



Topical workshop on:

Atomic-scale simulations in neutron scattering

20-21 January 2021

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Welcome!

- Practical information
- Background for this workshop



Welcome to all attendants

Here is the program:

Today	Tomorrow
Session 1: Biology <i>Chair: Wojciech Potrzebowski, ESS</i>	Session 3: Soft matter incl. biology <i>Chair: Andrew McCluskey, ESS</i>
Break	Break
Session 2: Nanomaterials and liquids <i>Chair: Peter Fouquet, ILL</i>	Session 4: Hard condensed matter <i>Chair: Gregory Tucker, ESS</i>

Organizers & hosts:

- Danielle Adonis, ESS
- Miguel Gonzalez, ILL
- Thomas H. Rod, ESS

20 presentations
– primarily by junior scientists
(2 withdrawals)

219 registrations



Practical instructions

The schedule is tight!

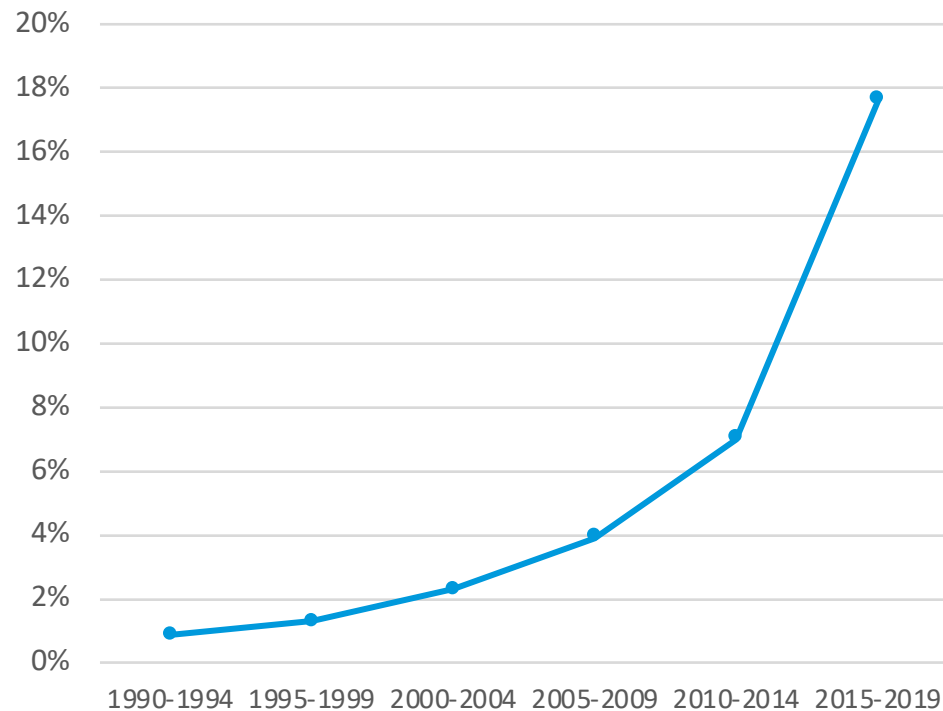
- There is only 5 minutes between presentations
- We only allow for typed questions:
 - Type your question using the **Q/A** feature in zoom (usually at the bottom of zoom)
 - Chair person will ask the speaker one or more of the questions raised **if** time allows for it
 - Speaker (or others) will have an opportunity to type answers to remaining questions after the Q/A session
- **Please**, use the chat function only for making the host(s) aware of **technical issues**
- If you have **technical issues**, try to disconnect and reconnect

Background for this workshop

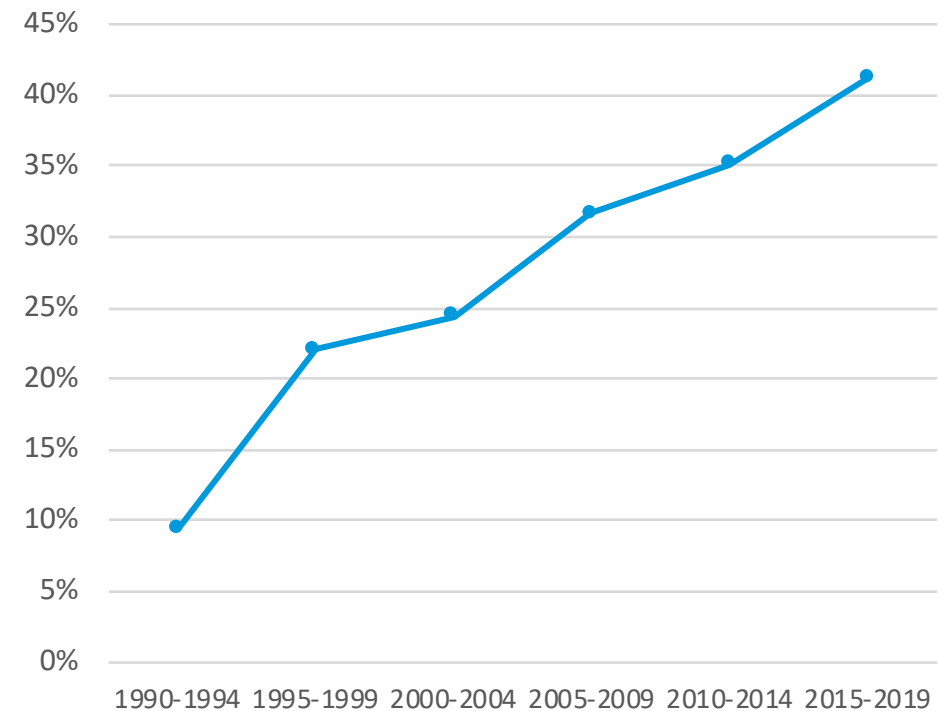


Increasing use of and request for supporting simulations

Fraction of publications with term
"neutron scattering"
that also contains
"DFT"



