I-VRESSE: A VRE for Integrative Modelling of Biomolecular Interactions with HADDOCK

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Computational Structural Biology

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EOSC-WeNMR

WeNMR is a worldwide e-infrastructure for Structural Biology

Computational methods developed by the academic groups are instrumentalized into applications and served as web services to the life sciences community

wenmr.eu

EOSC-WeNMR

> **37.000+** registered users

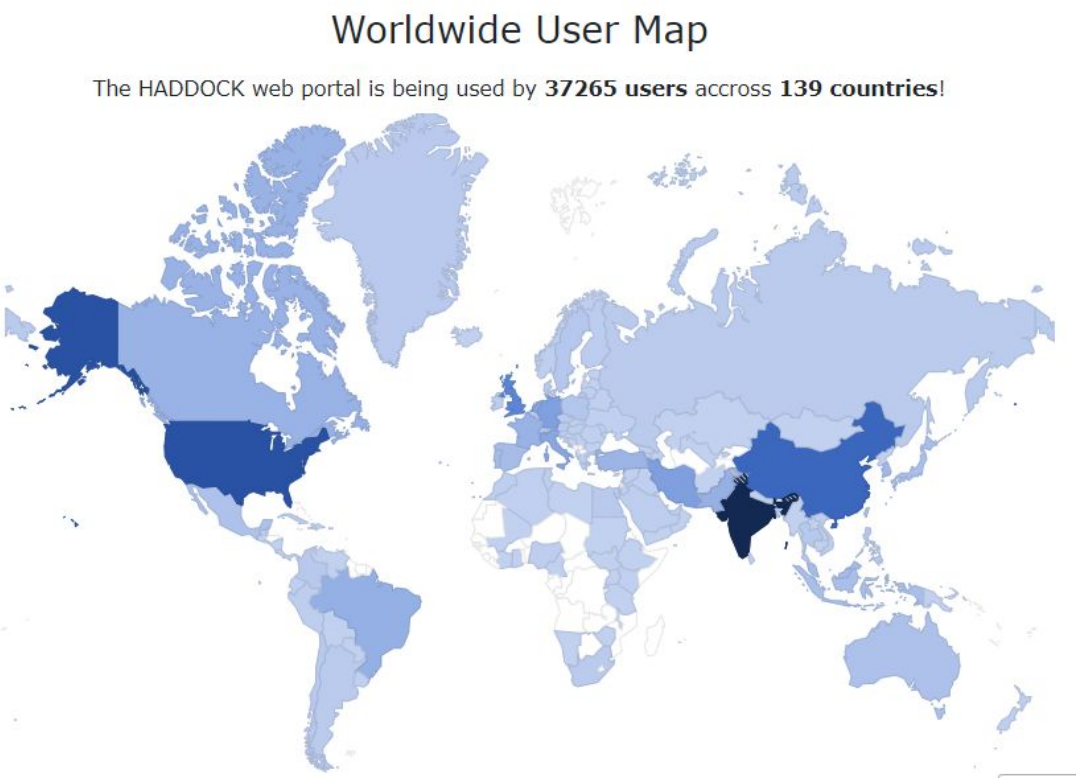
> **500.000+ served runs** since June 2008

>> 65% on the EGI GRID (total)

>> 80% for HADDOCK 2.4 service

>> Integrated in the EOSC marketplace

>> 14 Services in operation



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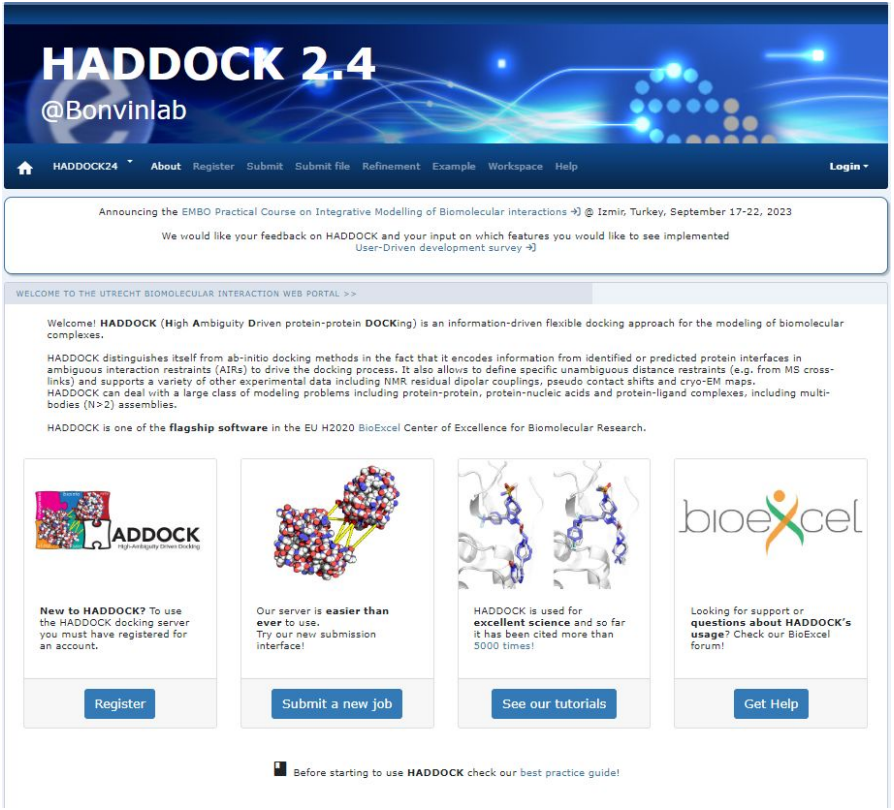
wenmr.science.uu.nl

