# Good Practice at IPAM: The Impact of Mathematics on other Sciences and Society

Christian Ratsch, Institute for Pure and Applied Mathematics, Deputy Director

## Mathematics is increasingly central to science

- Increasing reliance on algorithms, e.g. signal processing, data analysis
- Increasing importance and feasibility of simulation and modeling
- Machine Learning (ML) and Artificial Intelligence (AI) are used everywhere

## Mathematics is increasingly central for society

- Increasing reliance on ML, AI, and algorithms, e.g. privacy, encryption, decision-making
- Imperfect and biased data
- Uncertainty quantification, reliability

## Progress depends on developing math tools and approaches

- Math as a whole (pure and applied) plays a significant role

To address these challenges, the National Science Foundation supports a number of Math Institutes in the United States. One of them is IPAM.

# Why a Math Institute IPAM?

## IPAM programs bring together mathematics and domain sciences or multiple areas of mathematics

- Break down linguistic barriers and ensure there is a common language
- Highlight important mathematical problems and issues, explore possible approaches
- Start new communities and collaborations, bring together ideas from different fields
- Develop human resources, serve as a point of crystallization

## IPAM programs highlight the value of mathematics

- Use of mathematics in applications, as well as applications driving math research
- Mathematics as a viable career path, with many alternatives, including industry careers
- Mathematics as a driving force of innovation

# IPAM's Mission

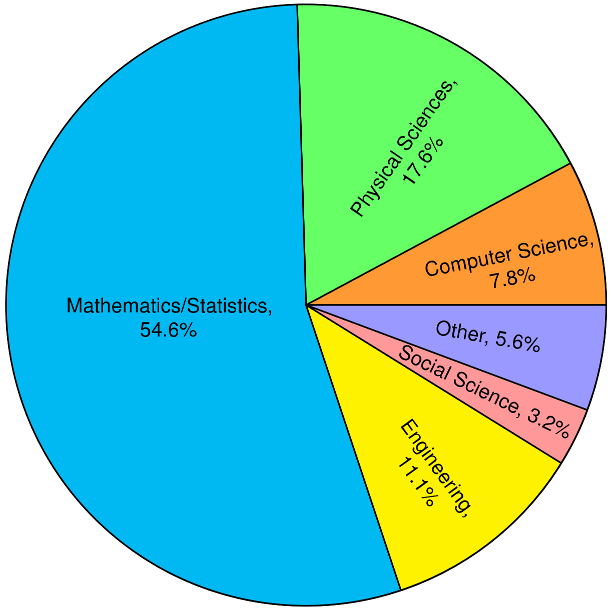
## IPAM's Mission Statement

- Foster the interaction of mathematics with a broad range of science and technology
- Create inclusive communities of mathematicians, statisticians and other scientists that find innovative ways of using mathematics to advance scientific knowledge
- Promote mathematical innovation
- Engage and transform the world through mathematics

## How does IPAM fulfill its mission?

We create new research communities through

- Long programs (3 months)
- Workshops and Exploratory Workshops
- Summer Schools




math changes everything™

# Long Programs

## Long Programs: Structure

- Core: approx. 40-50 people for 3 months
- 3 or 4 focused workshops
- Tutorials
- Culminating workshop at Lake Arrowhead
- Structured activities between workshops
  - Postdoctoral and other research seminars
  - Workgroups
  - Career panels, mentoring
- White paper
- 2-2.5 year lead time

