

Date: 16 November 2022 1:00-2:30 p.m.

Venue: 1520-731 (Sea View)

Topic: Research Committee at Nat – 5th meeting 2022

Participants: David Lundbek Egholm/DLE (NAT, chair), Anders Møller/AM (CS), Kurt Vesterager Gothelf/KVG (iNANO), Michael Møller Hansen/MMH (BIO), K. Brad Wray/KBW (MATH), Ove Christiansen/OC (CHEM), Steen Hannestad/SH (PHYS), Søren Munch Kristiansen/SMK (GEO), Torben Heick Jensen/THJ (MBG), Astrid Klungen/ARK (NAT, minutes)

Cancelations: --

Guest: Rasmus Handberg/RH (NAT) for item 3

Minutes

13:00 – 13:05 (5 min)

1. Welcome and approval of agenda

Attachment: Referat fra 21. september 2022 (godkendt)

DLE opened the meeting by welcoming KBW, who will represent MATH for the time being. All participants introduced themselves. The agenda got approved.

13:05 – 13:20 (15 min)

2. New Research at MBG by THJ

THJ presented MBG and two recent research projects (slide deck attached).

13:20 – 13:50 (30 min)

3. Data Management at Nat by RH

DLE introduced RH, newly assigned Data Management Coordinator at Nat (50% position, while he continues with 50% as Data and Systems Manager at PHYS. RH will tour all departments in the beginning of 2023.

RH presented the framework for Data Management/Open Science at AU, and gave an introduction to ERDA/SIF (slide deck attached).

Upon questions from the participants, RH added that:

- ERDA/SIF is physically located in Stilling and hooked to the Danish Research Network. Data traffic speed should thus be high, but upload of large amounts of data will anyway take a considerable amount of time.
- It will not be mandatory to use ERDA/SIF. Researcher groups which have other FAIR-compliant solutions in place, are welcome to keep using these.
- ERDA/SIF will not be searchable before implementation of DeIC's dataverse (tentatively scheduled for Q2/2023). ERDA/SIF does however allow for data showcasing via websites pointing at an archived data set's DOI.
- ERDA/SIF will run a monthly backup, but there is no version control in place.
- It is possible to share access to data with e.g. external collaboration partners or students via ERDA's workgroup feature. Access to SIF will however require an au-ID.

- Financing on the long run will likely become an issue. The solution will be to classify data storage as a marginal project cost and get funding agencies to cover these via a “bench” fee approach (cf. Nat’s ongoing work with full cost).

13:50 – 14:25 (35 min)

4. News from members

- DLE did draw attention to Nat’s revised [recruitment criteria for scientific positions](#) (aka “ABC-criteria”). Many have contributed making the document more readable, also for external candidates and members of evaluation committees. The revision focusses less on quantitative criteria, more and on leadership and collaboration. International mobility, experience and network are a requirement, but the criteria do now focus more on the actual qualifications, than the mean by which to achieve them.

To enhance transparency even more, Nat has developed descriptions of the most standard scientific positions and their use at Nat. The descriptions are temporarily accessible via [this link](#) and will soon be published at Nat’s new web portal “Career at Nat”.

Nat’s guidelines for the professor promotion programme have also been published.

This recent [news feature summarizes](#) Nat’s career development actions and ambitions here.

- The departments will be drivers for continued focus on responsible conduct of research, and will be asked to account for their activities (01/22-08/23) beginning of September 2023.
- AU’s Data Protection Officer (DPO) and colleagues in TTO has launched a [GDPR awareness campaign](#), featuring instructive [videos](#). Nat and Tech will invite to information meetings in cooperation with AU’s DPO in the beginning of 2023.
- AU’s working group on cross-disciplinary research will produce a report with recommendations for AU’s Management Team in the beginning of 2023. iNANO and Dandrite will be show-cased. DLE will share the report with the committee in due time.

14:25 – 14:25 (0 min.)

5. Written briefings

Attachment: Upcoming funding deadlines

14:25 – 14:30 (5 min.)

6. AOB

- Meetings scheduled for 2023: Monday 30 January, Thursday 23 March, Tuesday 6 June, Monday 25 September, Thursday 30 November (all 12:30-2:00 p.m.)

- Next meeting Monday 30 January 2023 at CHEM, feat. a research presentation by OC, and a presentation of AUFF's 2023 calls, and AUFFs selection procedures, by MMH.

Department of Molecular Biology and Genetics (+ BiRC)



Staff and Students

- Prof	11
- Assoc prof	25
- Assist prof	13
- Postdocs	85
- Tech. & adm.	66
- PhD stud.	80

Organization of the Department



The research at the Department of Molecular Biology and Genetics (MBG) at Aarhus University spans from basic to applied research within molecular biology. The department is organised in five research sections (Plant Molecular Biology, Neurobiology, RNA Biology and Innovation, Protein Science and Cellular Health, Intervention and Nutrition), a number of centres of excellence and various interdisciplinary centres.

The research takes place largely in collaboration with researchers from other laboratories, both in Denmark and abroad, and often in collaboration with researchers from other areas of research. Several of the department's researchers also have a collaboration with industry.

Plant Molecular Biology



Group leaders



Neurobiology



All scientific staff



RNA Biology and Innovation



Research centres



Protein Science



Publications



Cellular Health, Intervention and Nutrition



Dissemination of research



Core-facilities

Mass-spectrometry research group with state of the art equipment

Biophysics facility

Bioimaging facility

Zebrafish facility

Mouse facility with Bio-med

FACS facility with Bio-med

Cryo-EM. 300 kDa Titan Krios with direct detector. A second 300 kV microscope is expected up and running this fall.

Greenhouse facilities and growth cabinets.



The Department established an education in Molecular Biology in 2003



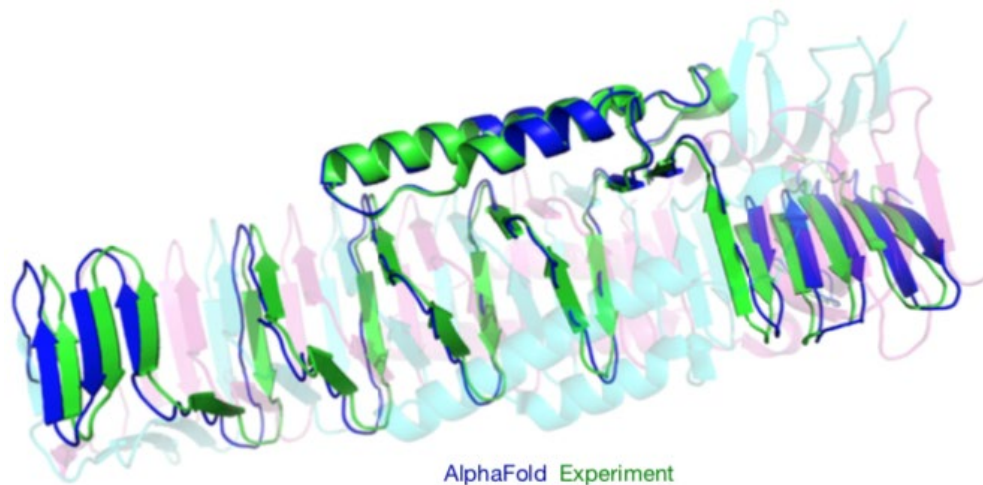
**Together with the Faculty of Health an education in
Molecular Medicine was established in 2007**



AlphaFold

a solution to a 50-year-old challenge in biology?

Protein structure prediction using machine learning



DeepMind (google owned company) developed AlphaZero, AlphaGo and AlphaStar defeating grandmasters in the games of Chess, Go and Starcraft II. 2021 released AlphaFold for predicting protein 3D structure

Crystallography, cryo-EM and NMR have produced ~181k experimental structures of macromolecules

- Available via PDB
- A few 1000 unique folds
- 17% of aa residues in the human proteome covered
- Experimental structure determination is often slow and resource demanding
- 3D structure prediction?

The screenshot shows the RCSB PDB homepage. At the top, it displays the PDB logo and statistics: 182624 Biological Macromolecular Structures, enabling breakthroughs in Research and Education. A search bar is present with the text 'Enter search terms or PDB ID(s)'. Below the header, there are links for 'Advanced Search' and 'Browse Annotations'. A banner celebrates 'Fifty Years of Protein Data Bank' with a 'Fifty Years of Open Access to PDB Structures' tagline. The main content area is divided into several sections: 'Welcome' with a sidebar for 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', and 'Learn'; 'A Structural View of Biology' which describes the PDB's role in molecular biology and mentions its membership in the wwPDB; 'October Molecule of the Month' featuring a 3D model of a protein complex; 'COVID-19 CORONAVIRUS Resources'; and 'Pairwise Structure Alignment'. The bottom section includes 'Latest Entries' with a 3D model of a protein, 'Features & Highlights' with a green 'id' icon, and 'News' with a link to 'The Nobel Prize in Physiology or Medicine 2021'.

