Chemistry - HPC - Pomona

http://mercuryconsortium.org/mc17/molssi-coding-workshop/

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Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY) is an NSF-funded consortium composed of 27 computational chemistry faculty from 25 primarily undergraduate institutions (PUIs) across the US. Aside from providing shared computational resources to these institutions, it promotes undergraduate research through the annual MERCURY conference. This is the 16th annual MERCURY conference and the first one held at Furman University in Greenville, SC. The last five were hosted at Bucknell University in Lewisburg, PA and the first ten were at Hamilton College in Clinton, NY.

http://mercuryconsortium.org/members/

MERCURY is a consortium of 27 computational chemistry faculty at predominantly undergraduate institutions across the country. The researchers share computational resources and use the consortium as a venue to collaborate and increase the visibility of their work.

2001 –

- Maria Gomez, Mount Holyoke College
- Carol Parish, University of Richmond
- George Shields, Furman University
- Marc Zimmer, Connecticut College

2008 –

- Maria Nagan, Adelphi University
- Tricia Shepherd, St. Edward's University
- Mauricio Cafiero, Rhodes College

- Kelling Donald, University of Richmond
- Becky Eggimann, Wheaton College
- Eric Patterson, SUNY, Stony Brook
- Adam Van Wynsberghe, Hamilton College

2012 –

- Kelly Anderson, Roanoke College
- Sudeep Bhattacharyay, U. of Wisconsin-Eau Claire
- Daqing Gao, Central State University
- Jim Phillips, U. of Wisconsin-Eau Claire
- Aimée Tomlinson, U. of North Georgia

2016 –

- Mychel Varner, Iona College
- Chrystal Bruce, John Carroll University
- Bill Miller, Truman State University
- JiaJia Dong, Bucknell University
- Joshua Schrier, Haverford College
- Ashley Ringer McDonald, Cal Poly San Luis Obispo
- Dmytro Kosenkov, Monmouth University
- Juan Navea, Skidmore College
- Nick Boekelheide, Colby College
- Isaiah Sumner, James Madison University
- George Barnes, Siena College

Others

- Berhane Temelso, Furman University, research scientist and system administrator
- Steve Young, Hamilton College and SlyMedia, System administrator and research support specialist
- Lori Law, Furman University, Executive Assistant, Office of the Vice President for Academic Affairs and Provost
- Lisa Aversa, Bucknell University, Executive Assistant to the Dean of Arts and Sciences at Bucknell

https://mercuryconsortium.org/Skylight/

Chemistry

The following applications are freshly compiled and tested to run on Skylight. The applications' capability to run on GPUs has not been tested extensively yet except for the case of AMBER16. We'll add GPU support for all capable applications over time.

1. Gaussian16 A.03
2. Gaussian09 A.02 + D.03
3. Orca 3.0.3 + 4.0.0
4. GAMESS 2016
5. AMBER 12, 14
6. AMBER 16 w/ GPU support for both NVIDIA GTX 1080 and P100 cards
7. LAMMPS 03-31-2017
8. NAMD 2.12 w/ GPU support
9. CP2K 2.6 + 3.0 + 4.1
10. Desmond 2016
11. libEFP

The following will be available shortly:

1. NWchem
2. PSI4
3. CFOUR
4. GROMACS
5. OpenMM
6. Quantum Espresso
7. Siesta
8. CPMD
9. DFTB+
10. cluster

General Tools

If you want to compile your own code, these general libraries are available.

