High performance computing in Norway

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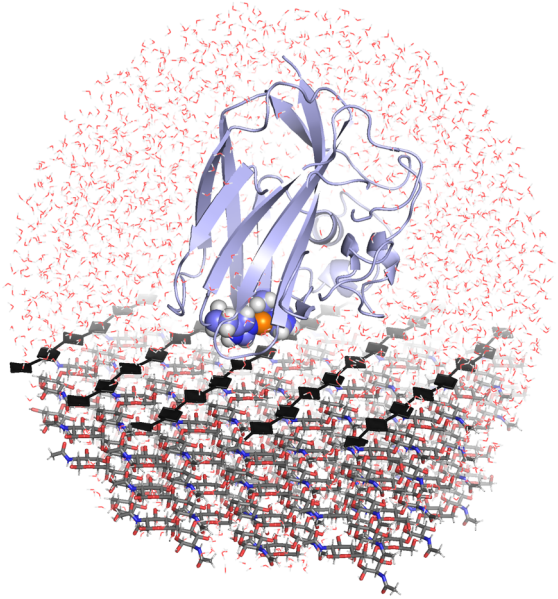
Overarching theme

"Develop understanding of protein structure, function and catalysis"

Enzymes – molecular machines

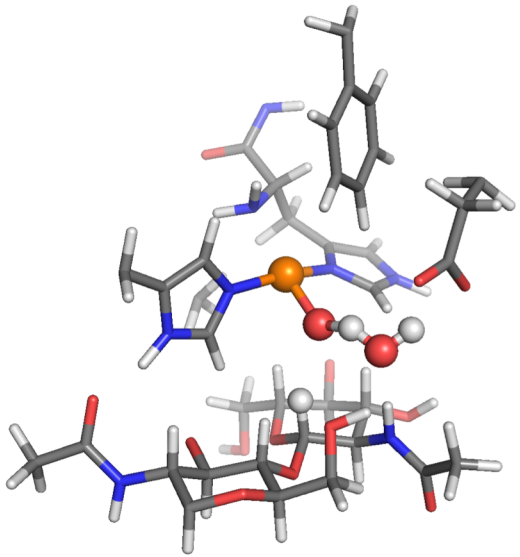
Ver. 1

Ver. 2



190 000 atoms!

Ver. 3



Increasing complexity when moving towards atomic scale

Supercomputers in biology

- ✓ Complicated research models may require **extensive computational resources.**
- ✓ Extensive computations may result in **huge amounts of raw data.**

National computational resources in Norway

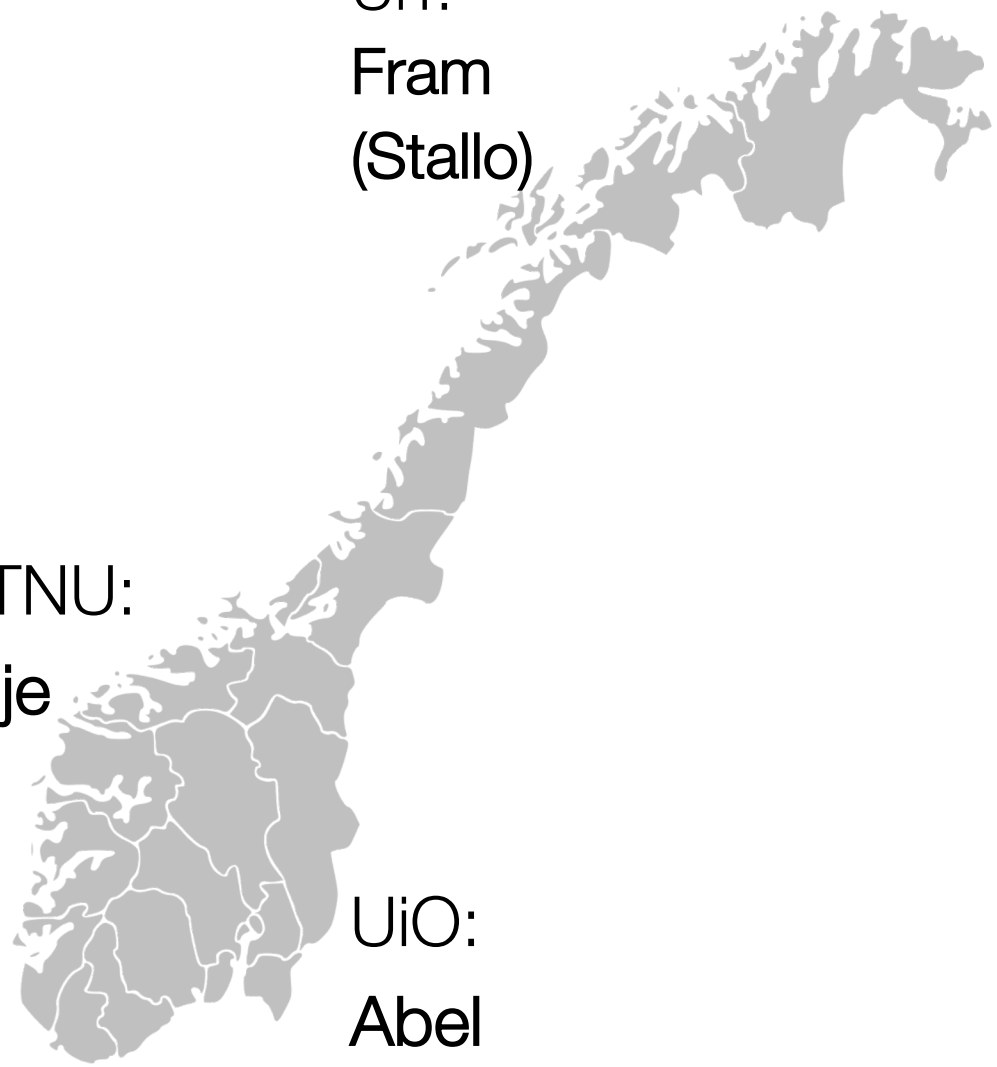
UNINETT Sigma2 AS is a non-commercial company that manages the national infrastructure for computational science in Norway.

