

Hands-on introduction to HPC for life scientists

-

PRACE & BioExcel

Center of Excellence for Computational Biomolecular Research

Vera Matser

EMBL-EBI

Training and Dissemination

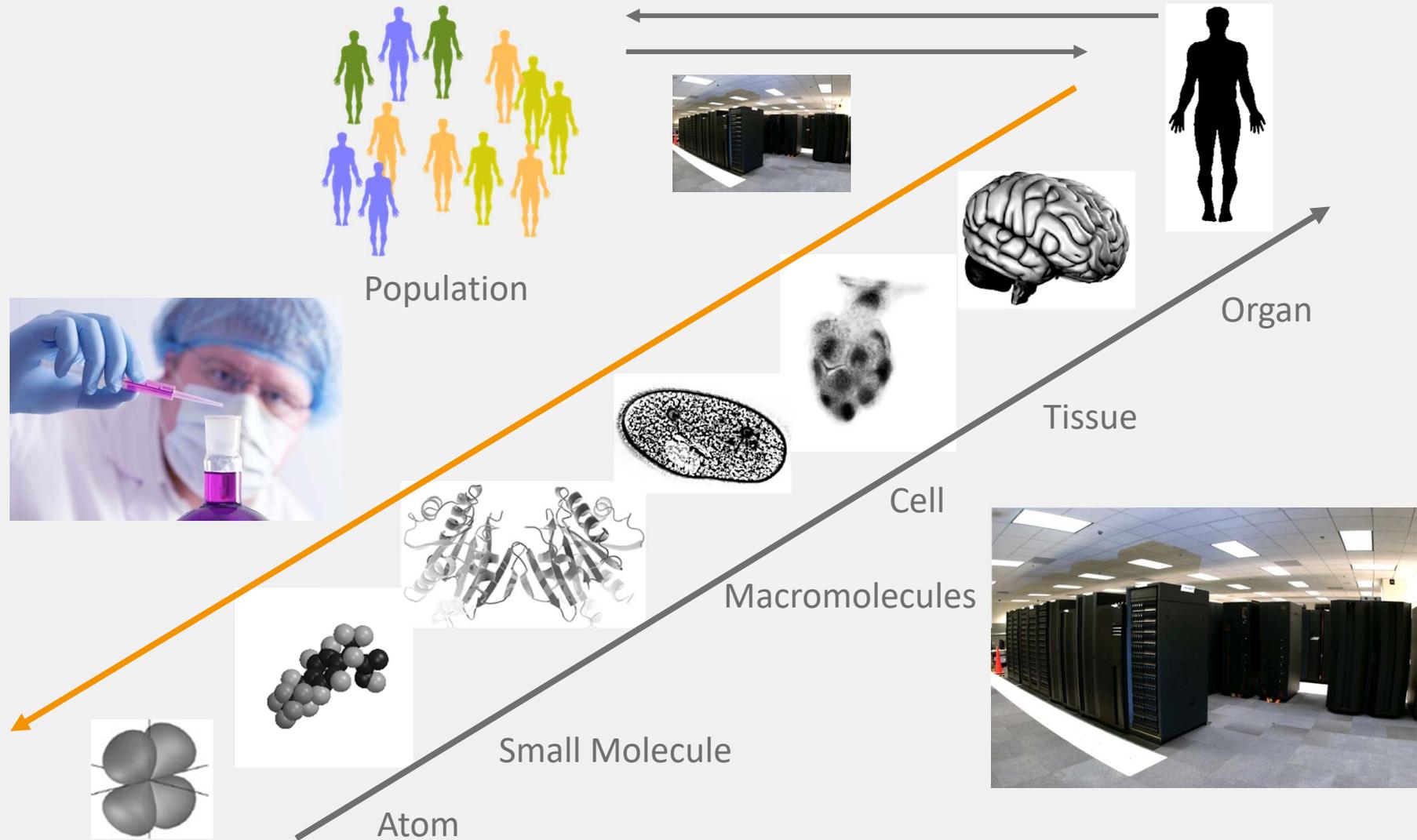
Partners



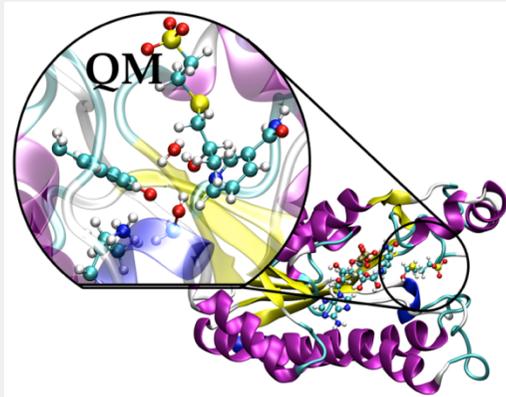
Funding



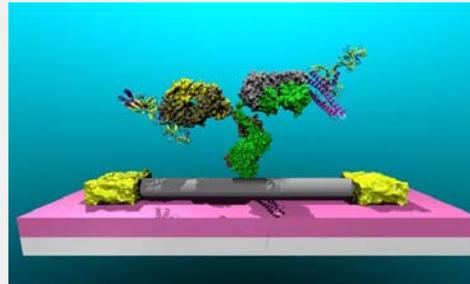
Life Science and HPC



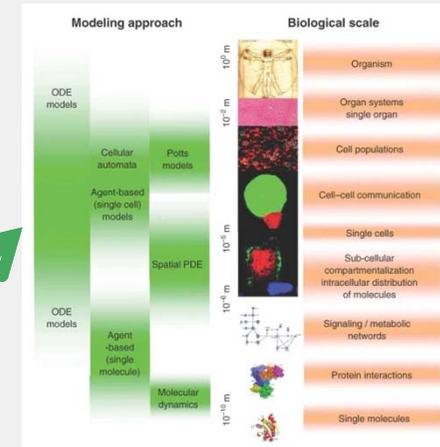
Electronic structure



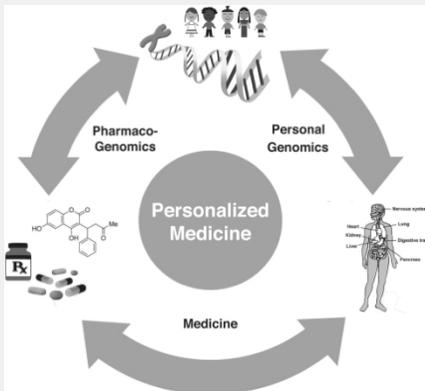
Biomarkers design



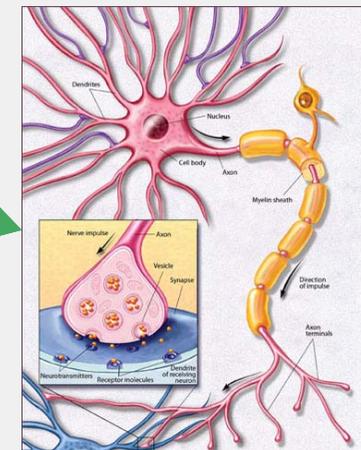
Physiology



Biomolecular Modeling and Simulations



Personalized medicine



Neuroinformatics



Biomaterials science and nanotechnology

BioExcel Center of Excellence

SOLUTIONS

SOFTWARE

Widely used, fast and scalable codes for integrative modelling and molecular simulations

CORE DEVELOPERS

The scientists who wrote the code and know it best work with us!

