

A Virtual Research Environment for Integrative Modelling of Biomolecular Complexes with the new Modular Version of HADDOCK

Prof. Alexandre M.J.J. Bonvin

Bijvoet Center for Biomolecular Research

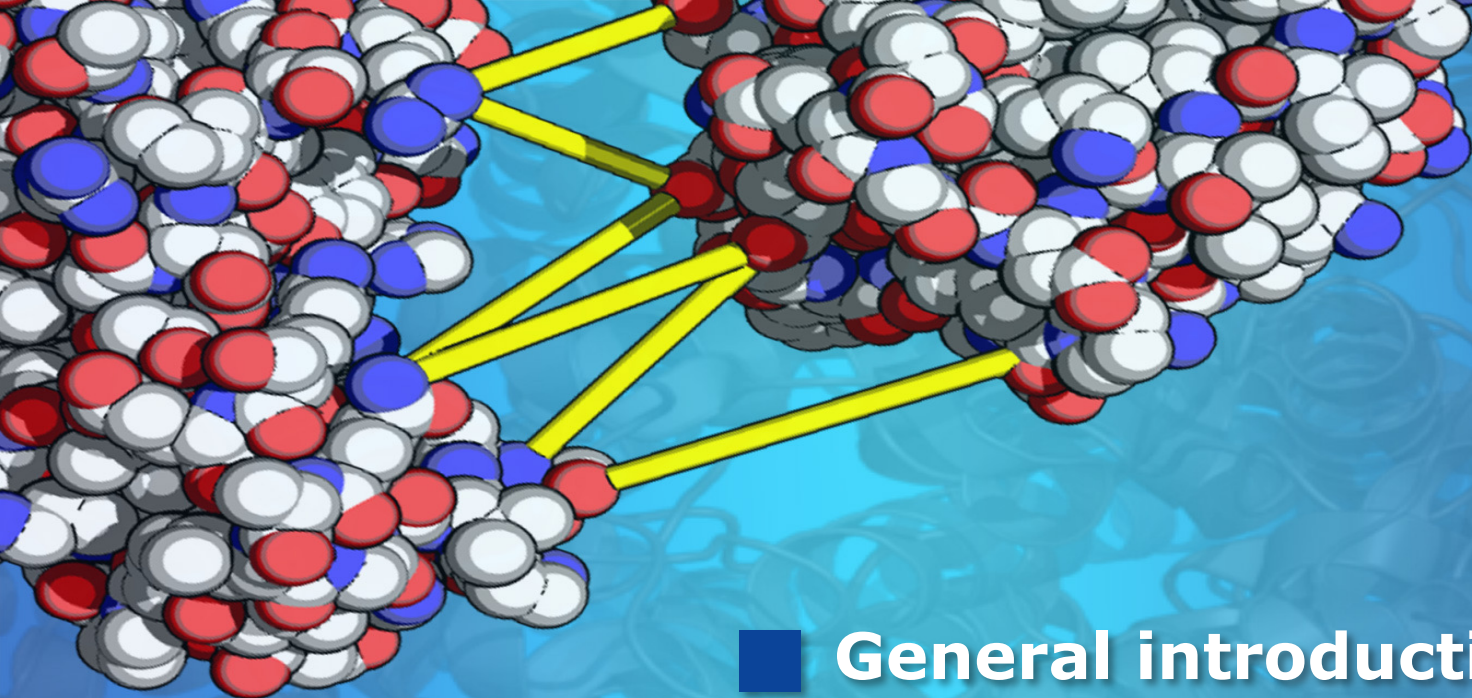
Faculty of Science, Utrecht University

the Netherlands

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

@amjjbonvin



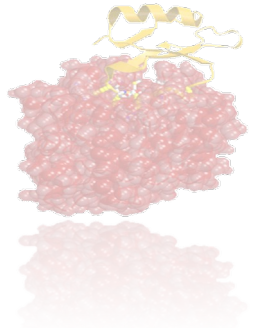


Overview

- General introduction
- Introducing the new modular HADDOCK3
- Towards a virtual research environment for HADDOCK3 – i-VRESSE
- Conclusions