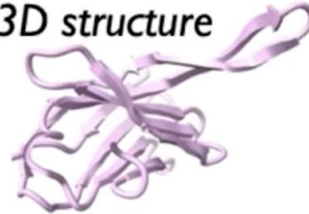
AlphaFold was trained to extract the information required to go from a MSA to a 3D structure using 180.000 structures in the PDB

Training

- Sequence
- Multiple sequence alignment
- 3D structure

180,000 protein structures in the PDB

```
EVQLVESGGGLVQPGGSLRLSCAASGFNIYSSSIHWVRQAPGKGLEWVAYI
.....F.....M.....Q.....
.....K.....Y.....L.....A.....V.....
.....A.....L.....V.....E.....Q.....
```



21 million parameters

Prediction

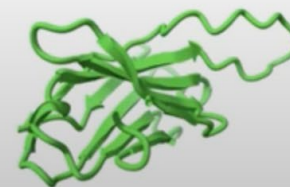
- Sequence
- Multiple sequence alignment

```
EVQLVESGGGLVQPGGSLRLSCAASGFNIYSSSIHWVRQAPGKGLEWVAYI
.....F.....M.....Q.....
.....K.....Y.....L.....A.....V.....
.....A.....L.....V.....E.....Q.....
```

21 million parameters

Focus attention on important relationships

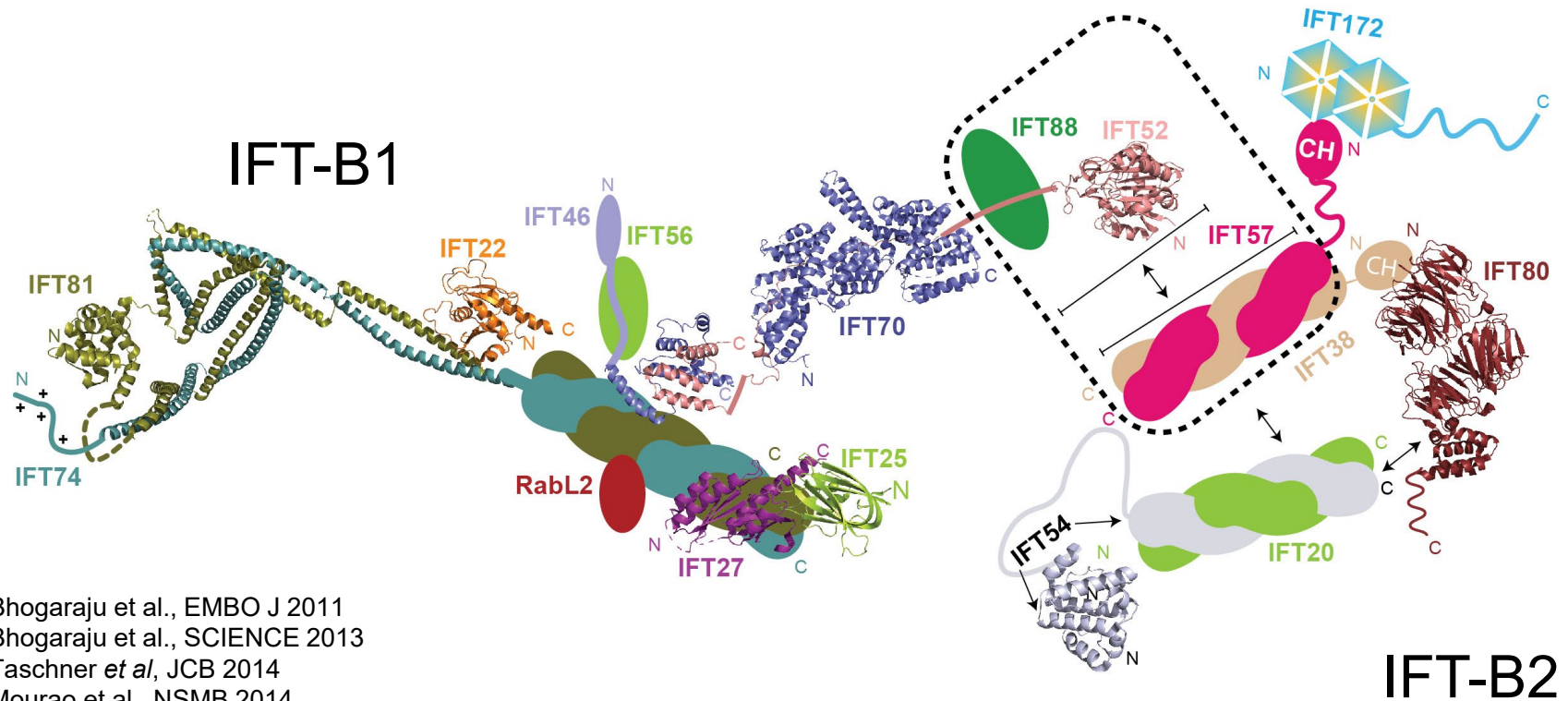
3D prediction



Confidence estimates (pLDDT)

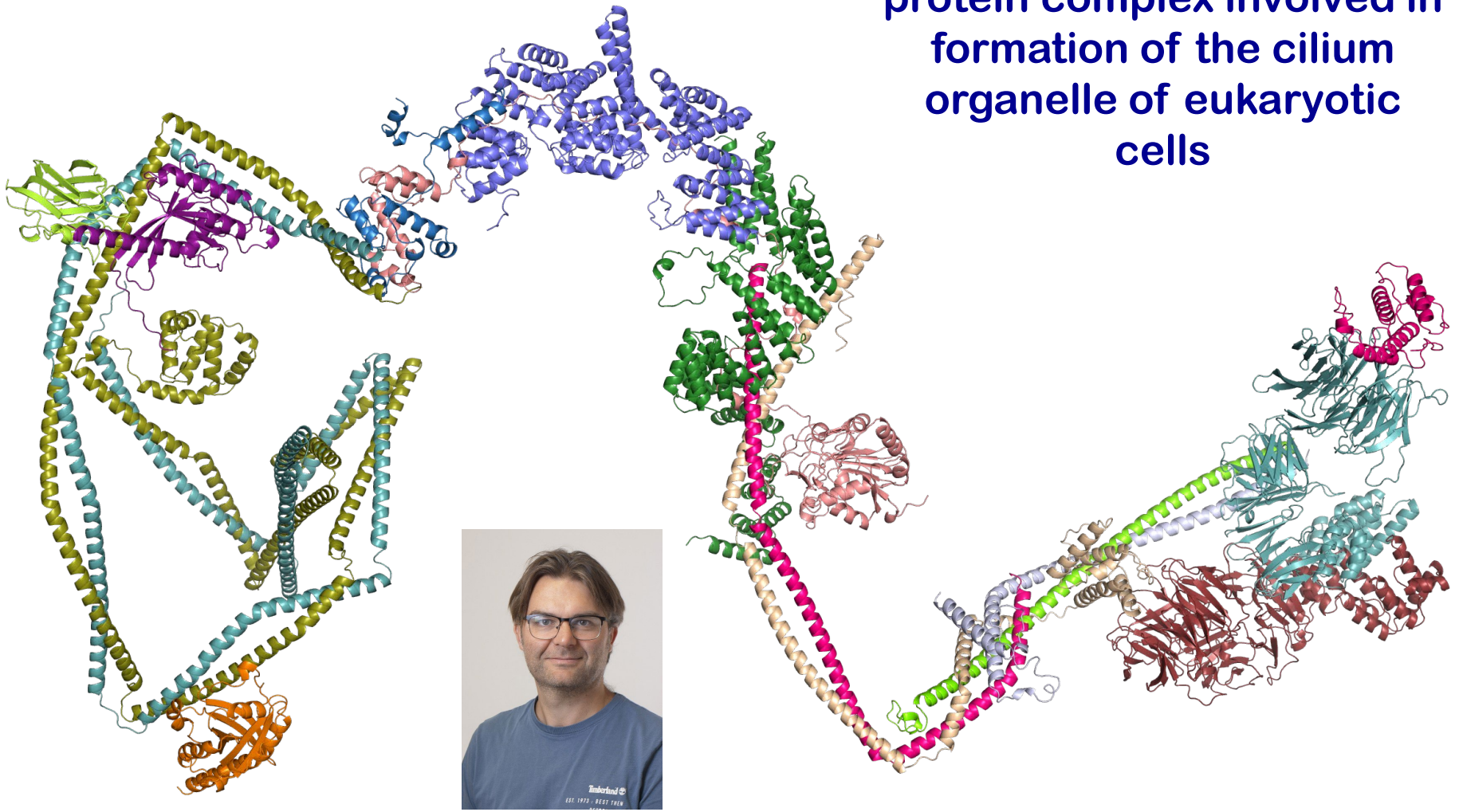
Slide from:
Tom Terwilliger
Los Alamos
National Laboratory

The IFT-B complex – pre-AlphaFold architectural overview



Bhogaraju et al., EMBO J 2011
Bhogaraju et al., SCIENCE 2013
Taschner *et al*, JCB 2014
Mourao et al., NSMB 2014
Vetter et al., NSMB 2015
Taschner *et al*, EMBO J 2016
Taschner *et al*, JBC 2017
Taschner et al., ELIFE 2018
Wachter et al., EMBO J 2019

