IOCB SERVICE DAYS 2023

Presentation of services by:
Research-Service Groups / Service Groups / Core Facilities

High Performance Computing Service Group

Hector Martinez-Seara

ÚOCHB AV ČR
IOCB PRAGUE

What do we offer?

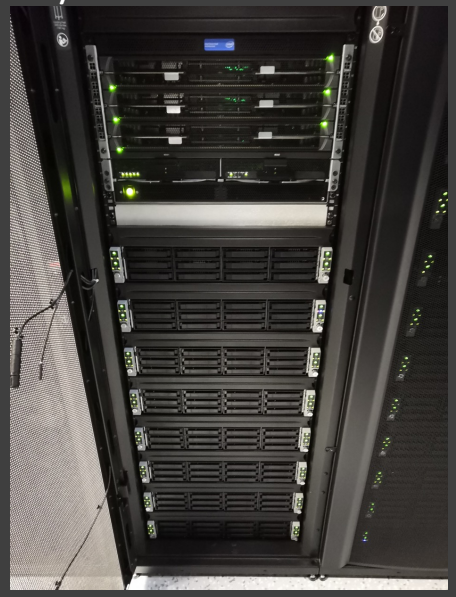
- High performance computing hardware/software
- Computational expertise
- Molecular modeling
- Image Processing
- “Bioinformatics”
- Mathematical modelling
- Training Courses

ALL OUR SERVICES ARE FREE FOR IOCB EMPLOYEES!!

Hardware:
The Aurum cluster

- Computing nodes: 291
- Number of cores: 10764
- Total Memory: 52TB
- Number GPUs: 84
- Omnipath/25 Gb network

Partition name	Nodes	count	cores	cpu	RAM (GiB)	RAM (MiB)	GPU	scratch	Network
a36_96	a[001-204]	204	36	intel-skylake[4]	87	89280			100 Gb[1]
a36_192	a[205-224]	20	36	intel-skylake[4]	181	186120		1 TB nvme	100 Gb[1]
a36_768	a[225-232]	8	36	intel-skylake[4]	748	766440		1 TB nvme	100 Gb[1]
a36_96_gpu	a[233-237]	5	36	intel-skylake[4]	82	84600	2x RTX 5000 [2]	1 or 8 TB nvme	100 Gb[1]
b32_128_gpu	b[001-003]	3	32	amd-zen3[5]	~120		2x RTX 3080 [9]	2 TB nvme	25 Gb
b32_128_gpu	b[004-029]	26	32	amd-zen3[5]	~120		2x RTX 3090 [3]	2 TB nvme	25 Gb
b32_128_gpu	b[030-032]	3	32	amd-zen3[5]	~120		4x RTX 3090 [3]	2 TB nvme	25 Gb
b64_1024	b[033-048]	16	64	amd-zen3[6]	~1000			2 TB nvme	25 Gb
b64_2048	b049	1	64	amd-zen3[6]	~2000			2 TB nvme	25 Gb
c24_32_gpu	c[001-005]	5	24	intel-broadwell[7]	~28		2x GTX 1080 [8]	1 TB ssd	1 Gb



- [1] Omnipath 100 Gb PCIe x8 Adapter
- [2] Quadro RTX 5000 16GB GDDR6
- [3] GeForce RTX 3090 24GB GDDR6
- [4] 2x Intel Xeon Gold 6140 CPU @ 2.30GHz
- [5] 1x AMD EPYC 7543, 32 cores @ 2.8 GHz
- [6] 2x AMD EPYC 7543, 32 cores @ 2.8 GHz
- [7] 2x Intel Xeon CPU E5-2650 v4 @ 2.20GHz
- [8] GeForce GTX 1080 8GB
- [9] GeForce RTX 3080 10GB GDDR6

https://hpcg.uochb.cas.cz/cluster/index.html

Our people

- The service group has a total of 3 FTEs
  - We have grown by 2 FTEs in the last year.
- Each member has 0.5 FTE in the HPCg service group