EOSC-WeNMR



High Ambiguity Driven protein-protein DOCKing is an information-driven flexible docking approach for the modeling of biomolecular complexes

Flagship software of EU H2020 *BioExcel Center of Excellence for Biomolecular Research*

Offered as open source code and web service

User friendly interface and free access to EGI computing resources via the WeNMRVO

HADDOCK3

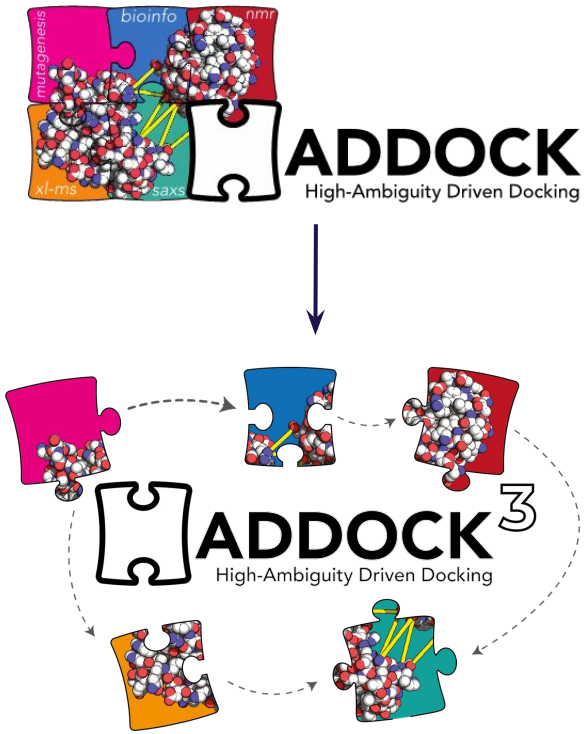
> Re-work of the HADDOCK2+ series, in production for over 20 years

> Breakdown of main subroutines into **modules**

> Modern development practices

> Open development and **FAIR**

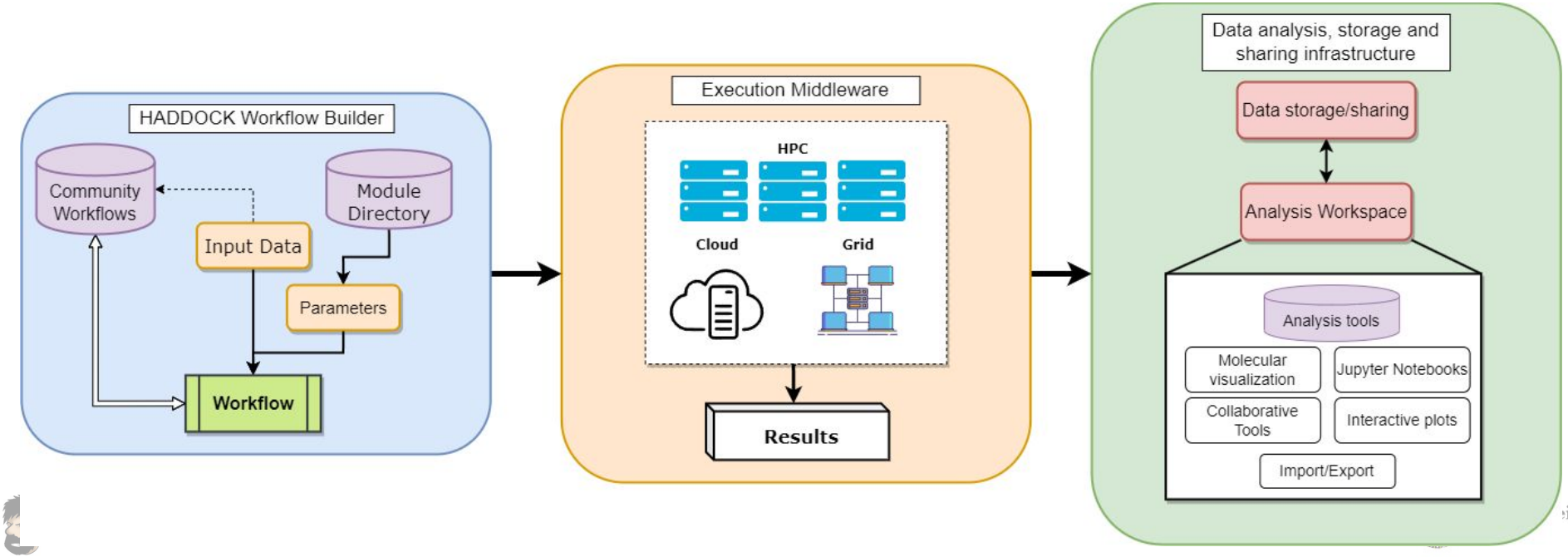
> Community engagement: development of new modules and HADDOCK workflows



