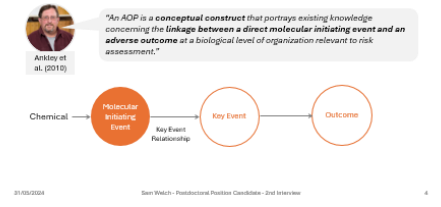
Aggregate Exposure Pathways for Source to Outcome pollution assessment

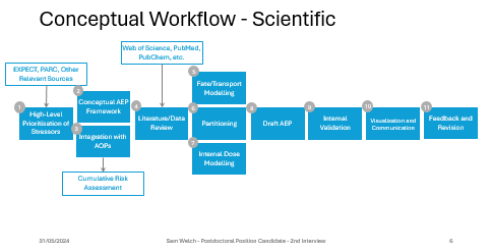
Sam Welch – Postdoctoral Position Candidate

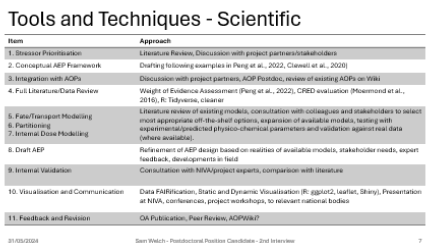
2nd Interview – 31/05/2024

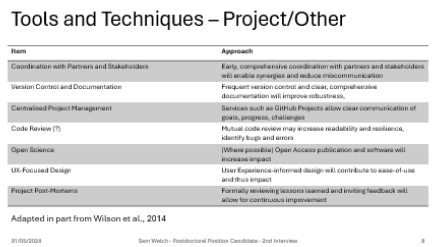
Link to GitHub repo containing slides, references, etc.

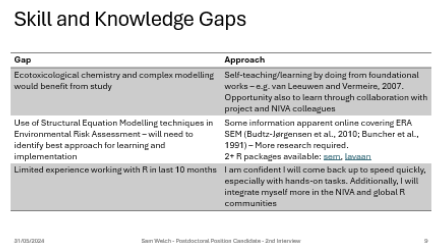
Presentation Content

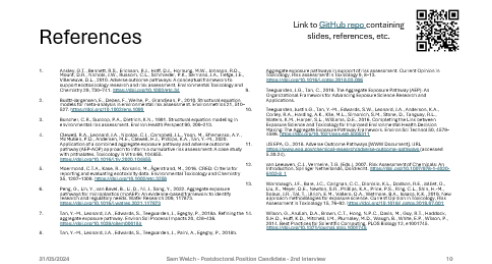


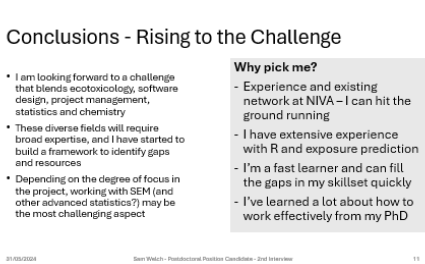












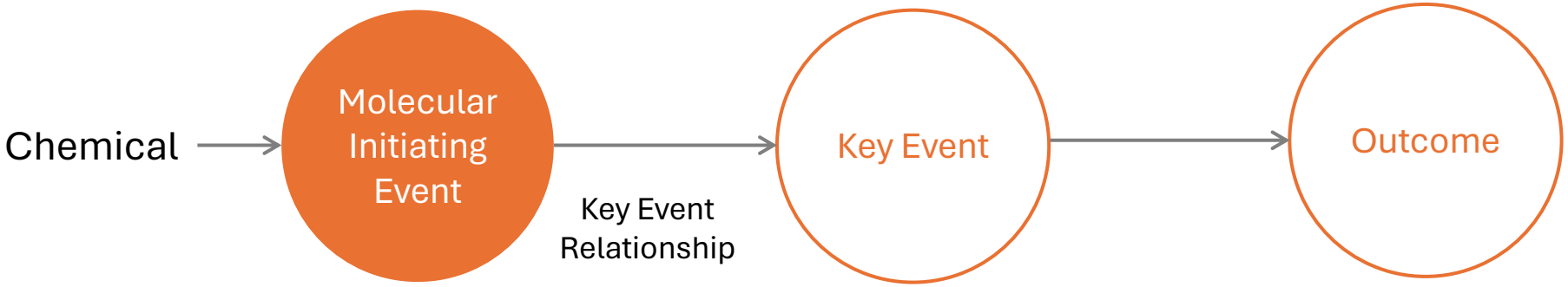
Problem Statement

- *Assess organism and population impacts from key Arctic industries* (EXPECT)
- *Develop next-generation chemical risk assessment to protect human health and the environment* (PARC)
- *Assessment of […] exposure to support research and regulatory needs* (PARC)
- *Development of Source to Outcome Pathways to characterise […] pollutants and their mixtures for use in subsequent Cumulative Risk Assessment*

