

# The McMahon Research Group

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We are a theoretical and computational physics group. Our focus is on **computational condensed matter physics**, but our interests are interdisciplinary.

This is a broad, but succinct statement; in general:

- **What we do:** condensed matter physics
- **How we do it:** computational physics

Specific **examples** of recent interest:

- The properties of solids and liquids that compose planetary interiors
- Quantum phases of matter that exhibit simultaneous types of order
- Ordered quantum phases that constitute new, exotic states of matter
- The development and use of theories and techniques from the emerging field of data science to solve intractable problems

- Condensed matter physics:
  - Solids and liquids
  - Quantum fluids and solids

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- Computational physics:
  - First-principles simulations
  - High performance computing
  - Methods development

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- Closing remarks

# Condensed Matter Physics

**Condensed matter physics** is a branch of physics that deals with the physical properties of condensed phases of matter, and their understanding using fundamental physical principles.

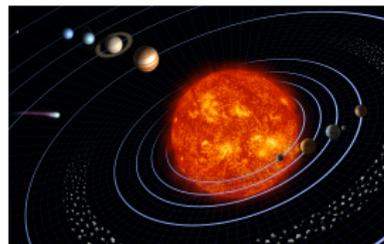
## Outline:

- Solids and liquids
- Quantum fluids and solids

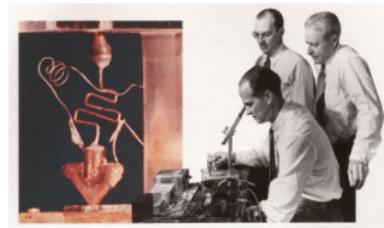
# Solids and Liquids

Condensed matter physics arose out of the (sub)field of **solid**-state physics, after interest in the study of **liquids** increased.

The properties of **solids and liquids** are key to understanding the major fraction of (ordinary) matter in the Universe.



Many of our most important technologies have come from such studies (e.g., semiconductor devices).



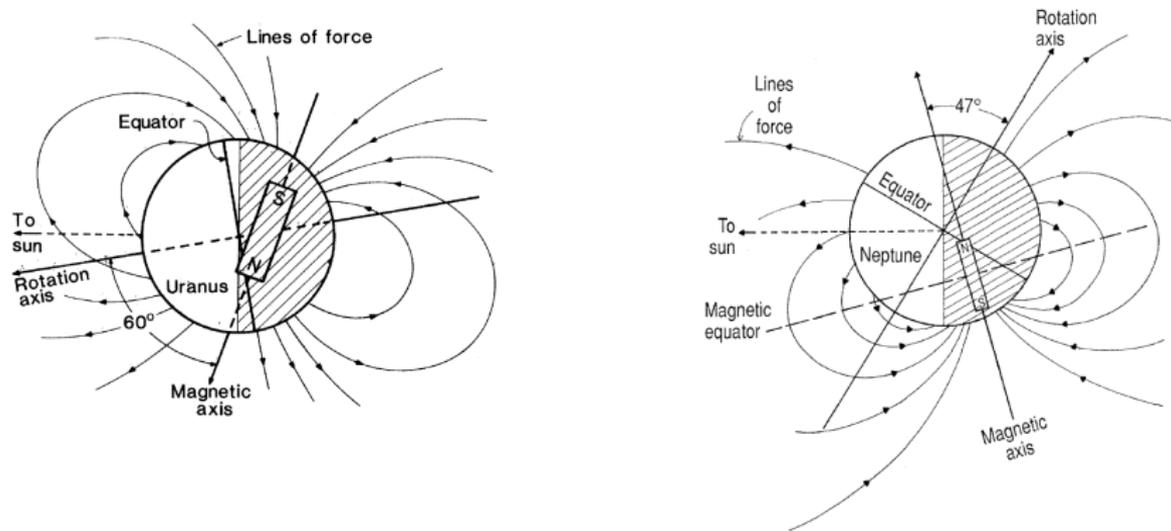
We're interested in the fundamental properties of **solids and liquids**.