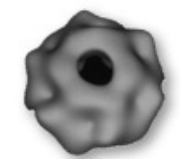
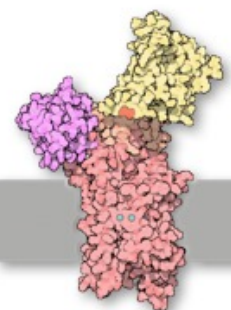
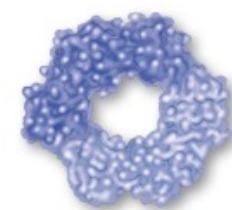
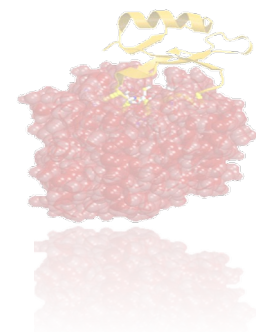
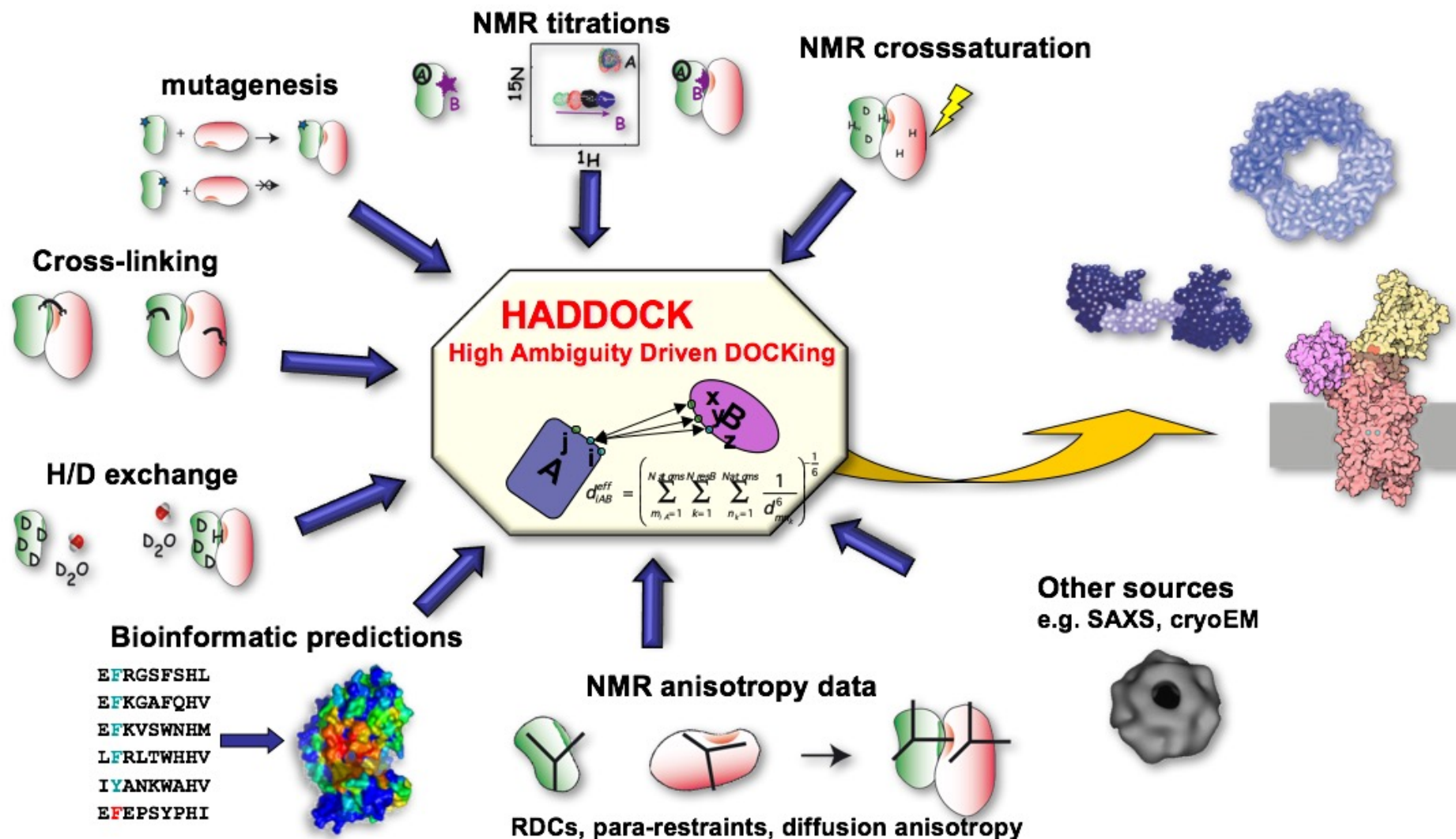
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100011010101000101111010110101  
10100001000111101010101110000110101  
0001010101011110010100110010101010100  
010101111111010101000010101010100000101010100  
0010110101011101010001111010101010001010010101011111  
0001111111010101011001100010111000101011010100010101000101
```

The social network of proteins

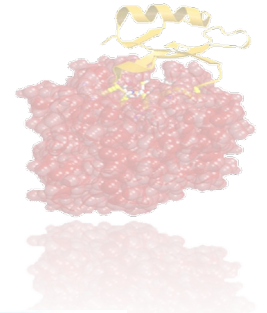


Majority of 'life' depends on interactions, particularly protein-protein

HADDOCK: An integrative modeling platform

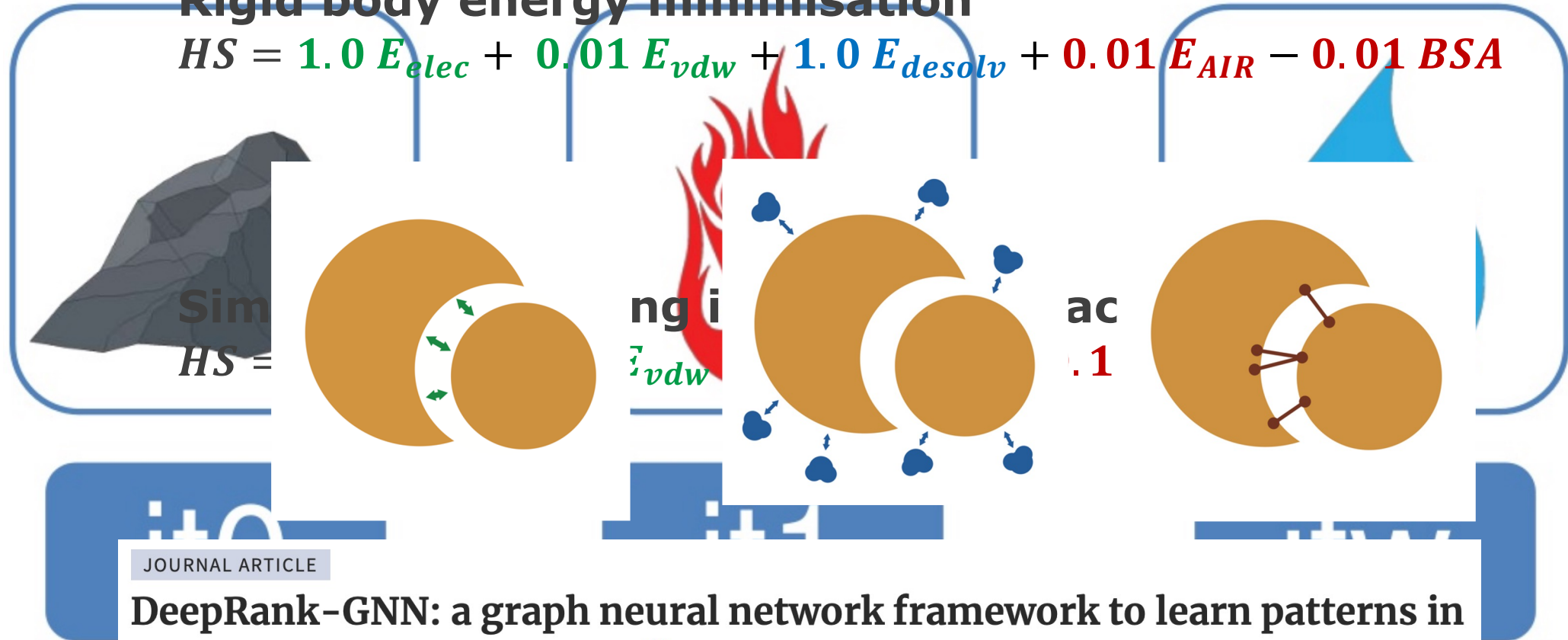


HADDOCK



Rigid body energy minimisation

$$HS = 1.0 E_{elec} + 0.01 E_{vdw} + 1.0 E_{desolv} + 0.01 E_{AIR} - 0.01 BSA$$

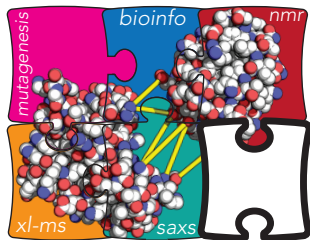


JOURNAL ARTICLE

DeepRank-GNN: a graph neural network framework to learn patterns in protein–protein interfaces

Manon Réau, Nicolas Renaud, Li C Xue, Alexandre M J J Bonvin  Author Notes

Bioinformatics, Volume 39, Issue 1, January 2023, btac759, <https://doi.org/10.1093/bioinformatics/btac759>

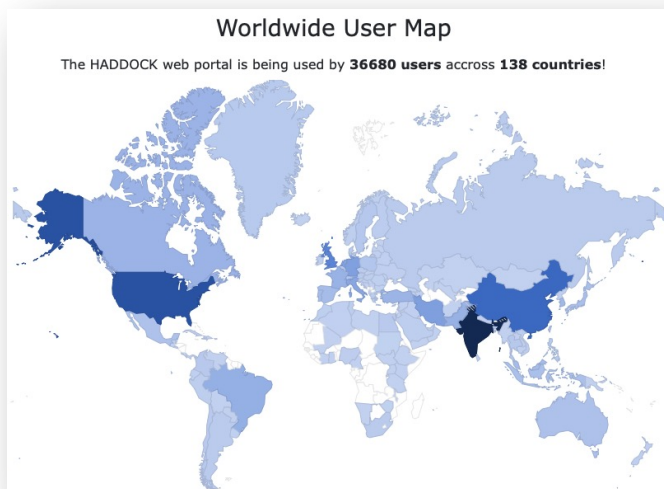


HADDOCK
High-Ambiguity Driven Docking

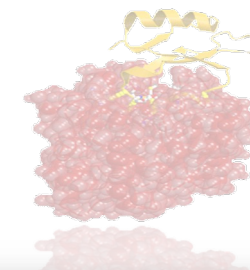
- > 35000 registered users
- > 530000 served runs since June 2008
- 65% on the EOSC HTC resources (>80% for 2.4)
- Integrated in the EOSC marketplace

De Vries *et al.* Nature Prot. 2010

Van Zundert *et al.* J.Mol.Biol. 2016



HADDOCK web portal (WeNMR)



HADDOCK 2.4
@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

Welcome! **HADDOCK** (High Ambiguity Driven protein-protein **DOCK**ing) is an information-driven flexible docking approach for the modeling of biomolecular complexes.

HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. It also allows to define specific unambiguous distance restraints (e.g. from MS cross-links) and supports a variety of other experimental data including NMR residual dipolar couplings, pseudo contact shifts and cryo-EM maps.

HADDOCK can deal with a large class of modeling problems including protein-protein, protein-nucleic acids and protein-ligand complexes, including multi-bodies (N>2) assemblies.

HADDOCK is one of the **flagship software** in the EU H2020 **BioExcel** Center of Excellence for Biomolecular Research.

New to HADDOCK? To use the HADDOCK docking server you must have registered for an account.

[Register](#)

Our server is **easier than ever** to use.
Try our new submission interface!

[Submit a new job](#)

HADDOCK is used for **excellent science** and so far it has been cited more than 5000 times!

[See our tutorials](#)

Looking for support or **questions about HADDOCK's usage**? Check our BioExcel forum!

[Get Help](#)

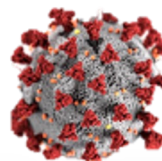
<https://wenmr.science.uu.nl>



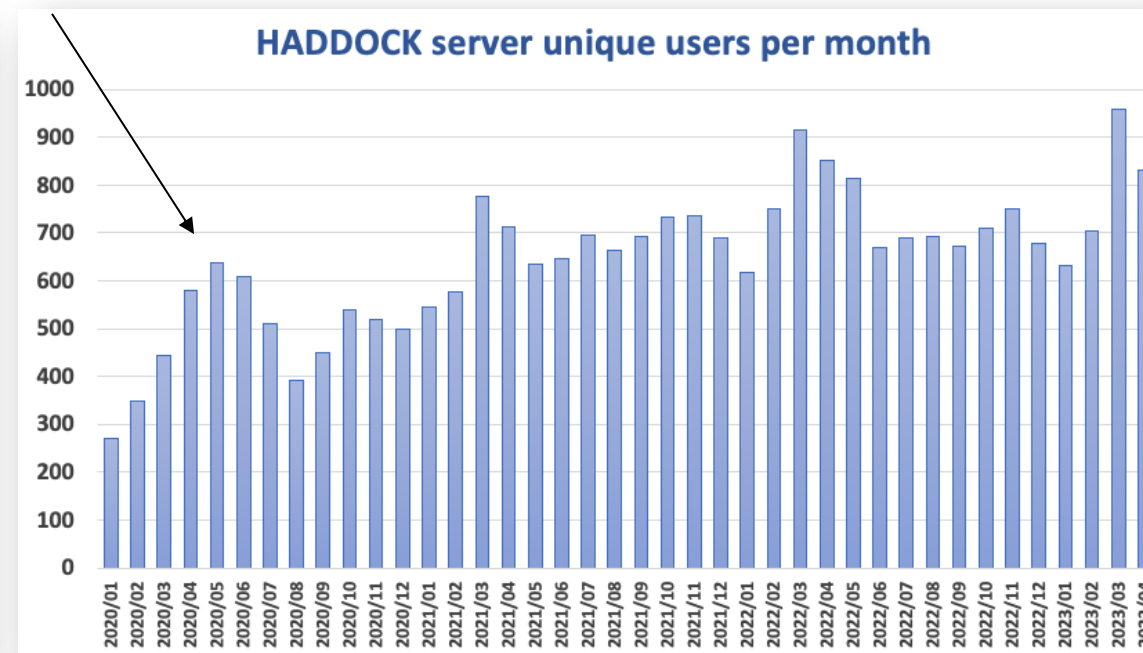
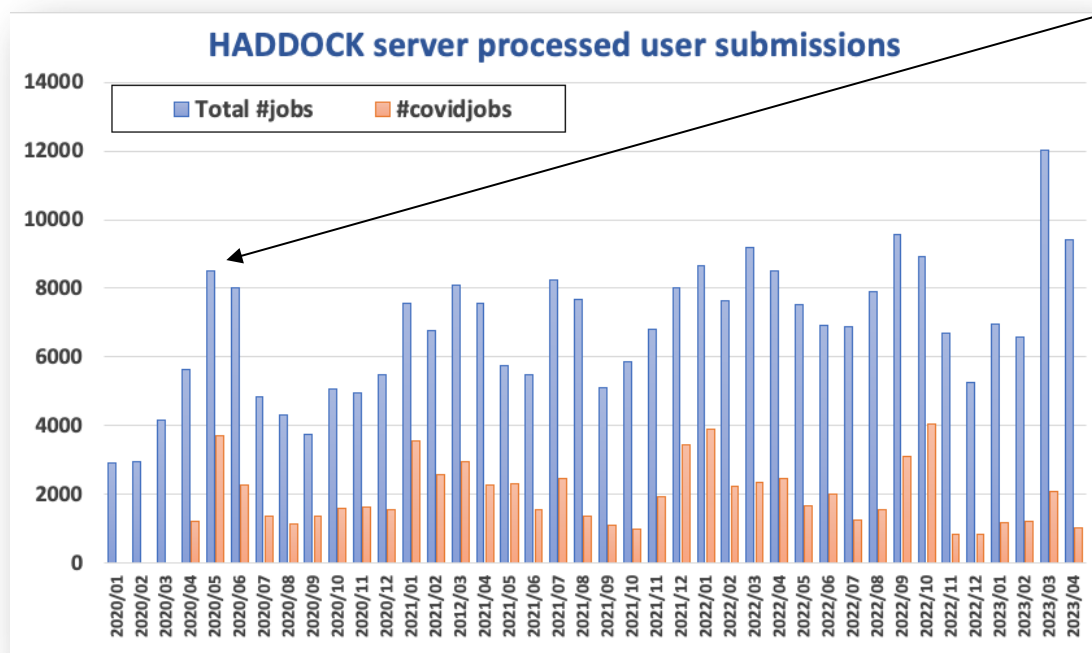
HADDOCK: Meeting the increased demand

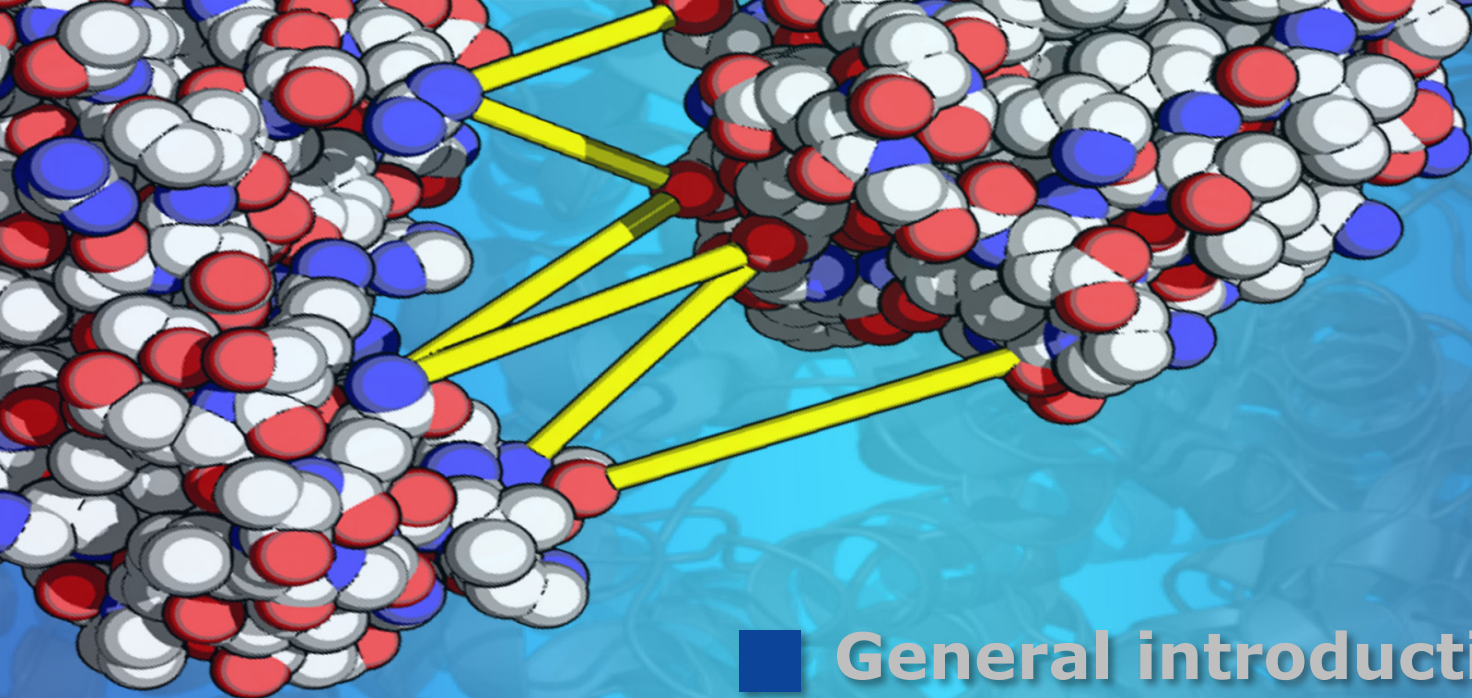


The HADDOCK workflow machinery was modified to improve its efficiency and meet the increased demand (and more resources were allocated thanks to EGI/EOSC/OSG).



COVID19 effect



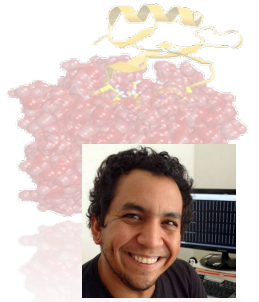
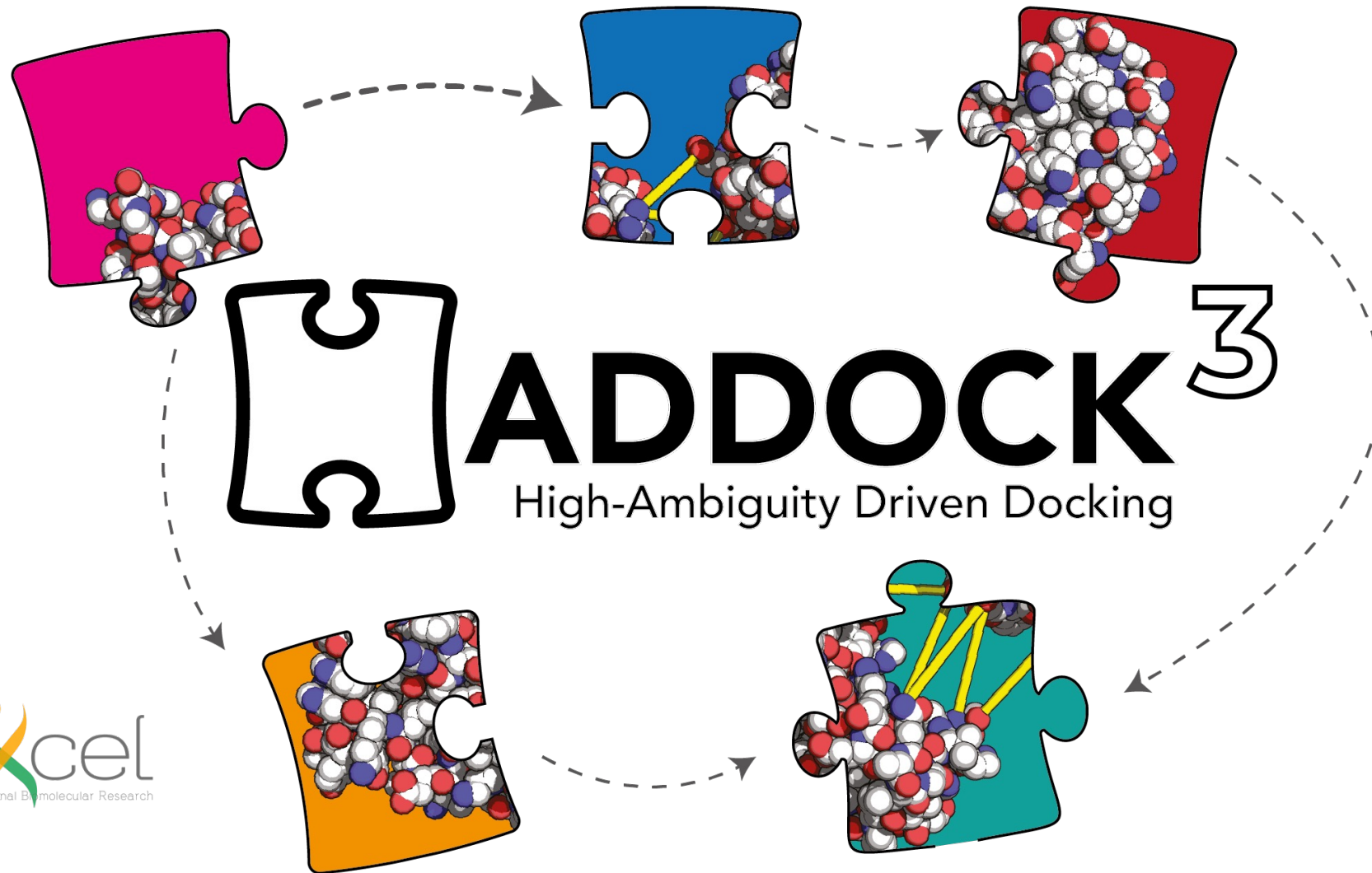


Overview

- General introduction
- **Introducing the new modular HADDOCK3**
- Towards a virtual research environment for **HADDOCK3 – i-VRESSE**
- Conclusions

