

Workshop on
Strengthening Computational Science in Europe

Programme

(Final Version, 13 January 2006)

Monday, 16 January 2005		
	<i>Session 1</i>	
09:00 - 09:15	The Research Centre Jülich and the European Initiative of the NIC	R. Wagner, FZJ
09:15 - 09:45	The Scientific Profile of the NIC	G. Münster, Münster
09:45 - 10:15	Supercomputing at NIC	Th. Lippert, NIC
10:15 - 10:30	Becoming Active in the NIC Initiative	N. Attig, NIC
10:30 - 11:00	Break	
	<i>Session 2 Chair: Th. Lippert</i>	
11:00 - 11:45	High Performance Computing in the Czech Universities and the Academy of Sciences METACentrum - Czech National Grid Environment	J. Nadrchal, Prague J. Kmunicek, Brno
11:45 - 12:15	Numerical Modelling of Geodynamo	P. Hejda, Prague
12:15 - 12:45	High Performance Computing in the Czech Technical University in Prague	P. Pospisil, Prague
12:45 - 14:00	Lunch	
	<i>Session 3 Chair: C. Alexandrou</i>	
14:00 - 14:45	Supercomputing in Poland	M. Bubak, Cracow
14:45 - 15:15	Bio-Algorithms and Med-Systems	I. Roterman-Konieczna, Cracow
15:15 - 15:45	Modelling and Interpretation of Complex Systems and Processes	B. Lesyng, Warsaw
15:45 - 16:15	Break	

	<i>Session 4</i> <i>Chair: J. Kertesz</i>	
16:15 - 16:45	Computational Protein Biophysics at NIC	U. Hansmann, NIC
16:45 - 17:15	Ab initio Simulation of Complex Chemical Systems: Achievements and Challenges	N. Doltsinis, Bochum
17:15 - 17:45	Simulation of transport and chemistry in the atmosphere	R. Müller, FZJ-ICG
17:45 - 18:15	Materials Science at the Computational Cutting Edge	S. Blügel, FZJ-IFF
18:30 - 19:30	Computer Centre Tour	
19:30	Bus Transfer to Burg Obbendorf	
20:00	Conference Dinner at Burg Obbendorf	
22:00	Bus Transfer to the Stadthotel in Jülich	

Tuesday, 17 January 2005		
	<i>Session 5</i> <i>Chair: J. Nadrchal</i>	
09:00 - 09:30	HPC in Cyprus - Applications from Basic Sciences	C. Alexandrou, Nicosia
09:30 - 10:00	HPC in Cyprus - Applications from Engineering	S. Kassinos, Nicosia
10:00 - 10:45	Some Aspects of Supercomputing in Hungary Grid Activities in Hungary	J. Kertesz, Budapest T. Maray, Budapest
10:45 - 11:15	Break	
	<i>Session 6</i> <i>Chair: B. Lesyng</i>	
11:15 - 11:45	High Level Quantum Chemical Calculations in Hungary	P. Szalay, Budapest
11:45 - 12:15	Magnetic Simulations from First Principles	L. Udvardi, Budapest
12:15 - 12:45	Investigating QCD on the Lattice	Z. Fodor, Wuppertal
12:45 - 13:15	Large Scale Computer Simulations of Biopolymers and Soft Matter	C. Holm, Frankfurt
13:15	Closing Remarks	Th. Lippert, NIC