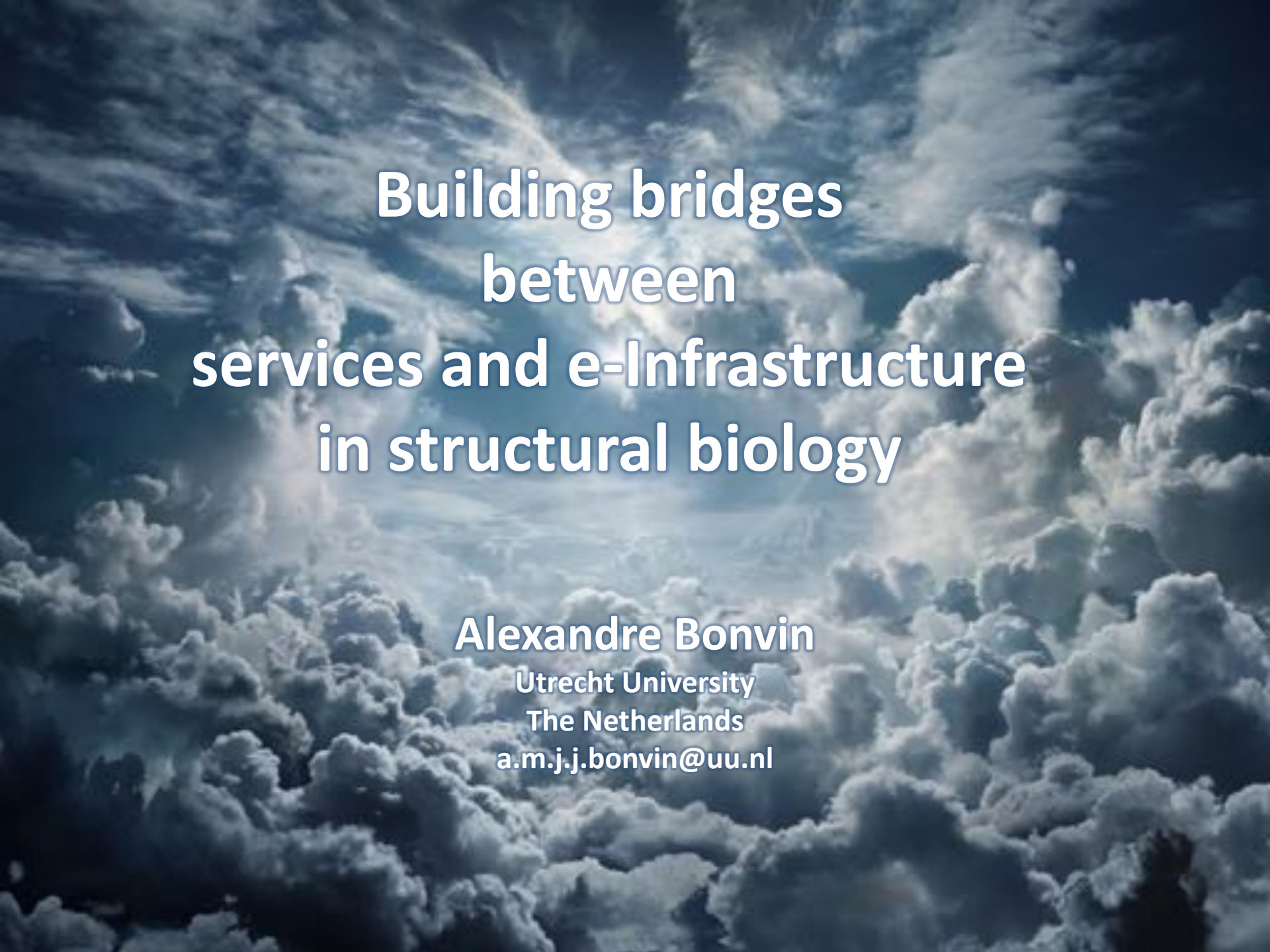


Building bridges between services and e-Infrastructure in structural biology

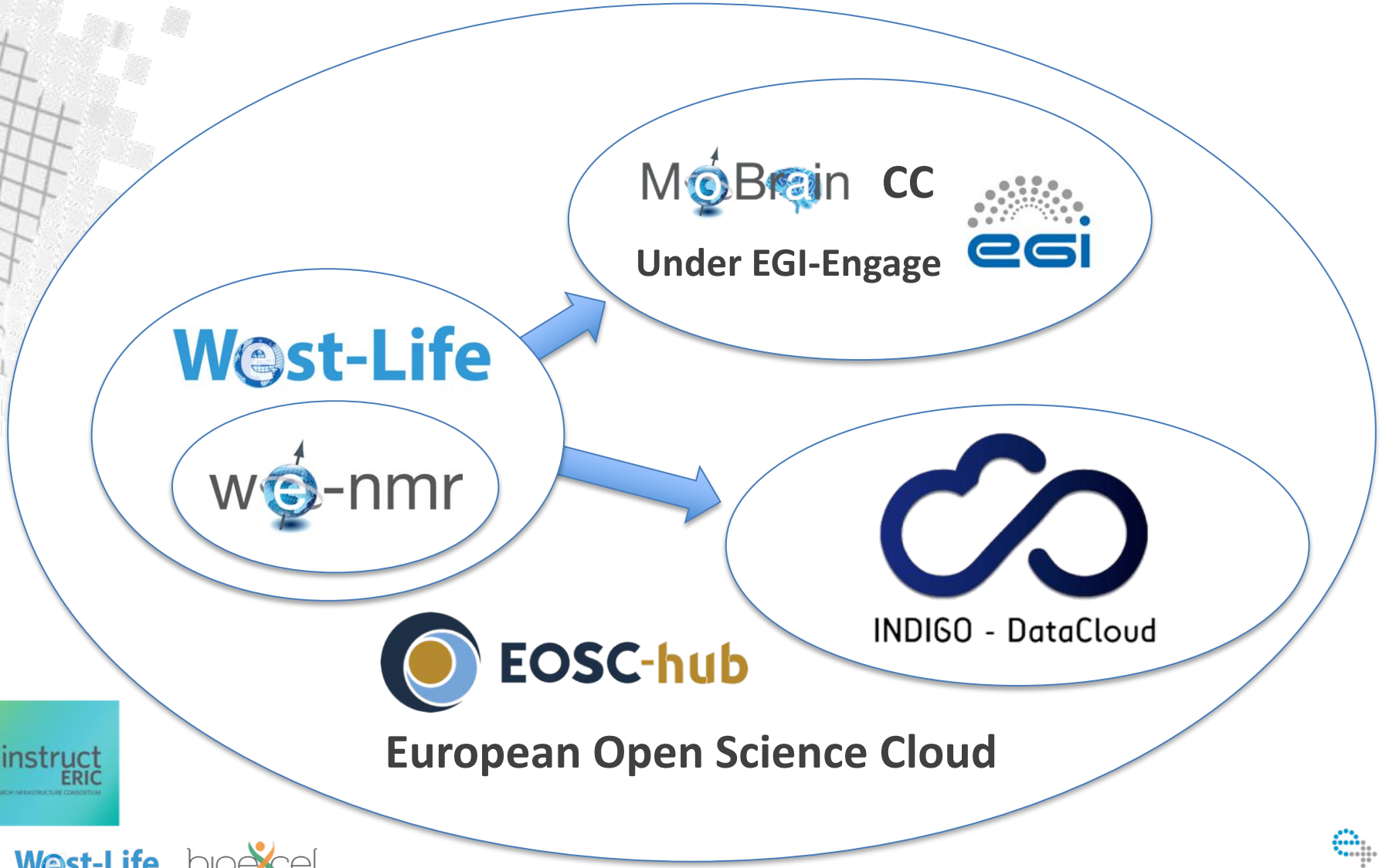
Alexandre Bonvin

Utrecht University

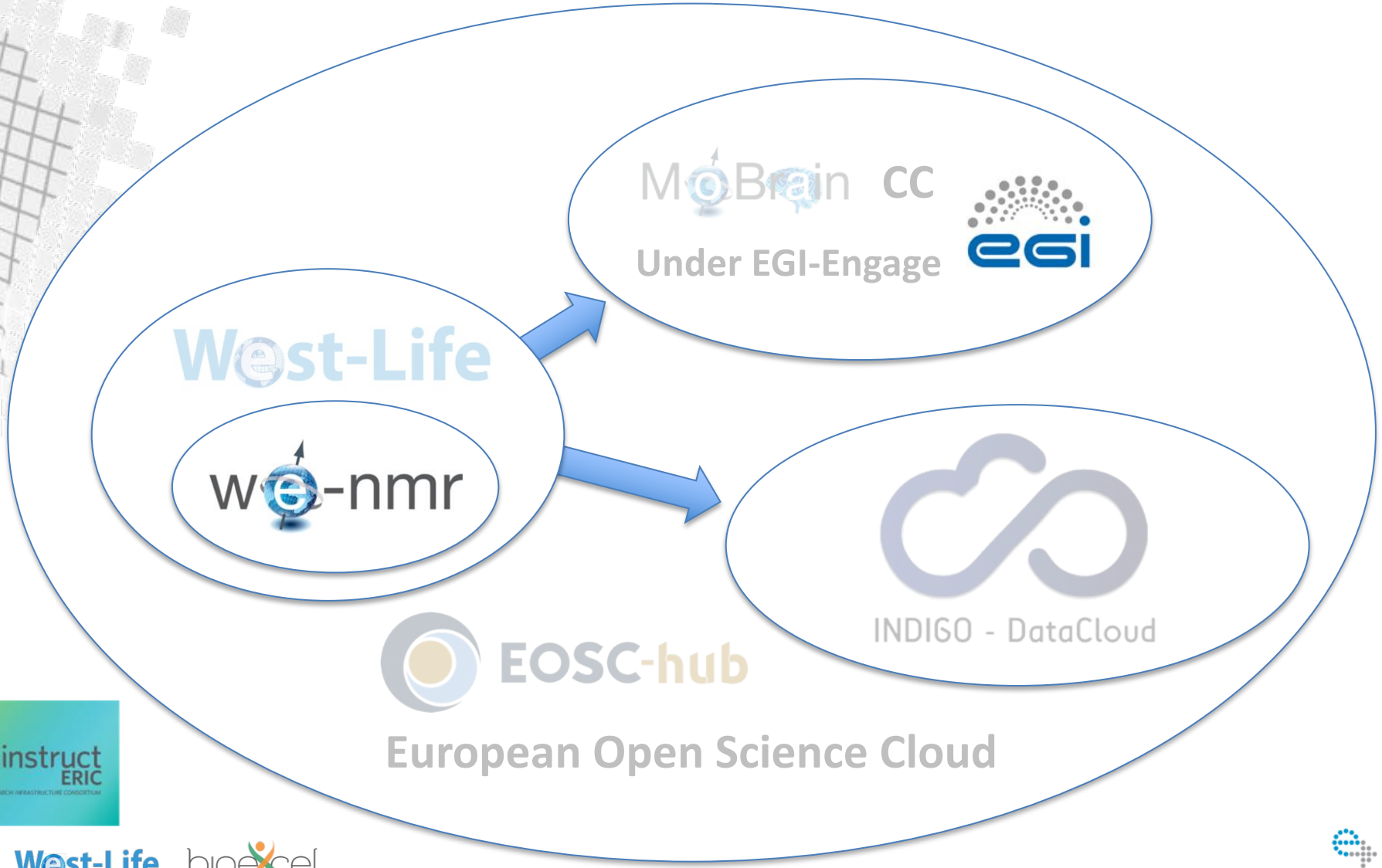
The Netherlands

a.m.j.j.bonvin@uu.nl

The structural biology e-Infrastructure landscape over the years



The structural biology e-Infrastructure landscape over the years



EOSC-hub

Virtual Research Community

INDIGO - DataCloud

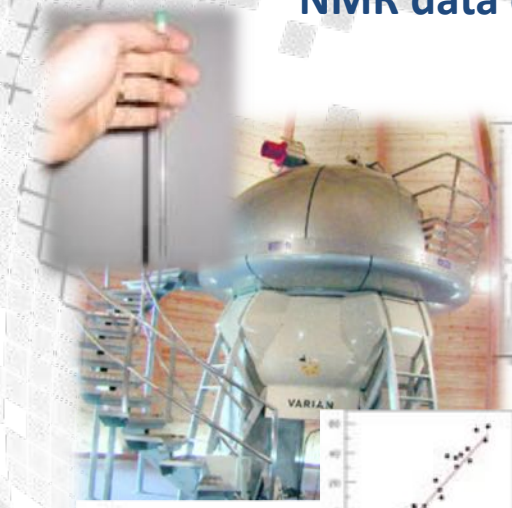
West-Life Structures for Life

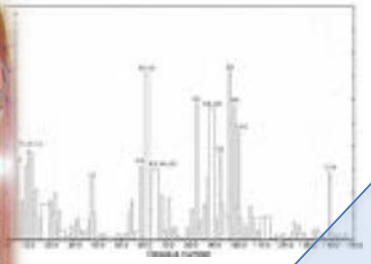
bioexcel Center of Excellence for Computational Biomolecular Research