```
111000100101010110101010
100011010101000101111010110101
10100001000111101010101110000110101
0001010101011110010100110010101010100
0101011111110101010000101010100000101010100
0010110101011101010001111010101010001010010101011111
0001111111010101011001100010111000101011010100010101000101
```


Introducing HADDOCK v3



Rodrigo
Vargas Honorato



Brian Jimenez

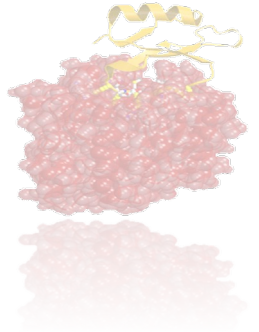


João MC Teixeira



Marco Giulini

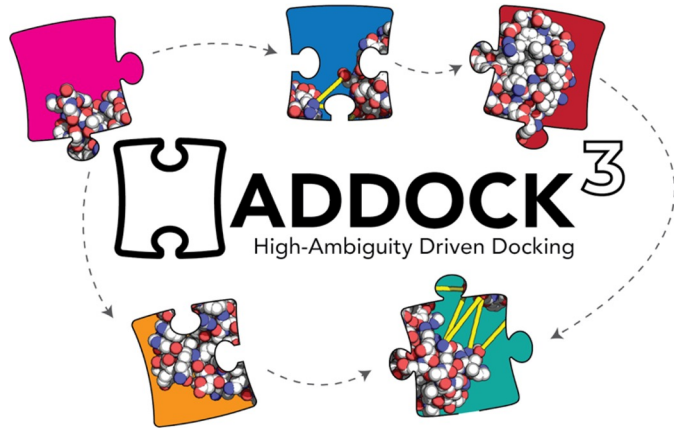
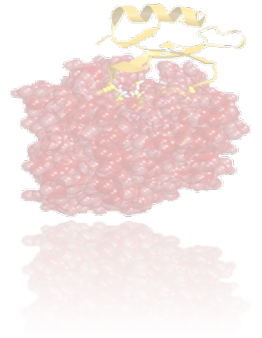
From static workflow ...



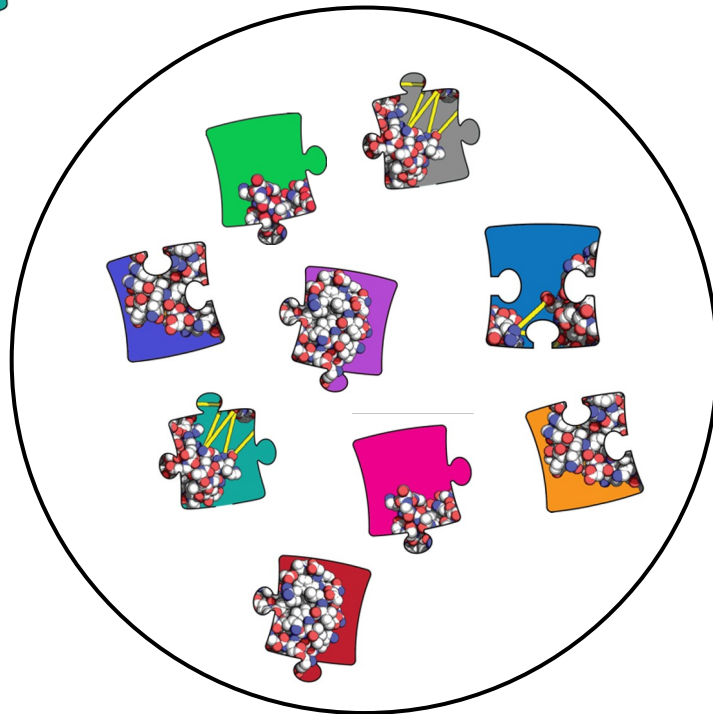
HADDOCK 2

Parameterizable pipeline

... to a modular workflow architecture

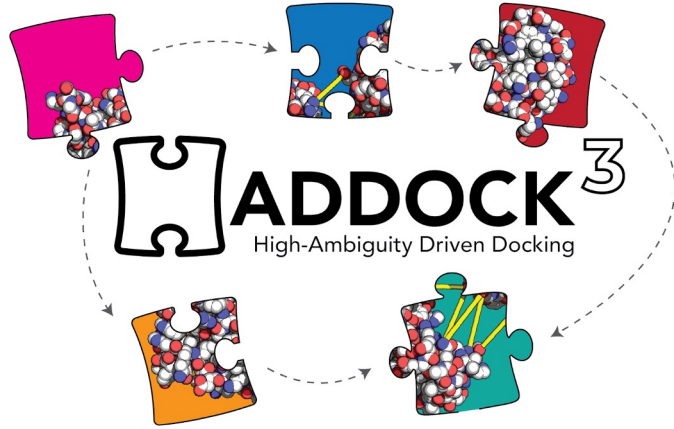


Catalogue of independent modules

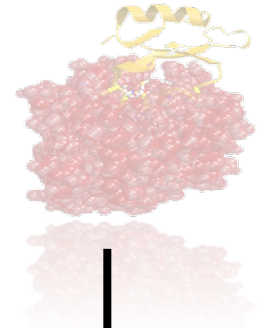
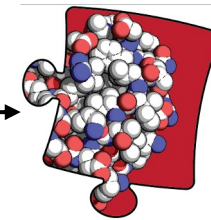
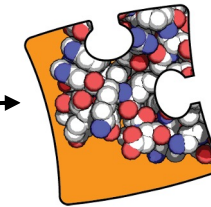
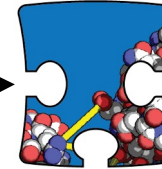
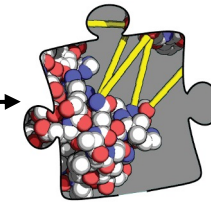
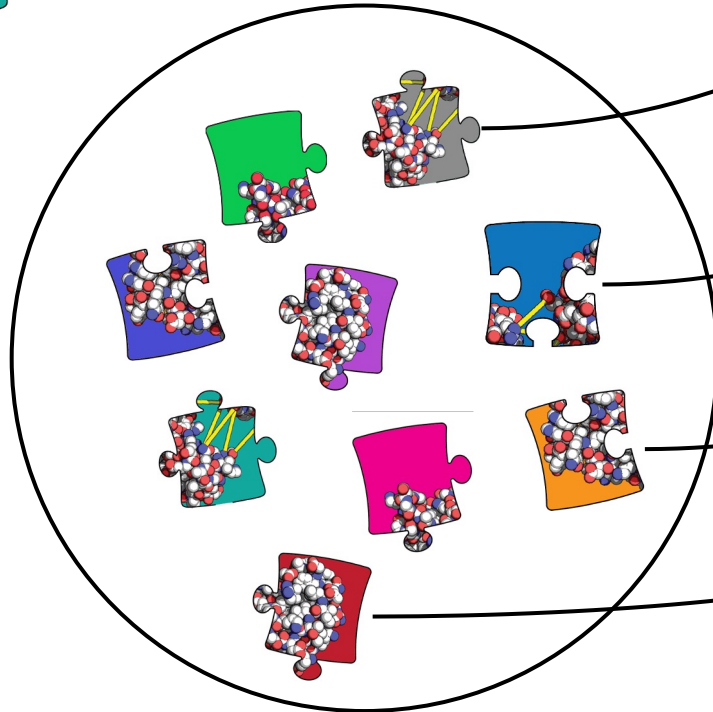


HADDOCK 2

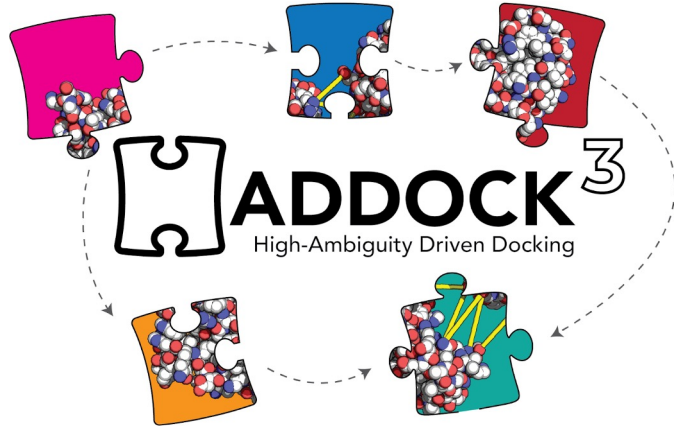
Combining the different pieces



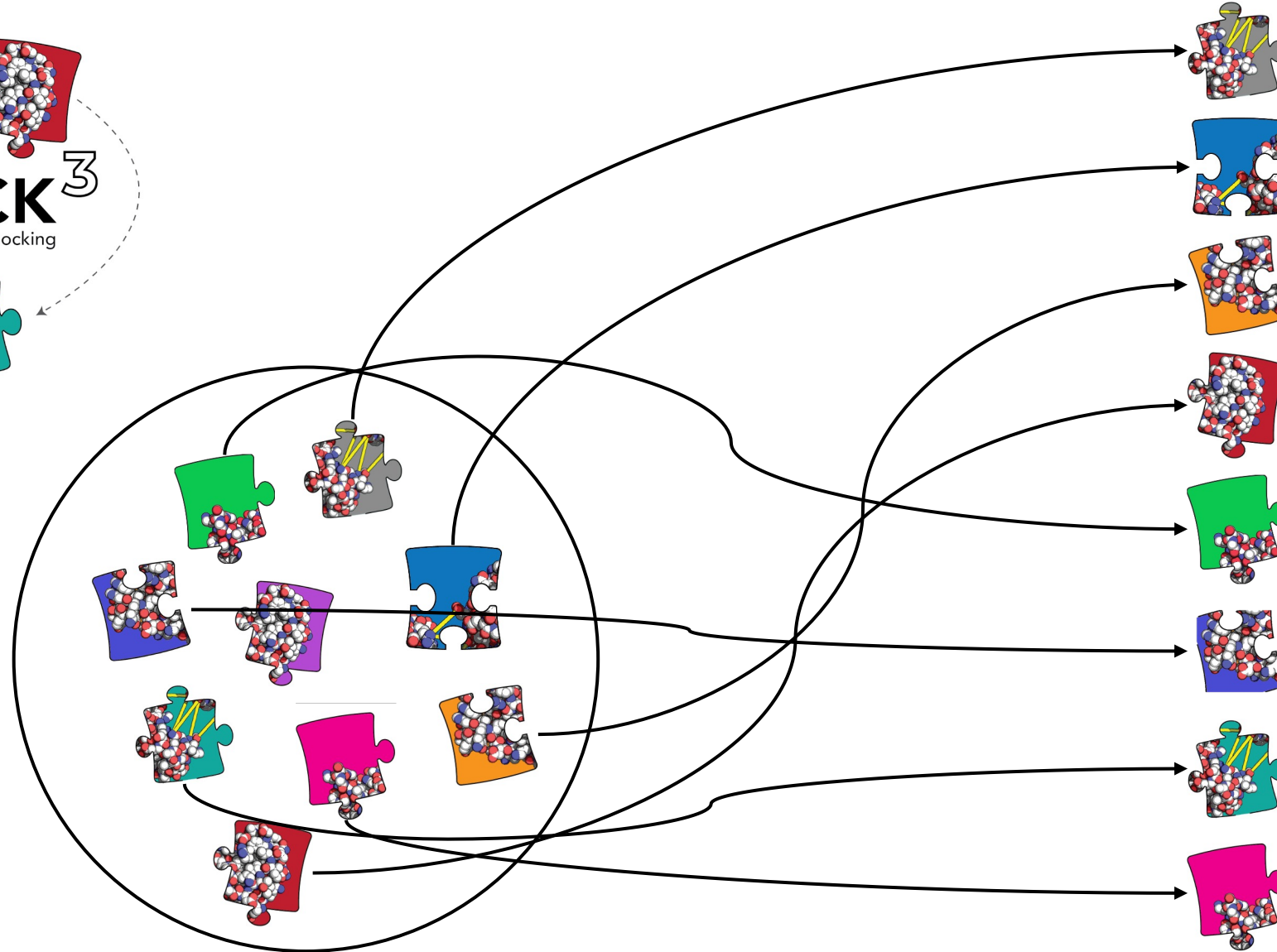
Catalogue of independent modules

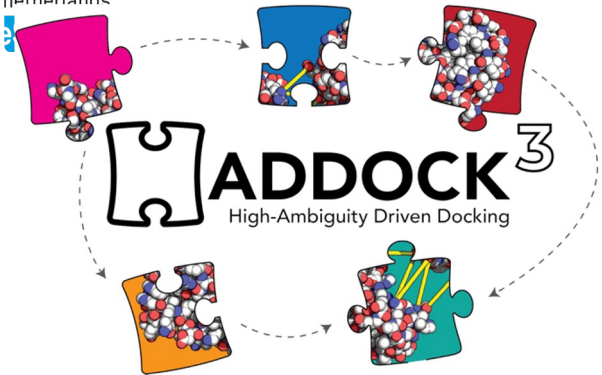


Combining the different pieces



Catalogue of independent modules





Mix and match modules to build custom workflows



topology

All-atom topology

analysis

- CAPRI eval
- RMSD matrix
- Clust by FCC
- Clust by RMSD
- Select top model
- Select top cluster
- DeepRank

sampling

- Rigid Body
- lightdock
- gdock

refinement

- Semi-Flexible ref.
- Energy minimization
- Short MD w/ explicit water
- openMM

scoring

- All-atom scoring
- All-atom scoring w/ MDexp. water

```
# =====
# Protein-protein docking example with
# NMR-derived ambiguous interaction restraints

# directory in which the scoring will be done
run_dir = "run1"

# molecules to be docked
molecules = [
  "data/e2aP_1F3G.pdb",
  "data/hpr_ensemble.pdb"
]

# =====
[topoaa]

[rigidbody]
ambig_fname = "data/e2a-hpr_air.tbl"
sampling = 1000

[seletop]
select = 200

[flexref]
ambig_fname = "data/e2a-hpr_air.tbl"

[emref]
ambig_fname = "data/e2a-hpr_air.tbl"

[caprieval]

[clustfcc]

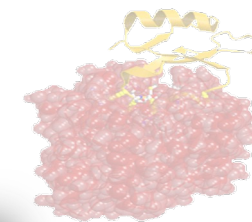
[seletopclusts]

[caprieval]

# =====
```



HADDOCK3's open-source repository



main ▾ 24 branches 6 tags

Go to file Add file <> Code ▾

mgiulini Merge pull request #639 from i-VRESSE/add_mol_viewer ... ✓ 0996f0c last week ⌚ 2,377 commits

.github	change codecov fail_ci_if_error	last week
devtools	Merge pull request #520 from haddocking/module_template	10 months ago
docs	Update INSTALL.md sementic on various haddock3	last month
examples	Merge pull request #632 from haddocking/adjust_clustrmsd	3 months ago
src	Merge pull request #639 from i-VRESSE/add_mol_viewer	last week
tests	use cluster rank instead of id, replace structure with model, fix test	3 weeks ago
varia	Update README.md	7 months ago
.bumpversion.cfg	name	last year
.gitignore	add haddock3-docs to .gitignore	last year
.gitmodules	add FCC submodule	2 years ago

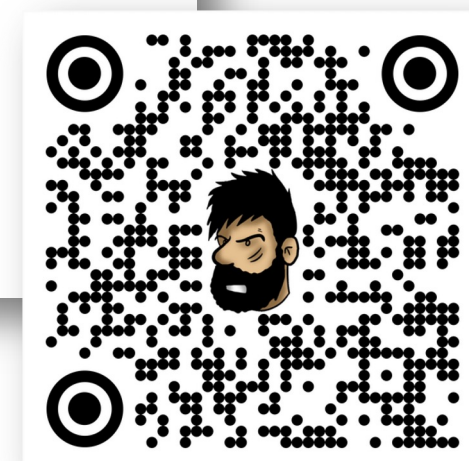
About

The official repo of the new modular BioExcel2 version of HADDOCK

www.bonvinlab.org/haddock3

bioinformatics proteins python3
modelling docking workflows
complexes integrative-modeling
utrecht-university

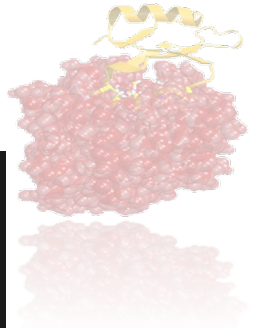
📖 Readme
📄 Apache-2.0 license
📈 Activity
★ 55 stars
👁 14 watching
🍴 22 forks
Report repository



<https://github.com/haddocking/haddock3>



HADDOCK3 development time line

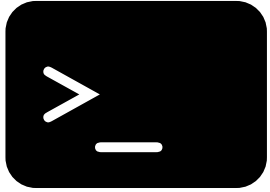


13/03/2019

HADDOCK3 Development Timeline



How to run?



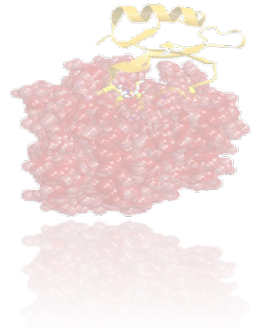
```
$ haddock3 m y-file.tom 1
```



Config file

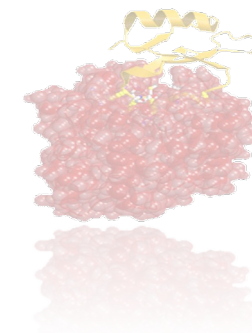


results folder



Current state: Only command line

Current execution modes



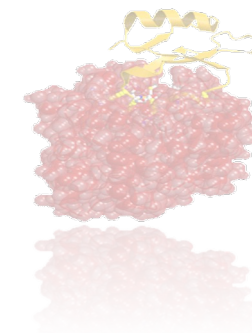
- **Local**

```
# compute mode  
mode = "local"  
ncores = 40
```

- **HPC (slurm & torque currently supported)**

