

WIP: PHYSICAL SENSING COUPLED WITH PHYSICS BASED MACHINE  
LEARNING

by

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WIP: PHYSICAL SENSING COUPLED WITH PHYSICS BASED MACHINE  
LEARNING

by

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DISSERTATION

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for the Degree of

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The University of Texas at Dallas, 2024

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Update required!

## TABLE OF CONTENTS

ACKNOWLEDGMENTS . . . . .	v
ABSTRACT . . . . .	vi
LIST OF FIGURES . . . . .	viii
LIST OF TABLES . . . . .	ix
CHAPTER 1 INTRODUCTION . . . . .	2
1.1 Goals of this Dissertation . . . . .	4
1.2 Global Change . . . . .	5
1.3 The Role of Sensing . . . . .	8
1.4 The Role of Computational Modelling . . . . .	10
1.5 Key Technologies . . . . .	11
1.5.1 Julia for Scientific Computing . . . . .	11
1.5.2 Scientific and Physics-based Machine Learning . . . . .	13
1.6 Machine Learning, Physics-Informed Machine Learning, Scientific Machine Learning . . . . .	15
1.6.1 overview of types of ML . . . . .	15
1.6.2 explain NN (i.e. neural network as a function + universal approximator) . . . . .	15
1.6.3 explain Physics Informed NN(s) . . . . .	15
1.6.4 explain SciML + UDE framework . . . . .	15
1.6.5 use RLC circuit instead of Spring mass to introduce the concept . . . . .	15
1.6.6 methods I've developed . . . . .	15
CHAPTER 2 PHYSICAL CONTEXT . . . . .	16
2.1 Pollution and Particulate Matter . . . . .	16
2.2 Optical Properties of Aqueous Solutions . . . . .	16
2.3 Chemical Reaction Kinetics . . . . .	16
2.4 Photolysis . . . . .	16
2.5 Indoor Air Quality . . . . .	16
2.6 Hyperspectral Imaging . . . . .	16

2.7	Remote Sensing . . . . .	16
2.8	Solar Geometry . . . . .	16
CHAPTER 3 PHYSICAL SENSING . . . . .		17
3.1	Low Cost Sensors for (Outdoor) Air Quality . . . . .	17
3.2	Sensing Chemical Concentration in Aqueous Environments . . . . .	17
3.3	Coordinated Robot Teams for Data Acquisition . . . . .	17
3.4	The HEART Chamber . . . . .	17
CHAPTER 4 COMPUTATIONAL TOOLS . . . . .		18
4.1	The Julia Programming Language . . . . .	18
4.2	Reproducible Research . . . . .	18
4.3	Eigen-stuff and the Singular Value Decomposition . . . . .	18
4.4	Optimization Methods . . . . .	19
4.5	High Performance Computing . . . . .	19
CHAPTER 5 THEORETICAL TOOLS . . . . .		20
5.1	Automatic Differentiation . . . . .	20
5.2	Dual Numbers . . . . .	20
5.3	Embedding Theorems . . . . .	20
5.4	Koopman Operator Theory . . . . .	20
5.5	Elements of Bayesian Statistics . . . . .	20
5.6	Maximum Likelihood Estimation . . . . .	21
5.7	KL Divergence . . . . .	21
5.8	A Survey of Relevant Mathematical Structures . . . . .	21
5.9	Uncertainty Propagation . . . . .	21
5.10	Kernelization . . . . .	21
5.11	Dynamical Systems . . . . .	21
CHAPTER 6 MACHINE LEARNING AND DATA-DRIVEN METHODS . . . . .		22
6.1	Data Sampling . . . . .	23
6.2	Neural Networks . . . . .	23
6.3	Decision Trees . . . . .	23



6.4	Gaussian Process Regression . . . . .	23
6.5	Model Ensembling . . . . .	23
6.6	Super Learners . . . . .	23
6.7	Self Organizing Maps . . . . .	24
6.8	Generative Topographic Maps . . . . .	24
6.9	Data Assimilation . . . . .	24
6.10	Conformal Prediction . . . . .	24
6.11	Generative Methods . . . . .	25
6.12	Topological Data Analysis . . . . .	25
6.13	Auto Encoders . . . . .	25
6.14	Physics Informed Neural Networks . . . . .	25
6.15	Universal Differential Equations . . . . .	25
CHAPTER 7 ROBOT TEAM . . . . .		26
7.1	Georectification . . . . .	26
7.2	georectification . . . . .	26
7.3	supervised ML for concentration . . . . .	26
7.4	super resolution if we have time (and open data cube) . . . . .	26
7.5	solar geometry . . . . .	26
7.6	reflectance/radiance . . . . .	26
7.7	unsupervised methods . . . . .	26
7.8	synthetic data generation . . . . .	26
7.9	RobotTeam Papers . . . . .	26
7.9.1	Robot Team II: Electric Boogaloo (title w.i.p.) . . . . .	26
7.9.2	Unsupervised Classification of Hyperspectral Imagery for Rapid Characterization of Novel Environments with Autonomous Robotic Teams . . . . .	27
7.9.3	Spectral Indices for Rapid HSI Surveys: Unsupervised and Supervised Methods via SciML . . . . .	28
7.9.4	Synthetic Data Generation for Hyperspectral Imaging with Autonomous Robotic Teams . . . . .	29
7.9.5	Uncertainty Quantification via $\partial P$ . . . . .	29

7.10	Supervised Methods . . . . .	30
7.11	Unsupervised Methods . . . . .	30
CHAPTER 8	SUPER RESOLUTION . . . . .	31
8.1	Cloud & Shadow Mask for Sentinel-2 . . . . .	31
8.1.1	ML Type . . . . .	31
8.1.2	ML Methods . . . . .	31
8.1.3	Features . . . . .	31
8.1.4	Targets . . . . .	31
8.2	Cloud & Shadow Fill . . . . .	31
8.2.1	ML Type . . . . .	31
8.2.2	ML Methods . . . . .	32
8.2.3	Features . . . . .	32
8.2.4	Targets . . . . .	32
8.3	Sentinel 2 RGB <i>Spatial</i> Super Resolution . . . . .	32
8.3.1	ML Type . . . . .	32
8.3.2	ML Methods . . . . .	32
8.3.3	Features . . . . .	33
8.3.4	Targets . . . . .	33
8.3.5	Loss Function Terms . . . . .	33
8.3.6	Notes . . . . .	33
8.4	Sentinel 2 Multiband <i>Spatial</i> Super Resolution . . . . .	34
8.4.1	ML Type . . . . .	34
8.4.2	ML Methods . . . . .	34
8.4.3	Features . . . . .	34
8.4.4	Targets . . . . .	34
8.4.5	Loss Function Terms . . . . .	34
8.5	Sentinel 2 Multiband <i>Spectral</i> Super Resolution . . . . .	34
8.5.1	ML Type . . . . .	34
8.5.2	ML Methods . . . . .	35

