NFDI4Chem Consortium Meeting 4.0

22/23 November 2023 (Jena)

Panel Discussion: Steering Committee and Advisory Boards

22 November: 11:45 - 13:00
Moderation: John D. Jolliffe

Summary of the discussion with the Advisory Boards (ABs):

Question 1: What is the feedback about the environment in NFDI4Chem?
- NFDI4Chem as large, collaborative team with passion and impressive output
- Specifically Chemotion ELN and outreach activities are central elements in order to push a culture change towards electronic data management; a wide knowledge of NFDI4Chem is being observed, confirming the impressive communication activities

Question 2: How can we achieve more collaboration from the Advisory Boards and the Steering Committee ? And what do we want to see from this collaboration?
- Personal meetings are preferred over virtual ones, but a combination can work; meeting frequency depends on project progress
- More meetings in the preparation for phase 2 would be useful to get proper feedback in the decision-making phase; after Community Workshop
- Whenever questions arise, contact ABs, and ABs will do vice-versa

Question 3: How can NFID4Chem increase collaboration with industry? How to avoid double work?
- Involves whole NFDI: send message that NFDI and industry work on the same topics and need to collaborate; leverage PCI
- We need to set up a forum that allows industry to work constructively
- Difference between (pharma) industry and academia: driven by patents vs. publications
- Security of data is a big issue for industry, we need to think more of that
- Standardization is important: ask vendors to deliver specific standards; coming together will raise the pressure on companies to deliver these standards
- Licenses: negotiate a German-wide Chemdraw license for all universities?

Question 4: How can we increase the collaboration between academia and industry?
- Currently there is no systemic information flow, but mutual exchange is essential in order to join forces in the first place
- ELN usage in industry: security and immediate bug fixes are crucial

- Exchange platforms within NFDI4Chem could be expanded to reach industry
- International perspective is important, e.g. for standards; global funding would be helpful; the global effort that already is taken has to be made visible to the communities: presence at international meetings (e.g. ACS), international data week, organise hackathons bringing various sides together, more self-confidence
- Challenge: leaving the RDM bubble - can we connect bubbles and initiate exchange?
- Possibility for industry engagement in academia: offer visiting lectures at universities

Question 5: What do you want to see from NFDI4Chem in the future?
- Outreach and communication has to be even stronger, to make chemists aware of the initiative and reduce insecurities (e.g. RDM section in DFG proposals); ambassadors
- More input from NFDI4Chem and RDM planned for Chemiedozententagung 2024
- Feedback after some workshops: "there is so much to plan and set up and they do not have time for that.
- "Constant drop makes the hole"-strategy is sustainability but too slow
- Editors of journals, especially big players, have to be on board and should push more the use of FAIR tools; Editors4Chem Workshop already established, 4Chem services already showing up in the author guidelines
- Pre-competition among publishers in developing standards

Question 6: What are the challenges and could we avoid them?
- Scalability of services, nation-wide implementation of chemotion difficult; Chemotion as a service (no need to host it), working together with FIZ as experienced institution
- Keep it simple! Acceptance rate in the lab has to be high. don't over-engineer your software; Chemotion is not user-friendly at some points, but fast to install and update
- Long-term financing and sustainability cannot be achieved in a 3-year-funding cycle; not sure if this is possible in Germany? Maybe commercialisation could be a solution
- Complete commercialization is against the philosophy of NFDI, but parts of it could be moved into a startup for example; or business model like wikipedia is desirable
- Exit plan for repos: depositing data in an archive
- A good example: Pipeline Pilot -> KNIME; now even Sanofi wants to move from pipeline pilot to KNIME, as it is cheaper. This is a business model you could think about.
- be more self-confident, it's not only vapor ware that you sell here, this is rock-solid. think outside the box, . e.g., find users in the US; 4Chem repos are open internationally