Bioexcel Workshop

SHARING DATA FROM MOLECULAR SIMULATIONS

Sunday 25th November - Tuesday 27th November

Bioexcel Workshop

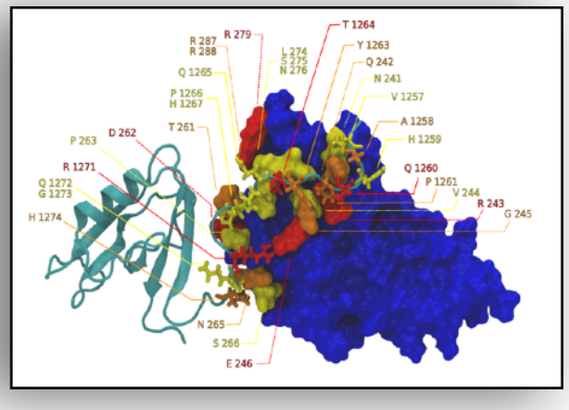
SHARING DATA FROM MOLECULAR SIMULATIONS

WELCOME!

Sunday 25th November - Tuesday 16th November

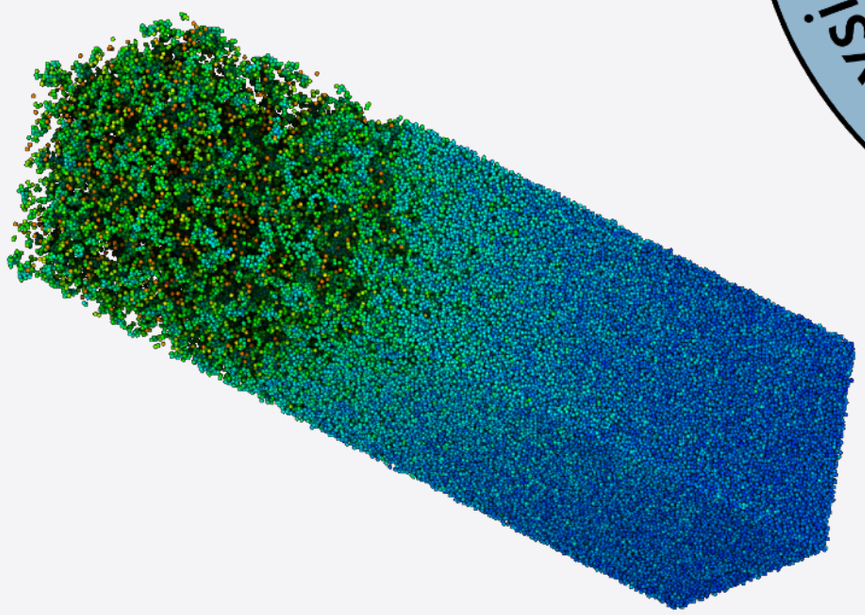
ME, MYSELF AND I

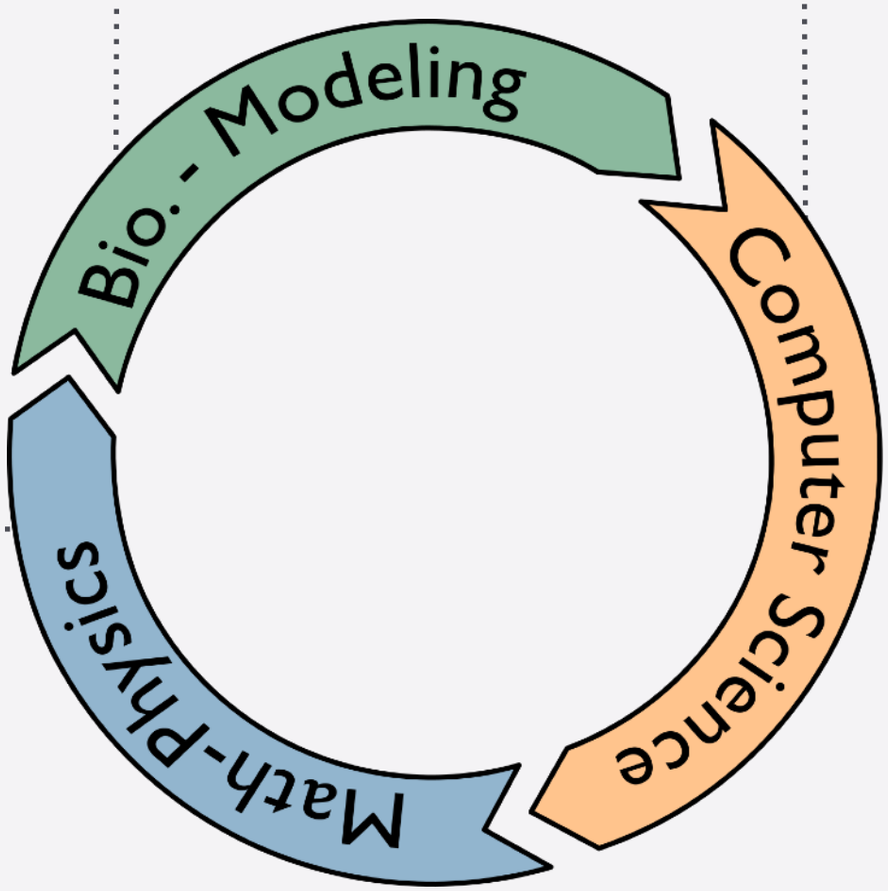
PROTEIN DOCKING



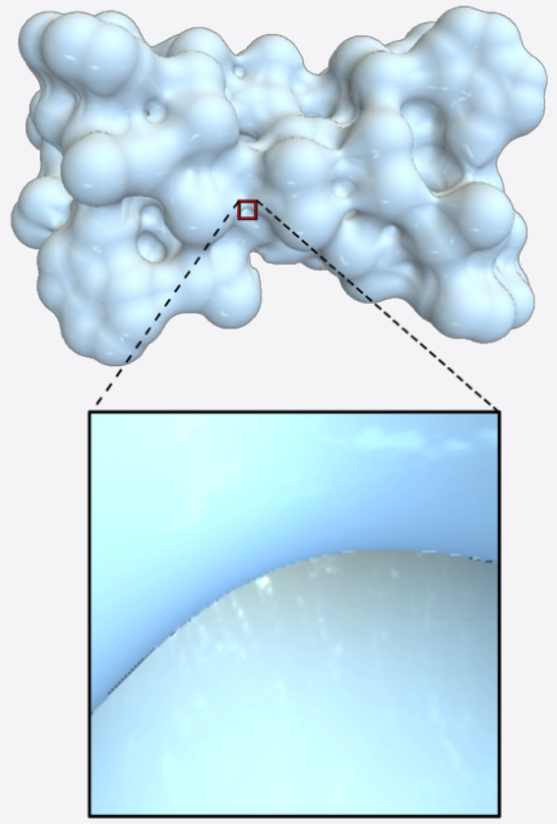
Déliot*, **Chavent*** *et al.* , *BBRC*, ***2009***

MATERIAL PHYSICS





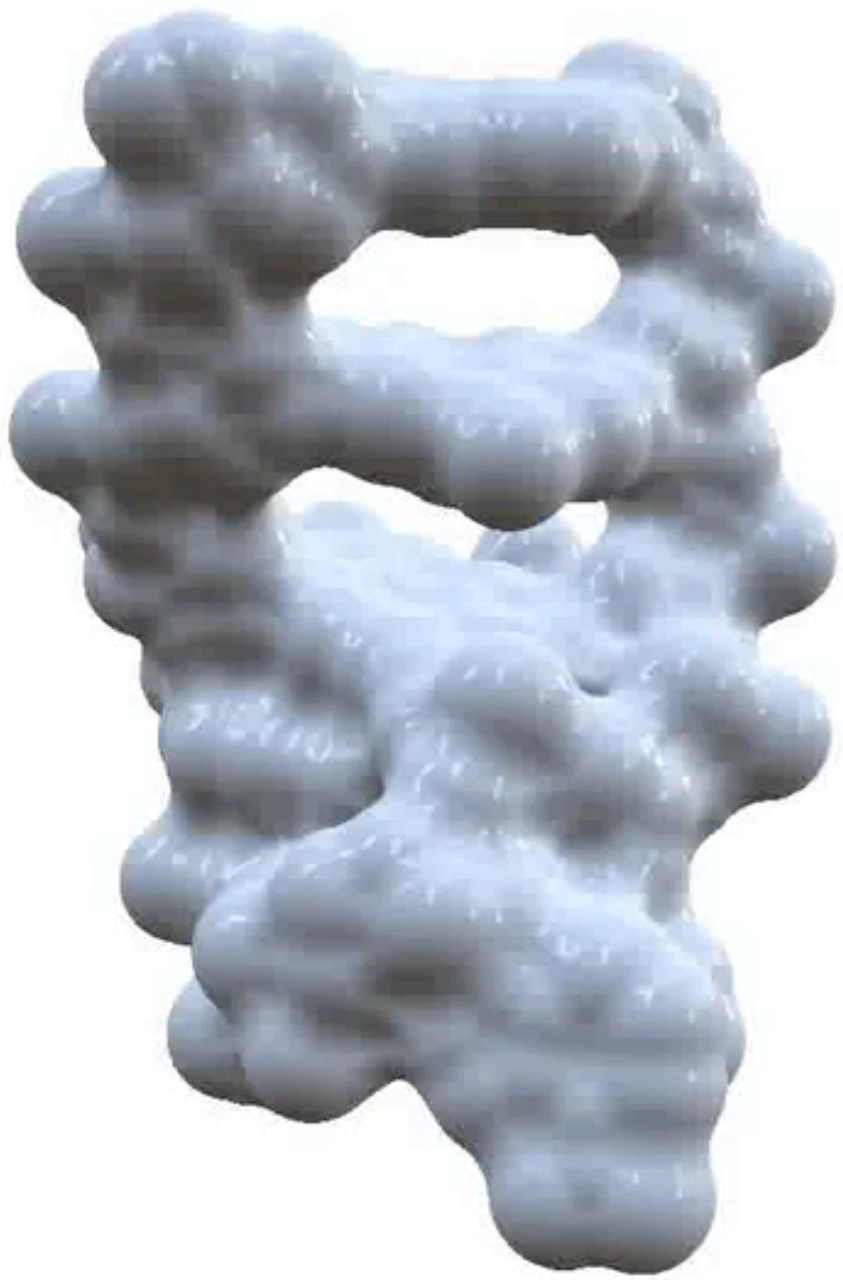
MOLECULAR SURFACE



Chavent *et al.* , *J. Mol. Graph. Mod.* , ***2008***

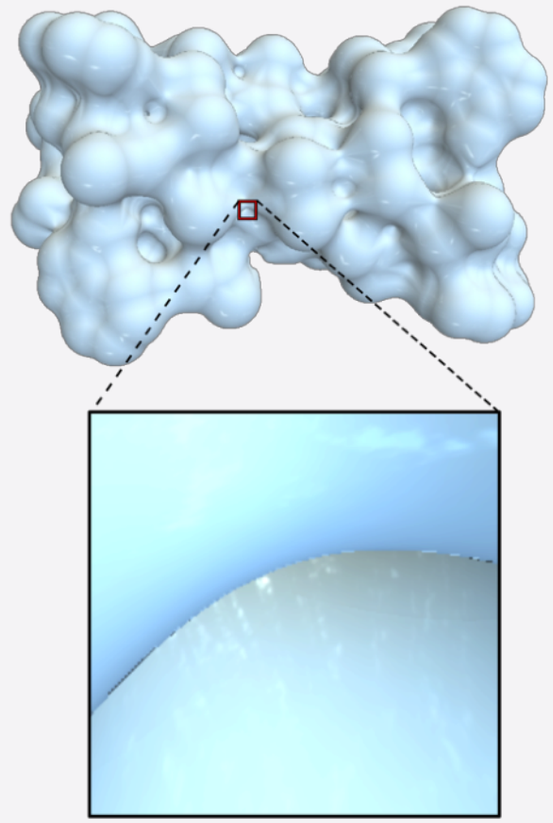
Chavent *et al.* , *J. Comp. Chem.*, ***2011***