```
# compute mode  
mode = "hpc"  
# Batch queue to use  
queue = "short"  
# Concatenate models inside each job  
concat = 5  
# Limit the number of concurrent submissions to the queue  
queue_limit = 250
```

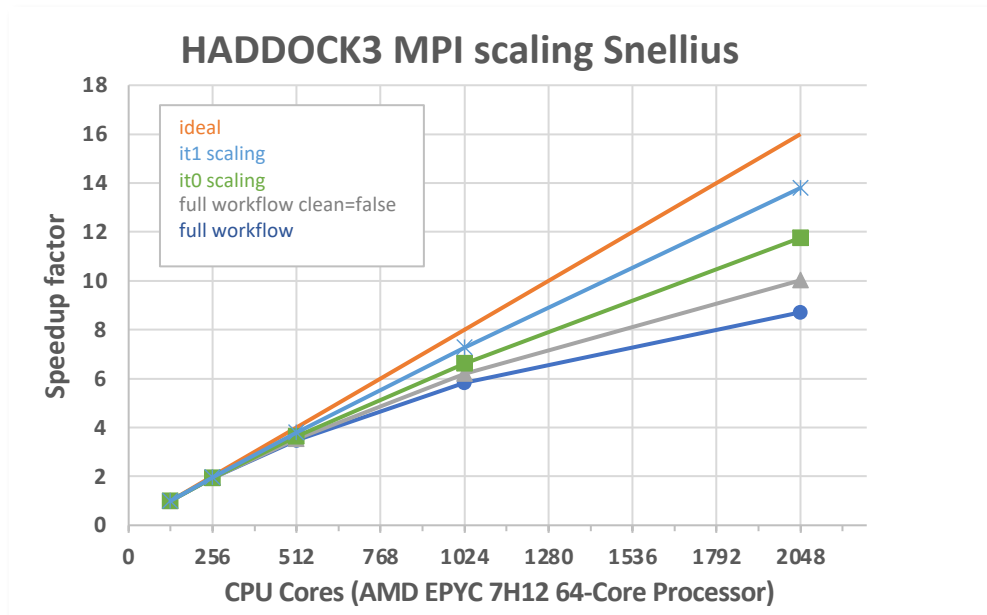
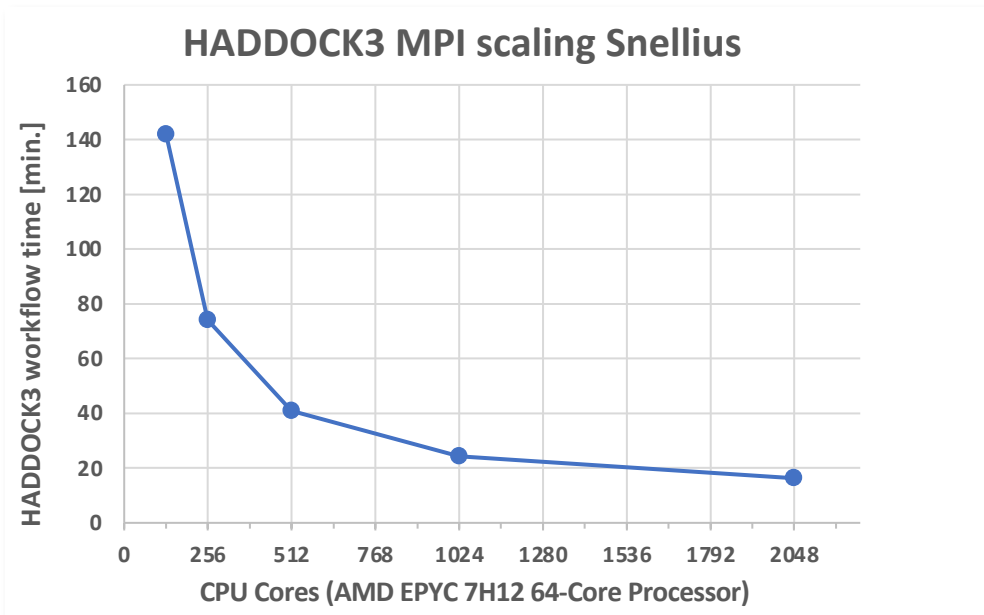
Current execution modes



- MPI

```
# compute mode
mode = "mpi"
# 5 nodes x 50 tasks = ncores = 250
ncores = 250
```

Antibody-antigen surface example
Sampling: 10240/2048/2048
rigidbody/flexref/emref



haddock-runner

Run large scale HADDOCK simulations using multiple input molecules in different scenarios



Rodrigo
Vargas Honorato



- ❑ Supports HADDOCK2.4, HADDOCK2.5 and HADDOCK3.0
- ❑ Scenarios are defined in standard YAML file
- ❑ Standalone executable
- ❑ Replicable and easily shared data generation blueprint
- ❑ Enables high throughput by leveraging HADDOCK's internal scheduling routines
- ❑ Free, Open and FAIR

User-guide: bonvinlab.org/education/haddock-runner

Source-code: github.com/haddock/haddock-runner

License Apache 2.0 linting passing unittests passing coverage 100% code quality A fair-software.eu sqaas software bronze

About ⚙️

Run large scale HADDOCK simulations using multiple input molecules in different scenarios

bonvinlab.org/education/haddock-run...

benchmark bioinformatics structural-biology high-performance-computing haddock large-scale utrecht-university

📖 Readme
📄 Apache-2.0 license
📄 Code of conduct
📈 Activity
⭐ 0 stars
👁 11 watching
🍴 2 forks
Report repository

Releases 10

📦 v1.5.0 Latest
on Feb 28

[+ 9 releases](#)

Contributors 4

rvhonorato Rodrigo V Honorato

dependabot[bot]

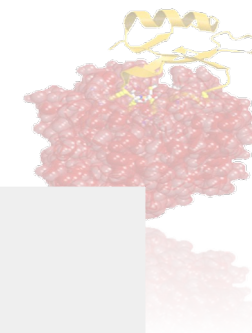
amjbonvin Alexandre Bonvin

mgiulini Marco Giuliani

Languages

Go 98.6% Shell 1.4%

Examples of runner config files

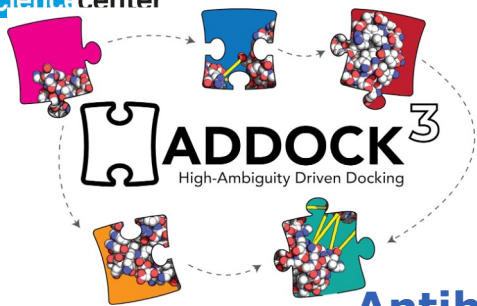


HADDOCK2.4

```
scenarios:
- name: true-interface
  parameters:
    run_cns:
      noecv: false
      structures_0: 1000
      structures_1: 200
      waterrefine: 200
    restraints:
      ambig: ambig
      unambig: restraint-bodies
      hbonds: hbonds
    custom_toppar:
      topology: _ligand.top
      param: _ligand.param
- name: center-of-mass
  parameters:
    run_cns:
      cmrest: true
      structures_0: 10000
      structures_1: 400
      waterrefine: 400
      anastruc_1: 400
    custom_toppar:
      topology: _ligand.top
      param: _ligand.param
```

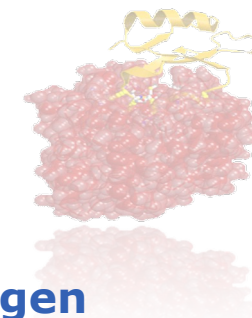
HADDOCK3.0