WORKFLOWS

User-friendly and efficient systems for workflow executions and data processing



SERVICES

TRAINING

Webinars, "ask-me-anything" sessions, hands-on workshops for everyone from newbies to advanced users

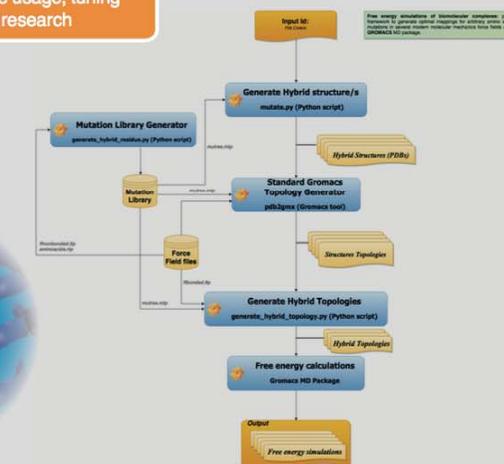
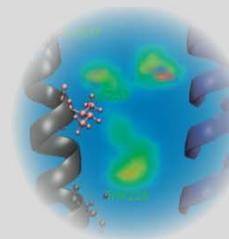
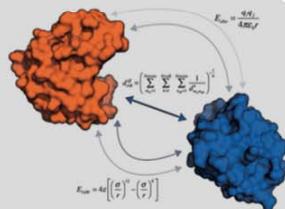
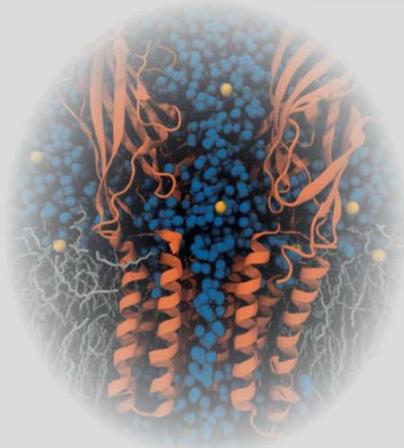
CUSTOMISATION

Tailored solutions adapted to your needs

CONSULTANCY

Personalized support with software usage, tuning and scientific aspects of the research

ACADEMIA
INDUSTRY

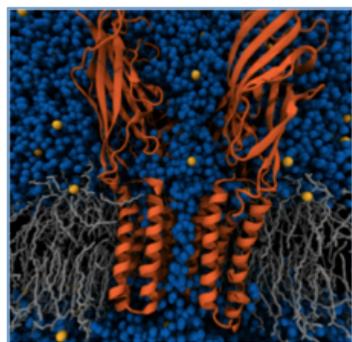


Objectives of BioExcel

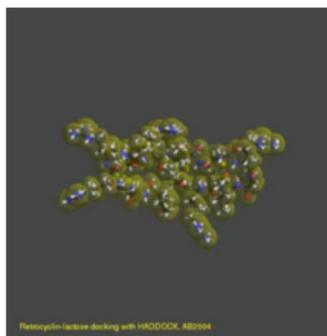
Excellence in Biomolecular Science

Improve the performance, efficiency and scalability of key codes

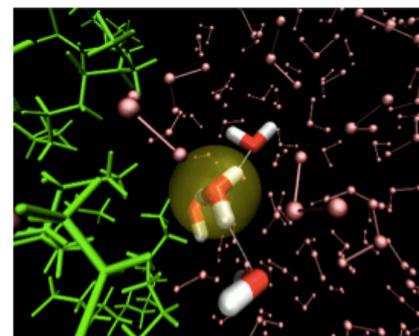
- GROMACS (Molecular Dynamics Simulations)
- HADDOCK (Integrative modeling of macro-assemblies)
- CPMD (hybrid QM/MM code for enzymatic reactions, photochemistry and electron transfer processes)