MOLECULAR SKIN SURFACE



Edelsbrunner , *Disc. Comp. Geom.*, ***1999***

MOLECULAR SURFACE



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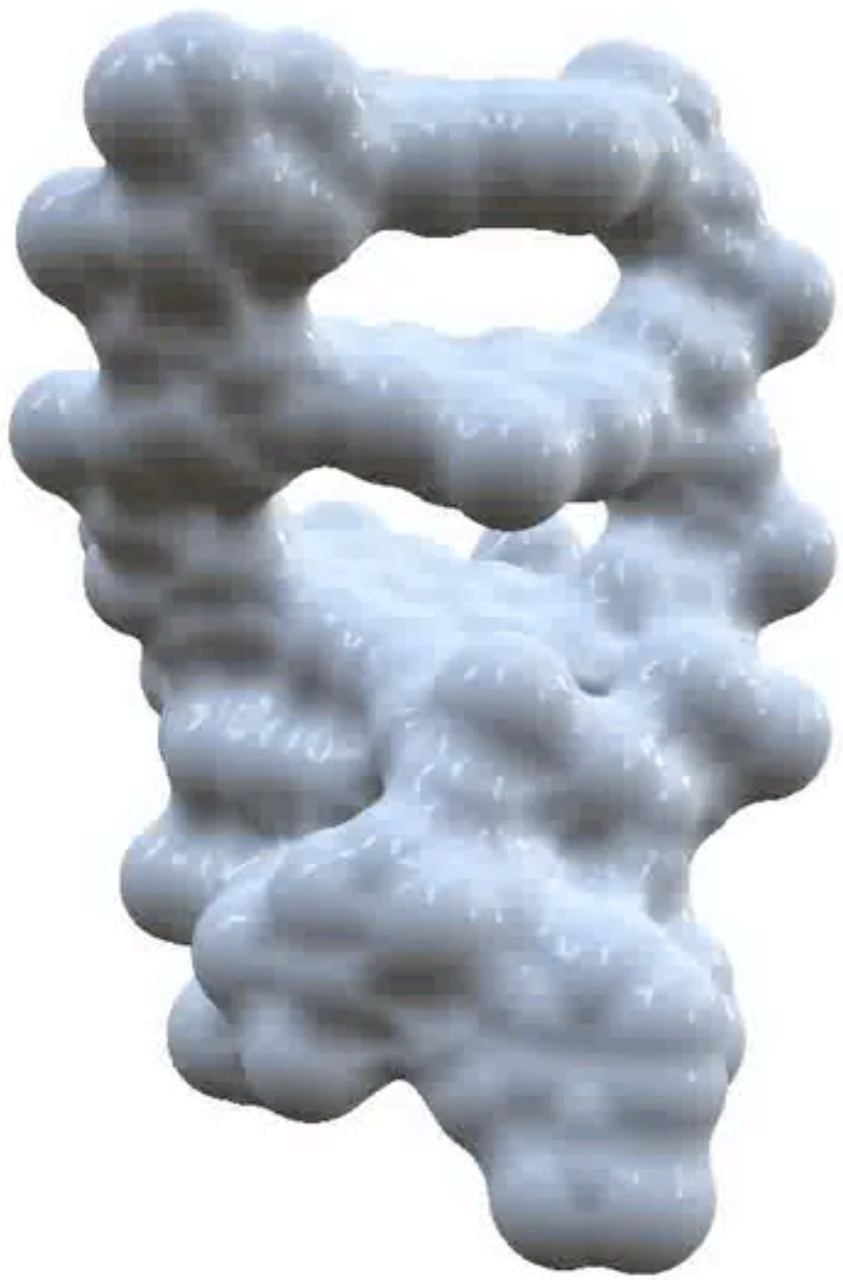

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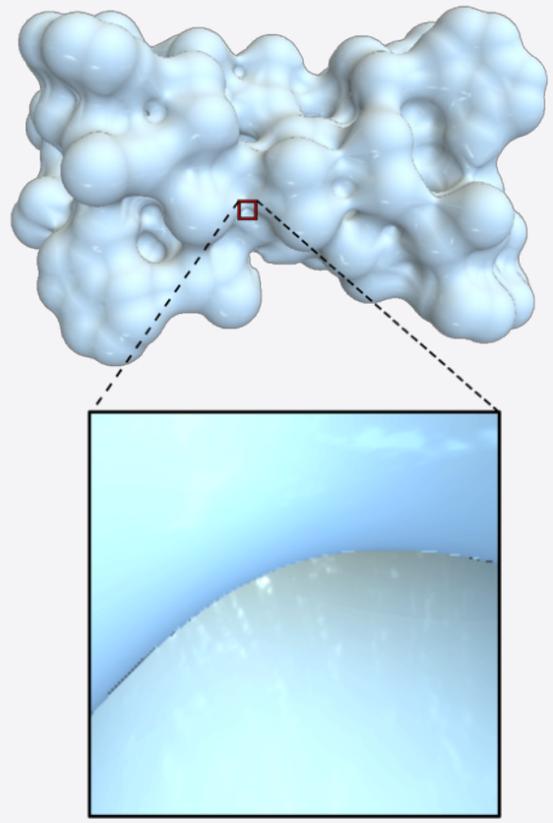

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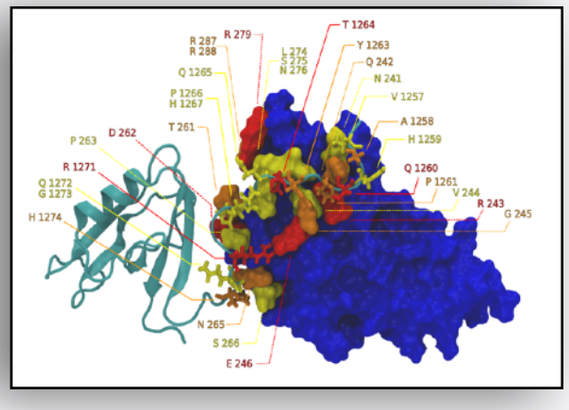

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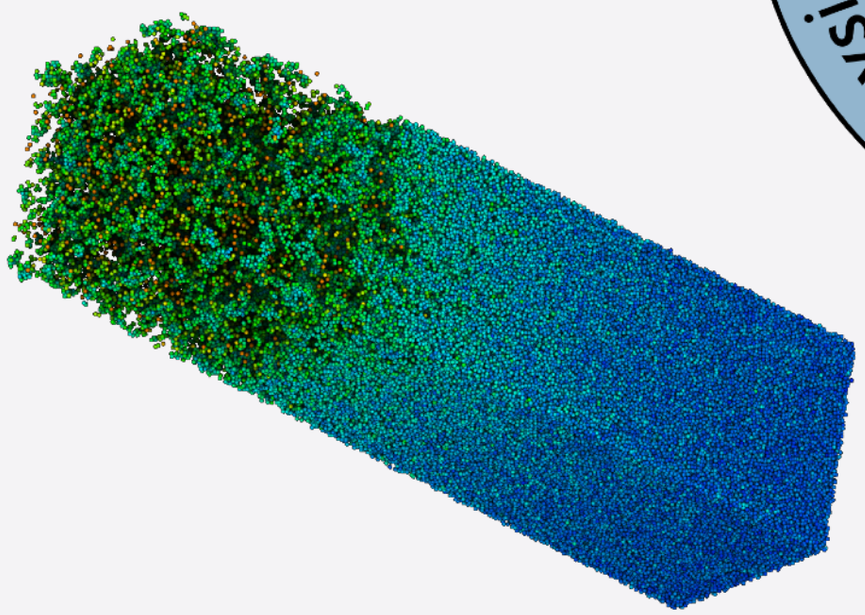