```
scenarios:
- name: true-interface
  parameters:
    general:
      mode: hpc
      queue: short
      queue_limit: 100
      concat: 5
    modules:
      order: [topoaa, rigidbody, seletop, flexref, emref, clustfcc, seletopclusts]
      topoaa:
        autohis: true
      rigidbody:
        ambig_fname: _ambig.tbl
        unambig_fname: _restraint-bodies.tbl
        ligand_param_fname: _ligand.param
        ligand_top_fname: _ligand.top
      seletop:
        select: 200
      flexref:
        ambig_fname: _ambig.tbl
        unambig_fname: _restraint-bodies.tbl
        ligand_param_fname: _ligand.param
        ligand_top_fname: _ligand.top
      emref:
        ambig_fname: _ambig
      clustfcc:
      seletopclusts:
```

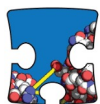


Example workflow

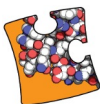
(not possible in HADDOCK2.X)



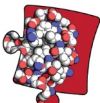
Antibody-antigen modelling with only CDR info and full surface on the antigen



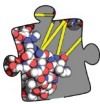
1. Build topo



2. Rigid-body (10000)



3. CAPRIeval



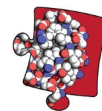
4. FCC clustering



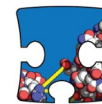
5. Select clusters (min size 4)
(max. 20 models per cluster)



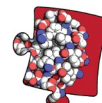
6. Flexref



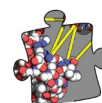
7. CAPRIeval



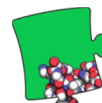
8. EMref



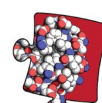
9. CAPRIeval



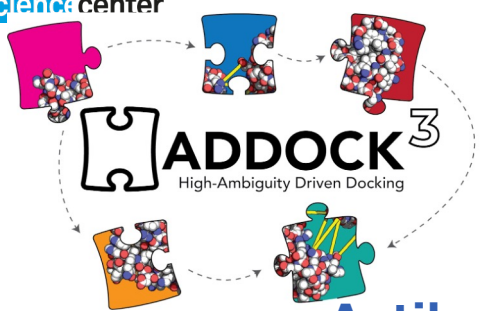
10. FCC clustering



11. Select clusters (min size 4)

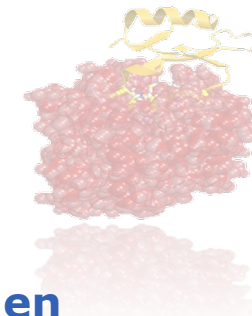


12. CAPRIeval



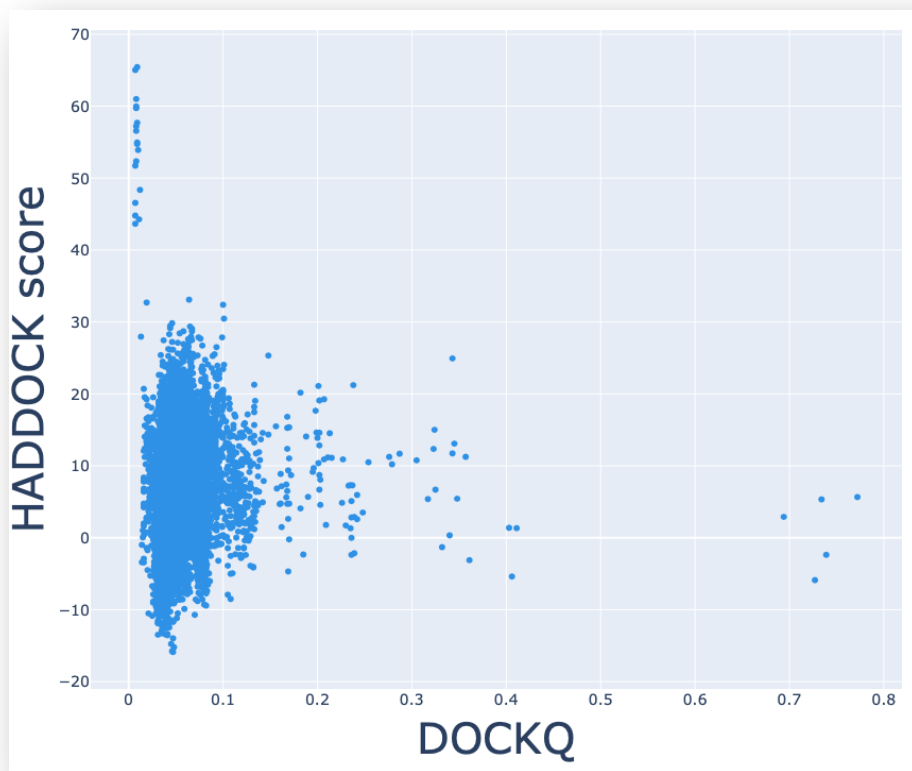
Example workflow

(not possible in HADDOCK2.X)

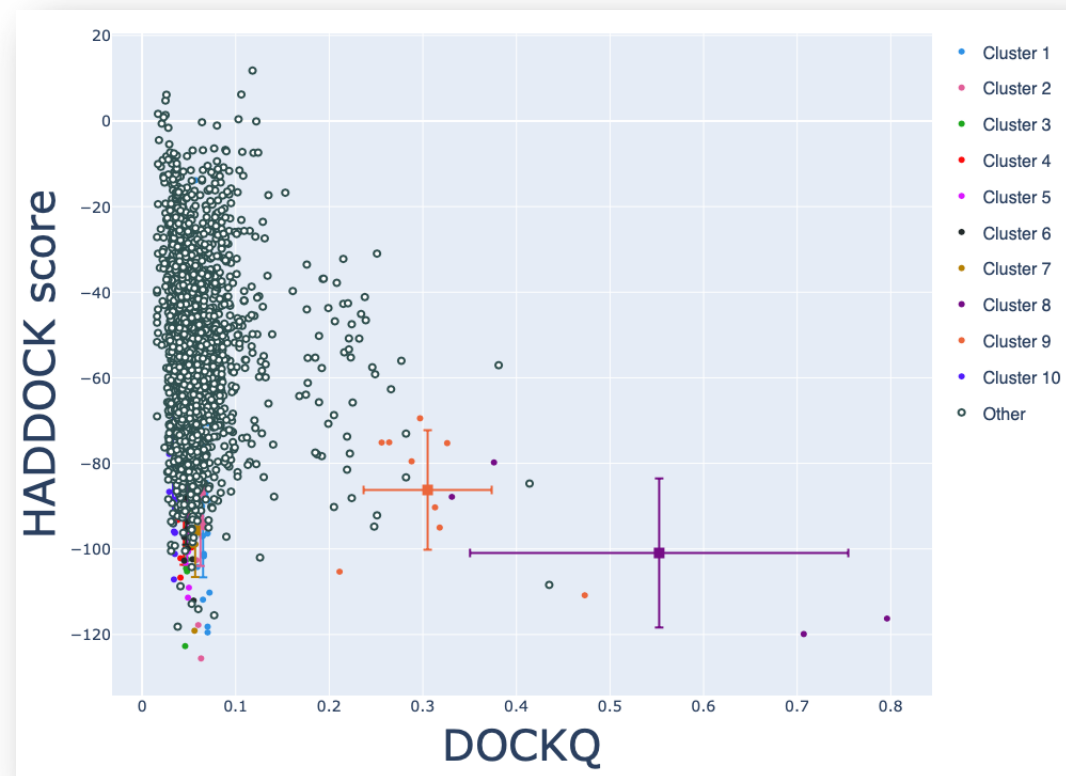


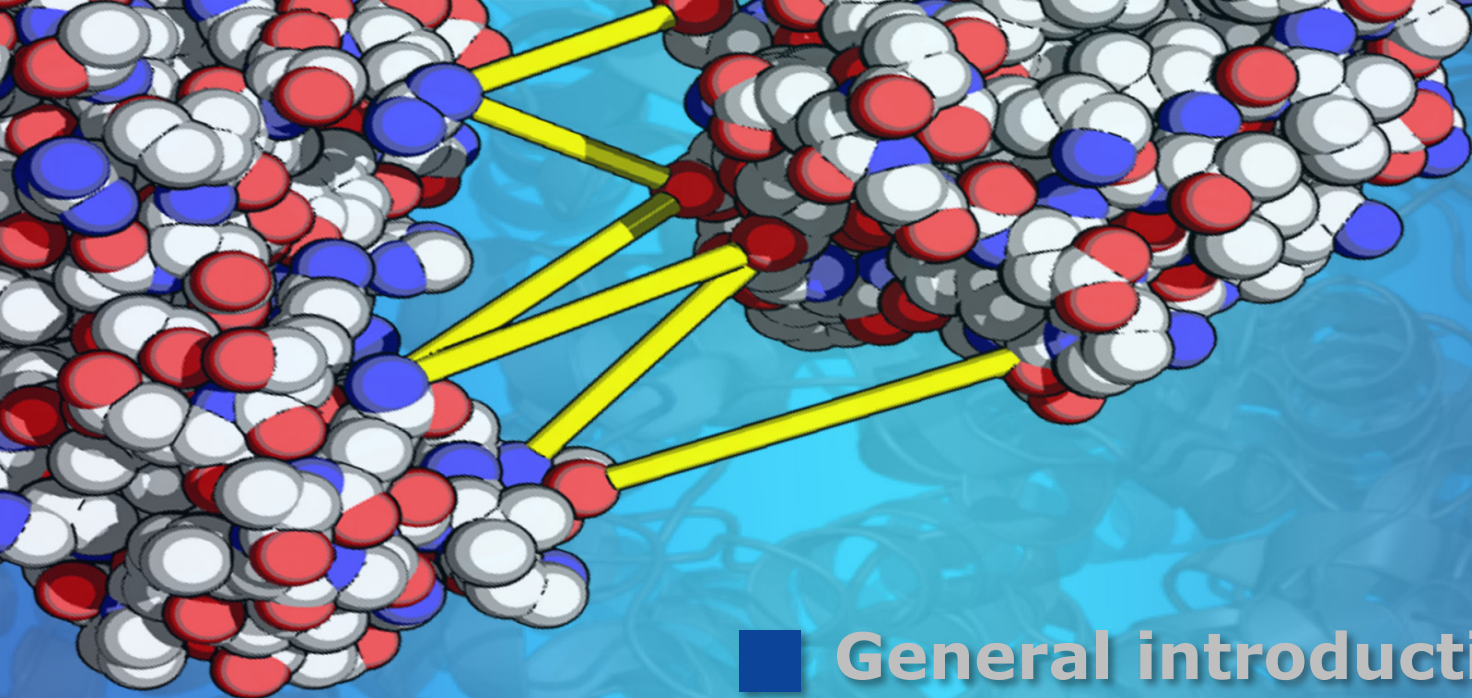
Antibody-antigen modelling with only CDR info and full surface on the antigen

Rigid body



Final refinement clusters



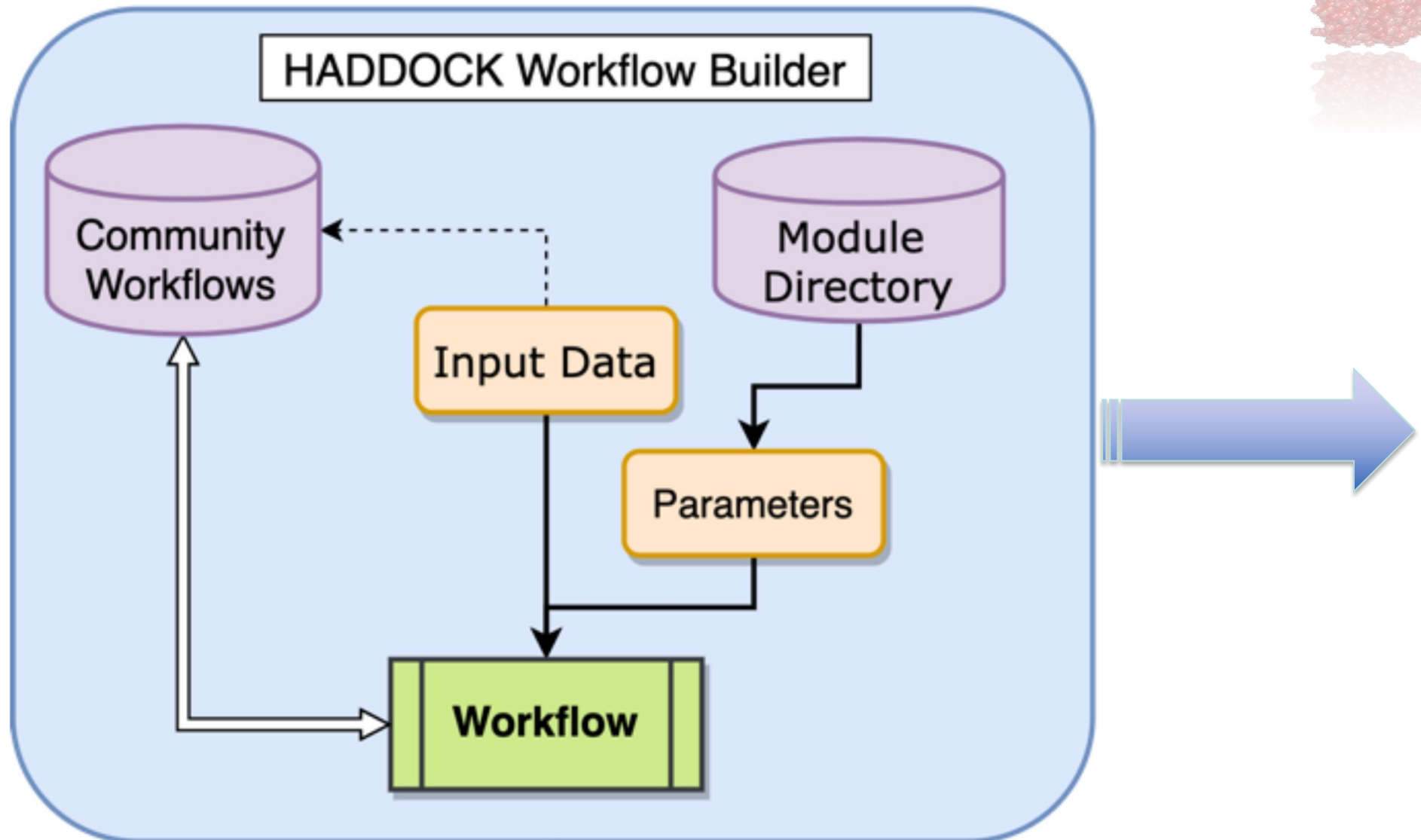
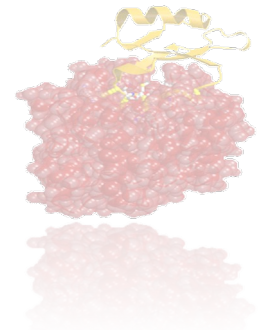


Overview

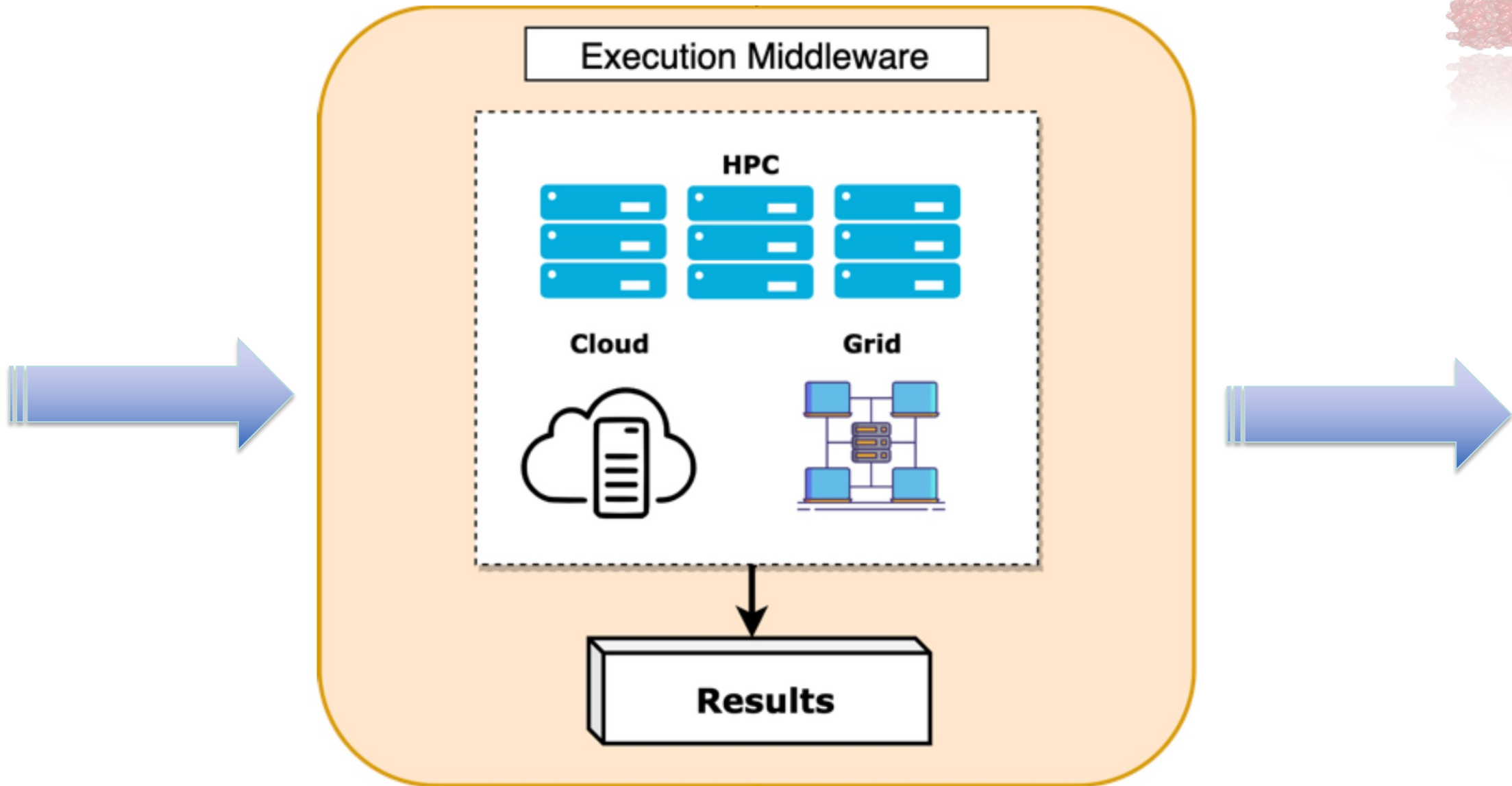
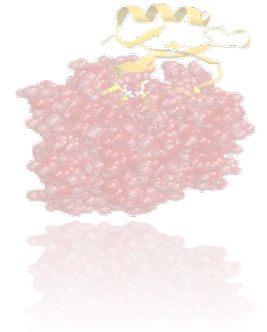
- General introduction
- Introducing the new modular HADDOCK3
- Towards a virtual research environment for HADDOCK3 – i-VRESSE
- Conclusions

```
111000100101010110101010
100011010101000101111010110101
10100001000111101010101110000110101
0001010101011110010100110010101010100
0101011111110101010000101010100000101010100
0010110101011101010001111010101010001010010101011111
0001111111010101011001100010111000101011010100010101000101
```

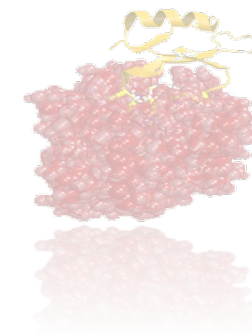
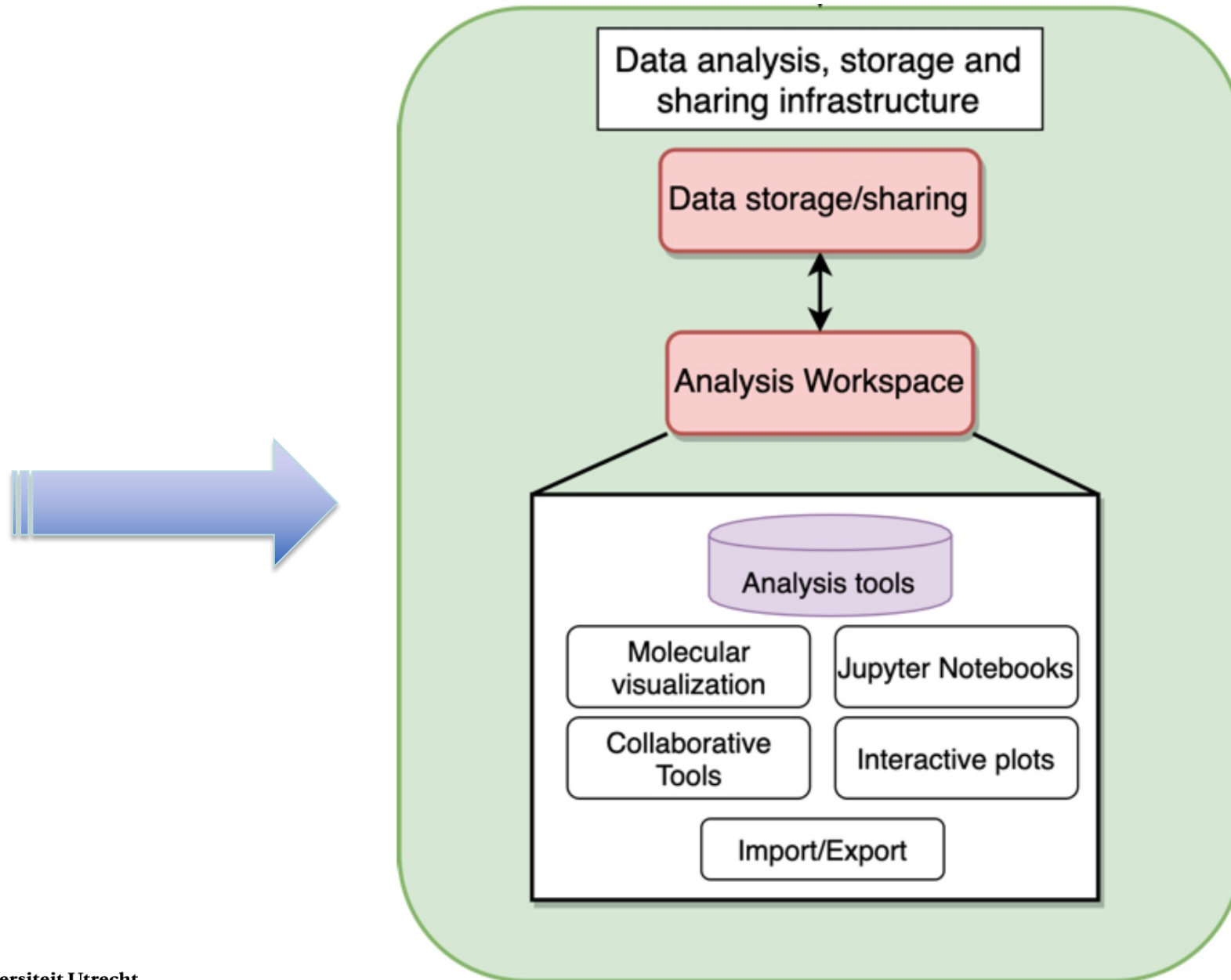

The plan...



The plan...

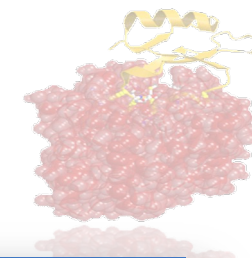


The plan...





Toward a new interface for HADDOCK3



Web application to build and execute HADDOCK3 workflows and manage, view and analyze results

Haddock3 Build Upload Manage About Help

Bonvin Lab

Build

Use the workflow builder to create and submit a job.

Upload

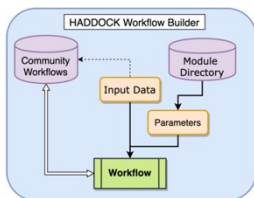
Upload a workflow and submit as job.

Manage

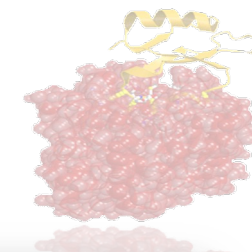
Explore and analyse the results of completed jobs.

github.com/i-VRESSE/bartended-haddock3





The workflow builder

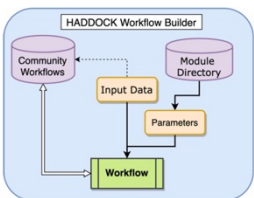


Haddock3 Build Upload Manage About Help **Bonvin Lab** Login

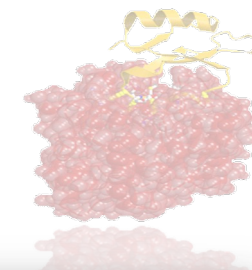
Build
Use the workflow builder to create and submit a job.

Upload
Upload a workflow and submit as job.

Manage
Explore and analyse the results of completed jobs.



Workflow builder



Workflow builder is dynamically configured based on HADDOCK3's modules definitions and parameters

Drag and drop workflow builder

Haddock3 Build Upload Manage About Help

Bonvin Lab

computational structural biology Login

Catalog Nodes

- ▼ topology
 - topoaa
- ▼ sampling
 - gdock
 - rigidbody
 - lightdock
- ▼ refinement
 - mdref
 - flexref

Workflow

Global parameters Upload

Visual Text

- topoaa
- rigidbody
- caprieval**
- seletop
- flexref
- caprieval

Submit Download archive

Node

Calculate CAPRI metrics. (caprieval)
HADDOCK3 module to calculate the CAPRI metrics.

analysis

Reference structure

Choose File No file chosen

data/target.pdb (chemical/x-pdb, 229768 bytes)
Structure to be used when calculating the CAPRI metrics.

Calculate I-RMSD
Performs Interface RMSD calculations.

Calculate FNAT
Performs FNAT calculations.

Save Cancel Delete

i-VRESSE workflow builder: Haddock 3 on easy level

haddock3easy

Nodes

▼ topology

- o topoa

▼ sampling

- o gdock
- o rigidbody
- o lightdock

▼ refinement

- o mdref
- o flexref
- o emref

▼ scoring

- o mdscoring
- o emscoring

▼ analysis

- o seletopclusts
- o clustrmsd
- o caprieval
- o rmsdmatrix
- o clustfcc

Workflow

Global parameters Upload

Visual Text

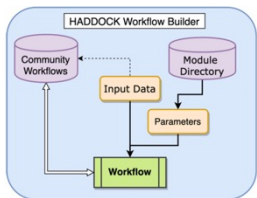
Append node to workflow by clicking node in catalog
 or by dragging node from catalog to here.

Download archive Clear

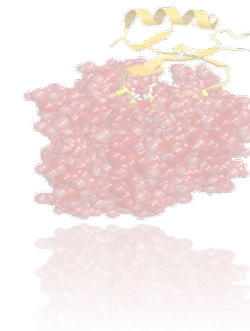
Node

No node or global parameters selected for configuration.





Easy integration: E.g. Galaxy



Galaxy Workflow Visualize Shared Data Admin Help User Using 196.7 MB

Tools: search tools, Upload Data

Get Data, Send Data, Collection Operations, Text Manipulation, Docking, Filter and Sort, Join, Subtract and Group, Built-in Converters, **WORKFLOWS**, All workflows

i-VRESSE workflow builder on guru level

Calculation completed successfully
Goto results (opens in new window)

Catalog: haddock3guru

Nodes:

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

Global parameters:

```

molecules = [
  'data/e2aP_1F3G.pdb',
  'data/hpr_ensemble.pdb',
]
ncores = 12
run_dir = 'run1-test'
[topoaa]
autohis = false
[topoaa.mo1]
nhisd = 0
nhise = 1
hise_1 = 75
[topoaa.mo2]
nhisd = 1
hisd_1 = 76
nhise = 1
hise_1 = 15
[rigidbody]
tolerance = 20
ambig_fname = 'data/e2a-hpr_...'
sampling = 20
[caprieval]
reference_fname = 'data/e2a-hpr_...'
[seletop]
select = 5
[flexref]
tolerance = 20
  
```

Path to the CNS executable: Choose File (No file chosen)

Number of CPU cores: 12

Mode of execution: local

Batch system: slurm

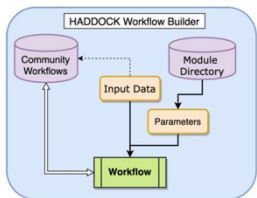
Queue name: [empty]

Number of jobs to submit to the batch system: 100

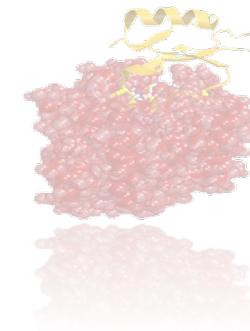
Number of models to produce per job: [empty]

Submit Clear Submit Cancel

History: 23.6 MB, 2: index.html, 1: docking-protein-ligand.zip



Easy integration: E.g. JupyterLab



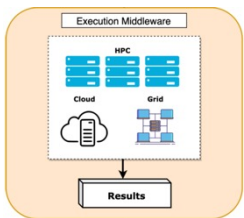
The screenshot shows the JupyterLab interface for configuring a HADDOCK3 workflow. The main window is titled 'untitled1.cfg' and contains the following sections:

- Catalog Nodes:** A tree view of workflow nodes including topology (topoaa), sampling (gdock, rigidbody, lightdock), refinement (mdref, flexref, emref), scoring (mdscoring, emscoring), and analysis (seletopclusts, clustrmsd, caprieval, rmsdmatrix, clustfcc, seletop).
- Global parameters:** A tab for editing workflow parameters. The 'Text' view shows:

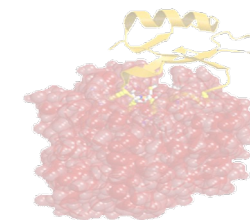

```

      run_dir = 'x'
      molecules = [
        '2oob.pdb',
      ]
      [gdock]
      ambig_fname = 'pyproject.toml'
      