MD simulations
/GROMACS/



Docking
/HADDOCK/

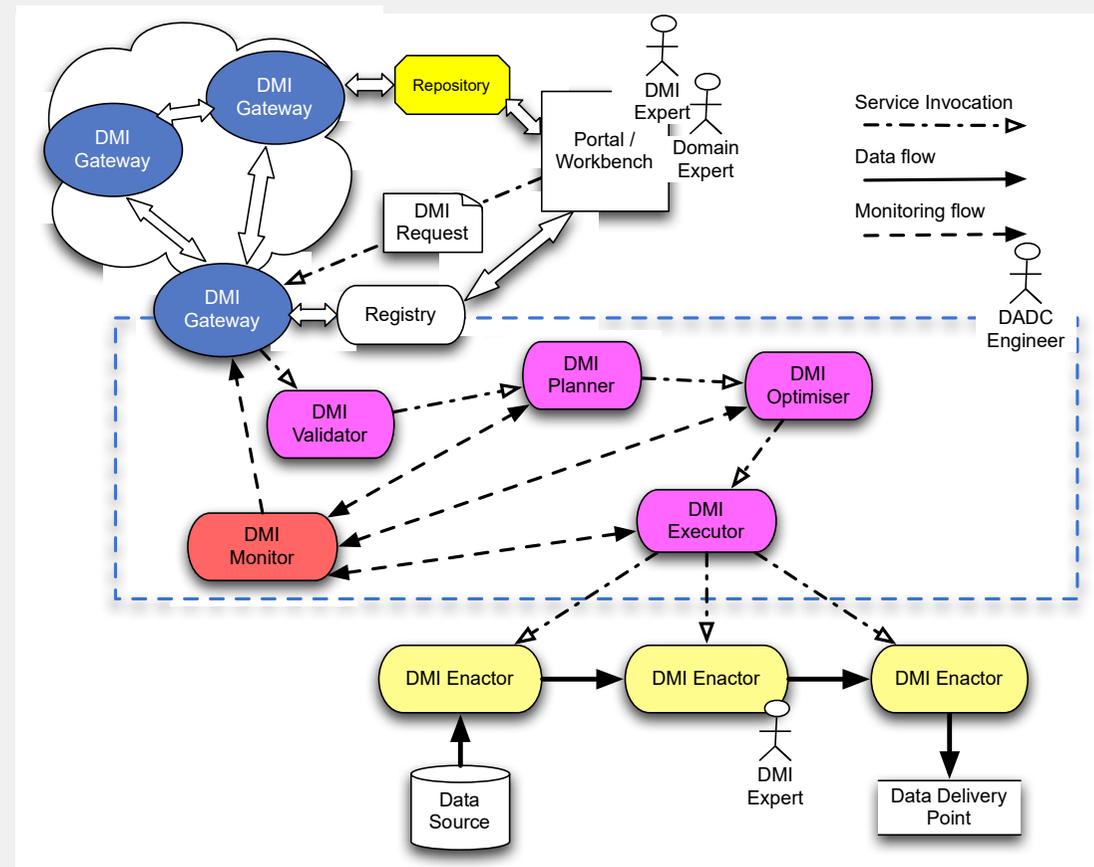


QM/MM
/CPMD/

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

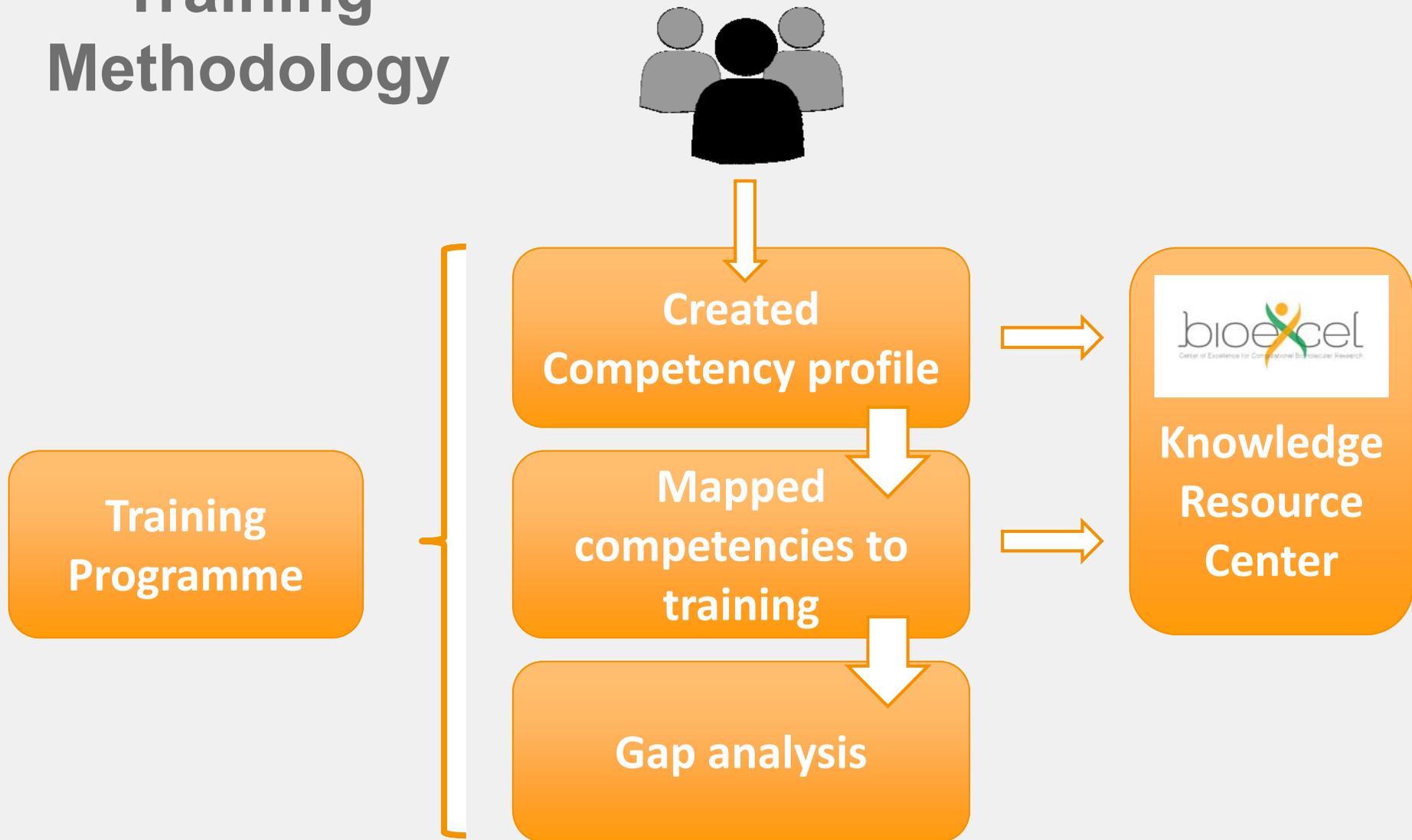
Competence-building among academia and industry

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



Training Methodology



A Competency is an observable ability of any professional, integrating multiple components such as knowledge, skills and behaviours

"Write his/her own scripts to perform tasks in context of biomolecular research"

Knowledge	Skills	Behaviour
Knowledge of existing commands/libraries to re-use	Is able to automate the process of executing processes remotely	Uses appropriate scripting languages
Judges when a task should be automated	Write & debug scripts	

