Internationaler Workshop

des DFG-Sonderforschungsbereichs 393

Numerische Simulation auf massiv parallelen Rechnern

Energy Landscapes

Zeit: Freitag, 24.11.2000, 9:00 Uhr - Samstag, 25.11.2000, 17:00 Uhr

Ort: Straße der Nationen 62, 208 A

Tentative Schedule:	
Do, 23 November:	
20.00	Informal get-together
Fr, 24 November:	
9.00- 9.15	Welcome
9.15-10.00	D. Heidrich (Leipzig) Potential energy surface analysis: The RP in chemistry
10.00-10.45	W. Quapp (Leipzig) Potential energy surface analysis: mathematical foundations and algorithms for small molecules
10.45-11.15	Coffee break
11.15-12.00	D. Wales (Cambridge) Energy landscapes: from glasses to biomolecules via clusters
12.00-12.45	J. Doye (Cambridge) Global optimisation and the relation to the underlying energy landscape
12.45-17.00	Lunch break and sightseeing
17.00-17.45	C. Tsallis (Rio de Janeiro) Nonextensive statistical mechanics, metaequilibrium and optimization techniques
17.45-18.30	P. Jund (Montpellier) Computer investigation of the energy landscape of amorphous silica
18.30-19.15	S. Woodley (London) Crystal structure prediction using a genetic algorithm
20.00	Conference dinner
Sa, 25 November:	
9.00- 9.45	P. Sibani (Odense) Aging and SOC in driven dissipative systems: a model study

9.45-10.30	P. Blaudeck/K.H. Hoffmann (Chemnitz) Simplifying energy landscapes
10.30-11.00	Coffee break
11.00-11.45	C. Schoen (Stuttgart) Structure prediction of crystalline and amorphous systems
11.45-12.30	A. Heuer (Münster) Computer simulation of glass-forming liquids
12.30-14.00	Lunch break
14.00-14.45	J. Hesser (Mannheim) Protein structure prediction
14.45-15.30	S. Kobe (Dresden) Walking in the energy landscape of +-J spin glass
15.30-16.00	Coffee break
16.00-16.45	O. Kirillova (St Petersburg) A model of communication networks with emergent dynamical structure
16.45-17.00	Closing