# **CCP**2018

XXX IUPAP Conference on Computational Physics
July 29 – August 3
University of California, Davis, USA

## **Abstracts /** Plenary Sessions

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# Monday, 09:30AM-10:15AM, Plenary Session

*Conference Center, Ballroom ABC*

## Cosmology Data Analysis Opportunities and Challenges in the LSST Sky Survey

**J. Anthony Tyson**
*University of California, Davis, USA*

Fueled by advances in software, microelectronics, and large optics fabrication, a new type of sky survey will soon begin. In a relentless campaign of 15 second exposures with a 3 gigapixel camera, the 8.4m Large Synoptic Survey Telescope will cover the sky deeply every week for ten years. LSST will chart billions of remote galaxies, providing multiple probes of the mysterious Dark Matter and Dark Energy. Multiple probes of the effects of dark energy over an unprecedented volume of the universe will allow us to measure how dark energy behaves over time to high precision. Hundreds of petabytes of high dimensional complex data will be mined and compared with Exascale simulations. After reviewing the LSST project, I will describe some of the computational challenges and opportunities.

# Monday, 10:45AM-12:15PM, Plenary Session

*Conference Center, Ballroom ABC*

## A quantum future for computational physics

**Matthias Troyer**
*Microsoft Quantum, Redmond, USA. ETH Zurich, Zurich, Switzerland*

A century after the discovery of quantum mechanics we are on the verge of building devices based on quantum mechanical principles that have the potential to vastly outperform any classical computer. Like past advances in computing hardware, quantum computers are eagerly awaited by many computational physicists to solve problems that are so far intractable. Looking forward to this quantum future, I will discuss connections between computational physics and quantum computing. Computational physics already now plays an important role in the design of quantum computers, and the simulation and testing of quantum computers. Even more, the skills of computational physicists will be important to bridge the gap between theoretical work in quantum computer science and real-world applications. I will present a number of examples illustrating the importance of algorithm development and optimization, and the comparison to state of the art classical methods for the growing field of quantum computing.

## The era of variational quantum algorithms

**Alan Aspuru-Guzik**
*Department of Chemistry and Computer Science, University of Toronto, Toronto, Canada. Vector Institute, Toronto, Canada. Zapata Computing, Cambridge, USA*

In this talk, I will describe the general area of variational quantum algorithms. These algorithms are very suitable to be employed in the Noisy-Intermediate Scale Quantum (NISQ) era. In this family of algorithms, an iterative loop between classical computers and quantum computers leads to the optimization of quantum states against a loss function. These algorithms include several variants. The simulation of chemistry and materials, and in general, any quantum system with an interesting Hamiltonian of reasonable locality can be carried out using the variational quantum eigensolver (VQE). The compression of quantum states for machine learning and communications purposes can be achieved by the quantum autoencoder (QAE) algorithm. Machine learning can be achieved by the quantum neuron (QN). Finally, error mitigation can be achieved by the quantum variational error correction (QVECTOR). Our group is actively working on all these algorithms. I will provide a summary of the state of the art for each and the prospects for new algorithms belonging to this family.

# Tuesday, 09:00AM-10:30AM, Plenary Session

*Conference Center, Ballroom ABC*

## Hydrogen-rich materials under high pressure: clue and route towards high-temperature superconductors

Tian Cui, **Defang Duan**
*State Key Laboratory of Superhard Materials, College of physics, Jilin University, Changchun, China*

The realization of room temperature superconductivity has always been the ultimate goal of scientists. Hydrogen-rich materials are potential high temperature superconductors, which are expected to be a new member of superconductor family: hydrogen-based superconductors.