## Long Programs 2022 – 2015

- Advancing Quantum Mechanics with Mathematics and Statistics (spring 2022)
- Mathematical and Computational Challenges in the Era of
- Gravitational Wave Astronomy (Fall 2021)
- Tensor Methods and Emerging Applications to the Physical and Data Sciences (Spring 2021)
- Mathematical Challenges and Opportunities for Autonomous Vehicles (Fall 2020)
- High Dimensional Hamilton-Jacobi PDEs (Spring 2020)
- Machine Learning in Physics & Physics of Learning (Fall 2019)
- Geometry and Learning in 3D and Beyond (Spring 2019)
- Big Data and High Performance Computing (Fall 2018)
- Quantitative Linear Algebra (Spring 2018)
- Complex High-dimensional Energy Landscapes (Fall 2017)
- Computational Issues in Oil Exploration (Spring 2017)
- Understanding Many-Particle Systems with Machine Learning (Fall 2016)
- Culture Analytics (Spring 2016)
- New Directions in Mathematical Approaches for Traffic Flow Management (Fall 2015)

# Outreach and Workforce Development

## Research in Industrial Projects for Students

Basic structure: a team of 4 students works for 8-9 weeks on a project that is sponsored by an industrial partner

- RIPS, Los Angeles
  - 2019 Sponsors: Aerospace Corporation, Airforce, Alibaba, Amazon, AMD, Google, Gumgum, HRL Laboratories, Lawrence Livermore
- RIPS, Singapore
  - 2019 Sponsors: Google, Grab, Nvidia
- G-RIPS Sendai
  - 2019 Sponsors: Toyota, Fujitsu, NEC
- G-RIPS Berlin, Germany
  - 2019 Sponsors: Deutsche Bahn, 1000 Shapes, Deloitte Germany

## Special Programs

- Outreach to women, underrepresented minorities
- Industry Short Courses
- Public lectures

# IPAM Growth

## IPAM "Universe" is expanding

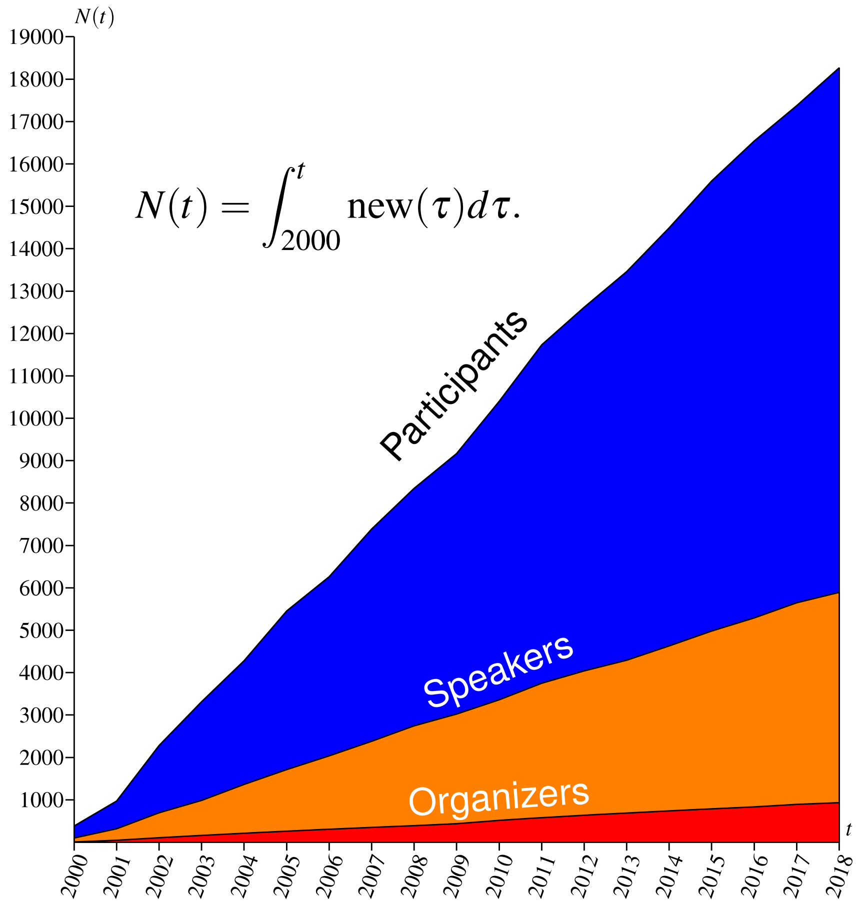
- New scientific themes and directions translate into new researchers coming to IPAM
- Approx. 2/3 of visitors are new

