived to have impact on the photovoltaic industry sector and on policy makers.

From March 30 to April 2, 2015, the prestigious EUROMECH Colloquium 575 on Contact Mechanics and Coupled Problems in Surface Phenomena co-chaired by Prof. M. Paggi and Prof. D.A. Hills (University of Oxford) took place in the campus of IMT Lucca under the auspices of the European Mechanics Society and the patronage of the following public authorities and associations: Città di Lucca, Provincia di Lucca, Regione Toscana, Associazione Industriali Lucca, Lucense ScpA. The conference website is permanently displayed at http://575.euromech.org/. The Colloquium has featured 49 participants from Czech Republic (3), Denmark (1), France (9), Germany (4), Italy (17), Russia (4), Spain (3), Sweden (1), Switzerland (2), United Kingdom (4), USA (1). The complete Book of Abstracts can be downloaded from http://musam.imtlucca.it/euromech575/Book_of_abstracts.pdf and the production of two special issues, one for the Journal of Strain Analysis for Engineering Design and another for the Journal of Mechanical Engineering Science, is in progress and will be finalized in 2016.
The logo of the EUROMECH Colloquium 575

Group photo
Moments of discussion in the IMT campus during the EUROMECH Colloquium 575

The research unit has also contributed to the organization of the workshop *Innovative Startups and Open Innovation: which opportunities with the new Italian regulation* (IMT Lucca, June 12, 2015) with invited presentations by Mattia Corbetta (Member of the Technical Secretariat of the Italian Ministry of Economic Development), Eugenio Telleschi (Euro Inn Advisory Srl) and Marco Paggi, see https://www.imtlucca.it/news-events/files/poster/000917_95_poster.pdf. The video of the event is also permanently available in streaming at https://www.youtube.com/watch?v=cmufGwTMIHw.

Moreover, the unit has co-organized the workshop *ERC Grants for the Excellence of European Research* (IMT Lucca, November 11, 2015), in collaboration with the European Research Council and APRE–Agency for the Promotion of the European Research, see https://www.imtlucca.it/news-events/files/poster/000976_111_poster.pdf. The video of the event is also permanently available in streaming at https://www.youtube.com/watch?v=ltT32iej2vU&feature=youtu.be.

Finally, the research unit has organized a stand on *Pannelli solari, carta e adesivi: cosa hanno in comune? Ce lo spiega la meccanica* at BRIGHT! Night of Researchers in Tuscany, an event promoted by Marie Curie Actions and Tuscany Region (Lucca, Italy, September 25, 2015).
The members of the research unit have also co-organized special sessions in international conferences, have served as members of scientific committees, and have delivered seminars and lectures at conferences and universities disseminating research results and promoting the visibility of the School in the field of mechanics, see the list below.

6.1 Special sessions and workshops


- Special Session *Phase field and enhanced finite element formulations for fracture mechanics*, ECCOMAS Thematic Conference on eXtended Discretization MethodS, Ferrara, Italy September 9-11, 2015. Organized together with T. Rabczuk (University of Weimar) and J. Reinoso (University of Seville).

6.2 Invited seminars and lectures


- Computational methods for nonlinear fracture mechanics problems with large displacements. Seminar by M. Paggi at the Solid and Structural Mechanics Group of the University of Trento, Trento, Italy, September 28, 2015.

- Modelling decohesion phenomena in thermo-elastic structures. Seminar by P. Lenarda at the group by Prof. F. Quarteroni at the École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, May 24, 2015.

- Multi-physics Modelling of Photovoltaic Laminates. Seminar by M. Paggi at the MUSIC Graduate School on Multiscale Methods for Interface Coupling, Institute of Continuum Mechanics, Leibniz University of Hannover, Hannover, Germany, May 18, 2015.


7 Funding and technology transfer

7.1 Funding

Two projects, one supported by the European Research Council and another by the Italian Ministry of Education, University and Research are currently ongoing. The ERC Starting Grant CA2PVM on Multi-scale and Multi-Physics Computational Methods for the Design and Durability of a Photovoltaic Modules will end in December 2017 and a list of scientific results is continuously updated on the project web-site http://musam.imtlucca.it/CA2PVM.html. The mid-term report, approved by the European Research Council, is also available for download at http://musam.imtlucca.it/Mid-term-report.pdf
The FIRB Future in Research Project on Structural Mechanics Models for Renewable Energy Applications involving Politecnico di Torino, the University of Salento and the University of Trento as partners is currently at its fourth year and will end in March 2016, see http://musam.imtlucca.it/FIRB.html.

7.2 Technology transfer

The research unit has carried out joint research activities with Applied Materials Inc., San Biagio di Callalta (Italy), and with Jabil Defense and Aerospace Services LLC, part of Jabil Circuit Inc., St. Petersburg (FL, USA), in the field of durability of photovoltaics. The joint publication [B.1] is the result of this international collaboration.

Activities aiming at fostering technology transfer to the local industries in the sectors of paper tissue, mechanical and naval engineering, and photovoltaics have also been carried out during 2015. In particular, articles [A.1, A.8] on computational modelling of adhesion between layers of paper tissue have been motivated by industrial research.