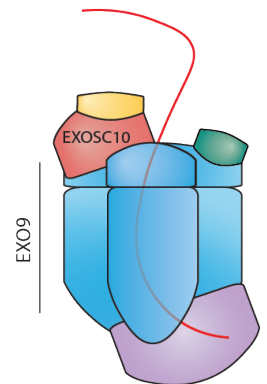
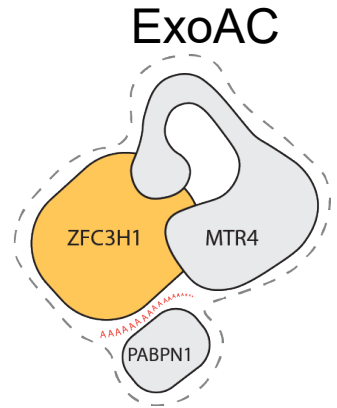
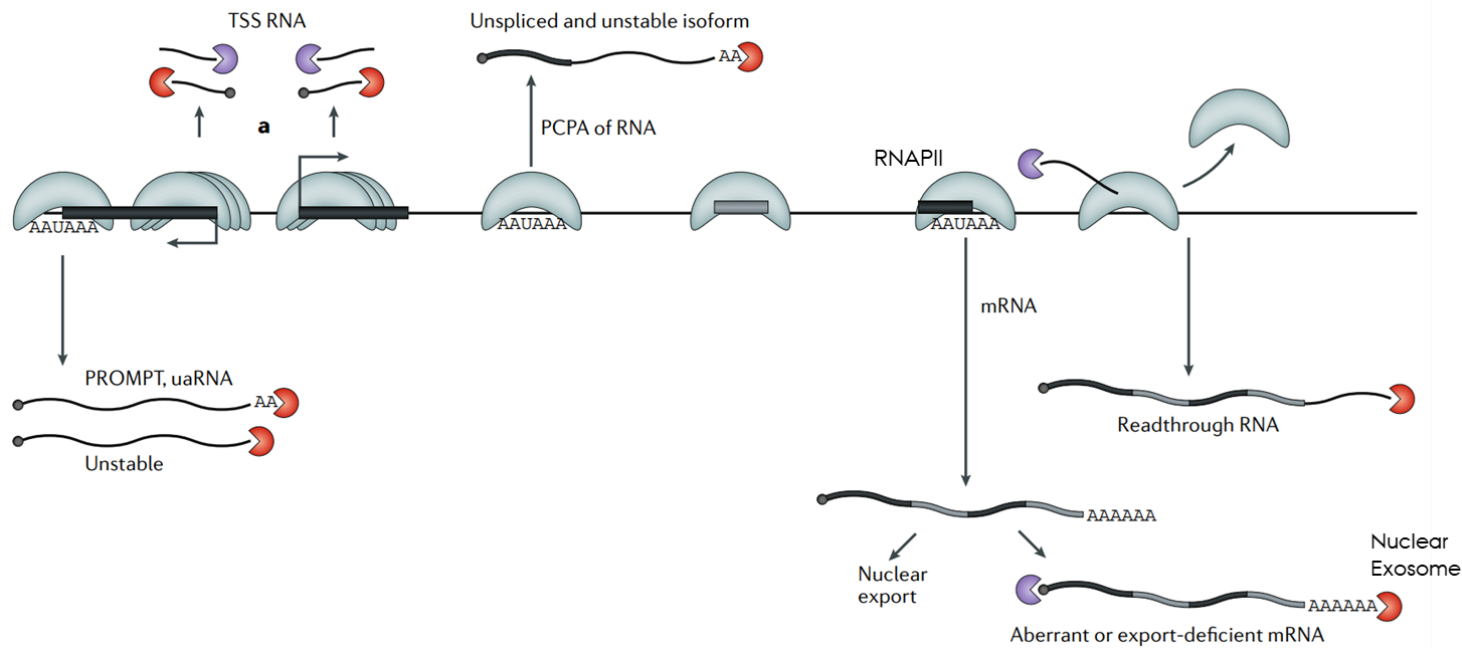
Alphafold prediction of the
3D structure of a 15 subunit
protein complex involved in
formation of the cilium
organelle of eukaryotic
cells



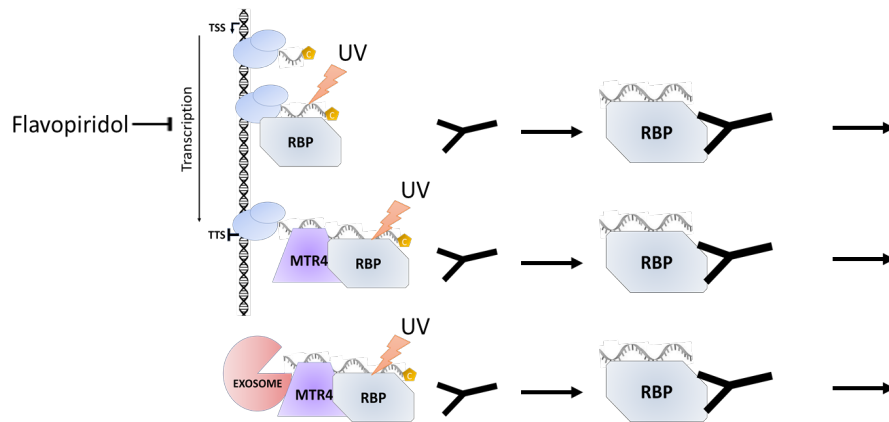
Esben Lorentzen, MBG
Petrman et al., EMBO
J, *in press*

High resolution profiling of protein- RNA complexes

Massive RNA turnover in the nucleus

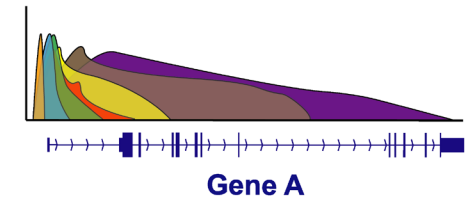


Accessing RNA-protein binding in cells



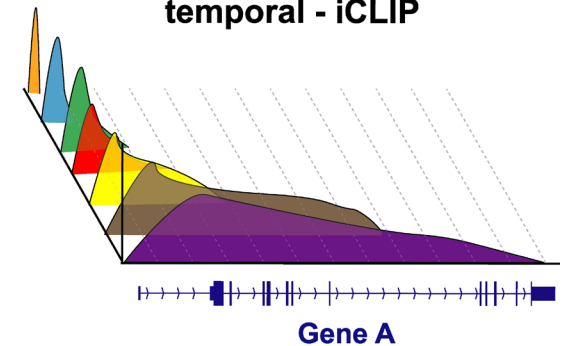
CLIP Library preparation
Protein interactions

'steady-state' iCLIP



average RNA binding profile

temporal - iCLIP

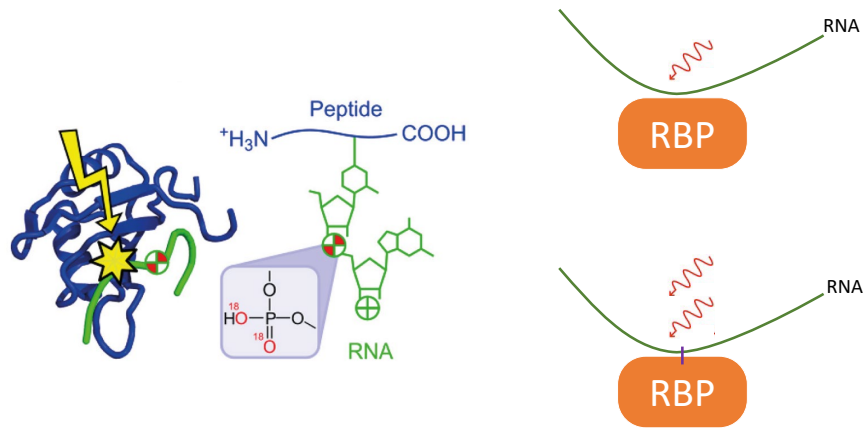


dynamic RNA binding profile

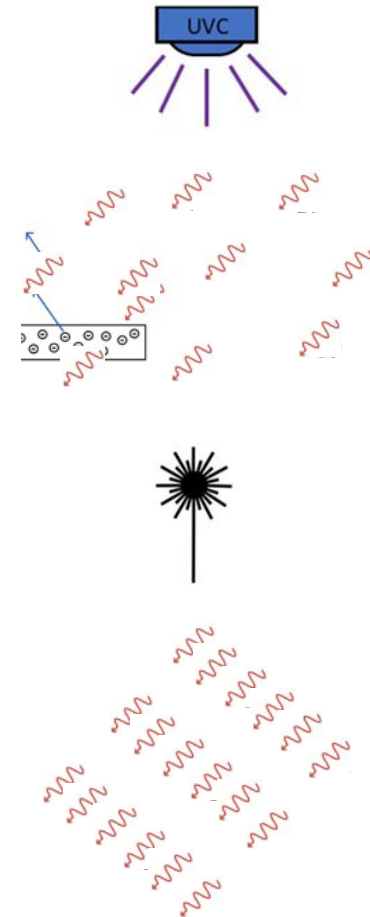
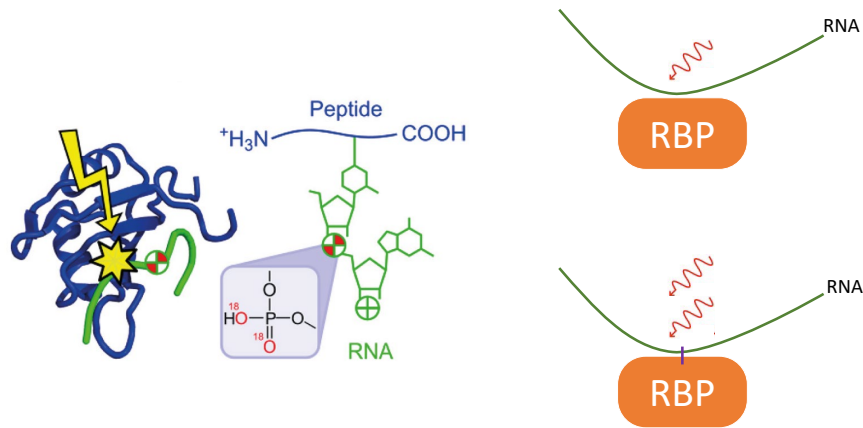
- ❖ Ti-CLIP (previously developed in the lab) allows to track protein interaction with nascent RNA in time and space
- ❖ Comparative analysis of several RBPs

