

**ECCOMAS Thematic Conference on
Computational modeling of Complex
Materials across the Scales**

CMCS 2017

Paris, France, November 7-9, 2017

Technical Program

Welcome to CMCS 2017, welcome to Paris!

The international Thematic Conference “**Computational modeling of complex materials across the scales (CMCS)**” will take place on 7 - 9 Nov. in Paris, France under the auspices of the European Community on Computational Methods in Applied Sciences (**ECCOMAS**).

The objectives of the international CMCS 2017 conference are to present recent state-of-the-art developments in multiscale modeling of complex materials with computational approaches. This thematic conference focuses on one hand on the modeling of complex (i.e. multiphysics, realistic microstructures) microstructural phenomena and on the other hand on the upscaling of these phenomena at coarse (engineering) scales to determine their effective or emergent behavior. The goal is to gather scientists from different disciplines working on scale bridging problems in materials and structures to make a step forward in the development of these approaches and to target integration in future engineering tools. We hope that this conference will be the opportunity for fruitful and inspiring discussions.

On behalf of the organizing committee,



Julien Yvonnet
Chairman



Marc Geers
Co-chairman



Paul Steinmann
Co-chairman

Acknowledgements

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TECHNICAL PROGRAM - CMCS 2017

Computational Modeling of Complex Materials Across the Scales

November 7-9, 2017 - Paris, France

Technical sessions

TS	Topics	Room
S01	Concurrent multi-scale simulations	Auditorium
S02	Microcracks, interfaces and localization	Denderah
S03	Advanced effective and mean-field methods	Louxor
S04	Stochastic and statistical approaches	Louxor
S05	Generation of microstructures	Denderah
S06	Microscale-based material models	Denderah (S06a - S06b)
		Auditorium (S06c)
S07	Advanced numerical methods	Louxor (S07a - S07b - S07d)
		Auditorium (S07c)
S08	Dynamic homogenization	Auditorium
S09	Multiphysical couplings	Louxor
S10	Experiments and microscale parameters identification	Denderah
S11	Atomistic and discrete simulations	Auditorium

Program Overview - Tuesday, November 7

8:00 - 8:45	Registration and welcome		
8:45 - 9:00	Auditorium Introduction to CMCS 2017 <i>J. Yvonnet</i>		
9:00 - 9:45	Auditorium Plenary lecture <i>M. Ortiz</i>		
9:45 - 10:30	Auditorium Plenary lecture <i>W.A. Curtin</i>		
10:30 - 11:00	Coffee break		
11:00 - 12:40	Auditorium S01a - Concurrent multi-scale simulations	Louxor S03 - Advanced effective and mean-field methods	Denderah S02a - Microcracks, interfaces and localization
12:40 - 14:00	Philae Lunch		
14:00 - 15:40	Auditorium S01b - Concurrent multi-scale simulations	Louxor S04a - Stochastic and statistical approaches	Denderah S02b - Microcracks, interfaces and localization
15:40 - 16:10	Coffee break		
16:10 - 17:25	Auditorium S01c - Concurrent multi-scale simulations	Louxor S04b - Stochastic and statistical approaches S07a - Advanced numerical methods (Discretization)	Denderah S05 - Generation of microstructures

Lectures - Tuesday, November 7 - Morning

Room	Auditorium
	Plenary lectures <i>chair: M.G.D. Geers</i>
9:00	The anomalous yield behavior of fused silica glass from a multiscale perspective <i>M. Ortiz</i>
9:45	Coupled Atomistics and Discrete Dislocations in 3D (CADD-3D) <i>W.A. Curtin</i>

Room	Auditorium	Louxor	Denderah
TS	S01a - Concurrent multi-scale simulations <i>chair: J. Yvonnet</i>	S03 - Advanced effective and mean-field methods <i>chair: N. Takano</i>	S02a - Microcracks, interfaces and localization <i>J. Clayton</i>
11:00	Modeling of micro-heterogeneous magneto-electric composites: an algorithmic scale-bridging scheme <i>J. Schröder, M. Labusch, V. Lemke</i>	Modelling skeletal muscle tissue across multiple scales <i>C. Bleiler, P.P. Castaneda, O. Röhrle</i>	Microstructural pattern evolution in magnesium by stabilized spectral homogenization <i>A. Vidyasagar, A. Tutcuoglu, D.M. Kochmann</i>
11:25	Computational Multiscale Stability Analysis of Periodic Magnetorheological Elastomers <i>E. Polukhov, D. Vallicotti, M-A. Keip</i>	Texture dependent approximation of Hashin-Shtrikman type for viscoplasticity based on the linear-comparison-material-method <i>M. Lobos, T. Böhlke</i>	Localization of plastic deformation in a stretching metal sheet: a mesoscopic approach <i>J-L. Dequiedt</i>
11:50	Magnetorheological elastomers as magneto-electric transducers: micro- and macrostructural effects <i>M. Rambausek, M-A. Keip</i>	Consistent algorithmic treatment and Finite-Element implementation of the incremental Mori-Tanaka model <i>P. Sadowski, K. Kowalczyk-Gajewska, S. Stupkiewicz</i>	Advanced micro-boundary conditions for single crystal plasticity at small scales <i>E. Husser, C. Soyarslan, S. Bargmann</i>
12:15	Microstructural modeling of functional properties of porous shape memory alloy <i>M.E. Evard, A.E. Volkov, E.N. Iaparova</i>		

