Title: “New Developments in Coupled-Cluster Theory”

Organizers: Anna Krylov, Jürgen Gauss
Location: Telluride Elementary School, 477 West Columbia Ave Telluride CO 81435
TSRC Hosts: Mark Kozak (970) 708-4426, Kristen Redd (970) 708-0827

ALL TALKS ARE 30 min + 15 min discussion

Sunday, August 2
Arrival, no-host drinks and dinner at Smugglers (7:30 pm)

Monday, August 3

MORNING:
7:30 Breakfast

Session Chair: Anna Krylov
8:00 Opening remarks
8:15 Jürgen Gauss, TBA
9:00 Cristina Puzzarini, "Coupled-cluster theory in rotational spectroscopy: Where we are and wish list"
9:45 Sonia Coriani, "CC response methods for NEXAFS, photoionisation and more”
10:30 BREAK

11:00 Dipayan Datta, "Spin-adapted coupled-cluster calculations of properties for open-shell molecules"
11:45 Lan Cheng, "Relativistic exact two-component coupled-cluster calculations of molecular properties"
12:30 END

EVENING:
Session Chair: Sonia Coriani
7:30 John Stanton, “Alternatives to EOM-CCSD, above and below. An honest assessment of what works and what doesn't”
8:15 Daniel Crawford, “Linear scaling coupled-cluster response theory"
9:00 END

Tuesday, August 4

AFTERNOON:
Session Chair: Ksenia Bravaya
1:25 Announcements
1:30 Anna Krylov “From EOM-CC wave functions to experimental observables”
2:15 Thomas Jagau, "Equation-of-motion coupled-cluster methods for metastable states"

3:00 BREAK

3:30 Devin Matthews "Accelerating the convergence of higher-order coupled cluster methods"
4:15 Ilya Kaliman, "Speeding up CCSD calculations on multi-core CPUs, GPUs, and accelerators: a new tensor contraction algorithm"
5:00 Ed Valeev, "Using separated representation to avoid the curse of dimensionality in non-LCAO coupled-cluster"
5.45 END

6:00 Town Talk, Telluride Conference Center, Mountain Village

Wednesday, August 5

AFTERNOON:
Session Chair: Andreas Koehn
1:55 Announcements
2:00 Gerald Knizia, "Permutation group techniques for the generation and simplification of coupled cluster equations"
2:45 Alex Auer, "Tensor decomposition techniques for coupled-cluster methods and Full CI"

3:30 BREAK

4:00 Ksenia Bravaya, “Approximate CAP/EOM-CCSD models: Towards accurate description of electronic resonances in medium-size molecules”
4:45 Stella Stopkowicz, “Coupled Cluster theory for atoms and molecules in strong magnetic fields”

5:30 END

6:00 TSRC Picnic @ Telluride Elementary School, under the tent

Thursday, August 6

AFTERNOON:
Session Chair: Mihaly Kallay
1:55 Announcements
2:00 Michael Hanrath, "Weak and strong correlation: Thoughts from the coupled-cluster perspective"
2:45 Andreas Koehn, “Some new adventures with internally contracted multireference coupled-cluster theory”

3:30 BREAK

4:00 Zoltan Rolik "Efficient implementation of the quasiparticle-based multi-reference coupled-cluster theory"
4:45 Marcel Nooijen, “Multireference equation of motion coupled cluster theory: Applications to transition metal spectroscopy including spin-orbit-coupling”
5:30 END

EVENING:
Session Chair: Marcel Nooijen
7:30 Janus Eriksen, “Various aspects of non–iterative coupled cluster perturbation theory
8:15 Simen Kvaal, “The bivariational principle and coupled-cluster theory”
9:00 END

Friday, August 7

MORNING:
Session Chair: Juergen Gauss
7:30 Breakfast
8:00 Kasper Kristensen, "Recent advances in the divide-expand-consolidate local coupled-cluster approach"
8:45 Christof Haettig, “Coupled-cluster response theory in a pair natural orbital basis”

9:30 BREAK

10:00 Michael Harding, "Systematic construction of auxiliary basis sets from and for atomic natural orbitals basis sets"
10:45 Mihaly Kallay, “Efficient fragmentation-based local coupled-cluster approaches”

11:30 Closing

Notes:

The workshop will begin with an informal no-host dinner on Sunday, August 2, at 7:30 PM at Smugglers Brew Pub.

Breakfast will be available at 7:30 AM, July 20-24, at the workshop venue (Telluride Elementary School, 477 West Columbia Ave).

ALL TALKS ARE 30 min + 15 min discussion.