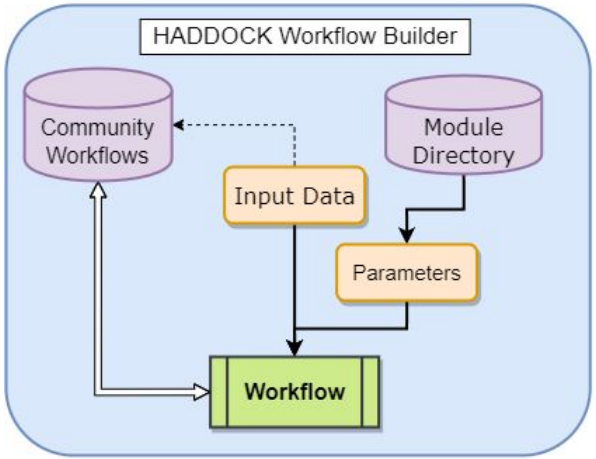
github.com/haddocking/haddock3

I-VRESSE: **I**nteractive **V**irtual **R**esearch **E**nvironment for **S**cientific **S**oftware **E**xecution

Enable researchers to design and run *custom HADDOCK workflows* for the prediction and analysis of macromolecular complexes, efficiently distributing the computations to cloud (or HPC) resources.



I-VRESSE - Workflow Builder



> Modern web GUI (React + WASM)

> Easily embedded in Galaxy, JupyterNotebooks and web native applications

> Automatic retrieval of HADDOCK parameters and modules

> Input parsing and validation with WebAssembly

i-vresse-workflow-builder.netlify.app

i-VRESSE workflow builder: Haddock 3 on easy level

haddock3easy

Nodes

- topology
  - topoaa
- sampling
  - gdock
  - rigidbody
  - lightdock
- refinement
  - mdref
  - flexref
  - emref
- scoring
  - mdscoring
  - emscoring
- analysis
  - seletopclusts
  - clustrmsd
  - caprieval
  - rmsdmatrix
  - clustfcc

Workflow

Global parameters | Upload

Visual | Text

Append node to workflow by clicking node in catalog

or by dragging node from catalog to here.

Download archive | Clear

Node

No node or global parameters selected for configuration.

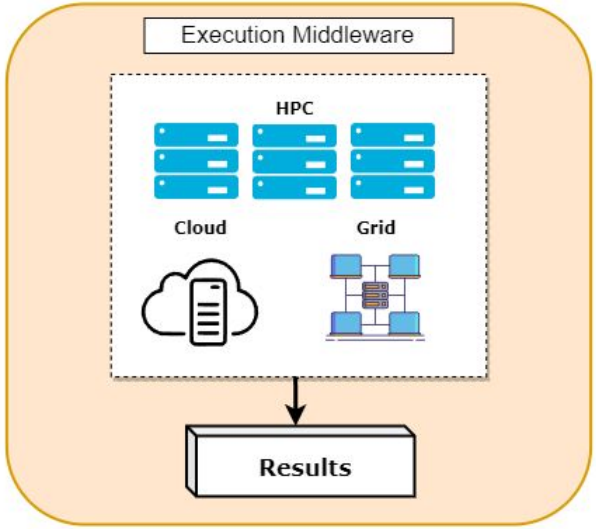
i-vresse-workflow-builder.netlify.app

I-VRESSE - Bartender

> Middleware web service to schedule jobs on various infrastructures

> Can run applications on: HPC (Slurm) / GRID (DIRAC) / CLOUD (soon!)

> Social + EGI Check-in (almost!)



i-vresse-bartender.readthedocs.io

application

- GET /api/application/ List Applications
- GET /api/application/{application} Get Application
- PUT /api/application/{application}/job Upload Job

users

- GET /api/users/profile Profile
- GET /api/users/ List Users
- GET /users/me Users:Current User
- PATCH /users/me Users:Patch Current User
- GET /users/{id} Users:User
- DELETE /users/{id} Users:Delete User
- PATCH /users/{id} Users:Patch User