## Full use of resources

- More exploratory workshops
- Regular summer schools (synergy with upcoming programs)
- Industry short courses
- Leverage NSF support to expand

## Diversity

- Approximately 23% of participants are female
- Approximately 14% or participants are minorities



# Selected Success Stories at IPAM

**2004**

"Multiscale Geometry and Analysis in High Dimensions"

- Candes-Tao, Donoho: compressed sensing

**2005**

"Multiscale Physics in Material Sciences and Biophysics"

- Connected Applied Math to Materials Science

**2011**

"Navigating Chemical Compound Space"

- Link between Machine Learning and materials and molecular physics, high throughput screening "

**2012**

Summer School on Deep Learning

- Helped end "AI Winter"
- 2018 workshop on DL over 150 participants

**2015**

"New Directions in Mathematical Approaches for Traffic Flow Management "

- Modeling of the Effect of Autonomous Vehicles

**2016**

"Culture Analytics"

- Connected math and social sciences; spotlight opportunities for mathematicians

**2016 and 2019**

"Understanding Many Particle Physics with Machine Learning (2016)" and "Learning of Physics and Physics of Learning (2019)"

- Solidified connection between physics, materials, and machine learning

# Compressed Sensing

The main ideas for Compressed Sensing were developed by Candes, Romberg, Tao, and Donoho during the IPAM program on "Multiscale Geometry and Analysis in High Dimensions".

- Compressed sensing is a signal processing technique for efficiently acquiring and reconstructing a signal.
- The sparsity of a signal can be exploited to recover it from far fewer samples than required by the Nyquist-Shannon sampling theorem.

Applications:

- Photography
- Magnetic Resonance imaging
- Holography
- Facial Recognition
- Network Tomography

