Machine Learning methods for multi-disciplinary multi-scales problems

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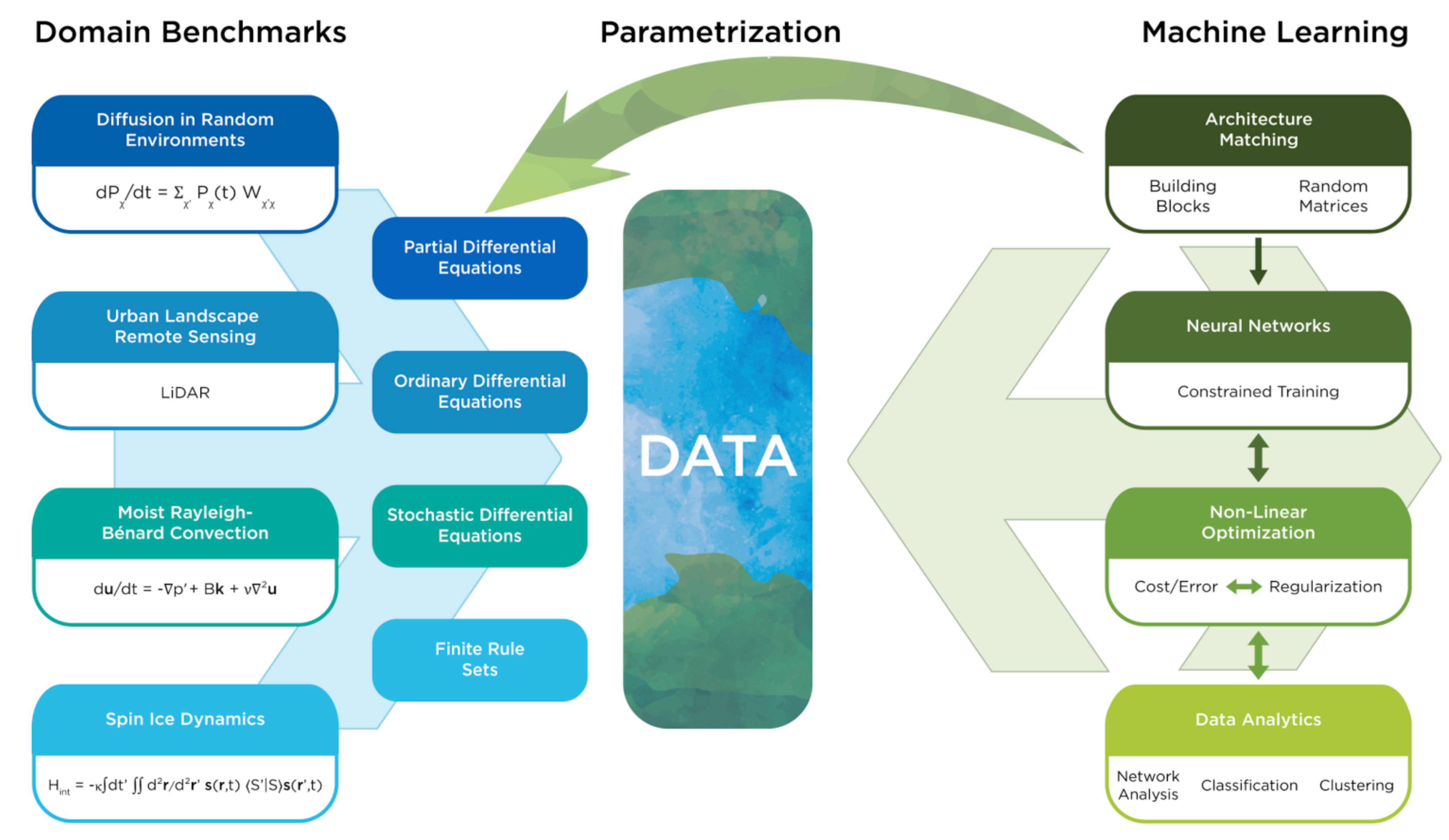
Project Overview:

Our goal: Develop new interpretable Machine Learning (ML) methods for scientific computing to tackle multi-scale problems across a wide array of scientific disciplines.
Our method: Use ML to train mathematical representations of small-scale processes in benchmark problems, then implement and evaluate them in coarse grained models.
Our plan: Establish 'best practice' methodologies for how to build and integrate ML within a computational framework.
A central part of our approach is to identify **benchmarks problems** within different disciplines and develop specific data science approach to tackle them.



