



Ruprecht-Karls-Universität Heidelberg

Interdisziplinäres Zentrum für
Wissenschaftliches Rechnen

Graduiertenkolleg „Complex Processes:
Modelling, Simulation and Optimization“

Universität Heidelberg • IWR • Im Neuenheimer Feld 368 • 69120 Heidelberg

Programme for the colloquium on Wednesday, February 20, 2002

9.00-9.15 Welcome

9.15-10.45 1st Session (Chairman Hannes Neuweiler)

Boris Vexler Mesh Adaptation for Parameter
Identification Problems

Joachim Gronki Optimization of Diesel Combustion

Christian Reichert Modelling and Simulation of Catalytic Surface
Reactions

10.45-11.15 Coffee Break

11.15-12.45 2nd Session (Chairman Boris Vexler)

Hannes Neuweiler Development and Simulation of fluorescent
peptide-based molecular probes for cancer
diagnostics

Ileana Tecuatl Methods for finding the conformational
pathways between known structures of
macromolecules

Jens Eberhard Coarse Graining of permeability of
heterogeneous porous media

12.45-14.15 Lunch Break

14.15-15.45 3rd Session (Chairman Joachim Gronki)

Somporn Chuai-Aree Modelling, Simulation and Visualization
of Plant Growth

Simona Scheit-Briganti A quantum dynamical description of mole-
cular Auger decay

Hoang Duc Minh Numerical Modelling of Catalytic Reactions
for efficient Simulation and Optimization

15.45-16.15 Coffee Break

16.15-17.15

4th Session (Chairlady Simona Scheit-Briganti)

Frank Otto	Quantum Molecular Dynamics with many degrees of freedom: Development and Implementation of efficient algorithms
Sebastian Sager	Mixed-integer nonlinear dynamic optimization
Werner Korb	Development of Surgical Manipulator: Modelling, Simulation, Control
18.00-...	Dinner