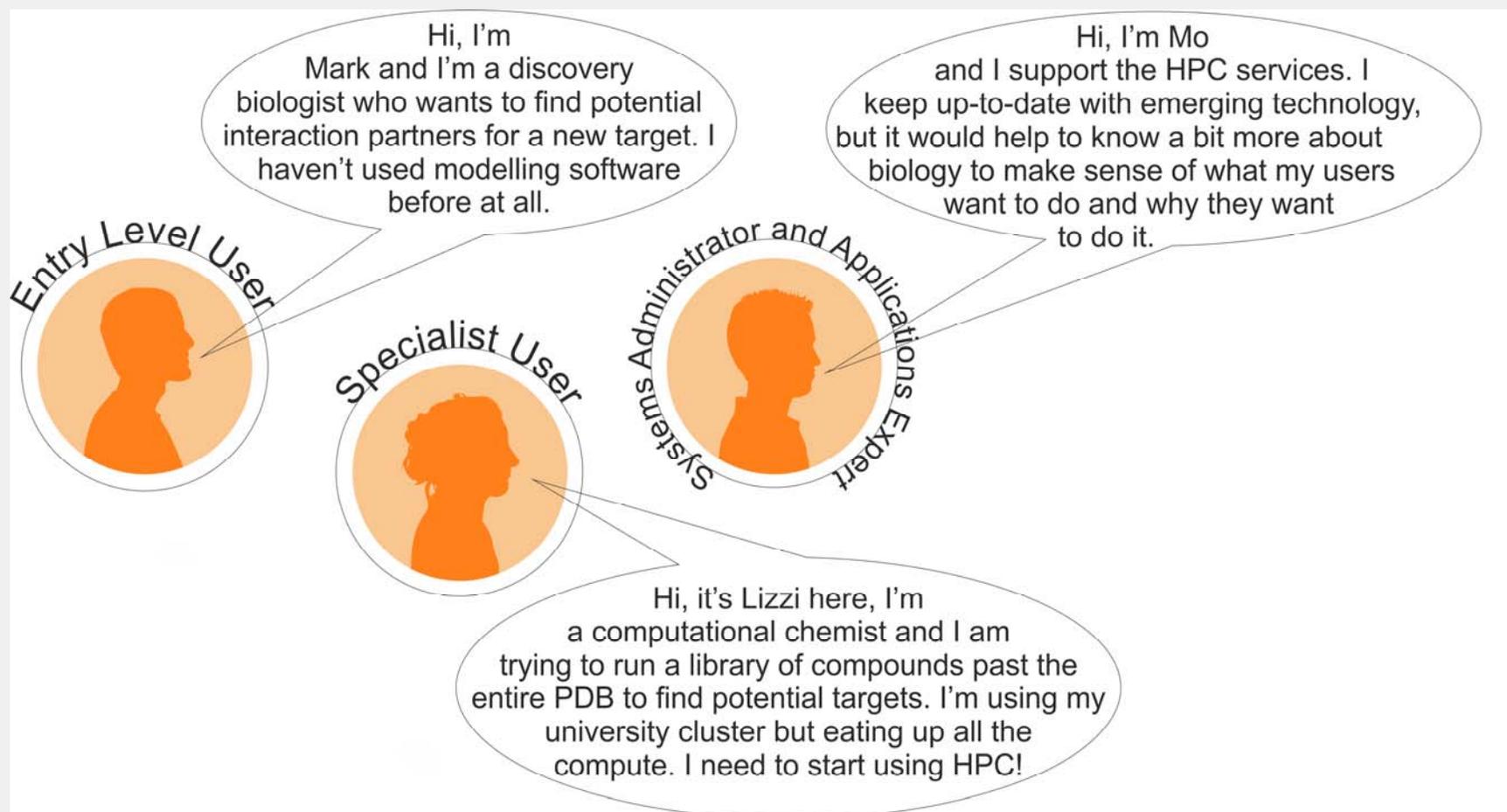
BioExcel Competency Profile

Group related competencies together into areas

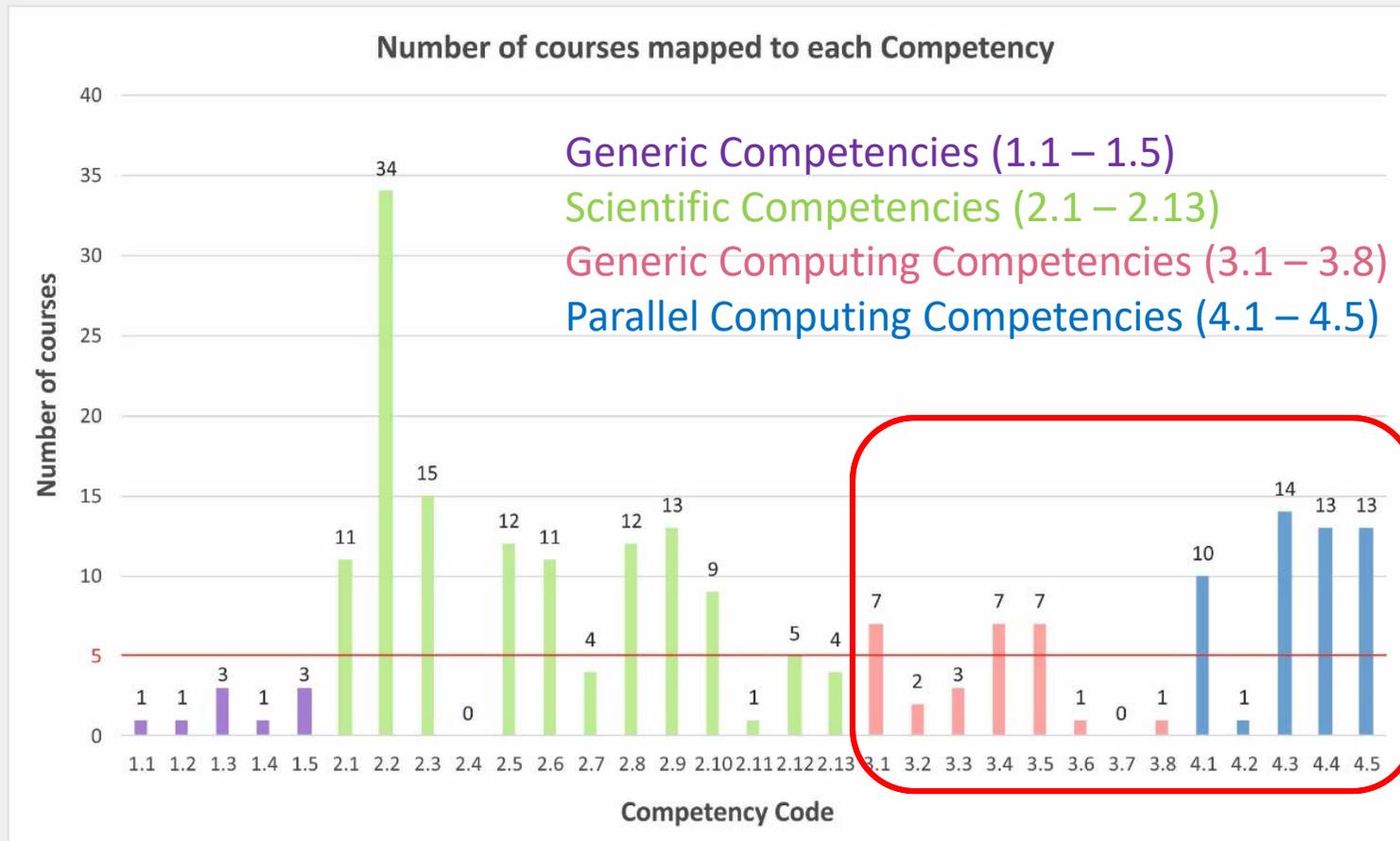
<p>Generic 5</p>	<p>Scientific 13</p>
<p>Generic Computing 8</p>	<p>Parallel Computing 5</p>