8.5.3	Features	35
8.5.4	Targets	35
8.5.5	Loss Function Terms	35
CHAPTER 9 CHEMICAL DATA ASSIMILATION		36
9.1	Photolysis	36
9.2	HEART Chamber	36
CHAPTER 10 MASTER CHEMICAL MECHANISM		37
10.1	sensor fusion	37
10.2	photolysis	37
10.3	docker ingestion framework	37
10.4	master chemical mechanism	37
10.5	data assimilation	37
10.6	Chemical Data Assimilation & ActivePure Work	37
10.6.1	ActivePure Research Lab	37
10.6.2	Kinetics and Chemical Data Assimilation	38
10.7	CRI Mechanism	38
10.8	AutoChem	38
10.9	Ion Chemistry	38
10.10	Evaluation Indoor Air Quality via Chemical Data Assimilation	38
10.11	Photocatalytic Ionization	38
CHAPTER 11 TIME SERIES METHODS		39
11.1	Uncertainty Estimation Via Time Series Sampling	40
11.1.1	Types Of Uncertainty	40
11.1.2	Instrument Uncertainty	40
11.1.3	Representativeness Uncertainty	40
11.1.4	Variograms	40
11.1.5	Mutual Information	40
11.1.6	Auto-correlation	40
11.2	Time Series Chaos	40

11.2.1	What is Chaos?	40
11.2.2	Lyapunov Exponents	40
11.2.3	Fractal Dimension	40
11.3	Koopman Operator Theory	40
11.4	Time Series Modeling Methods	40
11.4.1	Token-Hankel Delay Embeddings	40
11.4.2	Embedding Theorems (are magic)	40
11.4.3	Determination of Optimal Lag	40
11.4.4	Determination of Intrinsic Dimension (kind of unnecessary given <i>large enough</i> embedding)	40
11.4.5	DMD and HAVOK	40
11.4.6	Hamiltonian Neural Networks	40
11.5	Time Series Classification	40
11.5.1	Considerations for Batching of Time Series for ML Models	40
11.5.2	K-means Clustering	40
11.5.3	Self Organizing Maps	40
11.5.4	Generative Topographic Maps	40
11.5.5	Chaos Classification via HAVOK	40
11.5.6	Symplectic and Normal Gradients for HNN	40
11.6	Motivating Example: Lorenz63 System	40
11.6.1	Origin of Lorenz System	40
11.6.2	Time Scale Analysis and Variography	40
11.6.3	Embedding	40
11.6.4	Modeling	40
11.6.5	Classification	40
11.7	Real Example 1: PM Data	40
11.7.1	Origin of Lorenz System	40
11.7.2	Time Scale Analysis and Variography	40
11.7.3	Embedding	40

11.7.4	Modeling	40
11.7.5	Classification	40
11.8	Real Example 2: Biometric Data	40
11.8.1	Origin of Lorenz System	40
11.8.2	Time Scale Analysis and Variography	40
11.8.3	Embedding	40
11.8.4	Modeling	40
11.8.5	Classification	40
11.9	Real Example 3: Stock Market Analysis	40
11.9.1	Origin of Lorenz System	40
11.9.2	Time Scale Analysis and Variography	40
11.9.3	Embedding	40
11.9.4	Modeling	40
11.9.5	Classification	40
11.10	LoRa wan devices	40
11.11	Docker, NodeRed, InfluxDB, Grafana	40
11.12	Hamiltonian NN stuff	40
11.13	neural ode	40
11.14	TDA	40
11.15	Sensor Network + SciML	41
11.15.1	Evaluation of local chaos in SharedAirDFWNetwork	41
CHAPTER 12	DISCUSSION	43
12.1	Limitations	43
12.2	Future Work	43
CHAPTER 13	CONCLUSIONS	44
CHAPTER 14	TECHNICAL NOTES	45
14.1	Real Time Georectification of Drone Based Imagery	45
14.2	Self Organizing Maps	45
14.3	Bayesian Optimization with Gaussian Process Regression	45

14.4 Gaussian Process Regression / Classification in MLJ . . . . .	45
CHAPTER 15 OTHER TOPICS . . . . .	46
REFERENCES . . . . .	47
References . . . . .	47
Appendices . . . . .	54
APPENDIX A ADDITIONAL STUFF . . . . .	54
APPENDIX B EEG BAND DISCOVERY WITH DECISION TREES . . . . .	55
BIOGRAPHICAL SKETCH . . . . .	56
CURRICULUM VITAE	

## LIST OF FIGURES

## LIST OF TABLES



## TABLE OF CONTENTS

# CHAPTER 1

## INTRODUCTION

*NOTE:* For the proposal in particular, we should add a new section with timelines and a table of currently completed tasks.

*NOTE:* We want to emphasize the need for reproducible research paradigms. This motivates

*NOTE:* for the area of uncertainty quantification via statistical machine learning methods we should emphasize the fact that uncertainty is challenging to quantify in physical systems but in the age of big data, we need not really on the assumption of conveniently shaped normal distributions— we can do better. Instead, we let the data be our guide, deriving improved uncertainty bounds (in the statistical sense) with methods to track key diagnostic characteristics such as the relevant time scale. Further, in the domain of low-cost sensing, a key challenge is accurately quantifying uncertainty bounds for measurements as manufacturer provided estimates are almost always overly conservative (to minimize responsibility for variance, perhaps?)

*NOTE:* We should also mention (in our goals for the dissertation) that reproducibility is of critical importance (in physics, in machine learning, in scientific code, in analysis, etc...) with relevant statistics quoted (perhaps that nice interview from )

*NOTE:* explain Dr. Lary’s principle of “Do the obvious thing: ask the obvious question, run the obvious experiment, perform the obvious analysis” as a guiding principle for the logical organization of this dissertation.

The goal of this thesis is advancing physical sensing in service of society to provide actionable insights. This goal is pursued by applying physics informed approaches together with a suite of sensing and computational technologies, implementing the reusable paradigm of software

defined sensors, i.e. physical sensing elements wrapped in a software layer. This software layer can serve a variety of purposes such as calibration and the provision of enhanced or derived data products. It is part of a broader effort in the MINTS-AI laboratory at the University of Texas at Dallas. Where MINTS-AI is an acronym, **M**ulti-**S**cale **M**ulti-**U**se **I**ntegrated **I**ntelligent **I**nteractive **S**ensing in **S**ervice of **S**ociety for **A**ctionable **I**nsights.