```
- Global parameters configuration:**
 - Run directory*: x
 - Input Molecules: 0 (with a 'Choose file' button and '2oob.pdb' selected)
 - Execution options: 'clean' and 'execution' are checked.
- Files:** A list of files including '2oob.pdb' and 'pyproject.toml'.

The right sidebar contains various tool icons: Notebook, Python 3 (ipykernel), Console, Python 3 (ipykernel), Terminal, Haddock3 config, Text File, Markdown File, and Python File.



The bartender



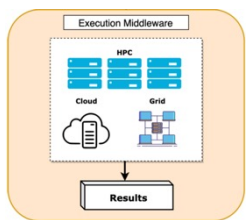
Backend to schedule jobs on various infrastructures and user management with social logins

Generic:
Can be configured as scheduler for any kind of service (requires CLI or container)

The screenshot shows the Bonvin Lab website interface. The header includes 'Haddock3', 'Build', 'Upload', 'Manage', 'About', and 'Help'. The main content area features three cards: 'Build' (gear icon), 'Upload' (folder icon with an arrow, circled in red), and 'Manage' (analysis workflow diagram). The 'Bonvin Lab' logo is visible in the top right.

github.com/i-VRESSE/bartender

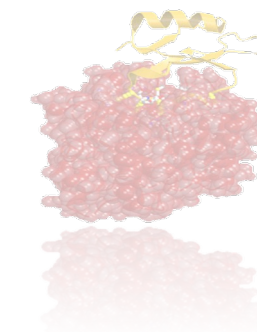


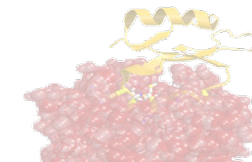


RESTful
application with
dynamic
documentation of
its APIs

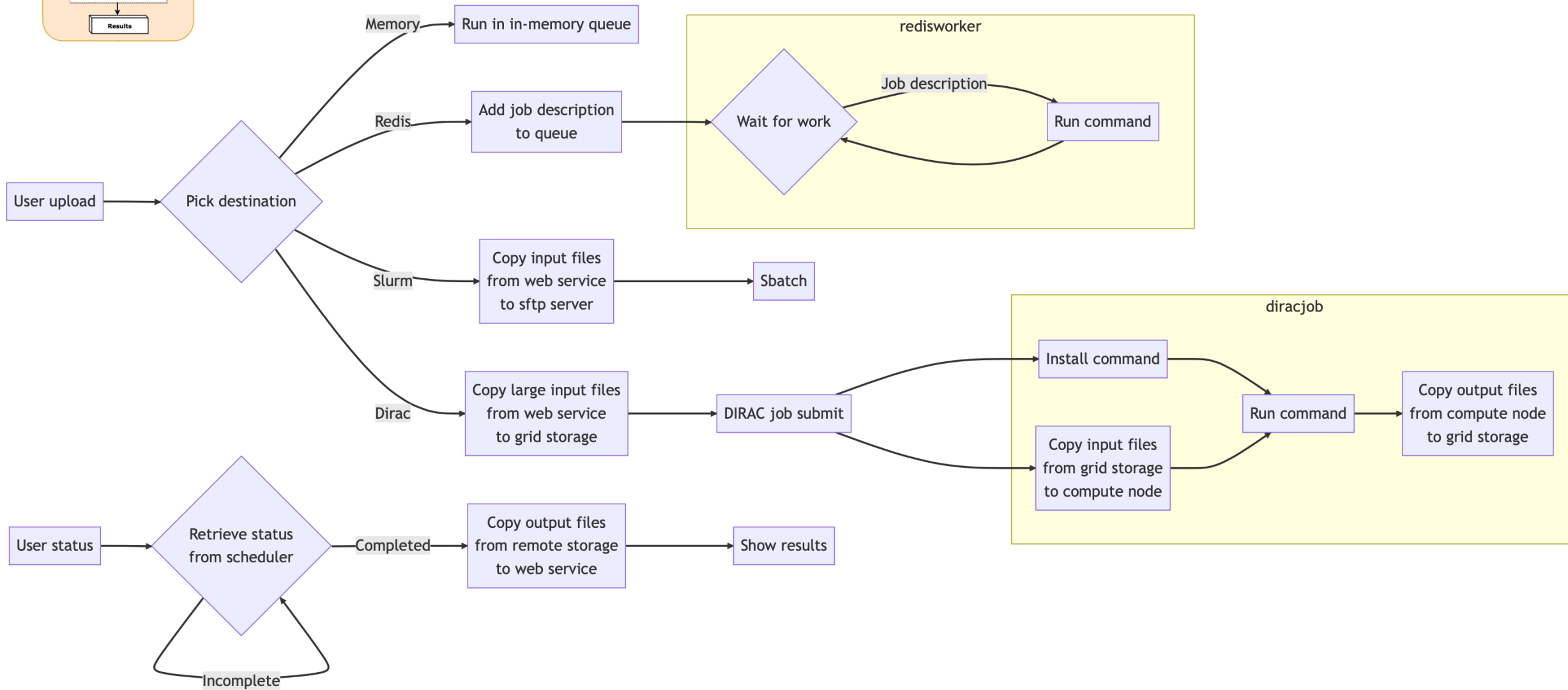
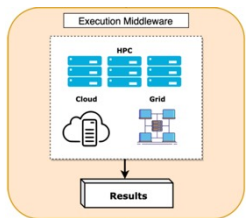
Needs to be
configured on
some (remote)
server(s)

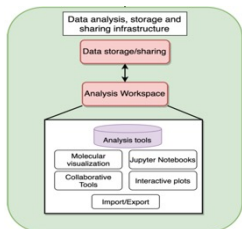
default		
GET	/api/health	Health Check
job		
GET	/api/job/	Retrieve Jobs
GET	/api/job/{jobid}	Retrieve Job
GET	/api/job/{jobid}/files/{path}	Retrieve Job Files
GET	/api/job/{jobid}/stdout	Retrieve Job Stdout
GET	/api/job/{jobid}/stderr	Retrieve Job Stderr
application		
GET	/api/application/	List Applications
GET	/api/application/{application}	Get Application
PUT	/api/application/{application}/job	Upload Job
users		
GET	/api/users/profile	Profile
GET	/users/me	Users:Current User
PATCH	/users/me	Users:Patch Current User
GET	/users/{id}	Users:User



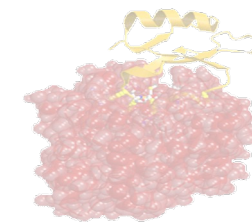


Bartender - Job flow

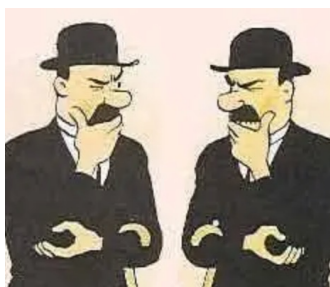




Management and analysis platform



Will provide data management, analysis and visualization tools



Haddock3 Build Upload Manage About Help

Bonvin Lab

Login

Build

Use the workflow builder to create and submit a job.

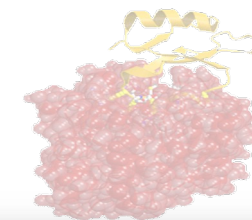
Upload

Upload a workflow and submit as job.

Manage

Explore and analyse the results of completed jobs.

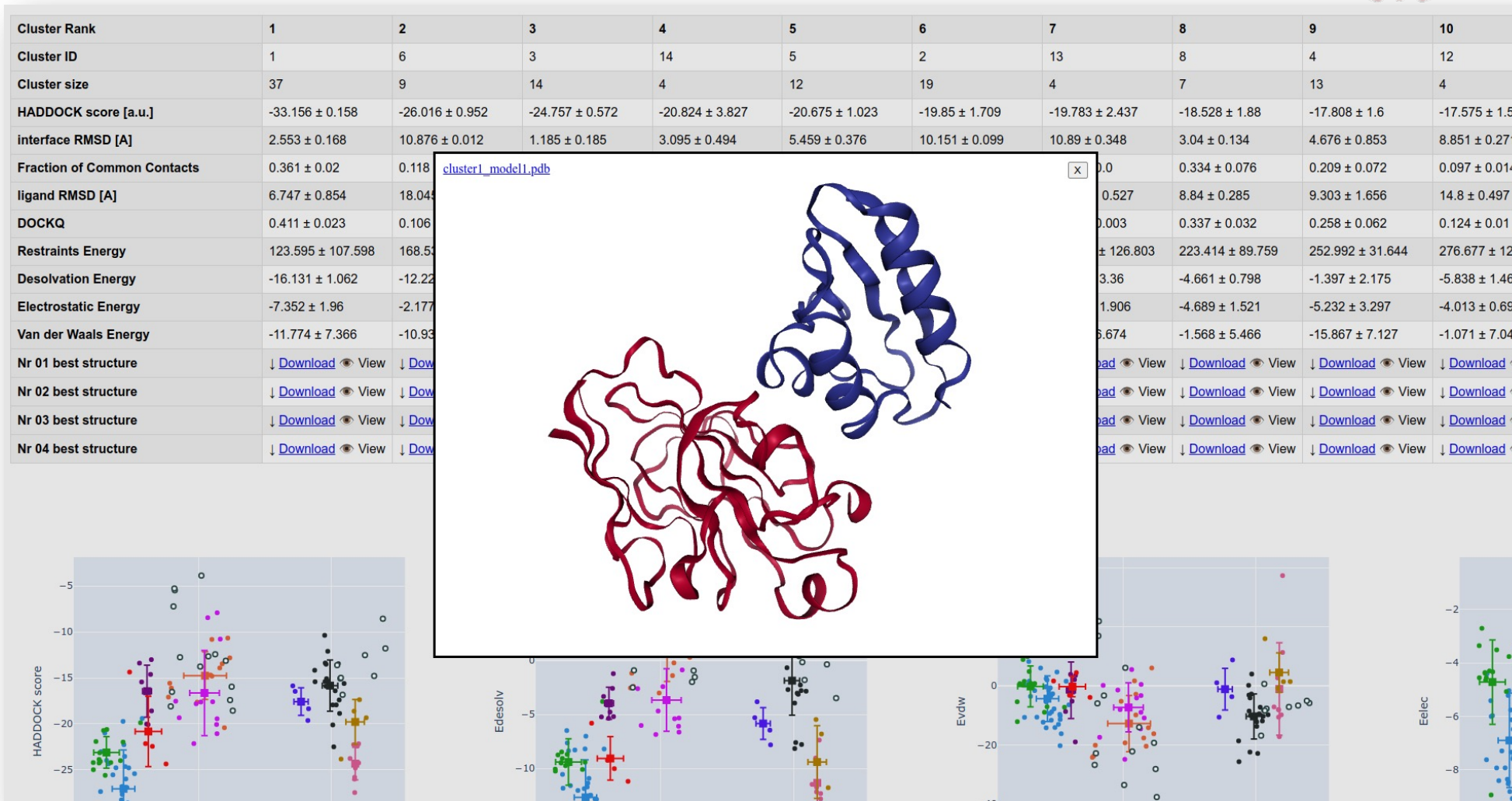
[github.com/i-VRESSE/...](https://github.com/i-VRESSE/)



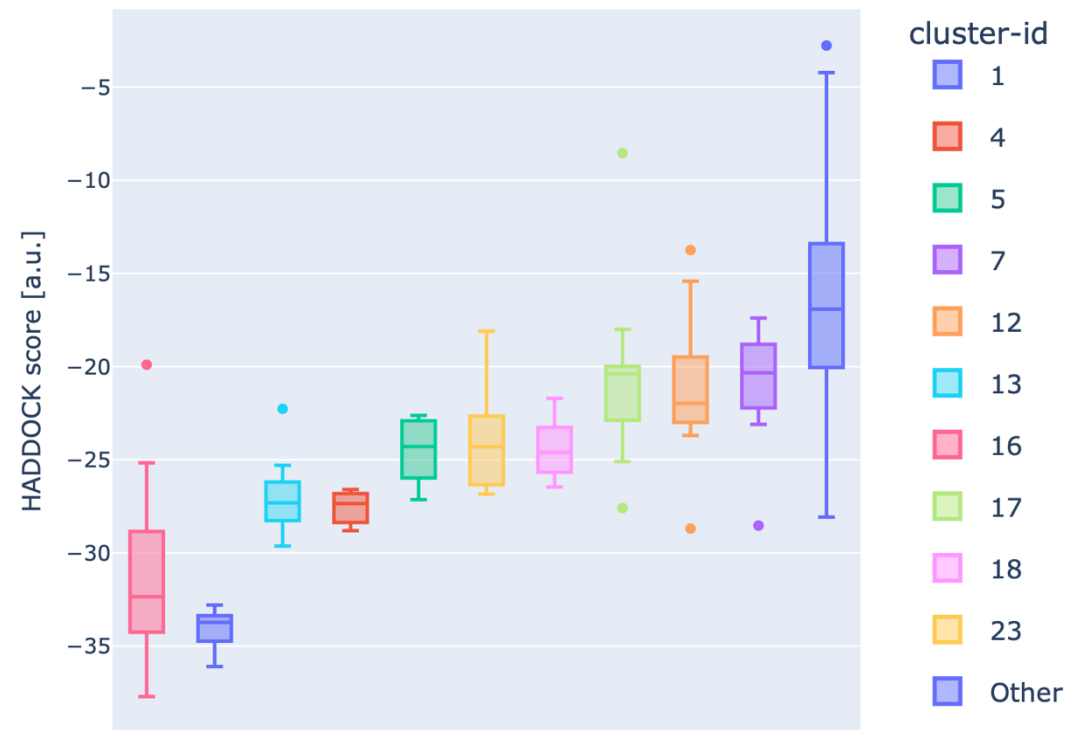
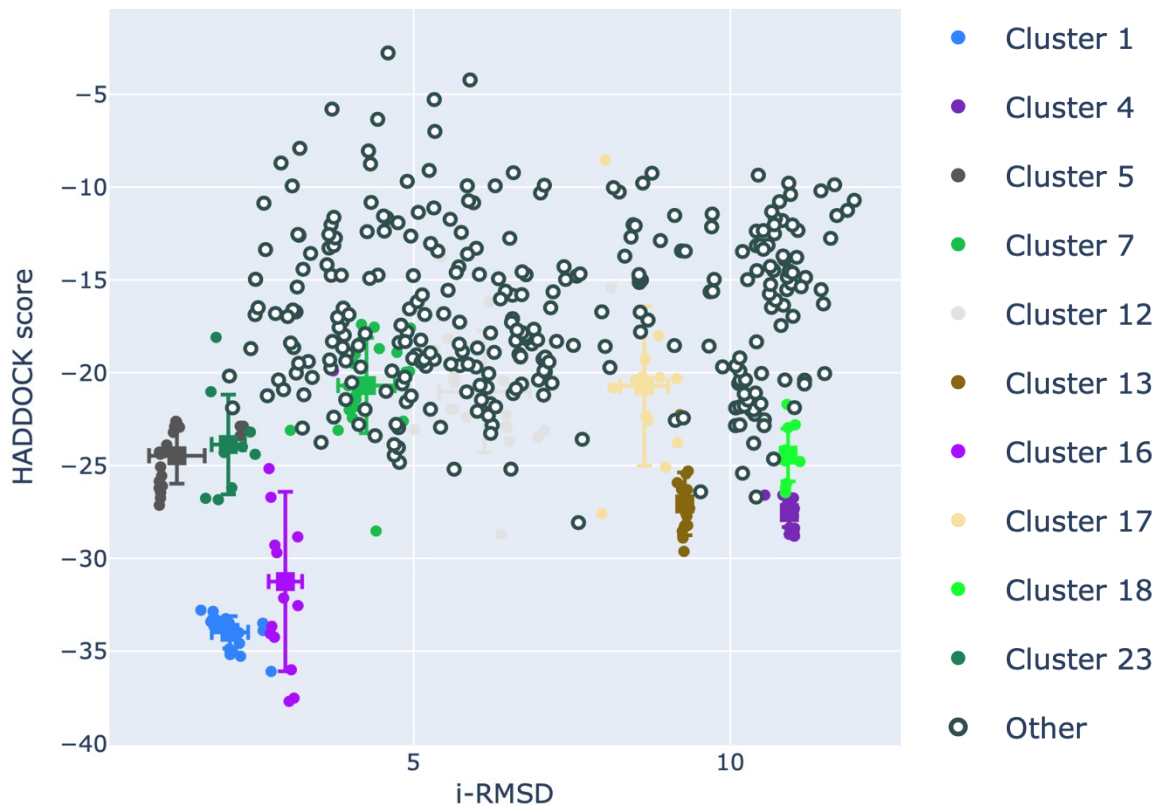
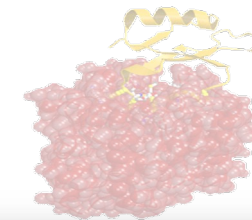
HADDOCK3 analyse report

HADDOCK3 can automatically generate interactive analysis plots (similar to what the 2.4 server gives)

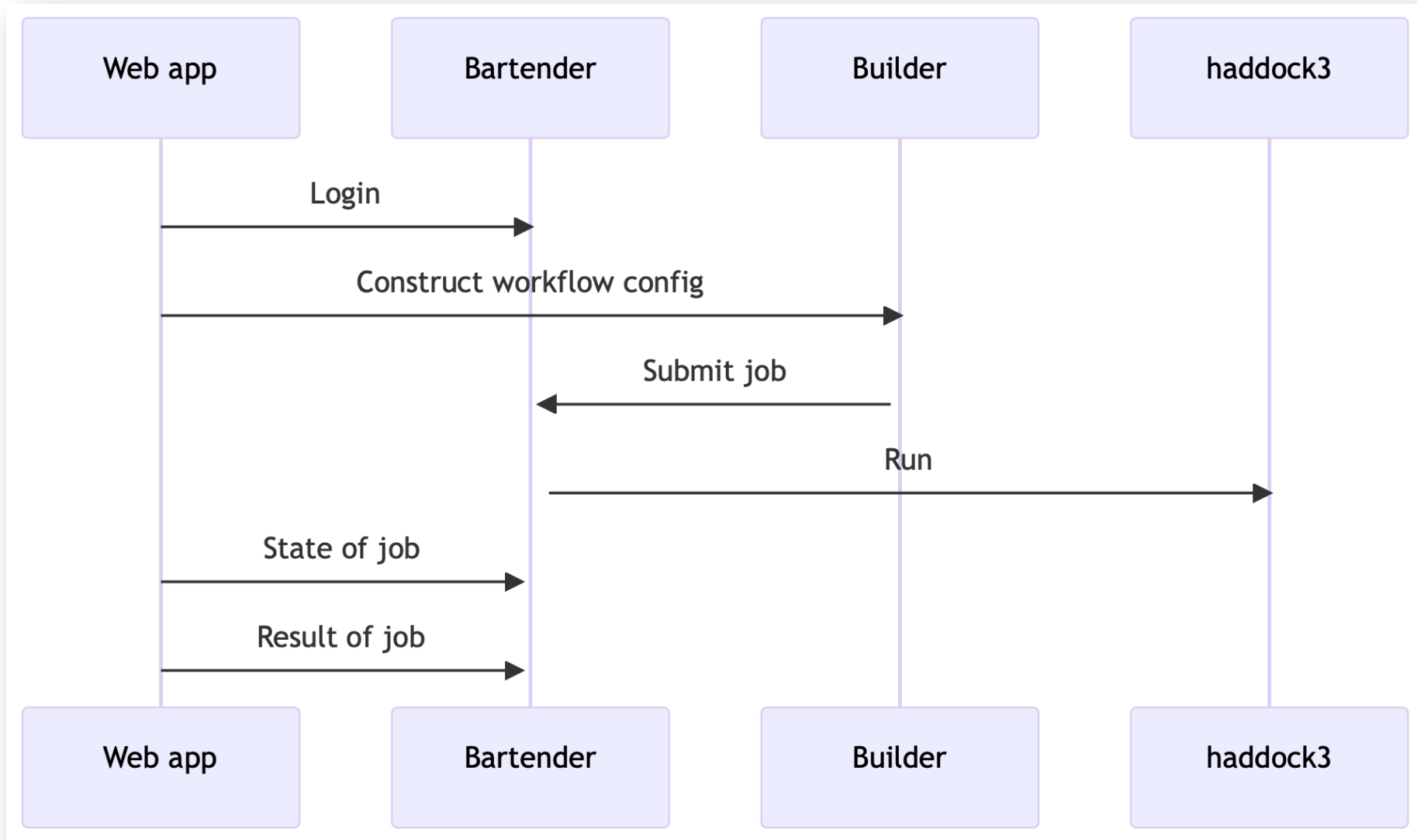
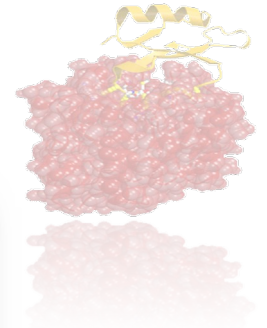
Will form the basis for the analysis interface



HADDOCK3 analyse report

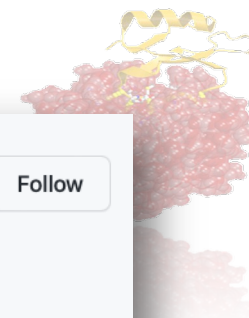


Bartended HADDOCK3 overall workflow





i-VRESSE



Interactive Virtual Research Environment for Scientific Software Execution

Project with Netherlands eScience Center and Bonvin Lab

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Popular repositories

[workflow-builder](#)

Public

Graphical interface to build a workflow file

TypeScript ☆ 2

[workflow-comparison](#)

Public

Python

[pdbtbx](#)

Public

Forked from douweschulte/pdbtbx

A library to open/edit/save (crystallographic) Protein Data Bank (PDB) and mmCIF files in Rust.

Rust

[pdbtbx-ts](#)

Public

JS wrapper around pdbtbx rust crate

Rust 🔗 1

[jupyterlab-haddock3-configurator](#)

Public

Jupyter Lab extension to create/edit haddock3 configuration file

TypeScript

[bartender](#)

Public

Middleware web service to schedule jobs on various infrastructures

Python

View as: **Public** ▾

You are viewing the README and pinned repositories as a public user.

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Discussions

Set up discussions to engage with your community!

[Turn on discussions](#)

People

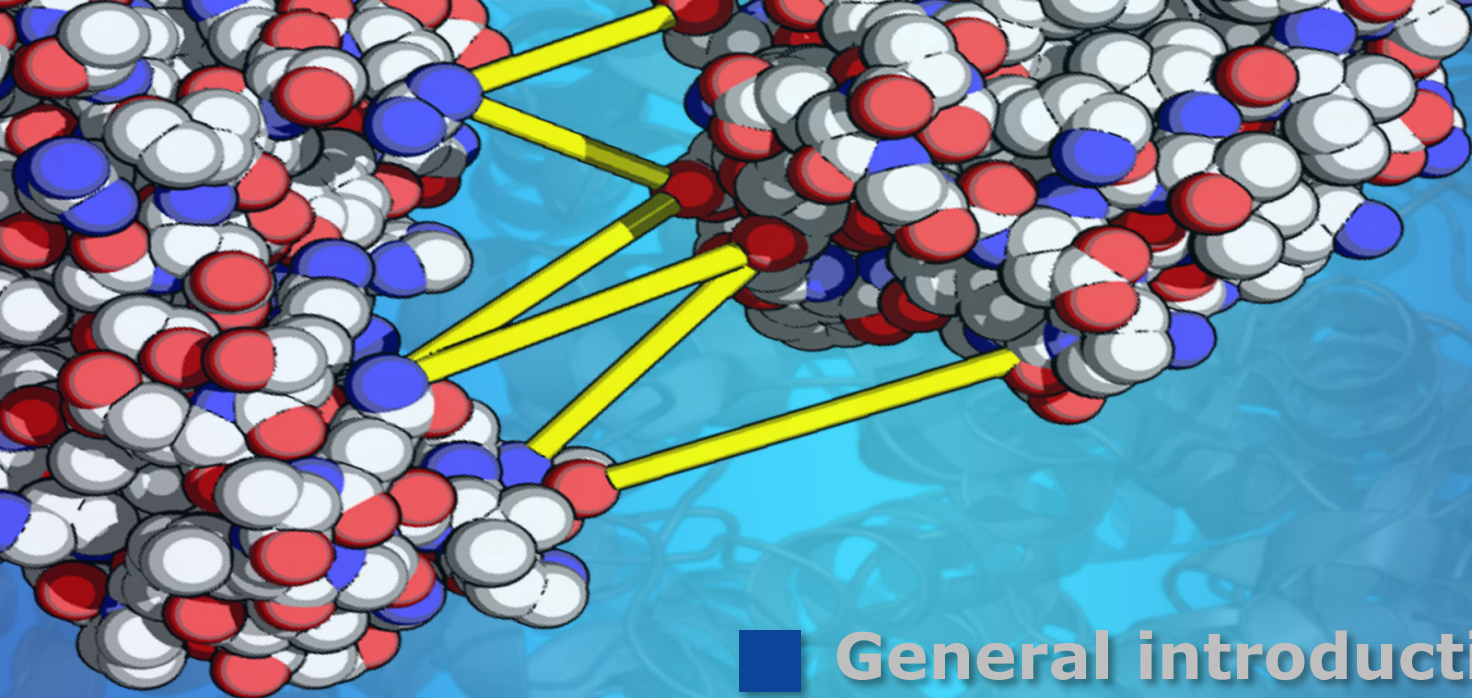


<https://github.com/i-VRESSE>



Universiteit Utrecht

[Faculty of Science
Chemistry]

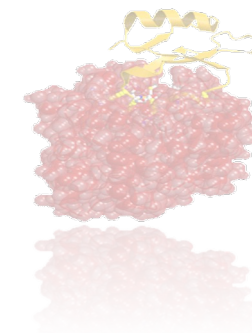


Overview

- General introduction
- Introducing the new modular HADDOCK3
- Towards a virtual research environment for HADDOCK3 – i-VRESSE
- Conclusions