BioExcel Competency Profile

Different types of users

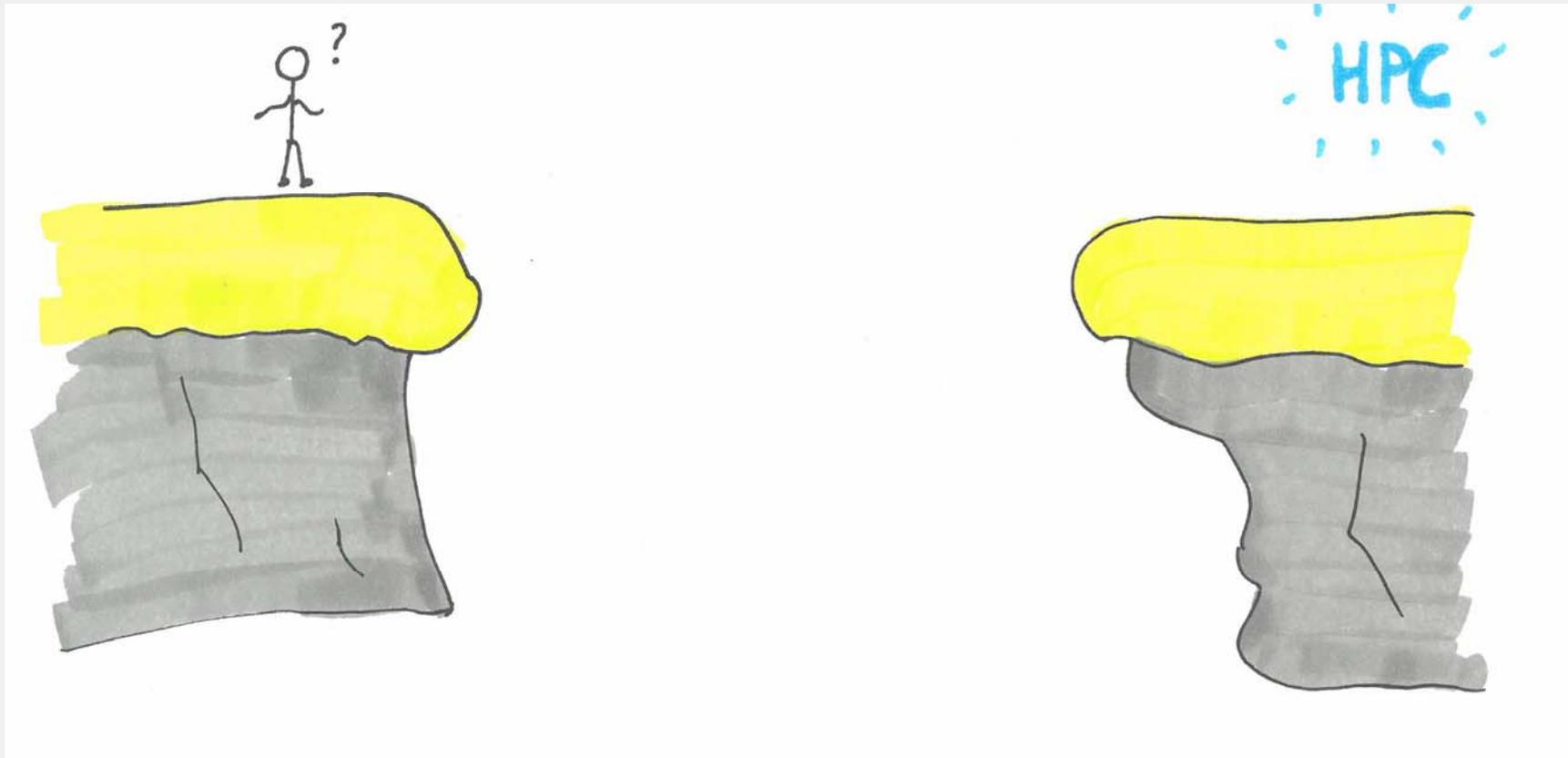


Mapping & Gap analysis

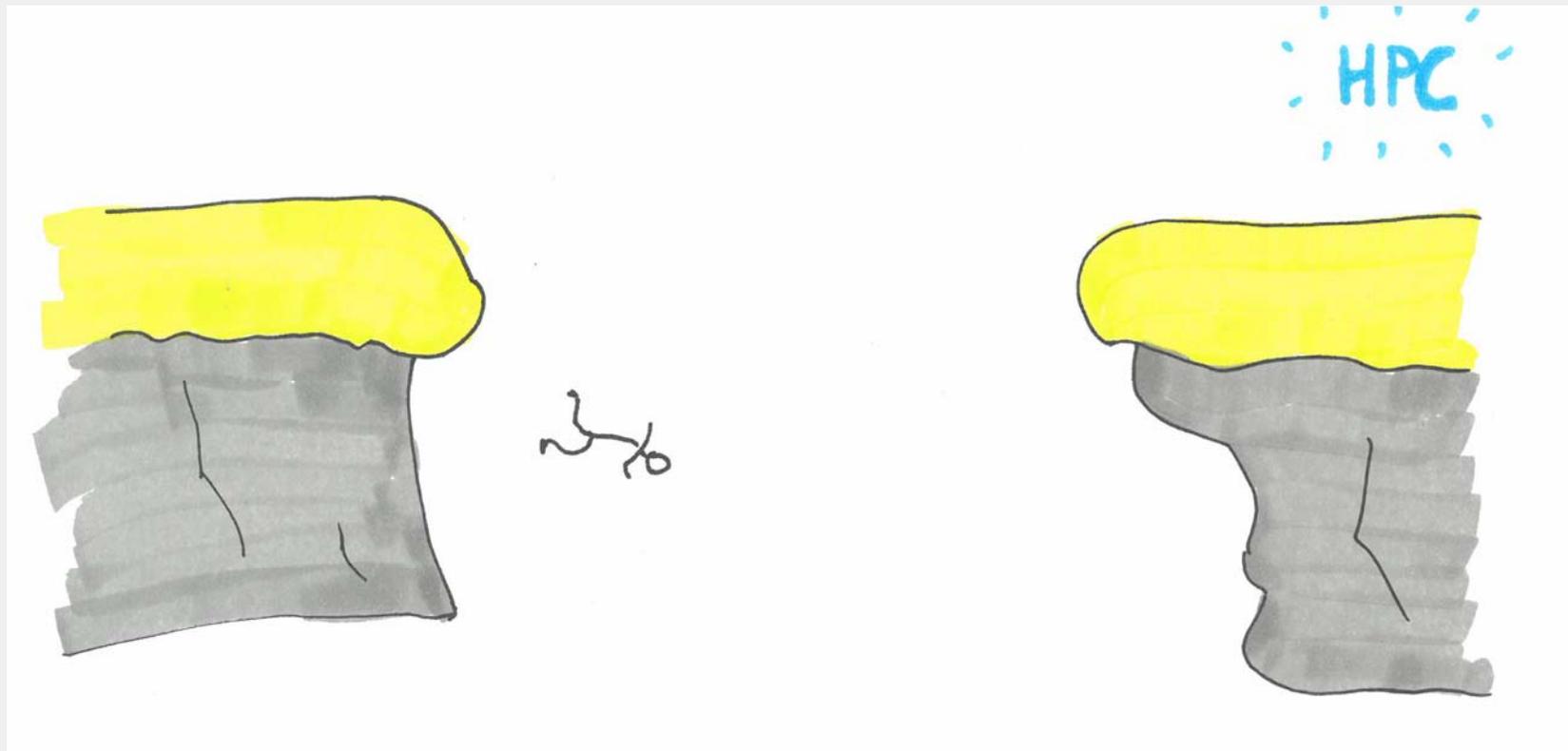


5 (total training resources) picked as a minimum viable number for coverage

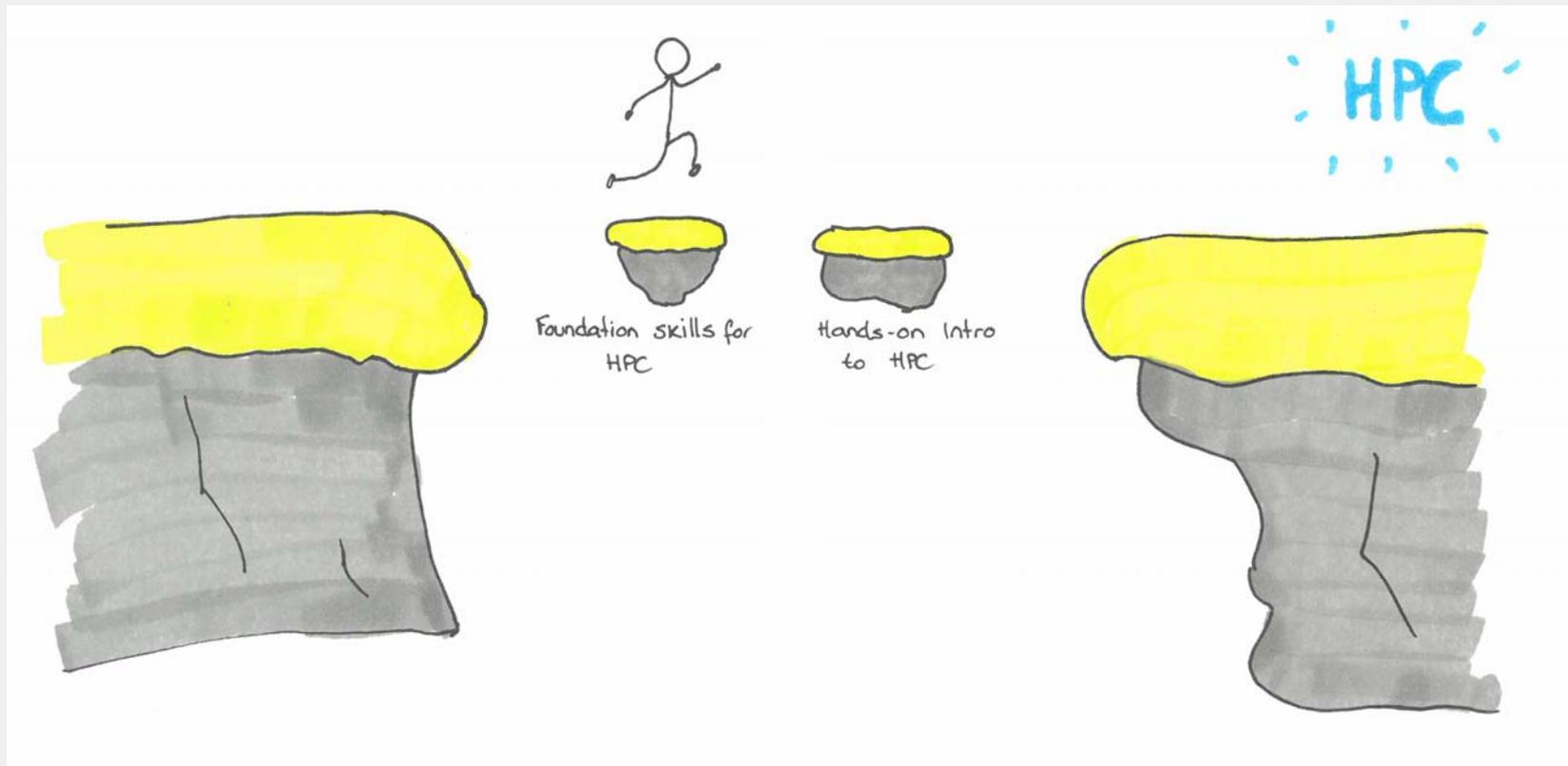
HPC training for life scientists



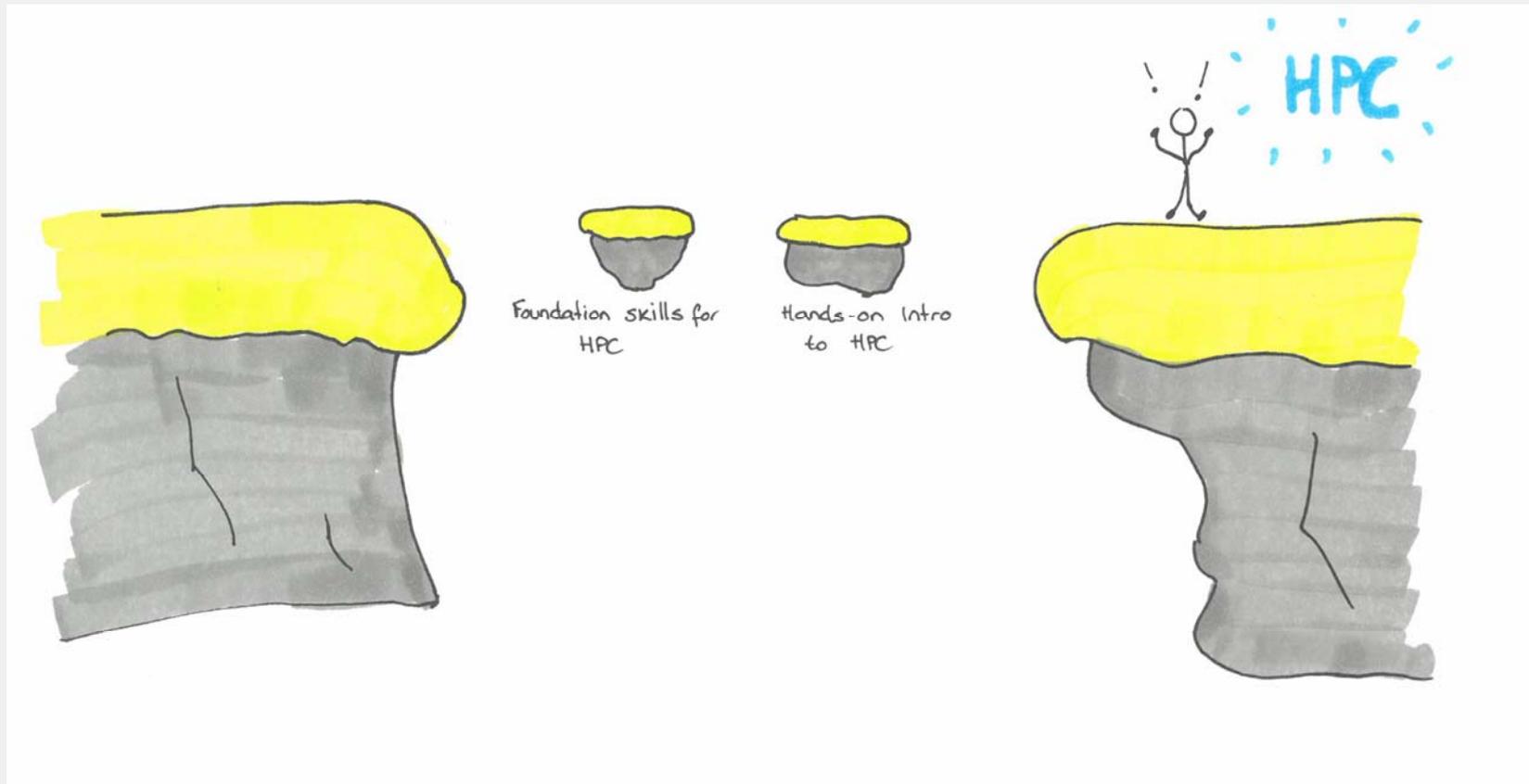
HPC training for life scientists



HPC training for life scientists



HPC training for life scientists



Parallel Computing Competencies

- Assess computational workflow systems and their potential benefits
- Apply knowledge of batch system
- Write computer programs that can run on a parallel computer
- Assess advantages and limitations for deploying, executing and optimising computations in a cloud/grid/HPC environment
- Apply knowledge of performance profiling to measure suitability of computing platforms

Activity - Benchmarking



How are your skills developing over time?