Comprehensive environmental sensing is a timely and beneficial endeavor for a variety of reasons. The growing awareness of major environmental issues such as climate change, pollution, and habitat loss necessitates effective environmental monitoring and management. Comprehensive environmental sensing can provide real-time data on air and water quality, weather patterns, and other environmental factors, assisting in the identification and resolution of environmental issues. This assists in the development and implementation of policies and strategies aimed at reducing environmental impact and increasing sustainability. Given that, for instance, air quality can have significant effects on human health, this has particular societal value.

Exposure to air pollution has been linked to a wide range of health effects (Brook et al. 2010; Kelly and Fussell 2011; Xu et al. 2017), including respiratory and cardiovascular diseases, cancer, and adverse birth outcomes. Further, physical sensing provides valuable data and the basis for international assessments such as the Intergovernmental Panel on Climate Change (IPCC), which seeks to assess the science related to climate change and its impacts on natural and human systems (Houghton, Jenkins, and Ephraums 1990; Houghton et al. 1996, 2001; Solomon et al. 2007; Parry et al. 2007; Metz et al. 2007; Stocker et al. 2013; Field et al. 2014; Edenhofer et al. 2014; Masson-Delmotte et al. 2018; Friedlingstein et al. 2020; Huang et al. 2017).

Comprehensive sensing of the environment can improve decision-making. The real-time and accurate data provided by environmental sensors can aid in informed decision-making regard-

ing various aspects such as traffic management, industrial regulation, and crop planning. For instance, data on air quality can be used to inform decisions about reducing pollution levels, while data on weather patterns can help farmers to plan their crops and reduce water usage. Comprehensive sensing of the environment can be instrumental in emergency response. Real-time data on weather patterns, air quality, water levels and resources, and seismic activity can help emergency responders to prepare for and respond to natural disasters such as hurricanes, floods, and earthquakes. The quick and accurate information can enable effective and timely response, potentially saving lives and reducing the impact of the disaster.

Many advances in technology have enabled the creation of comprehensive sensing systems that can monitor and analyze data from various sensors and devices in real-time. In this thesis we use a range of technologies including autonomous robotic teams (Dunbabin and Marques 2012; Rubenstein, Cornejo, and Nagpal 2014; Y. Chen et al. 2017), hyperspectral imaging (Plaza et al. 2009; Li et al. 2018; Zhu et al. 2017), mesh networks utilizing the Internet of Things (IoT) (Gubbi et al. 2013; Atzori, Iera, and Morabito 2010; Al-Fuqaha et al. 2015), machine learning (ML) (Goodfellow, Bengio, and Courville 2016; LeCun, Bengio, and Hinton 2015; Jordan and Mitchell 2015), edge computing, high-performance computing, wearable sensors and modern high-performance dynamic programming languages such as Julia (Bezanson et al. 2017) designed for numerical and scientific computing. These technologies have facilitated the collection and processing of large amounts of data from multiple sources, resulting in more accurate and comprehensive environmental monitoring.

## **1.1 Goals of this Dissertation**

Test text

## 1.2 Global Change

Global change refers to the significant and long-term alterations in the Earth's physical, chemical, and biological systems, resulting from natural and human-induced processes (Edenhofer et al. 2014; Masson-Delmotte et al. 2018; United Nations 2015). This includes changes in the climate, land use, biodiversity, and biogeochemical cycles, as well as interactions among these systems. Global change can have profound impacts on natural and human systems, including altered weather patterns, sea level rise, increased frequency and severity of extreme events, loss of biodiversity and ecosystem services, and effects on human health and well-being. Understanding and managing global change is a critical challenge facing society today, requiring interdisciplinary approaches and collaboration across sectors and regions.

Global change can have a range of impacts on society, including environmental, social, and economic effects. Some of the aspects of global change that have the biggest impact on society include:

- **Climate Change:** Climate change, driven by human activities such as burning fossil fuels, deforestation, and land-use changes, has impacts on natural systems such as ocean acidification, sea level rise, and changes in precipitation patterns. These impacts can have cascading effects on human systems, including impacts on food security, water availability, and health.
- **Biodiversity Loss:** Global change can lead to the loss of biodiversity, which can have impacts on ecosystem functioning and services, such as pollination, pest control, and carbon storage. These impacts can have indirect effects on human well-being, including impacts on food security, health, and cultural heritage.
- **Land Use Change:** Land use change, such as deforestation, urbanization, and agriculture, can have impacts on natural systems such as soil quality, water availability, and

biodiversity. These impacts can have direct and indirect effects on human systems, including impacts on food security, water availability, and cultural heritage.

- **Economic and Social Inequality:** Global change can exacerbate economic and social inequality, with impacts on access to resources, health, and well-being. These impacts can have cascading effects on the ability of societies to adapt and respond to global change.
- **Human Health:** Global change can have significant impacts on human health (World Health Organization 2018; Costello et al. 2009; Haines et al. 2006), both directly and indirectly, for example:
  - **Heat-related Illness:** As temperatures increase due to global warming, there is an increased risk of heat-related illness, including heat exhaustion and heat stroke, particularly in vulnerable populations such as the elderly, young children, and outdoor workers.
  - **Air Pollution:** Global change can lead to increased air pollution, including from sources such as wildfires and fossil fuel combustion. Exposure to air pollution can increase the risk of respiratory and cardiovascular diseases, including asthma, chronic obstructive pulmonary disease (COPD), and heart disease.
  - **Vector-borne Diseases:** Changes in temperature and precipitation patterns can affect the distribution and abundance of disease vectors such as mosquitoes and ticks, leading to increased risks of vector-borne diseases such as dengue fever, malaria, and Lyme disease.
  - **Waterborne Diseases:** Changes in precipitation patterns and water quality can increase the risk of waterborne diseases, including cholera and other diarrheal diseases.

- Food Security: Global change can affect food production and availability, leading to food shortages and malnutrition, particularly in vulnerable populations such as children and pregnant women.

Effectively addressing these aspects of global change requires interdisciplinary approaches and collaboration across sectors and regions, as well as a commitment to sustainable development and equitable solutions. Adaptation and mitigation are two strategies for addressing global change, which differ in their focus and approach.

Adaptation involves taking measures to adjust and respond to the impacts of global change that are already occurring or are expected to occur in the future. This can include actions such as building sea walls to protect against sea level rise, developing drought-resistant crops, and improving public health infrastructure to address the increased risk of vector-borne diseases. Adaptation strategies aim to reduce the vulnerability of human and natural systems to the impacts of global change and increase their resilience.

Mitigation involves taking measures to reduce the drivers of global change, such as greenhouse gas emissions, land use change, and deforestation. This can include actions such as increasing energy efficiency, shifting to renewable energy sources, and reducing waste and consumption. Mitigation strategies aim to address the root causes of global change and reduce its severity and impact.