auth

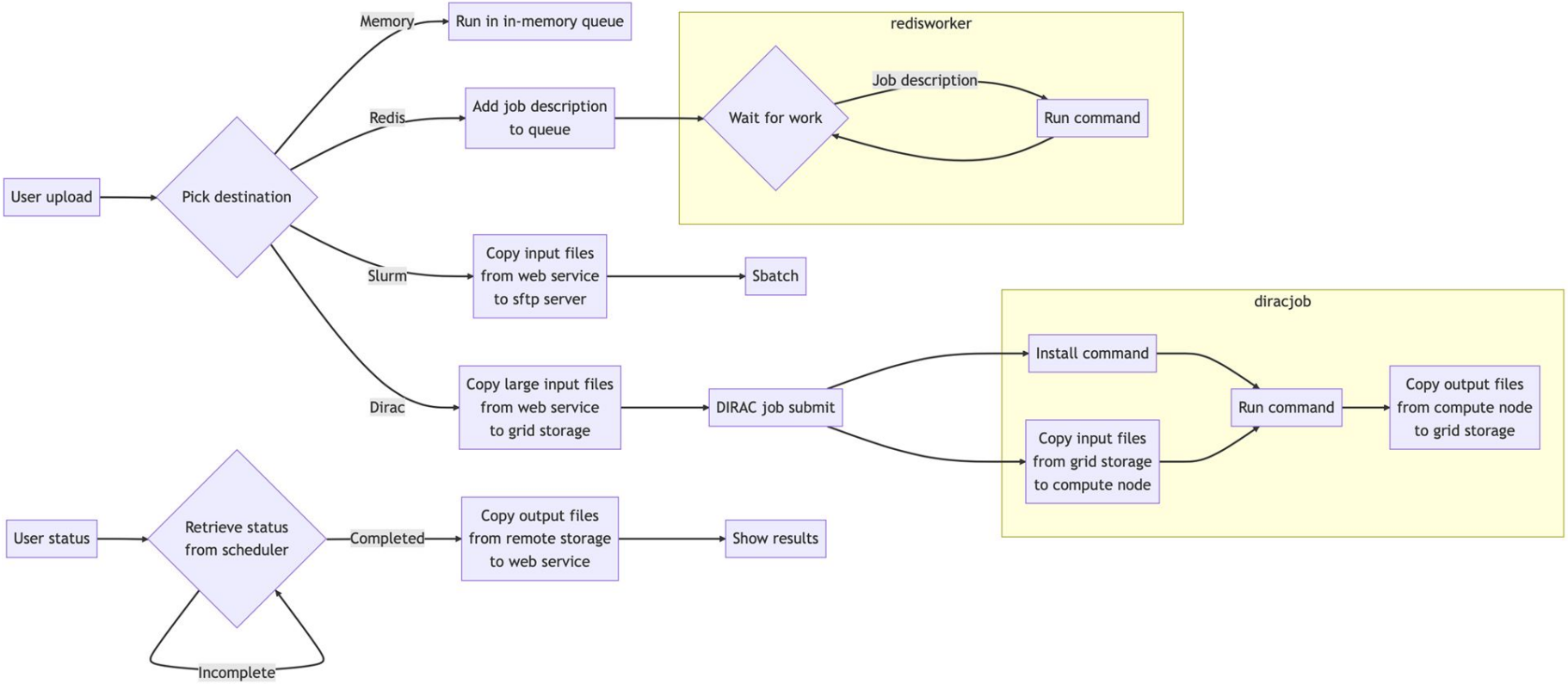
- POST /auth/jwt/login Auth:Local.Login
- POST /auth/jwt/logout Auth:Local.Logout
- POST /auth/register Register:Register

default

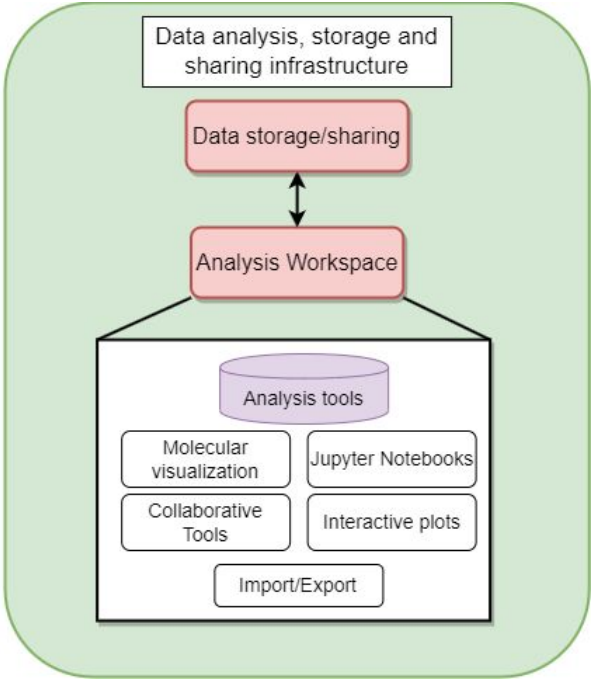
- GET /api/health Health Check

job

- GET /api/job/ Retrieve Jobs
- GET /api/job/{jobid} Retrieve Job
- GET /api/job/{jobid}/files/{path} Retrieve Job Files
- GET /api/job/{jobid}/stdout Retrieve Job Stdout
- GET /api/job/{jobid}/stderr Retrieve Job Stderr
- GET /api/job/{jobid}/directories Retrieve Job Directories
- GET /api/job/{jobid}/directories/{path} Retrieve Job Directories From Path