Interpreting Machine Learning and Neural Nets

- Solve a PDE *normally* via grids & matrices

$$\frac{\partial u(\vec{r},t)}{\partial t} = \kappa\nabla^2 u(\vec{r},t) \quad (\text{homo } \kappa) \qquad u(t+\Delta t) = u(t) + \frac{\partial u}{\partial t}\Delta t + \mathcal{O}(\Delta t^2)$$

$$\frac{\partial u(\vec{r},t)}{\partial t} = \nabla\cdot\kappa(\vec{r})\nabla u(\vec{r},t) \quad (\text{inhomo } \kappa) \qquad u(t+\Delta t) \approx u(t) + \left(\kappa\nabla^2 u(\vec{r},t) + \nabla\kappa\cdot\nabla u\right)\Delta t$$

$$\begin{pmatrix} | \\ u(t_1) \\ | \end{pmatrix} = \left(\begin{pmatrix} \kappa_1 & & \\ & \kappa_2 & \\ & & \kappa_3 \end{pmatrix}\begin{pmatrix} \underset{\sim}{\mathcal{I}} \end{pmatrix}\right) \begin{pmatrix} \begin{pmatrix} \underset{\sim}{D}_{Lap} \end{pmatrix} & \begin{pmatrix} \underset{\sim}{\emptyset} \end{pmatrix} \\ \begin{pmatrix} \underset{\sim}{\emptyset} \end{pmatrix} & \begin{pmatrix} \underset{\sim}{\mathcal{I}} \end{pmatrix} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \Delta t\, \underset{\sim}{\mathcal{I}} \end{pmatrix} \\ \begin{pmatrix} \underset{\sim}{\mathcal{I}} \end{pmatrix} \end{pmatrix} \begin{pmatrix} | \\ u(t_0) \\ | \end{pmatrix}$$

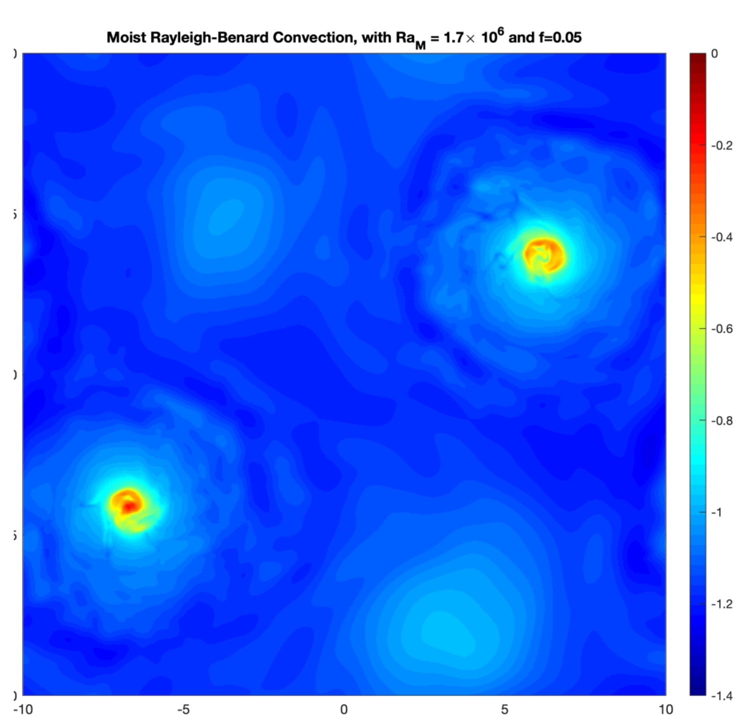
- Create a Neural Net matching the **form** of the *normal* approach, this allows the NN to arrive at its final result, and allows us to **interpret** the form it takes

