

Linear Scaling Electronic Structure Methods

Monday April 1, 2002

- 12:00 *Tutorials*
- 8:30 *Chair: Emily Carter (UCLA)*
- 8:30–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:50–9:00 *Welcome and Opening Remarks*
- 9:00–10:15 **Richard Martin** (University of Illinois)
Density Functional Theory for Interacting Electrons
- 10:15–10:30 *Break*
- 10:30–11:45 **Martin Mohlenkamp** (Ohio University)
A Tutorial on Wavelets and their Applications
- 11:45–12:45 *Lunch (on your own)*
- 12:45 *Chair: Roi Baer (Hebrew University)*
- 12:45–2:00 **Trygve Helgaker** (University of Oslo)
Quantum Chemistry Methods
- 2:00–3:00 **Danny Neuhauser** (UCLA)
Efficient Eigenvalue Methods
- 3:00–3:30 *Coffee Break*
- 3:30–4:45 **Tanja Füllenbach** (FhG-SCAI)
Tutorial on Multigrid and Local Refinement Methods
- 4:45–5:45 **Martin Head-Gordon** (University of California at Berkeley)
Fast methods for coulomb and exchange interactions in DFT calculation
- 5:45–7:00 *Wine/Cheese Reception (Hosted by IPAM)*



Tuesday April 2, 2002

- 12:00 *Research Presentations*
- 8:00 *Each talk will be 30 minutes with 15 minutes for discussion*
- 8:30 *Chair: Achi Brandt (Weizmann Institute)*
- 8:30–9:00 *Continental Breakfast*
- 9:00–9:45 **Jerry Bernholc** (North Carolina State University)
Multigrid DFT calculations, optimized localized orbitals and nearly $O(N)$ calculations of quantum transport
- 9:45–10:30 **Roi Baer** (Hebrew University, Jerusalem, Israel)
Phase coherent molecular electronics: challenges for linear scaling
- 10:30–11:00 *Coffee Break*
- 11:00–11:45 **Philip Sterne** (Lawrence Livermore National Laboratory)
A Finite-Element Approach for Electronic Structure Calculations
- 11:45–12:30 **Stefan Goedecker** (CEA DRFMC/SP2M)
Extensions of the traditional linear scaling concepts
- 12:30–2:00 *Lunch (on your own)*
- 2:00 *Chair: Emilio Artacho (Cambridge)*
- 2:00–2:45 **Michael J. Gillan** (University College, London)
Linear Scaling DFT with b-splines
- 2:45–3:30 **Peter Haynes** (Cambridge University)
Linear-scaling DFT using localised spherical-waves and real-space grids
- 3:30–4:00 *Coffee Break*
- 4:00–4:45 **Matt Challacombe** (Los Alamos National Laboratory)
An Irregular Approach to Parallelism in Linear Scaling Quantum Chemistry
- 4:45–5:45 *Panel Discussion*

Wednesday April 3, 2002

- 12:00 *Each talk will be 30 minutes with 15 minutes for discussion*
- 8:30 *Chair: Gregory Beylkin (University of Colorado, Boulder)*
- 8:30–9:00 *Continental Breakfast*
- 9:00–9:45 **Yan Wang** (University of British Columbia, Vancouver)
O(M InM) Orbital-Free Density Functional Theory
- 9:45–10:30 **Achi Brandt** (Weizmann Institute of Science)
Systematic upscaling: linear complexity and beyond
- 10:30–11:00 *Coffee Break*
- 11:00–11:45 **David Mazziotti** (Princeton University)
Linear Scaling and the 1,2-Contracted Schrodinger Equation
- 11:45–12:30 **Duane Johnson** (University of Illinois)
Green's function O(N) DFT method
- 12:30–2:00 *Lunch (on your own)*
- 2:00 *Chair: Emily Carter (UCLA)*
- 2:00–2:45 **Danny Sorensen** (Rice University)
Implicitly Restarted Krylov Projection Methods for Large Eigenvalue Problems
- 2:45–3:30 **Gustavo Scuseria** (Rice University)
Linear scaling DFT, Hartree-Fock, MP2 and coupled cluster theories
- 3:30–4:00 *Coffee Break*
- 4:00–4:45 **Derek Walter** (UCLA)
Weak-Pairs Pseudospectral Multireference Configuration Interaction
- 4:45–5:30 **Martin Schuetz** (University of Stuttgart)
Linear scaling coupled cluster theory
- 5:30–5:45 *Social Time (Beverages available)*
- 5:45–7:00 *Dinner (Hosted by IPAM)*

Thursday April 4, 2002

- 12:00 *Each talk will be 30 minutes with 15 minutes for discussion*
- 8:30 *Chair: Yousef Saad (University of Minnesota)*
- 8:30–9:00 *Continental Breakfast*
- 9:00–9:45 **Oren Livne** (Weizmann Institute of Science)
 $O(N \ln N)$ Calculation of N Eigenfunctions of Differential Operators
- 9:45–10:15 *Coffee Break*
- 10:15–11:00 **Arne Luechow** (University of Duesseldorf)
Linear scaling in quantum Monte Carlo
- 11:00–11:45 **Randy Hood** (Lawrence Livermore National Laboratory)
Linear Scaling Quantum Monte Carlo
- 11:45–1:15 *Lunch (on your own)*
- 1:15 *Chair: Achi Brandt (Weizmann Institute)*
- 1:15–2:00 **Weitao Yang** (Duke University)
Linear Scaling Methods and Applications with the Divide-and-Conquer Method and with Localized Orbitals
- 2:00–3:00 *Discussions and Conclusion*

