Seminar schedule

We will rely on Google Drive and slido to share information. The shared public link is:
https://tinyurl.com/DagstuhlBioML

This living document will contain a summary of the discussions and activities planned for each day, alongside links to the relevant notes.

Typical schedule:

7:30– 8:45	Breakfast (cafeteria)
9:00–10:30	First morning session
10:30	Coffee and tea (in front of lecture hall)
11:00–12:00	Second morning session
12:15–13:00	Lunch (cafeteria)
13:00–14:00	Free time (?)
14:00–15:30	First afternoon session
15:30–16:00	Afternoon tea (cafeteria)
16:00–17:30	Second afternoon session
18:00–19:00	Dinner (cafeteria)
19:00–	Free time (drinks, discussions, table tennis, pool, table football, sauna, music)
22:00–	Cheese platter (castle)

More general info about Schloss Dagstuhl here:
https://www.dagstuhl.de/en/program/planning-your-visit/
https://www.dagstuhl.de/en/seminars/dagstuhl-seminars/infos-for-organizers

Sunday Nov 3 - arrival day

Attendees will be trickling in throughout the day and should check into their rooms. There will be a light dinner served at 6 pm. We will have an informal meet and greet between 7pm-9pm in the main castle break room next to the snacks.

Monday Nov 4

9:00–10:30 Introduction (large conference room)

- Logistics (location of meeting rooms, food, amenities, outing, etc.)
- Intro about the Seminar and the scientific theme
- Intro slides from each person - one slide bios

11:00-12:00 Brainstorming and organization of topics

14:00-15:30 **Protein language models, foundation models**

- 30-min Introduction talk on Protein Language Models by Burkhard Rost
- Discussion - notes here
- Session chair / co-chair: Anne-Flo / Ilia

16:00-17:30 **Reliable protein-protein interaction prediction and benchmarking**
- 30-min Introduction talk on Protein-Protein Interaction prediction (including over-estimate of performance) by Arne Elofsson
- Discussion - notes here
- Session chair / co-chair: Simona / Alexandre

20:00 Beer/wine sessions:
- MSAs vs. LLMs – lounge
- OpenScience and biosecurity – Kaiserslautern, notes here

Tuesday Nov 5

9:00-10:30 Parallel discussion sessions preceded by joint talks in the lecture room
- Evolution and evolutionary paths – intro by Simona Cocco, chair: Martin W, lecture room, co-chair: Alex S

  Notes here
- Defining similarity between biomolecular interactions, fast search – intro by Anton & Roman, chair: Josef, co-chair: Roman, small room Kaiserslautern

  Notes here

11:00-12:00 Parallel discussion sessions preceded by joint talks in the lecture room
- Enzymes (Enzymatic reaction prediction) - Intro talk on enzymes by Simon, chair: Tomas, co-chair: Simon - small room Kaiserslautern

  Notes here
- Injection of laboratory constraints into ML models and workflows - Introductory words by Bruce, chair: Bruce, co-chair: Hunter – lecture room

  Notes here

14:00-15:30 Parallel discussion sessions
- Protein binder design: are we there yet? Protein-small molecules – chair: Andrew, co-chair: Ilia - small room Kaiserslautern

  Notes here
- Protein binder design: are we there yet? Protein-protein – chair: Armita, co-chair: Petr – lecture room

  Notes here

16:00-17:30 Wrap-up of all sessions and feedback, finalize next day schedule

20:00 Beer/wine sessions
Random groups

Wednesday Nov 6

9:00-9:30 **Joint intro talks for parallel sessions of the whole morning, max 5 minutes each** (Saarbrücken, large lecture room, new building)
9:30-10:30 **Parallel discussion sessions:**

- Protein tokenization in foundation models + Data representation for proteins and small molecules - Julius/Sergei short intro presentation - Julius: chair, Sergei: co-chair
  Random split in 2 subgroups + collective wrap-up at the end
  Saarbrücken (large lecture room, new building)
  Notes for sub-session 1 (Saarbrücken) here
- Enzymes de novo - Tomáš short intro presentation, notes here
  Kaiserslautern (castle building)

10:30 group photo

11:00-12:00 **Parallel discussion sessions:**

- Uncertainty estimation in models / Uncertainty estimation in ML for small molecules
  Hunter/Jessica short intro presentation
  Saarbrücken (large lecture room, new building)
- Enzymes engineering - Simon short intro presentation
  Kaiserslautern (castle), notes here
- Coevolution at the scale of PPI networks - Cyril short intro presentation
  S006 (lounge castle ground floor)

Afternoon:
14:00 Outing, free afternoon

Beer sessions

- Symmetries and equivariance

Thursday Nov 7

9:00-9:30 **Joint intro talks for whole morning, max 5 minutes each** (Saarbrücken, large lecture room, new building)
9:30-10:30 **Parallel discussion sessions:**

- Efficient training and small language models. Linear transformers. Linear-scaling models (mamba, hyena). - Chris short intro presentation - Saarbrücken
  - Notes
  - https://patmcguinness.substack.com/p/beyond-transformers-with-mamba
- Predicting graph-structured output - Juho short intro presentation - Kaiserslautern - Notes here

11:00-12:00

- Protein dynamics as input (and/or output?) for machine learning - Arne/Sergei
  - Notes Here
  - Saarbrücken (large lecture room, new building)
- Inductive bias injection - Hunter/Bruce - Kaiserslautern - Notes here
- Importance of homology and of multiple sequence alignments - Anne-Flo - Lounge - Notes here

14:00-14:30 **Joint intro talks for whole afternoon, max 5 minutes each** (Saarbrücken)
14:30-15:30 **Parallel discussion sessions:**

- Small molecules: Deep Learning for Molecular Property and Activity Prediction - Andrea - - Saarbrücken
- ML guided directed evolution - Bruce - Kaiserslautern

16:00-17:30

- Fine-tuning foundation models - Saarbrücken
- Protein symmetries; 3D alignments - Sergei - Kaiserslautern

20:00 Beer/wine sessions

Friday Nov 8 - departure day

9:00 - 10:30 Reporting back from Wednesday and Thursday sessions

11:00 - 12:00 General conclusion: lessons learned, both scientifically and organizationally. Future Dagstuhl seminars?

Attendees will be leaving at different times throughout the day, most expected to leave after lunch.