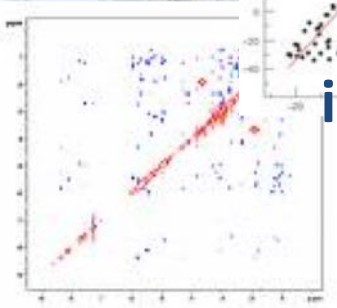
e-infrastructure

Exploiting GRID resources in structural biology…

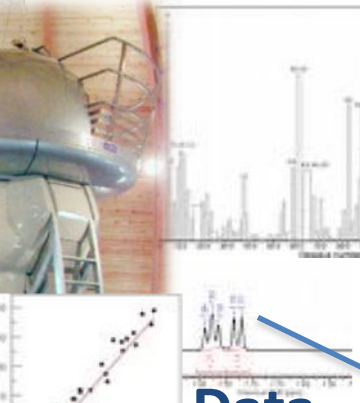
NMR data collection and processing





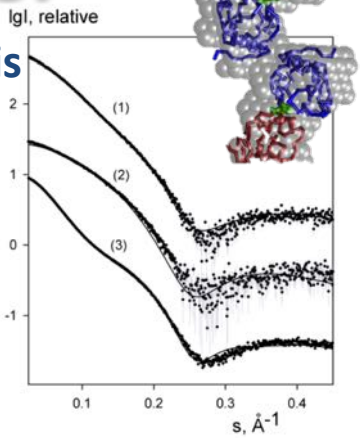


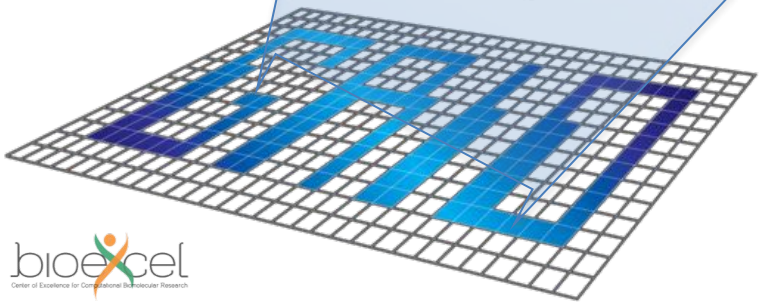
Data interpretation



Computations

SAXS data analysis





Structure, dynamics & interactions

➔ impact on research and health:

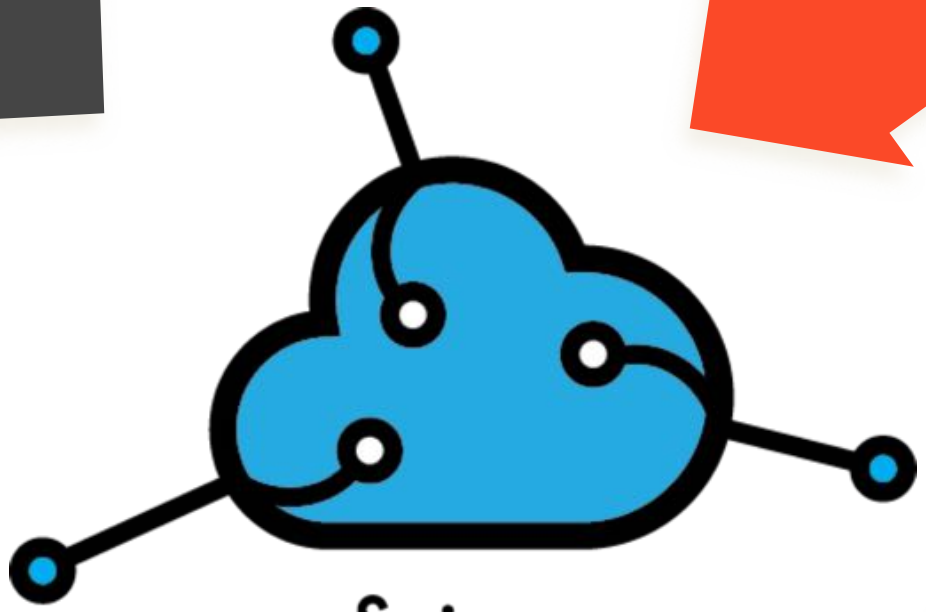
- origin of disease
- design of new experiments
- drug design…

EOSC hub
INDIGO - DataCloud
West-Life Structures for Life
bioexcel Center of Excellence for Computational Biomolecular Research
e-infrastructure

The WeNMR VRC

Community

Infrastructure



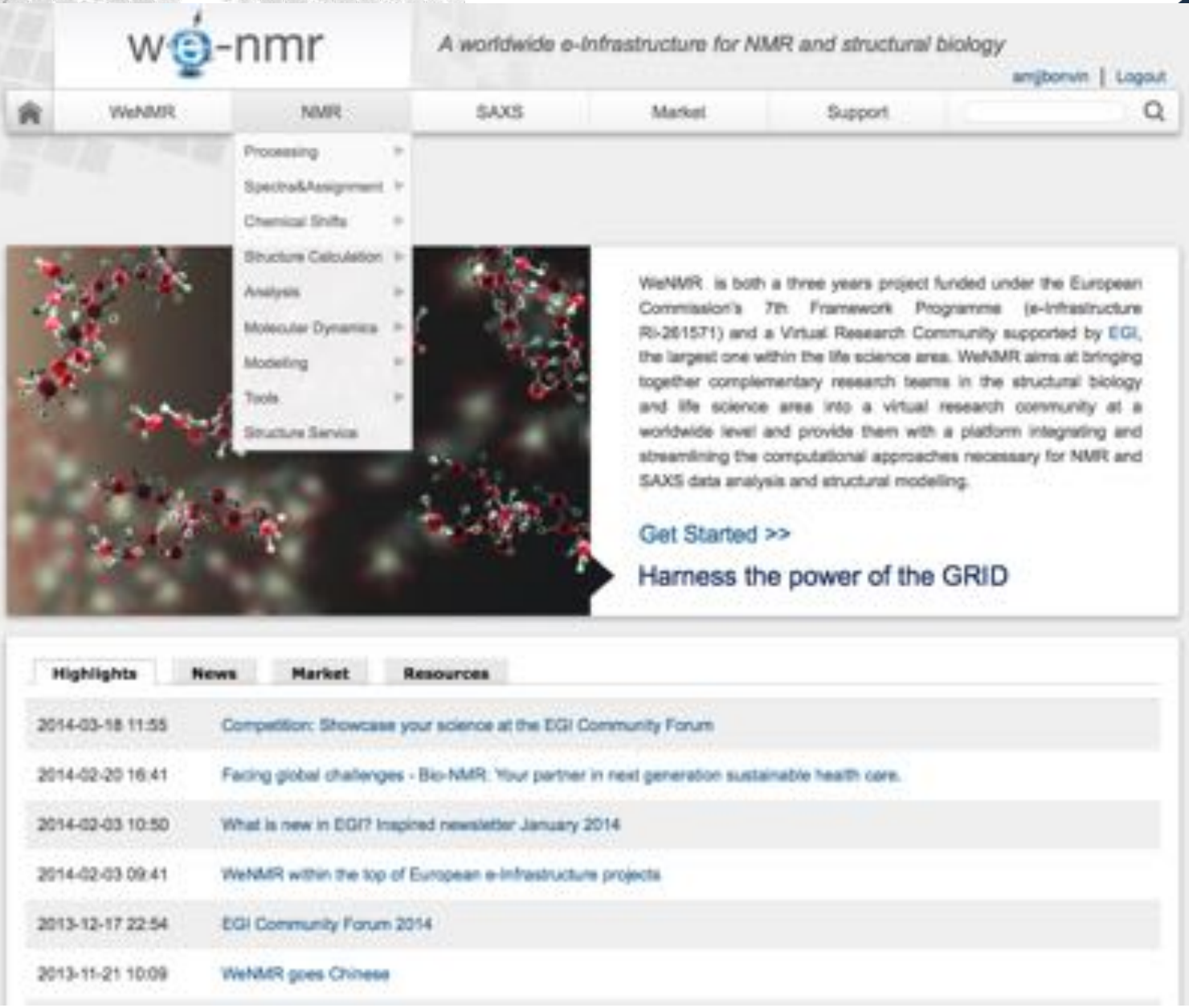
eScience
hub in the Cloud

Science

Knowledge

eScience hub for NMR and structural biology

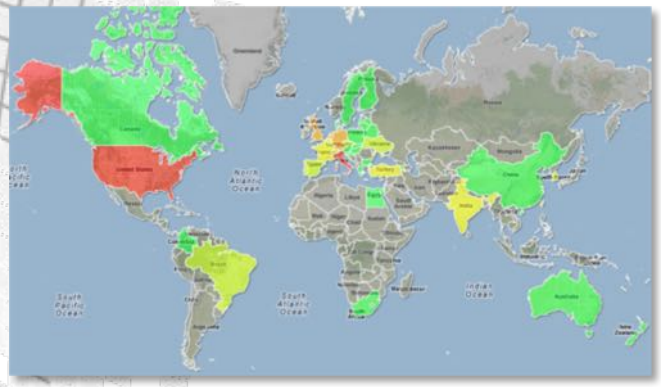
t-Life Structures for Life
bioexcel Center of Excellence for Computational Biomolecular Research
e-in

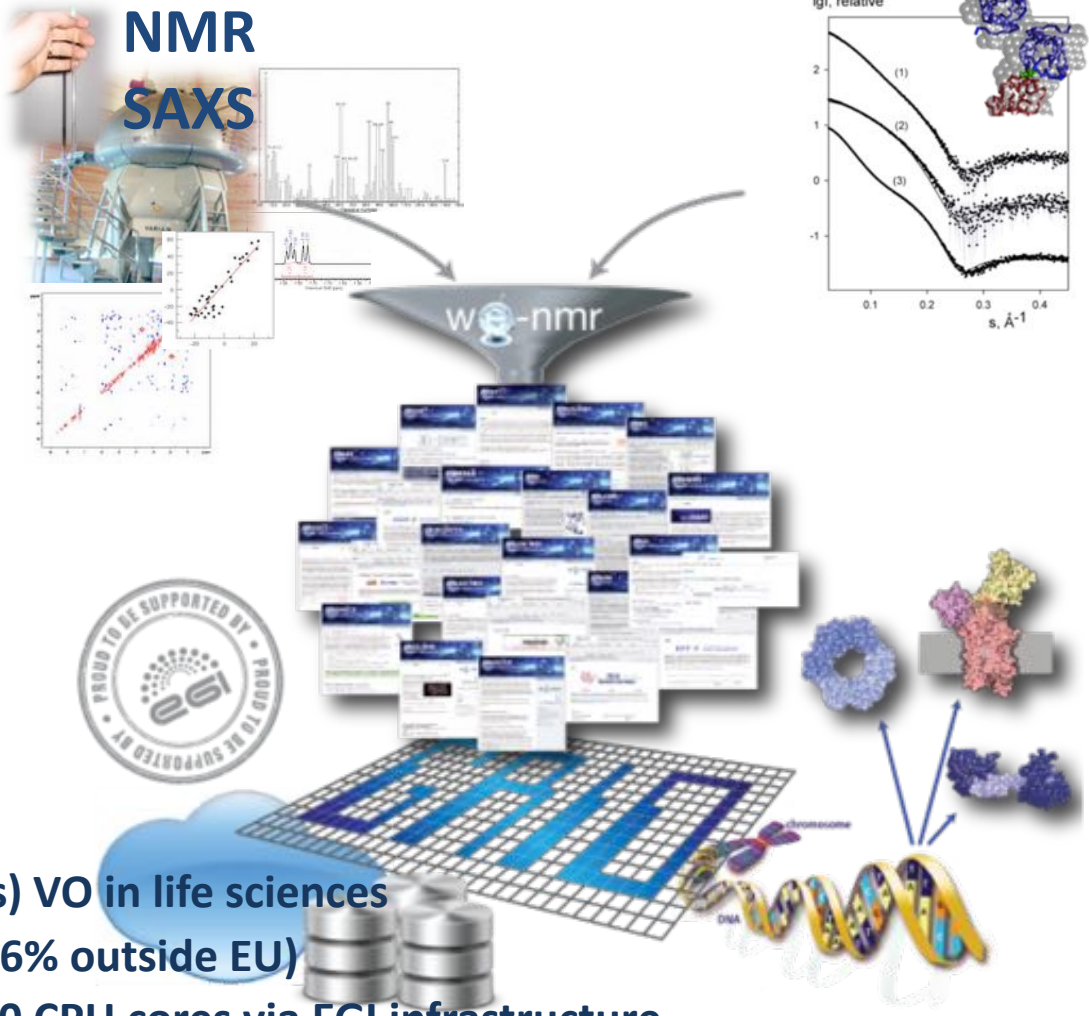


www.wenmr.eu

INDIGO - DataCloud
West-Life Structures for Life
bioexcel Center of Excellence for Computational Biomolecular Research
e-infrastructure