- ✓ High performance computing (HPC)
- ✓ Data storage

Collaboration between RCN, UiO, UiB, UiT and NTNU.
Linked to European computational infrastructure.

High performance computing

UiT:
Fram
(Stallo)



NTNU:
Vilje

UiB:
Hexagon

UiO:
Abel

UNINETT
Sigma2

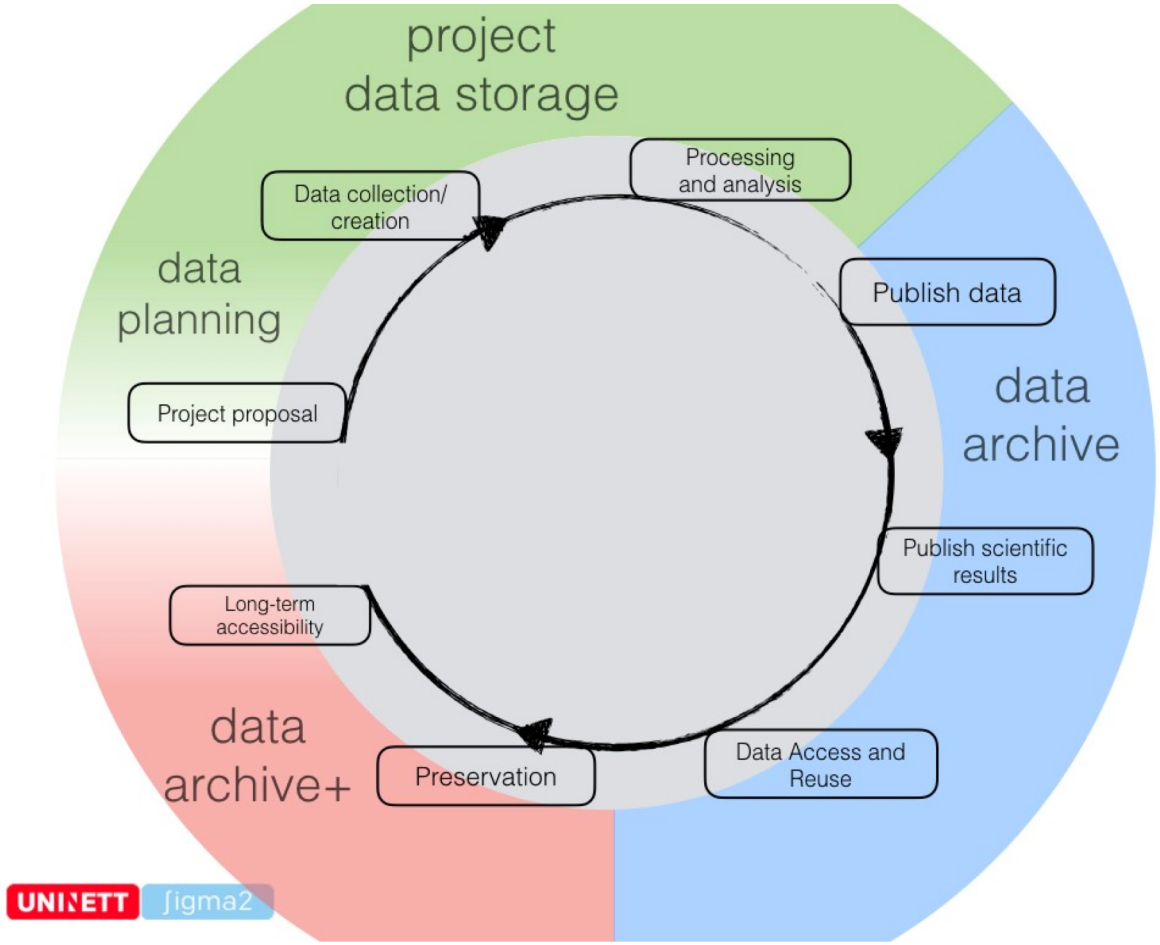
Data storage

National e-Infrastructure for Research Data (NIRD)