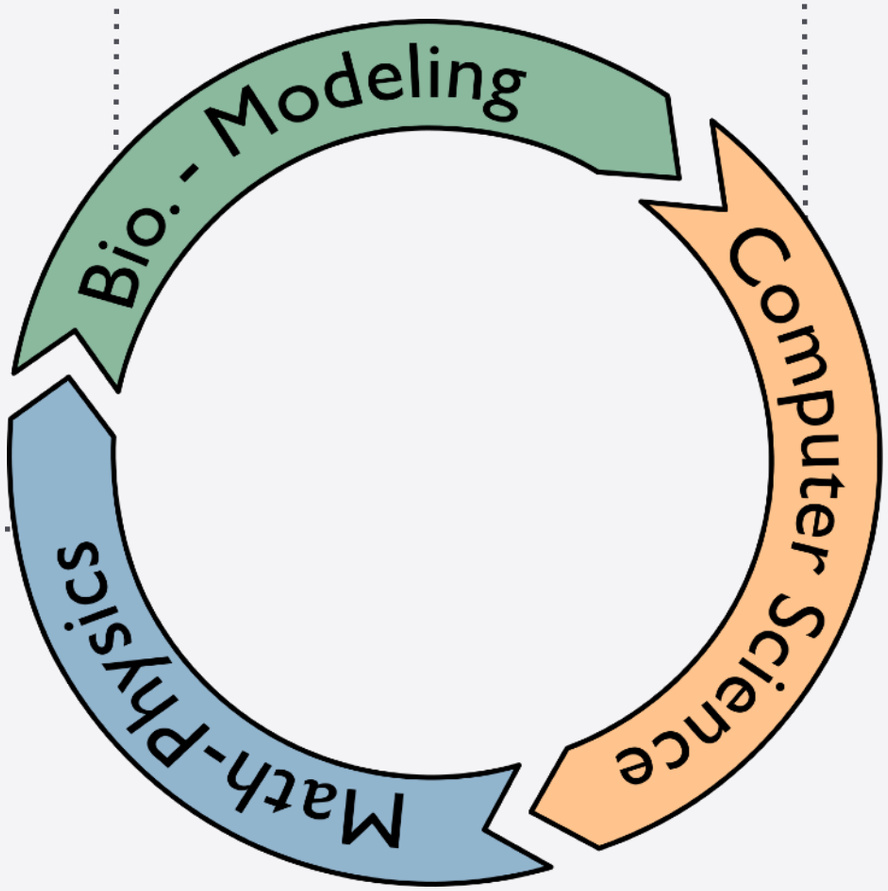

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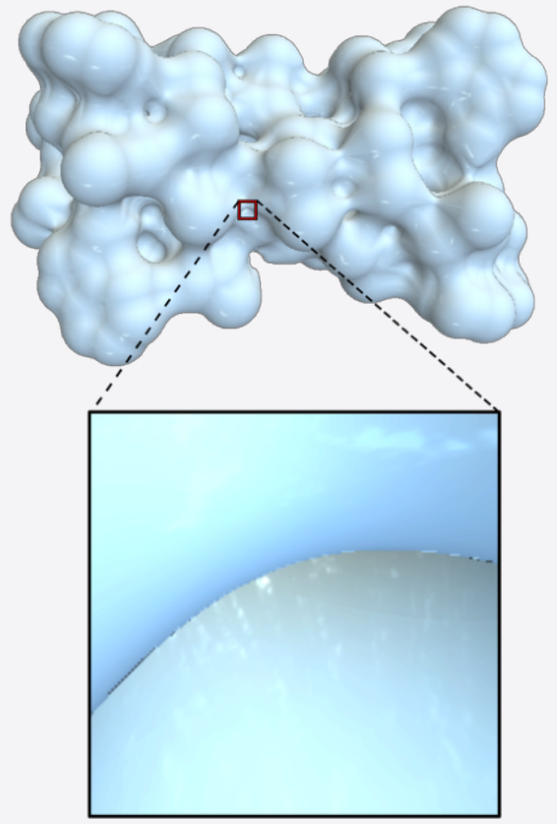

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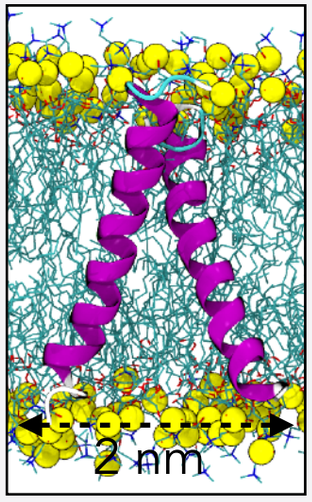

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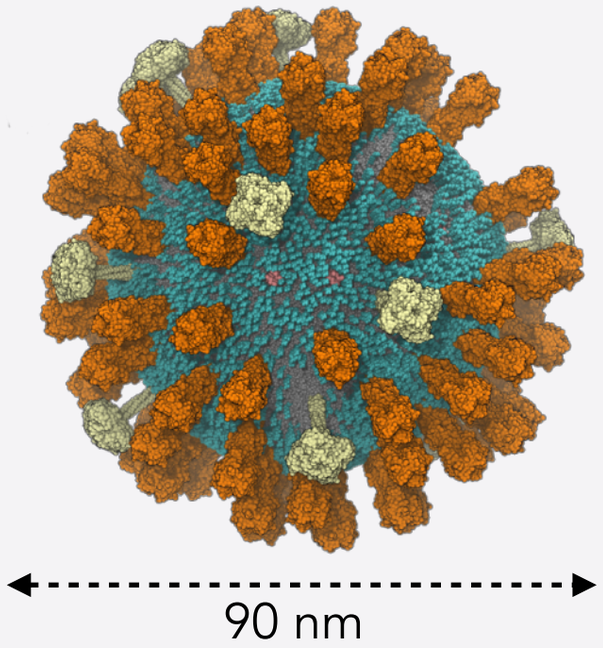
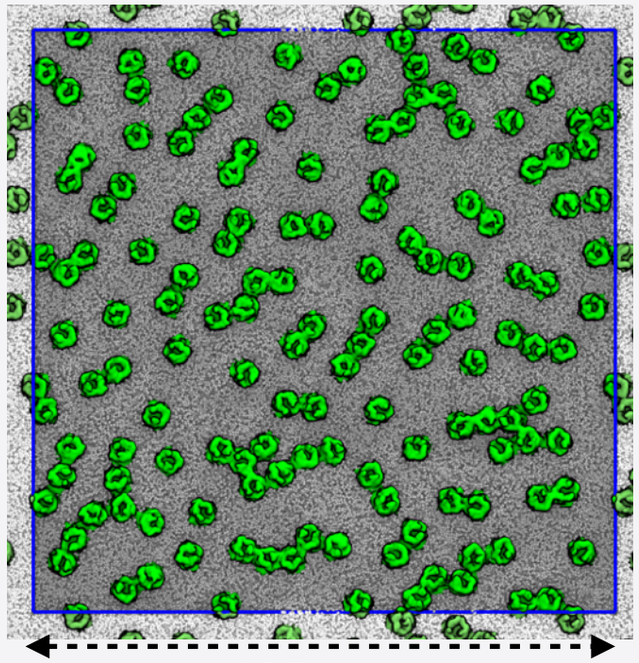
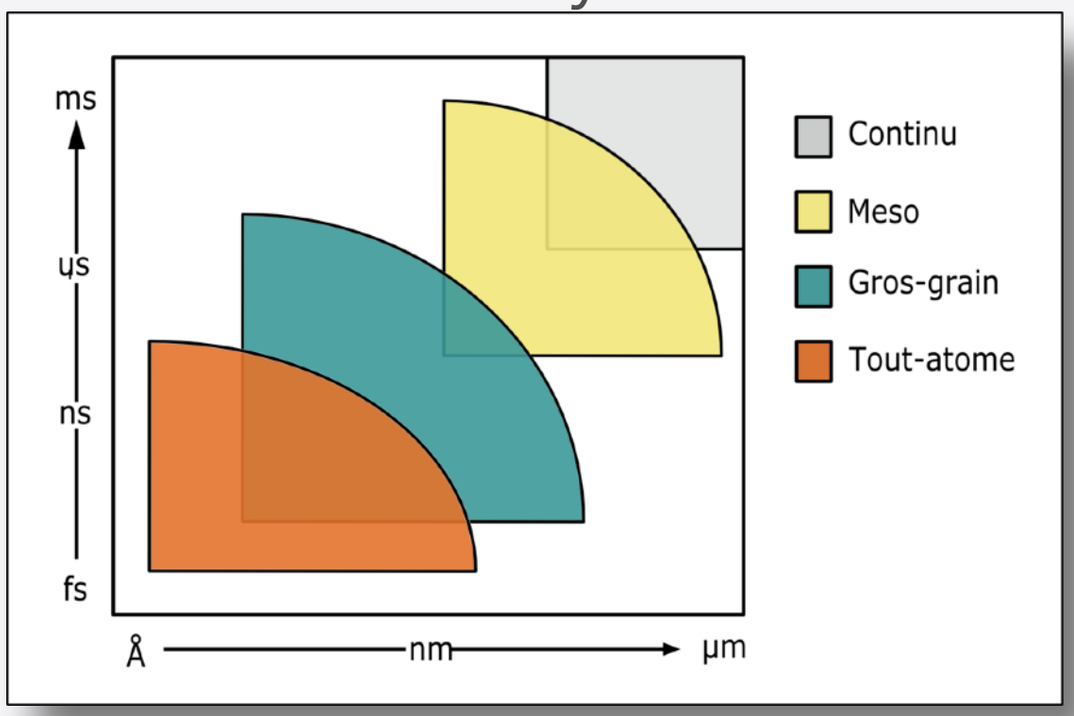
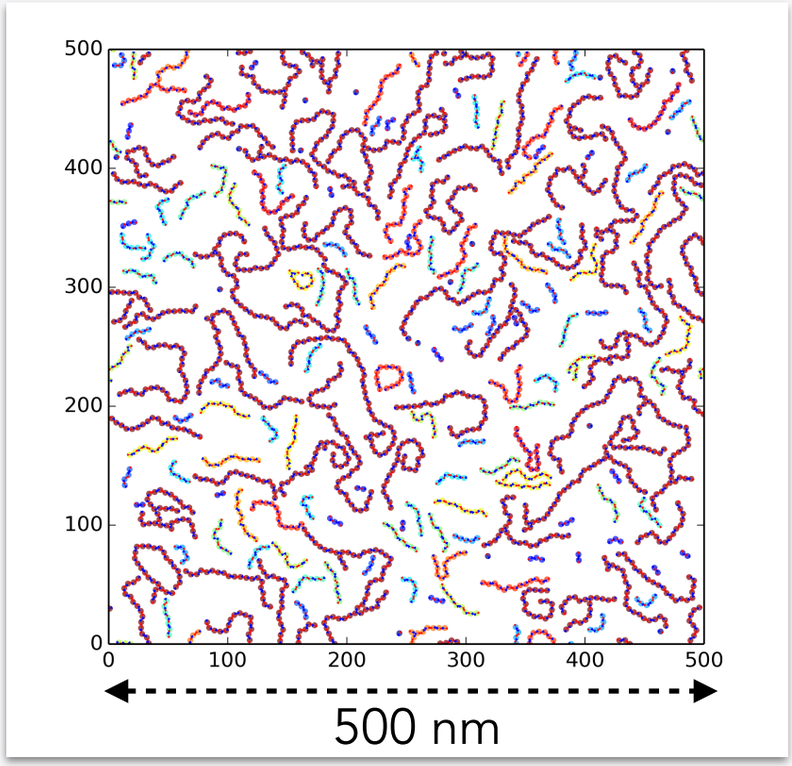