… and more

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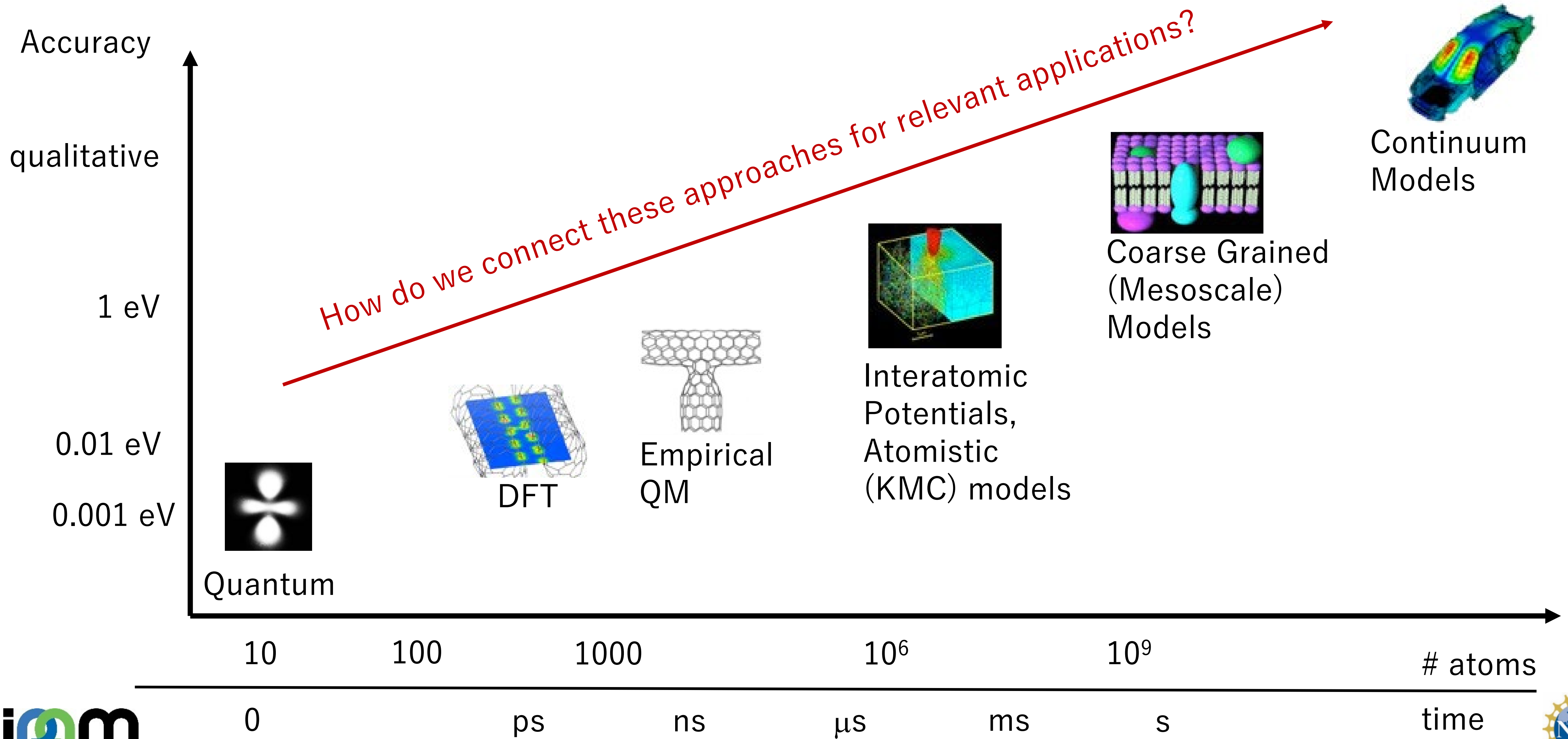
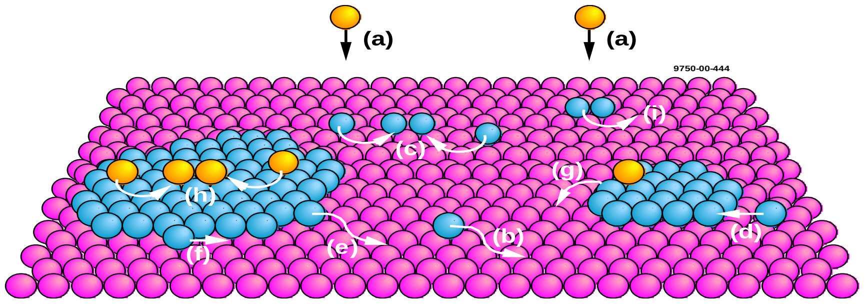
# Multiscale Modeling in Materials Science:



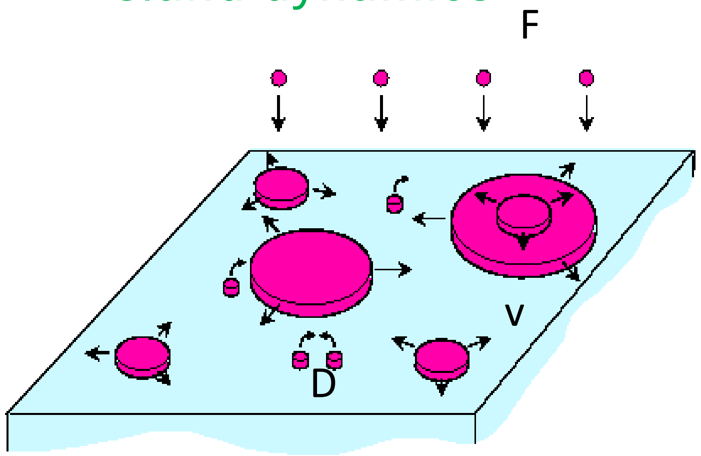
# Modeling Epitaxial Growth

## Atomistic picture
(i.e., kinetic Monte Carlo)




- Identify all possible processes for all atoms.
- Compute a rate for each of these processes.
    - For example with DFT accuracy
- Run a kinetic Monte Carlo simulation.