Ross Cordiner

Introducing laser-assisted crosslinking for studies of kinetic RNA-ExoAC interactions



Introducing laser-assisted crosslinking for studies of kinetic RNA-ExoAC interactions



Article

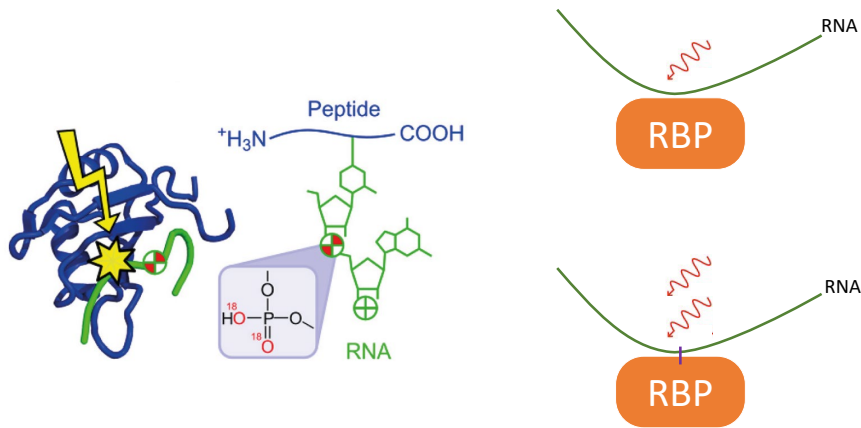
The kinetic landscape of an RNA-binding protein in cells

<https://doi.org/10.1038/s41586-021-03222-x>

Received: 19 May 2020

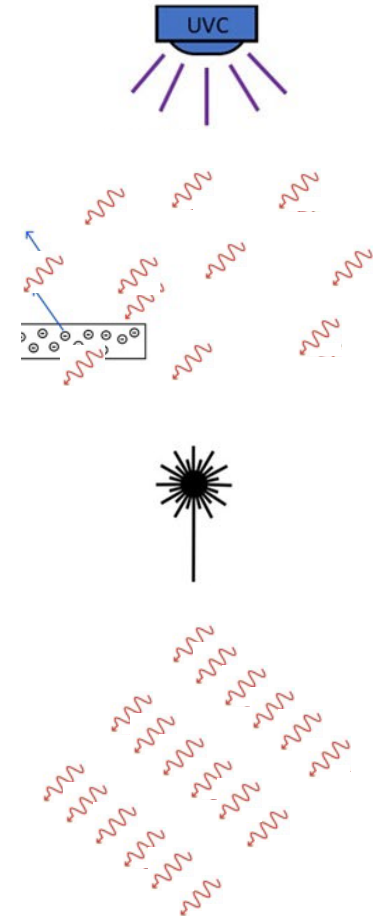
Deepak Sharma^{1,2}, Leah L. Zagore^{1,2}, Matthew M. Brister³, Xuan Ye^{1,2}, Carlos E. Crespo-Hernández³,
Donny D. Licatalosi^{1,2,5} & Eckhard Jankowsky^{1,2,4,5}

Introducing laser-assisted crosslinking for studies of kinetic RNA-ExoAC interactions

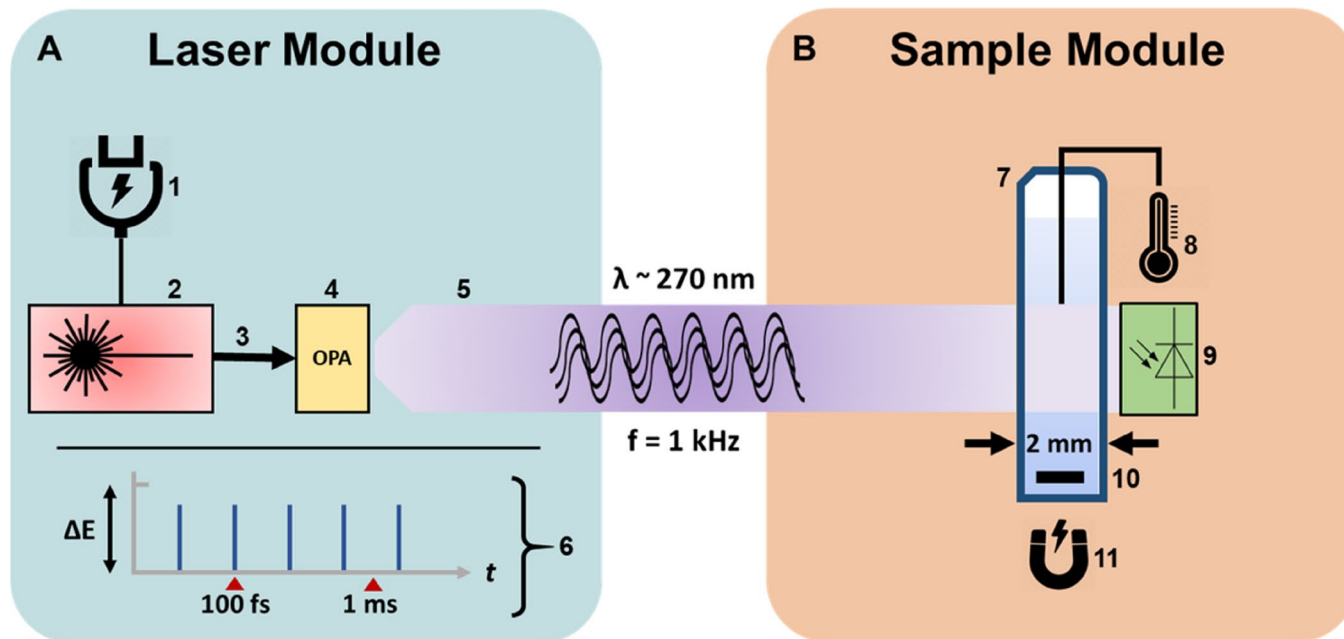


Why laser?

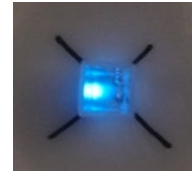
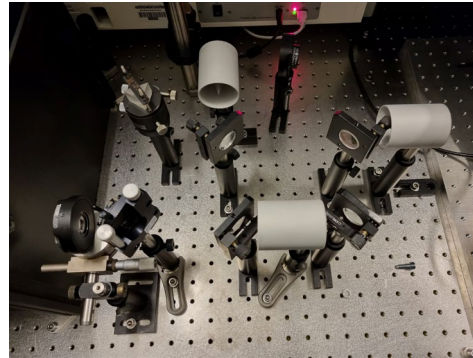
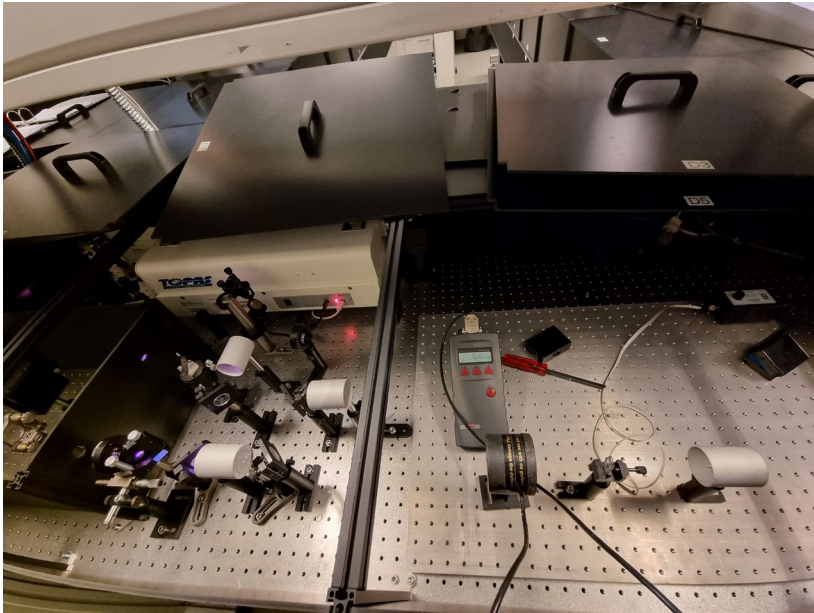
- ❖ yields a maximum number of multiphoton events while reducing total energy hitting the sample
- ❖ conformational transitions of the biomolecular complexes require more than 100 μ s, a femtosecond UV laser freezes interactions in real time.