Both adaptation and mitigation are important strategies for addressing global change, but they differ in their focus and approach. Adaptation strategies focus on responding to the impacts of global change that are already occurring or are expected to occur in the future, while mitigation strategies focus on reducing the drivers of global change and preventing its impacts from occurring in the first place. A comprehensive approach to global change will require both adaptation and mitigation strategies, as well as efforts to promote sustainable development and equitable solutions.

### 1.3 The Role of Sensing

Sensing technologies can play a critical role in both adaptation and mitigation efforts by providing data and information that can inform decision-making and improve the effectiveness of strategies (United Nations Environment Programme 2017; National Research Council 2010; Centre for Ecology and Hydrology 2017).

In adaptation efforts, sensing technologies can provide real-time data on environmental conditions such as temperature, precipitation, sea level, air quality, as well as on the status and health of ecosystems and wildlife. This information can be used to inform early warning systems for natural disasters, to track the spread of vector-borne diseases, and to monitor the impacts of climate change on biodiversity and ecosystem services. Sensing technologies can also provide data on the effectiveness of adaptation measures, such as the performance of sea walls and other infrastructure.

In mitigation efforts, sensing technologies can provide data on greenhouse gas emissions and other drivers of global change, as well as on the effectiveness of mitigation measures such as renewable energy and carbon capture and storage. Sensing technologies can also be used to monitor and manage land use changes such as deforestation and urbanization, and to track the impacts of these changes on ecosystems and carbon storage.

Overall, sensing technologies can provide critical data and information for both adaptation and mitigation efforts, helping to improve decision-making and increase the effectiveness of strategies. The integration of sensing technologies with other tools such as modeling and data analysis can also help to identify new strategies and solutions for addressing global change. There are various sensing technologies and approaches used for monitoring the global environment. Here are some of the key ones:



- Remote Sensing: This technology involves using satellites and other airborne platforms to collect data on the Earth’s atmosphere, land, and oceans. Remote sensing provides information on environmental parameters such as temperature, humidity, air quality, land use and land cover, and ocean temperature, salinity, and sea level (Thenkabail 2019; Buyantuyev and Wu 2017; Gamon et al. 2016; Wang et al. 2017; Pasher et al. 2019). Some examples of remote sensing include:
  - Lidar: This technology uses laser pulses to measure distance and can be used to create detailed three-dimensional maps of the environment. Lidar is commonly used to measure forest canopy height, but can also be used to measure atmospheric conditions such as cloud cover and aerosol concentrations.
  - Imaging Spectroscopy: This technology uses a combination of imaging and spectroscopy to measure the reflectance of different wavelengths of light. Imaging spectroscopy can be used to identify and map different types of vegetation and minerals, and can provide information on the health of plant communities.
  - Unmanned Aerial Vehicles (UAVs): These are remote-controlled or autonomous aircraft that can be equipped with sensors for remote and in-situ environmental monitoring. UAVs can be used for mapping and monitoring of large areas, and can collect high-resolution data on environmental conditions.
- In-Situ Sensors: These sensors are used to collect data directly from the environment at the location of interest. They can measure environmental parameters such as temperature, pressure, and humidity, as well as water quality and soil moisture. In situ sensors are commonly used in marine environments to measure ocean temperature, salinity, and other properties. Some examples of in-situ sensing include:
  - Weather Stations: These are automated weather monitoring systems that collect data on atmospheric conditions such as temperature, humidity, barometric

pressure, wind speed and direction, and precipitation. Weather stations can be installed on land or in the ocean to provide continuous monitoring of environmental conditions.

- Ground-Based Sensors: These sensors are used to monitor the quality of air, water, and soil. They can detect and measure pollutants such as carbon dioxide, nitrogen dioxide, ozone, sulfur dioxide, and particulate matter. Ground-based sensors are installed in various locations such as cities, industrial sites, and rural areas to provide localized environmental monitoring.
- Acoustic Sensors: These sensors are used to monitor environmental noise levels, including noise from traffic, industrial sources, and natural sources such as wind and waves. Acoustic sensors can provide information on noise levels over time and across different locations.

Overall, these sensing technologies play a critical role in monitoring the global environment and can provide valuable information for environmental research, management, and policy-making.

## **1.4 The Role of Computational Modelling**

Computer modeling can play a valuable role in both understanding and predicting global change (J. Chen et al. 2019; Hantson et al. 2016; DeLucia et al. 2021; Oleson et al. 2013; Clark et al. 2016). For example:

- Climate Modeling: Computer models can be used to simulate the Earth’s climate system and predict future climate conditions. These models can incorporate data on greenhouse gas emissions, land use changes, and other factors to project how the Earth’s climate will change over time.

- **Ecosystem Modeling:** Computer models can be used to simulate how ecosystems will respond to changes in environmental conditions, such as changes in temperature, precipitation, and atmospheric composition. These models can help predict how changes in ecosystems will impact biodiversity, ecosystem services, and human well-being.
- **Carbon Cycle Modeling:** Computer models can be used to simulate the global carbon cycle, which is the exchange of carbon between the Earth's atmosphere, land, and oceans. These models can help predict how changes in carbon emissions and land use will impact atmospheric carbon dioxide concentrations and global climate.
- **Air Quality Modeling:** Computer models can be used to simulate air quality, including the dispersion of pollutants in the atmosphere. These models can help predict how changes in emissions and atmospheric conditions will impact air quality and human health.
- **Hydrological Modeling:** Computer models can be used to simulate the movement of water through the Earth's hydrological cycle. These models can help predict how changes in precipitation, land use, and other factors will impact water availability, quality, and distribution.

Overall, computer modeling can provide valuable insights into the complex processes and interactions that drive global change. These insights can inform policy decisions and help guide efforts to mitigate and adapt to the impacts of global change.

## **1.5 Key Technologies**

### **1.5.1 Julia for Scientific Computing**

Julia is designed to combine the ease of use and high-level abstractions of languages like Python with the performance of compiled languages like C++, achieving a unique combination of speed and productivity for numerical and scientific computing. Julia is a high-level,

high-performance programming language designed for numerical and scientific computing. It combines the ease of use and readability of Python with the speed and efficiency of Fortran or C. Julia has a wide array of scientific computing functionality, making it a powerful language for numerical analysis, data science, and engineering. It has built-in support for arrays and linear algebra, as well as packages for differential equations, optimization, probabilistic programming, data analysis and visualization, parallel and distributed computing, and machine learning. Julia's combination of performance, expressiveness, and flexibility make it an excellent choice for scientific and engineering applications, allowing for high-level abstractions and rapid prototyping, while still providing low-level control and efficient execution.