A worldwide e-Infrastructure for NMR and structural biology





WeNMR VRC (February 2018)

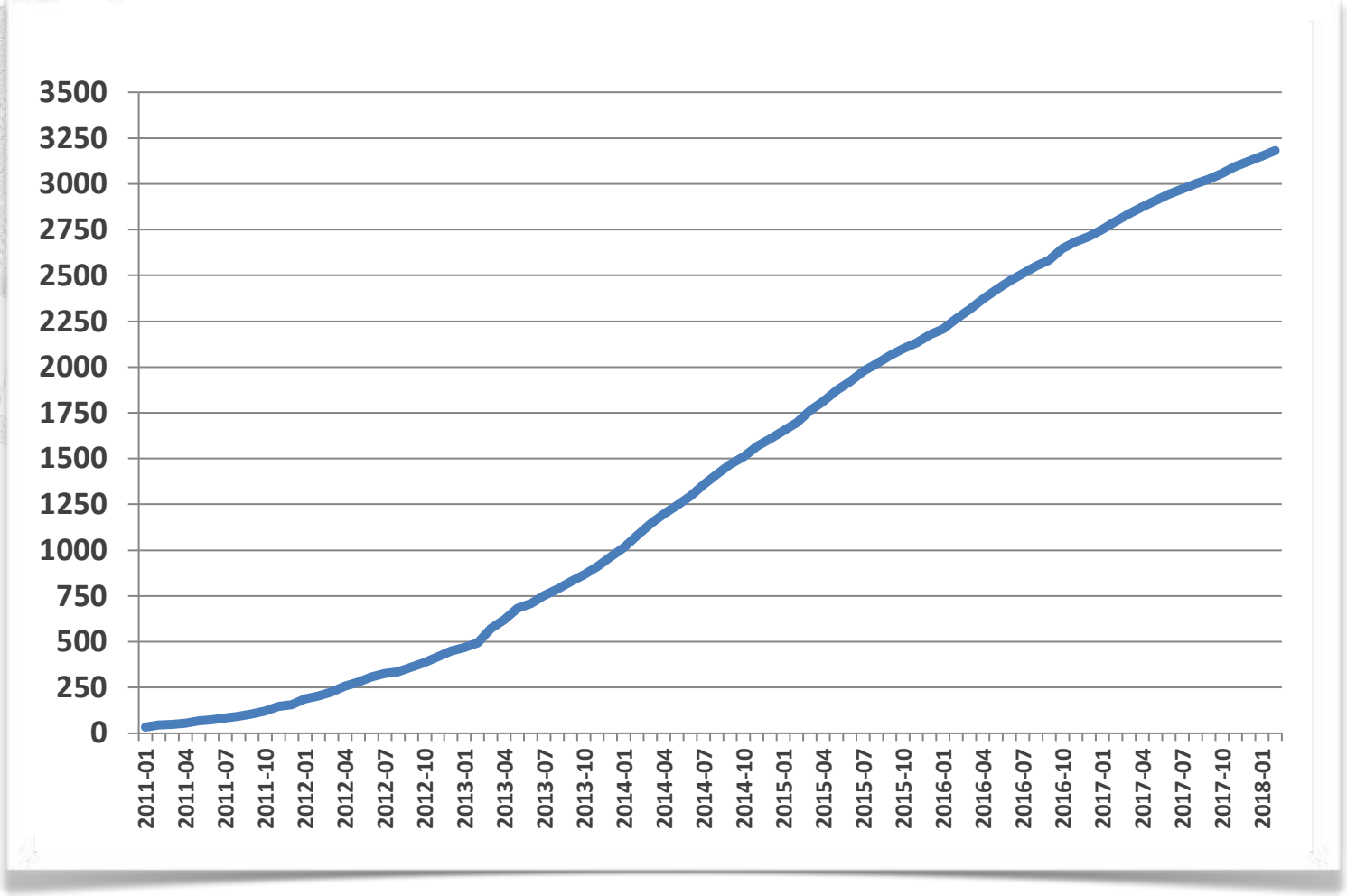
- enmr.eu: One of the largest (#users) VO in life sciences
- >830 users have registered so far(36% outside EU)
- Support from >40 sites for >200'000 CPU cores via EGI infrastructure
- User-friendly access to Grid via web portals
- Supported by an SLA (2016, updated in 2017) with EGI and NGIs

www.wenmr.eu

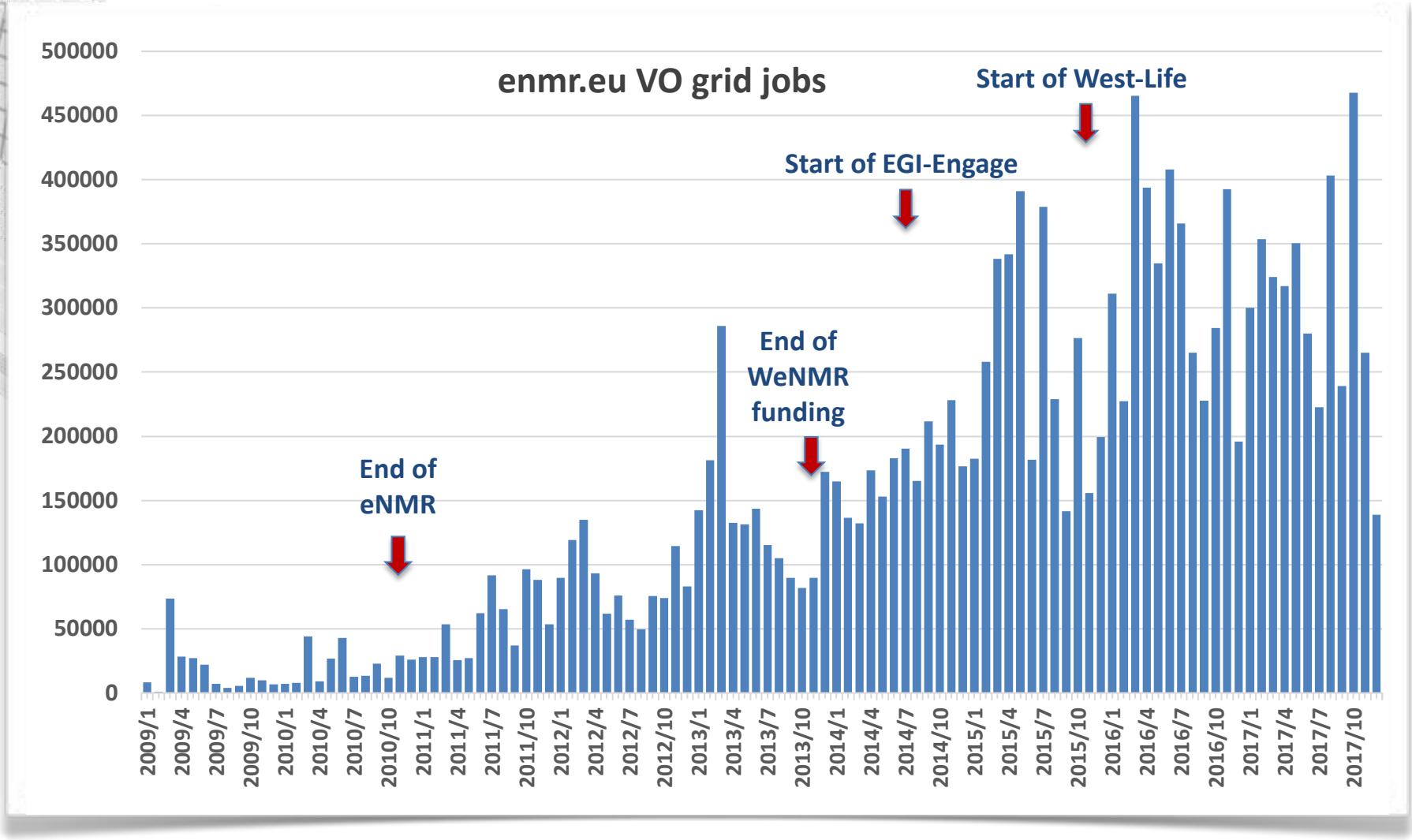
we-nmr

INDIGO - DataCloud · West-Life Structures for Life · bioexcel Center of Excellence for Computational Biomolecular Research · e-infrastructure

Sustained growth of the WeNMR VRC



Operational since 10 years



~2400 normalized CPU years over 2017

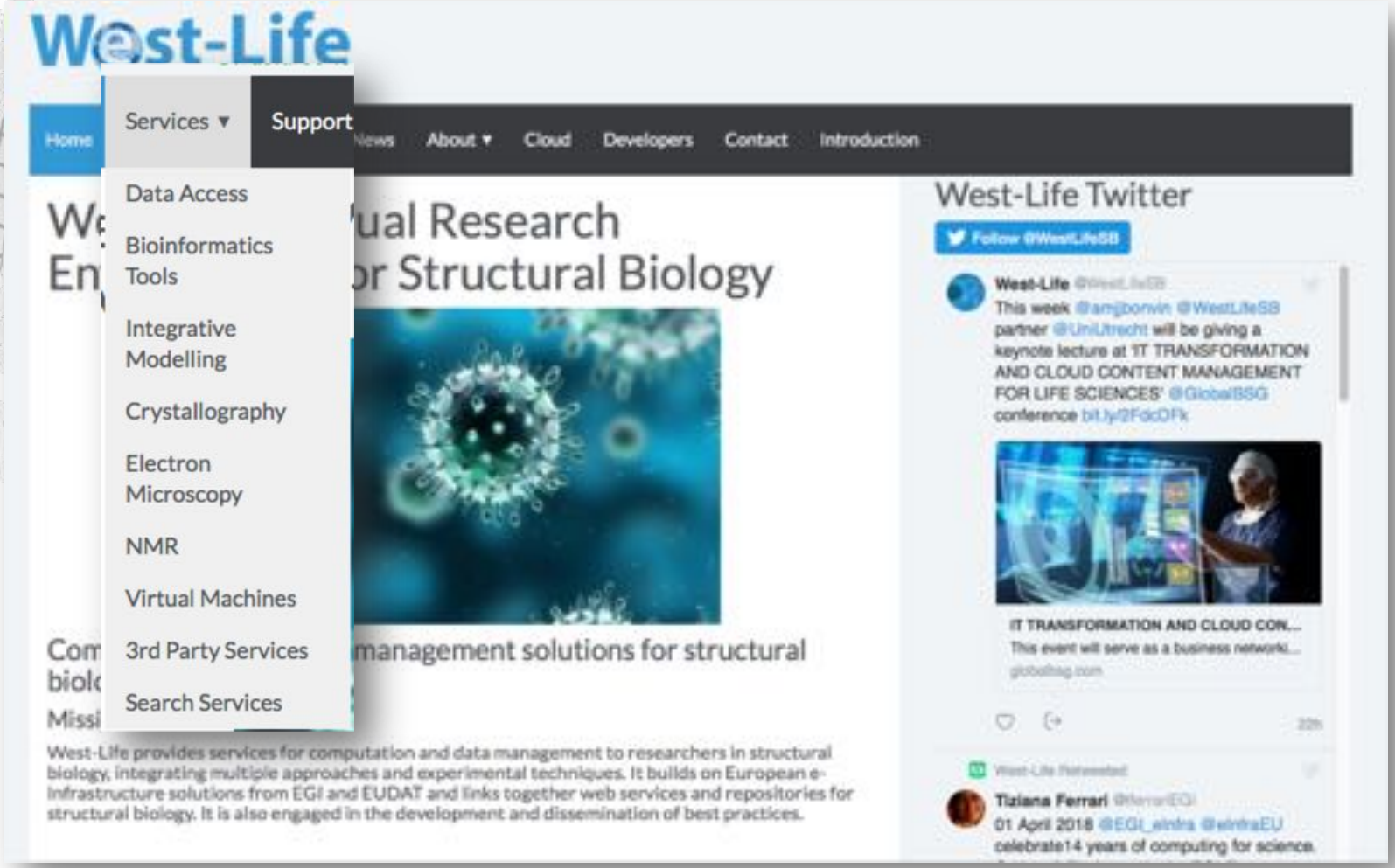
The West-Life VRE

west-life.eu

Challenges & e-Solutions

- Attract users!
  - Offer them top of the line eScience solutions for their research ... which means top of the line software

