

BioExcel

Center of Excellence for Computational Biomolecular Research

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Partners



Funding



BioExcel Consortium



KTH Royal Institute of Technology



MAX-PLANCK-GESELLSCHAFT

INSTITUTE
FOR RESEARCH
IN BIOMEDICINE

Universiteit Utrecht

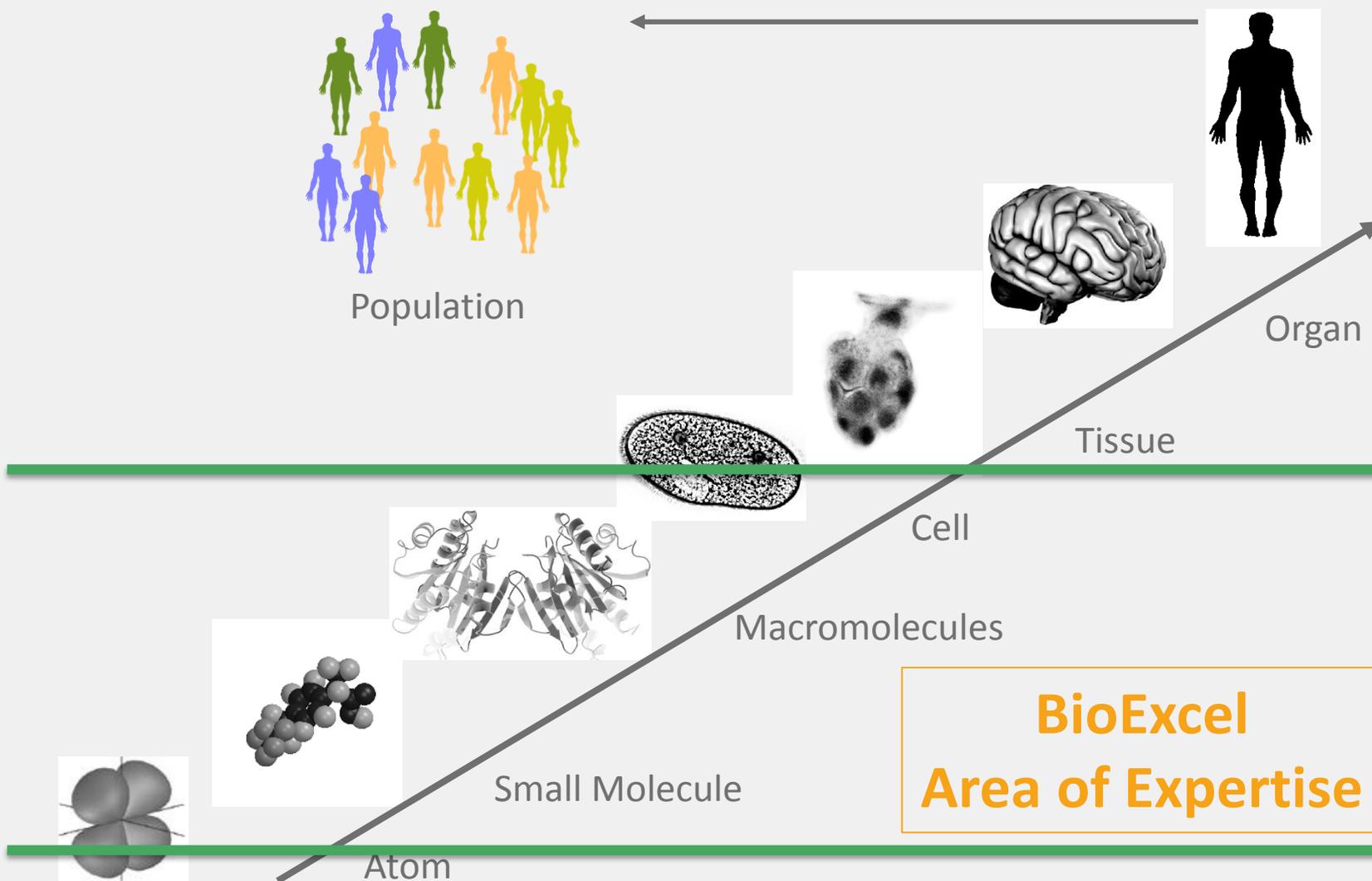
**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación

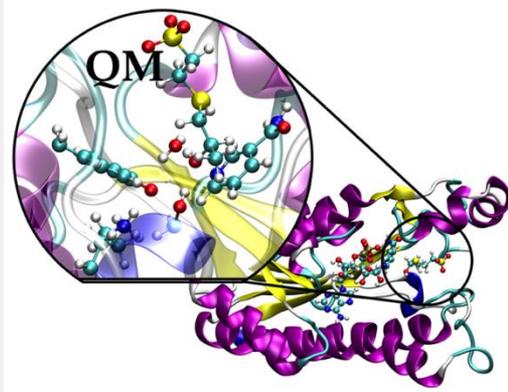
EMBL-EBI



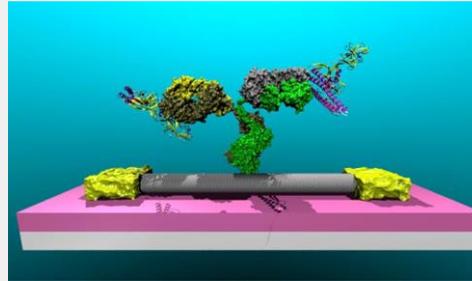
Life Science and HPC



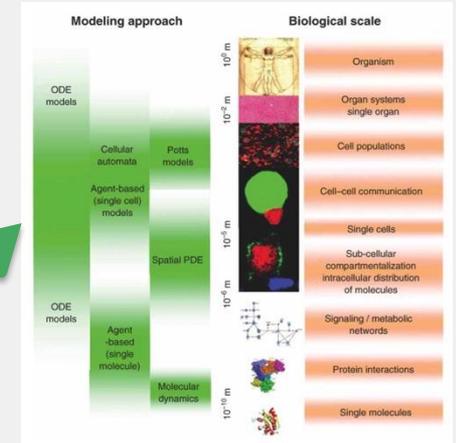
Electronic structure



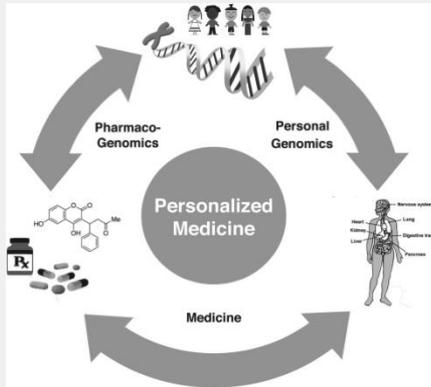
Biomarkers design



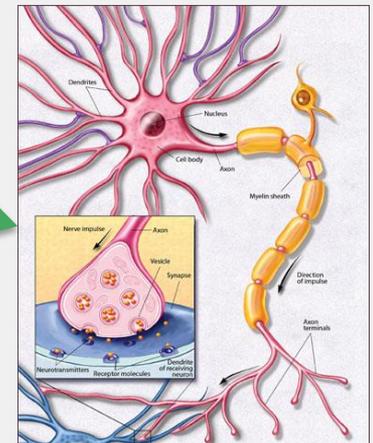
Physiology



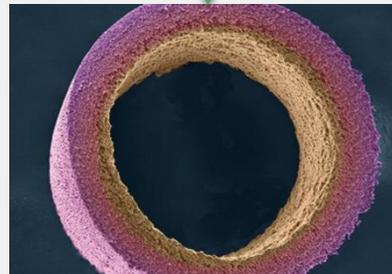
Biomolecular Modeling and Simulations