Reddy, *et al.* , *Structure*, ***2015***



Molecular dynamics





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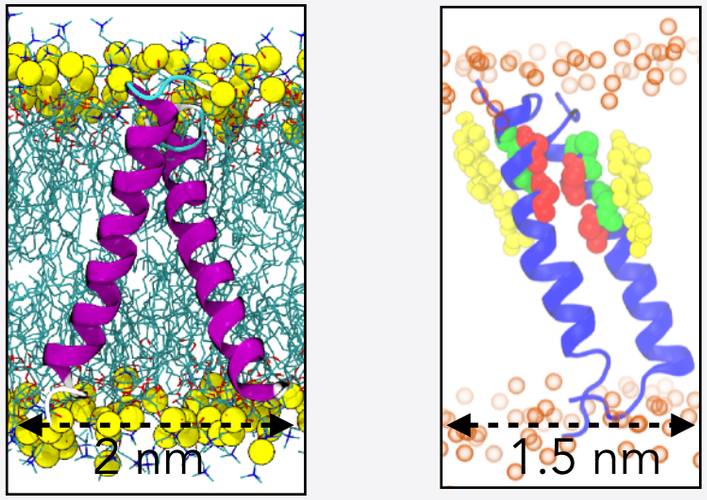
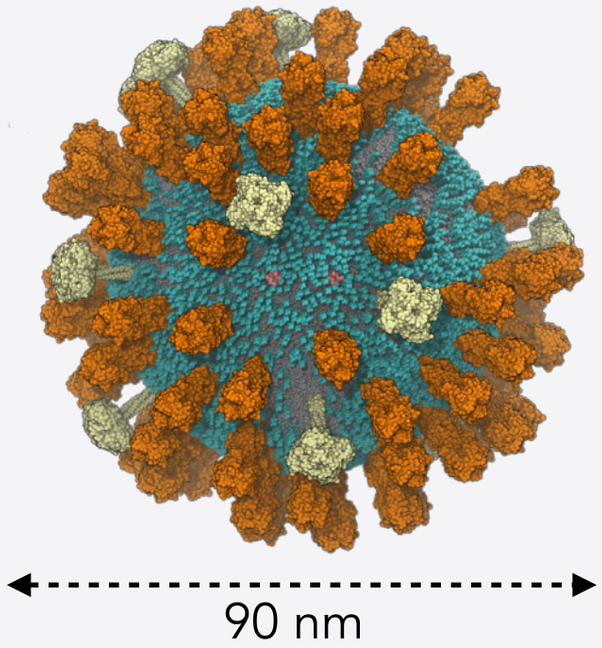


Chavent, *et al.* , *Biochemistry*, ***2014***

Atomistic (AT)



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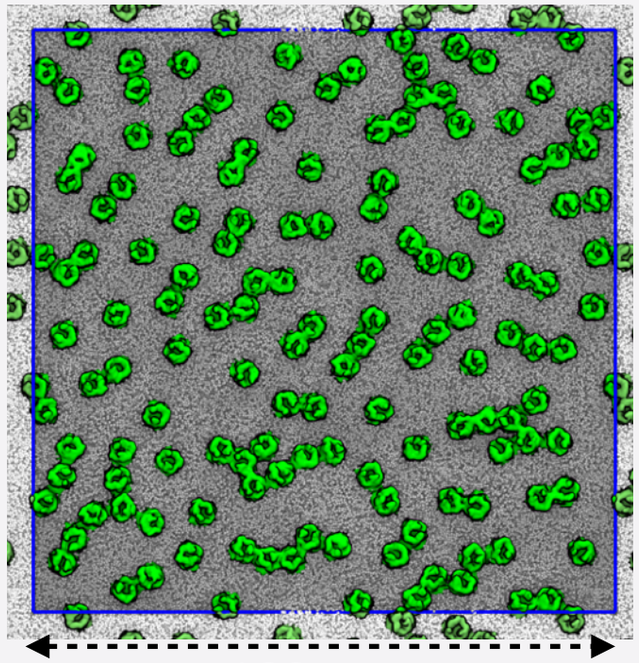

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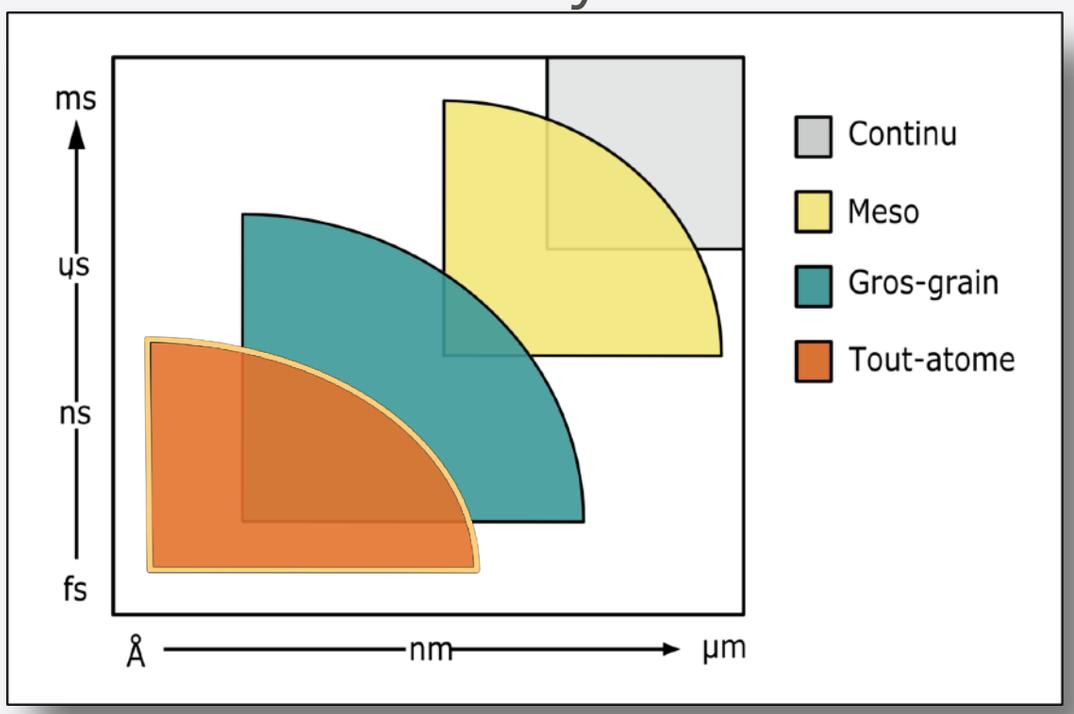

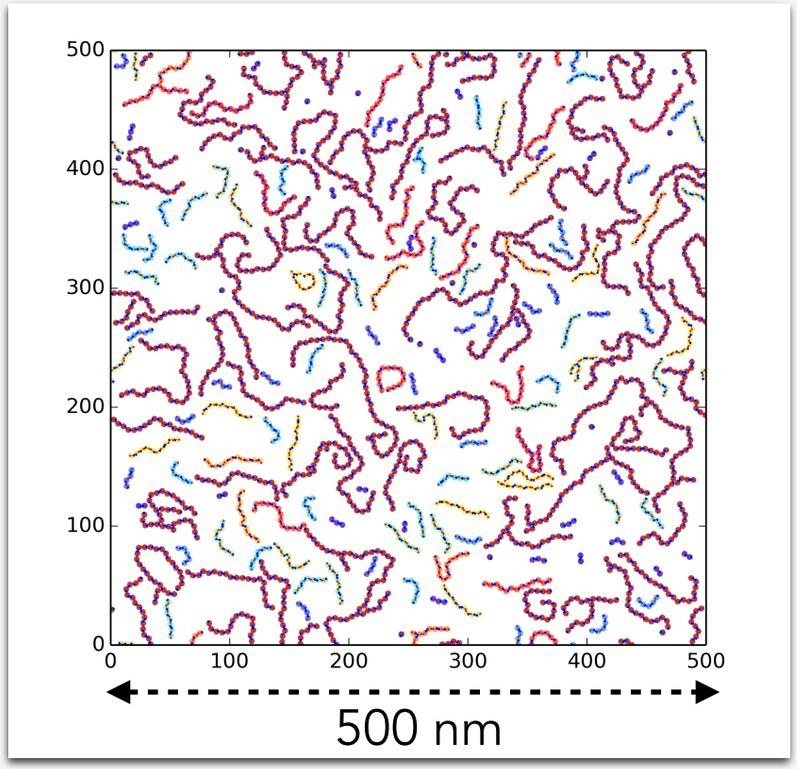

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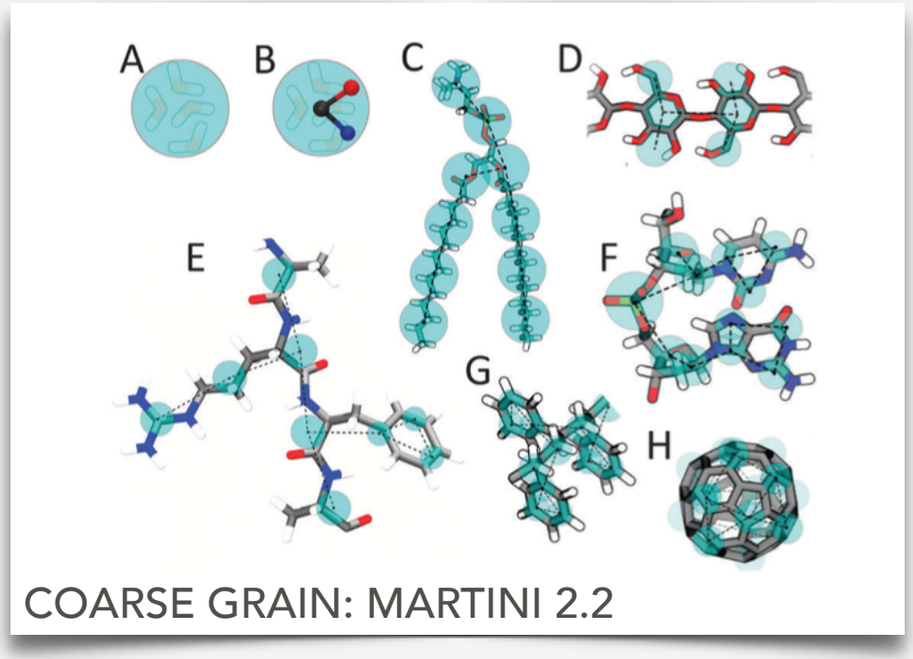
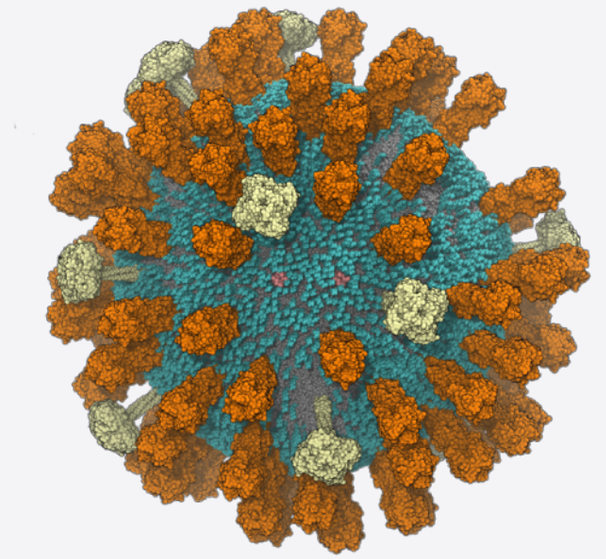
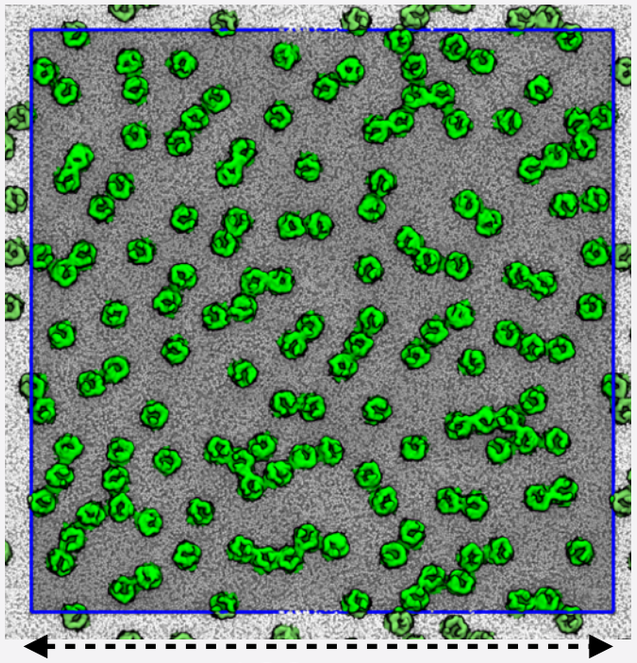