We discovered a few high-temperature superconductors in hydrogen-rich materials at high pressure by means of theoretical exploration. In binary hydrogen-rich materials, some high-$T_c$ superconductors have been triggered at high pressure. We first theoretically predicted $H_3S$ with *Im*-3*m* symmetry with $T_c$ reaching as high as 200 K at high pressure[1], which have been confirmed by in situ high pressure experiments[2-4]. It is also predicted that $SbH_4$ and $BiH_5$ are proposed as the stable hydrides, with high $T_c$ above 100 K at high pressures. Furthermore, we also explored high temperature superconductivity in ternary hydrides at high pressures. For ternary hydrides $LiAlH_6$, it can stabilize above 200 GPa with high $T_c$ of 160 K. Particularly, we have found that high-temperature superconductivity is closely associated with H structures of hydrogen-rich materials. Theoretical explorations call for experimental efforts to focus on the synthesis of hydrogen-rich materials consisted of atomic H, in which the quasi-molecular H units are absent and high-temperature superconductivity will be realized.

References:

[1] T. Cui, et al. Sci. Rep.,**4,** 6968 (2014); T. Cui, et al. Phys. Rev. B,**91,** 180502 (2015).

[2] M. I. Eremets, et al. Nature, **252**, 73-76 (2015).

[3] K. Shimizu, et al. Nature Phys., **12**, 835-838 (2016).

[4] T. Cui, et al. arXiv:1610.02630 (2016).

## Data-Driven Materials-Science – Rethinking the Pursuit of Understanding

**Matthias Scheffler**
*Fritz-Haber-Insitut der Max-Planck-Gesellschaft, Berlin, Germany. UCSB, Santa Barbara, USA*

The discovery of

• improved or even novel - not just new - materials or

• hitherto-unknown properties of known materials

to meet a specific scientific or industrial requirement is one of the most exciting and economically important applications of high-performance computing to date. In this talk I will discuss methods and applications how to extract knowledge from the resulting data immensity. Specifically I will describe how to spot yet unseen patterns or structures in the data, by identifying ***the key atomic and collective physical actuators*** by compressed sensing and machine learning. This enables us to build ***maps of materials*** where different regions correspond to materials with different properties. As the connections between actuators and materials properties are intricate, attempts to describe the relationship in terms of an insightful physical model may be pointless.

I will demonstrate our methodology for describing and predicting 2D topological insulators, the metal/insulator classification, catalytic $CO_2$ activation, and more.

This work was supported by the NOMAD CoE (Novel Materials Discovery Center of Excellence: https://nomad-coe.eu).

# Tuesday, 11:00AM-12:30PM, Plenary Session

*Conference Center, Ballroom ABC*

## Machine Learning and Materials Discovery

**Gus Hart**
*Brigham Young University, Provo, USA*

The relative accuracy and speed of density functional calculations have transformed computational materials science and enabled the creation of large databases of computed materials properties. But true ”materials by design” or in-silico materials discovery has not yet been realized, though there are isolated success stories. It seems likely that into make computional discovery of new materials possible, or to discover materials engineering routes to improve already-deployed materials, a brute force approach will not be practical—some other paradigm will be required. Machine learning, so successful in some other application areas, is an intriguing and promising idea, but there are hurdles to overcome. There are two important differences between the standard machine learning problems of image recognition, voice recognition, etc., and materials prediction. In the first instance, we cannot afford the typical accuracy tradeoff—materials predictions are not useful without meeting a high accuracy target; the energy difference of competing phases is often very small, requiring high fidelity in the models. The second difference is the amount of training data—we don’t have ”big data”. How do we move forward? In this talk I will review the state of the art in this emerging discipline and show some results from BYU’s Materials Simulation Group efforts in this area.

This work is supported by ONR (MURI N00014-13-1-0635).

## GW170817: The Multi-Messenger Observation of a Binary Neutron Star Merger

**Duncan Brown**
*Syracuse University, Syracuse, USA*

On August 17, the U.S. Laser Interferometer Gravitational-wave Observatory (LIGO) and the French-Italian Virgo gravitational-wave detector observed the ripples in spacetime from a neutron star merger. Two second later NASA’s Fermi Gamma Ray Burst Monitor detected a flash of gamma rays from the collision. LIGO and Virgo localized the source to a 30 square degree patch of the sky in the constellation Hydra. Twelve hours later, the optical counterpart to the merger was detected. I will present the detection of the neutron star merger, the associated kilonova, and the implications that this multi-messenger observation has for our understanding of the universe. I will also discuss the future path for gravitational-wave astronomy beyond the second-generation Advanced LIGO detectors.

