Introducing High Performance Computing to Chemists in Africa with the DevCloud

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Outline

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- Virtual Conference on Chemistry and its Applications
- The Carpentries and HPC Carpentry
- Workshop Outline
- Reflections

Virtual Conference on Chemistry and its Applications

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- Annual online conference organized by the Computational Chemistry Group, University of Mauritius since 2013
- Poster and/or video presentations in an online forum
- Daily focus on presentations within a theme for discussion
- A few interactive sessions and invited live presentations
- Post-conference proceedings

Virtual Conference on Chemistry and its Applications

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- Participation in 2021
 - 400 participants
  - 197 presented abstracts

Virtual Conference on Chemistry and its Applications

- Ramasami, Ponnadurai. Volume 1-3, Chemical Sciences for the New Decade. Vol 1-3, De Gruyter, 2022.
    - Volume 1: Organic and Natural Product Synthesis
    - Volume 2: Biochemical and Environmental Applications
    - Volume 3: Computational, Education, and Materials Science Aspects

Virtual Conference on Chemistry and its Applications

Word cloud from 14 abstracts in Volume 3: Computational, Education, and Materials Science Aspects

Virtual Conference on Chemistry and its Applications
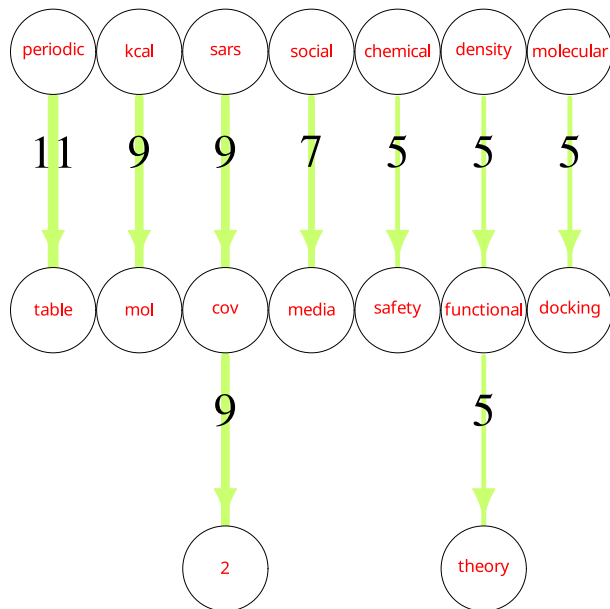
Most common bigrams from 14 abstracts in Volume 3: Computational, Education, and Materials Science Aspects

The Carpentries and HPC Carpentry

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- Bridge early career computational skills gap
- First Software Carpentry Workshop in 1998 by Greg Wilson and Brent Gorda
- Three established tracks:
  - Software Carpentry
  - Data Carpentry
  - Library Carpentry
- Track in incubation:
  - HPC Carpentry

The Carpentries and HPC Carpentry

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- Open access community developed materials
- In-person, online, and hybrid workshops
- Hands-on, low-stress, learn-by-doing approach
- A good way to develop teaching experience
- Helpful for working professionals
- Covers coding and data science skills
- Voluntary instructors and helpers

Online VCCA HPC Carpentry Workshop

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- Post-conference workshop
- Material discussed
    - Linux Shell Introduction
    - Introduction to Git, GitHub, and GitLab
    - Job queue submission
    - Introduction to molecular dynamics using SYCL
    - Introduction to GROMACS
    - Collaborative Software Development with GROMACS by Mark Abraham

Online VCCA HPC Carpentry Workshop

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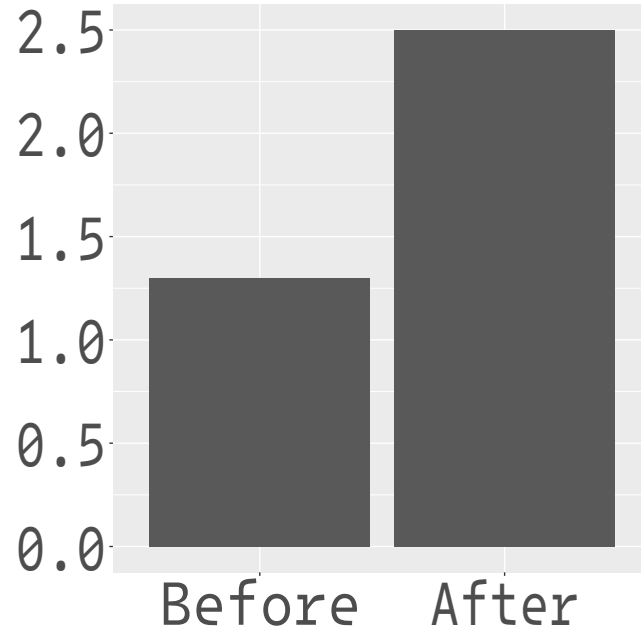
Participant feedback on average linux knowledge on a scale of 0 (none) to 5 (expert)

Online VCCA HPC Carpentry Workshop

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- Using the Intel® DevCloud
    - HPC environment
    - CPUs, GPUs and FPGAs available
    - Helpful for teaching and to measure node level performance
    - Useful to demonstrate installation and setup of software
    - SYCL is understandable to chemists

Online VCCA HPC Carpentry Workshop

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- Lessons learned
  - DevCloud environment is helpful
  - Commercial cloud costs would not be prohibitive if tools were available
  - Most challenging part is using the commandline, but helpful for automation
- 2 new Certified Carpentries Instructors
  - Rashid Hussain
  - Samuel Tetteh

Reflections

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- Virtual workshops can be a good way to build communities
- Domain-specific computational workshops can bring people with specific interests together
- Many tools are used in computational chemistry, though some shared infrastructure
- Growing the computational chemistry Carpentries community may be a feasible way for lesson production and maintenance
- Teaching chemists HPC will lead to its increased efficient utiliziation

Acknowledgements

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- BioExcel
- University of Mauritius
- Workshop participants
- Kavita Aroor

Bibliography

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- VCCA2021 summary
- VCCA websites
- Workshop website
- Workshop participant repositories
- The Carpentries website