Personalized medicine

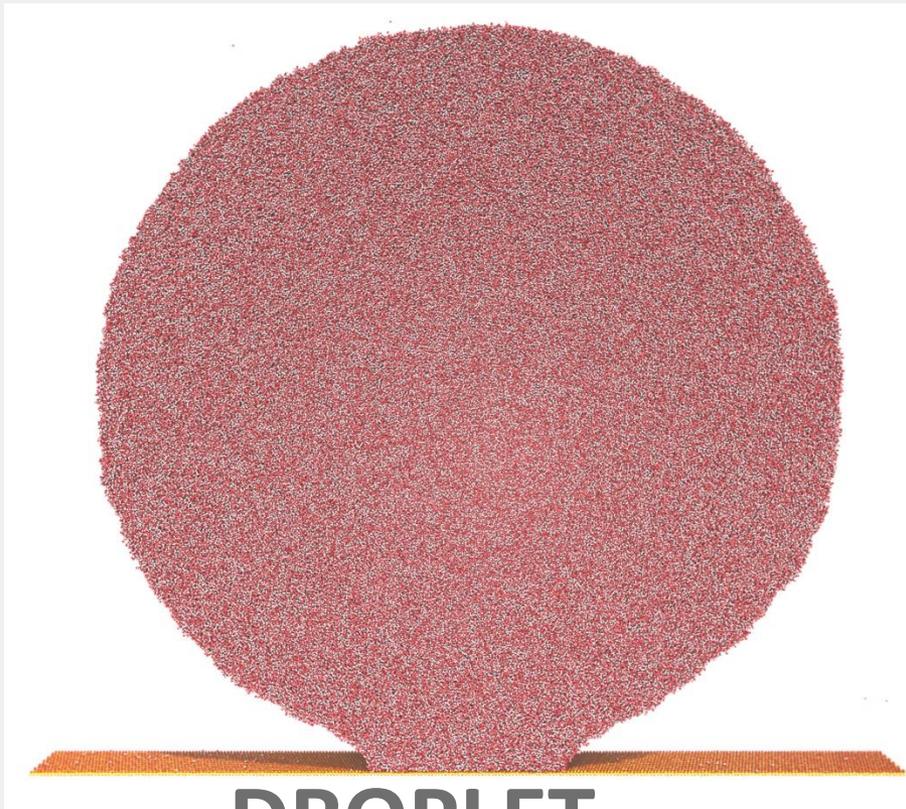


Neuroinformatics

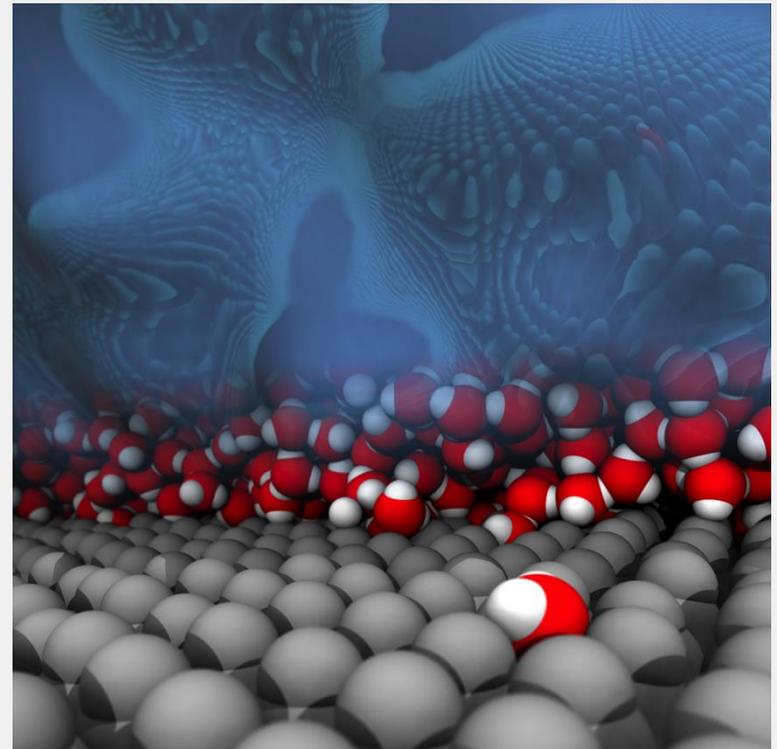


Biomaterials science and nanotechnology

Bio-Molecular Modeling and Simulations

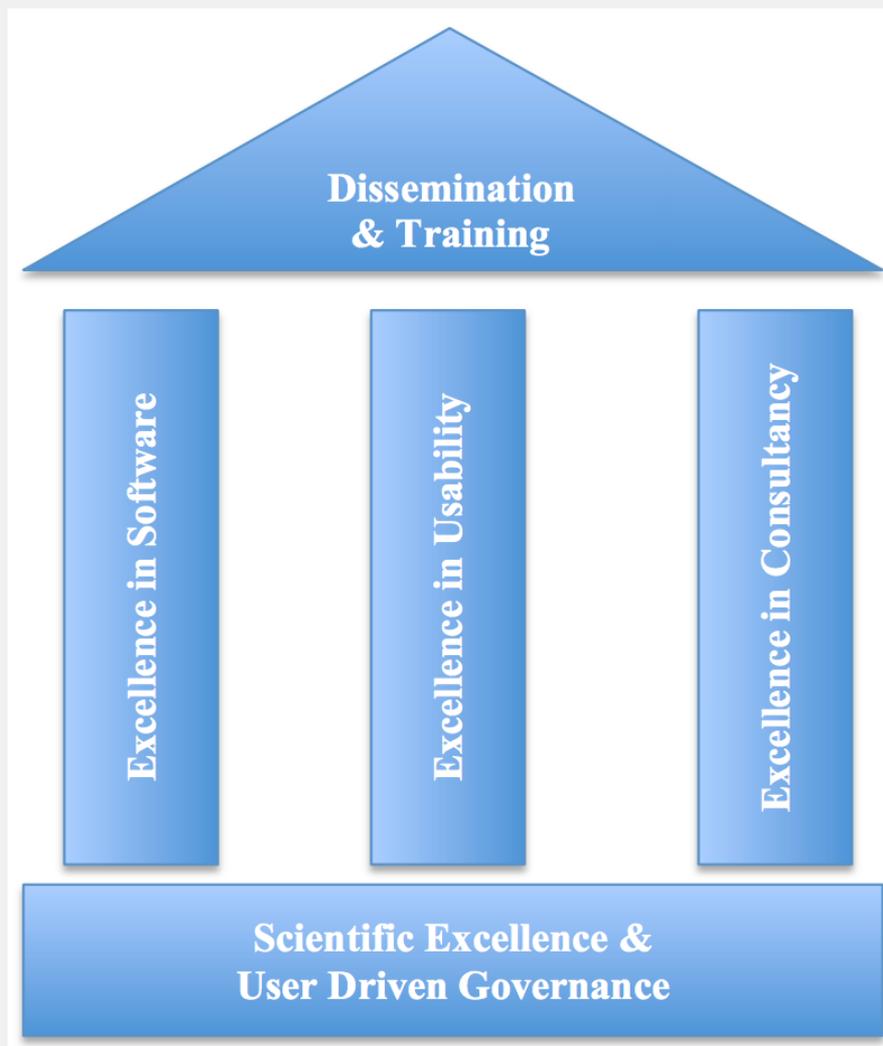


DROPLET



SURFACE

BioExcel Pillars of Excellence

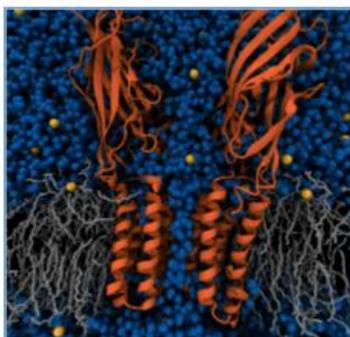


Objectives of BioExcel

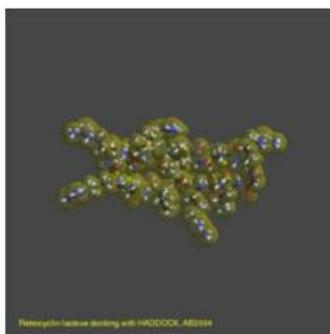
Excellence in Biomolecular Science

Improve the performance, efficiency and scalability of key codes

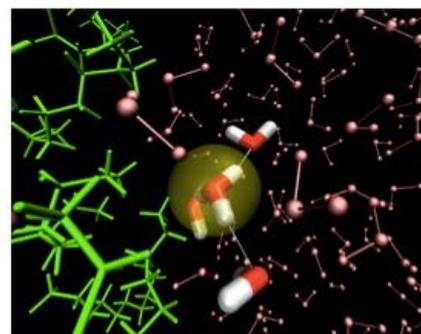
- GROMACS (Molecular Dynamics Simulations)
- HADDOCK (Integrative modeling of macro-assemblies)
- CPMD (hybrid QM/MM code for enzymatic reactions, photochemistry and electron transfer processes)



