

# Practical aspects of software for MD simulations

## workshop

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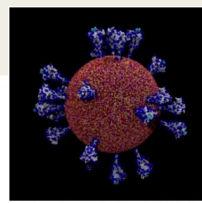
PhD student

Laboratory for molecular structural dynamics

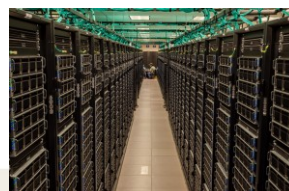
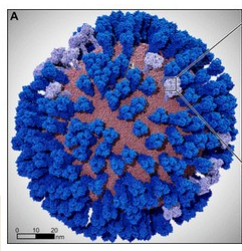


### GORDON BELL PRIZE

- Special prize for HPC Covid-19 research
- NAMD - winner in 2020
  - System size 305 million atoms
  - Summit and Frontera supercomputers
- Influenza virus simulations
  - 160 million atoms



The resulting model of SARS-CoV-2  
Image courtesy of Rommie Amaro and  
Lorenzo Casalino



## AŽMAN COMPUTATIONAL CENTRE

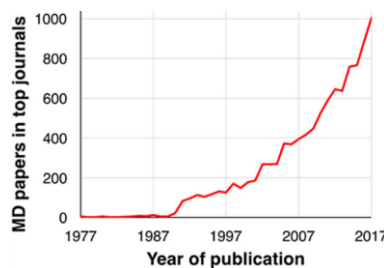
- Located inside the National chemistry institute
- Prof. dr. Andrej Ažman – pioneer of computational quantum chemistry in Slovenia (former Yugoslavia)
- > 15 Tflops
- Employed in various fields:
  - Biosciences
  - Material sciences
  - Engineering



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## MD SOFTWARE

- > 50 different software which enable MD simulations
- Typically free to use for academic users
- The need to efficiently parallelise on HPC infrastructure
- Most popular software packages:
  - CHARMM
  - NAMD
  - GROMACS
  - AMBER
  - LAMMPS



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## CHARMM IN NAMD

- CHARMM: one of the oldest programs for molecular dynamics of biological systems. Name implies both the software suite and the forcefield
- Easy to use scripting language:
  - A lot of ready made modules for analysis etc.
- Interoperable with NAMD:
  - Scripts for analysis can be reused

```

extracting selected frame
*
homlev -1
! Read topology and parameter files
stream toppar.str
open read unit 1 card name step5_assembly.psf
read psf card unit 1
open read unit 1 card name step6.6_equilibration.cor
read coor card unit 1
open read unit 11 file name recentrd.dcd
trajectory iread 11 nread 1 skip 5000 begin 175000
(traj read
open write card unit 10 name frame175k.pdb
write coor pdb unit 10
stop

```

NAMD  
Scalable Molecular Dynamics

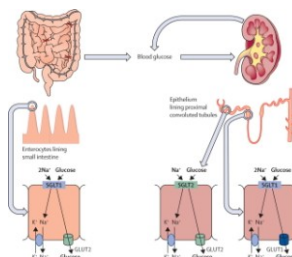
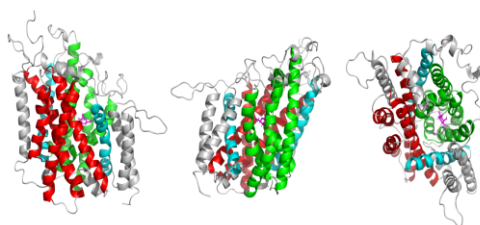
CHARMM  
Chemistry at HARvard Macromolecular Mechanics



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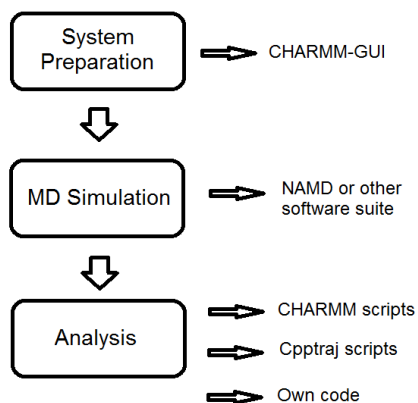
## SYSTEM OF INTEREST

- SGLT1 – sodium glucose cotransporter 1
- Physiological and pathophysiological importance
  - Oral rehydration therapy
  - Therapeutics for diabetes
  - Other diseases



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## BASIC WORKFLOW



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## REFERENCES

- <https://www.acm.org/media-center/2020/november/gordon-bell-special-prize-covid-research-2020>
- <https://www.olcf.ornl.gov/summit/>
- <https://www.tacc.utexas.edu/-/frontera-named-5th-fastest-supercomputer-in-the-world>
- <https://pubs.acs.org/doi/10.1021/acscentsci.9b01071>
- <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6209097/>
- [https://www.thelancet.com/journals/landia/article/PIIS2213-8587\(13\)70050-0/fulltext](https://www.thelancet.com/journals/landia/article/PIIS2213-8587(13)70050-0/fulltext)
- <https://www.ki.si/>



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