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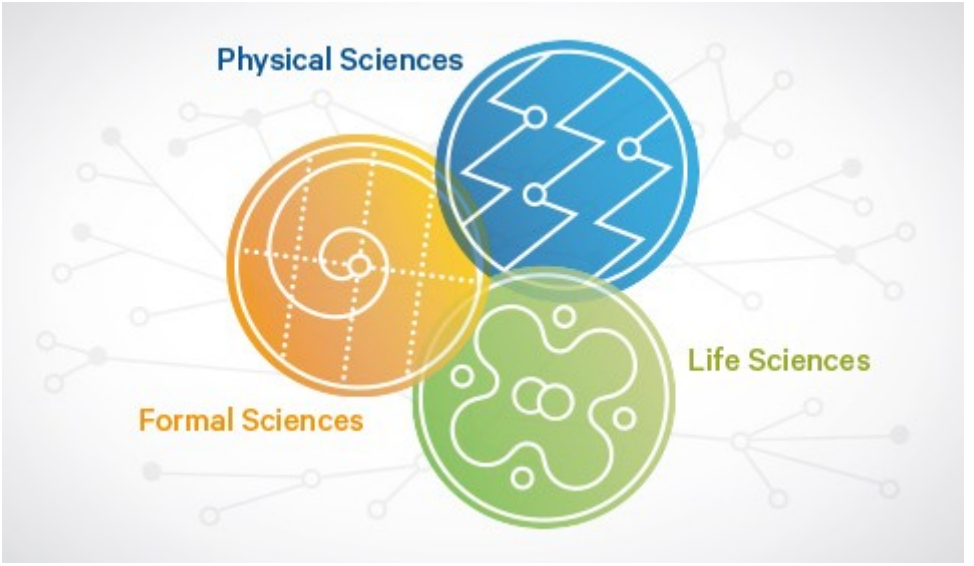
HPC @ IST



Alois Schlögl
IST Austria, Klosterneuburg

AHPC 2018
Linz, 20. Feb. 2018
Session: Beyond the usual suspects - get to know HPC in Austria

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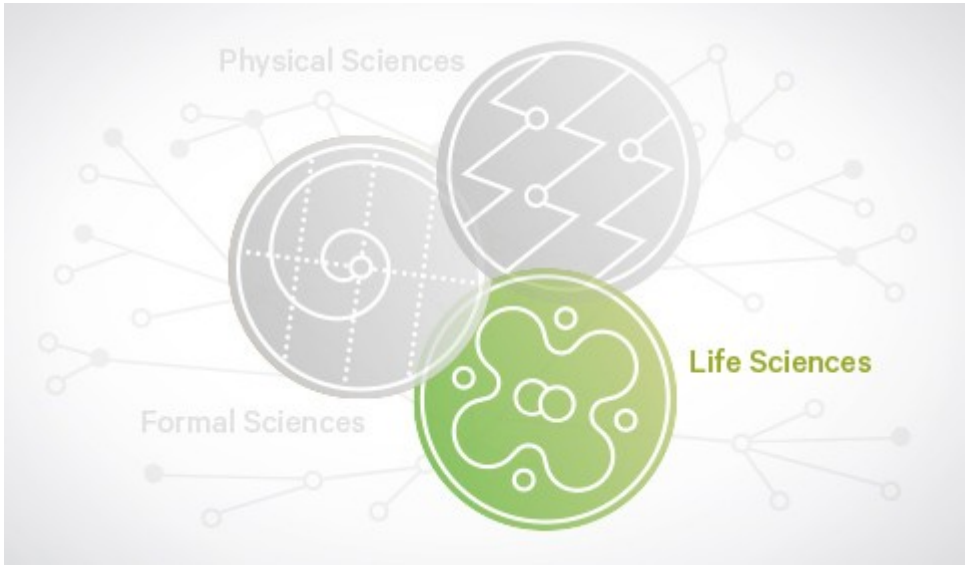

- 24 Groups in Life Sciences (Biology and Neuroscience)

~100 users (i.e. scientists) per year, from 15 different research group
Majority of users do work on non-IT topics like biology, neuroscience, physics, etc.

Main characteristics of the system(s) and services

- HPC is run by of the „Scientific Computing“ which is one out of eight „Core Facilities “(Scientific Service Units) at IST
  - Implications: charges, user group meeting, …
- Heterogeneous Hardware (Intel, AMD, GPU, Infiniband,)
- OS: common OS on all machines
- Scheduling system: Slurm v16
- Software (OS level - module system - user space)

  Packages from Debian Stable repository

  176 packages (363 released versions) in the module system

IST Cluster: Hardware (2018-01)

- 6 GPU machines with 28 GPU's
  - 5 x 4 x GTX1080Ti
  - 1 x 8 x GP100
  - 256 GB RAM
- BigMem machines
  - 2 x 1 TB
  - 5 x 0.5 TB
- several user machines
  - Common design:
  - connected with QDR Infiniband and Ethernet

- 35 x Bjoern [2013]
  - 16C/32T (2 x E5-2670)
  - 64 GByte RAM
  - QDR (40 GB/s)
- 16 x Leo [2015]
  - 16C/32T (2 x E5-2630 v3)
  - 128 GByte RAM
  - FDR (56 GB/s)
- 4 x Bea [2016]
  - 12 Core / 24 threads (2 x E5-2680 v3)
  - 2 x 256 + 2 x 512 GByte RAM
  - FDR (56 GB/s)
- 28 x Epsilon [2016]
  - 20 Core / 40 threads (2 x E5-2630 v4)
  - 128 GByte RAM
  - EDR (100 GB/s Infiniband)

Total: ~100 nodes, ~200 CPU's, ~3400 CPU cores
Shared among 100 users and 10 research groups

Nobel Prize 2017 for chemistry refers to work performed on HPC Cluster at IST

KUNGL. VETENSKAPS-AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

4 OCTOBER 2017

Scientific Background on the Nobel Prize in Chemistry 2017

THE DEVELOPMENT OF CRYO-ELECTRON MICROSCOPY

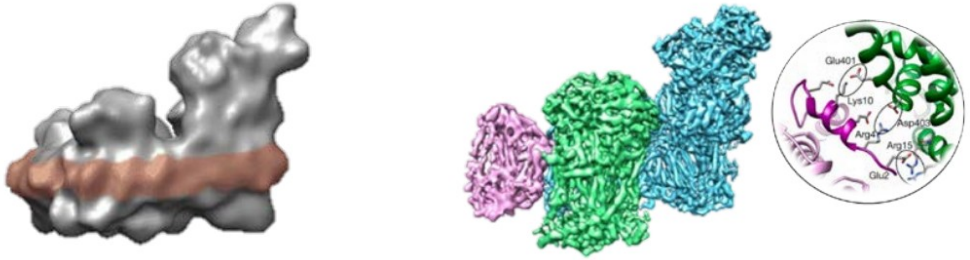

Fig. 1. Models of the electron-transport chain components in a mitochondrial supercomplex $I_1III_2IV_1$, determined in 2011 (left, from (3), resolution ~2 nm) and 2016 (right, from (4), resolution ~6 Å), respectively. On the left, the coloured shape indicates the position of amphipols used for solubilization. On the right, complexes I, III and IV are shown in blue, green and pink, respectively. The encircled inset shows a model of a putative CIII-CIV interface.

4. Letts, J. A., Fiedorczuk, K., and Sazanov, L. A. (2016) The architecture of respiratory supercomplexes. *Nature* **537**, 644-648

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The architecture of respiratory supercomplexes

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