Computational expertise

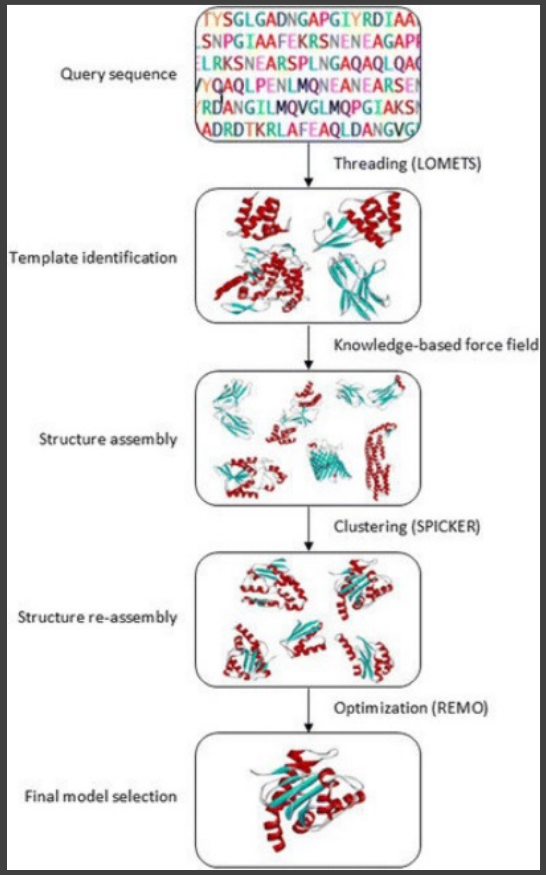
- General support
  - Cluster tenders
  - Maintanace of the cluster
  - Installation of commonly used software

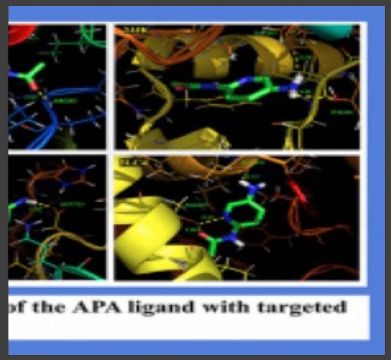
- Personalized support
  - Personalizing the cluster experience to match user needs
    - Software and hardware
  - Help with tenders and grants
  - Help people using cluster (Kiran)

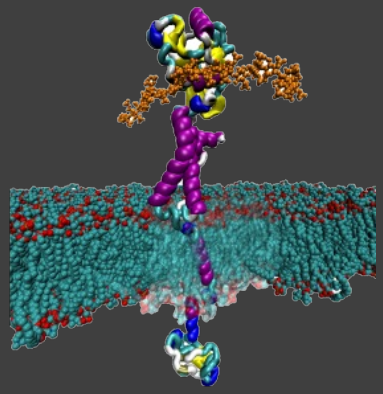
Molecular modelling techniques

Quantum mechanics	Molecular dynamics	QM/ MM	Docking & scoring	Big data	Image processing	Machine learning	Optimization & clustering	Calculations & statistics

- Molecular dynamics simulations involving all sort of biomolecules
- Ligand docking and scoring
- Reaction mechanism
- Generation of conformers
- pKa predictions
- Structure prediction methods
- Protein design
- Parametrization of molecules
- Understanding macromolecular interactions