The West-Life VRE



west-life.eu

Thematic services under EOSC-Hub

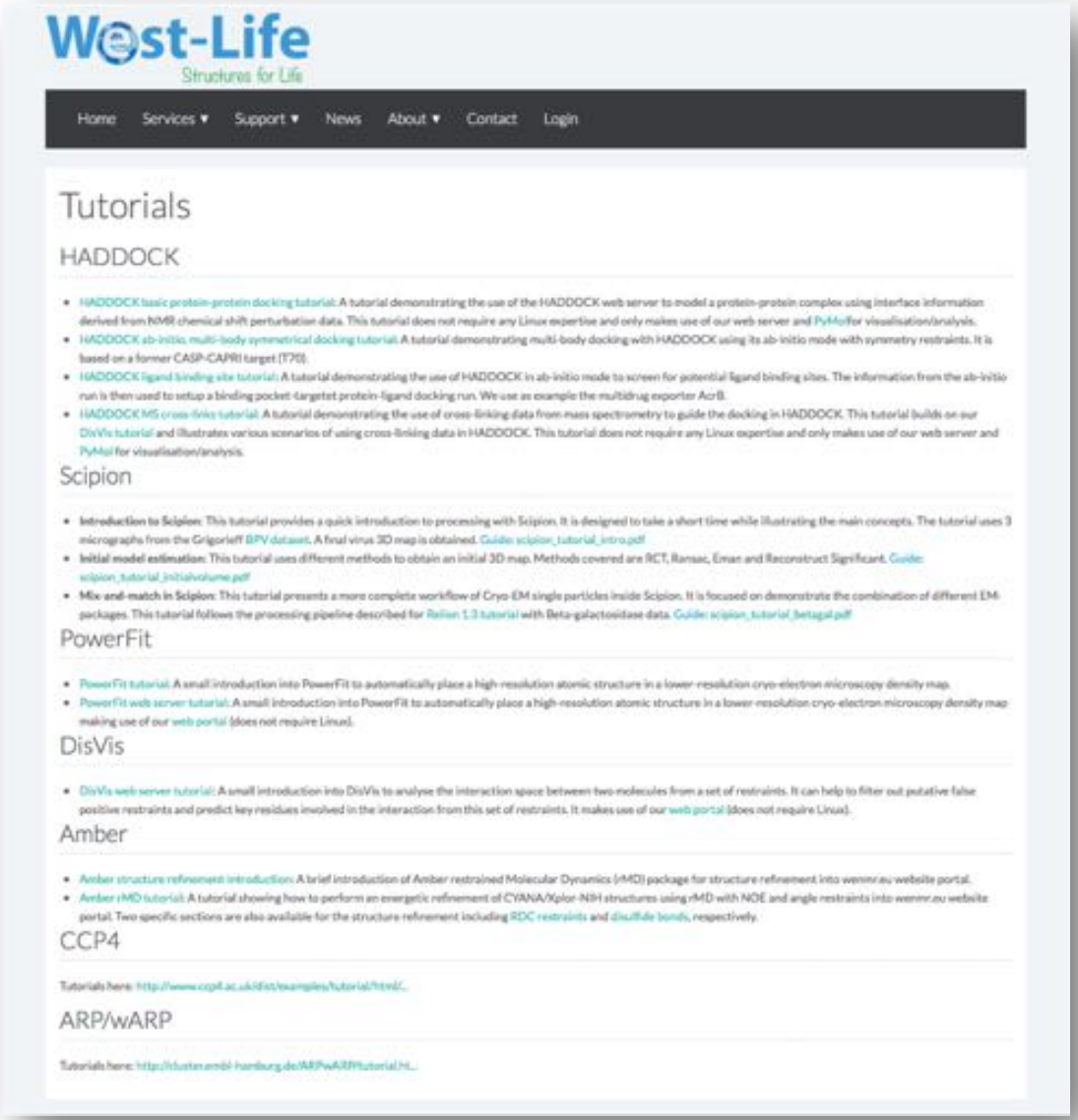
https://www.egi.eu/use-cases/scientific-applications-tools/

Challenges & e-Solutions

- **Attract users!**
  - **Offer them top of the line eScience solutions for their research ... which means top of the line software**
  - **Provide them training, tutorials and support**

West-Life knowledge and support center

- Various online tutorials aggregated in the support center



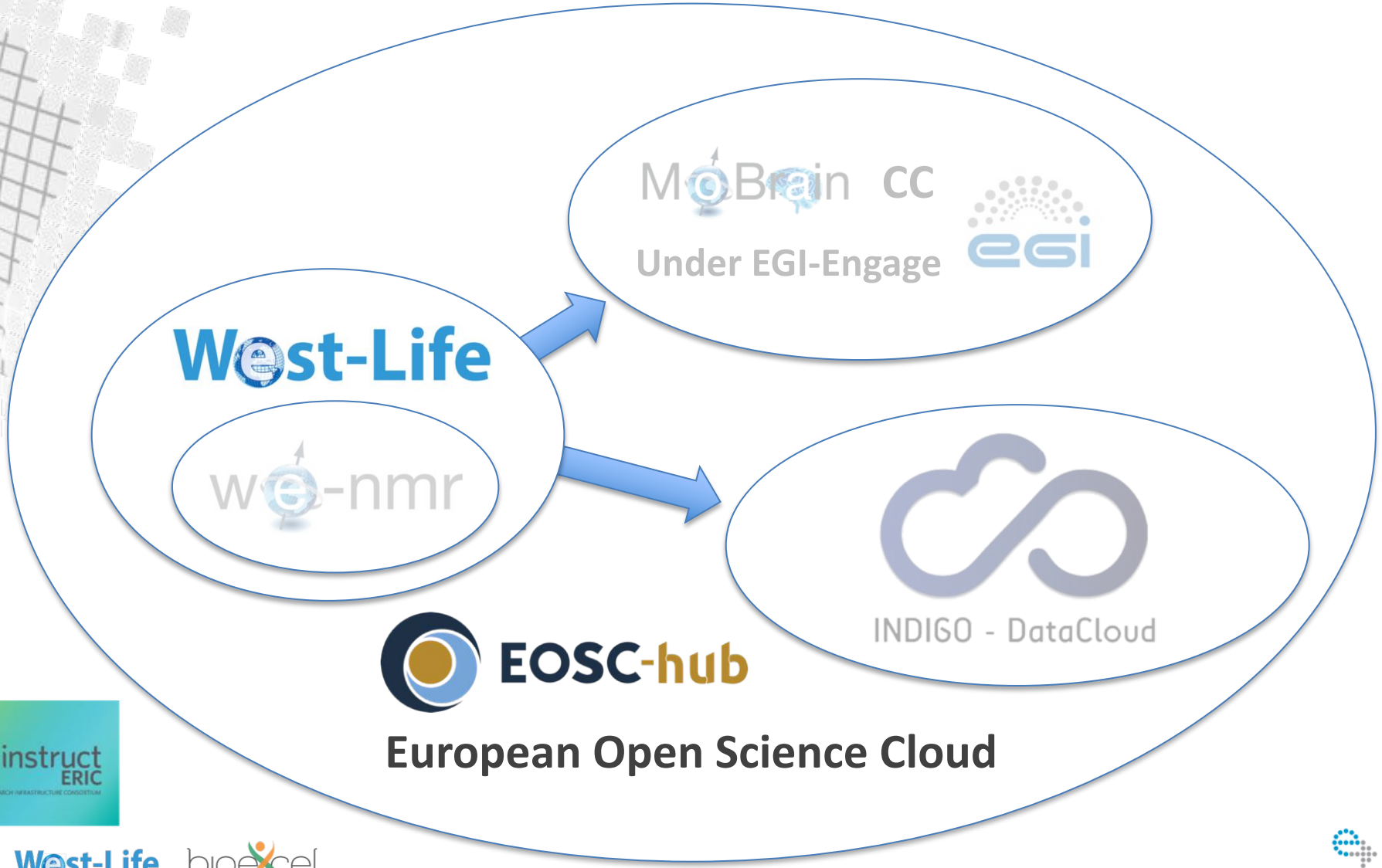
Challenges & e-Solutions

- **Attract users!**
  - Offer them top of the line eScience solutions for their research ... which means top of the line softwares)
  - Provide them training, tutorials and support
  - Make their life easier