Laser crosslinking system: schematic

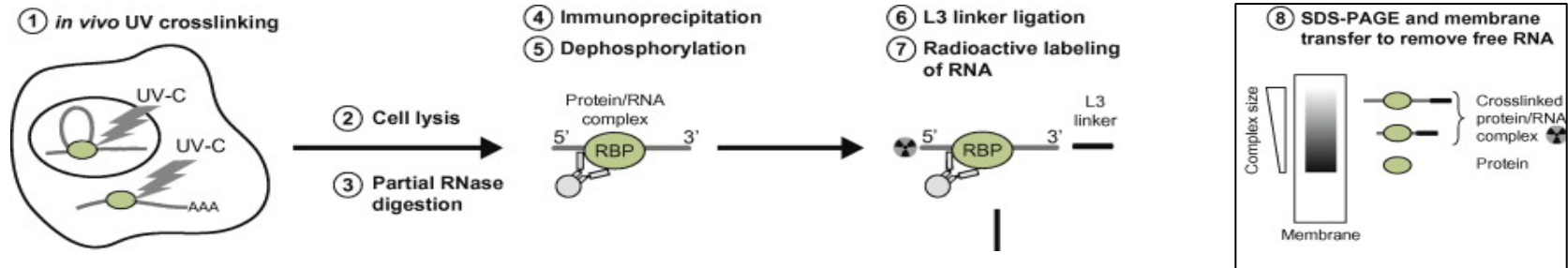


Laser crosslinking system: in real life



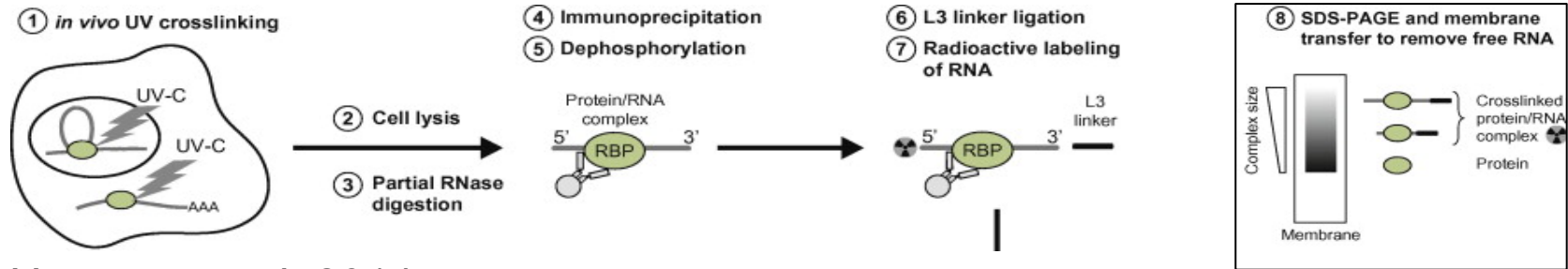
Rune Thomsen
Jan Thøgersen

Optimising fs-laser crosslinking in vivo

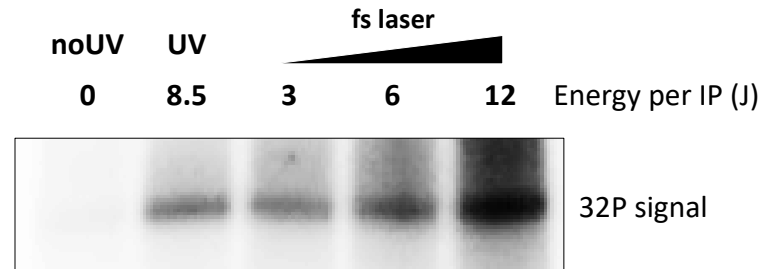


Huppertz et al. 2014

Optimising fs-laser crosslinking in vivo



Huppertz et al. 2014





Andrii Bugai + Rune Thomsen



Key collaborators:

Michael Drewsen

(Physics)

Jan Thøgersen

(Chemistry)

Thomas Breitenbach

(Chemistry)

Tobias Weidner

(Chemistry)



THJ LAB



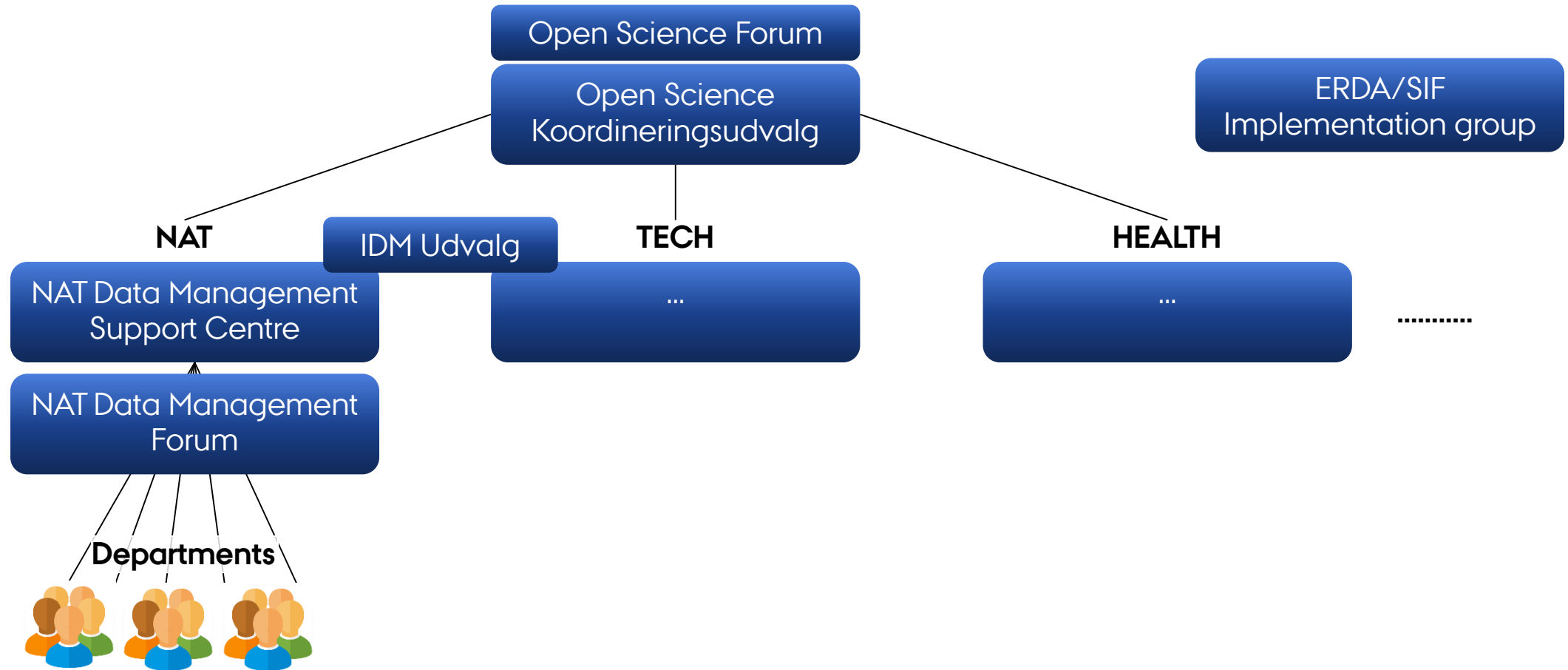
**novo
nordisk
fonden**



DATA MANAGEMENT ERDA / SIF

Electronic Research Data Archive
Sensitive Information Facility

NAT DATA MANAGEMENT

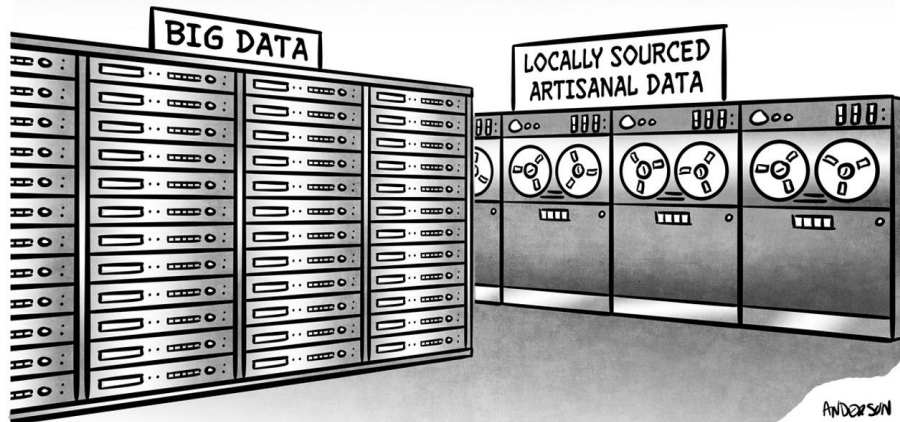


RESEARCH DATA MANAGEMENT

RDM is a part of all steps in research...



