Spatiotemporal Exposure and Toxicology {SET} Group

2024 Tenure Track Advisory Committee Meeting

Kyle P Messier, PhD

National Institute of Environmental Health Sciences - Division of Translational Toxicology - Predictive Toxicology Branch

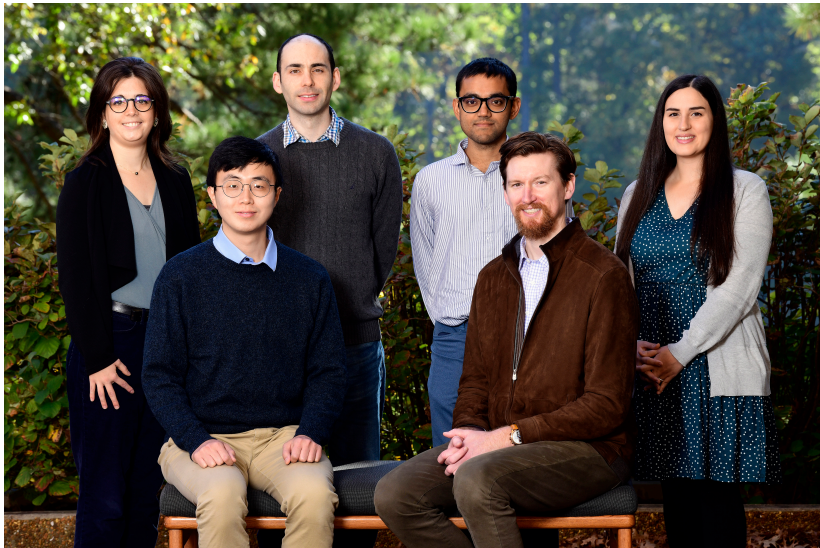**Spatiotemporal Exposures and Toxicology (SET) Group**

Contents I

Overview

About Us

Spatiotemporal Exposures and Toxicology {SET} group

- Geospatial Exposure Mapping: Spatiotemporal exposure mapping of environmental and climate variables (e.g. chemical mixtures, social, behaviorial, environmental, and climate factors)
- GeoTox: Otherwise known as **source to outcome continuum** modeling, GeoTox is the integration of geospatial exposures, toxicokinetic modeling, and non-animal toxicological data such as high-through *in vitro* screen assays to develop mechanistically-informed risk maps of chemical mixtures
- Software Development: Developing and promoting software and computational best-practices such as test driven development (TDD) and open-source code for the environmental health sciences

About Us

CHORDS Project

- I am a co-lead on the CHORDS project with Aubrey Miller, Charles Schmitt, and Trisha Castranio.
- David Reif, Alison Motsigner-Reif, David Fargo, among many others involved a regular contributors
- The project represents a major NIEHS initiative for climate change and health research that I am involved in. It has come with additional monies for postdocs and data analysts in my group
- It also comes with significant time commitments and responsibilities
- A lot of the CHORDS work/deliverables are folded into my group's work and manuscripts

Group Management

- In late 2023/ early 2024, with help from the new CHORDS funding, my group was poised to expand from 2 postdocs to 5 postdocs and a data analyst.
- I took 30 hours of project management courses to prepare
- I adopted software best practices as both a technique to help manage the group and to improve the quality of our software products, as well as increase software as a product of our research group
- Software best practices will help ensure that I have knowledge retention, reproducibility, and extensibility built into the core of my group
  - You'll see why this is important in the next few slides

Software and Computational Best Practices

- Test Driven Development
- Continuous Integration
- Build Checks
- Style/Linting
- Workflows/Pipelines

Group Personnel Updates

Daniel Zilber

- Postdoc with me ~2.5 years
- 1 first/last author publication (Zilber and Messier, 2024)
- 1 first/second author publication (me 2nd, Matt Wheeler last) in major revisions
- 1 last/second (me last, Daniel 2nd) in press
- Daniel is now a staff scientist with Shanshan Zhao as of July 7, 2024 (BCBB)
- Overall, Daniel has been an excellent postdoc and demonstrated how providing flexibility and intellectual freedom can lead to high-impact research

