

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

Lectures are in Scripps, posters are in Heather.

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): "TiledArray: A composable massively parallel block-sparse tensor framework"

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): "Many-body toolkit in re-designed Massively Parallel Quantum Chemistry package"

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 (University of Florida), Overview of ACES4 project
8:35-8:55 Robert Harrison: "Sustaining innovation --- look forward!"

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 Ben Pritchard (MolSSI): Overview of integral projects
9:10-9:30 Edmond Chow (Gatech): "Simint: Vectorized Obara-Saika Integral Library"
9:30-9:50 Ed Valeev (VT): "The Libint compiler for Gaussian integrals"
9:50-10:10 Evgeny 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 Ilya Kaliman (USC): Libxm: Efficient tensor contraction in a single node and GPU
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 cases"

9:20-9:40: Moderated discussion

Topic 1: "Integrals", Lead: Ben Pritchard

Topic 2: "Tensor Libraries", Lead: Anna Krylov

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"

Ed Valeev/Peng Chong (VT): "MPQC overview"

Ed Valeev/Peng Chong (VT): "Libint and TiledArrays"

Ilya Kaliman (USC): "Libpt: a distributed-parallel implementation of various non-iterative coupled cluster triples corrections"

Anastasia Gunina (USC): "Dyson orbitals implementation within ccman2 module of Q-Chem"

Robert Harrison: "Task-based Environment for Scientific Simulation at Extreme Scale (TESSE)"

Xintian Feng (UC Berkeley): "Using density fitting and Cholesky decomposition within EOM-CC framework"

Evgeny Epifanovsky (Q-Chem): "Libqint and libtensor projects"

List of participants

- Edmond Chow, Georgia Tech
- Johannes Dieterich, Princeton University
- Evgeny Epifanovsky, Q-Chem
- Xintian Feng, University of California, Berkeley
- Anastasia Gunina, Iowa State

- Jeff Hammond, Intel
- Florian Hampe, University of Mainz
- Robert Harrison, MolSSI Board of Directors, SUNY Stony Brook
- Khaled Ibrahim, Lawrence-Berkeley National Lab
- Andrew James, Virginia Tech
- Ilya Kaliman, University of Southern California
- Karol Kowalski, Pacific Northwest National Lab
- Roland Lindh, Uppsala University
- Devin Matthews, University of Texas
- Adrian Morrison, Ohio State University
- Kaushik Nanda, University of Southern California
- Chong Peng, Virginia Tech
- Pavel Pokhilko, University of Southern California
- Dirk Rehn, University of Heidelberg
- Saday Sadayappan, Ohio State University
- Beverly Sanders, University of Florida
- Edgar Solomonik, University of Illinois at Urbana-Champaign
- John Stanton, University of Florida
- Qiming Sun, California Institute of Technology
- Ruslan Tazhigulov, Boston University
- Eduard Valeyev, Virginia Tech
- Theresa Windus, MolSSI Board of Directors, Iowa State