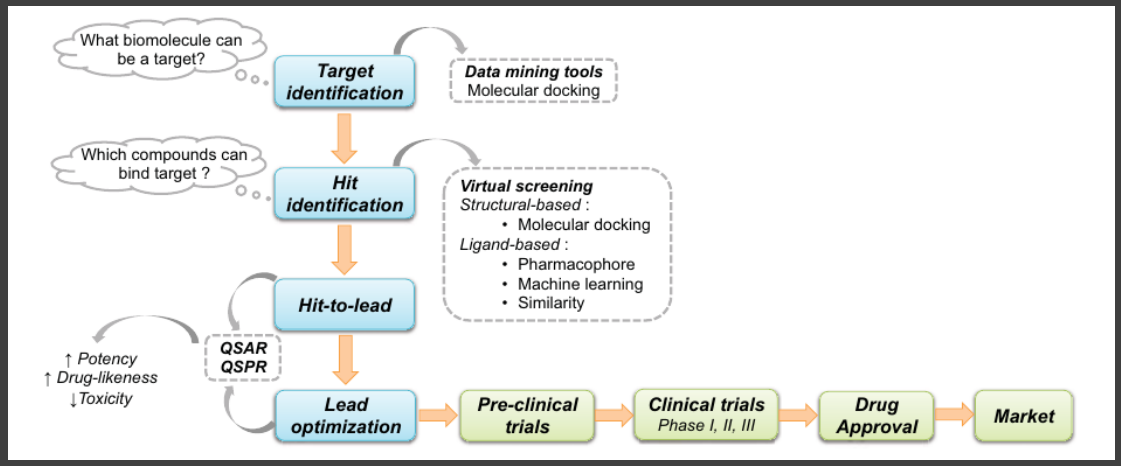
- Coordinated by Dr. Martin Lepšík (0.5 FTE)
- Dr. Petro Khoroshyy (0.5 FTE)
- MSc. Miguel Riopedre (0.5 FTE since 2023)

“Bioinformatics”

Quantum mechanics	Molecular dynamics	QM/ MM	Docking & scoring	Big data	Image processing	Machine learning	Optimization & clustering	Calculations & statistics

- Data mining
- High throughput techniques
- Querying databases
- Virtual screening

- Proteomics
- Genomics
- Lipidomics



We are not experts in everything, but if there is demand we are ready to try.

- Dr. Kiran Kumar Telekunta (0.5 FTE since Nov 2022)
- MSc. Miguel Riopedre (0.5 FTE since 2023)
- In collaboration with other facilities:
  - CryoEM (Dr. Tomáš Kouba)
  - Mass spectrometry (Dr. Josef Cvačka)
  - Next generation sequencing (Dr. Ondřej Lukšan)

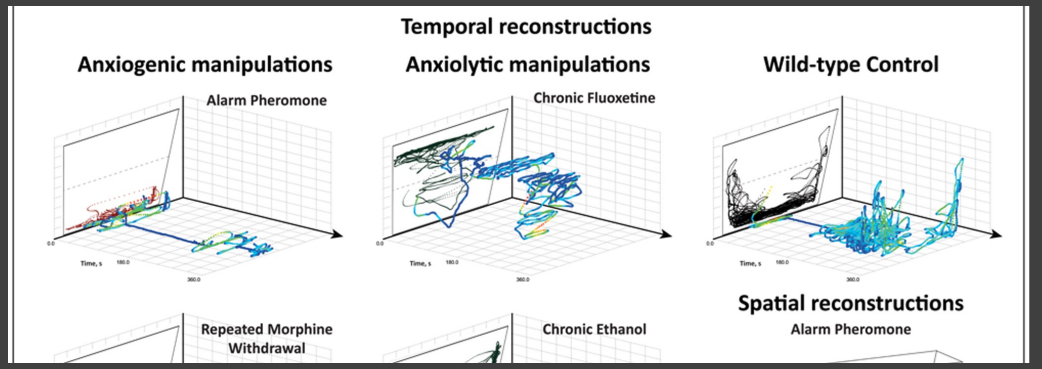
New in-house virtual screening pipeline

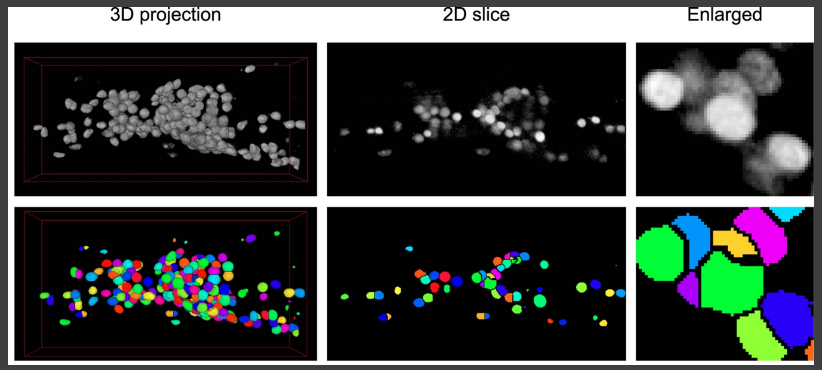
Do you want to try?