<http://www.cedmagic.com/history/transistor-1947.html>

<http://solarsystem.nasa.gov/>

## Example: Dense Water-ice

In 1986 and 1989, Voyager 2 revealed non-dipolar and non-axisymmetric magnetic field structures of Uranus and Neptune:



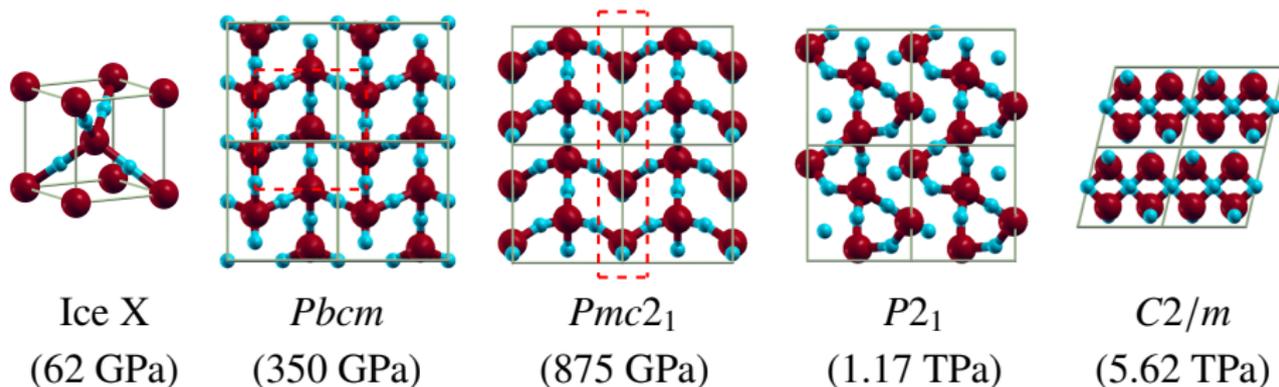
The properties of **dense water-ice** are key to understanding the ice giants.

N. F. Ness, M. H. Acuna, K. W. Behannon, L. F. Burlaga, J. E. P. Connerney, R. P. Lepping, and F. M. Neubauer, *Science* **233**, 85 (1986)

N. F. Ness, M. H. Acuna, L. F. Burlaga, J. E. P. Connerney, R. P. Lepping, and F. M. Neubauer, *Science* **246**, 1473 (1989)

# Example: Dense Water-ice

A number of groups have recently found that at high (planetary) pressures, water-ice goes through a series of phase transitions ...



... characterized by rearrangements of the hydrogen-bond network, in order for the oxygen sub-lattice to better close pack.

J. M. McMahon, *Phys. Rev. B* **84**, 220104(R) (2011)

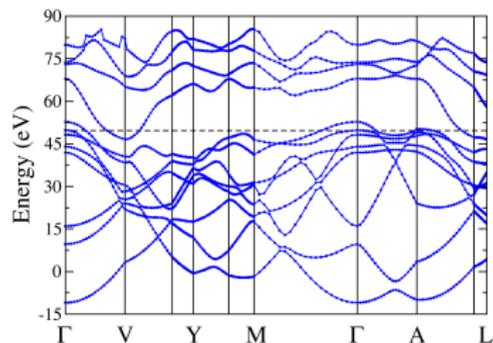
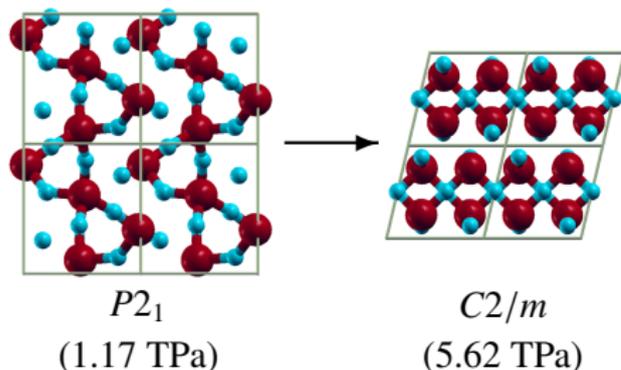
Y. Wang, H. Liu, J. Lv, L. Zhu, H. Wang, and Y. Ma, *Nature Comm.* **2**, 563 (2011)