1. Intel Compilers (16, 17)
2. Intel MKL libraries (16, 17)
3. Intel MPI (17)

4. GCC (4.8.5)
5. OpenMPI (1.6, 1.8, 2.0)
6. MVAPICH2 (2.2)
7. MPICH (3.3)
8. Python (2.7.5, 3.3)
9.

https://mercuryconsortium.org/marcy/

Chemistry

1. Gaussian09 A.02 + D.01
2. Gaussian03 A.01
3. NWchem 6.5, 6.3
4. PSI 4
5. Gamess 2013(+cuda), 2011
6. Cfour 1.0
7. AMBER 9, 12 (+cuda)
8. NAMD 2.9 (+cuda)
9. GROMACS 5.0
10. LAMMPS
11. OpenMM
12. ORCA 3.0.2/3.0.3
13. Openbabel 2.3.2
14. libEFP
15. Espresso
16. Siesta 3.2
17. cp2k 2.5
18. cpmd 3.17
19. cluster 1.0/1.1
20. dftb+

General Tools

1. Intel Compilers (12, 13)
2. Intel MKL libraries (10.3, 13)
3. OpenMPI (1.3.3, 1.6.4)

4. Mvapich2 (1.9)
5. Fftw (3.1.5, 3.3.3)
6. Python (2.6, 2.7, 3.3)
7. cmake 2.8
8. cuda 5.5, 5.0, 4.2, 6.0
9. Jre 1.8.0
10. swift

https://insidehpc.com/2017/10/accelerating-quantum-chemistry-drug-discovery/

This sponsored post from NVIDIA is the third of five in a series of case studies that illustrate how AI is driving innovation across businesses of every size and scale. This article explores how the University of Florida and University of North Carolina developed an anakin-me neural network engine to produce computationally fast quantum mechanical simulations with high accuracy at a very low cost.

https://ulhpc-tutorials.readthedocs.io/en/latest/advanced/MultiPhysics/

The objective of this session is to exemplify the execution of several common, parallel, Computational Fluid Dynamics, Molecular Dynamics and Chemistry software on the UL HPC platform.

Targeted applications include:

- OpenFOAM: CFD package for solving complex fluid flows involving chemical reactions, turbulence and heat transfer
- NAMD: parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems
- ASE: Atomistic Simulation Environment (Python-based) with the aim of setting up, steering, and analyzing atomistic simulations
- ABINIT: materials science package implementing DFT, DFPT, MBPT and TDDFT

- Quantum Espresso: integrated suite of tools for electronic-structure calculations and materials modeling at the nanoscale

The tutorial will cover:

1. Basics for parallel execution with OAR and SLURM
2. different MPI suites available on UL HPC
3. running simple test cases in parallel
4. running QuantumEspresso in parallel over a single node and over multiple nodes
5. running OpenFOAM in parallel over a single node and over multiple nodes
6. running ABINIT in parallel over a single node and over multiple nodes
7. the interesting case of the ASE toolkit

https://www.aspsys.com/solutions/hpc-applications/mpi-applications/

https://aws.amazon.com/solutions/case-studies/novartis/

https://www.hpcwire.com/1998/03/13/germany-hosts-first-hpc-chemistry-conference/

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 The Central Institute for Applied Mathematics (ZAM, Zentralinstitut fuer
Angewandte Mathematik) at Research Center Juelich, Germany, organized the
first "Conference on High-Performance Computing in Chemistry" from February
16 to 18.

  About 180 participants made this first effort at Juelich a big success --
surely there will be follow-ups. The themes covered the broad spectrum of
computer usage in chemistry: material sciences, polymer simulation,
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catalysis, membranes, drug design, bioinformatics, combinatorial chemistry and process and plant optimization.

The German Ministry of Research (BMBF), the Society of German Chemists and the Working Group of Theoretical Chemists supported this event actively. The proceedings of the talks and posters -- two-page abstracts -- are available on the Web (see URL below).

ZAM at Juelich

Professor Friedel Hofeld, Director of ZAM, and Johannes Grotendorst highlighted the structure, the organizational aspects and the offerings of the computing center. It is equipped with a SGI/Cray ensemble. ZAM operates them and provides expertise in vector and parallel processing, porting, and chemistry applications. As 15% of the computing capacity is reserved for industrial projects, ZAM is open for, and interested in industrial projects. Its expertise can often shorten the product cycle, improve quality and reduce costs for high-performance computing.