Lectures - Tuesday, November 7 - Afternoon

Room	Auditorium	Louxor	Denderah
TS	S01b - Concurrent multi-scale simulations <i>chair: J. Schröder</i>	S04a - Stochastic and statistical approaches <i>chair: R. Cottreau</i>	S02b - Microcracks, interfaces and localization <i>chair: X. Oliver</i>
14:00	Influence of bimodal microstructure morphologies on local and macroscopic mechanical responses <i>B. Flipon, C. Keller, F. Barbe</i>	A stochastic 3-scale method to predict the thermo-elastic behaviors of polycrystalline structures <i>L. Wu, V. Lucas, J-C. Golinval, S. Paquay, L. Noëls</i>	Modeling of complex inelastic deformation mechanisms in crystalline solids with phase field and geometric concepts <i>J. Clayton, J. Knap</i>
14:25	Thermomechanical multiscale modeling of materials embedding phase change particles <i>K-M. Kodjo, J. Yvonnet, K. Sab, M. Karkri</i>	Stochastic multiscale modeling and analysis of three-dimensionally woven CMC considering many random parameters <i>N. Takano, K. Hagiwara, D. Haruyama</i>	Numerical identification of homogeneous phase field models to quasi-brittle fracture in heterogeneous periodic media <i>N. Nguyen, J. Yvonnet, J. Réthoré</i>
14:50	Nonlinear Multi-Scale Simulations of Fabric Laminate Components <i>T. Ceglár, M. Schwab, A. Wagner, H. Pettermann</i>	Quantitative sensitivity of properties to microstructural characteristics in cement paste <i>J-S. Kim, T-S. Han</i>	Aspects of micro-to-macro transition accounting for general imperfect interfaces <i>S. Saeb, P. Steinmann, A. Javili</i>
15:15	Application of the submodeling technique for analyzing cord-rubber composites <i>N. Heinrich, J. Ihlemann</i>	Considerations on the stochastic time homogenization method <i>A. Moreira De Oliveira Filho, G. Puel, K. Sab</i>	Modelling Interfaces in Nanostructured Composite Actuators <i>J. Wilmers, A. McBride, S. Bargmann</i>

Lectures - Tuesday, November 7 - End of afternoon

Room	Auditorium	Louxor	Denderah
TS	S01c - Concurrent multi-scale simulations <i>chair: E. Husser</i>	S04b - Stochastic and statistical approaches <i>chair: G. Puel</i>	S05 - Generation of microstructures <i>chair: V.G. Kouznetsova</i>
16:10	Microstructural evolution of neutron-irradiated tungsten under high temperature loading <i>A. Mannheim, H.V. Dommelen, M.G.D. Geers</i>	Modeling the effects of crystal disorientation in turbine blades and other highly directional loading situations <i>T. Rose, A. Boucicaud, S. Gourdin, F. Coudon, G. Cailletaud</i>	Generation of unidirectional composite stochastic volume elements from micro-structural statistical information <i>L. Wu, B. Bidaine, Z. Major, C.N. Chung, L. Noëls</i>
TS		S07a - Advanced numerical methods (Discretization) <i>chair: G. Puel</i>	
16:35	Minimalist two-scale model for the Payne and Mullins effects in filled elastomers <i>M. Semkiv, P. Anderson, D. Long, M. Hütter</i>	Isogeometric homogenization analysis with microscopic contact behavior <i>S. Nishi, K. Terada, I. Temizer</i>	An automated procedure for the generation and discretization of 3D woven composites RVEs <i>B. Wintiba, B. Sonon, K. Ehab Moustafa Kamel, T.J. Massart</i>
17:00	Two-Scale Anisotropic Damage Modeling of Debonding and Matrix Damage in SMC <i>M. Schemmann, J. Görthofer, T. Böhlke</i>	Modeling the response of fibrous networks under hygroscopic swelling <i>P. Samantray</i>	Computational modeling and analysis of complex cellular material RVEs <i>N. Gopala Kilingar, K. Ehab Moustafa Kamel, B. Sonon, L. Noëls, T.J. Massart</i>