M. Ji, K. Umemoto, C.-Z. Wang, K.-M. Ho, and R. M. Wentzcovitch, *Phys. Rev. B* **84**, 220105(R) (2011)

A. Hermann, N. W. Ashcroft, and R. Hoffmann, *Proc. Natl. Acad. Sci. USA* **109**, 745 (2012)

# Example: Dense Water-ice

Water-ice remains a wide bandgap insulator until the  $P2_1 \rightarrow C2/m$  phase transition<sup>1</sup>:



Since metallization occurs at finite-temperature also near 5 TPa<sup>2</sup>, these results imply that metallization does *not* play a role in understanding the ice giants.<sup>3</sup>

<sup>1</sup>J. M. McMahon, *Phys. Rev. B* **84**, 220104(R) (2011)

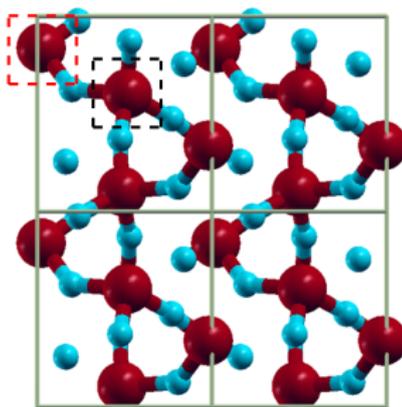
<sup>2</sup>M. French, T. R. Mattsson, and R. Redmer, *Phys. Rev. B* **82**, 174108 (2010)

<sup>3</sup>B. Militzer and H. F. Wilson, *Phys. Rev. Lett.* **105**, 195701 (2010)

# Example: Dense Water-ice

The  $P2_1$  phase (1.17 to 5.62 TPa) partially overcomes a large proton-transfer barrier to adopt a partially-ionic ground state<sup>1-3</sup>:

Alternating layers of  $\text{OH}^{-\delta}$   
and  $\text{H}_3\text{O}^{\delta}$  with  $\delta \approx 0.62$



## Approximate energy scales:

- Proton transfer: 1.5 eV
- Concerted proton diffusion: 0.7 eV/H
- Zero-point motion: 1.5 eV/H<sub>2</sub>O

This behavior is consistent with dynamo simulation that show a stably stratified fluid interior surrounded by a convective thin shell produces magnetic fields similar in morphology to those of Uranus and Neptune.<sup>4</sup>

<sup>1</sup>J. M. McMahon, *Phys. Rev. B* **84**, 220104(R) (2011)

<sup>2</sup>Y. Wang *et al.*, *Nature Comm.* **2**, 563 (2011)

<sup>3</sup>A. Hermann, N. W. Ashcroft, and R. Hoffmann, *Proc. Natl. Acad. Sci. USA* **109**, 745 (2012)

<sup>4</sup>S. Stanley and J. Bloxham, *Nature* **428**, 151–153 (2004)

In modern condensed matter physics, much of the fundamental research is driven by the search for exotic phases of matter.

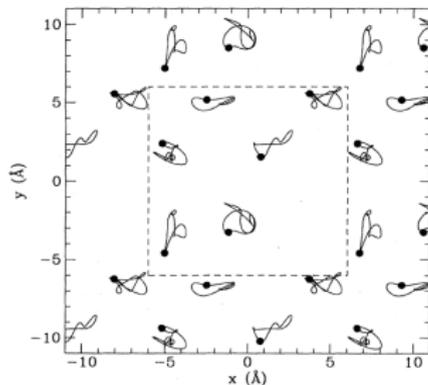
**Example: Quantum fluids and solids:** substances in which the interaction between the constituent atoms or molecules is governed by the laws of quantum mechanics.

- The study of exotic phases has and continues to play a pivotal role in the development of key concepts and ushering paradigm shifts in quantum many-body physics.
- Exotic phases will probably be at the center of the important technologies of tomorrow.

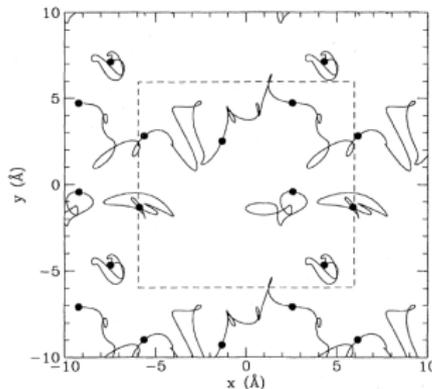
# Example: Superfluidity

A **superfluid** is perhaps the most well known quantum fluid<sup>1</sup>: a state of matter that behaves like a fluid with zero viscosity.

