

# Programme for the colloquium on Friday/Saturday, November, 21/22, 2003

Friday 21, 2003

09.20 - 09.30	Welcome	
<b>09.30 - 11.00</b>	<b>1<sup>st</sup> Session (Chair: Katja Mombaur)</b>	
Tecuatl, Ileana	Smith, Bock	<i>On the connection of stable conformations of macromolecules</i>
Krachtus, Dieter	Smith, Lesyng	<i>Study of the Dark Adaptation Process in Bacteriorhodopsin</i>
Noé, Frank <sup>a</sup>	Smith, Reinelt	<i>Methods for finding alternative conformational transition pathways in proteins</i>
11.00 - 11.15	Coffee break	
<b>11.15 - 12.45</b>	<b>2<sup>nd</sup> Session (Chair: Boris Vexler)</b>	
Tutuianu, Monika	Warnatz, Rudnicki	<i>Quantum mechanical calculations for chemical surface reactions in catalytic processes</i>
Ishmurzin, Anton	Warnatz, Schlöder	<i>On dynamical dimension reduction of one biochemical reaction mechanism</i>
Shaik, Osman	Warnatz, Gorecki	<i>Control of chemical and biochemical reaction systems</i>
12.45 - 14.00	Lunch Break	
<b>14.00 - 16.00</b>	<b>3<sup>rd</sup> Session (Chair: Jens Prager)</b>	
Ge, Hai-Wen	Gutheil, Wolfrum	<i>PDF Simulation of Turbulent Spray Flows</i>
Sager, Sebastian	Reinelt, Bock	<i>Optimal control with integer control functions</i>
Toma, Monika	Bock, Jäger	<i>Motion Optimization of Multi-legged Dynamic Walking Mechanisms</i>
Mombaur, Katja <sup>b</sup>	Postdoc	<i>Self-stabilizing motions in robotics and biomechanics</i>
16.00 - 16.15	Coffee Break	
<b>16.15 - 17.45</b>	<b>4<sup>th</sup> Session (Chair: Thomas Dunne)</b>	
Doktorski, Igor	Jäger, Niezgodka	<i>Mathematical Modelling of Biofilms</i>
Heuser, Phillip	Jäger, Roth	<i>Homogenization of thin structures with applications to soil physics</i>
Lacharme, Severine	Jäger, Bastian	<i>Homogenization Techniques for Reactive Flows and Catalysis in Industrial Reactor</i>
<b>18.45 - ...</b>	<b>Dinner</b>	

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<sup>a</sup> ungefördert

<sup>b</sup> gefördert vom 01.02.2003 bis 31.10.2003

Saturday 22, 2003

<b>09.15 - 10.45</b>	<b>1<sup>st</sup> Session (Chair: Sebastian Sager)</b>	
Bönisch, Sebastian	Rannacher, Wolfrum	<i>Numerical simulation of the free fall problem</i>
Stricker, Thomas	Rannacher, Warnatz	<i>The Reduction method ILDM in dynamical systems</i>
Richter, Thomas <sup>a</sup>	Rannacher, Warnatz	<i>Simulation of nonsteady flames</i>
10.45 - 11.00	Coffee break	
<b>11.00 - 13.00</b>	<b>2<sup>nd</sup> Session (Chair: Imke Müller)</b>	
Dunne, Thomas <sup>a</sup>	Rannacher, Becker	<i>Fluid Structure Interaction</i>
Montes, Pau <sup>a</sup>	Jäger, Bock	<i>Dynamic CT for the visualization of organ perfusion</i>
Hartmann, Dirk	Jäger, Niezgodka	<i>Multiscale Modelling Analysis and Simulation of Mechano-Chemical Properties of Cells</i>
Diehl, Moritz <sup>a</sup>	Postdoc	<i>Optimal Periodic Control of the Simulated Moving Bed Process</i>
13.00 - 14.00	Lunch Break	
<b>14.00 - 15.00</b>	<b>3<sup>rd</sup> Session (Chair: Moritz Diehl)</b>	
Eberhard, Jens	Wittum, Jäger	<i>Generalized Coarse Graining Procedures</i>
Scheit-Briganti, Simona	Cederbaum, Bock	<i>Molecular multi-mode quantum dynamics of decaying states: algorithms and applications</i>
Müller, Imke	Cederbaum, Dahlhaus	<i>Electronic decay following valence ionization of micro-solvation clusters</i>
Friedman, Elfriede	Jäger, Wittum	<i>Shape Design and its Application to Microstructures and Homogenization</i>
Reichert, Christian	Jäger, Wolfrum	<i>Deterministic and stochastic Modelling of CO oxidation on platinum surfaces</i>
Chuai-Aree, Somporn <sup>a</sup>	Jäger, Bock	<i>Modeling, Simulation and Visualization of Plant Growth</i>
15.00 - 15.10	Coffee Break	
<b>15.10 - 16.00</b>	<b>4<sup>th</sup> Session (Chair: Pau Montes)</b>	
Otto, Frank	Meyer, Bock	<i>Application of the MCTDH method to the Standard Generic Quantum Computer model</i>
Vexler, Boris	Rannacher, Bock/Wolfrum	<i>Adaptive Finite Element Methods for Parameter Identification Problems</i>
Prager, Jens	Warnatz, Bastian	<i>Modellierung und Simulation der Funkenzündung in mageren Brennstoffgemischen</i>
Minh, Hoang Duc	Bock, Warnatz	<i>Modeling, simulation and optimization of complex processes in catalytic monoliths with detailed chemistry</i>
Brandt-Pollmann <sup>a</sup> Ulrich	Bock, Warnatz	<i>Optimization of discontinuous dynamical models</i>

<sup>a</sup> ungefördert

<sup>b</sup> gefoerdert vom 01.02.2003 bis 31.10.2003