Program Overview - Wednesday, November 8

9:00 - 9:45	Auditorium Plenary lecture <i>K. Terada</i>		
9:45 - 10:30	Auditorium Plenary lecture <i>S. Forest</i>		
10:30 - 11:00	Coffee break		
11:00 - 12:15	Auditorium S08 - Dynamic homogenization	Louxor S07b - Advanced numerical methods (Discretization)	Denderah S06a - Microscale-based material models
12:15 - 13:15	Philae Lunch		
13:15 - 14:55	Auditorium S07c - Advanced numerical methods (Saving CPU time)	Louxor S09 - Multiphysical couplings	Denderah S06b - Microscale-based material models
14:55 - 15:25	Coffee break		
15:25 - 16:40	Auditorium S06c - Microscale-based material models	Louxor S07d - Advanced numerical methods (Coupling)	Denderah S10 - Experiments and microscale parameters identification
17:30 - 19:30	Bus visit tour		
20:00 - 23:00	Le Procope restaurant Banquet		

Lectures - Wednesday, November 8 - Morning

Room	Auditorium
	Plenary lectures <i>chair: P. Steinmann</i>
9:00	Enhancing microstructural analyses in computational homogenization <i>K. Terada</i>
9:45	Combining large scale simulations and experiments for the understanding of plasticity and cracking phenomena in metal polycrystals <i>S. Forest</i>

Room	Auditorium	Louxor	Denderah
TS	S08 - Dynamic homogenization <i>chair: M. Rambausek</i>	S07b - Advanced numerical methods (Discretization) <i>chair: A. Salvadori</i>	S06a - Microscale-based material models <i>chair: M. Hütter</i>
11:00	A general homogenization framework towards the computation of complex emergent elastodynamics of metamaterials <i>A. Sridhar, V.G. Kouznetsova, M.G.D. Geers</i>	Numerically robust two-scale simulations of heterogeneous microstructures <i>J. Kochmann, S. Wulfinghoff, B. Svendsen, S. Reese</i>	A Multi-scale Simulation of Ferroelastic Phase Formation in LSCF Polycrystal Based on Phase-field Method <i>M. Muramatsu, K. Yashiro, T. Kawada, K. Terada</i>
11:25	On multiscale modeling of materials accounting for inertial effects. Application to acoustic materials design <i>X. Oliver</i>	A filter-based computational homogenization method for composite structures without scale separation assumption <i>L. Minh Vuong, J. Yvonnet, N. Feld, C. Combescure</i>	Discussion of Flow Stress and Strain Hardening in a Dislocation Density-based Continuum Model <i>K. Schulz, M. Sudmanns, P. Gumbsch</i>
11:50	Computational homogenization for transient phenomena in linear and non-linear locally resonant metamaterials <i>V.G. Kouznetsova, A. Sridhar, P. Brandão Silva, T.F.W. Van Nuland, M.G.D. Geers</i>	The role of kinematic boundary conditions and their (in)accuracy in micromechanical parameter identification <i>O. Rokos, J.P.M. Hoefnagels, R.H.J. Peerlings, M.G.D. Geers</i>	