# Wednesday, 09:00AM-10:30AM, Plenary Session

*Conference Center, Ballroom ABC*

## Molecular Crystal Structure Prediction with GAtor and Genarris

**Noa Marom**
*Carnegie Mellon University, Pittsburgh, USA*

Molecular crystals are bound by dispersion interactions, whose weak nature produces potential energy landscapes with many local minima. Hence, they often exhibit polymorphism, whereby the same molecule crystallizes in several structures, which may exhibit different properties. Crystal structure prediction is challenging because it requires searching a high-dimensional space with high accuracy. We present the genetic algorithm (GA) code, GAtor, and its associated structure generation package, Genarris. Both rely on dispersion-inclusive density functional theory (DFT) for geometry relaxations and energy evaluations.

Genarris generates random structures with physical constraints and uses a Harris approximation to construct the electron density of a molecular crystal by superposition of single molecule densities. The DFT energy is then evaluated for the Harris density without performing a self-consistent cycle, enabling fast screening of initial structures. Genarris creates a maximally diverse initial population by using machine learning for clustering based on structural similarity with respect to a relative coordinate descriptor.

GAs rely on the evolutionary principle of survival of the fittest to perform global optimization. GAtor offers a variety of crossover and mutation operators, designed for molecular crystals, to generate offspring by combining/ modifying parent structural genes. GAtor achieves massive parallelization by spawning several GA replicas that run in parallel and read/write to a common population. GAtor performs evolutionary niching by using machine learning to dynamically cluster the population. A cluster-based fitness function is used to steer the GA to under-sampled low-energy regions of the potential energy landscape. This helps overcome initial pool biases and selection biases.

## Diagrammatic and Continuous Time Quantum Monte Carlo

**Emanuel Gull**
*University of Michigan, Ann Arbor, USA*

This talk will give an overview of several techniques that use Feynman diagrammatic series to describe correlated quantum systems. We will introduce diagrammatic Monte Carlo, continuous time Monte Carlo, bold line techniques and inchworm techniques. We will then give examples of how diagrammatic methods can be used to compute single- and two-particle response functions that can directly be related to experiment and simpler theories.

# Wednesday, 11:00AM-12:30PM, Plenary Session

*Conference Center, Ballroom ABC*

## First principles calculations for materials with strong electronic Coulomb correlations – where do we stand?

**Silke Biermann**
*Centre de Physique Theorique Ecole Polytechnique, France*

Assessing excited states properties of materials with strong electronic Coulomb correlations is a challenge to computational solid state physics. Dynamical mean field techniques, in conjunction with electronic structure methods, have led to tremendous progress over the last years.

We will illustrate the current state of the art by discussing spectral properties of 3d, 4d, and 5d transition metal compounds, which are compared to experimental photoemission data.

We conclude with an outlook on current construction sites in the field and recent progress on the development of parameter-free interfaces of electronic structure and many-body theory, within the quest of quantitatively accurate predictive schemes.

[1] Martins, et al., Phys. Rev. Mat. Rapid, 2018.

## Developments in Quasi-Lagrangian Moving-Mesh and Mesh-Free Methods: Applications to Fluid Dynamics, Cosmology, Plasmas, Collisionless and Elastic Dynamics

**Philip Hopkins**
*California Institute of Technology, Pasadena, USA*

I will review developments (primarily coming from astrophysics) of novel mesh-free and moving-mesh algorithms which combine historical advantages of smoothed-particle hydrodynamic methods with the accuracy, convergence and superior shock-capturing advantages of higher-order finite-volume methods. These methods have been widely applied to simulate highly-compressible fluid dynamics and magneto-hydrodynamics, self-gravitating collapse and cosmology, kinetic effects in diffuse plasmas, elasto-dynamics and solid-body material collisions, relativistic dynamics, and more. I'll discuss generalizations to follow collisionless or weakly-collisional systems in high-dimensional phase space at tractable computational cost, relevant for radiation-hydrodynamics and collisionless self-gravitating systems (e.g. dark matter in cosmological simulations), and show some examples of how these methods have enabled dramatic resolution improvements in astrophysical simulations.