A full list of experimental testing and numerical simulation facilities for technology transfer is available at: http://musam.imtlucca.it/MUSAM-LAB.pdf and it has been distributed via Assindustria Lucca to all the industries active in the district. Moreover, the research unit and MUSAM-Lab collaborates with Lucense SCpA to the R&D and technology transfer activities of the Distretto Cartario Lucchese.
8 Scientific results

The members of the research unit have co-authored 15 articles printed or in press in peer-reviewed international journals and 3 in conference proceedings. Articles co-authored by PhD students are 6 over 18. Articles A.1, A.2 and A.8 are the result of the collaboration with Dr. Reinoso, visiting professor of the research unit at IMT Lucca. Overall, 8 articles over 18 are the outcome of international collaborations. Articles A.3 and A.9 are the result of the cooperation between the research units DYSCO and MUSAM.

The key results are summarized in the following items:

- Numerical modelling and experimental testing of adhesive properties of cellulose fibers joining paper tissues [A.1, A.8]. The computational model is based on a novel cohesive zone approach where the interface tractions are the result of the peeling force of each individual fibril integrated over the statistical distribution of their in-plane and out-of-plane orientations. This constitutive model has been implemented within a novel interface finite element whose kinematics is suitable for mechanical problems governed by large displacements and moderate rotations.

![Large displacement formulation for fibrillar interfaces.](image)

Large displacement formulation for fibrillar interfaces.
Examples of fibrillar crack propagation in paper tissue and in polymers.

- Study of the interplay between delamination and wrinkling in functionally graded thermal barrier coatings [A.2]. This work has required the integration of the new interface element for large displacements developed in [A.8] with solid shell finite elements to model thin stiff layers bonded onto a soft substrate.

Wrinkling of a stiff layer bonded onto a soft substrate.

- Proposal of a new interface finite element for interface fracture able to deal with non matching finite element discretizations of the bulk [A.4].
Proposal of a fatigue crack growth equation able to model the anomalous behaviour of short cracks and validation with experiments [A.5].

Crack growth velocity vs. stress-intensity factor curve, showing the anomalous behaviour of short cracks
• Investigation of the distribution of residual thermo-elastic stresses in photovoltaic modules considering for the very first time the visco-elastic behaviour of the polymeric encapsulant and the transient regime during cooling [A.6]. The thermo-visco-elastic constitutive response has been modelled via fractional calculus based on the results in [A.14].

• Experimental testing and simulation of an innovative approach to produce thin film solar cells via thermo-mechanically induced spalling [A.7].

• Proposal of new optimization algorithms for the solution of the frictionless normal contact problem between rough surfaces, with a significant speed-up in computation time with respect to the state-of-the-art literature [A.9].

Speed-up in computation time of the proposed optimization algorithms with respect to the Greedy conjugate gradient (CG) method

• Investigation of the topological features of the free volume between rough surfaces in contact, with applications to sealing [A.10].
Free volume domains for different threshold values

- Development of a power and energy procedure suggesting new standards for determining the sources of losses in a photovoltaic plant and thus minimizing poor performance in the energy production [A.11].

Example of crack pattern in a photovoltaic modules detected by the electroluminescence technique

- Development of a numerical tool for the multi-resolution statistical and spectral characterization of textured surfaces such as antireflective coatings and hydrophobic surfaces sampled by a confocal profilometer [A.13].
Comparison between experimental and theoretical joint probability density functions

8.1 Peer-reviewed journal publications


8.2 Peer-reviewed conference publications

B.1 V. Gade, S. Narendra, M. Paggi, J. Opalewski (2015) Predicting the long term power loss from cell cracks in PV modules, Photovoltaic Specialist Conference (PVSC), 2015 IEEE 42nd, 14-19 June 2015, New Orleans (LA) USA, 1–6, http://dx.doi.org/10.1109/PVSC.2015.7355665


9 Future perspectives

The target of the research unit is to promote fundamental research in mechanics and the integration between materials science and computational methods. In the School context, the natural role of the unit is to provide quantitative methods, mathematical and numerical modelling and simulation for problems governed by partial differential equations, common to physics, engineering and economics. Therefore, if on the one hand the highest level of specialization in the classical topics of mechanics should be cultivated, on the other hand it is desirable to increase the impact on interdisciplinary applications. In 2016, the collaboration with Dr. Alessio Gizzi and his LAB at the Università Campus Bio-Medico di Roma will be strengthened towards the study of problems governed by complex interactions between biological objects.

Further international cooperations will be exploited via the research periods of the PhD students supported by the ERASMUS Plus programme: Valerio Carollo will spend a research period in the group by Prof. J. Llorca at the IMDEA Materials Institute in Madrid, Vigneswaran Govindarajan will have an internship in the group by Prof. T. Rabczuk at the University of Weimar, and Paolo Cinat will collaborate with Dr. V. Yastrebov at the CNRS in Paris. Pietro Lenarda will apply his methods for partial differential equations to problems of common interest to the Mathematical Institute of the University of Oxford, with an internship under the guidance of Dr. R. Ruiz Baier.

Finally, thanks to the support of the ERC StG, the research unit composition will increase of 4 people in 2016, with one new post-doctoral fellow, Dr. Lorenzo Morini, from the middle of January, and three new research collaborators from the beginning of March. This will assure the completion of the activities of the ERC StG project and further positive impact on the quality of the research.