

Utilizing ToUCH Modules in a Carpentries Workshop

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HPC Carpentry.

- Collaboratively developed materials for introducing high performance computing to a broad audience
- Focus on linux skills and using a remote cluster
- Many users need some notion of heterogeneous programming

ToUCH Modules of Interest

- [A2 Task Mapping on Soft Heterogeneous System](#)
- [B1 Hybrid Algorithms](#)
- [D1 Introduction to CUDA Programming](#)

Current Teaching Plan

- Interactive hands on sessions where participants enter code and execute it
- [Workshop webpage](#)
- Aim is to demonstrate enough about heterogeneous computing that computational chemists can understand why it is useful for molecular dynamics
- Evaluate understanding by questionnaire

Further Work

- Port some of the modules to use [SYCL](#) in addition to OpenMP/CUDA
- Will likely use [hipSYCL](#)
- [Vulkan](#) would also be nice, but one step at a time
- Add a module on [stochastic gradient descent](#) for linear and/or logistic regression
- Make such a module use real world data sets
- Possibly also add [PageRank](#)

Datasets

- [Human Activity Recognition](#)
- [Network Intrusion Dataset](#)
- [Diabetes Dataset](#)
- [Boston House Price Dataset](#)
- [Burkardt Regression Datasets](#)
- [Malicious Smartphone Apps](#)
- [Fake News](#)
- [SherLock smartphone dataset](#)