## Island dynamics




- Treat each atomic layer as continuum in the plane
- Evolve island boundaries with level set method:

$$\frac{\partial \varphi_i}{\partial t} + v_i |\nabla \varphi_i| = 0$$

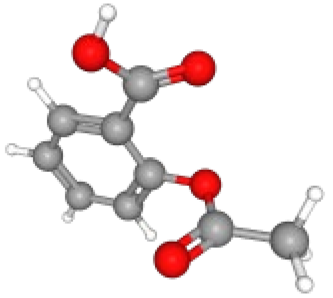
- Treat adatoms as a mean-field quantity and solve diffusion equation:

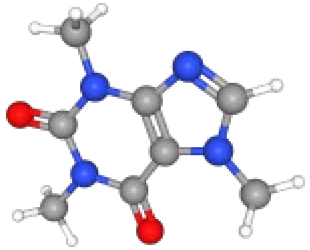
$$\frac{\partial \rho}{\partial t} = F + \nabla \cdot \mathrm{D}(\nabla \rho) - 2\frac{dN}{dt}$$

- Boundary condition: $\nabla \rho \cdot \mathbf{n} = \frac{D'}{D-D'}(\rho_{eq} - \rho)$

# Chemical Compound Space for Materials and Drug Design

- Chemical Compound Space is Huge
- It is argued that up to $10^{60}$ small molecules exist (molecules with no more than 20 heavy atoms)
- For rational design of materials and molecules (drug design), we need
  - Efficient sampling methods
  - Efficient methods to calculate properties of these molecules with quantum mechanical accuracy
- DFT calculations can take around 1 CPU hour per molecule
- Navigating Chemical Compound Space was the topic of the 2011 long program at IPAM