- Pre-course
- Post-course
- 6 – 12 months

Note:

- Survey in email also rates generic computing Competencies
- [Link to full profile](#)

Long-term Feedback & Impact

Competency development over time

Post-course impact survey (6-12 months)

Impact interviews

- Will send invite later today and explain in one of the coffee breaks
- Short skype conversation with individuals

Why is this important?

- For us to improve our courses
- Report to funding agencies
 - Anonymous data as part of future funding proposals
- For you – benchmark of where you started from



Activity: Human barometer

Sticky dots

Have you ever been to Edinburgh before?

1 – No first time ever, London is the furthest North I generally go

2

3

4

5 – I grew up here

* – Wildcard - Where is Edinburgh, aren't we in London?

How familiar are you with linux?

1 - Linux.. what?

5 - Linux commands are my primary way of communicating

What is your programming expertise?

1 – I only used existing code/software that is ready to run

5 – I would never use someone else's code, only my own!

Have you attended any previous courses dedicated to HPC (or with a large HPC component)?

1 – No, just starting out with HPC

5 – I've lost count, so much to learn..

How freaked out are you about the prospect of working in an HPC environment

1 – Very! Help

5 – I'm cool, just here to dot the i's and cross the t's

How much support do you have in your home institute?

1 – None, I have to do this by myself or find outside support

5 – My group is heavily into HPC and I'll be supported every step of the way

Have you used an HPC machine before?

1 – Never, I wouldn't even know where to start

5 – Every day, I live in the HPC environment

Do you know how to gain access to time on an HPC machine?

1 – No!

5 – I have allocated time on multiple HPC machine

Online resources

BioExcel webinar series

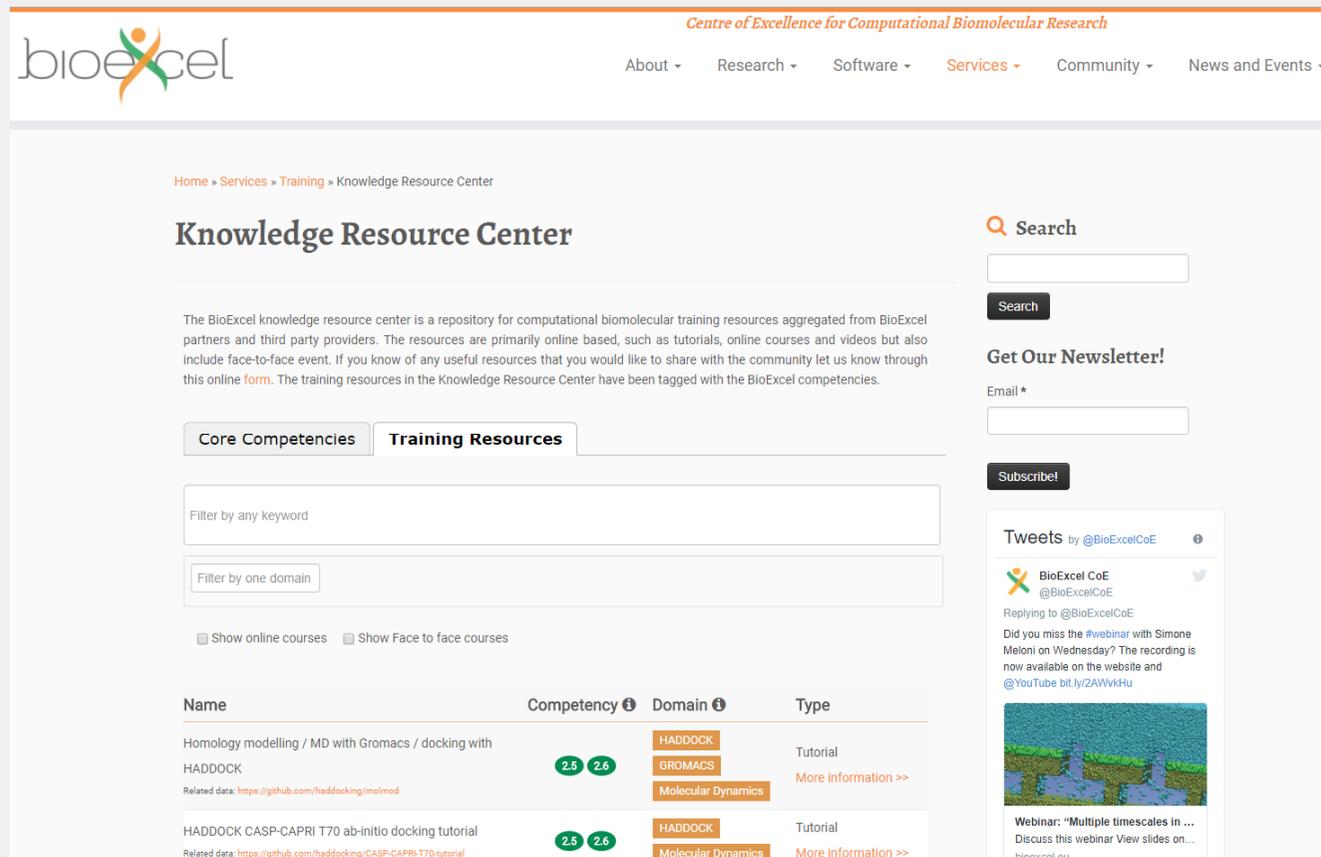
- Wednesday 14:00 GMT / 15:00 CET
- Video on the website afterwards
<http://bioexcel.eu/category/webinar/>

Knowledge Resource Center

- Relevant F2F courses (internal & external)
- Relevant tutorials, courses, best practice docs
- Beta version
- Content review

BioExcel Knowledge Resource Center

<http://krc.bioexcel.eu/>



The screenshot shows the BioExcel Knowledge Resource Center website. At the top, there is a navigation bar with the BioExcel logo and menu items: About, Research, Software, Services, Community, and News and Events. The main content area is titled "Knowledge Resource Center" and includes a breadcrumb trail: Home » Services » Training » Knowledge Resource Center. A paragraph describes the center as a repository for computational biomolecular training resources. Below this, there are tabs for "Core Competencies" and "Training Resources". A search bar and a "Search" button are present. A "Get Our Newsletter!" section includes an email input field and a "Subscribe" button. A "Tweets" section shows a tweet from BioExcel CoE (@BioExcelCoE) replying to another tweet, mentioning a webinar recording. At the bottom, a table lists training resources with columns for Name, Competency, Domain, and Type.

Centre of Excellence for Computational Biomolecular Research

bioexcel

About ▾ Research ▾ Software ▾ Services ▾ Community ▾ News and Events ▾

Home » Services » Training » Knowledge Resource Center

Knowledge Resource Center

The BioExcel knowledge resource center is a repository for computational biomolecular training resources aggregated from BioExcel partners and third party providers. The resources are primarily online based, such as tutorials, online courses and videos but also include face-to-face event. If you know of any useful resources that you would like to share with the community let us know through this online [form](#). The training resources in the Knowledge Resource Center have been tagged with the BioExcel competencies.