Feynman's path-integral formulation of quantum mechanics gives us a simple classical picture of a superfluid<sup>2</sup>; **example**: 6 <sup>4</sup>He atoms<sup>3</sup>:



$T = 2\text{K}$



$T = 0.75\text{K}$

<sup>1</sup>1/2 Nobel Prize in Physics 1978; 1996 Nobel Prize in Physics; 1/3 Nobel Prize in Physics 2003

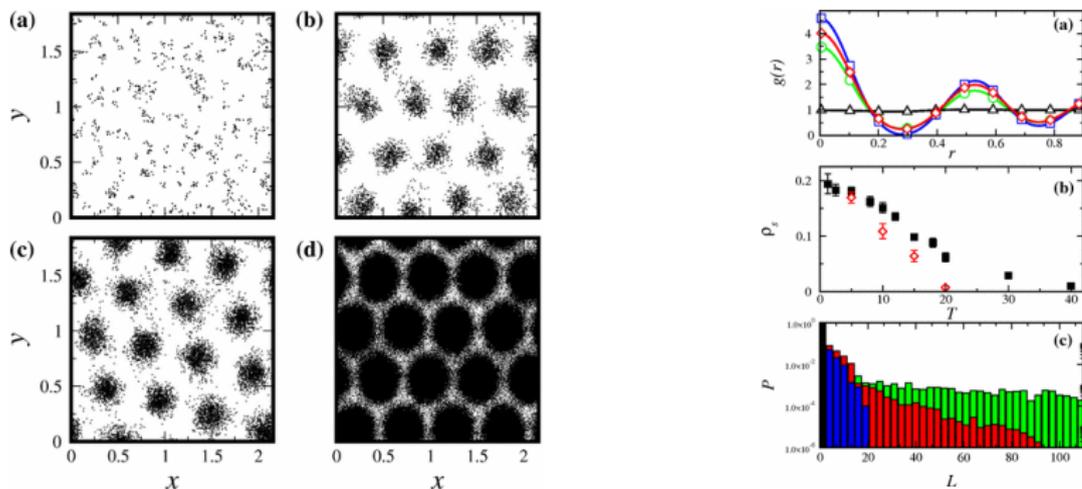
<sup>2</sup>R. P. Feynman, *Phys. Rev.* **90**, 1116 (1953); *ibid.* **91**, 1291 (1953); *ibid.* **91**, 1301 (1953)

<sup>3</sup>D. M. Ceperley, *Rev. Mod. Phys.* **67**, 279–355 (1995)

# Example: Supersolidity

Significant recent interest has been on phases of matter exhibiting simultaneous types of order; a standard **example** is the so-called **supersolid**.

**Example:** Bosons interacting via a modified power-law potential:



Temperatures of  $T^* = 200$  [(a) – left, triangles, black], 20 [(b), squares, blue], 1.0 [(c), diamonds, red], and 0.1 [(d), circles, green]

F. Cinti, P. Jain, M. Boninsegni, A. Micheli, P. Zoller, and G. Pupillo, *Phys. Rev. Lett.* **105**, 135301 (2010)

# Example: Liquid Metallic Hydrogen

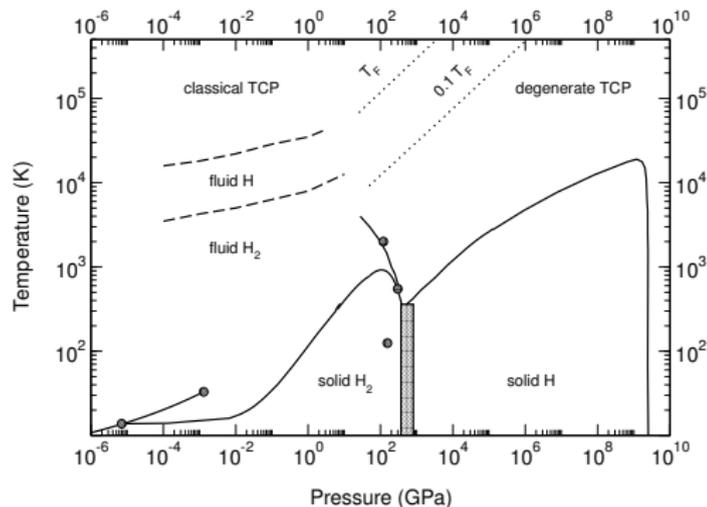
Calculations suggest that dense **hydrogen** will become a quantum fluid ...