Adverse Outcome Pathways

Ankley et al. (2010)

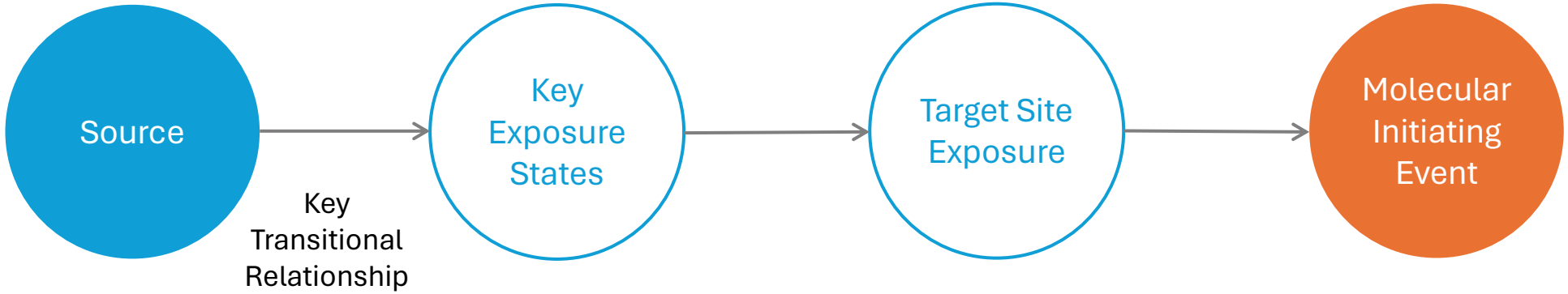
*"An AOP is a **conceptual construct** that portrays existing knowledge concerning the **linkage between a direct molecular initiating event and an adverse outcome** at a biological level of organization relevant to risk assessment."*