User upload
Pick destination
Memory
Run in in-memory queue
Redis
Add job description to queue
redisworker
Wait for work
Job description
Run command
Slurm
Copy input files from web service to sftp server
Sbatch
Dirac
Copy large input files from web service to grid storage
DIRAC job submit
diracjob
Install command
Copy input files from grid storage to compute node
Run command
Copy output files from compute node to grid storage
User status
Retrieve status from scheduler
Completed
Incomplete
Copy output files from remote storage to web service
Show results

I-VRESSE - Analysis



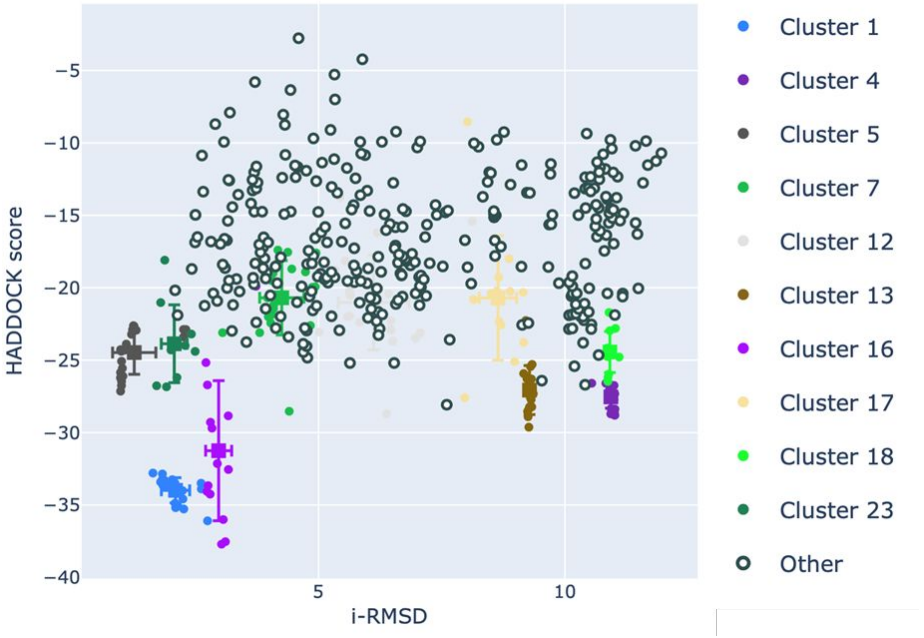
> WIP: github.com/i-VRESSE/UI-analysis

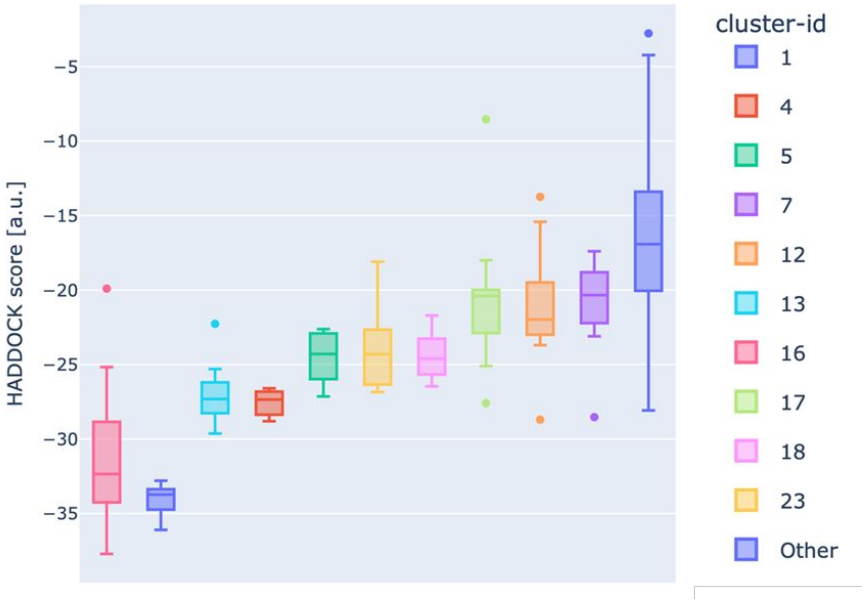
> Workspace will be a GUI integrated with an array of microservices containing analysis tools

> WebAssembly for the core functions

I-VRESSE - Analysis

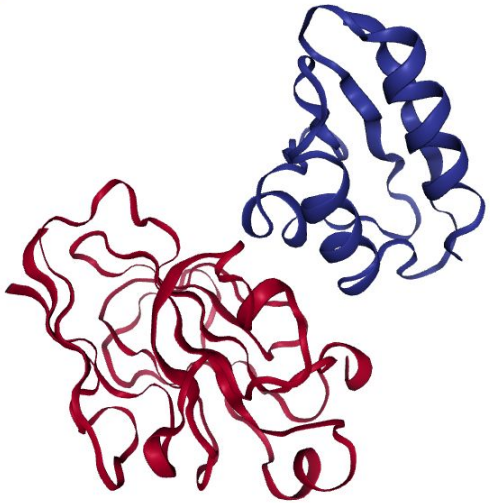
> Can embed graphical elements produced by the applications ex: HADDOCK3