## A quantum fluid of metallic hydrogen suggested by first-principles calculations

Stanimir A. Bonev, Eric Schwegler, Tadashi Ogitsu & Giulia Galli

Lawrence Livermore National Laboratory, University of California, Livermore, California 94550, USA

It is generally assumed<sup>1-3</sup> that solid hydrogen will transform into a metallic alkali-like crystal at sufficiently high pressure. However, some theoretical models<sup>4,5</sup> have also suggested that compressed hydrogen may form an unusual two-component (protons and electrons) metallic fluid at low temperature, or possibly even a zero-temperature liquid ground state. The existence of these new states of matter is conditional on the presence of a maximum in the melting temperature versus pressure curve (the 'melt line'). Previous measurements<sup>6-8</sup> of the hydrogen melt line up to pressures of 44 GPa have led to controversial conclusions regarding the existence of this maximum. Here we report *ab initio* calculations that establish the melt line up to 200 GPa. We predict that subtle changes in the intermolecular interactions lead to a decline of the melt line above 90 GPa. The implication is that as solid molecular hydrogen is compressed, it transforms into a low-temperature quantum fluid before becoming a monatomic crystal. The emerging low-temperature phase diagram of hydrogen and its isotopes bears analogies with the familiar phases of <sup>3</sup>He and <sup>4</sup>He (the only known zero-temperature liquids), but the long-range Coulomb interactions and the large component mass ratio present in hydrogen would result in dramatically different properties<sup>9</sup>.



S. A. Bonev, E. Schwegler, T. Ogitsu, and G. Galli, *Nature* **431**, 669 (2004)

J. M. McMahon, M. A. Morales, C. Pierleoni, and D. M. Ceperley, *Rev. Mod. Phys.* **84**, 1607 – 1653 (2012); Cover Article

# Example: Liquid Metallic Hydrogen

... and exhibit properties such that it cannot be classified exclusively as either a superconductor or superfluid.

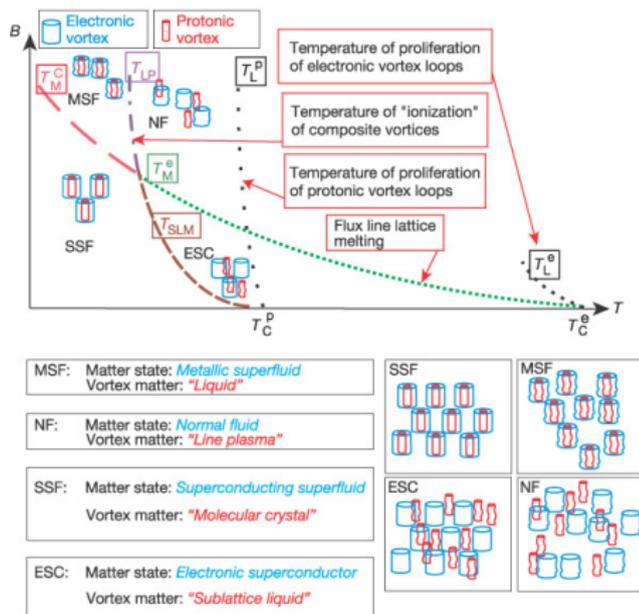
## A superconductor to superfluid phase transition in liquid metallic hydrogen

Egor Babaev<sup>1,2</sup>, Asle Sudbø<sup>2</sup> & N. W. Ashcroft<sup>1</sup>

<sup>1</sup>Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York, 14853-2501, USA