Here are some examples of what can be done easily in Julia that may not be as easy or efficient in other widely used scientific computing languages such as Python or Fortran:

- Multiple dispatch: Julia has a powerful multiple dispatch system that allows for generic programming and efficient function overloading. This allows for more flexible and expressive code compared to traditional object-oriented programming (OOP) in Python. Multiple dispatch allows a function to behave differently based on the types and/or number of arguments passed to it. In other words, the behavior of a function can be 'dispatched' based on the specific types and/or number of arguments passed to it.
- Just-in-time (JIT) compilation: Julia's JIT compiler translates high-level Julia code into optimized machine code, making Julia programs run nearly as fast as C or Fortran. In contrast, Python code is interpreted, and Fortran requires pre-compilation.
- Distributed computing: Julia has built-in support for distributed computing, making it easy to parallelize and scale up computations across multiple processors or machines. This is not as easy to do in Python or Fortran.
- Units and Error Propagation: The Units package in Julia provides a powerful and flexible framework for handling physical units in computations, useful for error propagation

and dimensional analysis, helping to ensure that the results are accurate, consistent, easy to interpret, and dimensionally consistent.

- Built-in unit testing: Julia has a built-in testing framework that makes it easy to write and run unit tests for your code, ensuring that it works correctly.
- ISO characters: Julia supports the use of Greek and other ISO characters in variable and function names, which can make code more readable and expressive, especially in mathematical or scientific contexts.
- Interactive data visualization: Julia has a number of powerful data visualization packages, such as Plots.jl and Makie.jl, that allow for interactive, high-performance data visualization.
- Package management: Julia has a sophisticated package manager that makes it easy to install, manage, and use third-party packages in your code. This is not as easy to do in Fortran, and while Python has a package manager, Julia’s package manager is faster and more reliable.
- Inline C/Fortran/Python/R/Matlab code: Julia allows for inline C, Fortran, Python, R or Matlab code, making it easy to use existing libraries and code written in these languages without having to rewrite everything in Julia.

### 1.5.2 Scientific and Physics-based Machine Learning

Scientific machine learning (SciML) refers to the application of Machine Learning (ML) techniques to scientific problems, where the goal is not only to make predictions but also to gain insights into the underlying physical processes (Raissi, Perdikaris, and Karniadakis 2019; Rackauckas et al. 2020; Carleo et al. 2019). SciML involves the integration of domain-specific knowledge and physical models with data-driven techniques, and it has the potential to revolutionize many areas of science and engineering. In this thesis we explore the use of Physics-based machine learning (PBML) (Raissi and Karniadakis 2021; Wu and Zhang 2021) for a variety of applications.

Recent examples include a paper by (Raissi, Perdikaris, and Karniadakis 2019) that introduces a physics-informed neural network (PINN) framework for solving nonlinear partial differential equations, a paper by (Rackauckas et al. 2020) that proposes a universal differential equation (UDE) approach to scientific machine learning, and a review article by (Carleo et al. 2019) that discusses the use of machine learning in various fields of physics, including condensed matter physics, high-energy physics, and quantum physics. PBML has several advantages over purely data-driven approaches, including:

- Improved generalization: PBML models incorporate prior knowledge of the underlying physics, resulting in models that are more interpretable and generalizable. This enables the models to make accurate predictions even with limited training data.
- Incorporation of physical constraints: PBML models can be designed to incorporate physical constraints, such as conservation laws, which can help to ensure physically consistent predictions.
- Improved interpretability: PBML models are more interpretable than purely data-driven models since they are designed to incorporate physical principles. This can enable scientists and engineers to gain deeper insights into the underlying mechanisms of the systems they are studying.
- Reduced data requirements: PBML models require less training data than purely data-driven models since they leverage the physics-based priors, reducing the need for large datasets to train accurate models.
- Better extrapolation: PBML models are better equipped to extrapolate beyond the training data since they incorporate knowledge of the underlying physics, enabling them to make more accurate predictions in new and unseen scenarios.

Overall, PBML has several advantages over purely data-driven approaches, including improved generalization, reduced data requirements, better extrapolation, incorporation of

physical constraints, and improved interpretability, making it a valuable tool for scientific and engineering applications.

## **1.6 Machine Learning, Physics-Informed Machine Learning, Scientific Machine Learning**

### **1.6.1 overview of types of ML**

### **1.6.2 explain NN (i.e. neural network as a function + universal approximator)**

### **1.6.3 explain Physics Informed NN(s)**

### **1.6.4 explain SciML + UDE framework**

### **1.6.5 use RLC circuit instead of Spring mass to introduce the concept**

### **1.6.6 methods I've developed**

- Ensembling and Super Learners
- Self Organizing Maps
- Generative Topographic Mapping

NOTE: perhaps add section on increasing concerns about indoor air quality (use EPA RFI document). I think ideally we should break down the introduction by sensing domain

## CHAPTER 2

### PHYSICAL CONTEXT

test text

#### 2.1 Pollution and Particulate Matter

#### 2.2 Optical Properties of Aqueous Solutions

#### 2.3 Chemical Reaction Kinetics

#### 2.4 Photolysis

#### 2.5 Indoor Air Quality

#### 2.6 Hyperspectral Imaging

#### 2.7 Remote Sensing

mention different types of satellite data platforms (mostly optical), differences in orbits, coverage, etc... Also good to discuss the increasing use of drones for a variety of applications including intelligent agriculture, geophysics, mapping, etc...

#### 2.8 Solar Geometry

An explanation of relevant solar angles as well as their determination (i.e. the code I ported to Julia from Matlab script Dr. Lary supplied). We should also comment on the importance of



## **CHAPTER 3**

### **PHYSICAL SENSING**

#### **3.1 Low Cost Sensors for (Outdoor) Air Quality**

The outdoor part here is optional. Here I seek to provide specific details of the classes of low cost sensors used for PM (optical particle counters based on Mie scattering), thermistors (for tempature), humidity sensors, pressure sensors, gas sensors, etc... This can be a rough outline for those that specifically are used in my research projects.

#### **3.2 Sensing Chemical Concentration in Aqueous Environments**

Here we can give an overview of the sensors utilized on the boat for the robot team studies... We should include any information about the uncertainties. We can also comment on their use in fresh v.s. salt water environments.

#### **3.3 Coordinated Robot Teams for Data Acquisition**

Here we can discuss the drone, boat, and walking robot as well as long range communication setup with wifi router, transferring of files, MQTT protocol, and real time mapping with Grafana.

#### **3.4 The HEART Chamber**

For specifics of sensing equipment, see EPA RFI we did for Mr. Urso

## CHAPTER 4

### COMPUTATIONAL TOOLS

#### 4.1 The Julia Programming Language

Overview of key features of Julia that made it attractive for this work:

- reproducibility
- composability
- readability (greek symbols as variables and operators)
- speed

#### 4.2 Reproducible Research

*principles & implementation:* version control, CI-CD, test-driven-development, containerization

We should also discuss how *this dissertation is built* using quarto and github workflows. Similarly, we can discuss the process of building quarto templates via pandocs to target specific journals as well as pdf, web, and slides formats.