Image processing techniques

Quantum mechanics	Molecular dynamics	QM/ MM	Docking & scoring	Big data	Image processing	Machine learning	Optimization & clustering	Calculations & statistics

- Processing large data sets
  - Confocal microscopy
  - Electron microscopy
- Automatic image tracking and analyzing





Course at Charles University (Faculty of Natural Sciences) - *Methods and applications in computational cell biology and biophysics*.

Starting in 8th of March

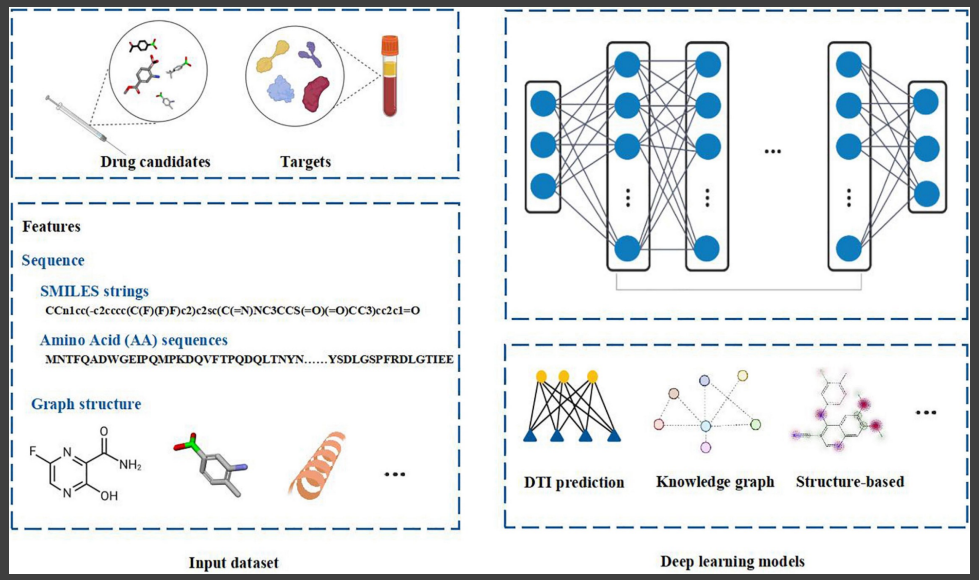
(IOCB employees welcome – write to hseara@uochb.cas.cz)

- Dr. Petro Khoroshyy (0.5 FTE)

Mathematical modelling

Quantum mechanics	Molecular dynamics	QM/ MM	Docking & scoring	Big data	Image processing	Machine learning	Optimization & clustering	Calculations & statistics

- Machine learning
  - Supervised
  - Deep learning
- Advanced optimization methods
  - Genetic algorithms
  - Differential evolution
- Markov models and variants
- Cluster analysis
- Statistical models



- MSc. Ondřej Ticháček (0.5 FTE since 2023)

Our roles

Hector Martinez-Seara

Head, Aurum, Mol. Modelling, Courses

Ondřej Ticháček

Aurum, Mathematical modelling, ML

Kiran Kumar Telukunta

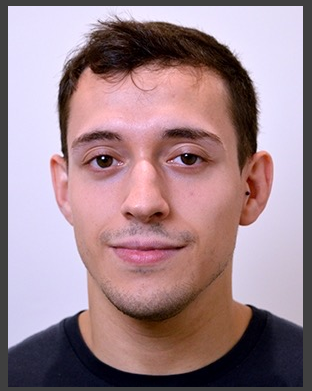
Aurum, Cryo, programing Bioinformatics

Martin Lepšík

Modelling, Virtual screening, Bioinformatics, Courses

Petro Khoroshyy

Imaging, Virtual screening, Modelling, Courses, MS



Miguel Riopedre

Modelling, Programing, NGS

Courses

We organize 1 week of courses twice a year.