ZAM is equipped with massively parallel computers of Cray T3E-type with different Alpha processors, a T3E with 512 processors, 64 GB memory (307 Gflop/s peak), a T3E with 256 processors, 32 GB memory (230 Gflop/s peak). For vectorized applications a Cray T90 with 16 CPUs, 8 GB memory (30 Gflop/s peak) is the workhorse. Two Cray J90s are installed, one with 16 CPUs and 8 GByte, the other with 12 processors and 2 GByte is used as a fileserver. In total there are 50 central servers, 200 X-terminals, 1100 workstations and 3400 PCs. All the machines are connected via JuNet, Ethernet, FDDI, ATM, HIPPI and the Cray-based GigaRing. The external access to the central computers is possible via B-WIN, the German Research Network, 34 GBit/s or ISDN, 64KBit/s.

A broad spectrum of chemistry software is installed, UniChem, Gaussian, Molpro, DGauss and others; on the T3E one finds DGauss, CPMD, Amber and more. Furthermore, DFT, Hartree Fock, CADPAC, GAMESS, MNDO, MOPAC, GROMOS (SYBILL) are available on different machines. Grotendorst underlined the usability of UniChem, a software environment for quantum chemistry applications on distributed applications, a close interaction between

workstations and compute servers.

The Conference

The Conference was opened by Professor Rolf Theenhaus, member of the Board of Directors. He listed kernel competencies of the Research Center and mentioned that the different topics, such as the operation of the machines, the mathematical-scientific environment (parallel algorithms for example) and science and research within and outside of the Research Center have to be combined.

Via the HLRZ (High-Performance Computing Center) -- a joint effort of Juelich, DESY in Hamburg and GMD in St. Augustin, in theoretical physics and chemistry -- the Research Center is actively involved in chemistry, as a lot of projects come from this area. Theenhaus mentioned a recently published report from the German Ministry of Education, Science, Research and Technology on "Chemistry Location in Germany, strengthening of education and research for assuring future development", which is published in German (Chemiestandort Deutschland -- Staerkung von Bildung und Forschung zur Zukunftssicherung). It is available at BMBF, Referat Oeffentlichkeitsarbeit, D-53170 Bonn, email: information@bmbf.bund400.de In it, a lot of strategies are listed to start a chemistry initiative.

As mentioned, ZAM has reserved 15% of its computing capacity for projects and collaborations with industry. Thus, this conference underlined their efforts. As computing time alone nowadays is not an ideal offer, scientific competence and advising is extremely necessary. ZAM and the Research Center with its chemistry-oriented institutes are attempting to build bridges between the sciences, industry and applications, offering a neutral platform for an information and experience exchange between academia, research and industry.

Chemistry Talks

The first topic, drug design, was covered by two speakers from industry and one from academia. They discussed computer-aided tools for drug design. These consist of elements such as analysis of protein structure, ligands

docking, search in commercially available structure data bases, de-novo ligand design, estimation of the binding affinity of ligands, and analysis of the electronic and conformity properties of ligands.

Hans-Joachim Boehm (Hoffmann-La Roche Ltd., Basel) presented and explained different approaches and examples. The 3D-structures of proteins and protein-ligand-complexes are used to identify the essential interactions. The researcher can look for binding areas that have not been entered by the ligands. New strategies and new drugs are the result which aid in the fight against AIDS and HIV viruses.

Gerhard Barnickel (Merck, Darmstadt) discussed combinatorial chemistry. The "synthetic" chemist is faced with the problem of choosing -- out of a very large number of compounds -- those which can go into production. This requires the use of high-performance computers and results in new perspectives and approaches for molecular modeling. Another aspect is the close interaction and integration of modeling and experiment.

The next topic was computer-aided polymer simulation and synthesis. Some of the tools and their performance have been presented: molecular modeling, force field-based methods, semi-empirical quantum chemical and first-principle methods.