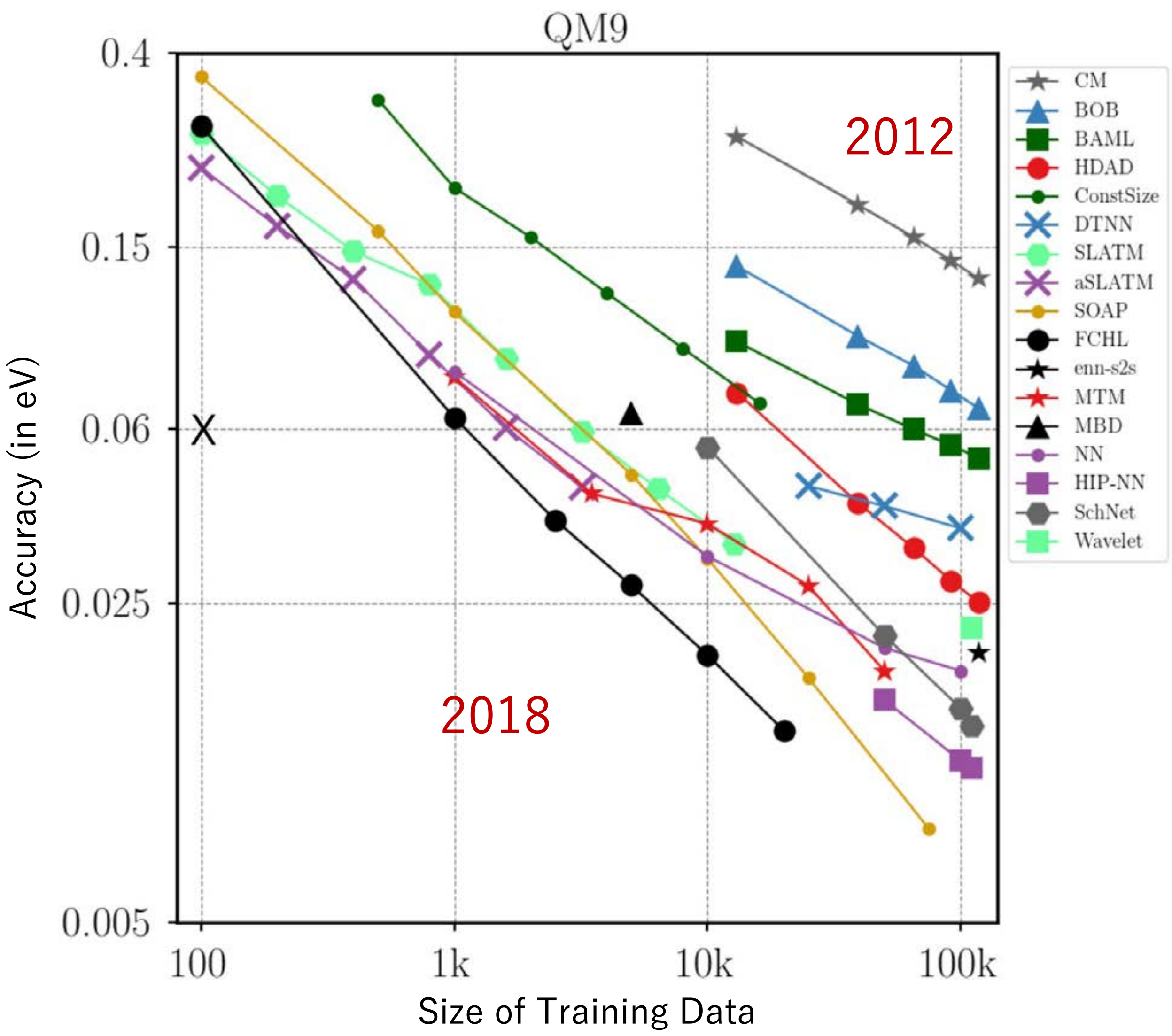




# Machine Learning for Materials Design

- The QM9 data set contains 134K small molecules
- Calculating properties with ML take about 1 ms (or less)
- This is a speedup of more than 6 order of magnitude
- Similar results exist for calculating forces, or other properties.
- The next step is to use ML for wave functions, or the XC functional in DFT:
- 2022 IPAM program:

"Advancing Quantum Mechanics with Mathematics and Statistics"



