NATIONAL ACADEMIES Sciences Engineering Medicine

BOARD ON LIFE SCIENCES

Navigating the Benefits and Risks of Publishing Studies of In Silico Modeling and Computational Approaches of Biological Agents and Organisms - A Workshop

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THURSDAY- FRIDAY, APRIL 3-4, 2025

Workshop Description

This workshop aims to explore the opportunities and biosecurity risks associated with communicating studies involving computational modeling and generative AI in biological systems, particularly dual-use research of concern and pathogens of pandemic potential, during the dissemination and publication stages. This project was developed following the release of the U. S. Government Policy for Oversight of DURC and PEPP, asking for the development of voluntary guidance for research involving in silico models and computational approaches. The implementation of this policy is planned for May 2025. The activity aims to strike a balance between scientific advancement and security risks through the active engagement of experts and policy discussions.

The different activities will convene a diverse group of U.S. and international stakeholders from the scientific research and medical communities, the publishing industry, experts in biosecurity, biotechnology, artificial intelligence, professional societies, and policymakers across the government, among others.

During this interactive hybrid workshop, participants will consider existing policies and guidelines for various communication outlets, discuss challenges and needs to safeguard the benefits of communicating such studies while mitigating risks as illustrated in case examples, review the relevance of ongoing AI safety efforts, and explore policy options and norms at the national and international levels.

Submit Your Questions in Advance:

The audience is invited to submit questions in advance of the meeting to better inform the discussions. Please submit your questions on our Slido platform.

Day 1–Thursday, April 3

Goal: Gain a comprehensive understanding of the challenges and gaps in existing statements, policies, guidance, and safeguards related to dual-use research of concern and pathogens with pandemic potential, specifically in the context of disseminating life sciences studies, models, and tools using in silico modeling and computational approaches.

12:00pm–12:20pm ET

Welcome and Meeting Overview

- **Alex John London**, Carnegie Mellon University
- **Valda Vinson,** Science
- **Audrey Thévenon,** National Academies of Sciences, Engineering, and Medicine

12:20pm–1:30pm ET

Session 1: Setting the Stage – Context and Scope

Goal: Frame and define the scope of the workshop, focusing on the research's benefits, potential for innovation, and dual-use research concerns/biosecurity risks in the context of disseminating research and resources using computational modeling, foundation models, and generative AI

Moderator: Alex John London, Carnegie Mellon University

Invited Speakers

- **Gigi Gronvall**, John Hopkins University
- **Lynda Stuart**, Fund for Science and Technology
- **Sara Del Valle**, Los Alamos National Laboratory
- **Feilim Mac Gabhann**, John Hopkins University
- **Valda Vinson,** Science

Questions & Answers

1:30pm–2:30pm ET

Session 2: Benefits and risks of disseminating studies, models, and tools involving computational approaches: What's hype, and what's reality?

Goal: Illustrate theoretical discussions through real-world examples, highlighting the complexity of biological systems, particularly when involving computational approaches, and the broad range of dissemination options**.**

Moderator: Jaspreet Pannu, Stanford University

Case Studies Speakers:

- **James Diggans,** Twist Bioscience
- **Anthony Gitter**, University of Wisconsin–Madison
- **Nick Sofroniew**, EvolutionaryScale
- **Jamie Yassif**, Nuclear Threat Initiative

Questions & Answers

2:30pm–2:40pm ET

Introduction Session 3: Challenges and Needs to Effectively Safeguard the Benefits and Mitigate the Risks of Disseminating Studies, Models, and Tools Involving Computational Approaches – Thematic Breakout Rooms

Moderator: Simone Bianco, Altos Labs Institute of Computation

Goal: To collaboratively identify known issues when disseminating studies, models, and tools involving in silico modeling and computational approaches in life sciences research, explore potential future challenges, and begin identifying what might be needed to effectively safeguard research benefits while mitigating the dual-use risks associated with disseminating these studies, models, and tools.

2:40pm–2:55pm ET

Break – Move to breakout rooms

2:55pm–4:15pm ET

Session 3: Thematic Breakout Rooms – Challenges and Needs to Effectively Safeguard the Benefits and Promote Advances

During the breakout room discussion, the groups will aim to address challenges and needs to effectively safeguard the benefits and mitigate the risks of disseminating studies, models, and tools involving computational approaches through the following overarching research themes:

1. Molecules & Proteins – Padlet Board Room 1
2. Systems Biology & Genetic/Cellular Engineering - Padlet Board Room 2
3. Epidemiological Modeling & Biosecurity - Padlet Board Room 3

General Guidance for the Breakout Room Discussion:

- The group will first review the relevant **outputs** for in-silico research, their dissemination **outlets,** and **stakeholders** associated with each output and outlet.
- The group will then answer a series of questions:
    - What **criteria** should be used to assess and evaluate the research **benefits** and **biosecurity risks**? This discussion will review the existing policies, guidance, and safeguards for physical research.
    - What **additional criteria** (if any) should be used to assess the **biosecurity risk** of in silico research in biological systems for each dissemination outlet?
    - Do the different dissemination outlets present different risks?
    - What do you see as current **challenges and gaps** in assessing and evaluating the benefits and the DURC and PEPP potential of disseminating in silico research in biological systems?
- The group will use an online platform to collect these answers
- If time allows, the group can brainstorm what could be implemented (now, near-term, long-term) to fill these gaps and overcome current barriers to implementing effective voluntary guidelines.