Lectures - Wednesday, November 8 - Afternoon

Room	Auditorium	Louxor	Denderah
TS	S07c - Advanced numerical methods (Saving CPU time) <i>chair: L. Noëls</i>	S09 - Multiphysical couplings <i>chair: S. Forest</i>	S06b - Microscale-based material models <i>chair: J. Wilmers</i>
13:15	Extended cyclic simulations in crystal plasticity - Mean field and hyper-reduced finite element simulations <i>H. Farooq, D. Ryckelynck, G. Cailletaud, S. Forest</i>	A Computational Homogenization Framework for Variational Phase-Field Modeling of Micro-Magneto-Mechanics at Finite Strains <i>D. Vallicotti, A. Sridhar, M-A. Keip</i>	Multiscale wear modelling of cemented tungsten carbide tools in hard rock drilling <i>D. Tkalich, V. Yastrebov, G. Cailletaud, A. Kane</i>
13:40	High-performance reduced-order computational homogenization <i>R.A. Van Tuijl, J.J.C. Remmers, M.G.D. Geers</i>	A computational homogenization approach for (Li-ion) battery cells: microscale analysis <i>A. Salvadori, M. Magri</i>	Multiscale modeling of the electromechanical properties of graphene-reinforced nanocomposites <i>X. Lu, J. Yvonnet, F. Detrez, J. Bai</i>
14:05	A revision of the algorithmic structure of two-scale finite element methods for nonlinear homogenization <i>B. Eidel, A. Fischer, A. Gote</i>	A coupled framework for modeling of concurrent viscoplastic deformation and grain boundary migration in metallic polycrystals <i>A. Ask, S. Forest, K. Ammar, B. Appolaire, O. Salman</i>	Multiscale Analysis and Realization of Photo-responsive Polymer <i>M. Cho</i>
14:30	Model-order reduction of nonlinear homogenization problems using a Hashin-Shtrikman type finite element scheme <i>F. Cavaliere, S. Wulfinghoff, S. Reese</i>		Finite element simulation of an intrinsic hybrid composite <i>R. Kießling, J. Ihlemann</i>

Lectures - Wednesday, November 8 - End of afternoon

Room	Auditorium	Louxor	Denderah
TS	S06c - Microscale-based material models <i>chair: L. Wu</i>	S07d - Advanced numerical methods (Coupling) <i>chair: M. Cho</i>	S10 - Experiments and microscale parameters identification <i>chair: M. Muramatsu</i>
15:25	Modelling of the mechanical behavior of the polyurethane foams by means micromechanical characterization and computational homogenization <i>M. Marvi Mashhadi, C.S. Lopes, J. Llorca</i>	Fully scalable implementation of a volume coupling scheme for the modeling of random polycrystalline materials <i>R. Cottureau, T. Milanetto Schlittler</i>	Mechanical behavior of 316L steel subjected to biaxial strain path changes: multi-scale modeling and experiments <i>M. Upadhyay, A. Patra, W. Wen, T. Panzner, S. Van Petegem, C. Tome, R. Lebensohn, H. Van Swygenhoven</i>
15:50	Simulation and inverse calculation of single metal foam pores <i>T. Bleistein, A. Jung, S. Diebels</i>	The Capriccio Method for Concurrent Continuum Mechanics and Particle-Based Simulations <i>S. Pfaller, P. Steinmann</i>	Microstructure-Based Mechanical Simulation of Dual-Phase Steel <i>F. Scherff, S. Scholl, S. Diebels</i>
16:15	Numerical and experimental identification of strain-rate effects in hybrid foams from the micro scale to the macro scale <i>A. Jung, J. Luksch, M. Felten, D. Sory, A. Pullen, W. Proud</i>		Meso-scale finite element model and experiments for impact damage prediction in three-dimensional rectangular braided composites <i>H. Tan, S. Xu, Y. Guan, L. Lulu, C. Wei</i>

Program Overview - Thursday, November 9

9:30 - 10:45	Auditorium S11 - Atomistic and discrete simulations	Louxor S06d - Microscale-based material models	Denderah
10:45 - 11:15	Coffee break		
11:15 - 12:00	Auditorium Plenary lecture <i>P. Wriggers</i>		

Lectures - Thursday, November 9

Room	Auditorium	Louxor	Denderah
TS	S11 - Atomistic and discrete simulations <i>chair: K. Schulz</i>	S06d - Microscale-based material models <i>chair: X. Lu</i>	
09:30	Atomic instabilities at the origin of failure initiation <i>S. Souguir</i>	Multiphase continuum models for fiber-reinforced media <i>J. Bleyer</i>	
09:55	Simulation of low-temperature sintering bonding for optics using silver particles <i>X. Wang, L. Benabou</i>	Multiscale Constitutive Models for the Prediction of the Microstructure Evolution and the Mechanical Properties of Fibre Based Materials <i>F. Martinez-Hergueta</i>	
10:20	Atomistic simulations at reduced strain rates of dislocation interactions in nanocrystalline Aluminium <i>M. Dupraz, Z. Sun, C. Brandl, H. Van Swygenhoven</i>	Anisotropic Elastoplastic model for Fiber Reinforced Laminates <i>S. Nagaraja, C. Schuecker, M. Pletz</i>	

Room	Auditorium
	Plenary lecture <i>chair: K. Terada</i>
11:15	Obituary in honor of Prof. Dr.- Ing. Christian Miehe <i>P. Wriggers</i>

Room list