<sup>2</sup>Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway

Although hydrogen is the simplest of atoms, it does not form the simplest of solids or liquids. Quantum effects in these phases are considerable (a consequence of the light proton mass) and they have a demonstrable and often puzzling influence on many physical properties<sup>1</sup>, including spatial order. To date, the structure of dense hydrogen remains experimentally elusive<sup>2</sup>. Recent studies of the melting curve of hydrogen<sup>3,4</sup> indicate that at high (but experimentally accessible) pressures, compressed hydrogen will adopt a liquid state, even at low temperatures. In reaching this phase, hydrogen is also projected to pass through an insulator-to-metal transition. This raises the possibility of new state of matter: a near ground-state liquid metal, and its ordered states in the quantum domain. Ordered quantum fluids are traditionally categorized as superconductors or superfluids; these respective systems feature dissipationless electrical currents or mass flow. Here we report a topological analysis of the projected phase of liquid metallic hydrogen, finding that it may represent a new type of ordered quantum fluid. Specifically, we show that liquid metallic hydrogen cannot be categorized exclusively as a superconductor or superfluid. We predict that, in the presence of a magnetic field, liquid metallic hydrogen will exhibit several phase transitions to ordered states, ranging from superconductors to superfluids.



E. Babaev, A. Sudbø, and N. W. Ashcroft, *Nature* **431**, 666 (2004)

# Open Questions in Quantum Fluids and Solids

There are considerable controversies and **open questions in the study of quantum fluids and solids** (from both theory/computation and experiment).

**Example<sup>1</sup>**: Evidence of nonclassical rotational inertia (supersolidity) in solid  $^4\text{He}$  was observed in 2004; in 2012, the same group found no such evidence.

**Example<sup>2</sup>**: In 2011, calculations suggested the possibility of supersolidity in 2D; calculations in 2012 suggested that this is only the result of numerical approximations.

**Example<sup>3</sup>**: Liquid metallic hydrogen and its ordered quantum states was suggested in 2004; calculations in 2015 suggested that atomic metallic hydrogen is stable to approximately 300K.

We are trying to provide definitive answers to these (and other) open questions, in order to understand the fundamental physics of quantum fluids and solids .

<sup>1</sup>E. Kim and M. H. W. Chan, *Nature* **427**, 225 (2004); E. Kim and M. H. W. Chan, *Science* **305**, 1941 (2004); D. Y. Kim and M. H. W. Chan, *Phys. Rev. Lett.* **109**, 155301 (2012)

<sup>2</sup>M. C. Gordillo, C. Cazorla, and J. Boronat, *Phys. Rev. B* **83**, 121406(R) (2011); Y. Kwon and D. M. Ceperley, *Phys. Rev. B* **85**, 224501 (2012)

<sup>3</sup>J. M. McMahon, M. A. Morales, R. Clay III, C. Pierleoni, and D. M. Ceperley, *Submitted* (2015); J. M. McMahon and D. M. Ceperley, *Phys. Rev. B* **84**, 144515 (2011); *ibid.* **85**, 219902(E) (2012)

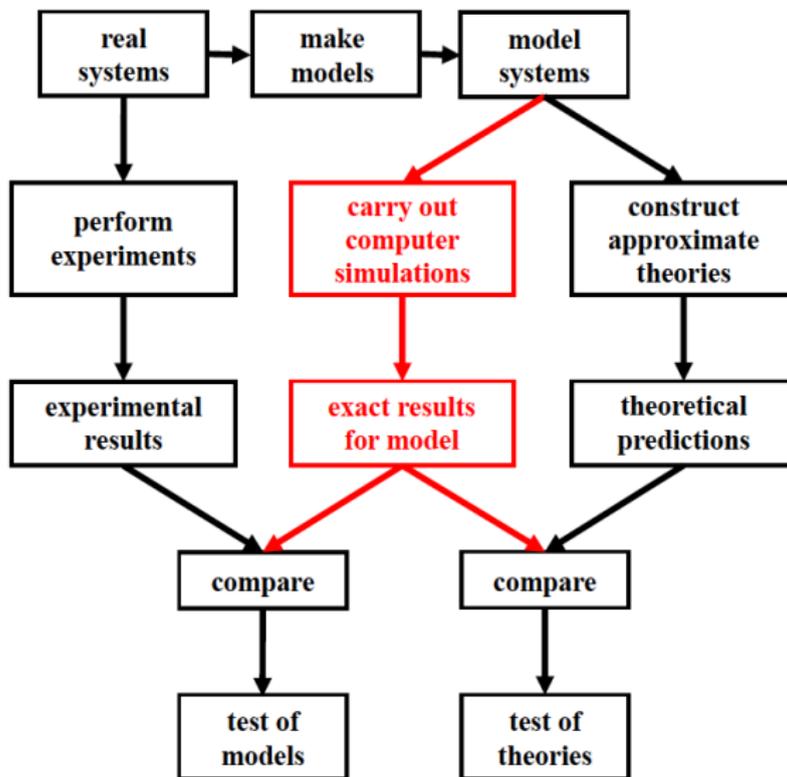
# Computational Physics

**Computational physics** is the study and implementation of numerical analysis to solve problems in physics for which a quantitative theory already exists.