MD simulations
/GROMACS/



Docking
/HADDOCK/

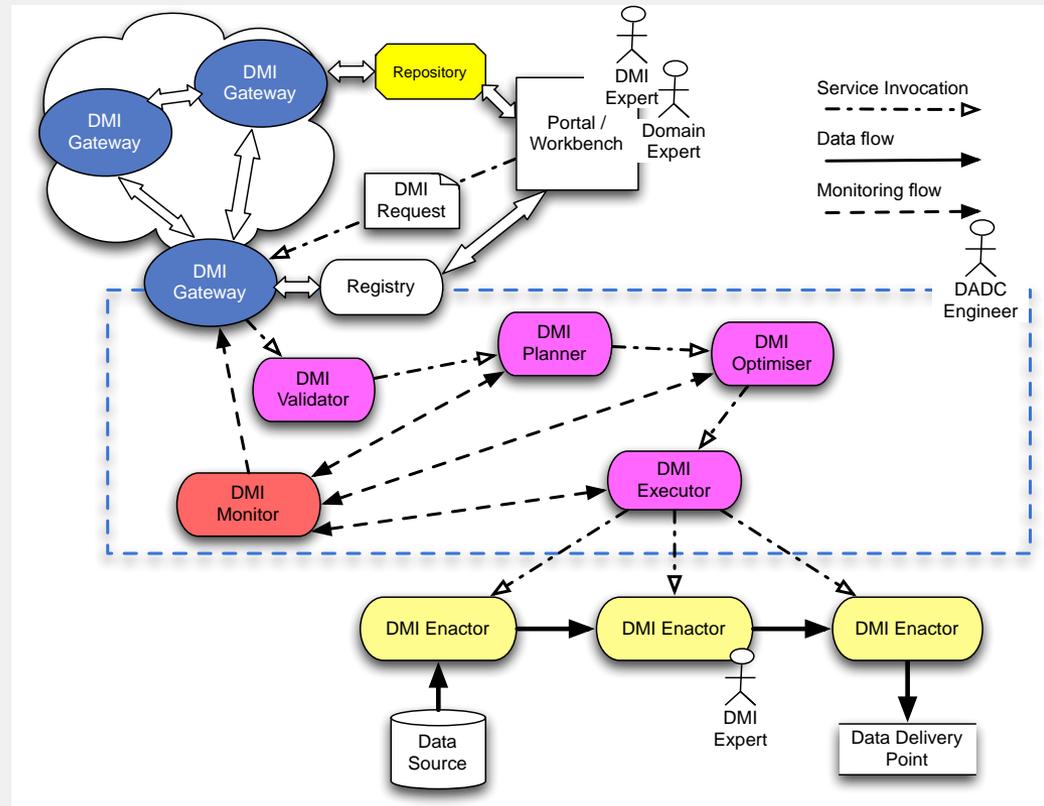


QM/MM
/CPMD/

Objectives of BioExcel

Excellence in Usability

- Make ICT technologies easier to use by biomolecular researchers, both in academia and industry
- Devise efficient workflow environments with associated data integration



Objectives of BioExcel

Competence-building among academia and industry

Promote best practices and train end users to make best use of both software and computational infrastructure

- academic and non-profit users
- industrial users
- independent software vendors (ISVs) and academic code providers of related software
- academic and commercial resource providers



Services: Application development

- Improving performance and scalability
- Porting to new architectures
- Code validation and benchmarking
- Extending the functionality

Services: Usability aspects

- Easier to use, tailor-made workflows
- Improved data management and integration
- Extending the functionality of portals and environments as needed
- Provisioning of pre-packaged solutions, e.g. VM images

Services: Consultancy and Training

- Workshops with hands-on and “surgery” sessions
- Online tutorials
- Webinar series
- One-to-one support
- Promotion of best practices for software development
- Knowledgebase

International Cooperation

- EU Initiatives and projects: ELIXIR, INSTRUCT, WestLIFE VRE, FET-HPC, IMIs, MuG-VRE
- International (non-EU) Centers: Oak Ridge, RIKEN
- Infrastructure projects: PRACE, EGI, EUDAT, HelixNebula
- Resource providers: Amazon etc.
- Industrial alliances: Pistoia Alliance, CEFIC, FoodDrinkEurope

Relations with HPC Projects

- Co-chairing EXDCI WP on Life Science software
- Contributed to the SRA
- Participation in the EsD
- Links with ExCAPE
- Links with CompBioMed, E-CAM, MaX CoEs