

# Program Schedule

**MMM** 2008  
*Fourth  
International Conference*  
**MULTISCALE MATERIALS MODELING**  
**OCTOBER 27-31, 2008 - TALLAHASSEE, FLORIDA, USA**

Organized and Hosted by  
The Department of Scientific Computing and  
Florida State University

DEPARTMENT OF  
**Scientific**  
COMPUTING





# Timetable

## Sunday (10/26/2008)

5:30 -8:30 pm    Registration and reception  
                         Tallahassee-Leon County Civic Center

## Monday (10/27/2008)

8:00 am	<b>Registration</b>							
8:20 am								
8:40 am	8:30-9:00	<b>Opening Remarks &amp; Announcements</b>						
<b>Session M-A (Plenary)</b>								
9:00 am	<p>50 minute plenary</p> <p>Sir <b>Harold Kroto</b>, Nobel Laureate for Chemistry &amp; Francis Eppes Professor of Chemistry and Biochemistry, Florida State University, USA</p> <p>Title: <b>Architecture in nanospace</b></p> <p>Room A3</p>							
9:20 am								
9:40 am								
	10:00 am	<b>20 min Coffee Break</b>						
<b>Session M-B (Parallel)</b>								
		<b>Room A3</b>	<b>Room A2</b>	<b>Room A1</b>	<b>Room B</b>	<b>Room C</b>	<b>Room D</b>	
		<b>S-3</b>	<b>S-4</b>	<b>S-5</b>	<b>S-1</b>	<b>S-9</b>	<b>S-7</b>	
10:20 am		Maenghyo Cho	Benoit Devincere	Peter Lee	Russel Cafilisch	Ronald Scattergood	Gregory A. Voth	1
10:40 am								2
11:00 am		Yuji Nakasone	Dennis Dimiduk	Raja Mishra	Endre Suli	Vaclav Vitek	Jonathan Wilke	3
11:20 am		Marino Arroyo	Dan Mordehai	Young-Min Kim	Petr Plechac	Bob Pond	Dmitry Kopelevich	4
11:40 am		Reza Naghdabadi	Siu Sin Quek	Duc Nguyen-Manh		Anna Serra	Shugo Yasuda	5
12:00 pm		Ted Vaughan	Daniel Weygand	Adam Kiejna	John H. Maddocks	Christian Brandl	Tahir Cagin	6
	12:20 pm	<b>Lunch Break (12:20 - 1:40 pm)</b>						
<b>Session M-C (Parallel)</b>								
		<b>S-3</b>	<b>S-4</b>	<b>S-5</b>	<b>S-1</b>	<b>S-9/S-6</b>	<b>S-7</b>	
1:40 pm		Sarah Ricker	Paul Dawson	Qiang Du	Gero Friesecke	Dane Morgan	Darrin Pochan	7
2:00 pm		Kenjiro	Somnath		Claude Le	Alexander	Andrea Liu	8

2:20 pm		Terada	Ghosh	Teck Tan	Bris	Barashev		9
2:40 pm		Anais Gaubert	Carmen Schaefer	Liming Xiong	Qiang Du	Christophe Domain	Martin Steinhauser	10
3:00 pm		Nicolas Nicaise	Aruna Prakash		Leonid Berlyand	Michael Jenkins	Lucio Colombi Ciacchi	11
	3:20 pm	<b>20 min Coffee Break</b>						
	<b>Session M-D (Parallel)</b>							
		<b>S-3</b>	<b>S-4</b>	<b>S-5</b>	<b>S-1</b>	<b>S-8</b>	<b>S-6</b>	
3:40 pm		Gerolf Ziegenhain	Dominique Jeulin	J-C Zhao	Eric Cances	Tomas de la Rubia	Alfredo Caro	12
4:00 pm		Yoshitaka Umeno						13
4:20 pm		Bo Yang	Vesselin Yamakov	Brent Adams	Carlos Garcia-Cervera	G. Robert Odette (Kurtz)	Kai Nordlund	14
4:40 pm			Botond Bako	Marius Stan	Frederik Heber	C H Woo	Arnoldo Badillo	15
	5:00 pm	<b>30 min break</b>						
	<b>Session M-E (Plenary)</b>							
5:30 pm		<p>50 minute plenary  <b>Subra Suresh</b>, Ford Professor and Dean of Engineering, Massachusetts Institute of Technology, USA</p> <p>Title: <b>Nanomechanics and the study of human disease states</b></p> <p>Room A3</p>						