## Outline:

- First-principles simulations
- High performance computing
- Methods development

# The Role of Computer Simulations



Adapted from: M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Oxford University Press: New York 1991)

# First-principles Simulations

We're interested in studying condensed matter starting from the fundamental many-body equations (**first-principles simulations**).

**Example:** The electronic problem:

$$\hat{H}_{\text{BO}}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E_{\text{el}}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$
$$\hat{H}_{\text{BO}} = -\sum_{i=1}^N \frac{1}{2} \nabla_i^2 + \sum_{j=1}^N \sum_{i<j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{n=1}^K \sum_{i=1}^N \frac{Z_n}{|\mathbf{r}_i - \mathbf{R}_n|}$$

*“The general theory of quantum mechanics is now almost complete ... The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”*

— Paul Dirac, 1929

# Example: Electronic Structure Methods

“... *It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.*”

— Paul Dirac, 1929

A number of **electronic structure methods** exist; **examples:**

- Exact diagonalization
  - ▶ Most exact method ...
  - ▶ ... but  $\mathcal{O}(e^N)$  scaling
- Mean field
  - ▶  $\mathcal{O}(N^3)$  scaling, small prefactor ...
  - ▶ ... but requires reformulating the problem to one that is not exact
  - ▶ Uncontrolled approximation(s)
- Quantum Monte Carlo
  - ▶  $\mathcal{O}(N^3)$  scaling, *large* prefactor
  - ▶ Stochastic sampling of the *actual* many-body wavefunction
  - ▶ The *only* highly-accurate method that scales reasonably with  $N$

It is often necessary to use high performance computing.

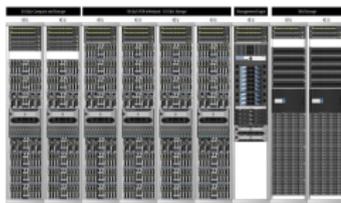
# High Performance Computing (HPC)

**HPC** is computing on a **supercomputer**: a computer with a high-level computational capability compared to a general-purpose computer.

Consider the **levels of HPC program development**:



**Development level:** Code development on a PC; toy systems (IBM 5150 PC)



**Test level:** Demonstration of scaling capabilities on HPC clusters; test systems (Kamiak HPC cluster at WSU)

**Production level:** Massive calculations at supercomputing facilities; realistic systems (Titan at ORNL)



**IBM 5150 PC image:** Photograph by Rama, Wikimedia Commons, Cc-by-sa-2.0-fr

**Titan image:** Courtesy of Oak Ridge National Laboratory, U.S. Dept. of Energy

# Scale of HPC Calculations

In HPC, calculations are (often) measured in **core hours**:

$$(1 \text{ x86 CPU core}) \times (1 \text{ hour}) \times (\text{scale}) = 1 \text{ core hour}$$

**Scale of HPC calculations** (in core hours):

- Development level: 0 – 12
- Test level: 500 – 10K
- Production level: 20K – 500K

In the past, we have been awarded hundreds of millions of core hours:

Awards:

- INCITE (DOE)
- XSEDE (NSF)
- PRACE (EU)

Internal:

- *Kamiak* (WSU)
- ALCF (ANL)
- CNM (ANL)
- Blue Waters (UIUC)

Even with HPC, solving the fundamental many-body equations is not possible for many systems.

