CECAM:

European center for simulation and modeling

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CECAM

A grassroot network of excellence in simulation & modeling

Gathers all relevant actors
- scientific institutions & researchers

Working on
- methods, algorithms & HPC
- leading edge applications & training

>50 years of activities

Leading the communities in Europe & beyond

17 Nodes: 10 European countries
           Funded locally

- CECAM HQ at EPFL - Central hub of the network
  - Funding from 25 partner institutions from Europe & China
  - Largest number of activities
  - General strategy & steering
  - Global visibility

cecam 2019

Community-driven:

Core activities:

- workshops & schools
- Online events
- Focus groups & activities in topics of emerging interest

Events:

- 50-70 Events/year in the network
  - Funded locally
- ~18 Events/year @ HQ
  - Funded from 25 partner institutions
- ~700 Participants to events @HQ/year
- 2000 Participants to events in the network/year

Scientific areas

- Electronic Structure Calculations
- Classical and Quantum Monte Carlo
- Molecular Dynamics
- First-principles Dynamics
- Coarse-grained Simulation Methods
- Multi-scale Modelling
- Quantum Computing
- Computational Fluid Dynamics
- System Biology Network Modelling
- Data Driven Science
- Scientific Machine Learning
- …

The importance of being H.P.C. Earnest - June 18 2020
3,691 views • Streamed live on Jun 18, 2020

Activities

Workshops ⟶ Frontiers of research

- address open challenges
- medium size to promote ideas exchange
- 3 days
- enforce discussions

Schools ⟶ Teaching at graduate postdoctoral level

Number of events

Legend:
- Schools nodes
- Workshops nodes
- Schools HQ
- Workshops HQ
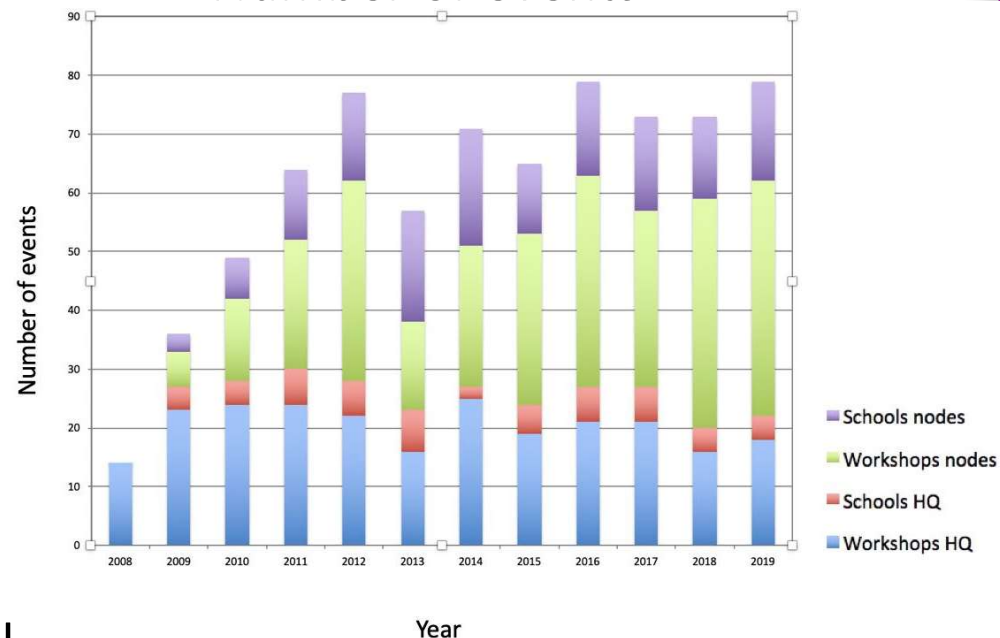
Alternative formats

- Visitor program
- Conferences
- Recurrent events
- Focus meetings
- Online & hybrid meetings
- Software development workshops

The Journal of Chemical Physics   ARTICLE   scitation.org/journal/jcp

The CECAM electronic structure library and the modular software development paradigm 🄵 🅂🄲🄸

🌐 View Online   ⬆ Export Citation   🔴 CrossMark

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LearnHPC: a mash-up of other projects
...where the credit is really due
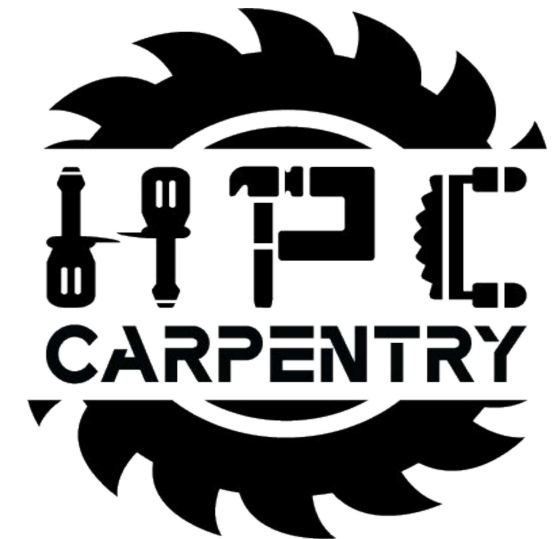
With resources provided by:

- "Real" systems come with strict security requirements and plenty of bureaucracy for the instructor/learner
  - These are all intimidating barriers to the learning experience (particularly for beginners)

- If I run a German HPC centre, would I seriously consider running training courses for arbitrary European institutions and companies?

- Cloud-based clusters are unencumbered
  - Bring them up, take them down, throw them away
  - Can agree in advance that nothing there is considered secure

- Cloud-based clusters don't have to be toys
  - Successfully tested with infiniband fabric on Azure and EFA fabric on AWS, also GPUs
  - Can be configured to run with scalable file systems (e.g., Lustre)

- Cloud-based clusters are reproducible, and reproducible means scalable (e.g. event specific)