**Tuesday (10/28/2008)**

8:00 am	<b>Registration</b>							
8:20 am								
8:40 am	8:50-9:00	<b>Remarks &amp; Announcements</b>						
<b>Session T-A (Plenary)</b>								
9:00 am	<p>50 minute plenary  <b>Nasr Ghoniem</b>, University of California Distinguished Professor, Mechanical And Aerospace Engineering Department &amp; Materials Science and Engineering Department, UCLA, USA   <b>Title: Multiscale modeling of the mechanical behavior of structural materials in nuclear energy systems</b>   Room A3</p>							
9:20 am								
9:40 am								
10:00 am	<b>20 min Coffee Break</b>							
<b>Session T-B (Parallel)</b>								
		<b>Room A3</b>	<b>Room A2</b>	<b>Room A1</b>	<b>Room B</b>	<b>Room C</b>	<b>Room D</b>	
		<b>S-3</b>	<b>S-4</b>	<b>S-5</b>	<b>S-1</b>	<b>S-8</b>	<b>S-7</b>	
10:20 am		Vasily Bulatov	Stephen Foiles	Christopher Woodward	J Tinsley Oden	Akiyuki Takahashi	Ulrich H E Hansmann	16
10:40 am		Michael Ortiz	Enrique Martinez	Jorg Neugebaue	Max Gunzburger	Jaafar El-Awady	Aaron Dinner	17
11:00 am						Christian Motz		Tapan Desai
11:20 am		Javier Llorca	Mukul Kabir	Yaroslav Shtogun	Denis Aubry	Michael Zaiser	Maxim Paliy	19
11:40 am		Ron Peerlings	Luis Sandoval	Zi-Kui Liu	Serge Prudhomme		S Adiga	20
12:00 pm								21
12:20 pm	<b>Lunch Break (12:20 - 1:40 pm)</b>							
<b>Session T-C (Parallel)</b>								
		<b>S-3</b>	<b>S-4</b>	<b>S-5</b>	<b>S-1</b>	<b>S-6</b>	<b>S-7</b>	
1:40 pm		G.V. Lasko	Gao Yingjun	Janina Zimmermann	Mitchell Luskin	Alain Chartier	Cecilia Clementi	22
2:00		Ryan	Giovanni	Yan Wang				

pm		Elliott	Bonny					
2:20 pm		Renald Brenner	Pär Olsson	Bandeep Singh	Ronald Miller	Ying Chen	Thomas Truskett	24
2:40 pm		Napo Bonfoh	<del>Kurt Scheerschmidt</del>	Dmitri Kilin	Jill Reese	Mikhail Lavrentiev	Jeffery Saven	25
3:00 pm		Ricardo Lebensohn	Edward Glaessgen	Michael Anisimov	Yanzhi Zhang	Duc Nguyen-Manh	Sergio Tafur	26
	3:20 pm	<b>Coffee Break and Poster Session</b> <b>Session T-D (Poster)</b> <b>Session T-D (Oral, S-9/S-6)</b>						
							<b>S-9/S-6</b>	
3:20 pm							C A English	
3:40 pm		Symposium 3: 37 Posters					David Stewart	
4:00 pm		Symposium 4: 30 Posters					Howard Heinisch	
4:20 pm		Symposium 7: 13 posters					Fei Gao	
4:40 pm							Rick Kurtz	
5:00 pm							C H Woo	
5:20 pm							Jaime Marian	
		<b>Session T-E (Plenary)</b>						
5:30 pm		50 minute plenary <b>Bennett C Larson</b> , Corporate Fellow, Materials Science and Engineering Division, Oak Ridge National Laboratory, USA  Title: <b>Linking multiscale materials modeling with experiment at the mesoscale using 3D X-ray microscopy</b>  Room A3						