In the material properties section, Michele Parinello (Max-Planck Inst. for Festkoerperforschung, Stuttgart) gave the overview talk on ab initio simulations of complex chemical processes.

A practical application, which can be seen daily in the kitchen, was presented by Robert Jones (Research Center Juelich). He analyzed the material behavior of Beta-Eukryptit, the material of Ceran cooking fields, in a broad temperature range, using density functional calculations.

As different disciplines grow together, bioinformatics will play a major role in the future of chemistry too. Reinhard Schneider (Lion biosciences, Heidelberg -- a new start-up company) discussed functional genome analysis. Other topics in this session have been the structure-based search for proteins that are relevant for illness and computer-aided protein design.

Herman Berendsen (University Groningen) highlighted the aspects of molecular dynamics simulations of biological membranes. Other talks covered the simulation of membrane proteins and the usage of FFT Particle-Mesh-Ewald methods in simulations of polyelectrolytes.

In the catalysis section the structure and the effects of catalysts have been computed with ab initio methods. In industry, quantum chemistry is used for the computation of molecular structures as well as for the simulation of chemical reactions.

Quite a different usage of high-performance computers in industry is plant and process simulation. Using mathematical models that might have up to 60,000 equations it is possible to optimize plants and production. The gain in one example came up to more than 100%, according to Rolf Bachmann (Bayer, Leverkusen).

The multidisciplinary aspect highlighted Juergen Warnatz (University Heidelberg), reactive flows, problems and applications. In combustion processes chemical reactions, heterogene catalysis and hypersonic flows are influencing factors. Warnatz reported that he needed 30 hours on 128-processors of the Juelich-Cray T3E, simulating the turbulent combustion in a two-dimensional geometry of 1 square cm with 250,000 equations.

Issues of Hardware and Software Vendors and Exhibition

In the more industrial-oriented part, Erich Wimmer (Molecular Simulations (MSI), Orsay Cedez) examined the role of high-performance computers in chemistry as a bridge between research and industrial usage. Broad applicability here is mostly hindered by the limits of theoretical approaches and numerical methods, the availability of software systems and education, as well as the understanding and experience of researchers and engineers. His own experiences at MSI have shown that customers not only need the software packages and computers but also qualified, chemistry-based advisory services. He mentioned that this opens chances for research centers like Juelich, to bring together theoretical and basic research and industrial usage.

Michael Schlenkrich (SGI, Grassbrunn) demonstrated web-integration in high-performance computing. Charles Henriet (NEC, Manno Switzerland) gave deeper insights into the achievement and perspectives of the CSCS/NEC SX-4 Task Force in Computational Chemistry. Together with users and CSCS, they optimized and parallelized -- thus significantly speeding-up -- several chemical programs such as MNDO94, CPV (Car-Parinello Method and Vanderbilt Pseudopotentials), GROMDO and DALTON, for example, with good results. Johannes Grotendorst (Research Center Juelich) demonstrated the ZAM-Cray computer systems as a catalyst for computer-aided chemistry.

In addition, the conference hall held an exhibition where hardware and software players presented their solution in chemistry. Pallas and Bruehl, showed parallelisation tools, while MSI, Baldham, Oxford Molecular, and Erlangen, showed software in chemistry. The four major scientific computing companies, Wuerzburg, Tripos, Munich, and Siemens Nixdorf were prominent. Munich, demonstrated solutions on a SNI Celsius personal workstation running LINUX. SGI, Grassbrunn, showed their web-solutions. NEC, Duesseldorf, and CSCS/SCSC, Manno, underlined the performance of their vector-parallel machine especially for chemistry applications and codes. GMD, St. Augustin, showed their activities as a German HPC Technology Transfer Node, especially in chemistry.

The proceedings are available on the WWW. The majority of the presentations are in German, but seven of the talks are in English: http://www.kfa-juelich.de/compchem/proceedings/proceedings.html

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