"Data" can be many things...



It needs to be organized and preserved...

Findable
Accessible
Interoperable
Reusable



ONE MAJOR PROBLEM SO FAR...

Aarhus University has been missing an efficient data storage solution for research data!



The solution:

ERDA / SIF

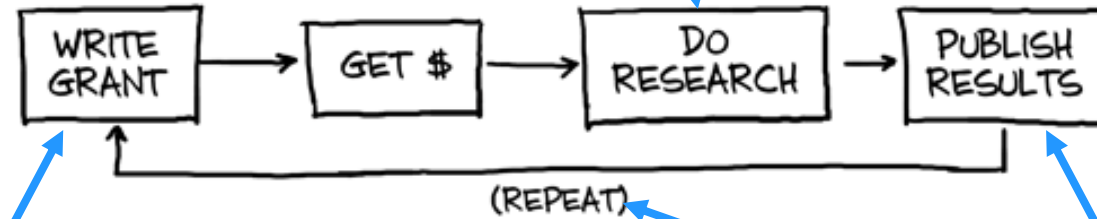
Electronic Research Data Archive
Sensitive Information Facility



ERDA / SIF

ERDA/SIF:

Safe data storage
Data sharing
Backups



Data Management Plan
(ERDA/SIF won't help here)

ERDA/SIF:

Make data available
Create DOIs

O-DRIVE, U-DRIVE, ONEDRIVE ... ???

It has been decided by the Aarhus University management that the cost for data storage on the U- and O-drive (personal and share-drives) is going to be passed to the departments.

Prize is calculated as **1.219 kr/TB/yr** for all data **exceeding the use on 31/12 2021**.

ERDA/SIF is free!

Plus it is going to have some nice features to help you during your research...



ERDA OR SIF

ERDA

erda-test.au.dk

NO sensitive information.

Full feature set.

SIF

sif-test.au.dk

Sensitive information!

In particular personal data requiring
special care under GDPR.

Fewer features (to protect data!)

VDI interface

Storage

Welcome to ERDA

AU Users	External Users	Advanced Access
Sign up to ERDA using your AU account? sign up		I'm already signed up to ERDA with my AU account! log in

About ERDA

ERDA or Electronic Research Data Archive at Aarhus University (AU) is meant for storing, sharing, analyzing and archiving research data. The intended audience is employees, their collaboration partners and students. ERDA delivers safe central storage space for own and shared files, interactive analysis tools in addition to archiving for safe-keeping and publishing. You can use ERDA as a secure network drive from anywhere and it also comes with a stand-alone file synchronization service similar to Dropbox, but with the data safely stored locally at AU. ERDA is delivered by [AU IT](#) and is currently for test use, but others have access mainly for data archiving and publication with AU DOIs. A roll-out to all of AU is underway to support the general AU [Data Management Guidelines](#).

Sensitive and Personal Data (GDPR)

Please note that while ERDA comes with a strong security focus, it is *only* a solution approved for general scientific data and *not* for highly sensitive data. In particular it is not for personal data classified as sensitive in the EU General Data Protection Regulation (GDPR). In case you need to work on such sensitive data we recommend the ERDA sister facility [SIF](#), which *is* intended and approved for exactly that purpose.

Getting Started

We've gathered information about ERDA in a few short intro guides and a more thorough user guide

- 💡 [Sign Up Intro](#) for AU and external users
- 💡 [Workgroup Intro](#) about creating, managing and accessing Workgroups
- 💡 [Network Drive Intro](#) about using ERDA as a network drive on your computer (only covers Windows for now)
- 💡 [Seafile Intro](#) about Seafile sign up and file synchronization
- 💡 [Seafile Collaboration Intro](#) about Seafile data sharing and exchange
- 💡 [ERDA Overview](#) if you're not sure whether to use ERDA's main storage or Seafile
- 📖 [User Guide](#) with general usage instructions

We strongly recommend reading and following at least the first intro guide if you want to use ERDA.

Status and News

You can always refer to our separate [status and news overview](#) for a.o. the latest ERDA system status as well as information about new or changed features.

Frequently Asked Questions (FAQ)

- + How much storage space do I have on ERDA?
- + Is My ERDA Data Replicated and Backed Up?
- + How do I Transfer Entire Folders to/from ERDA?
- + Can I Share, Exchange and Publish Data in e.g. a Read-only Fashion on ERDA?
- + Is it possible to get a DOI for my ERDA archive?
- + How Are Workgroups Managed?
- + Can I have a shared or separate account for our project?
- + Why can't I use certain characters in file names?
- + How do I install and run software XYZ in Jupyter?

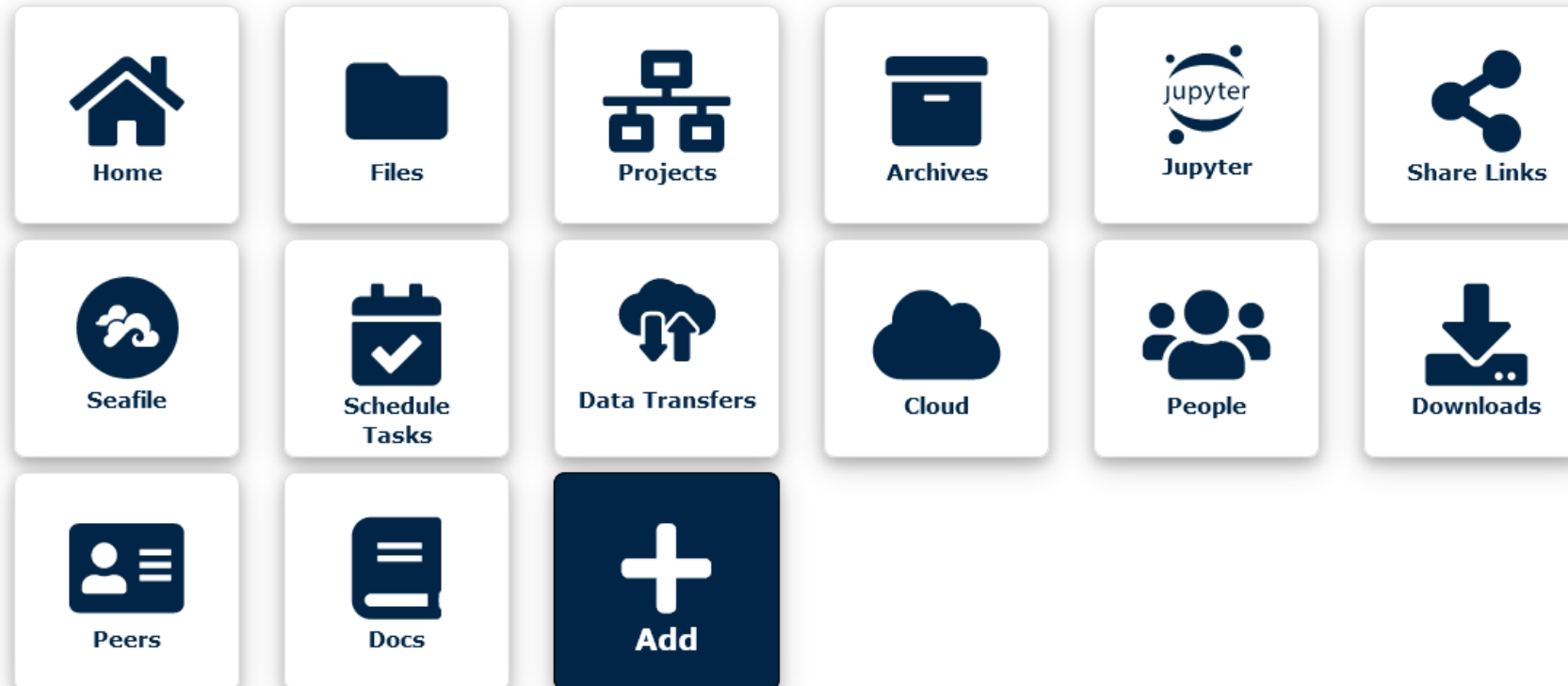


Welcome to ERDA!

Tools from ERDA helps you with storage, sharing and archiving of data. ERDA delivers centralised storage space for personal and shared files.

 **Quick Tip: 2-Factor Authentication (2FA) ...**

Your apps & app-setup



[Support](#)

[About](#)





- TASOC
- Trash
- private_base
- public_base



Name	Size	Type	Date Modified	...
TASOC	4.00 KB	dir	2022-11-14 14:18	...
Trash	11.50 KB	dir	2022-10-31 15:27	...
private_base	11.50 KB	dir	2022-11-14 14:12	...
public_base	11.50 KB	dir	2022-11-14 14:12	...
welcome.txt	218.00 B	txt	2022-11-14 12:38	...

Click to open upload helper

☐ Hidden files

10 files in current folder of total 84.74 KB in size.