#### 4.3 Eigen-stuff and the Singular Value Decomposition

Begin with a general description of the utility of eigen-stuff type analysis. Then explain how the SVD is the natural extension of this to non-square systems (rectangular matrices). Further expand by illustrating the application to principal component analysis. Make sure to comment on the general utility of decomposing a function/vector/signal into a (infinite) linear combination of (stationary) modes with simple time evolution.

#### 4.4 Optimization Methods

Describe standard gradient descent and its utility for machine learning. Expand to briefly describe the extensions used in our work:

- ADAM
- BFGS
- LBFGS

#### 4.5 High Performance Computing

Provide an overview of relevant concepts in high performance computing i.e.

- slurm
- multi-threading
- parallelization (distributed computing)
- Memory management (i.e. preallocating data containers and writing functions that mutate, not allocate)

## CHAPTER 5

### THEORETICAL TOOLS

#### 5.1 Automatic Differentiation

perhaps this can be moved to the **Computational tools** section instead.

Use Chris Rackauckas and Chris Olah blogs to start with chain rule and justify automatic differentiation. Then describe reverse mode via gradient tapes and the pullback operator.

#### 5.2 Dual Numbers

Describe dual numbers because they are cool (and by extension, forward mode AD)

#### 5.3 Embedding Theorems

Discuss Taken's embedding theorem and other relevant information for the time-series work.

#### 5.4 Koopman Operator Theory

Give an overview of continuous and discrete Koopman operator theory.

#### 5.5 Elements of Bayesian Statistics

Derive Baye's rule and other important concepts

## 5.6 Maximum Likelihood Estimation

## 5.7 KL Divergence

## 5.8 A Survey of Relevant Mathematical Structures

generic overview of role of mathematical structures in physics and machine learning

## 5.9 Uncertainty Propagation

Linear v.s. Nonlinear Techniques, measurements.jl

## 5.10 Kernelization

## 5.11 Dynamical Systems

can quote paper on origins of term *phase space*

## CHAPTER 6

### MACHINE LEARNING AND DATA-DRIVEN METHODS

NOTE: Good way to start is with the question: What is a model? We can discuss the differences between mechanistic models (i.e. physics equations), their free parameters (constants of nature) and other types of models such as the non-parametric, nonlinear models used in machine learning. Further, we can discuss how machine learning models often display have the desirable trait of being a *universal approximator*. This will naturally lead to a discussion of function expansions (Taylor, Fourier, other polynomial expansions, etc...) and how they scale poorly (exponential) with increasing dimension. Machine learning models essentially allow us to do the same thing: perform a function expansion given data but in a way that can scale well to arbitrary dimension (features) of data. This allows us to build predictive models without necessarily needing to prescribe *all* of the physics. From another perspective, this framework allows us to incorporate our physics knowledge from well-behaved or linearized domains in order to *fit the residual* behavior with a sophisticated data-driven approach.

discuss role in science in particular (i.e. calibration, modeling, etc...)

discuss pushback against use in science and need for methods which simultaneously provide uncertainty bounds. Also describe types of ML e.g. supervised, unsupervised, generative, etc...

this is a good place for the Chihuahua vs Muffin meme... and use this to motivate incorporating physical knowledge into the machine learning process as a key feature for scientific applications... we have more constraints!

also discuss statistical v.s. deep learning

## **6.1 Data Sampling**

cross-validation techniques

Dr. Lary's method (from Gaussian Process Code) for representative sampling to reduce data size

## **6.2 Neural Networks**

From a perspective of basic function composition... as in Rackauckas's blog

## **6.3 Decision Trees**

## **6.4 Gaussian Process Regression**

## **6.5 Model Ensembling**

Boosting vs Bagging

XGBoost vs RandomForest (and other implementations)

MLJ and SciKitLearn documentation sites will have good references for this, I think.

## **6.6 Super Learners**

Use the example of model stacking from MLJ documentation to describe our approach.

## 6.7 Self Organizing Maps

## 6.8 Generative Topographic Maps

## 6.9 Data Assimilation

## 6.10 Conformal Prediction

The focus of this section can be on the concept of uncertainty quantification. For many physics theories that are nicely linearized, uncertainty analysis can be easily accomplished at the level of first order sensitivities. That is, we can look at the Jacobian of our model to infer the behavior of small deviations about initial conditions. This approach does not easily extend to more complicated domains where the nonlinear effects dominate. Further, we also often want to establish ways to think about the fundamental instrument uncertainty for a measuring device. This can require meticulous calibrations which often assume a linear or polynomial fit... We can do better. Why not let the data tell us what the measurement uncertainty really is?

A good motivating example for the discussion of instrumental uncertainty is the use of a thermistor to measure temperature. One must assume a reasonable range of temperatures to establish the linear relationship between temperature and resistivity that is used to determine the temperature. However, the material characteristics of the thermistor that introduce nonlinearities at extreme temperatures don't necessarily mean we should have to throw out measurements that do not fall within this well-behaved range. Rather, we can perform a more sophisticated *calibration* to learn a model mapping resistivity to temperature that can account for these effects.

This is the bread-and-butter of the MINTS sensing efforts. Often low-cost sensing solutions provide decent measurements within a limited domain. With quality data from superior (but



often prohibitively expensive) reference instruments, we can improve the default calibration to improve the reliability of data (by reducing uncertainty) and extend it's domain of usefulness.

### **6.11 Generative Methods**

### **6.12 Topological Data Analysis**

### **6.13 Auto Encoders**

This is a good place to talk about dimensionality reduction in general, e.g. PCA and other linear methods...

### **6.14 Physics Informed Neural Networks**

### **6.15 Universal Differential Equations**

It may also be nice to add a section on model evaluation criteria. Similarly, we can have a section on *Feature selection and dimensionality reduction*

## CHAPTER 7

### ROBOT TEAM

#### 7.1 Georectification

#### 7.2 georectification

#### 7.3 supervised ML for concentration

#### 7.4 super resolution if we have time (and open data cube)

#### 7.5 solar geometry

#### 7.6 reflectance/radiance

#### 7.7 unsupervised methods

#### 7.8 synthetic data generation

#### 7.9 RobotTeam Papers

##### 7.9.1 Robot Team II: Electric Boogaloo (title w.i.p.)

- Discuss real time georectification, generation of reflectance data, etc...
- Combine Multiple days of observations
- Discuss need for both viewing geometry and solar geometry
  - make reference to highly nonuniform reflectance as a function of incident angle
  - make reference to Beer's law as justification for direct determination of concentration of concentration from spectra
  - in depth discussion of fluorometers (maybe save this for the dissertation)

## 7.9.2 Unsupervised Classification of Hyperspectral Imagery for Rapid Characterization of Novel Environments with Autonomous Robotic Teams

### 7.9.2.1 K-means / Fuzzy K-means

### 7.9.2.2 Self Organizing Maps

- fit an SOM model to the data
- for each pixel in entire map, assign best matching unit (use distinguishable colors for a  $10 \times 10$  or  $25 \times 25$  SOM grid)
- For class, investigate the learned “spectrum” representation and compare against known chemical spectra.
  - is there a database we could try to use to look up possible species in the reflectance spectra?