Core Competencies Training Resources

Filter by any keyword

Filter by one domain

Show online courses Show Face to face courses

Name	Competency	Domain	Type
Homology modelling / MD with Gromacs / docking with HADDOCK Related data: https://github.com/haddock/molmod	2.5 2.6	HADDOCK GROMACS Molecular Dynamics	Tutorial More information >>
HADDOCK CASP-CAPRI T70 ab-initio docking tutorial Related data: https://github.com/haddock/CASP-CAPRI-T70-tutorial	2.5 2.6	HADDOCK Molecular Dynamics	Tutorial More information >>

Search

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Subscribe!

Tweets by @BioExcelCoE

BioExcel CoE @BioExcelCoE
Replying to @BioExcelCoE
Did you miss the #webinar with Simone Meioni on Wednesday? The recording is now available on the website and @YouTube bit.ly/2AWvKHu

Webinar: "Multiple timescales in ...
Discuss this webinar View slides on...
bioexcel.eu

Summer school 2018

18-22nd June 2018

Cagliari, Sardinia



Use case based summer school

- Showcasing BioExcel resources
- Potentially expanded use case developed for community forum



Keep an eye on the website for details

How to get in touch with us

www.bioexcel.eu



@BioExcelCoE



Company Page



ask.bioexcel.eu

About < People

Announce updates,
training courses,
webinars & papers

Subscribe to mailing list

User support forum

Interest Groups

- BioExcel aims to foster a community around computational biomolecular research and **support existing communities**
- An important link with wider communities is through **Interest Groups**: Smaller groups of named individuals who have chosen to be members of the group

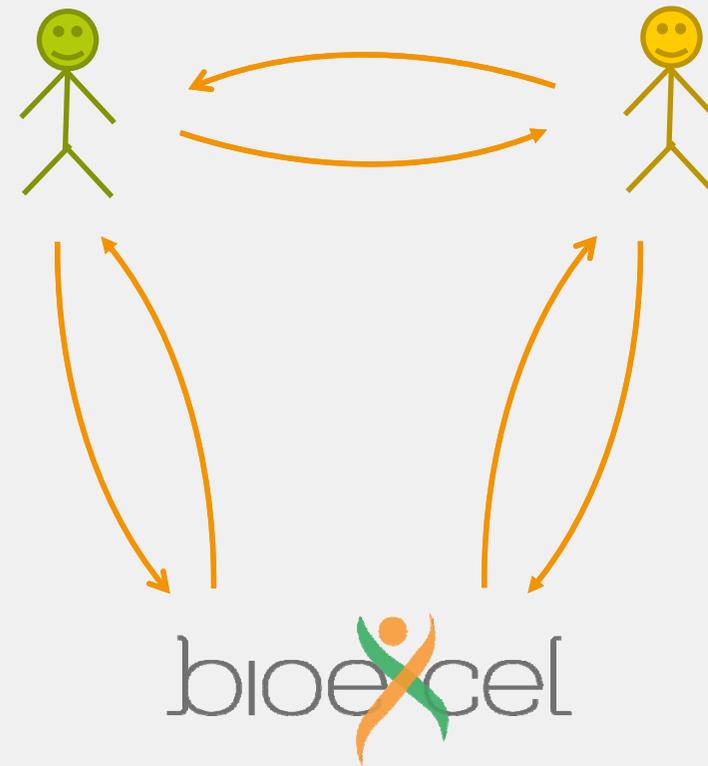
Interest Groups are **open to all**:
Sign up at bioexcel.eu/interest-groups.

Funding available to support face-to-face meetings

Interest Groups

Interest Groups will:

- Allow BioExcel to learn about its **users**
- Allow members to learn **from BioExcel**
- Aid communication **between** members
- Lead to user-driven **governance**



Interest Groups

- Entry Level Users
- Integrative Modeling
- Free Energy Calculations
- Hybrid methods
- Workflows
- Industry
- Training

www.bioexcel.eu/interest-groups

Support platforms

Forums



Code Repositories



Chat channel



Video Channel



Appendix

Home » Services » Training » Knowledge Resource Center

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HADDOCK CASP-CAPRI T70 ab-initio docking tutorial <small>Related data: https://github.com/haddock/CASP-CAPRI-T70-tutorial</small>	2.5 2.6	HADDOCK Molecular Dynamics	Tutorial More information >>

Search

Search

Get Our Newsletter!

Email *

Subscribe!

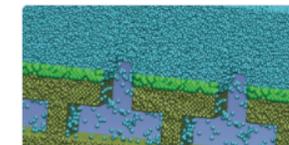
Tweets by @BioExcelCoE



BioExcel CoE
@BioExcelCoE

Replying to @BioExcelCoE

Did you miss the #webinar with Simone Meloni on Wednesday? The recording is now available on the website and @YouTube bit.ly/2AWvkHu



Webinar: "Multiple timescales in ...
Discuss this webinar View slides on...
bioexcel.eu

Filter by any keyword

Filter by one domain

Show online courses Show Face to face courses

Name

Competency **i**

Domain **i**

A domain allows us to cluster the related training resources into groups. You can filter on more than one domain.

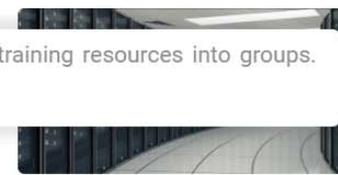
Homology modelling / MD with Gromacs / docking with HADDOCK Related data: https://github.com/haddock/molmod	2.5 2.6	HADDOCK GROMACS Molecular Dynamics	Tutorial More information >>
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WeNMR lecture on information-driven docking with HADDOCK	2.5 2.6	HADDOCK Molecular Dynamics	YouTube More information >>
Democratization of the WeNMR HADDOCK webportal (work in progress)		HADDOCK	YouTube

Subscribe!

Tweets by @BioExcelCoE



We were featured in this year's @etp #European #HPC handbook! bioexcel.eu/european-hpc-h...



BioExcel CoE Retweeted



Our first webinar, and free to all. Register here: register.gotowebinar.com/register/367 and join us next Wednesday with @CompSciOxford and in collaboration

Competency 2.6

Evaluate the ability of a computer-based system, process, component, or program to meet desired needs in a biomolecular context.

Knowledge

- Has a deep comprehension of biological problems
- Comprehend the capabilities and limitations of computer-based system, process, component and programs.

Skill

- Creative thinking & problem solving
- Has an interdisciplinary view

Behaviour

- Keeps up-to-date with emerging techniques and applications

[Go to competency profile](#)

Core Competencies

Training Resources

Filter by any keyword

Competency number

Name and description

1

Generic Competencies

Function effectively in teams to accomplish a common goal.

Knowledge

- Understanding of the context of the persons in the team
- Aware of cultural differences

Skill

- Communication
- Conflict management
- Time management

1.1

Behaviour

- Invites two-way communication; actively listens/pays attention; able to excite participation and commitment from others
- Delivers on his/her actions and inspires this behaviour in others
- Informs others of relevant information appropriately and on time

[View related training resources](#)

Core Competencies

Training Resources

1.1

Filter by one domain

Show online courses Show Face to face courses

Clear filters

Name	Competency ⓘ	Domain ⓘ	Type
Professional Skills in Drug Discovery <small>Related data: http://www.ed.ac.uk/</small>	1.1 1.4 2.12	Life Science	online More information >>