

Core Software Blocks in Quantum Chemistry: Tensors and Integrals Workshop Program

Start: Sunday, May 7, 2017 afternoon. Resort check-in at 4:00 pm.

Finish: Wednesday, May 10, noon

Sunday

6:00-7:00: Dinner

7:30-9:00 Opening session

7:30-7:45 Anna Krylov (USC): "MoISSI and some lessons from previous workshop, goals of the workshop"

7:45-8:00 Theresa Windus (Iowa): "Mission of the Molecular Science Consortium"

8:00-9:00 Introduction of participants: 2 min presentation, can have one slide (send in advance)

9:00-10:30 Reception and posters

Monday

Breakfast: 7:30-9:00

9:00-11:45 Session I: Overview of tensors projects and current developments (moderator Daniel Smith)

9:00-9:10 Daniel Smith (MoISSI): Overview of tensor projects

9:10-9:30 Evgeny Epifanovsky (Q-Chem): Overview of Libtensor

9:30-9:50 Ed Solomonik: "An Overview of Cyclops Tensor Framework"

9:50-10:10 Ed Valeev (VT): Overview of TiledArrays

10:10-10:30 Coffee break

10:30-10:50 Devin Matthews (UT Austin): "Aquarius and TBLIS: Orthogonal Axes in Multilinear Algebra"

10:50-11:10 Karol Kowalskii (PNNL, NWChem), "NWChem, NWChemEX, and new tensor algebra systems for many-body methods"

11:10-11:30 Peng Chong (VT): Current work on TiledArrays in MPQC4 (parallelism)

11:30-11:55 Moderated discussion: "What problems are we *still* solving?"

Lunch: 12:00-1:00

Free time for unstructured discussions

5:00 Posters (coffee/tea)

Dinner: 6-7:00

7:15-9:00 Session II: Computer science perspective (moderator Ben Pritchard)

7:15-7:35 Khaled Ibrahim (LBNL), "Scaling Tensor Contractions: A Programming Model Perspective"

7:35-7:55 Jeff Hammond (Intel), "Musings on the future of computational chemistry from a hardware perspective."

7:55-8:15 Saday Sadayyapan
8:15-8:35 Beverly Sanders
8:35-8:55 Robert Harrison

9:00-10:30 Posters and social (cash bar)

Tuesday

Breakfast: 7:30-9:00

Session III: Overview of integral projects and current developments (moderator Ben Pritchard)

9:00-9:10 Daniel Smith (MoISSI): Overview of integral projects
9:10-9:30 Ed Chow (Gatech): "Simint: Vectorized Obara-Saika Integral Library"
9:30-9:50 Ed Valeev (VT): Overview of Libint
9:50-10:10 Epifanovksy (Q-Chem): Overview of Libqint

10:10-10:30 Coffee Break

Session IV: Tensors and integrals in various packages and use cases (moderator Ben Pritchard)

10:30-10:50 Qiming Sun (Caltech, PySCF) "Analytical Gaussian integrals on Knights Landing coprocessor".
10:50-11:10 Roland Lindh (Uppsala, MOLCAS), "Integral libraries a redundant notion?"
11:10-11:30 Johannes Dieterich (Princeton, TigerCI), "TigerCI: Local multi-reference configuration interaction"
11:30-11:50: Moderated discussion

Lunch: 12:00 -1:00

Free time for unstructured discussions
5:00 Posters (coffee/tea)

Dinner: 6-7:00

7:15-9:00 Session V: Tensors and integrals in various packages and use cases (moderator Daniel Smith)

7:15-7:35 Xintian Feng (UC Berkeley/Q-Chem): Cholesky and RI in Q-Chem
7:35-7:55 Andrew James (VT): Direct Product Decomposition Library: Cholesky and RI in PSI
7:55-8:15 Dirk Rehn (Heidelberg), "GATOR program: Response properties based on the Algebraic Diagrammatic Construction of the Complex Polarization Propagator"
8:15-8:35 Florian Hampe (Mainz, CFOUR), "EOM-CC Methods in Strong Magnetic Fields: Implementation & Tools"
8:35-9:00: Moderated discussion

9:00-10:30 Posters and social (cash bar)

Wednesday

Breakfast: 7:30-9:00

9:00-11:00 **Session VI: Interoperability discussion (moderator Theresa Windus)**
9:00-9:20 Theresa Windus: "Interoperability and use discussion"

9:20-9:40: Moderated discussion
9:40-11:00 Working on use cases
Group 1: "Tensor Libraries", Lead: Daniel Smith
Group 2: "Integrals", Lead: Ben Pritchard

Lunch: 12:00

Departure

Posters (please put posters out on Sunday and keep for the entire workshop)

Pavel Pokhilko (USC), "Development of Frozen Natural Orbital approximation for EOM-SF method"
Kaushik Nanda (USC) "EOM-CCSD implementations for response properties in Q-Chem"
Florian Hampe (Mainz, CFOUR), "EOM-CC Methods in Strong Magnetic Fields: Implementation & Tools"
Quiming Sun (Caltech) "PySCF on Knights Landing coprocessor"
Ruslan Tazhigulov (BU), "Simulating electron transfer and spin chemistry in biological systems"
Johannes Dieterich (Princeton, TigerCI), "TigerCI: Local multi-reference configuration interaction"
Adrian Morrison (OSU), "Toward GPU Accelerated Integral Digestion for Novel Excited State Methods"
Dirk Rehn (Heidelberg), "RIXS scattering amplitudes in the ADC/ISR framework"
Ed Solomonik, "Recent Developments in Cyclops Tensor Framework"
Ed Solomonik, "Strassen-like Algorithms for Symmetric Tensor Contractions"
Devin Matthews, "Aquarius: Scalability and Extensibility by Design"
Devin Matthews, "Tensor Contraction without Transposition"

Contacts:

Kortni (VT): 540-231-2602
Raymond (Asilomar): 831-642-4225
Lectures: Scripps room, posters: Heather room.