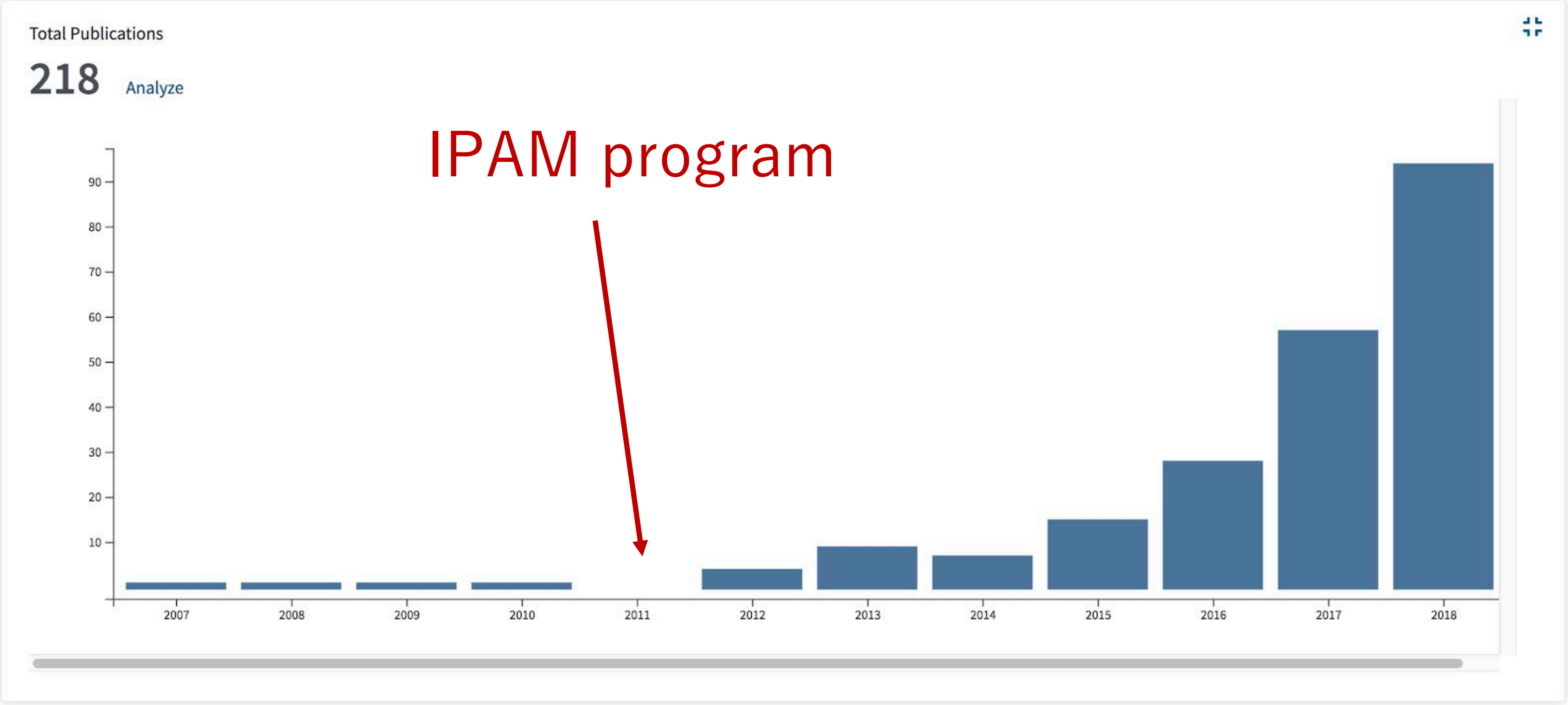

v. Lilienfeld, K. Mueller, A. Tkatchenko, 2019

# Impact of Machine Learning for Materials at IPAM on the Materials Community

Web of Science Data for papers on

Machine Learning and DFT

(Nov. 2018)




Until 2010, Machine Learning was essentially unheard of at the annual meetings of the Professional Societies (MRS, APS, SIAM).

Since 2011, many sessions and entire symposia are now dominated by the connection of Machine Learning and Materials Sciences with organizers and speakers from IPAM programs.

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# Traffic Flow Management:
# Mathematical Modeling of the Effect of Autonomous Vehicles on Traffic Flow

- Nagoya traffic experiment (2008) shows that cars on a ring road will lead to “phantom traffic jams”.
- This can be modeled by a set of coupled ODEs:
  - ODE for car driven by human

$$\ddot{y}_j = \alpha_1 \left( y_{J+1} - y_j \right) - \alpha_2 \dot{y}_j + \alpha_3 \dot{y}_{j+1}$$

- Introduce autonomous vehicle (AV) to stabilize flow (at t=120s)
  - ODE for AV

$$\ddot{y}_j = \beta_1 \left( y_{J+1} - y_j \right) - \beta_2 \dot{y}_j + \beta_3 \dot{y}_{j+1}$$

- Choice of right parameters avoids traffic jams
- This was verified in experiment conducted by a collaboration that formed at IPAM.

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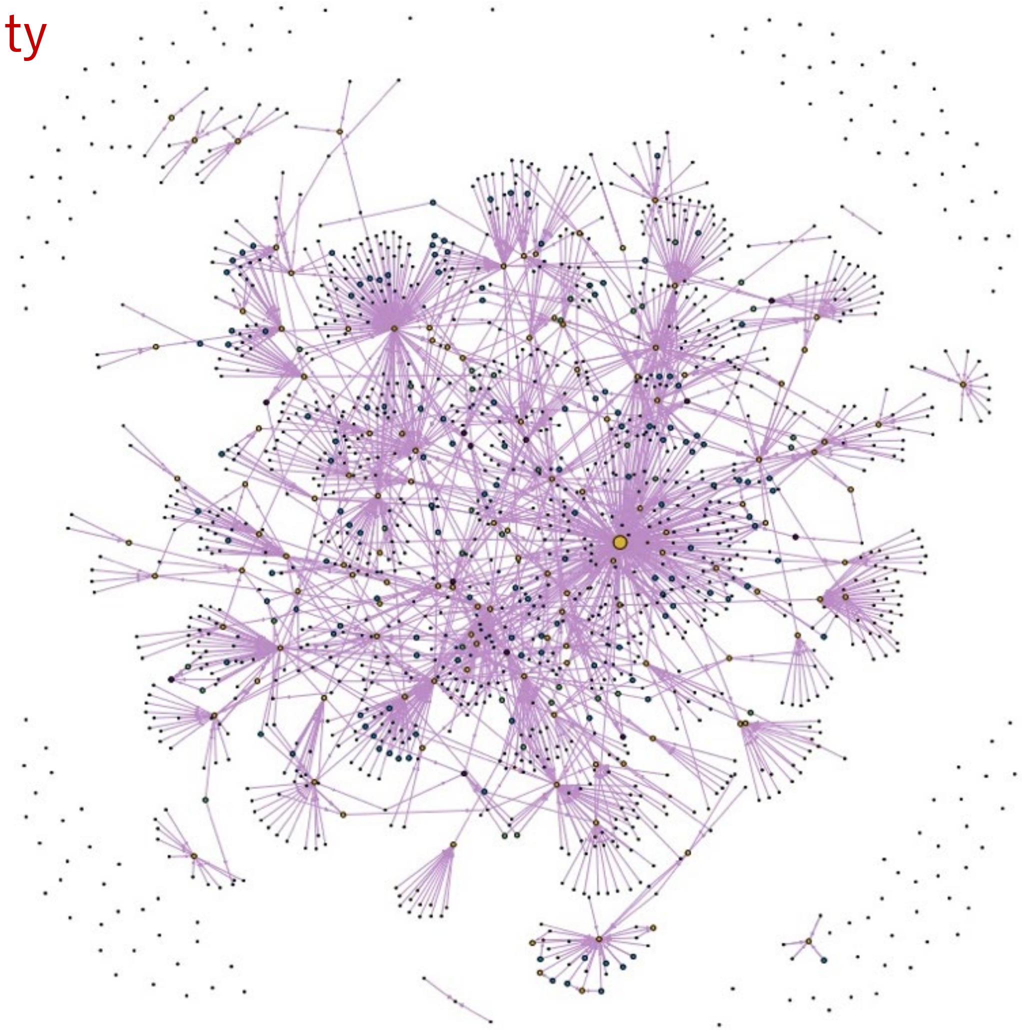
# Culture Analytics

- Connect researchers from the Humanities, Social Sciences, Mathematics, and Data Sciences
- The data driven analysis of culture is now a reality

Example

- Network analysis to understand the spread of news
- ··· and fake news ···
- Can we use network analysis for computational fact-checking?



# Conclusions

- IPAM fosters the interaction of mathematics with a broad range of science and technology.
- IPAM builds new interdisciplinary research communities.
- IPAM programs tackle a range of topics of high scientific and societal value.

- For more information visit

www.ipam.ucla.edu

- IPAM is funded by the National Science Foundation.