```
111000100101010110101010
100011010101000101111010110101
10100001000111101010101110000110101
0001010101011110010100110010101010100
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```

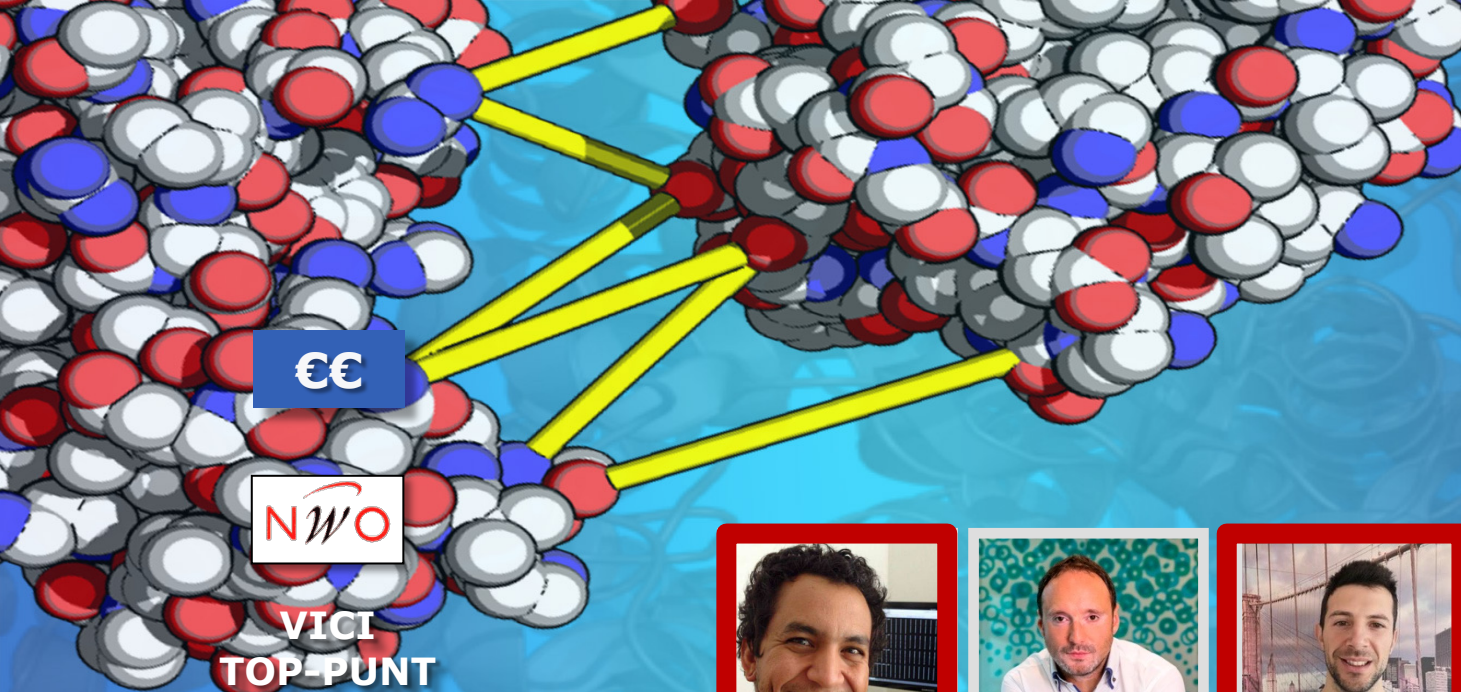
Conclusions



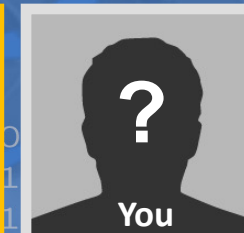
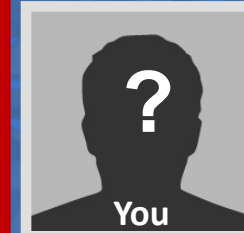
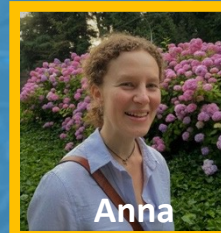
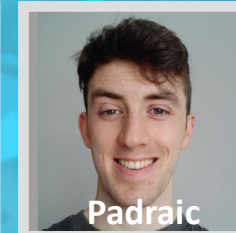
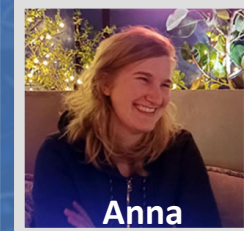
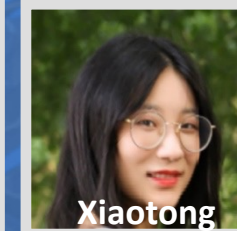
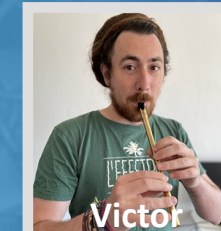
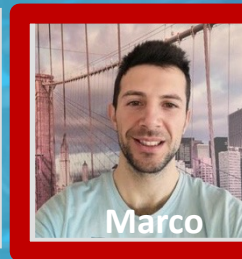
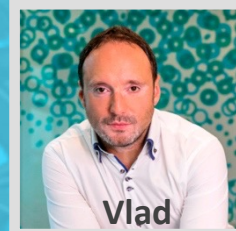
- **Finalizing the 1st production release of HADDOCK3**
 - Modularity and custom workflows
 - Integrated analysis tools that can be leveraged by the VRE (only offered until now via the web server for HADDOCK2.X)
 - Both HTC and HPC oriented (EuroHPC BioExcel CoE core software)
- **New VRE software for integrative modelling (i-VRESSE)**
 - Will provide the user-friendly interface and integrated backend to build/execute/analyze HADDOCK3 workflows
 - Easy off-site deployment with docker compose (next to centralized WeNMR service)
 - Generic technology that can be reused for other projects

Acknowledgments:

former and current
CSB group@UU

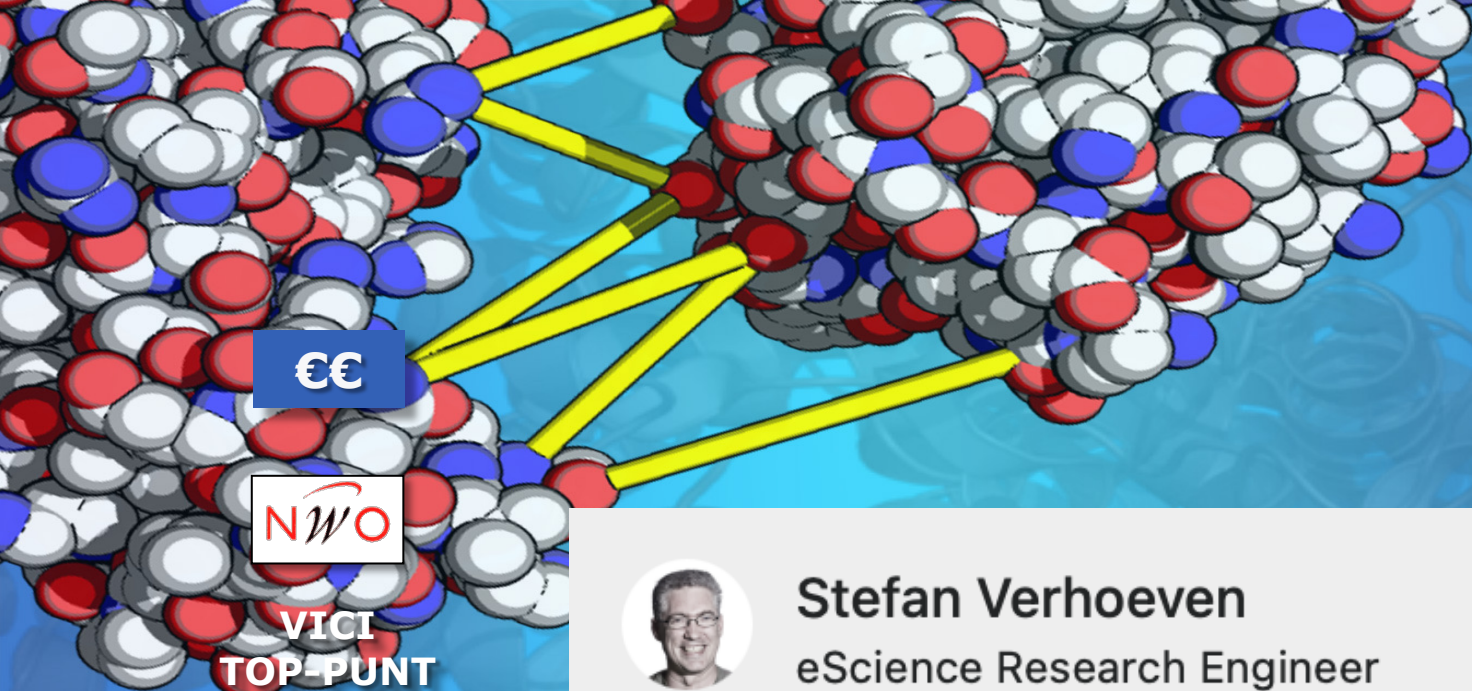


WeNMR
West-Life
EGI-Engage
INDIGO-Datacloud
BioExcel CoE
EOSC-Hub
EGI-Ace



bonvinlab.org/people

Acknowledgments: the eScience Center team



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



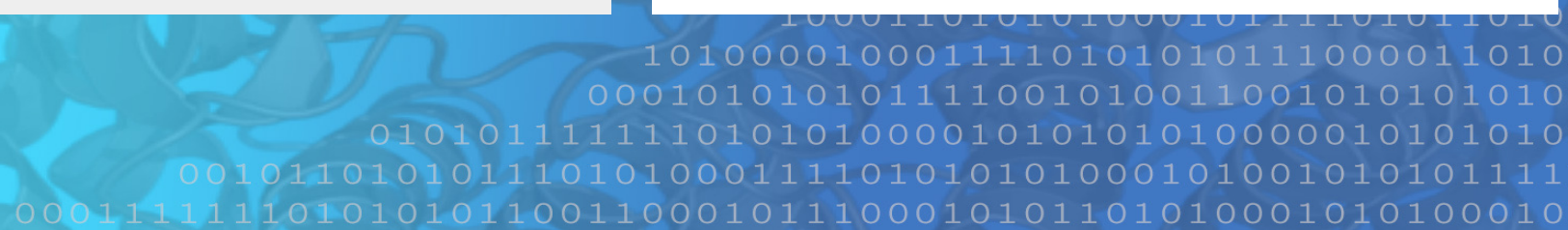
Stefan Verhoeven
eScience Research Engineer
Netherlands eScience Center
ID 0000-0002-5821-2060

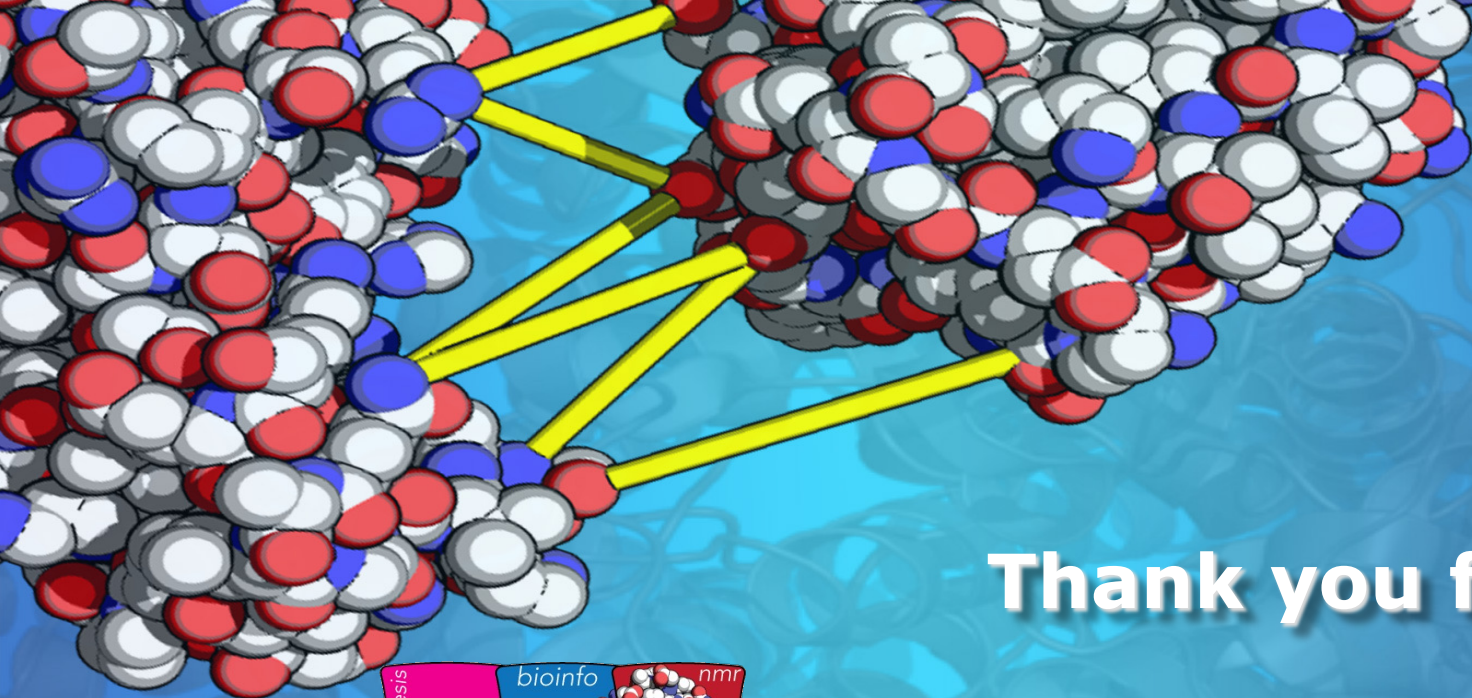


Peter Kalverla
Netherlands eScience Center
ID 0000-0002-5025-7862

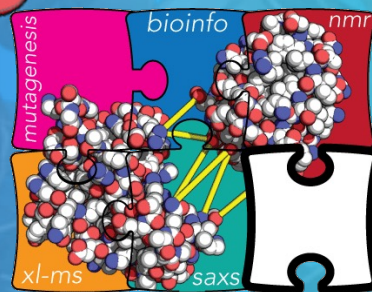


Fakhreh (Sarah) Alidoost
Netherlands eScience Center
ID 0000-0001-8407-6472





Thank you for your attention!



HADDOCK
High-Ambiguity Driven Docking

HADDOCK online:

- <https://wenmr.science.uu.nl>
- <https://bonvinlab.org/software>
- <https://github.org/haddocking>
- <https://github.org/i-VRESSE>
- <https://ask.bioexcel.eu>



Utrecht
Bioinformatics
Center

111000100101010110101010
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0001010101011110010100110010101010100
0101011111101010100001010101010000101010100
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0001111110101010110011000101110001010110101000101010001010