## SESSION GAMESTORMING

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horse

... OR HOW TO KEEP YOU FOCUS AND ENTERTAINED

WHILE YOU ARE CHANGING THE WORLD

Sharing Data for Molecular Simulations workshop 25/11/2018 – Stockholm



- PhD in Virtual Reality for exploration and analysis of molecular data
- Postdoc in the Computational Structural Biology team @ BonvinLab.org
  - Integration of scientific software (HADDOCK et al.) within efficient frameworks interfacing web portals and HTC resources



- Part of BioExcel EU project aiming to improve core software in biomolecular research and spreading best practices and expertise in the community.
- Part of the IHM (Integrative and Hybrid Methods) taskforce lead by RCSB/PDB and grouping SaliLab, ChimeraX and HADDOCK to design the new mmCIF extension
  → add metadata to make modelling process reproducible

#### https://pdb-dev.wwpdb.org/

#### **TOPIC-DRIVEN SESSIONS - OVERVIEW**

- 4 topics:
  - Standardization of file formats

- Monday 9h-11h45
- Tools for trajectory file sharing
  Monday 13h30-16h15
- Streamlining molecular simulations data

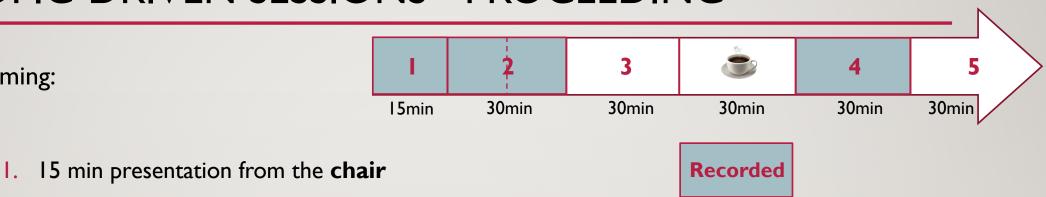
Monday 16h30-19h15

• Reproducibility of molecular simulations

Tuesday 8h30-11h

#### **TOPIC-DRIVEN SESSIONS - PROCEEDING**

• Timing:



- 2. 2\*15min talks from session guests
- 3. 30min group gamestorming (what?!) 4/5 people per group
- 4. 30min **debriefing** with one representative per group
- 5. 30min final discussion with key points for white paper

#### **ROLE OF THE CHAIRS**

• (Re-)introduce what is the goal of the topic, give some context

• **Briefly** introduce the speakers

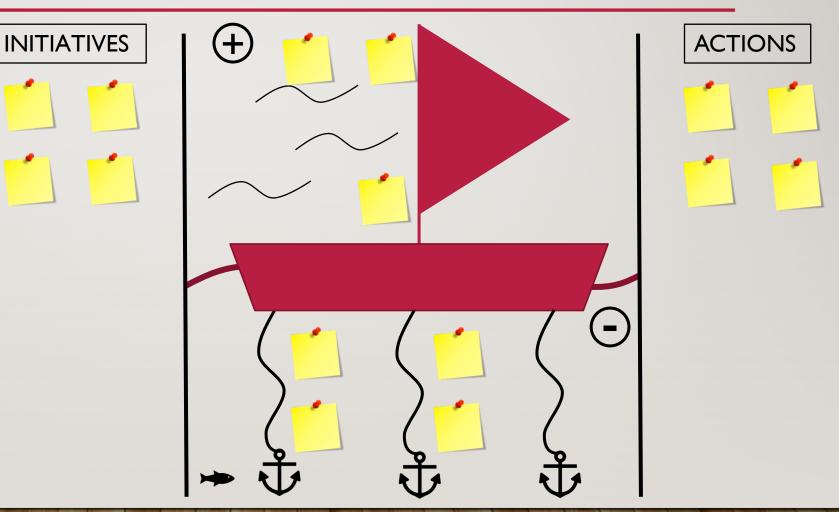
• Be careful with timing

• Merge group ideas during debriefing

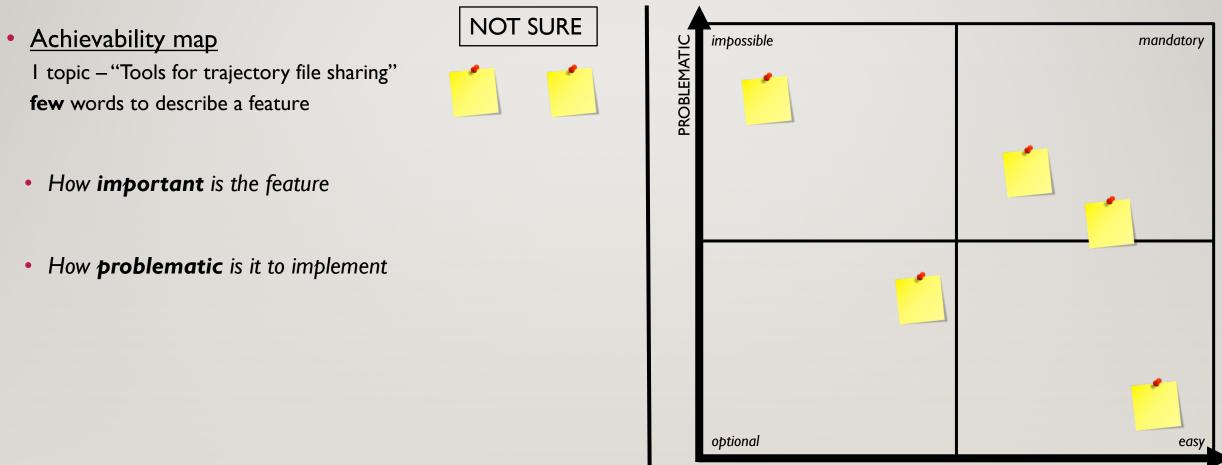
• <u>Lead</u> the final discussion

### GAMESTORMING..?!

- <u>Sailboat metaphor</u>
  3 out 4 topics
  few words to describe an idea
  - What makes it possible (+)
  - What makes it complex (-)
  - Initiatives going in this direction
  - Actions to be taken



#### **GROUP DISCUSSION PROCEEDING**



IMPORTANCE

#### LET'S PLAY!

- Get ready for an extra topic
  - In 5/10 minutes, let's gamestorm around the following topic

# How to have a fruitful workshop in Stockholm?

#### INITIATIVES



ACTIONS