### 7.9.2.3 Generative Topographic Mapping

### 7.9.2.4 analysis ideas

- The nice feature of both the SOM and the GTM is we can reinterpret them to be spectral-unmixing models. Each SOM node has a feature vector of identical length to the input vector. Similarly, the mean projection  $y(x; W)$  in GTM represents the center of a gaussian in *data space*. Thus, we can reinterpret these feature vectors and gaussian centers as representative endmember spectra for the dataset. Further, the topographic properties of these methods ensure we have similarity between classes (at least in the latent space). For the GTM we are guaranteed that the data space projections of our GTM nodes will be similar. **We should see if this holds for SOM.** We can also interpret the cluster means from K-means as our endmembers.
- For SOM and GTM once we have fit the models, we can look at the map of “winning nodes” (BMU for SOM and Mean for GTM) and perform a secondary clustering (via

K-means or DBSCAN). These new clusters can define our endmember-bundles for a spectral-unmixing model.

- Once we have these maps, we should color the point by which day the data came from to see if there are any interesting groups or if the data are distributed across observation days
- We should make sure we apply the method for unsupervised classification to the dye-released images (see if the maps mirror the diffusion of dye). Pick a day where we have >1 dye flight. Make a map for both cases to illustrate how rapidly fitting an unsupervised model on the fly can enable near real time tracking of plume evolution (good for defense, oil spills, etc...). -> can we then construct a vector field / flow field from the difference and predict the plume evolution? Maybe this would be a good excuse to try lagrangian particle tracking...
- Provided our GTM/SOM fits, we should try a secondary
- From nodes/node clusters, can we identify spectral endmembers that represent chemicals we measure (e.g. chlorophyll)?
- From node activations (SOM) or responsibilities (GTM) can we fit a good model that competes with predictions from full spectra? (dimensionality reduction demonstration)
- cluster viewing geometry separate from reflectances and use resulting viewing geo classes to color GTM/SOM map of reflectance data

### 7.9.3 Spectral Indices for Rapid HSI Surveys: Unsupervised and Supervised Methods via SciML

- Apply to PROSPECT database as a simple test case
- Apply to our own Data
  - [Multiple Endmember Spectral Mixture Analysis](#)

- generalize **Spectral Unmixing Models** unmixing models... with gaussian process we could think of an infinite basis of gaussians describing “peaks” in the spectrum”. Can we try to kernelize this procedure?

#### 7.9.4 Synthetic Data Generation for Hyperspectral Imaging with Autonomous Robotic Teams

- Variational Autoencoders
- Group transformations, e.g. rotations, reflections, translations, cropping, etc... (do these make sense if boat data is point observation)
- Advanced sampling methods for regions with

#### 7.9.5 Uncertainty Quantification via $\partial P$ .

- Categorize Methods into two categories:
  - quantifying uncertainty in collected data
  - quantifying model uncertainty
- Conformal Prediction (we have a NN code for doing this in flux. Just need to apply it)
- Representativeness Uncertainty i.e. when georectifying HSI images and reducing spatial extend via `ilat` and `ilon` settings, also compute the stdev for each grainy pixel
- `Measurements.jl forward mode` once we have the representativeness uncertainty.
- Need a way to quantify uncertainty from Boat sensors...
- Sensativity Analysis with w/ automatic differentiation

the stuff regarding the full robot team that appeared in our 2020 robot team paper that Dr. Lary was the first author on.

## **7.10 Supervised Methods**

stuff from paper # 1

## **7.11 Unsupervised Methods**

stuff from paper # 2

## **CHAPTER 8**

### **SUPER RESOLUTION**

#### **8.1 Cloud & Shadow Mask for Sentinel-2**

##### **8.1.1 ML Type**

- Supervised Classification

##### **8.1.2 ML Methods**

- Single Pixel w/ Tree Based Methods
- Deep NN with Convolutional Layers

##### **8.1.3 Features**

- Sentinel 2 Multi-band Imagery
- Land Type
- Viewing Geometry
- Solar Geometry

##### **8.1.4 Targets**

- Sentinel 2 Cloud Mask + Cloud Shadow Mask

#### **8.2 Cloud & Shadow Fill**

##### **8.2.1 ML Type**

- supervised regression

### 8.2.2 ML Methods

- pixel based (Would it make sense to do something else here?)

### 8.2.3 Features

- Sentinel 2 Multi-band Imagery
- Sentinel 2 Cloud Mask & Cloud Shadow Mask
- Sentinel 1 SAR Variables (GRD or SLC or both?)
- 10 m Digital Elevation Map
- Viewing Geometry
- Solar Geometry
- Land Type

### 8.2.4 Targets

- *Cloudless & Shadowless* Sentinel 2 Multi-band imagery

## 8.3 Sentinel 2 RGB *Spatial* Super Resolution

### 8.3.1 ML Type

- Supervised Regression

### 8.3.2 ML Methods

- This has to be a Deep NN method using convolution to get the upsampling. I don't think we can do this with pixel based models (using tree methods)
- Probably should use a GAN



### 8.3.3 Features

- High (spatial) Resolution NAIP RGB Image
- Sentinel 2 Multi-band Imagery
- Sentinel 1 SAR Variables (GRD or SLC or both?)
- 10 m Digital Elevation Map
- Viewing Geometry
- Solar Geometry
- Land Type

### 8.3.4 Targets

- Sentinel RGB Bands @ NAIP Resolution

### 8.3.5 Loss Function Terms

### 8.3.6 Notes

We could make a model that uses all 3 bands (RGB) simultaneously, or we can make a model for a single band that we validate against R, G, and B bands individually. This has the added perc of increasing the training samples. This will be much easier to then apply to *all* bands of the sentinel imagery (and perhaps Sentinel 1, etc...) independently. We could try:

- Red, Green, Blue bands separately
- Black and White converted RGB image
- Data Augmentation via Scaling / Rotation / Reflection

## 8.4 Sentinel 2 Multiband *Spatial* Super Resolution

### 8.4.1 ML Type

- Supervised Regression

### 8.4.2 ML Methods

- This has to be a Deep NN method using convolution to get the upsampling. I don't think we can do this with pixel based models (using tree methods)
- Probably should use a GAN