COARSE GRAIN: MARTINI 2.2

S. J. Marrink & P. T. Tielman, *Chem. Soc. Rev.* ***2013***



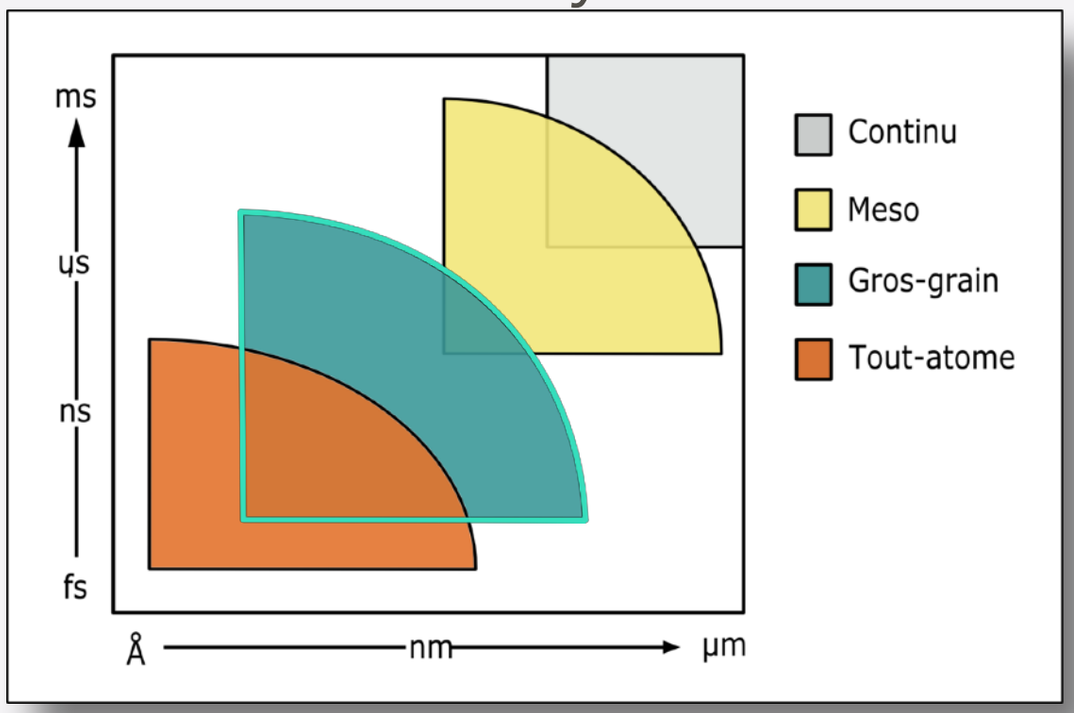
90 nm



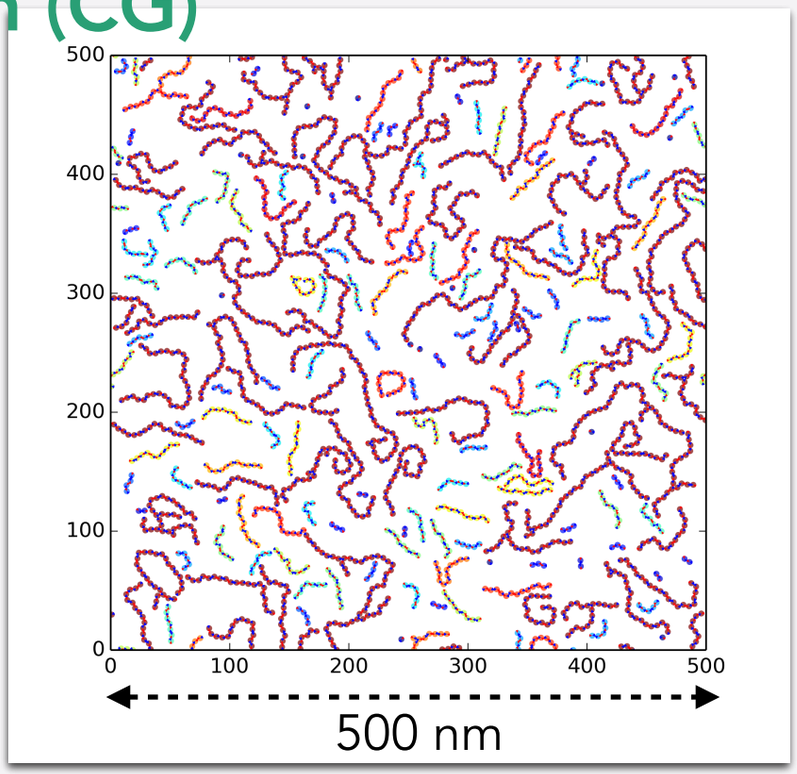
120 nm

Reddy, *et al.* , *Structure*, ***2015***

Molecular dynamics



Coarse-Grain (CG)



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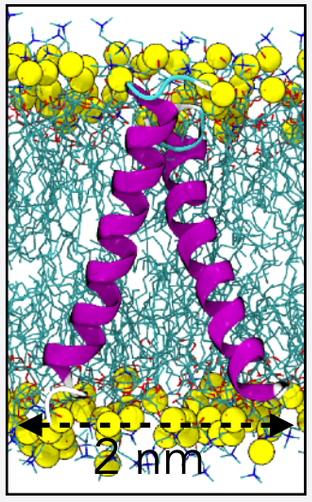

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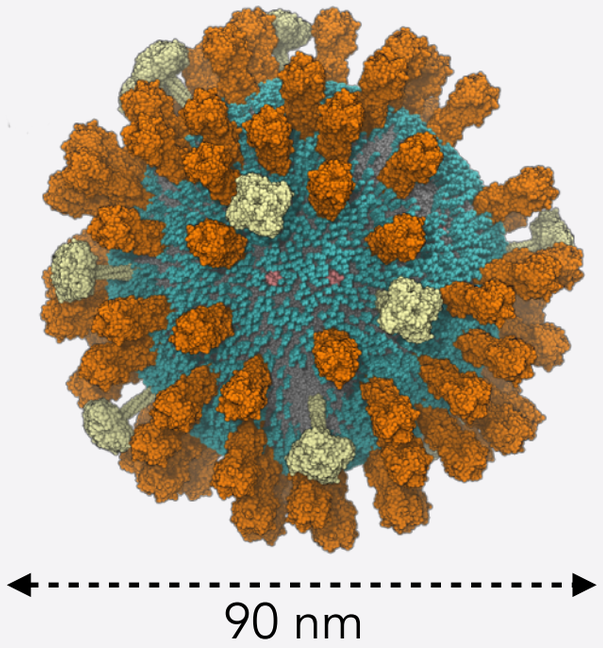

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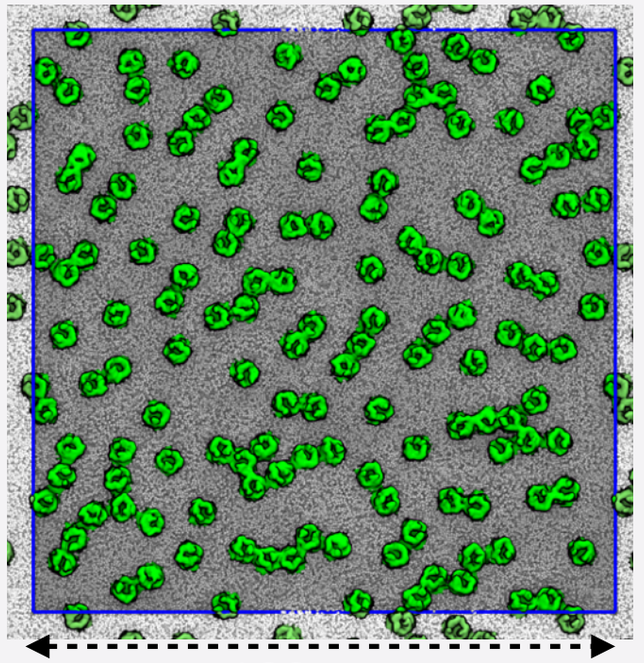