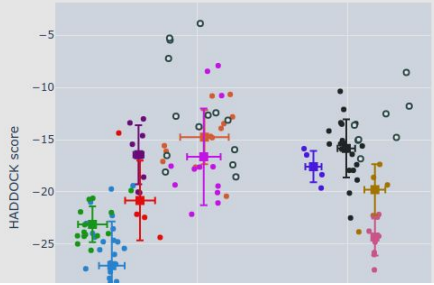


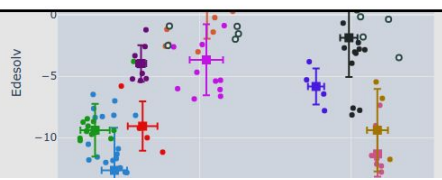


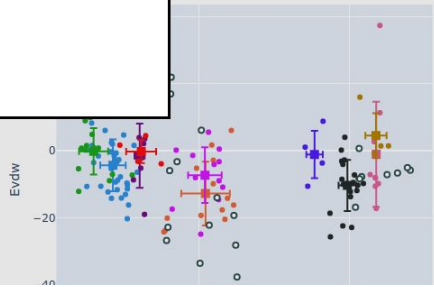
Cluster Rank	1	2	3	4	5	6	7	8	9	10
Cluster ID	1	6	3	14	5	2	13	8	4	12
Cluster size	37	9	14	4	12	19	4	7	13	4
HADDOCK score [a.u.]	-33.156 ± 0.158	-26.016 ± 0.952	-24.757 ± 0.572	-20.824 ± 3.827	-20.675 ± 1.023	-19.85 ± 1.709	-19.783 ± 2.437	-18.528 ± 1.88	-17.808 ± 1.6	-17.575 ± 1.5
interface RMSD [A]	2.553 ± 0.168	10.876 ± 0.012	1.185 ± 0.185	3.095 ± 0.494	5.459 ± 0.376	10.151 ± 0.099	10.89 ± 0.348	3.04 ± 0.134	4.676 ± 0.853	8.851 ± 0.271
Fraction of Common Contacts	0.361 ± 0.02	0.118					0.0	0.334 ± 0.076	0.209 ± 0.072	0.097 ± 0.014
ligand RMSD [A]	6.747 ± 0.854	18.04					0.527	8.84 ± 0.285	9.303 ± 1.656	14.8 ± 0.497
DOCKQ	0.411 ± 0.023	0.106					0.003	0.337 ± 0.032	0.258 ± 0.062	0.124 ± 0.01
Restraints Energy	123.595 ± 107.598	168.5					± 126.803	223.414 ± 89.759	252.992 ± 31.644	276.677 ± 125
Desolvation Energy	-16.131 ± 1.062	-12.22					3.36	-4.661 ± 0.798	-1.397 ± 2.175	-5.838 ± 1.466
Electrostatic Energy	-7.352 ± 1.96	-2.177					1.906	-4.689 ± 1.521	-5.232 ± 3.297	-4.013 ± 0.698
Van der Waals Energy	-11.774 ± 7.366	-10.93					6.674	-1.568 ± 5.466	-15.867 ± 7.127	-1.071 ± 7.044
Nr 01 best structure	↓ Download 👁 View	↓ Dow					ad 👁 View	↓ Download 👁 View	↓ Download 👁 View	↓ Download 👁
Nr 02 best structure	↓ Download 👁 View	↓ Dow					ad 👁 View	↓ Download 👁 View	↓ Download 👁 View	↓ Download 👁
Nr 03 best structure	↓ Download 👁 View	↓ Dow					ad 👁 View	↓ Download 👁 View	↓ Download 👁 View	↓ Download 👁
Nr 04 best structure	↓ Download 👁 View	↓ Dow					ad 👁 View	↓ Download 👁 View	↓ Download 👁 View	↓ Download 👁