# Thursday, 09:00AM-10:30AM, Plenary Session

*Conference Center, Ballroom ABC*

## Building quantum control solutions using filter functions as an efficient computational tool

**Michael Biercuk**
*The University of Sydney, Sydney, Australia. Q-CTRL, Sydney, Australia*

The development of quantum computing relies on computational tools for the simulation of fundamental devices and circuits. However, even at the level of single quantum bits, or qubits, computational techniques rapidly become unwieldy when considering the task of modelling quantum information subjected to realistic laboratory environments. Here, the presence of ambient time-varying Non-Markovian noise both complicates mathematical assumptions underlying many quantum information protocols, and induces degradation of quantum information. This noise-induced degradation, known as decoherence, represents the most significant challenge in the field and requires dramatic advances in error suppression for quantum computing to come to reality.

In this talk we provide an overview of the field of quantum control and the tools we have built to enable scientists and engineers to deploy efficient and effective decoherence-mitigation techniques at the physical hardware layer. We introduce the concept of the filter function, a simple computational tool to characterize arbitrary quantum operations performed on single or multi-qubit devices. We perform experiments with trapped ions to validate the predictive power of the filter functions and demonstrate how they can enable quantum control solutions for both noise characterization and noise suppression in quantum hardware. These concepts form the fundamental tools at the heart of our venture-backed quantum technology startup Q-CTRL.

## Using Artificial Intelligence to Discover New Materials

**Chris Wolverton**
*Northwestern University, EVANSTON, USA*

Rational, data-driven materials discovery has the potential to make research and development efforts far faster and cheaper. In such a paradigm, computer models trained to find patterns in massive chemical datasets would rapidly scan compositions and systematically identify attractive candidates. Here, we present several examples of our work on developing machine learning (ML) and deep learning methods capable of creating predictive models using a diverse range of materials data. As input training data, we demonstrate ML on both large computational datasets of DFT calculations, as implemented in the Open Quantum Materials Database (oqmd.org), and also experimental databases of materials properties. We construct ML models using a large and chemically diverse list of attributes, which we demonstrate can be used as an effective tool to automatically learn intuitive design rules, predict diverse properties of crystalline and amorphous materials, such as formation energy, specific volume, band gap energy, and glass-forming ability, and accelerate combinatorial searches.

# Thursday, 11:00AM-12:30PM, Plenary Session

*Conference Center, Ballroom ABC*

## Self-propelled topological defects in active matter

**Julia Yeomans**
*University of Oxford, Oxford, United Kingdom*

Active materials, such as bacteria, molecular motors and self-propelled colloids, are Nature's engines. They continuously transform chemical energy from their environment to mechanical work. Dense active matter shows mesoscale turbulence, the emergence of chaotic flow structures characterised by high vorticity and self-propelled topological defects.

The chaotic nature of active turbulence means that it is likely to be difficult to harness its energy. Hence it is interesting to consider ways to 'tame' active turbulence, channeling the energy input into coherent flows. This can be done by screening hydrodynamics through confinement or friction, and I will describe flow patterns and defect trajectories in active matter in confined geometries.

Moreover the ideas of active matter suggest new ways of interpreting cell motility and cell division. In particular recent results indicate that active topological defects may help to regulate turnover in epithelial cell layers and contribute to controlling the structure of bacterial colonies.

## Zero temperature phase diagrams of two dimensional quantum spin models

**Ribhu Kaul**
*University of Kentucky, Lexington, USA*

Just as classical spin models like the Ising model provide the paradigmatic examples of thermal phase transitions, lattice Hamiltonians of quantum spins harbor the simplest examples of T=0 phase transitions driven solely by quantum fluctuations. In this presentation, I review how the phase diagrams of quantum spin Hamiltonians on two dimensional spatial lattices determined by novel quantum Monte Carlo algorithms and interpreted with sophisticated field theoretic ideas contain a number of striking new features including deconfined critical points and fractionalized spin liquids.