    ➔ SSO mechanisms

    ➔ Build bridges between applications and with e-infrastructure solutions

Building bridges

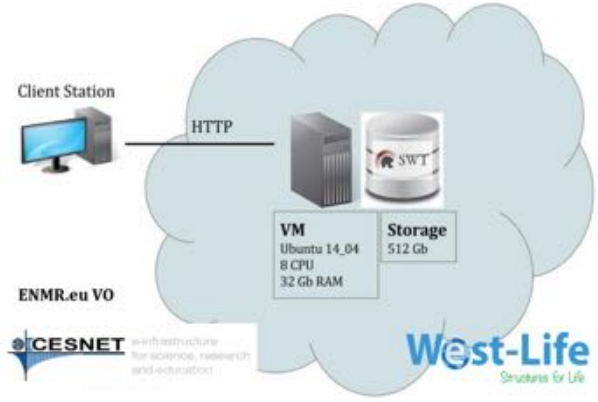


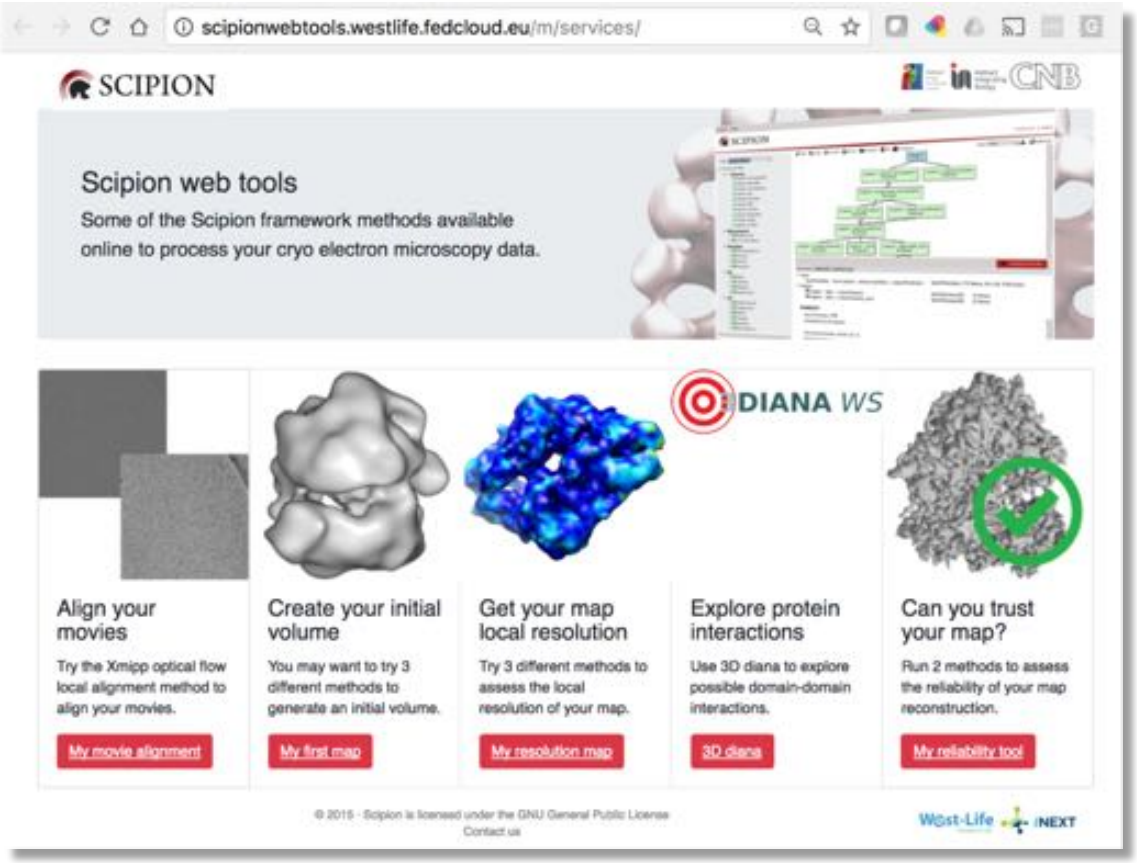
European Open Science Cloud

Building bridges between services

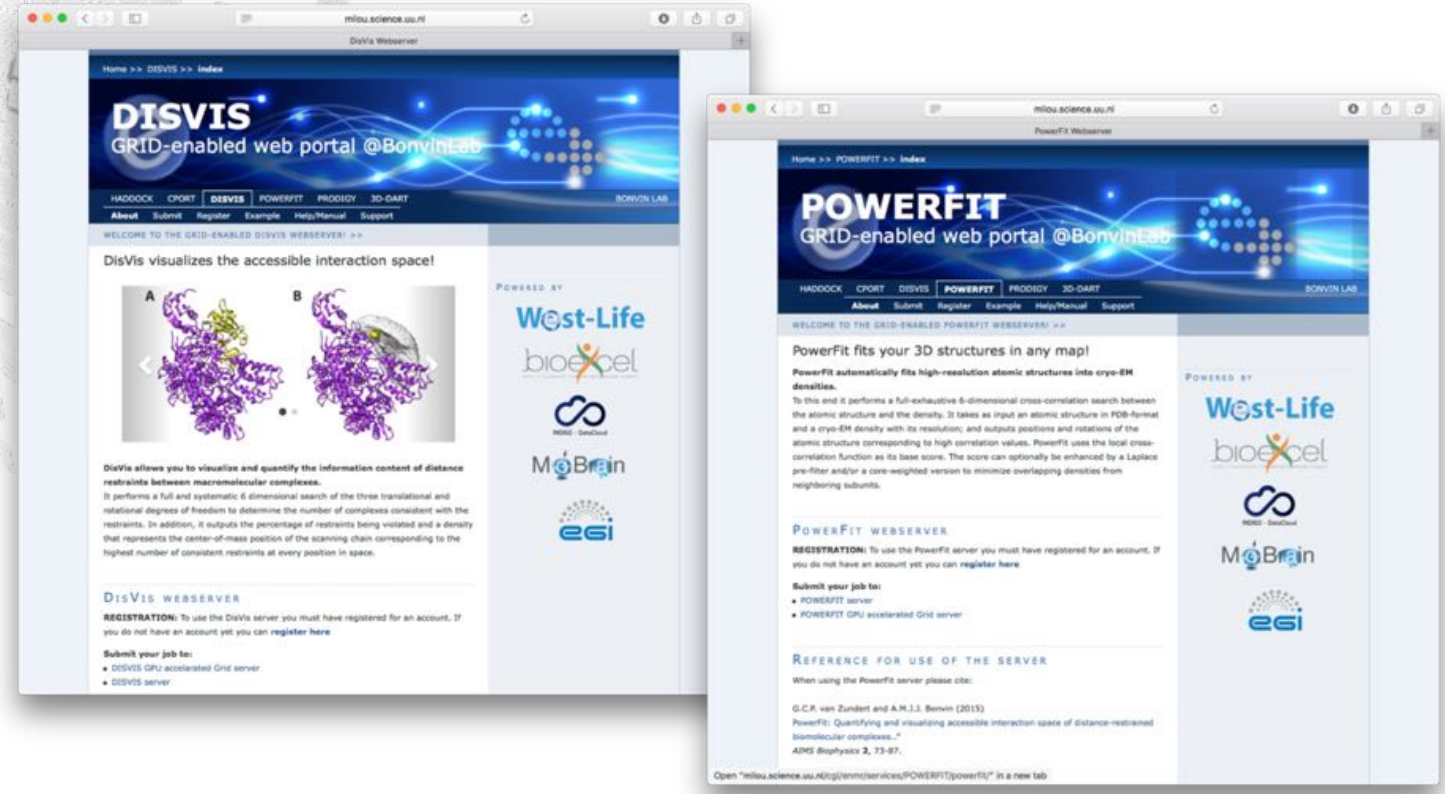
West-Life: Cryo-EM in the clouds

SCIPION cloud server in production





New grid, GPGPU-enabled web portals: DISVIS & POWERFIT



http://milou.science.uu.nl/enmr/services/DISVIS/

indigodatacloudapps/**disvis**

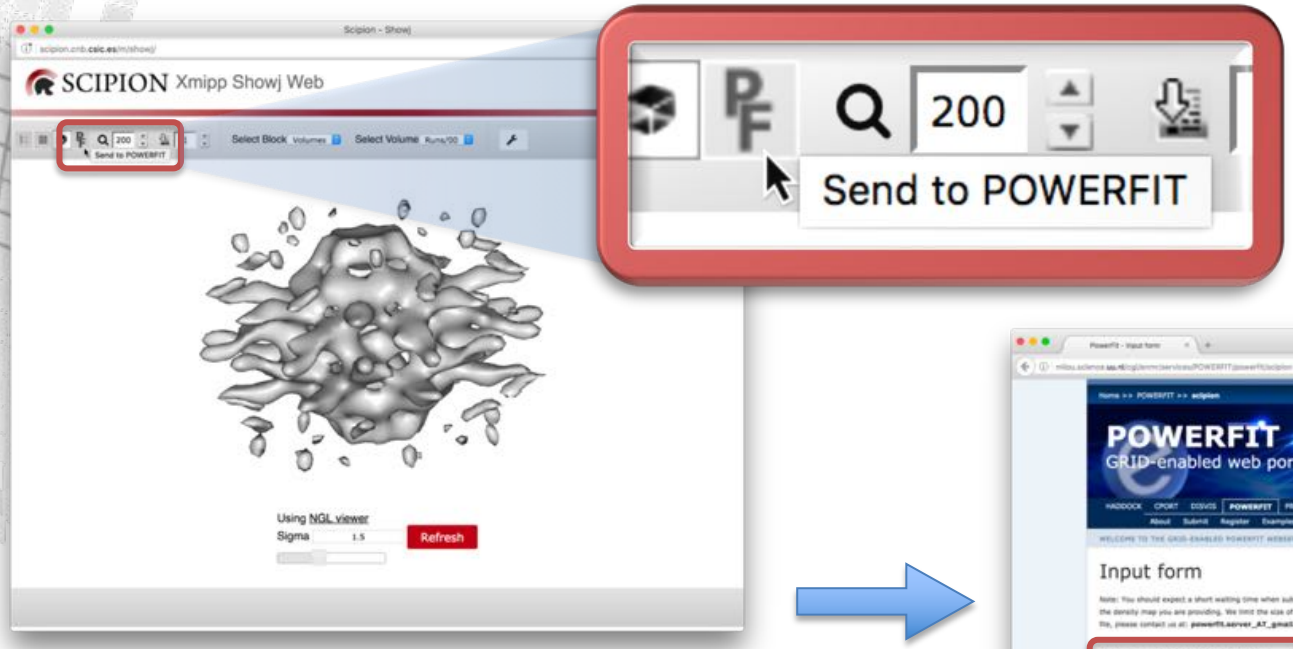
indigodatacloudapps/**powerfit**

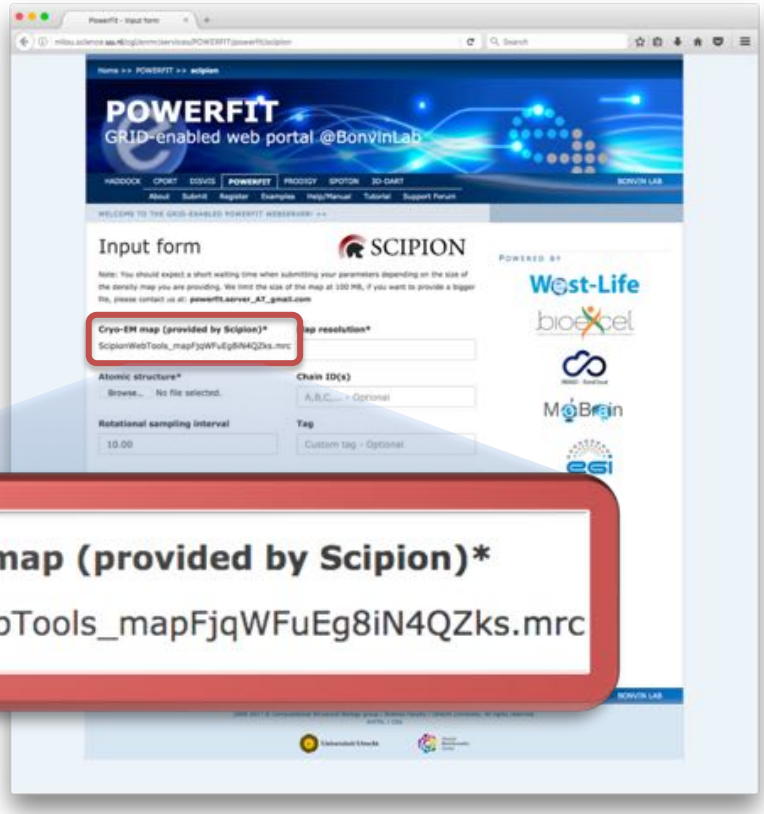
udocker
(Userspace Container Support)

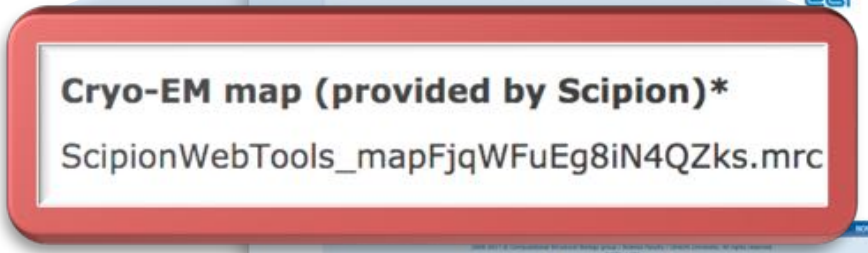
http://milou.science.uu.nl/enmr/services/POWERFIT/

- Hosted in Utrecht
- Implement INDIGO-Datacloud solutions
- Runs on GPGPU resources in Florence