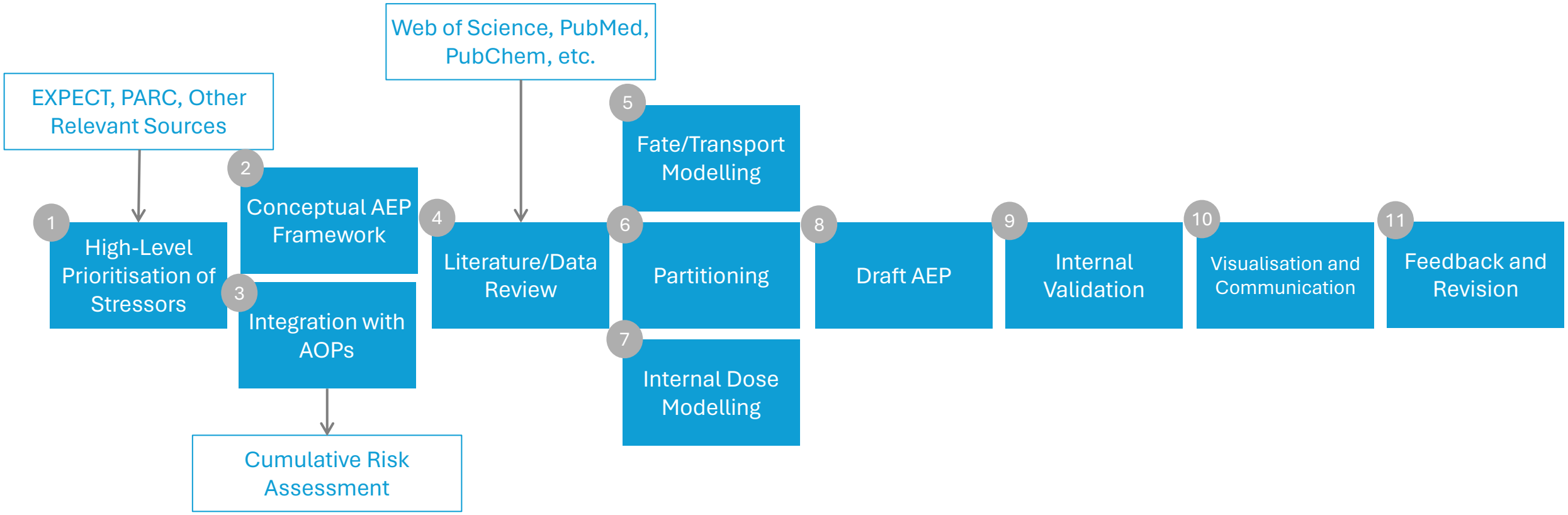
Aggregate Exposure Pathways

Teeguarden et al. (2016)

*"An AEP is the assemblage of existing knowledge concerning **biologically, chemically and physically plausible**, empirically supported **links** between **introduction of a chemical** or other stressor into the **environment** and its **concentration at a site of action**."*



Conceptual Workflow - Scientific



Tools and Techniques - Scientific

Item	Approach
1. Stressor Prioritisation	Literature Review, Discussion with project partners/stakeholders
2. Conceptual AEP Framework	Drafting following examples in Peng et al., 2022, Clewell et al., 2020)
3. Integration with AOPs	Discussion with project partners, AOP Postdoc, review of existing AOPs on Wiki
4. Full Literature/Data Review	Weight of Evidence Assessment (Peng et al., 2022), CRED evaluation (Moermond et al., 2016), R: Tidyverse, cleaner
5. Fate/Transport Modelling 6. Partitioning 7. Internal Dose Modelling	Literature review of existing models, consultation with colleagues and stakeholders to select most appropriate off-the-shelf options, expansion of available models, testing with experimental/predicted physico-chemical parameters and validation against real data (where available).
8. Draft AEP	Refinement of AEP design based on realities of available models, stakeholder needs, expert feedback, developments in field
9. Internal Validation	Consultation with NIVA/project experts, comparison with literature
10. Visualisation and Communication	Data FAIRification, Static and Dynamic Visualisation (R: ggplot2, leaflet, Shiny), Presentation at NIVA, conferences, project workshops, to relevant national bodies
11. Feedback and Revision	OA Publication, Peer Review, AOPWiki?

Tools and Techniques – Project/Other

Item	Approach
Coordination with Partners and Stakeholders	Early, comprehensive coordination with partners and stakeholders will enable synergies and reduce miscommunication
Version Control and Documentation	Frequent version control and clear, comprehensive documentation will improve robustness,
Centralised Project Management	Services such as GitHub Projects allow clear communication of goals, progress, challenges
Code Review (?)	Mutual code review may increase readability and resilience, identify bugs and errors
Open Science	(Where possible) Open Access publication and software will increase impact
UX-Focused Design	User Experience-informed design will contribute to ease-of-use and thus impact
Project Post-Mortems	Formally reviewing lessons learned and inviting feedback will allow for continuous improvement

Adapted in part from Wilson et al., 2014

Skill and Knowledge Gaps

Gap	Approach
Ecotoxicological chemistry and complex modelling would benefit from study	Self-teaching/learning by doing from foundational works – e.g. van Leeuwen and Vermeire, 2007. Opportunity also to learn through collaboration with project and NIVA colleagues
Use of Structural Equation Modelling techniques in Environmental Risk Assessment – will need to identify best approach for learning and implementation	Some information apparent online covering ERA SEM (Budtz-Jørgensen et al., 2010; Buncher et al., 1991) – More research required. 2+ R packages available: sem, lavaan
Limited experience working with R in last 10 months	I am confident I will come back up to speed quickly, especially with hands-on tasks. Additionally, I will integrate myself more in the NIVA and global R communities

References

Link to GitHub repo containing slides, references, etc.

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Conclusions - Rising to the Challenge

- I am looking forward to a challenge that blends ecotoxicology, software design, project management, statistics and chemistry
- These diverse fields will require broad expertise, and I have started to build a framework to identify gaps and resources
- Depending on the degree of focus in the project, working with SEM (and other advanced statistics?) may be the most challenging aspect

Why pick me?

- Experience and existing network at NIVA – I can hit the ground running
- I have extensive experience with R and exposure prediction
- I'm a fast learner and can fill the gaps in my skillset quickly
- I've learned a lot about how to work effectively from my PhD