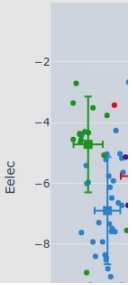
cluster1_model1.pdb





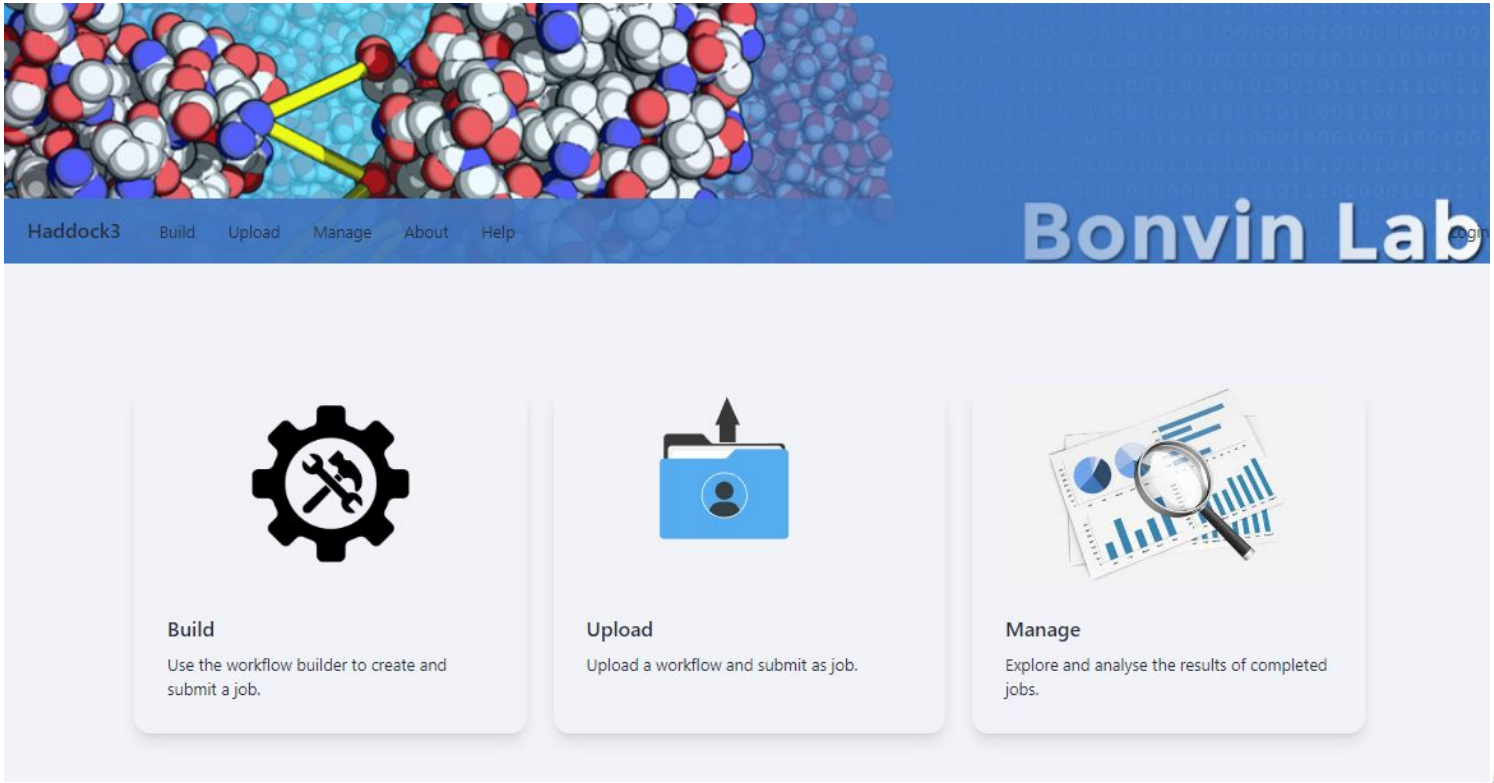






I-VRESSE + HADDOCK

github.com/i-VRESSE/bartended-haddock3



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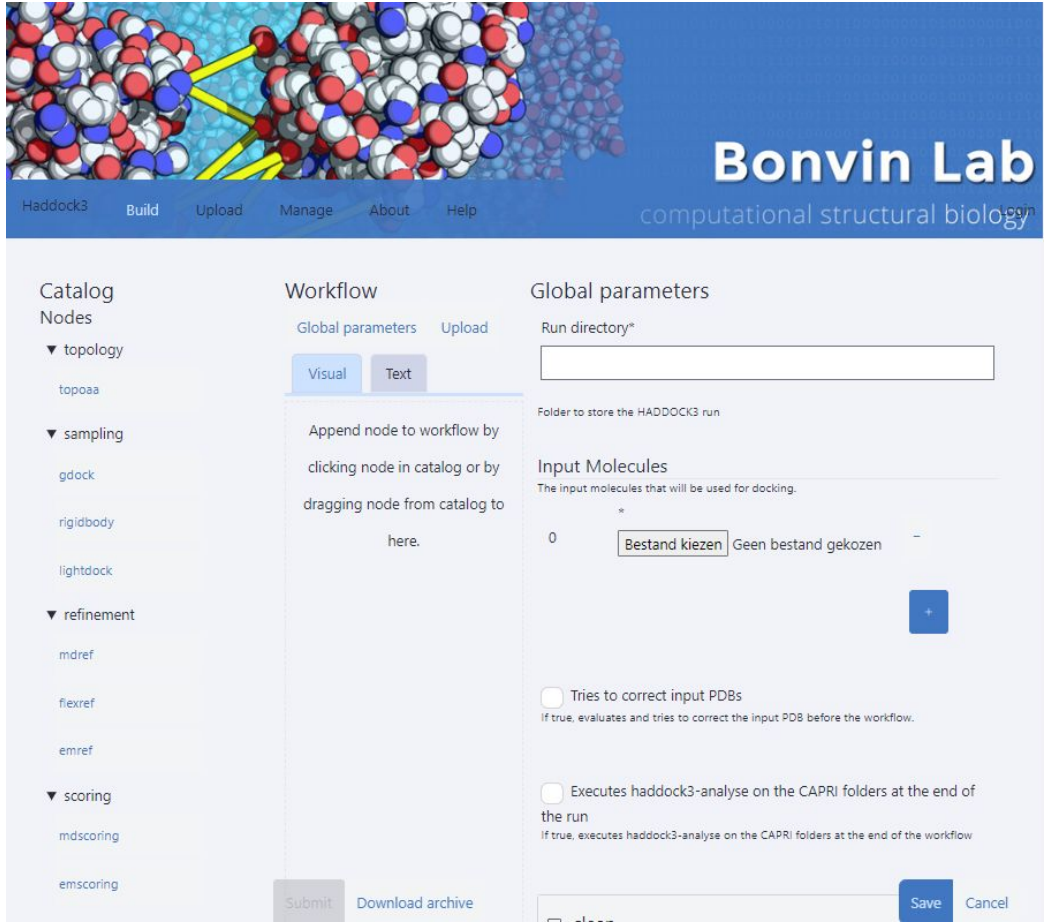

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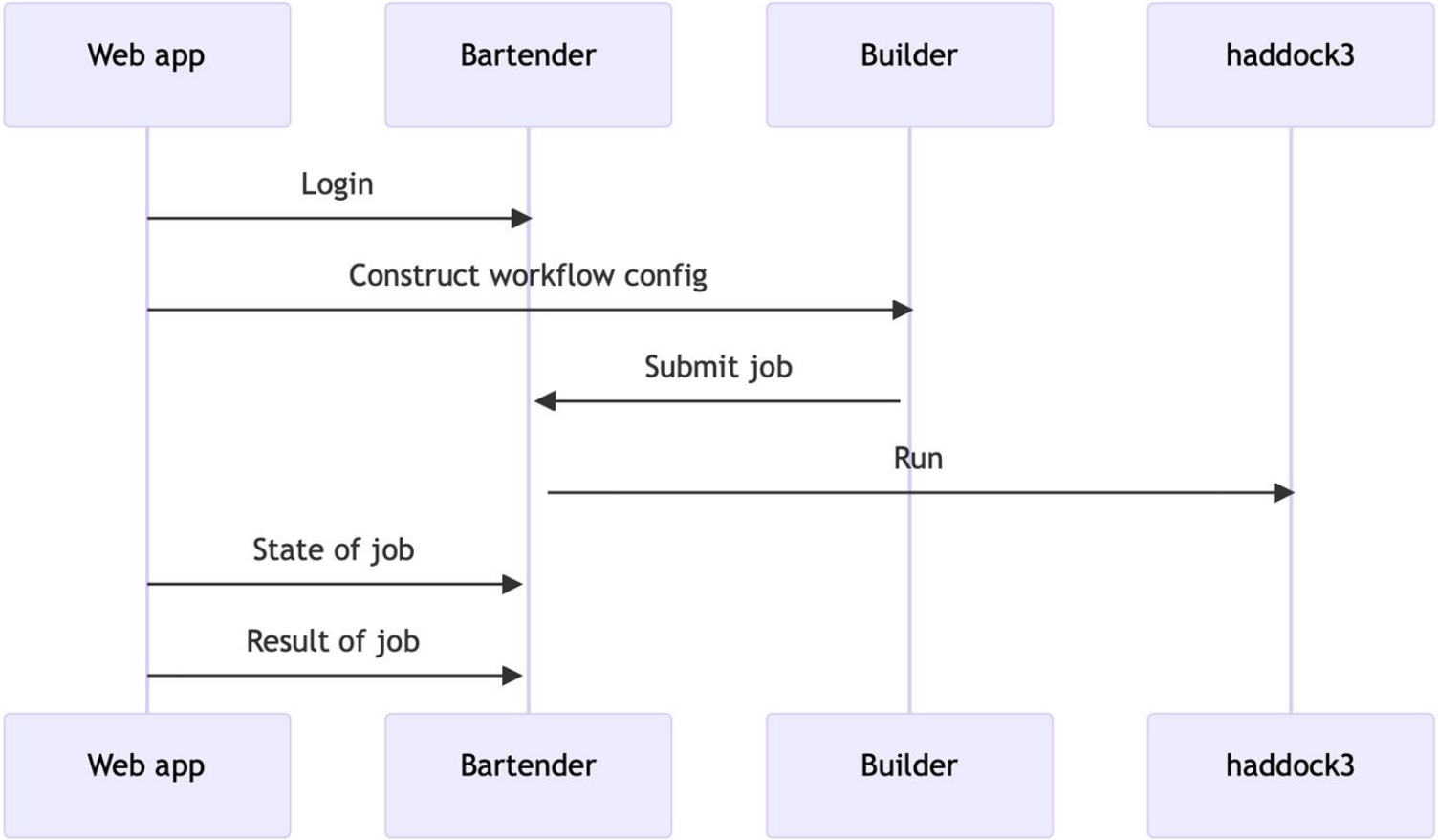

Thanks!

wenmr.science.uu.nl
github.com/haddocking
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