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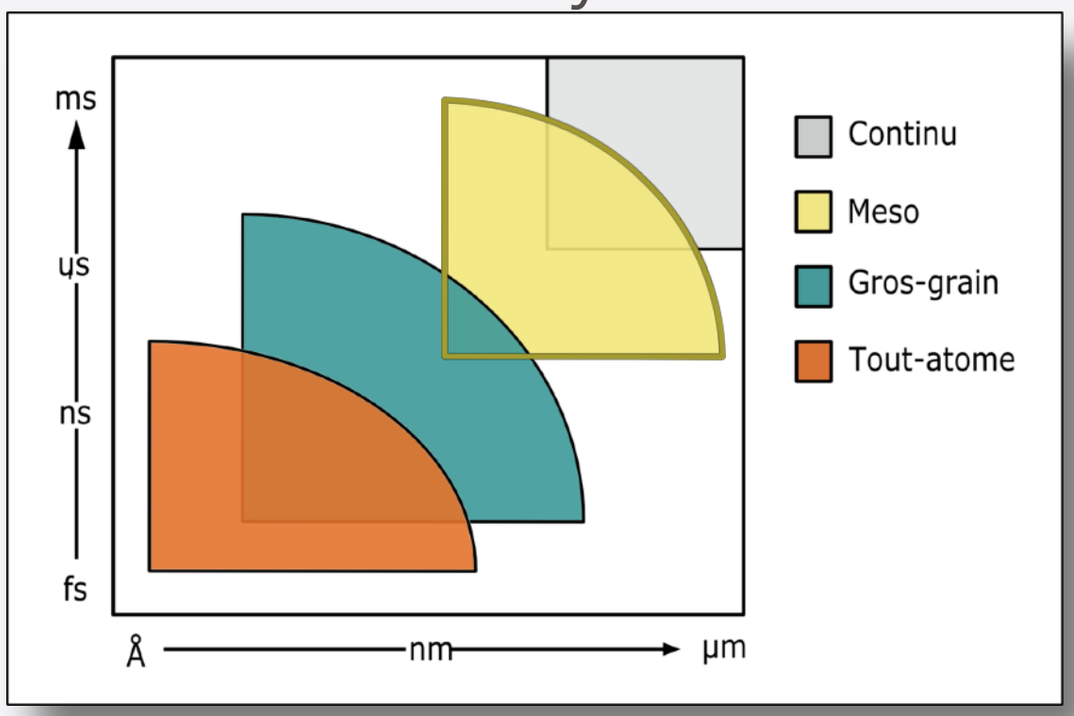
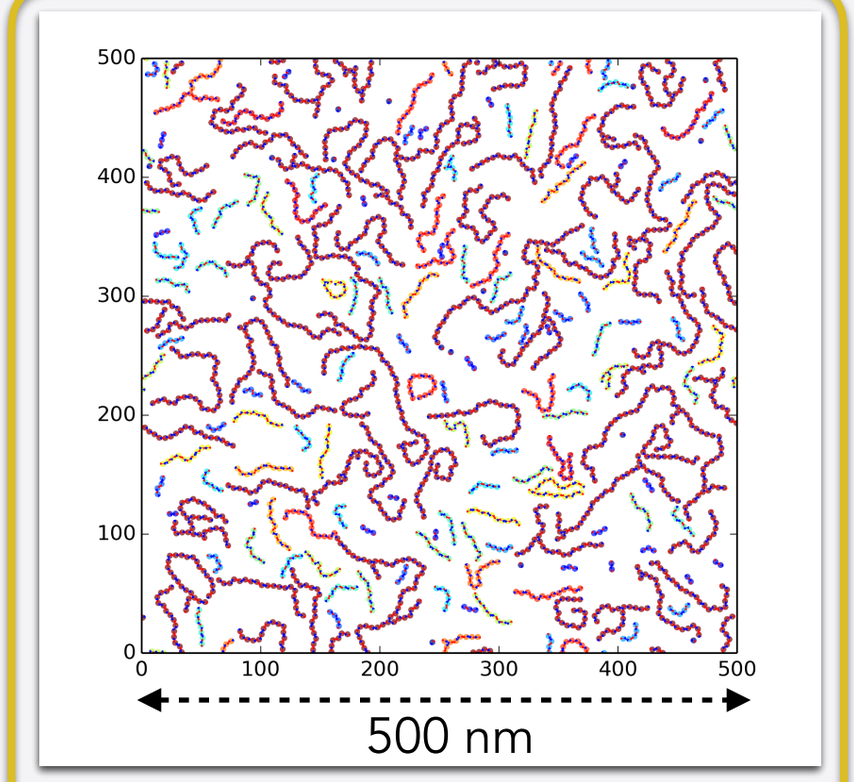


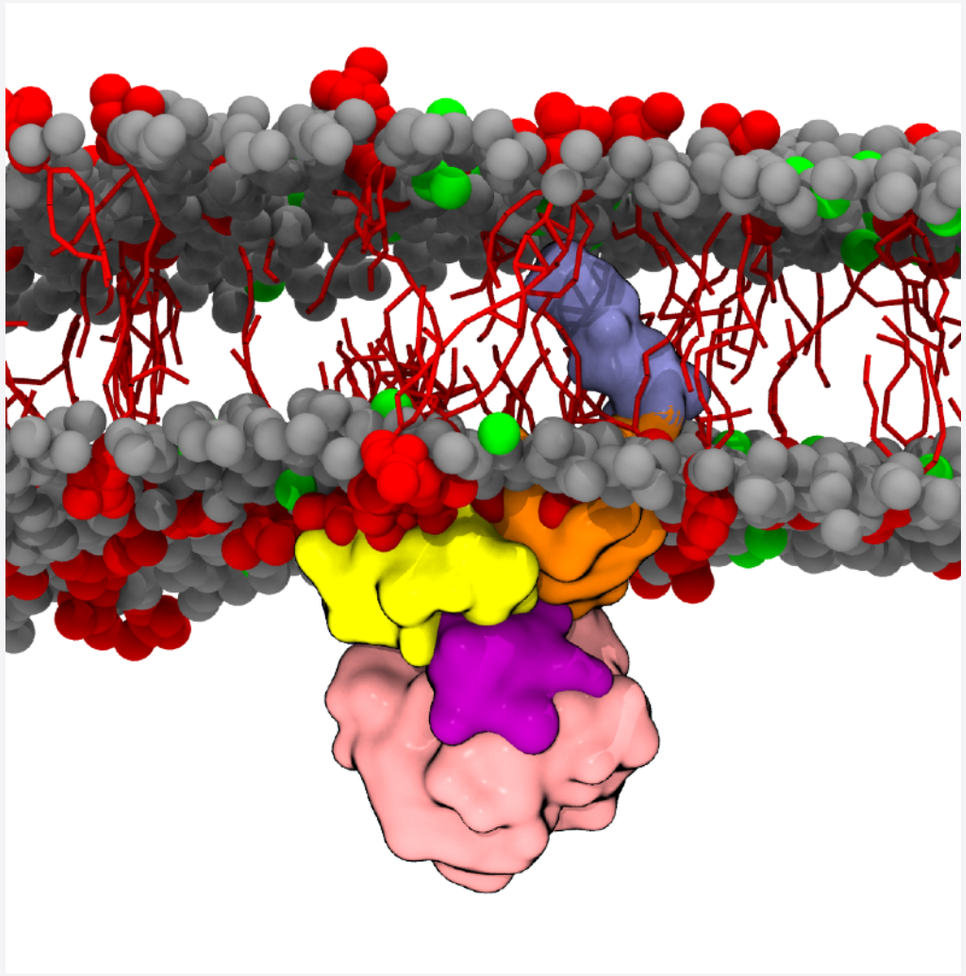
Meso



Chavent, *et al.* , *Nature Com.*, ***2018***

HOW TO SHARE MD DATA ?

EphA2 KINASE interacting with PIP2 molecules



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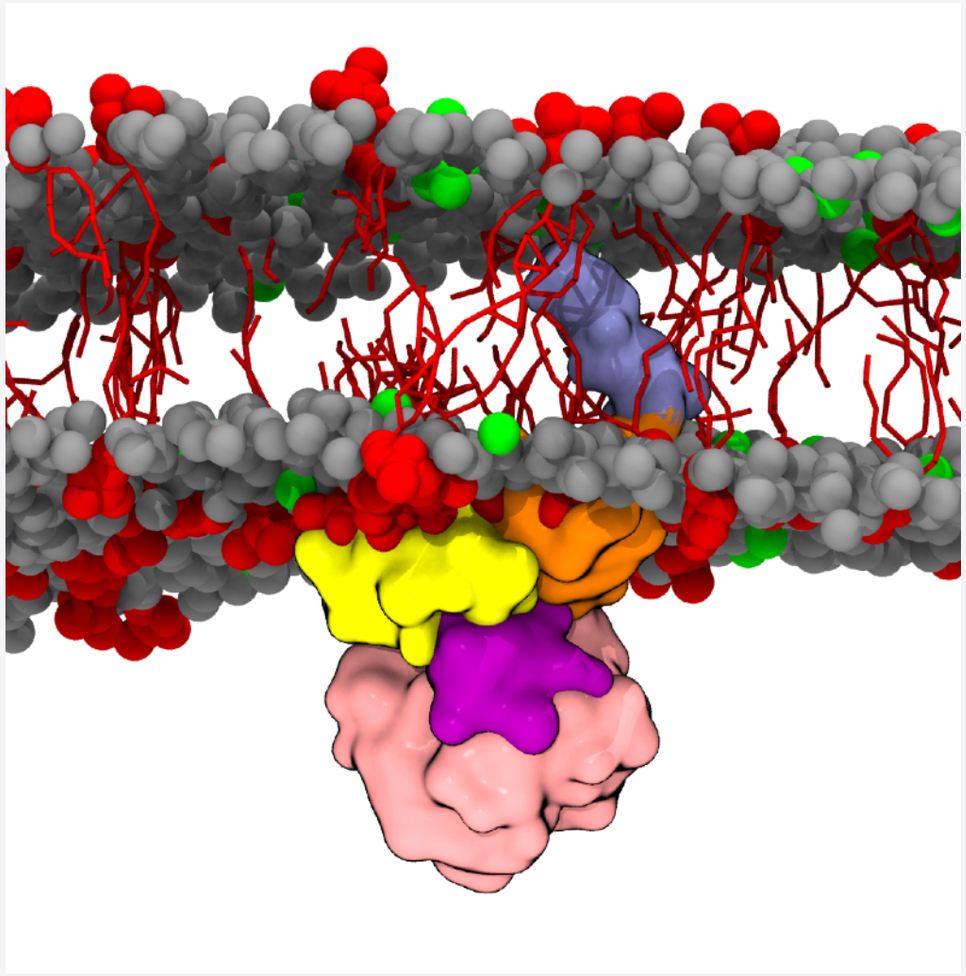

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Zenodo and link in SI

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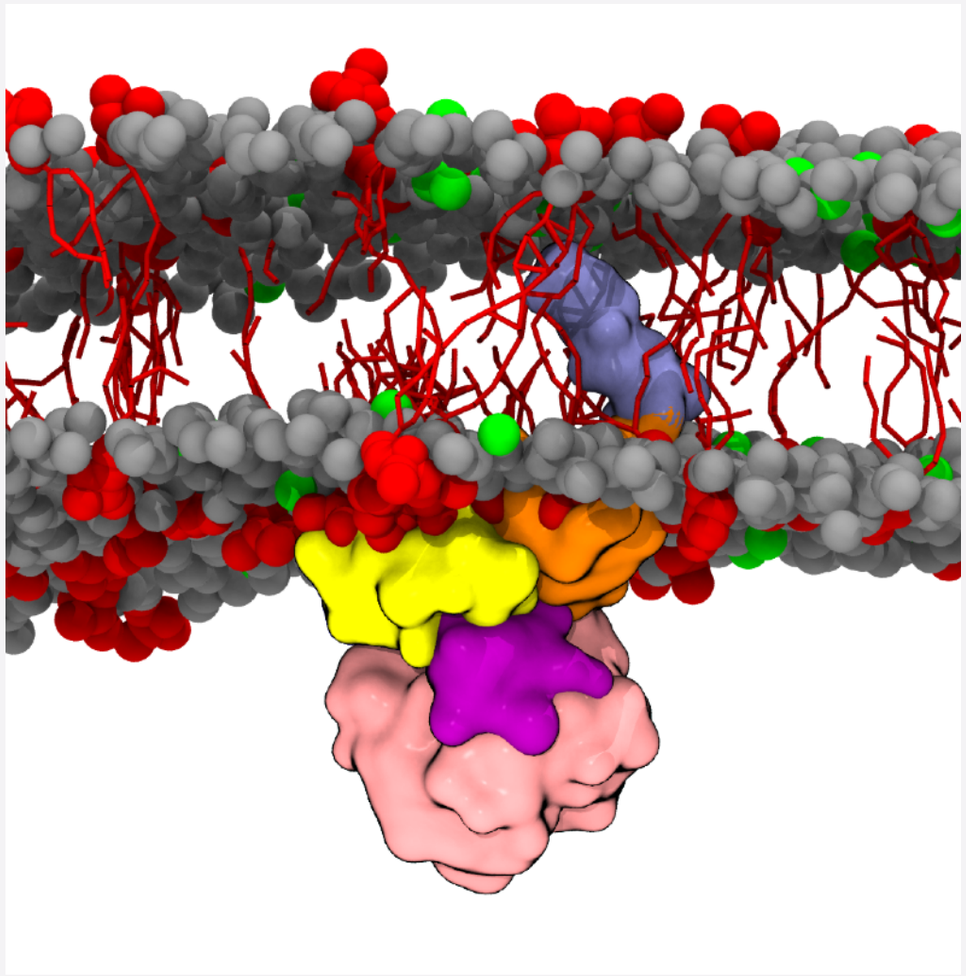

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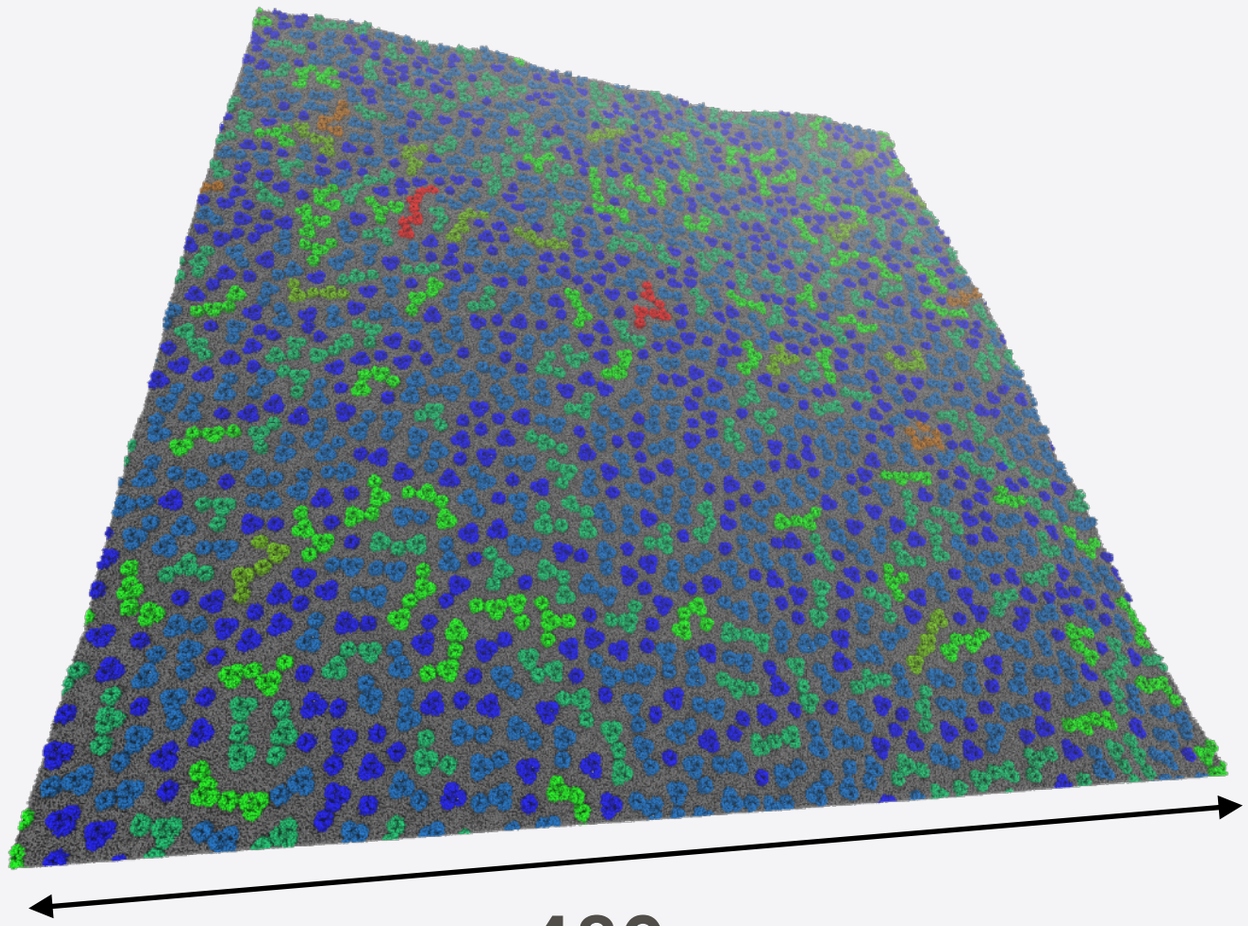
mix of BtuB and OmpF proteins

> 2000 proteins
~22M particles (with water)
1.5TB of data (2.5µs trajectory)
1 GB for 1 snapshot



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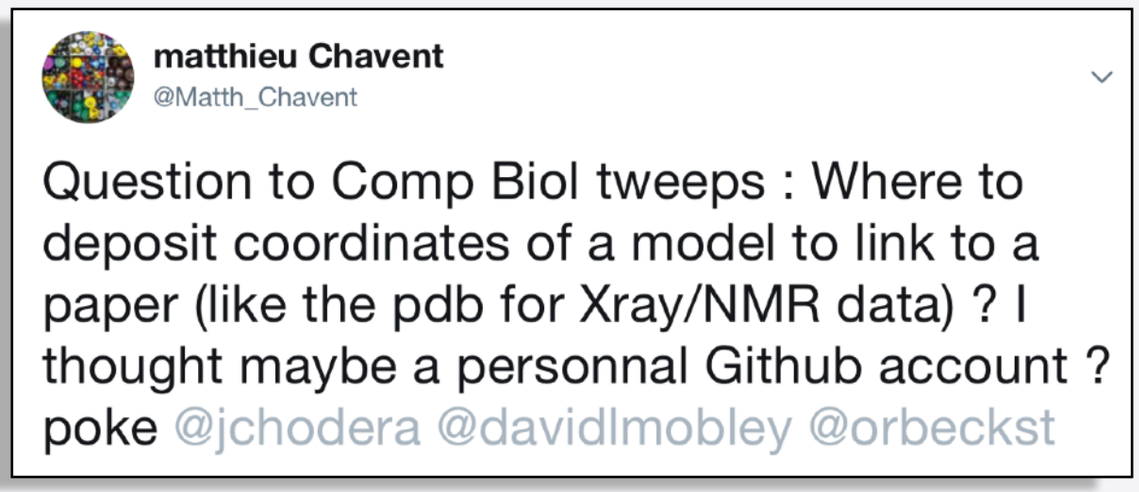
ASKING TWITTER



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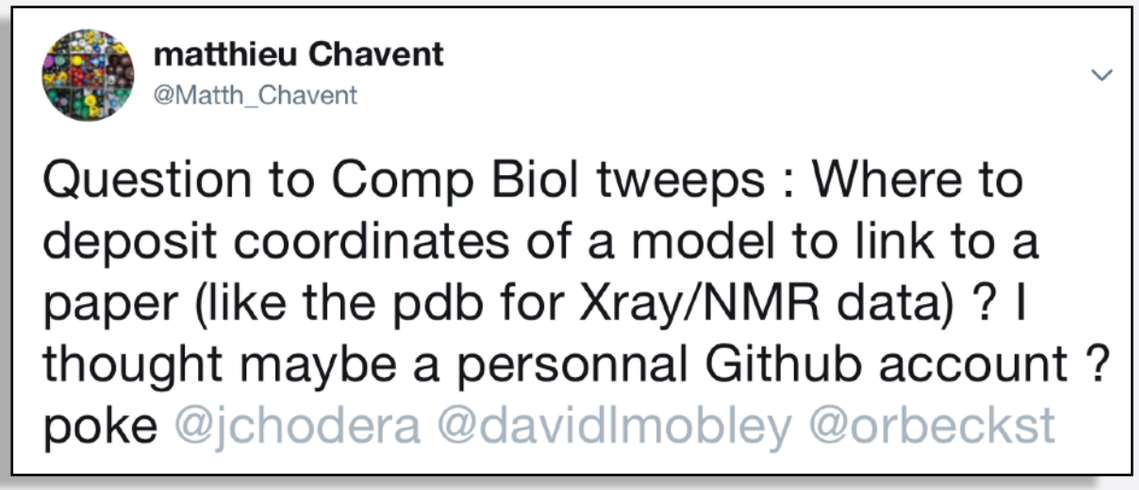

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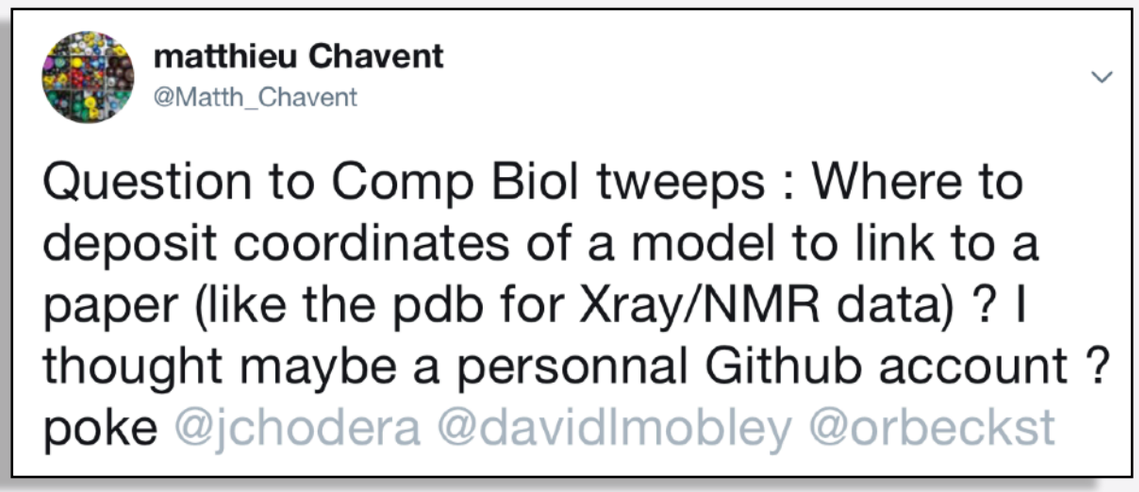

ASKING TWITTER

Andrew Marsh @marshgroup · 24 avr.