Fraction of publications with term
"QENS"
that also contains
"molecular dynamics simulations"



Based on searches using Google Scholar

Moore's Law



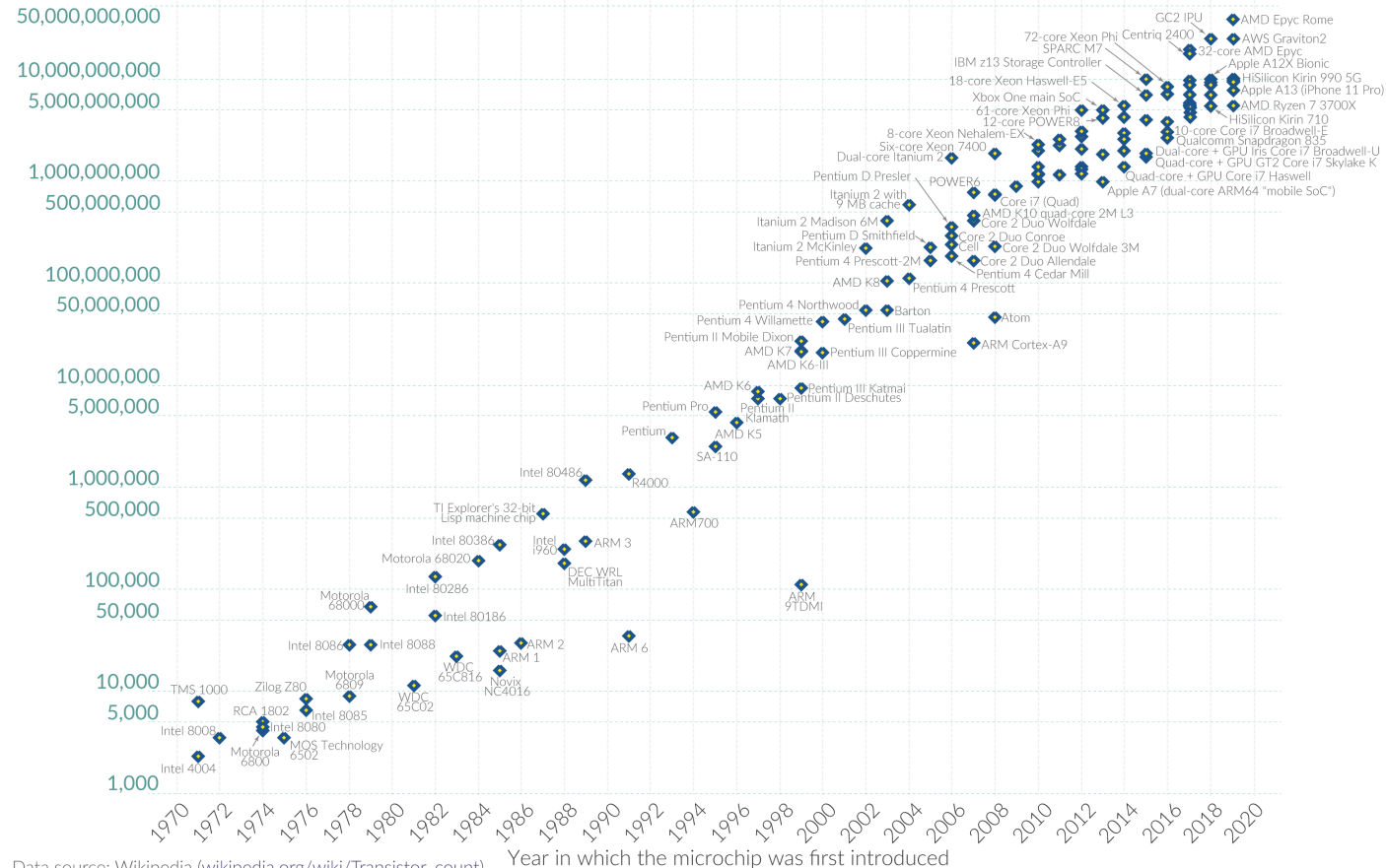
But more efficient software and algorithms are equally important

Moore's Law: The number of transistors on microchips doubles every two years



Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important for other aspects of technological progress in computing – such as processing speed or the price of computers.

Transistor count



Associated activities

MDANSE **Semi-regular summer school. Topics:
MD, lattice, spin dynamics
simulations and instrument
simulations**

LENS A new sub-group to Working Group 4
Computing and Data focuses on
atomic-scale simulations.

Speaker: Sanghamitra
Mukhopadhyay, ISIS

PaNOSC Atomic-scale simulations coupled
WP5 with instrument simulations

MDANSE 2018



Credit: Emmanuel Farhi



Send us a note

Please let us know if there is something you would like us to comment on or discuss in the concluding session.

Send an e-mail to Danielle: danielle.adonis@ess.eu

Happy workshop!



Danielle, Miguel, Thomas