

Recent Progress in Numerical Green's Functions Methods in Physics and Chemistry

Organizers: Emanuel Gull (egull@umich.edu) and Dominika Zgid (zgid@umich.edu)

Meeting dates: 08/01/2016 - 08/05/2016

TSRC Hosts: Mark Kozak, 970-708-4426

The meeting address: Telluride Elementary School located at 447 W Columbia Ave, Telluride, CO 81435

Welcome reception: at Arroyo Wine Bar from 6-8pm on Sunday, July 31

The Picnic address: under the tent outside of the Telluride Elementary School at 447 W Columbia Ave.

The Town Talk address: Conference Center in Mountain Village from 6:00 pm to 7:00 pm (cash bar starts at 5:30 pm). It is roughly a 30 minute commute from the Elementary School to the Conference Center.

Conference dinner will be held at 6:30 on Thursday (August 4) at La Marmotte, 150 W San Juan Ave, Telluride, CO 81435. Dinner cost is \$60 per person including tax and tip but not including alcohol. Participants will be billed after signing up. A signup sheet will be distributed on Monday and Tuesday during the workshop.

Breakfast is served everyday in the morning at the Telluride Elementary School (before the talks) from 8 to 9 am.

All talk slots are 1 hour long with 45-50 min presentation time and 15-10 min for questions. Telluride is in the Mountain Time Zone.

-----Monday-(Aug1)-----

8:00- 9:00 Breakfast at Telluride Elementary School

9:00-10:00 Guy Cohen, Tel Aviv University, The inchworm algorithm for quantum Monte Carlo: introduction and recent advances

10:00-11:00 Misha Galperin, U of California, San Diego, Transport, dynamics and optical spectroscopy at molecule-metal interfaces)

11:00 -11:30 Coffee break

11:30-12:30 Robert van Leeuwen, U of Jyvaskyla, Diagrammatic perturbation theory for positive spectral functions

12:30-2:30 Lunch on your own

2:30-3:30 Rafael Fernandez, U of Minnesota, Pairing promoted by quantum critical magnetic fluctuations: a Quantum Monte Carlo study

3:30-4:30 Martin Eckstein, MPI Munich, Nonequilibrium dynamical mean-field theory for photo-induced dynamics in strongly correlated systems

4:30-5:00 Coffee break

5:00-6:00 Tim Wehling, U of Bremen, Nonlocal interaction effects: How to describe and manipulate them

6:00 Dinner on your own

-----**Tuesday-(Aug2)**-----

- 8:00- 9:00 Breakfast at Telluride Elementary School**
9:00-10:00 Philipp Werner, U of Fribourg, Self-consistent GW+DMFT for correlated materials
10:00-11:00 Shiwei Zhang, College of William and Mary, Computation of ground-state observables and imaginary-time Green's functions with auxiliary-field quantum Monte Carlo
11:00-11:30 Coffee break
11:30-12:30 Dominika Zgid, U of Michigan, Green's function embedding for molecular problems
12:30- 2:30 Lunch on your own
2:30- 3:30 Michael Pothoff, U of Hamburg, Making use of self-energy functionals
3:30- 4:00 Coffee break
4:00- 5:00 Silke Biermann, Ecole Polytechnique, TBA
5:00 Town talks (optional) and dinner on your own

-----**Wednesday-(Aug3)**-----

- 8:00- 9:00 Breakfast at Telluride Elementary School**
9:00-10:00 Andrew J. Millis, Columbia University, Thoughts on DFT+DMFT
10:00-11:00 Daniel Neuhauser, U of California, Los Angeles, Stochastic methods for quantum chemistry
11:00-11:30 Coffee break
11:30-12:30 Bryan Clark, U of Illinois, Urbana-Champaign, TBA
12:30- 2:30 Lunch on your own
2:30- 3:30 Ed Valeyev, Virginia Tech, Explicitly-correlated electronic structure: from wave functions to Green's functions
3:30-4:00 Coffee break
4:00-5:00 Marco Govoni, U of Chicago, Large scale GW calculations: methodological developments in the computation of excited-state properties
5:00-6:00 Panel discussion: "Challenges and requirements for methods in realistic materials simulations". Discussion facilitators: Andrew J. Millis and Ed Valeyev
6:00-8:00 Conference picnic under the tent outside of the Telluride Elementary School

-----**Thursday-(Aug4)**-----

- 8:00- 9:00 Breakfast at Telluride Elementary School**
9:00-10:00 Felix Hummel, MPI Stuttgart, TBA
10:00-11:00 Nikolai Prokofiev, U of Massachusetts, Amherst, Dielectric function and thermodynamic properties of jellium in the GW approximation
11:00-11:30 Coffee break
11:30-12:30 Johannes Lischner, Imperial College of London, Including electron-plasmon, electron-spin wave and electron-phonon interactions into Green's function calculations
12:30- 2:30 Lunch on your own
2:30- 3:30 Brenda Rubenstein, Lawrence Livermore National Lab, Slater-Jastrow Wave Functions in Auxiliary Field Quantum Monte Carlo Simulations of the Hubbard Model
3:30- 4:00 Coffee break
4:00- 5:00 Emanuel Gull, U of Michigan, Numerical experiments on the Hubbard Model
6:30 Conference Dinner at La Marmotte restaurant

-----**Friday-(Aug5)**-----

- 8:00- 9:00 Breakfast at Telluride Elementary School**
9:00 Group hike with discussions