Scipion – PowerFit workflow



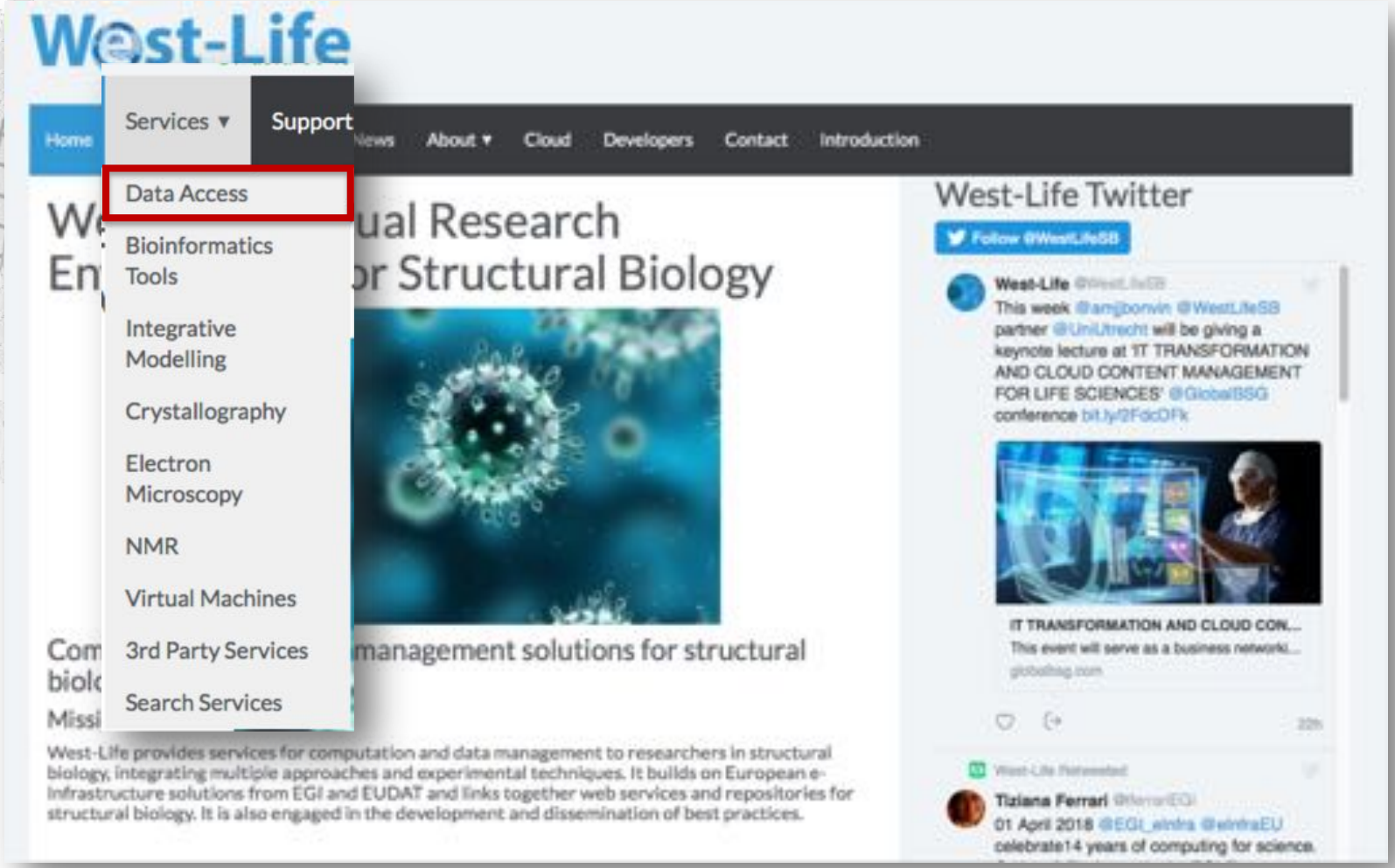




FANTEN – HADDOCK workflow

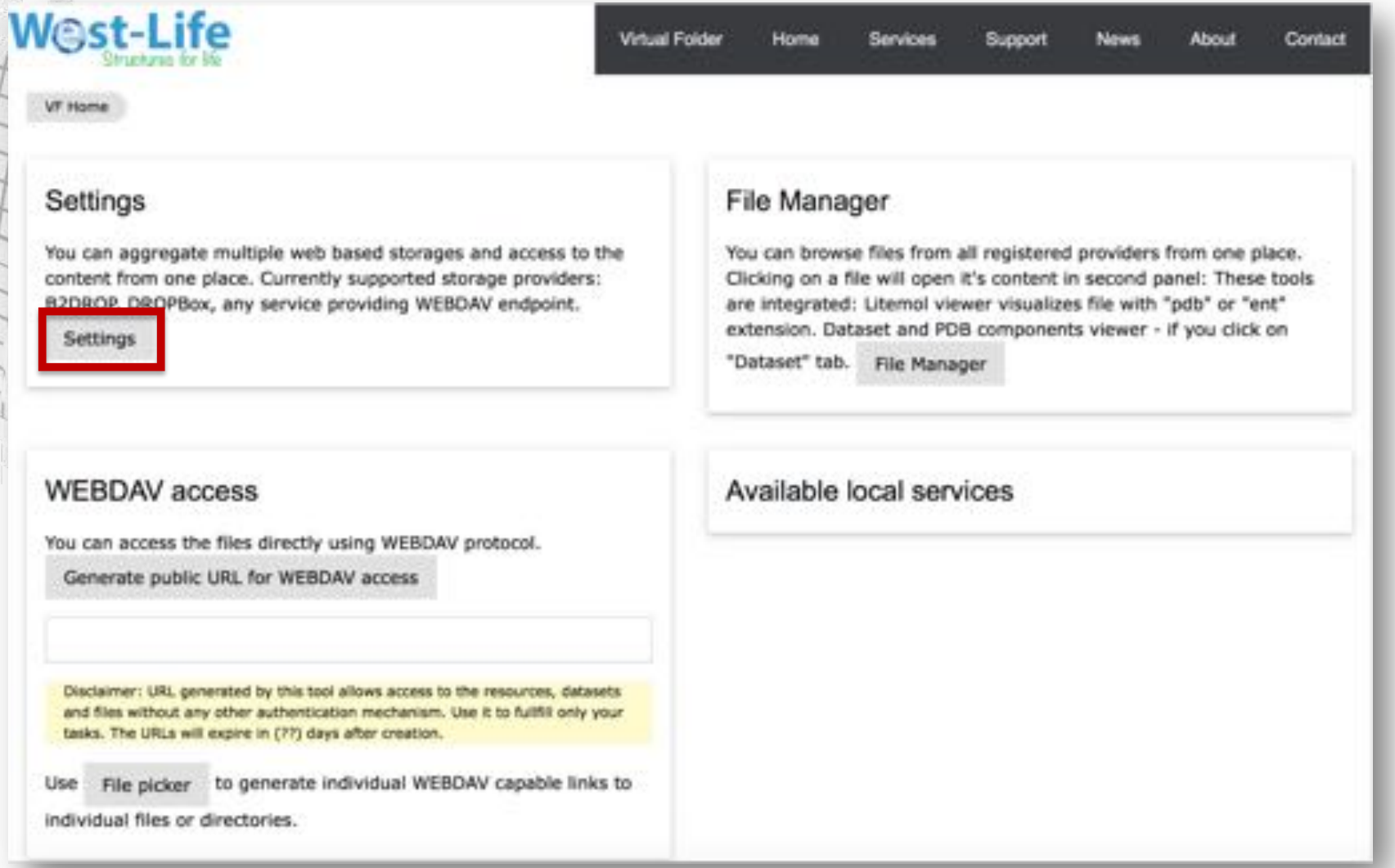
Building bridges with “cloud” storage

The West-Life VRE

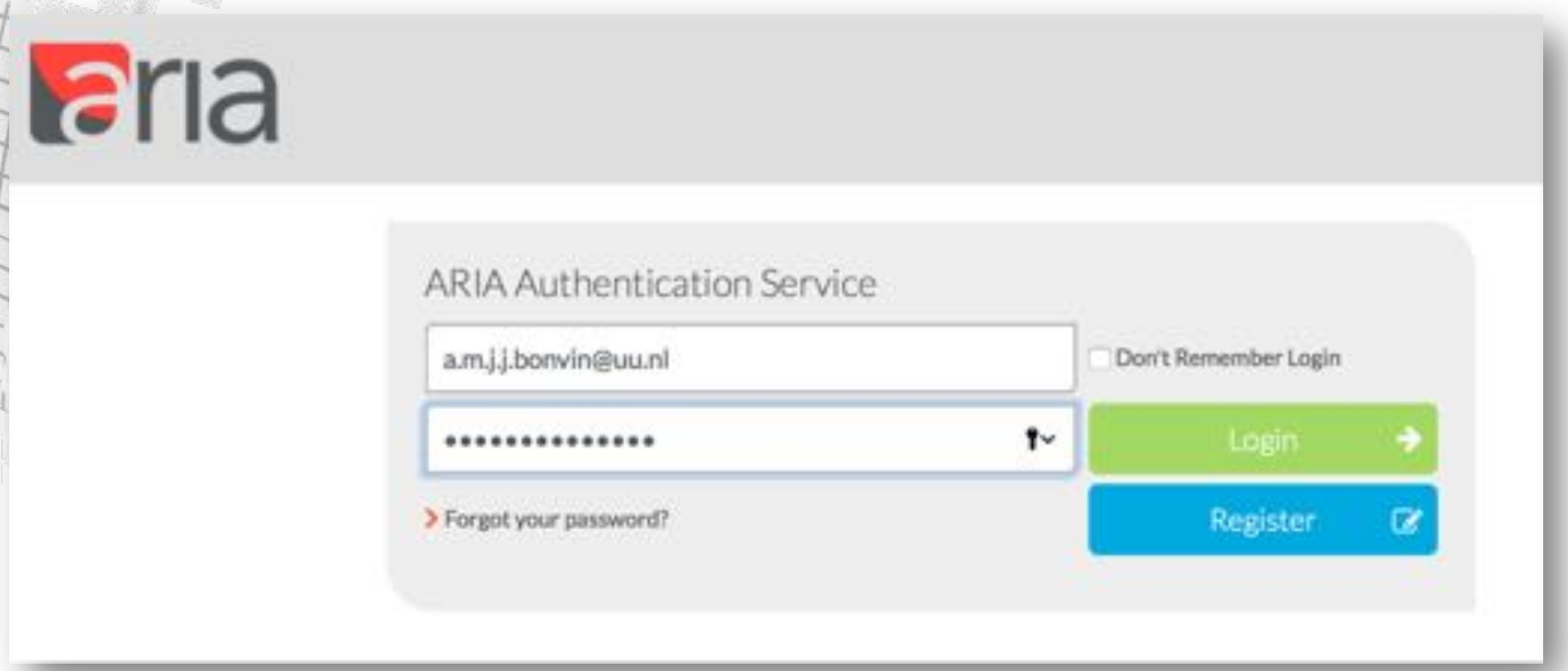


west-life.eu

The West-Life Virtual Folder

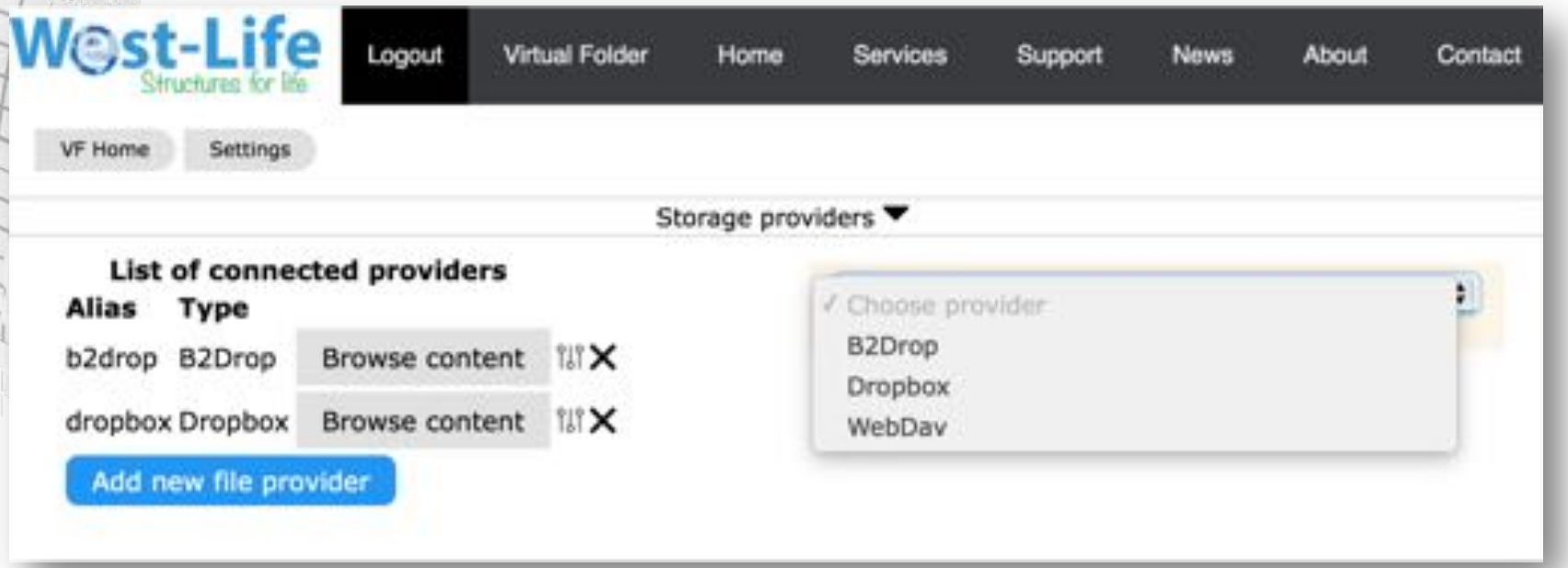


The West-Life Virtual Folder



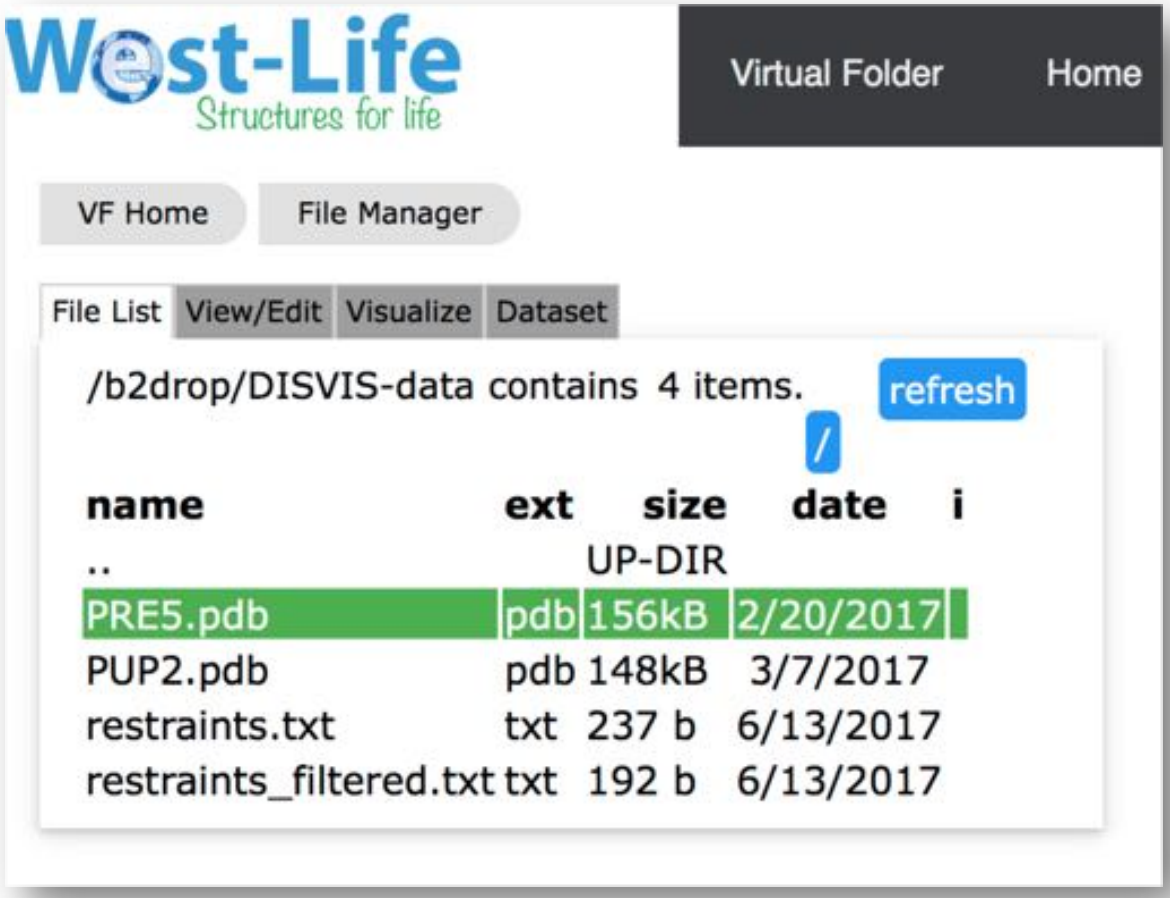
SSO authentification via INSTRUCT-ERIC

The West-Life Virtual Folder



Allows to aggregate storage providers