✓ Accommodates FAIR principles

Operating from 2017

~ 12 PB (12 000 terabyte)



The Abel computer cluster

- ✓ More than 10 000 cores (about 2500 desktop computers)
- ✓ More than 650 nodes (16 cores pr. node)
- ✓ About 64 GB RAM pr. node

Software parallelization (efficiency) varies …

Check out:
http://www.uio.no/english/services/it/research/hpc/abel/help/software/

Biology/bioinformatics software (Abel):

- 454apps
- alleleCount
- ABySS
- AmpliconNoise
- BEAGLE
- BEAST
- BLAST
- BLAST+
- bowtie2
- busco
- cdbfasta
- CD-HIT
- CEGMA
- Circleator
- Clearcut
- ClonalOrigin
- ClustalW
- denoiser
- dosageconverter
- FastTree
- flash
- fqgrep
- Freesurfer
- FSL
- GARLI
- GATK
- Geneid
- hisat2
- HMMER
- HUMAnN2
- IMPUTE2
- Infernal
- Interproscan
- Irreproducible Discovery Rate (IDR)
- LAMARC
- MAFFT
- MACS2
- MAGMA
- MaSuRCA
- MaxQuant
- mcmcphase
- metaxa2
- MGLTools
- Microbiome Utilities
- Migrate
- MIRA
- Molden
- mothur
- MrBayes
- MUSCLE
- NCL
- ngsplot
- Novoalign
- Orthograph
- PAML
- Pandaseq
- ParsInsert
- PAUP
- PennSNV
- PhyloBayes
- PhyML
- Picard-tools
- PLINK
- PLINKSEQ
- pplacer
- ProtTest
- QIIME
- RAxML
- rtax
- SHAPEIT
- SPAdes
- structure
- Stacks
- STAR
- Stringtie
- Subread
- swarm
- TransDecoder
- TREEFINDER
- Trinotate
- UCLUST
- UNPHASED
- USEARCH
- Velvet
- vsearch
- Wise2 (formerly GeneWise)
- VCFLIB

Other

Chemistry

- ADF
- AMBER
- AutoDock
- AutoDock Vina
- CP2K
- Gaussian
- LAMMPS
- MaterialsStudio
- NAMD
- QuantumEspresso
- VASP

Computational linguistics

- DyNet
- VISL CG-3

Geo Sciences

- ESyS-Particle
- FLEXPART
- OpenIFS
- WRF & WRF CHEM

Statistics

- R
- Stata

When do you need access to HPC

- ✓ When it feels like you laptop is melting
- ✓ When one program consumes ALL resources on your computer

CHECK THE ABEL SOFTWARE LIST!

How to get access?

- ✓ Visit: https://www.sigma2.no/content/apply-e-infrastructure-resources
- ✓ Write a short but consistent proposal.
- ✓ Estimate how long the project period should be.
- ✓ Do some test-calculations so you can estimate the number of cpu-hours to apply for (e.g. 12 hours on 10 cores = 120 cpu hours)
- ✓ Small projects (~50 000 cpu hours) may be granted on short notice for testing purposes.

Training/courses

- ✓ Training courses are given regularly at UiO. Check out the Sigma2 site!
- ✓ HPC staff are in general supportive!

Training events in 2018

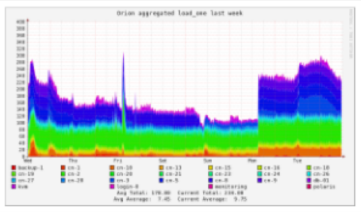
Python workshop, Tromsø, 4-6 September, 2018
PDC Summer School, KTH, Sweden, 13-24 August, 2018
CSC Summer School in HPC 2018, Espoo, Finland 26 June - 4 July 2018
Cross-national training workshop on HPC and applications, Iceland 13 - 15 June 2018
CodeRefinery Workshop, Oslo, 12 - 14 June 2018
Software Carpentry Workshop, UiO 7 - 8 June 2018
NORBIS course: HPC in Bioinformatics, UiO, 16 - 27 April 2018
HPC for research training course, Oslo, 21 - 23. March, 2018
CSC Spring School on Computational Chemistry, Finland, 13 - 16 March 2018
CodeRefinery Workshop, Trondheim, 27 February - 1 March 2018
Introduction to parallel programming, Trondheim, 06 - 15. February 2018
Research Bazaar 2018, Oslo, 7 - 9 February 2018
HPC course 2018.1, Bergen 25 - 26. January 2018

HPC at NMBU

CIGENE computational unit

Bioinformatics is an essential and integrated part of CIGENE operations. The rapidly reduced cost of sequencing has increased demand of computational storage and analysis, and CIGENE has during the last years invested in a local computer cluster to meet this demand.