En réponse à @AnthonyC1Nash @Matth_Chavent et 3 autres

.@figshare @datadryad also good places. Librarians have told me the more the better to maximise exposure and @altmetric impact.

John Chodera @jchodera · 24 avr.

En réponse à @Matth_Chavent @davidlmobley @orbeckst

Your friendly journal editors have thought about this question! @Naturepub suggests @figshare and @datadryad for cases that are not clearly handled by standardized databases. nature.com/authors/polici…

Anthony Nash
@AnthonyC1Nash

Abonné

En réponse à @Matth_Chavent @jchodera et 2 autres

Following. Wouldn't be interested to know.

Traduire le Tweet

10:46 - 24 avr. 2018

matthieu Chavent
@Matth_Chavent

Question to Comp Biol tweeps : Where to deposit coordinates of a model to link to a paper (like the pdb for Xray/NMR data) ? I thought maybe a personnal Github account ? poke @jchodera @davidlmobley @orbeckst

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Mikael Trellet @mika_trellet · 24 avr.

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Partial answer: if this is a model you got from integrative/hybrid methods have a look at pdb-dev.wwpdb.org

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David Mobley @davidlmobley · 24 avr.

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Pierre Poulain @pierrepo · 24 avr.

;-) no need to put the data elsewhere. @ZENODO_ORG is backed up in @CERN_FR cloud infrastructure and implements FAIR principles about.zenodo.org/principles/ Pretty safe!

Mikael Trellet @mika_trellet · 24 avr.

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10:46 - 24 avr. 2018

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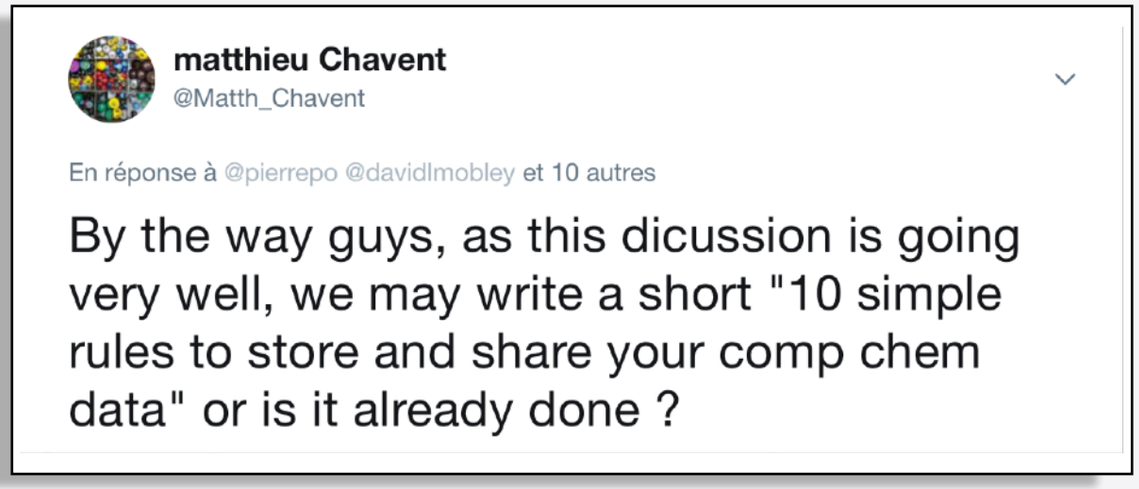

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Well, if I can find enough people to help I am happy to lead this. Please DM me if you want to participate to start this project

WORKSHOP FUNDING AND ORGANIZATION

Rossen Apostolov

bioexcel

Erik Lindahl

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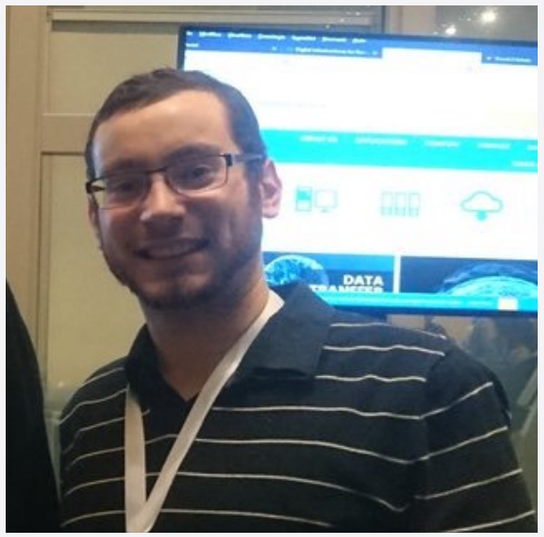
Lucie Delemotte
(SciLifeLab)

Reba Howard
(SciLifeLab)



Mikael Trellet
(Utrecht Uni)

Daniel Smith
(MolSSI)

WHAT ARE THE GOALS OF THIS WORKSHOP ?

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(during the session and before/after)

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(what are the solutions we already have?)

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(during the session and before/after)

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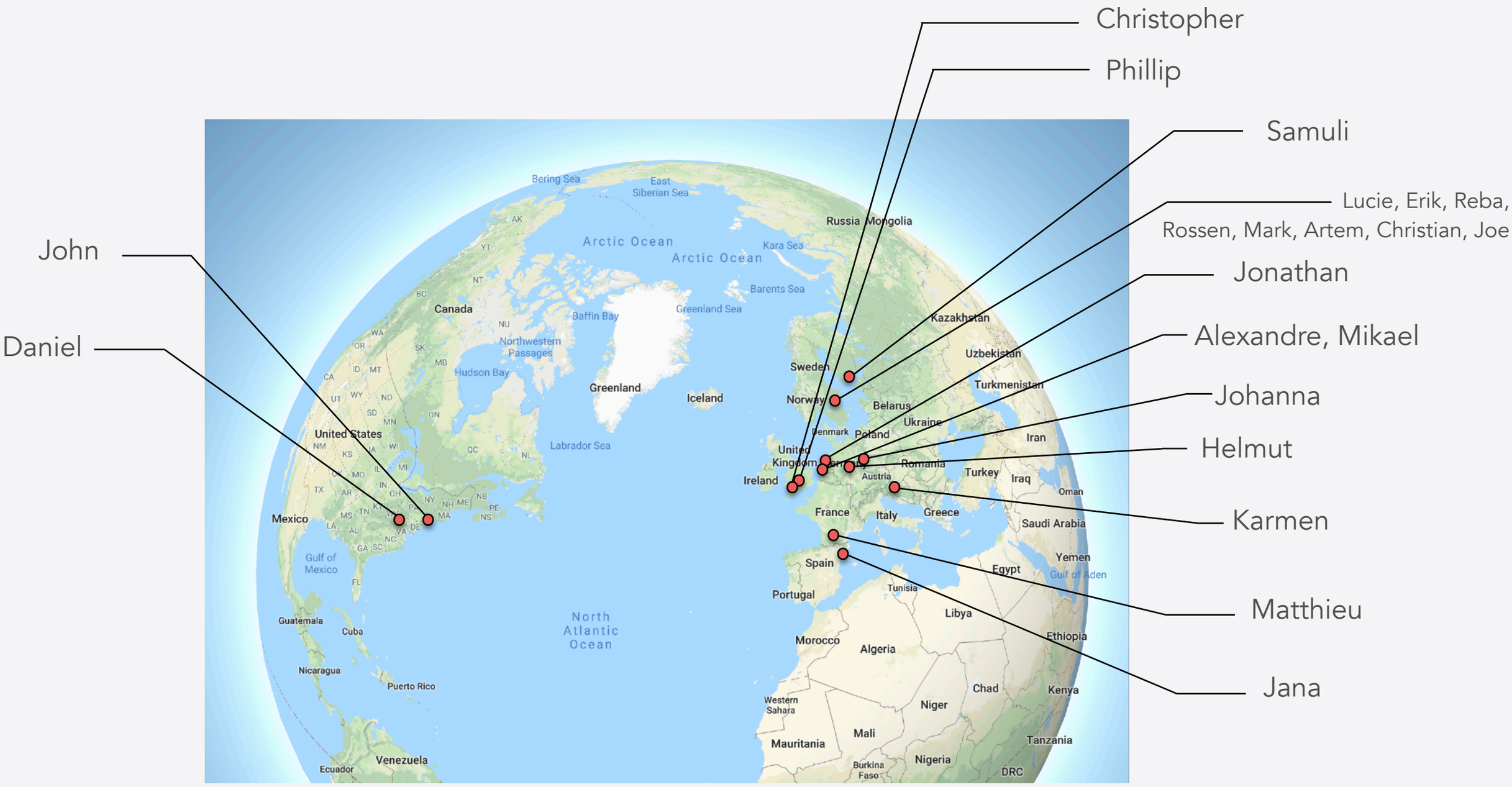
Highlight issues - find new solutions

(what can we develop in the future?)

Write - disseminate

(gather these pieces of information in a white paper)

WHO ARE WE ?


Christopher
Phillip
Samuli
Lucie, Erik, Reba,
Rossen, Mark, Artem, Christian, Joe
Jonathan
Alexandre, Mikael
Johanna
Helmut
Karmen
Matthieu
Jana
John
Daniel
Bering Sea
East Siberian Sea
Russia
Mongolia
Arctic Ocean
Kara Sea
Barents Sea
Canada
Baffin Bay
Greenland Sea
Northwestern Passages
Hudson Bay
Greenland
Iceland
Labrador Sea
United States
Mexico
Gulf of Mexico
North Atlantic Ocean
Kazakhstan
Uzbekistan
Turkmenistan
Sweden
Norway
Belarus
Ukraine
Poland
Denmark
Iran
Romania
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Oman
Saudi Arabia
Yemen
Egypt
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France
Italy
Greece
Spain
Portugal
Tunisia
Libya
Morocco
Algeria
Ethiopia
Chad
Kenya
Niger
Mali
Western Sahara
Mauritania
Nigeria
Burkina Faso
Tanzania
DRC
Guatemala
Cuba
Nicaragua
Puerto Rico
Venezuela
Ecuador

WHAT HAVE WE DONE ?

MemProt MD Search About

MemProtMD

GROMACS
FAST. FLEXIBLE. FREE.

GPCRMD

HOME ABOUT

EOSC-hub

MolSSI

mdbox

MDsrv

A fast & easy way of sharing MD simulations

bioexcel

BioSimSpace

Open Force Field Initiative

An open source, open science, and open data approach to better force fields

The NMRlipids project

HOW THIS WORKSHOP WILL WORK

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(no computing devices during the sessions
- except for taking notes or for tweeting)

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(Twitter: #SDMS18 , recordings)

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Few more things …

(Mikeal and Reba)