Ranadeep Daw

- Postdoc with me 1 year
- 0 publications or products. 1 manuscript in progress, but not holding my breath for seeing it completed
- Overall, disappointing, not meeting expectations, and negative attitude
- Complained about data set being too large for the proposed methodology, then complained about it being too small
- Nonetheless, a positive outcome as he accepted a position as a tenure-track assistant professor in Statistics at the University of West Florida

Insang Song

- Postdoc with me 1 year and as a contractor for 4 months before that
- 1st author publication in NIEHS internal review (`chopin` software manuscript).
- 1st author publication (`beethoven` group project) in preparation.
- 2nd author on `PrestoGP` manuscript in preparation
- **Recent Big News** He has been offered and accepted a tenure-track assistant professor position at Seoul National University (Top Public University in Korea- Top 30-50 Worldwide). It is a great opportunity for him for a highly competitive position. A bit bittersweet for me because he has been an amazing postdoc and extremely productive.
  - Start date is surprisingly soon, Sept 1 2024.

Eva Marques

- Postdoc with me 1 year
- Excellent group member and attitude
- Project on high-resolution heat exposure mapping is going well
    - 2 first author publications in progress. 1 first author publication in 2025 is realistic.

Mariana Alifa Kassien

- Postdoc with me 1 year
- Excellent group member and positive attiude
- Project goal is to develop a geospatial of $100+$ VOCs in air.
    - The methodology has changed from a physics-informed neural network to something more tractable that builds upon our previous spatial models and pipeline developments.
    - Additionally, we hope to integrate this into the **GeoTox** framework towards a geospatial mixtures risk assessment.
- Spends 10-20% of her time working with the CHORDS knowledge dissemination team and has some interest science communication and outreach.
- Was on maternity leave from Mar - May 2024.

Mitchell Manware

- With me 1 year as a fully-remote data analyst supported by the CHORDS project.
- Has been a great team member contributing to `amadeus` and `beethoven` software as well as leading the first-author for the `amadeus` manuscript (currently under internal NIEHS review).
- He is interested in doing a PhD with the goal of learning and developing ML/AI models for environmental exposure and risk assessment, but has a likely geographical constraint of New England. Will discuss the possibility of supporting a PhD at UNC ESE.

Postbac Outcomes

- **Taylor Potter**, BS, IRTA Postbac 2020-2022, now in MD program at Meherry Medical College

- **Melissa Lowe**, BS, MS, IRTA Postbac 2020-2022, 1st author publication, Biostatistician at Duke Cancer Center, Recently resigned to purse a JD and focus on environmental justice, I wrote her a recomomendation letter for law school.

Postdoc Outcomes

- **Dr. Kristin Eccles** - Research Scientist, Computational Toxicology Research group, Exposure and Biomonitoring Division, Health Canada

- **Dr. Ranadeep Daw** - Tenure Track Assistant Professor, Department of Mathematics and Statistics, University of West Florida

- **Dr. Daniel Zilber** - Staff Scientist, BCBB, NIEHS

- **Dr. Insang Song** - Tenure Track Assistant Professor, Seoul National University

Summer Intern Outcomes

- **Alvin Sheng**, PhD candidate, SIP 2021, NCSU Department of Statistics (Advisor: Brian Reich), Project manuscript is now in press in American Journal of Epidemiology, Included as 3rd chapter in dissertation.

- **Jennifer Kampe**, PhD candidate, SIP 2024, Duke Department of Statistics (Advisor: David Dunson), Project is on the development of a Bayesian latent variable model for chemical mixture prediction. She is hoping it can be incorporated into her dissertation.

Project Updates

PrestoGP

- `PrestoGP` and the application on US-wide groundwater pesticides is proceeding with steady progress. The publication is in preparation, but we are unlikely to get it done in 2024. Nonetheless, I am still excited at this development and the potential for a high-impact publication in late 2024 or 2025.

- Jump over to `PrestoGP` GitHub repo and website: https://niehs.github.io/PrestoGP/

beethoven SET Group Project

- Goal: Develop an air pollution model for the last 5 years that is updated bi-annually
- Entire SET group, Cavin Ward-Caviness, Lara Clark, Anisha Singh
- Test-Driven Development
- GitHub with strict rules
- Targets make-like pipeline
- Fine spatial and temporal resolution
- Post-processing for aggregated spatial and temporal resolutions