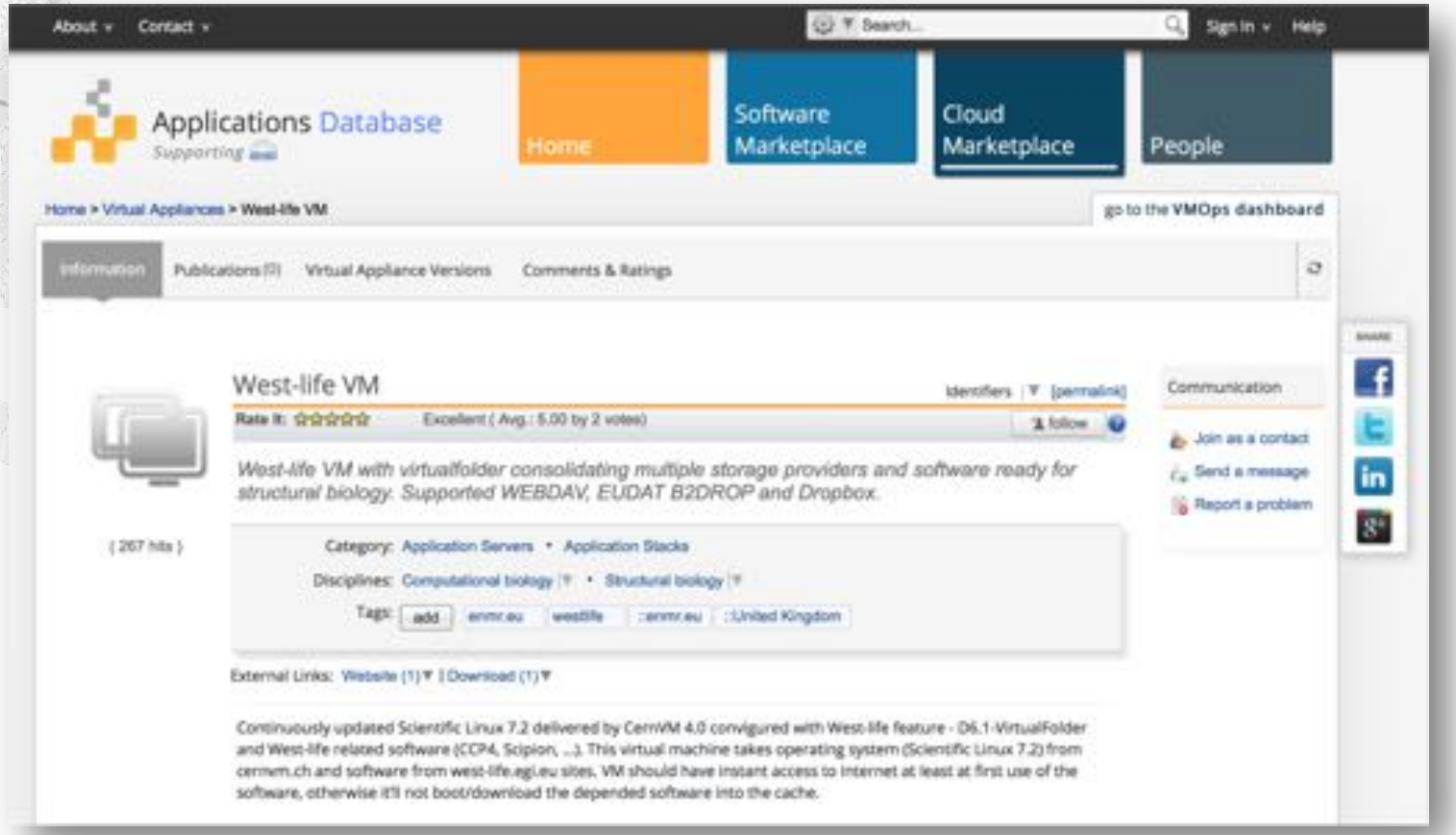
The West-Life Virtual Folder



Allows to browse storage

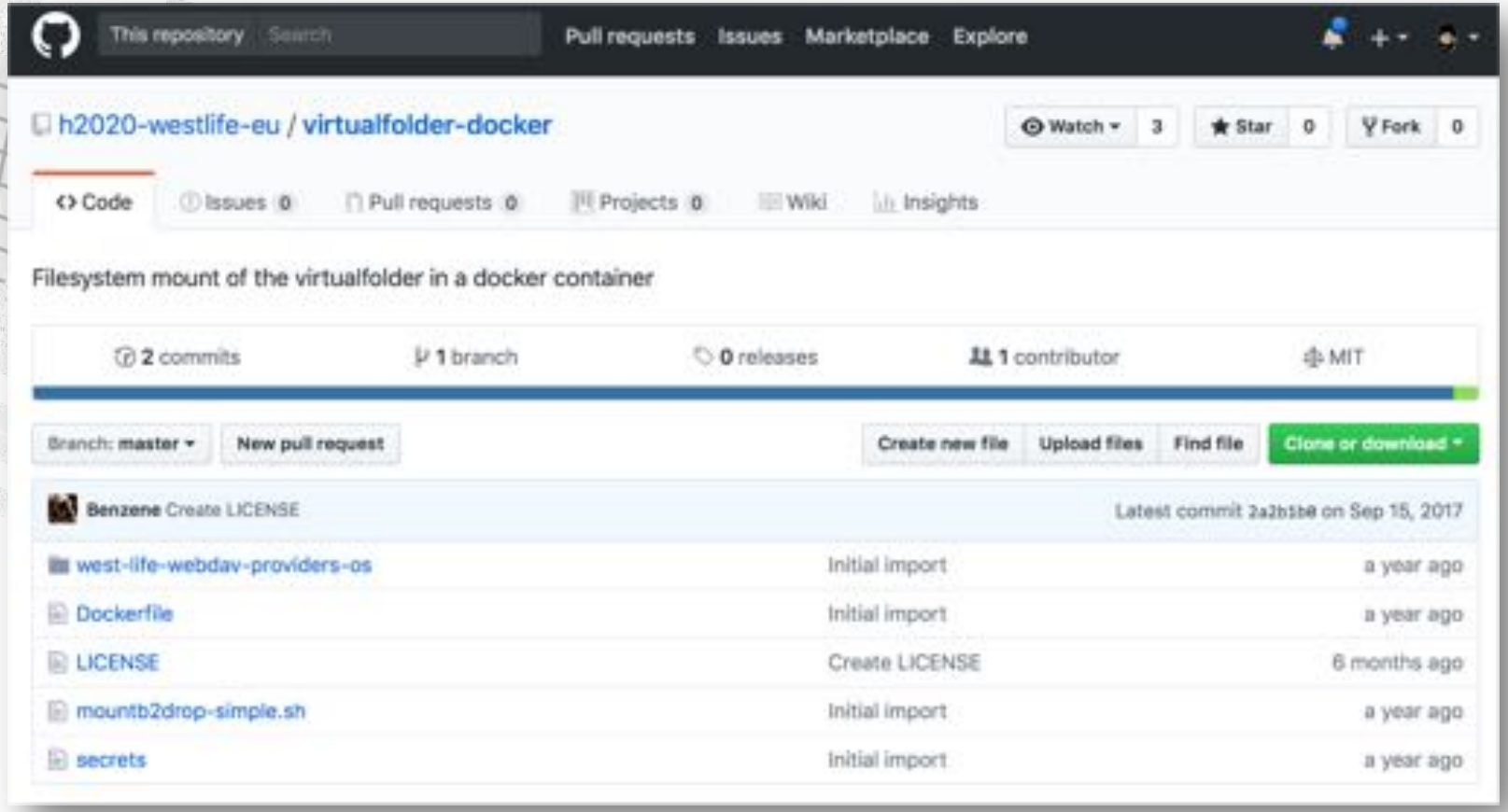
West-Life VMs

West-Life VMs



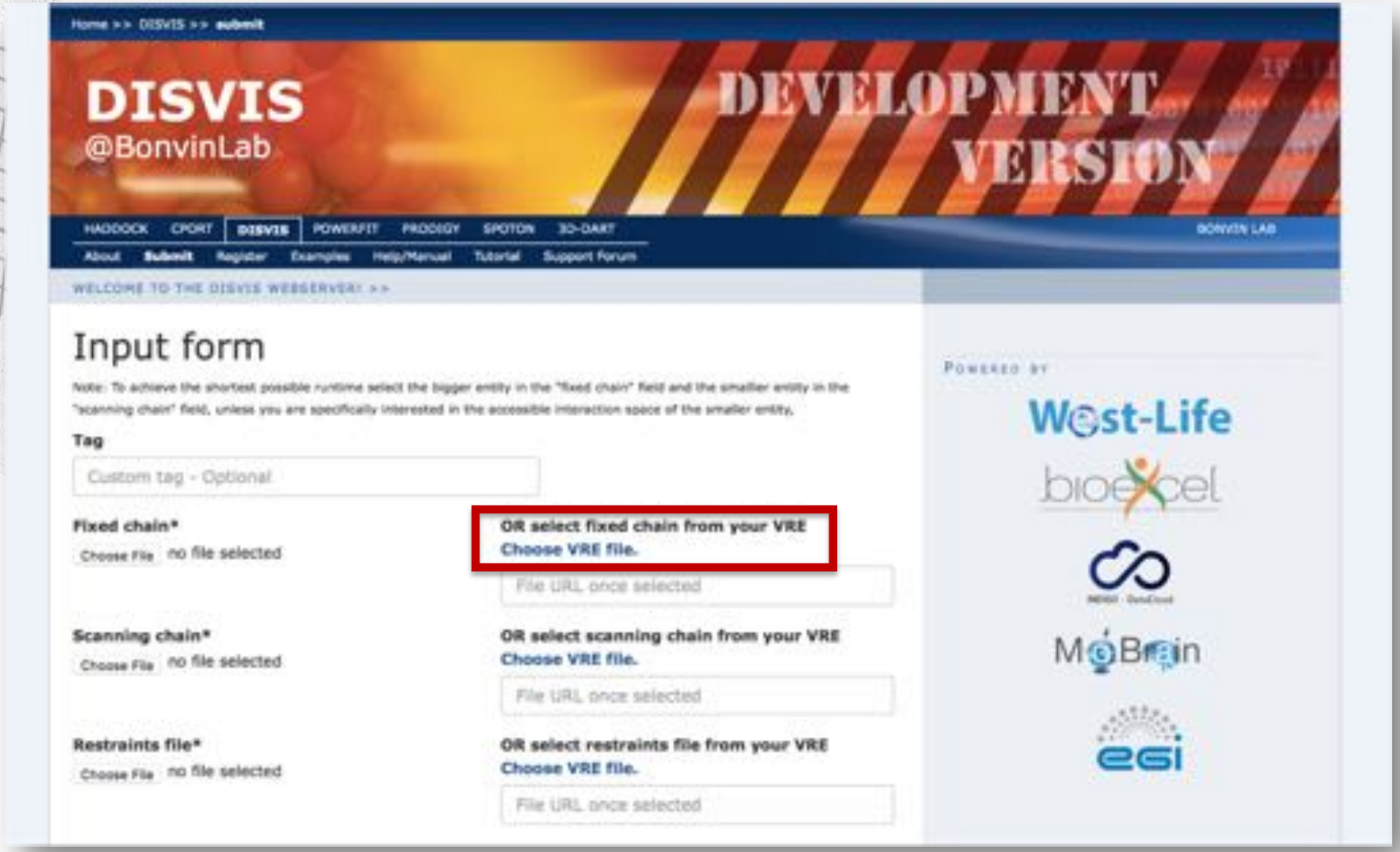
Available from EGI AppDB

West-Life Virtual Folder

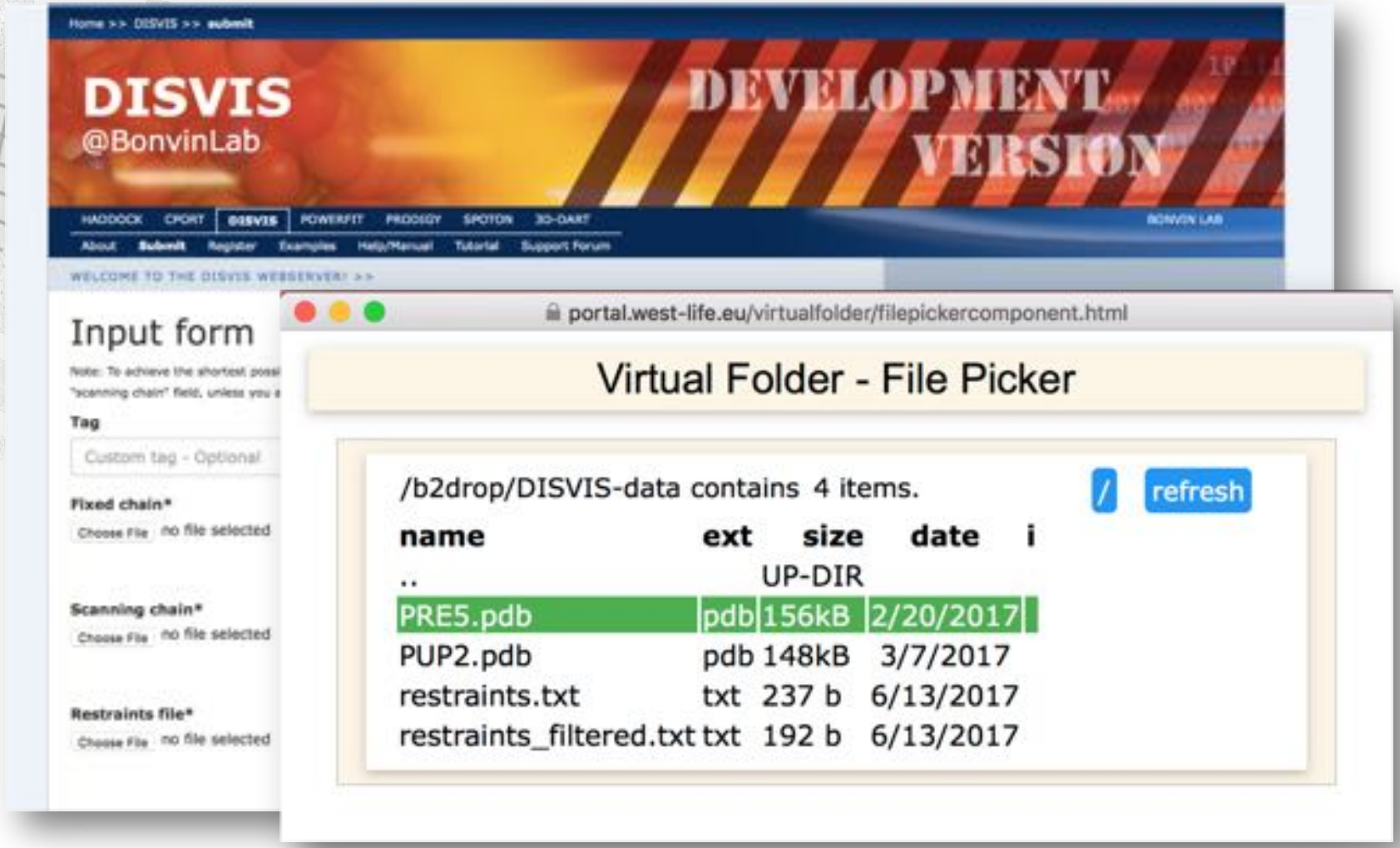


More on the West-Life GitHub repo

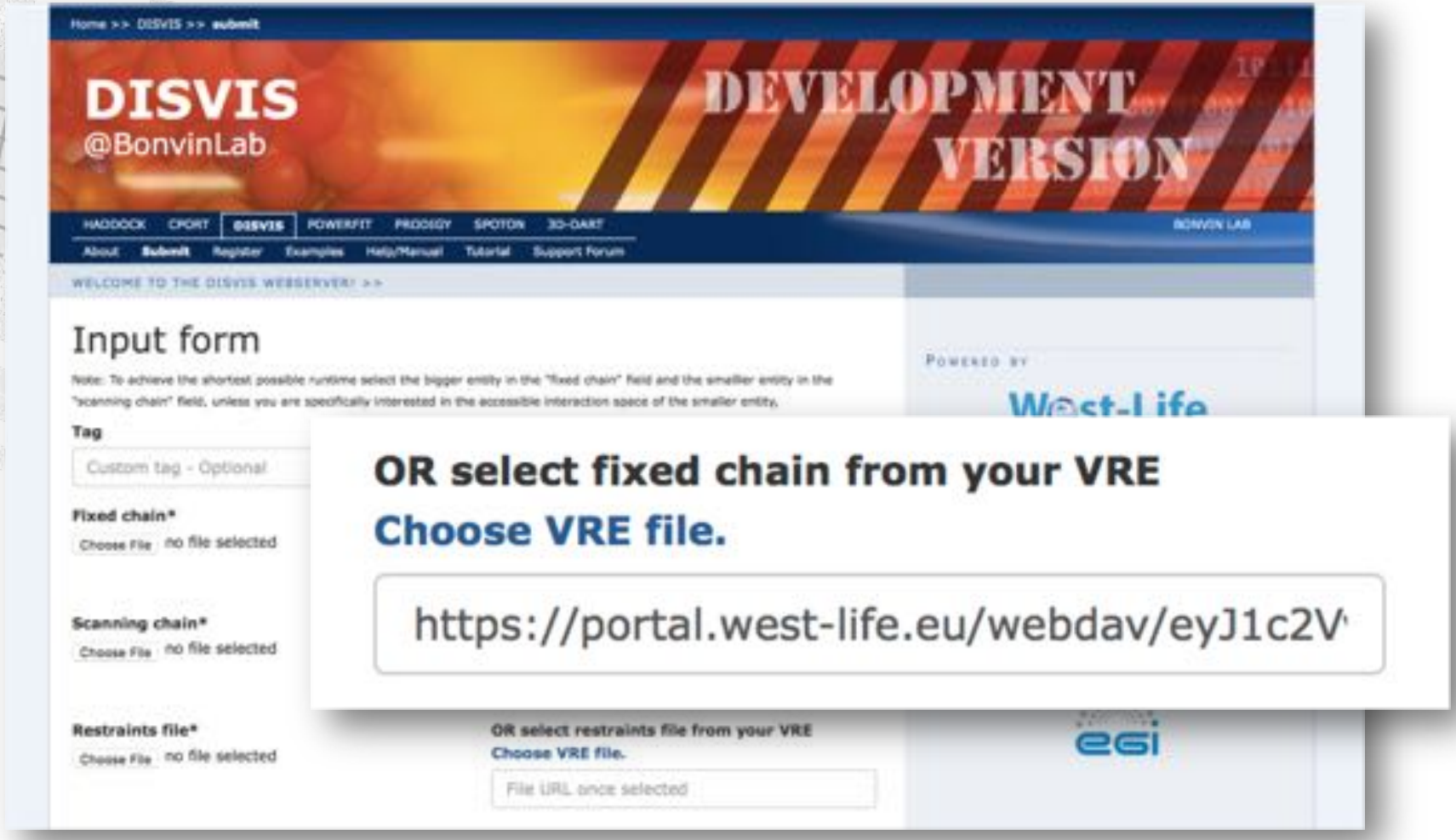
Implementation in a web portal



Implementation in a web portal



Implementation in a web portal



Conclusions

- Life of users made easier by offering direct connections between portals (no need to download and upload data)
- West-Life Virtual Folder solution
  - Aggregated view of data
  - Direct transfer to portal via webdav
- Future: Direct upload of results to Virtual Folder

Conclusions

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Implementation in a web portal

Acknowledgments:

the CSB group@UU

€€

NWO

VICI
TOP-PUNT

WeNMR
West-Life
EGI-Engage
INDIGO-
Datacloud
BioExcel CoE
EOSC-Hub
SURFSara

Thank you for your attention!
http://bonvinlab.org