### Wednesday (10/29/2008)

8:40 am	8:50- 9:00	<b>Remarks &amp; Announcements</b>						
<b>Session W-A (Plenary)</b>								
9:00 am	50 minute plenary							
9:20 am	Weinan E, Professor of Mathematics, Princeton University, USA							
9:40 am	Title: <b>Some mathematical and numerical issues on multiscale modeling</b>							
Room A3								
10:00 am	<b>20 min Coffee Break</b>							
<b>Session W-B (parallel)</b>								
		<b>Room A3</b>	<b>Room A2</b>	<b>Room A1</b>	<b>Room B</b>	<b>Room C</b>	<b>Room D</b>	
		<b>S-3</b>	<b>S-4</b>	<b>S-5</b>	<b>S-1</b>	<b>S-2</b>	<b>S-8</b>	
10:20 am		Ryo Kobayashi		Michael Gao	Pingbing Ming	Tom Lubensky	Elias Aifantis	27
10:40 am		Youping Chen	Thomas Bieler	Veera Sundararaghavan		Alfonso Ngan	Radan Sedlacek	28
11:00 am		<del>Cristina Arevalo</del>	Erik M. Lauridsen	Alireza Asgari	Rolf Krause			29
11:20 am		Don Nicholson		David McDowell	Richard Lehoucq	Roman Groger	Istvan Groma	30
11:40 am		Simon Gill	Susan Sinnott			Lasse Laurson	Anter El-Azab	31
12:00 pm		Peter Chung	<del>Alysson Diogenes</del>	Greg Olson	Michael Parks	Paolo Moretti	Richard LeSar	32
12:20 pm		Mihai Anitescu	Ling Yue	Aravind Asthagiri	Frederic Legoll	Adil Mughal	Hanchen Huang	33
12:40 pm	<b>Lunch Break (12:40 - 1:40 pm)</b>							
<b>Session W-C</b>								
		<b>S 3</b>	<b>S 4</b>	<b>S-9</b>	<b>S-6</b>	<b>S-2</b>	<b>S-8</b>	
1:40 pm		John Morris	Lucie Saintoyant	D Terentyev	François Willaime	James Sethna	Talat Rahman	34
2:00 pm			Anthony Rollett	Ghiath Monnet		Thomas Hochrainer		35
2:20 pm		Saurabh Puri	Byeong-Joo Lee	Christophe Domain	William J Weber	Jie Deng	Klaus Schwarz	36



2:40 pm	Camille Perrin	Martin Steinhauser	Lorenzo Malerba	Dilpuneet Aidhy	Ferenc F Csikor	Lizhi Sun	37
3:00 pm	Nicolas Cordero	D. Weygand or M. Verdier	Christophe Domain	Syo Matsumura		Mutasem Shehadeh	38
3:20 pm	<b>Coffee Break and Poster Session</b>						
	<b>Session W-D (parallel)</b>						
							<b>S-9/S-6</b>
3:20 pm							David Rodney
3:40 pm	Symposium 1: 9 Posters						Tomohito Tsuru
4:00 pm	Symposium 2: 5 posters						Y Osetskiy
4:20 pm	Symposium 5 : 8 Posters						Y Osetskiy
4:40 pm	Symposium 6: 12 Posters						Emmanuel Clouet
5:00 pm	Symposium 8: 11 Posters						Stanislav Golubov
5:20 pm							Aleksandar Donev
	<b>Session W-E (Plenary)</b>						
5:30 pm	<p>50 minute plenary  <b>Peter Gumbsch</b>, Head of the Fraunhofer Institute for Mechanics of Materials (IWM) &amp; Professor, Mechanics of Materials, University of Karlsruhe (TH), Germany</p> <p>Title: <b>Making and breaking of chemical bonds under mechanical loads</b></p> <p>Room A3</p>						