- Linux
- Python
- Pymol
- ImageJ
- Gromacs
- Gaussian
- **We accept suggestions for new courses**

So far more than 250 attendees.

Course at Charles University (Faculty of Natural Sciences) - *Methods and applications in computational cell biology and biophysics*.

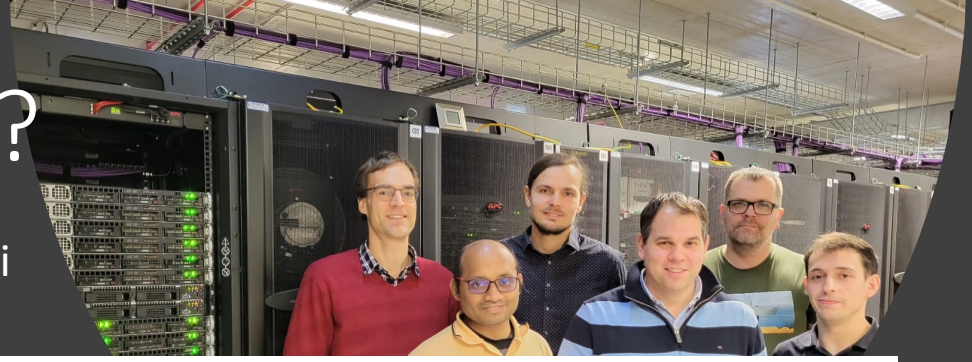
Starting in 8th of March

(IOCB employees welcome – write to hseara@uochb.cas.cz)

Something missing contact us

How to contact us?

https://intraweb.uochb.cas.cz/vypocetni-core-facility-510.html



ÚOCHB AV ČR
IOCB PRAGUE

Vyhledat

Rozcestník | Nástěnka | Události | Vedení | Administrativa | Věda | Personální & mzdy | ITS | Kontakty | Ostatní | Dokum

/ Úvod / Věda / Core facilities / Vysoce výkonné počítání

Core facilities
- Analytické laboratoře
- Biochemická farmakologie
- MS
- NMR
- Mikroskopie
- NGSf
- Radiochemie
- Virologie
- Vysoce výkonné počítání
  - Aurum cluster
  - Služby
- Granty
- Knihovna
- ORCID

Skupina **Podpory vysoce výkonného počítání** nabízí celou řadu služeb. Pro řešení problémů vyžadující velký výpočetní výkon zajišťujeme provoz clusteru Aurum. Poskytujeme též konzultace / pomoc s výpočetními projekty výzkumných pracovníků ÚOCHB. Témata pokrývají širokou oblast od zpracování obrazu, virtuálního screeningu, biomolekulárních výpočtů, manipulací s velkými daty, až po softwarovou a hardwarovou podporu pro simulaci molekulární dynamiky.

Lidé

- Hector Martinez-Seara (vedoucí), ☎ 187
- Martin Lepšík (podpora modelování), ☎ 523
- Petro Khoroshyy (podpora zobrazování a organizace kursů), ☎ 448/463
- Ondřej Ticháček (matematické a statistické modelování a design clusteru), ☎ 296

Aurum cluster
Služby

How to contact us?

https://hpcg.uochb.cas.cz

HPCg Home Cluster Services GitLab Contact

Podpora vysoce výkonného počítání
High Performance Computing

The High Performance Computing Support group offers a range of services. We ensure the operation of the Aurum cluster for solving problems that require a lot of computing power. We also provide consultations / help with computational projects of IOCB researchers. Topics cover a wide range from image processing, virtual screening, biomolecular computing, big data manipulation, to software and hardware support for molecular dynamics simulation.

Aurum cluster

Located in the basement of building B, the aurum cluster provides computational resources to all employees of IOCB.

Learn more | Documentation | Request user account | Issue tracker

HPCg GitLab

High Performance Computing Service Group (HPCg) maintains its own GitLab instance which is accessible only to IOCB employees.

HPCg GitLab

Other services

List of services which we provide, continue to improve and increase.

HPCg Services

How to contact us?

https://hpcg.uochb.cas.cz/gitlab