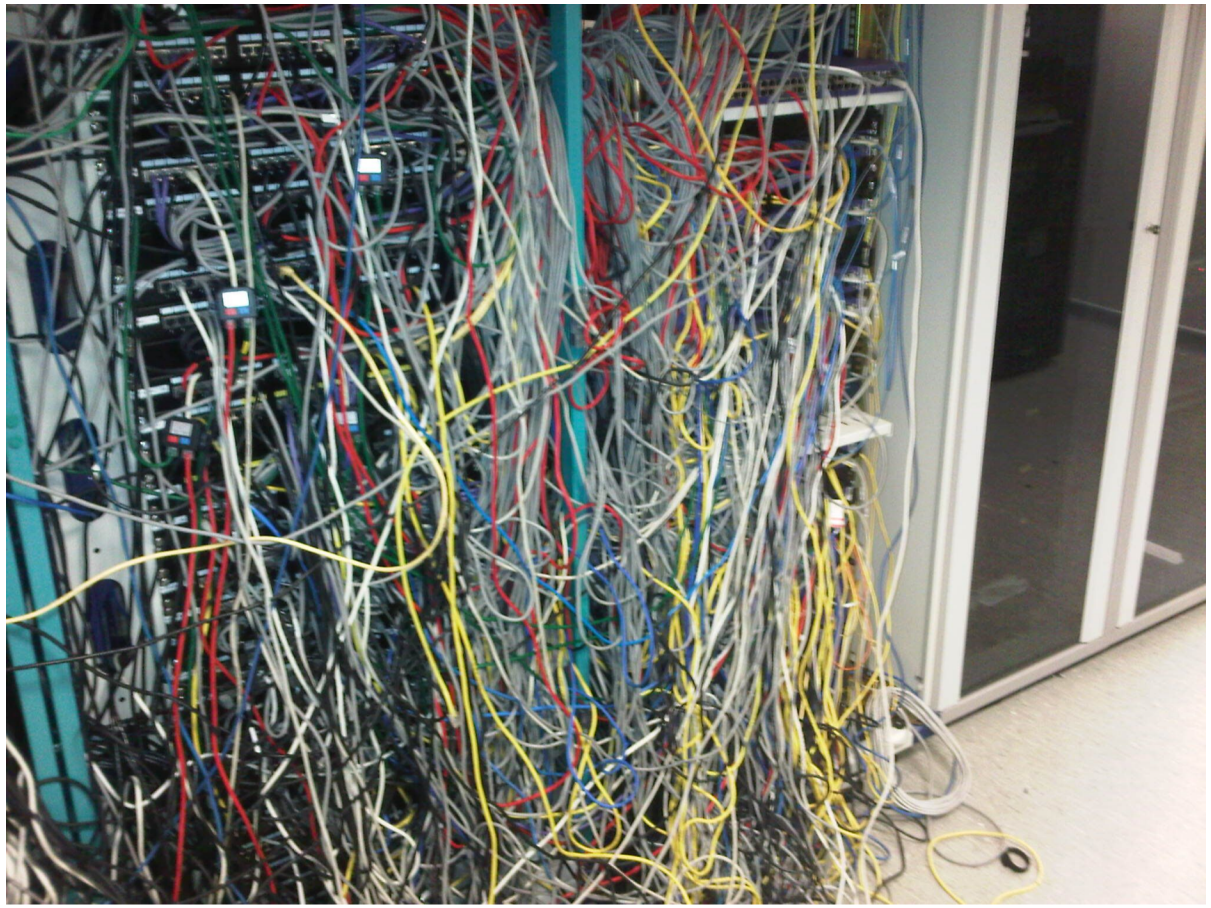
We currently maintain and administer a SLURM-based linux cluster called *Orion* with 580 CPUs, 4 TB RAM and 430 TB storage space. Access to Orion is provided to local users at the Norwegian University of Life Sciences (NMBU). CIGENE also hosts a Galaxy server to facilitate analysis of large-scale data in a friendly, reproducible environment; this is a collaboration with NMBU's node in ELIXIR Norway.



Who use HPC at NMBU?

- ✓ Share experiences?
- ✓ Expand HPC toolboxes?
- ✓ Arrange workshops?
- ✓ Preach HPC to potential users and expand the community?

My experience with Management of Research Data



during the project ….

At project termination: