



## WPI-NanoLSI Special Computational Workshop on Digital Solutions

**Date:** Wednesday February 8<sup>th</sup> 2023

**Time:** 9:30am – 4:30pm

**Location:** Seminar Hall 4<sup>th</sup> Floor NanoLSI Building

**Event:** In person / online

**Registration:** <https://forms.gle/tUNwZ5tVT1ccGPFRA>

**Contact:** nanolsi-office@adm.kanazawa-u.ac.jp



### Workshop Program

#### February 8<sup>th</sup> - Wednesday 9:30am – 12:30pm

Adam Foster: Workshop overview, digital workflows, open data, advanced analysis

David Gao: Introduction to digital data and machine learning tools

Filippo Canova: Highly optimized data management tools

#### February 8<sup>th</sup> - Wednesday 1:30pm – 4:30 pm

Adam Foster: Advanced analysis of AFM images

Niko Oinonen: Disease recognition from AFM adhesion measurements

Damien Hall: Computational AFM tools for biophysical measurements of dynamic surfaces

# Access to the NanoLSI building at Kakuma Campus

For information how to access Kanazawa university (Kakuma campus) from Kanazawa station please check the website <https://nanolsi.kanazawa-u.ac.jp/en/access/>

The Nano Life Science Institute is the building framed in red in the map below.  
The workshop venue is located on the 4th floor.



## Helpful Information

TAXI companies

Ishikawa Kintetsu Taxi phone 076-221-3265

Fuji Taxi phone 076-237-1020

Kamome Taxi phone 076-231-1128

## NanoLSI Administration

Office hours: 8:30am-5pm

Contact: [nanolsi-office@adm.kanazawa-u.ac.jp](mailto:nanolsi-office@adm.kanazawa-u.ac.jp)



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### Topics covered

- Introduction to digital data
- Data management tools
- Integration of machine learning techniques
- Case studies in AFM
- Open discussion of audience data issues and solutions.

### Digital data management, advanced analysis, and machine learning

Modern research efforts benefit from a rapidly increasing ability to generate a wealth of experimental and modelling data. Recent developments in data science, machine learning, and automation provide powerful opportunities to leverage this research data. To use scientific data as a resource beyond its initial publication, database infrastructures and digital workflows must be established to collect, store, organise and analyse the data, with records of how it was produced, and how it was processed or transformed afterwards. Good **management of research data** is of critical importance to knowledge-led discovery and innovation, and is increasingly embedded in the requirements of research journals and funding bodies. It is a prerequisite step in the application of data science and machine learning techniques in research. In this workshop, we highlight some examples of modern data management and discuss case studies involving the application of machine learning to scientific data. Emphasis is placed on applications to Scanning Probe Microscopy (SPM) in general and Atomic Force Microscopy (AFM) in particular.

### Instructors

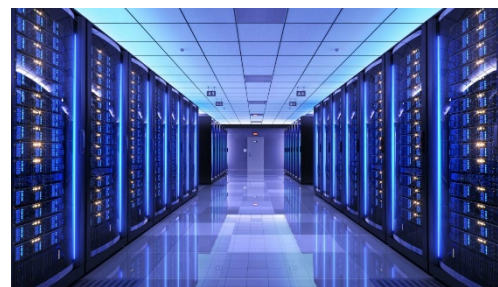
Adam Foster (Aalto University)

David Gao (NanoLayers Incorporated)

Filippo Canova (NanoLayers Incorporated)

Nikko Oinonen (Aalto University)

Damien Hall (Kanazawa University)



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## References

1. Data-driven materials science: status, challenges and perspectives - L. Himanen, A. Geurts, A. S. Foster and P. Rinke, *Adv. Sci.* (2019) 1900808
2. DDescribe: Library of Descriptors for Machine Learning in Materials Science - Lauri Himanen, Marc O Jäger, Eiaki V Morooka, Filippo Federici Canova, Yashasvi S Ranawat, David Z Gao, Patrick Rinke and Adam S Foster, *Comp. Phys. Comm.* **247** (2020) 106949
3. Machine Learning at the (Sub)Atomic Scale: Next Generation Scanning Probe Microscopy - Gordon, Oliver M., and Philip J. Moriarty, *Machine Learning: Science and Technology* **1** (2020) 023001
4. AtomAI Framework for Deep Learning Analysis of Image and Spectroscopy Data in Electron and Scanning Probe Microscopy, Ziatdinov, Maxim, Ayana Ghosh, Chun Yin (Tommy) Wong, and Sergei V. Kalinin, *Nature Machine Intelligence* **4** (2022) 1101
5. Precise atom manipulation through deep reinforcement learning - I-Ju Chen, Markus Aapro, Abraham Kipnis, Alexander Ilin, Peter Liljeroth and Adam S. Foster, *Nat. Commun.* **13** (2022) 7499
6. Generalised deep-learning workflow for the prediction of hydration layers over surfaces - Yashasvi S. Ranawat, Ygor M. Jaques and Adam S. Foster, *J. Mol. Liquids* **367** (2022) 120571
7. Electrostatic Discovery Atomic Force Microscopy - Niko Oinonen, Chen Xu, Benjamin Alldritt, Prokop Hapala, Filippo Federici
8. Canova, Fedor Urtev, Ondřej Krejčí, Juho Kannala, Peter Liljeroth and Adam S. Foster, *ACS Nano* **16** (2022) 89
9. Practical considerations for feature assignment in high-speed AFM of live cell membranes - Damien Hall and Adam Foster. *Biophysics and Physicobiology*. **19** e190016, 1-21

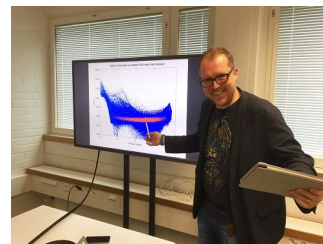
## Instructors

**Instructor:** Adam Foster

**Email:** [adam.foster@aalto.fi](mailto:adam.foster@aalto.fi)

**Position:** Professor

**Institution:** Department of Applied Physics, Aalto University



**Biography:** Adam Foster is an overseas PI at the WPI Nano Life Science Institute (WPI-NanoLSI) and leader of the Surface and Interfaces at the Nanoscale (SIN) group at Aalto University in Finland. He obtained his PhD in University College London in 2000, before moving to Helsinki University of Technology in the same year. He obtained a senior academy fellowship in 2004, followed by a professorship in Tampere University of Technology in 2009. He joined Aalto University in 2012 and has held a visiting position in Kanazawa since 2015. Foster is a computational physicist applying his expertise in simulations to a wide range of areas including molecular self-assembly, solid-liquid interfaces and quantum materials, often in conjunction with scanning probe microscopy research. The SIN group generally work at the atomistic level, looking from both the quantum and classical viewpoints and working closely with experimentalists. More recently, they have focused on developing and applying data intensive and machine learning approaches in materials research.

**Instructor:** David Gao

**Email:** [david@nanolayers.com](mailto:david@nanolayers.com)

**Position:** Director

**Institution:** Nanolayers Research Computing Ltd.



**Biography:** Director and founder of Nanolayers Research Computing LTD (UK) and Nanolayers OU (ES), David has a B.Sc. in chemistry from UC Berkeley, a Ph.D. in physics from University College London, and is currently an Assoc. Prof. in the Materials Theory group at the Norwegian Institute of Science and Technology. David also holds an Executive M.B.A. from the Quantic School of Business & Technology and has industrial experience working for Chevron Corp. as a chemical engineer and chemist and is acutely aware of the research and development needs of similar commercial entities. His career there was focused on bridging the gap between chemistry and engineering and now has turned his attention to bridging a similar gap between molecular modelling, machine learning, and industrial research and development. David has been a long-time member of the European Materials Modelling Council (EMMC) as a stakeholder, an active participant in CEN consortium workshop agreements, and contributed to developing EU standards for metadata, data management, and digital research. He has authored 32 papers in international, high impact, refereed journals and has ongoing industrial research projects funded by companies including Chevron, Applied Materials, and Nantero, and drives the research digitalization efforts of several international research projects including the Horizon Europe Mast3rboost and the joint iUK/NSERC ALANN projects.

**Instructor:** Filippo Federici Canova  
**Email:** [filippo.federici@aalto.fi](mailto:filippo.federici@aalto.fi)  
**Position:** Scientific Director at NanoLayers  
**Institution:** NanoLayers Incorporated



**Biography:** Filippo is the co-founder and scientific director for Nanolayers Research Computing, where he leads the business' development of scientific data management solutions, the design of lubricants, and image recognition and machine learning methods for materials science and image recognition. Filippo holds a M.Sc. in experimental physics and a doctorate in Computational Physics from the Tampere University of Technology in Finland. His main research focus was simulation of nc-AFM contrast formation and energy dissipation mechanisms. During his post doc he investigated the frictional dynamics of nanoconfined ionic liquids (AIMR, Tohoku University) and prediction of frictional properties with machine-learning methods (ASCI, Aalto University). With extensive knowledge of advanced experimental and computational systems, Filippo has been instrumental in the development of some of Nanolayers most significant solutions, including the Nature Conservancy wildlife image recognition system and Cassandra Scientific databasing system.

**Instructor:** Niko Oinonen  
**Email:** [niko.oinonen@aalto.fi](mailto:niko.oinonen@aalto.fi)  
**Position:** PhD Student D3  
**Institution:** Department of Applied Physics, Aalto University



**Biography:** Niko Oinonen is a doctoral student the Surfaces and interfaces at the Nanoscale group at Aalto University, Finland, where he also graduated with the degree of M.Sc. in 2019. The topic of his doctoral research is applying machine learning methods to the interpretation of high-resolution atomic force microscopy images. His work focuses on the design and development of neural networks for this task as well as the development of software for atomic force microscopy simulations.

**Instructor:** Damien Hall  
**Email:** [hall.damien@staff.kanazawa-u.ac.jp](mailto:hall.damien@staff.kanazawa-u.ac.jp)  
**Position:** Assistant Professor  
**Institution:** WPI - Nano Life Science Institute, Kanazawa University, Japan.



**Biography:** Damien Hall received an undergraduate degree in chemistry (1994) and a PhD in physical biochemistry in 2000 from the University of Queensland. In January of 2021 he was appointed as a Specially Appointed Assistant Professor at the WPI Nano Life Science Institute located at Kanazawa University, Japan. Prior to this he held a series of personal five-year research fellowships at the National Institutes of Health, Osaka University, The Australian National University, University of Tsukuba and the University of Cambridge. In addition to his direct research activities, Damien has been the Chief Editor of the International Union for Pure and Applied Biophysics (IUPAB) journal, 'Biophysical Reviews' since 2019.