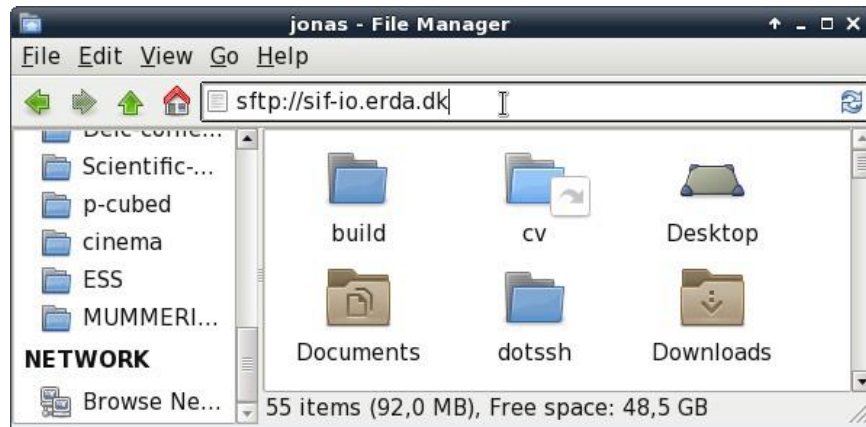
Support

About

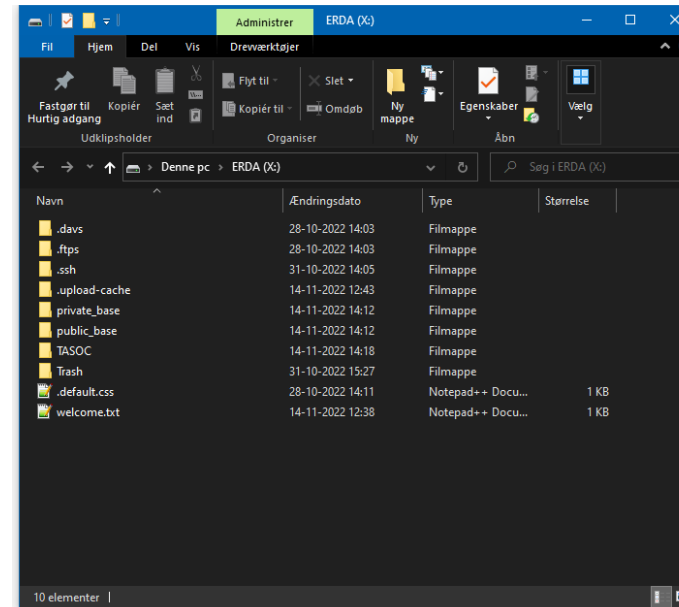


MOUNTING

You can also mount ERDA/SIF as a network drive on your computer
(SFTP / WebDAV / SSHFS)



Directly in File Manager



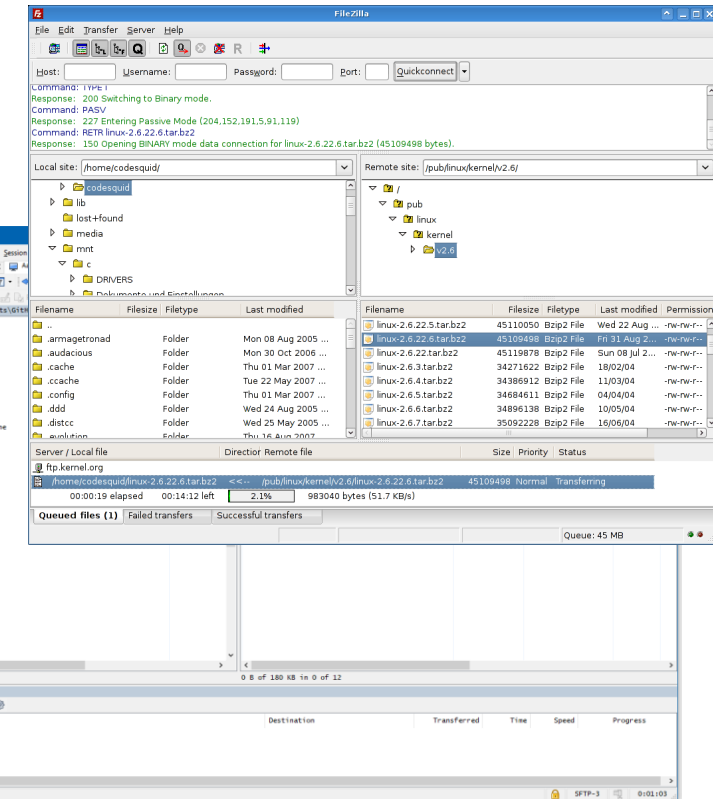
Windows network drive

Linux mount via sshfs

```
$ sshfs io.erda-test.au.dk:/ /mnt/erda -p 2222  
-o idmap=user,reconnect
```

```
$ ls /mnt/erda  
...all my files...
```

FileZilla, WinSCP



FILE SHARING

One of the very important feature of ERDA is the possibility to create "Share Links".

Create a link, and send it to your collaborator – they can now see (or even edit) your files.

You can also mount using the Share Link ID as username and password.







In SIF you can only share data within a project with other people who also have a SIF account (i.e. AU people).

Manage share links

Share Links

1 to 2 of 2 rows

25 share links per page

ID	Action	Path	Access	Created	Active	Invites
KQJ7Chbl9o	  	TASOC/archive_tda	read, write	Tue Nov 15 14:01:49 2022	Yes	
HGOAzekf8b	  	TASOC/archive_tda/TASOC_DR06	read	Mon Nov 14 14:22:19 2022	Yes	

Create Share Link

You can explicitly share files and directories with anyone using share links. That is especially useful when sharing data with people who do not have an account here, so that basic Project sharing is impossible. Individual files can only be shared read-only, but folders can additionally be shared with read-write or write-only access to allow recipients of the share link to write and upload in the share.

Please be careful about giving write access to anyone you do not fully trust, and note that you can always delete share links again later to limit the risks of abuse.

File/folder to share:

Read Access

☒

Write Access

☐

Create share link

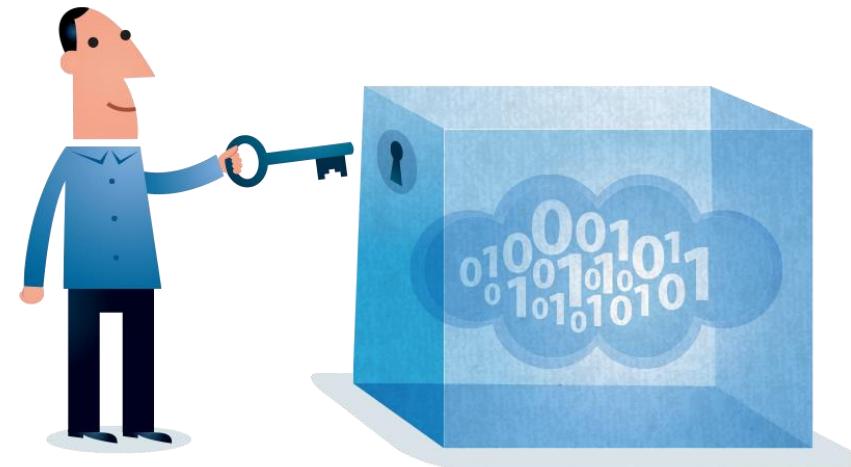
FREEZE ARCHIVE - DOI

In ERDA, you can create a "freeze archive" where you lock the files from further editing.

Then ERDA allows you to "mint" a Digital Object Identifier (DOI), which is a unique identifier for your dataset.

This DOI can then be referenced in subsequent publications.

Get credit for data.



BACKUP WITH ERDA

You can backup arbitrary (research) data to ERDA to protect against data-loss.

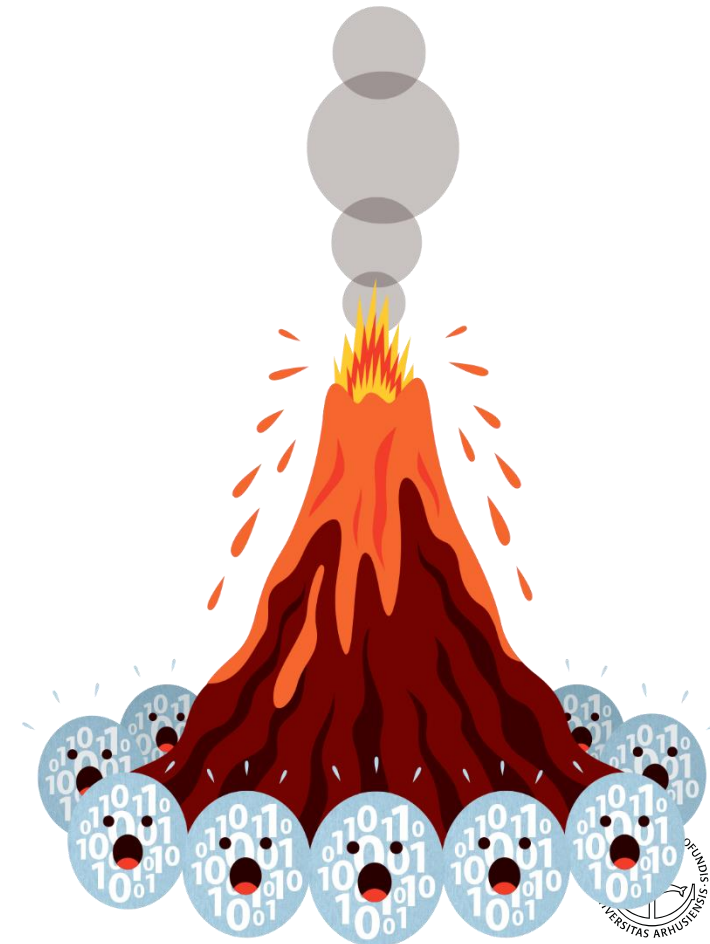
Recommended software is **Duplicati**, but in principle any backup software that can save to SFTP/WebDAV can be used...