## Examples:

- Large-scale and/or long-time simulations of solids and liquids
- First-principles particle interactions for quantum fluids and solids

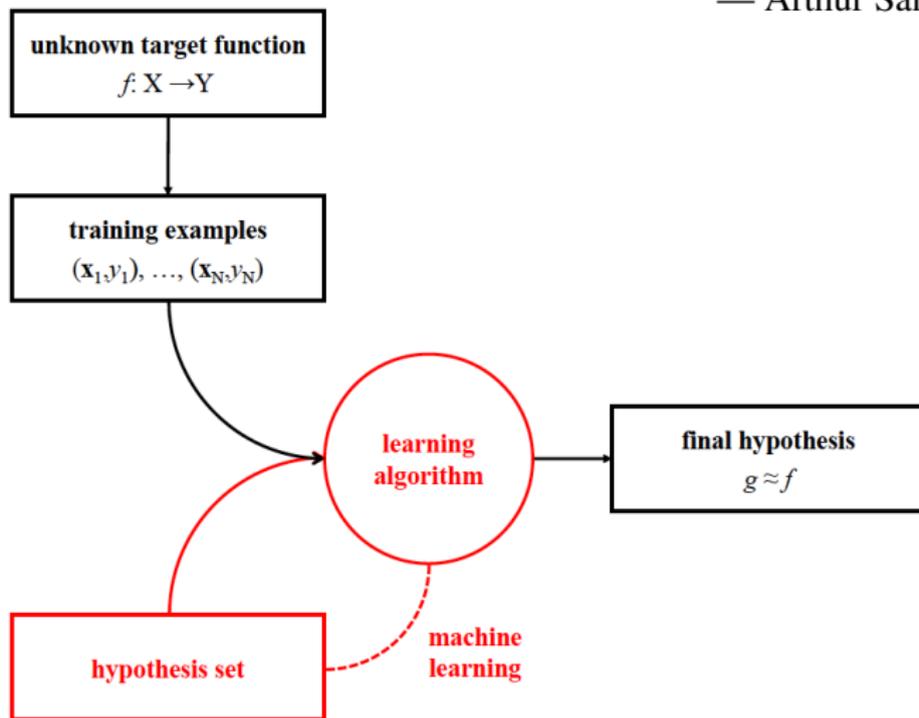
It is such intractable problems where open questions exist, and where a lot of exciting physics occurs.

We devote significant effort towards **methods development**.

# Example: Machine Learning

*“[Machine learning is the] field of study that gives computers the ability to learn without being explicitly programmed.”*

— Arthur Samuel, 1959



# Concluding Remarks

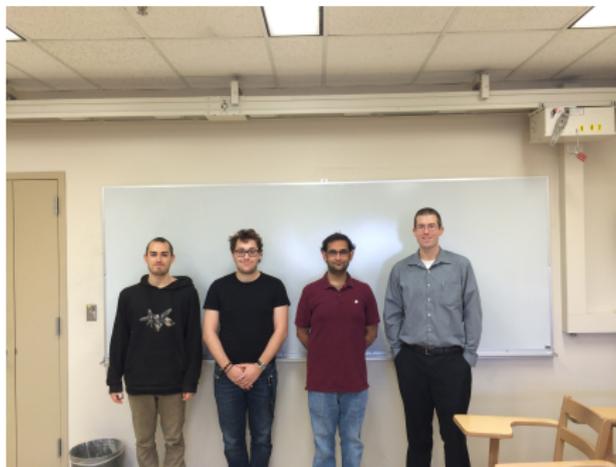
## Outline:

- Summary
- (Open) Positions

# Summary

- In the McMahon Research Group, we do theoretical and computational physics; our focus is on computational condensed matter physics.
- We address problems at the forefront of condensed matter physics; we study both “normal” and “exotic” phases of condensed matter.
- We carry out our studies by solving the fundamental many-body equations of quantum mechanics.
- Solving the many-body equations often requires HPC.
- Since we’re interested in problems that are currently intractable, this often requires the development of novel computational approaches.

# The McMahon Research Group



## Members (left to right):

- Thomas Badman
- Nikolas Steckley
- Jeevake Attapattu
- Jeffrey M. McMahon

## Resources:

- Personal HPC cluster (500 – 1000 cores) (tentative)
- Early access to Kamiak HPC cluster at WSU
- High-performance desktop computers
- Private server, copy machine, etc. (tentative)

There are several **open positions** in the McMahon Research Group.

I *strongly* encourage motivated students that are interested in any of the topics that I discussed to contact me:

- Email: [jeffrey.mcmahon@wsu.edu](mailto:jeffrey.mcmahon@wsu.edu)
- Office: Webster, Room 947D