## Thursday (10/30/2008)

8:40 am	8:50- 9:00	<b>Remarks &amp; Announcements</b>						
<b>Session Th-A (Plenary)</b>								
9:00 am	50 minute plenary							
9:20 am	<b>Stéphane Roux</b> , Professor, LMT, ENS-Cachan / CNRS-UMR 8535 / Université Paris 6, France							
9:40 am	Title: <b>Depinning transition in solid mechanics</b>							
<b>Room A3</b>								
	10:00 am	<b>20 min Coffee Break</b>						
<b>Session Th-B (parallel)</b>								
		<b>Room A3</b>	<b>Room A2</b>	<b>Room A1</b>	<b>Room B</b>	<b>Room C</b>	<b>Room D</b>	
		<b>S-3</b>	<b>S-4</b>	<b>S-8</b>	<b>S-2</b>	<b>S-6</b>	<b>S-1</b>	
10:20 am		Thomas Wright	Peter D Lee	Garani Ananthakrishna	Daniel Bonamy	D Schwen	Hamid Garmestani	39
10:40 am		Hua Jun	Corbett Battaile	J S Chen	Phani Nukala	Fei Gao		40
11:00 am		Gianpietro Moras	Marc Bernacki			Giovanni Bonny	Yan Wang	41
11:20 am		Oscar Rodriguez de la Fuente	James Belak	Javier Gil Sevillano	Michael Zaiser	Luis Sandoval	Valdemar Melicher	42
11:40 am		Tomoyuki Hirouchi	P W Voorhees	Nicholas Kioussis	Mikko Alava	Dmitry Terentyev	Catalin Picu	43
12:00 pm		Jaafar Ghanbari				Chaitanya Deo		44
	12:20 pm	<b>Lunch Break (12:20 - 1:40 pm)</b>						
<b>Session Th-C (parallel)</b>								
		<b>S-3</b>	<b>S-4</b>	<b>S-8</b>	<b>S-2</b>		<b>S9</b>	
1:40 pm		Erik Van der Giessen	Alphonse Finel	Gang Lu	Mark Robbins		Andy Calder	45
2:00 pm		William Curtin	Srujan Rokkam	S. Brochard	Peter Schall		Roger Stoller	46
2:20 pm				Catalin Picu		Alexander Barashev	47	
2:40 pm		N R Barton	Rashmi Ranjan Mohanty	Michal Benes	Craig Maloney		Alexandre Legris	48

3:00 pm		Ashwin Ramasubramaniam	Ke-Gang Wang	Zhiqiang Wang	Garani Ananthakrishna		Francois Willaime	49
	3:20 pm	<b>20 min Coffee Break</b>						
		<b>Session Th-D (parallel)</b>						
		<b>S-3</b>	<b>S-4</b>	<b>S-8</b>	<b>S-2</b>	<b>S-5</b>	<b>S9</b>	
3:40 pm		Mohamed Chabaat	Alexandre Viardin	<i>S. Sharafat</i>	Mitsuhiro Itakura	Moe Khaleel	Helmut Trinkaus	50
4:00 pm		Katerina Aifantis	Ramanarayan Hariharaputran		Stefano Zapperi	Dongsheng Li	Volker Mohles	51
4:20 pm		Shuji Ogata	Paul Millett	<i>Steve Zinkle</i>	Diego Gómez-García	Eunseok Lee	Laurent Proville	52
4:40 pm		Ismail Tirtom	Vikranth Racherla	S Bulent Biner	Isabel Corominas		Christophe Denoual	53
	5:00 pm	<b>30 min Break</b>						
		<b>Session Th-E (Plenary)</b>						
5:30 pm		<p>50 minute plenary  <b>Ted Belytschko</b>, Walter P. Murphy Professor and McCormick Professor of Computational Mechanics, Northwestern University, USA</p> <p>Title: <b>Multiscale computations of fracture: quantum to continuum</b></p> <p>Room A3</p>						
7:00 pm		<b>Reception &amp; Banquet</b>						
		<p>Dinner  Awards  Announcing MMM-2010  Other announcements</p> <p>Room A3</p>						

## Friday (10/31/2008)

8:10 am	8:10- 8:20	<b>Remarks &amp; Announcements</b>
<b>Session F-A (Plenary)</b>		
8:20 am		50 minute plenary
8:40 am		<b>David Bacon</b> , Professor of Materials Science Department of Engineering & former Dean of Engineering, The University of Liverpool, UK
9:00 am		<b>Title: In pursuit of imperfection: can modelling help?</b>  Room A3
	9:00 am	<b>20 min Coffee Break</b>
<b>Session F-B (Plenary)</b>		
9:20 am		50 minute plenary
9:40 am		<b>Jacob Fish</b> , The Rosalind and John J. Redfern Chaired Professor of Engineering; Director, Multiscale Science and Engineering Center, Rensselaer Polytechnic Institute, USA
10:00 am		<b>Title: Coupling atomistic and continuum scales commonalities and differences</b>  Room A3
	10:20 am	<b>20 min Coffee Break</b>
<b>Session F-C (Panels)</b>		
10:40 am		
11:00 am		Panel I: Future Directions in Multiscale Materials Modeling (40 min)
11:20 am		Room A3
11:40 am		
12:00 noon		Panel II: Applications of Multiscale Materials Modeling (40 min)
12:20 pm		Room A3
12:40 pm		<b>Closing Remarks</b>
1:00 pm		<b>MMM-2008 Ends</b>