Can be set up to run automatically (e.g. once a day) to keep a copy of important data.

No need to backup your Windows Documents and Desktop (they are already backed up!)



DUPLICATI



SEAFIRE / ONEDRIVE ⚠

A file synchronization tool like Dropbox, Google Drive, NextCloud, Box, OneDrive – using ERDA as the backend.

It is very clear that such a tool is a must-have!

SeaFile is being used in Copenhagen and is integrated in ERDA, but needs formal approval (Chinese company).

OneDrive is already available at AU – maybe it can be integrated with ERDA?

Exact details are still unclear... ⚠



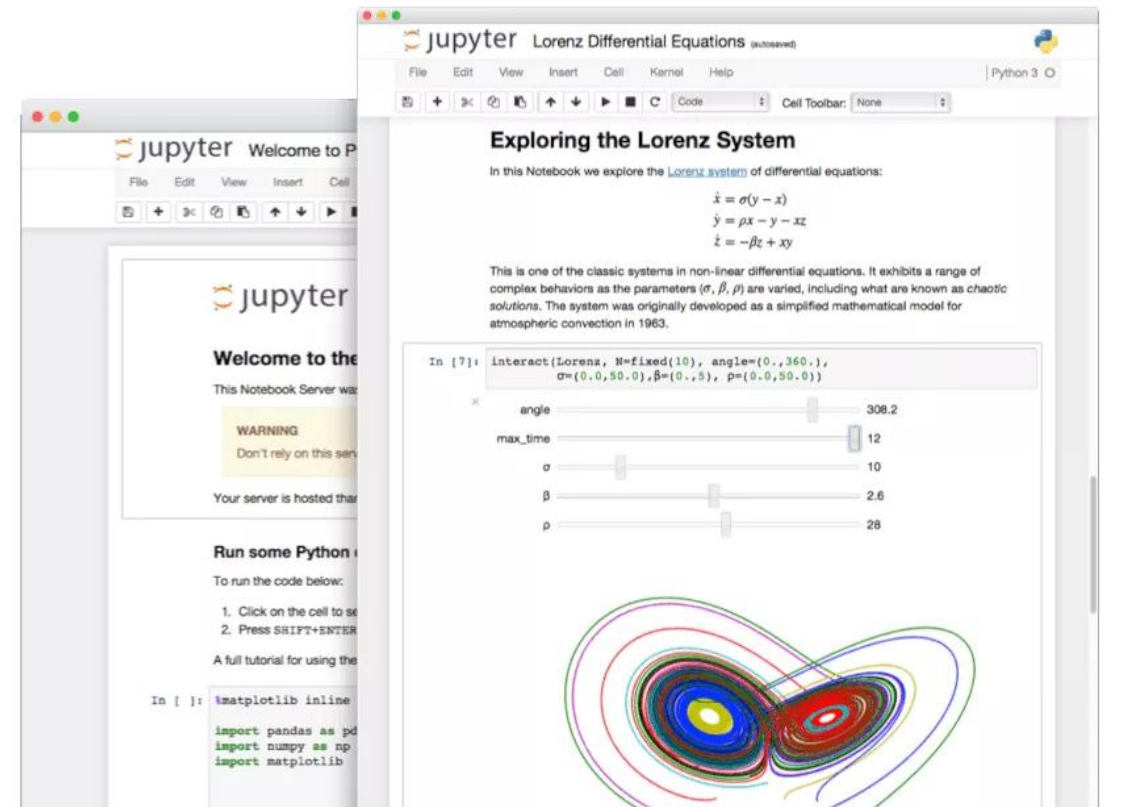
JUPYTER AND VDI ⚠

Play with your data directly in ERDA using Virtual Desktop Infrastructure (VDI) or Jupyter (Python, R).

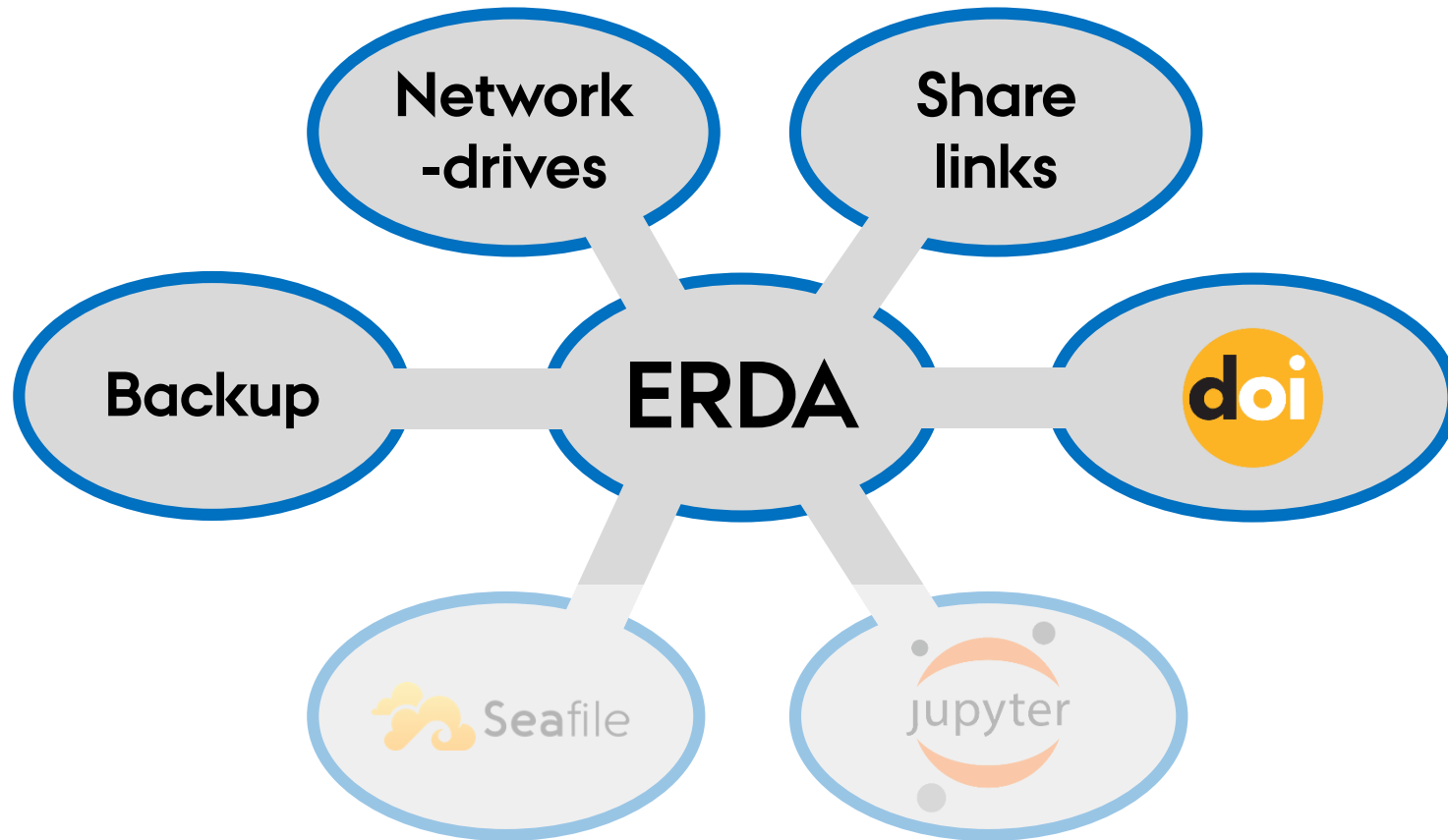
Interact with all your data on ERDA through Jupyter without having to download/mount them on your computer.

On SIF, VDI will be the only way to interact with the data.

Exact details are still unclear... ⚠



OVERVIEW



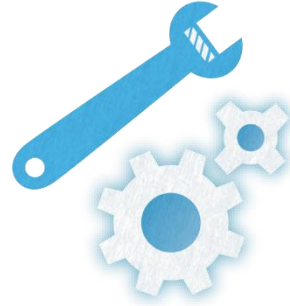
DeiC
Dataverse

ERDA/SIF
CPH

THE TAKEAWAYS

ERDA/SIF is here soon!

- Pilot-tests are happening right now.
- Manuals and guides are being written.
- Many features planned - some will be ready for launch.



NAT Data Management Support Centre

- Happy to help!
- Tour of the departments/groups to give introductions to ERDA/SIF.

Things to ask yourself:

- How can ERDA/SIF be integrated into my daily workflow?
- What issues does ERDA/SIF not solve for me?
- Do I really need to store all my data forever?





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