### 8.4.3 Features

- High (spatial) Resolution NAIP RGB Image
- Sentinel 2 Multi-band Imagery
- Sentinel 1 SAR Variables (GRD or SLC or both?)
- 10 m Digital Elevation Map
- Viewing Geometry
- Solar Geometry
- Land Type

### 8.4.4 Targets

- Sentinel RGB Bands @ NAIP Resolution

### 8.4.5 Loss Function Terms

## 8.5 Sentinel 2 Multiband *Spectral* Super Resolution

### 8.5.1 ML Type

- Supervised Regression

### 8.5.2 ML Methods

- This can be pixel based

### 8.5.3 Features

- Sentinel 2 Multi-band Imagery
- Sentinel 1 SAR Variables (GRD or SLC or both?)
- 10 m Digital Elevation Map
- Viewing Geometry
- Solar Geometry
- UAV Hyperspectral Image

### 8.5.4 Targets

- Sentinel *Hyperspectral* Imagery (i.e. Sentinel at all HSI Bands)

### 8.5.5 Loss Function Terms

if we get to it... probably with a focus on Scotty's Ranch

## CHAPTER 9

### CHEMICAL DATA ASSIMILATION

#### 9.1 Photolysis

#### 9.2 HEART Chamber

## CHAPTER 10

### MASTER CHEMICAL MECHANISM

10.1 sensor fusion

10.2 photolysis

10.3 docker ingestion framework

10.4 master chemical mechanism

10.5 data assimilation

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10.6 Chemical Data Assimilation & ActivePure Work

10.6.1 ActivePure Research Lab

- Overview of all sensor in sensor matrix
- Overview of measurement capabilities (list of species, uncertainty levels, etc...)
- Overview of containerized data acquisition pipeline
  - NodeRed
  - InfluxDB
  - Grafana
  - Quarto
  - Automatic Alerts
  - Automatic Reports

### **10.6.2 Kinetics and Chemical Data Assimilation**

- MCM Implementation in Julia
- Direct computation of Photolysis rates
- Combination with Dr. Lary's AutoChem
- Addition of Ion Chemistry from MIT Lightning dissipation
- Visualization of chemical cycles
- SciML methods to infer below detection limits

### **10.7 CRI Mechanism**

### **10.8 AutoChem**

### **10.9 Ion Chemistry**

### **10.10 Evaluation Indoor Air Quality via Chemical Data Assimilation**

This is where we put our non-ActivePure results

Specific testing done (e.g. in fourth floor lab space) sans-ActivePure technology

### **10.11 Photocatalytic Ionization**

This is where we put our ActivePure-specific results

Testing results done with ActivePure technology



## CHAPTER 11

### TIME SERIES METHODS

#### 11.1 Uncertainty Estimation Via Time Series Sampling

##### 11.1.1 Types Of Uncertainty

##### 11.1.2 Instrument Uncertainty

##### 11.1.3 Representativeness Uncertainty

##### 11.1.4 Variograms

##### 11.1.5 Mutual Information

##### 11.1.6 Auto-correlation

#### 11.2 Time Series Chaos

##### 11.2.1 What is Chaos?

##### 11.2.2 Lyapunov Exponents

##### 11.2.3 Fractal Dimension

#### 11.3 Koopman Operator Theory

#### 11.4 Time Series Modeling Methods

##### 11.4.1 Token-Hankel Delay Embeddings

##### 11.4.2 Embedding Theorems (are magic)

##### 11.4.3 Determination of Optimal Lag

##### 11.4.4 Determination of Intrinsic Dimension (kind of unnecessary given *large enough* embedding)

##### 11.4.5 DMD and HAVOK 40

##### 11.4.6 Hamiltonian Neural Networks

##### 11.5 Time Series Classification



## 11.15 Sensor Network + SciML

### 11.15.1 Evaluation of local chaos in SharedAirDFWNetwork

- This gives me an excuse to work with the sensor data
- Train GTM, SOM, and Variational Autoencoder to produce lower dimensional representation of all data from a central node, e.g. in  $\mathbb{R}^2$ .
  - For VAE, test a range of dimensions from the number of sensors down to 2 (better for visualization)
- Analyze the variety of methods from [DataDrivenDiffEq.jl](#) to infer dynamics in the low dimensional space
- Can we infer some kind of Hamiltonian from the data and do a HamiltonianNN approach?
  - Start of with a standard kinetic-energy style Hamiltonian e.g.  $\sum_i \frac{1}{2} \dot{x}_i^2$  where  $x_i$  is the
  - use DataDrivenDiffEq approach to learn the associated potential energy term
  - alternatively, attempt to capture diurnal cycle (or other relevant time scales) by *learning* coordinate representation that forces dynamics to be uncoupled harmonic oscillators a la Hamilton-Jacobi theory.
  - Test if this hamiltonian NN model can then be transfered to another central node with an appropriate shift in the “total energy”
- Attempt to analyze the 2d data to infer Koopman operator. We should treat the original sensor values as observables on which the learned koopman operator acts. This should be doable if the NN is just a function.

- use DMD approach to identify a “forcing” coordinate that can identify when we switch nodes as in [Chaos as an intermittently forced linear system](#)
- [video on Physics Informed DMD](#)
- [Deep Learning to Discover Coordinates for Dynamics: Autoencoders & Physics Informed Machine Learning](#)
- NOTE: we may need to impute missing values. We should do so with either my GPR code or with other ML methods + ConformalPrediction. Provided uncertainty estimates, we should then think about how to propagate errors through our analysis via [Measurements.jl](#), [IntervalArithmetic](#),

## CHAPTER 12

### DISCUSSION

#### 12.1 Limitations

#### 12.2 Future Work

**CHAPTER 13**  
**CONCLUSIONS**

## **CHAPTER 14**

### **TECHNICAL NOTES**

#### **14.1 Real Time Georectification of Drone Based Imagery**

- Georectification of pushbroom HSI
- Georectification of square visible + thermal FLIR imagery

#### **14.2 Self Organizing Maps**

#### **14.3 Bayesian Optimization with Gaussian Process Regression**

#### **14.4 Gaussian Process Regression / Classification in MLJ**

j ## Solar Geometry? (probably not necessary)

## CHAPTER 15

### OTHER TOPICS

- Sparse Nonlinear Models for Fluid Dynamics with Machine Learning and Optimization
- Residual Dynamic Mode Decomposition: A very easy way to get error bounds for your DMD computations
- Deep Learning of Dynamics and Coordinates with SINDy Autoencoders
- Identifying Dominant Balance Physics from Data

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## APPENDIX A

### ADDITIONAL STUFF

You might put some computer output here, or maybe additional tables. It is possible to have multiple appendices. Just list them in the appropriate place within `_quarto.yml`.

**APPENDIX B**

**EEG BAND DISCOVERY WITH DECISION TREES**

## BIOGRAPHICAL SKETCH

Update required!



## CURRICULUM VITAE