4:15pm–4:25pm ET

Reflection & Ah-ha moments

Audience - drop in the chat ONE challenge or barrier you have identified as critical to consider when co-producing policy options and norms

4:25pm–4:30pm ET

Wrap up and Adjourn

Valda Vinson, Science

END OF DAY 1

Day 2 – Friday, April 4

Goal of Day 2: Building on day 1 discussion and considering lessons learned from past biotechnology innovations and in silico modeling & AI safety and security from other domains (nuclear, chemistry, cybersecurity), discuss and refine collaboratively policy options, norms, guidance, and/or best practices for safeguarding the benefits and advances while reducing the risks posed by disseminating research information and resources on life sciences studies, models, and tools using in silico modeling and computational approaches, especially dual-use research of concern and pathogens of pandemic potential.

12:00pm–12:10pm ET

Welcome and Overview

- **Alex John London**, Carnegie Mellon University
- **Valda Vinson,** Science

12:10pm–12:40pm ET

Session 6: Challenges and Opportunities in Safeguarding Benefits - Lessons Learned from Past Biotechnology Governance

Moderator: Amina Ann Qutub, University of Texas, San Antonio

Goal: Highlight the ongoing challenge of balancing scientific openness with biosecurity concerns in biotechnology, illustrated by historical and current efforts by scientists, policymakers, and other stakeholders to navigate risks and opportunities in data sharing, model accessibility, and governance, and explore how safeguards can be effectively leveraged to promote responsible innovation without unnecessarily hindering scientific progress.

Speakers:

- **Diane DiEuliis**, National Defense University
- **Kenneth Oye,** Massachusetts Institute of Technology

Questions & Answers

12:40pm–1:25pm ET

Session 7: In Silico Modeling & AI Safety and Security – Lessons from Other Domains

Moderator: Richard Sever, Cold Spring Harbor Laboratory Press

Goal: Explore how in-silico modeling, foundation models, and principles and practices for generative AI safety have evolved to inform security and biosecurity efforts in other domains. The session will draw upon insights from various scientific domains and that guidelines, policies, norms, and best practices have been established to facilitate the dissemination of such information beyond DURC and PEPP.

Speakers:

- **Steinn Sigurðsson**, Pennsylvania State University
- **Sean Ekins**, Collaborations Pharmaceutical
- **Nandi Leslie**, RTX Corporation

1:25pm–2:45pm ET

Session 8: Policy Options and Norms for Responsible Dissemination - Interactive Cross-Sectoral and Transdisciplinary Solution-building Panel Discussions with Public Participation

Moderator: Sarah Carter, Science Policy Consulting LLC

Goal: During this **cross-sectoral panel discussion**, we aim to discuss strategies, best practices, policy options, and norms for safeguarding the benefits and advances of research while reducing the risks posed by funding and disseminating research information and resources involving dual-use research or research involving pathogens of pandemic potential. This session will build on Day 1.

After brief opening remarks from the panelists, the facilitators from the breakout rooms on Day 1 will briefly present a set of discussed complex barriers or challenges and their associated initial strategies to the panel.

The panel will have 10-15 minutes to debate and explore innovative, coordinated, and integrated strategies that align with the needs and capacity of all sectors represented.

In parallel, the audience can submit their ideas for strategies (not comments or challenges, nor questions) through an online platform if they are inspired while listening to the panel discussion. Other attendees are invited to upvote strategies they found particularly innovative and cross-cutting.

Panelists:

- **Jim Brase,** Lawrence Livermore National Laboratory
- **Jennifer Gibson,** Dryad
- **Michael Imperiale,** University of Michigan
- **Girish Patangay,** Chan Zuckerberg Initiative
- **Richard Sever,** Cold Spring Harbor Laboratory Press

2:45pm–2:55pm ET

Introduction Session 9: Promising Implementation Opportunities or Pitfalls of the Policies/Norms/Guidance/Strategies/Best Practices Proposed

Moderator: Héctor García Martín, Lawrence Berkeley National Laboratory

Goal: In breakout groups, discuss and refine collaboratively policy options, norms, guidance, strategies, and/or best practices for safeguarding the benefits and advances while reducing the risks posed by disseminating research information and resources.

2:55pm–3:10pm ET

Break – Move to breakout rooms

3:10pm–3:40pm ET

Session 9: Breakout Rooms - Promising Implementation Opportunities or Pitfalls of the Policies/Norms/Guidance/Strategies/Best Practices Proposed

During the breakout discussion, the groups will consider the landscape of dissemination outlets and the types of research outputs or resources disseminated (paper, code, dataset, weights, etc.).

Main Question: What approaches or strategies should be used to promote high-quality science, scientific progress, and the openness of science while mitigating

the biosecurity risks associated with disseminating in silico research in biological systems?

The groups will aim to:

- Highlight priority areas for guidance and policy development.
- Propose next steps for implementation and collaboration.
- Identify key stakeholders for follow-up actions or engagement.

3:50pm–4:15pm ET **Report out from each group**

4:15pm–4:30pm ET **Closing Remarks and Adjourn**

Alex John London, Carnegie Mellon University
Valda Vinson, Science

END OF DAY 2