$$\begin{pmatrix} | \\ \mathbb{O} \\ | \end{pmatrix} = f_M\left[\left(\begin{pmatrix} \underset{\sim}{W}_M \end{pmatrix}\begin{pmatrix} \underset{\sim}{\mathcal{I}} \end{pmatrix}\right)\begin{pmatrix} \begin{pmatrix} | \\ \mathbb{L}_M \\ | \end{pmatrix} \\ \begin{pmatrix} | \\ b_M \\ | \end{pmatrix} \end{pmatrix}\right] \qquad \begin{pmatrix} | \\ \mathbb{L}_M \\ | \end{pmatrix} = \ldots f_1\left[\left(\begin{pmatrix} \underset{\sim}{W}_1 \end{pmatrix}\begin{pmatrix} \underset{\sim}{\mathcal{I}} \end{pmatrix}\right)\begin{pmatrix} \begin{pmatrix} | \\ \mathbb{I} \\ | \end{pmatrix} \\ \begin{pmatrix} | \\ b_1 \\ | \end{pmatrix} \end{pmatrix}\right]$$

- Pre-seed NN to reflect a model approach with known properties to see whether the NN maintains that structure or finds a *new one*.

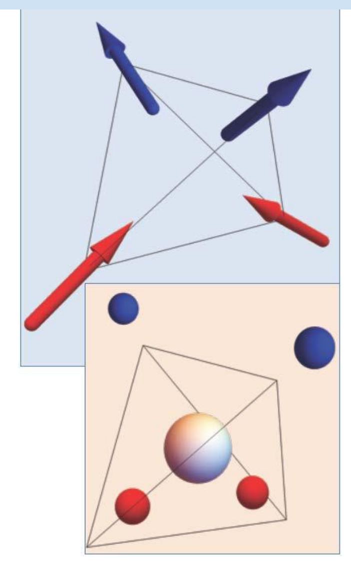
Climate Science:

Moist convection (aka clouds) remains a key challenge in climate and weather models. We use here a simplified formulation of the problems to assess the capability of machine learning approaches to assess regimes transition and improve the representation of convection in climate models.



Multiscale Materials

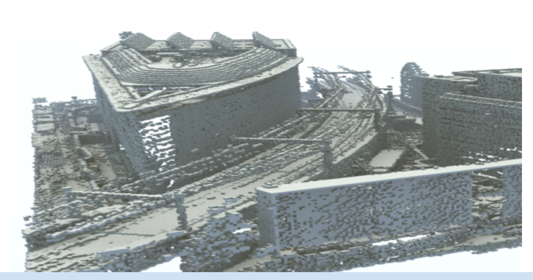
Slow monopoles in spin ice: Spin ice is an exotic magnet with long time scales and supercooled liquid behavior.



Diffusion in random media: a ubiquitous problem in materials, controlling the kinetics of materials processing. The multiscale nature spans from atomic to micrometer scales. Structural patterns introduce superbasins in trajectory information.

LIDAR - Full waveform analysis

Light Detection and Ranging (LiDAR) is a line-of-sight remote sensing technique that relies on capturing the return signal from a laser beam to capture the geometry of the existing environment. The resulting point cloud is derived from a full waveform version of the data that has only recently become accessible to researchers. As full waveform is a rawer and more high dimensional form of the data, machine learning approaches hold the potential for both better and faster processing that data into point clouds over traditional Gaussian fitting.



Ongoing activities:

- Training solver for the heat equation from data (generated from the heat equation itself, but with some noise added
- Development of neural net taylored for advection/diffusion problems.
- Evaluation of different ML approach in idealized PDE's.
- Spin ice Monopole dynamics generated by Markov chain.
- Uncertainty quantification in learning systems under constraints.
- Uncertainty quantification in deep learning systems with variational autoencoders using normalization flows.
- Development training framework for machine learning across physical sciences
- Undergrad & HS students selected for summer placements (to be done remotely at most places)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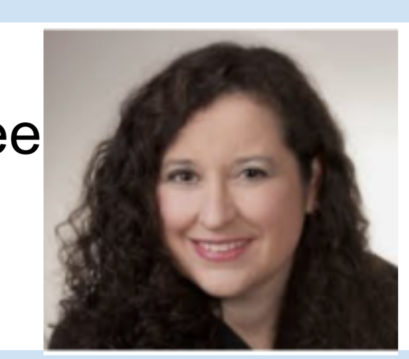
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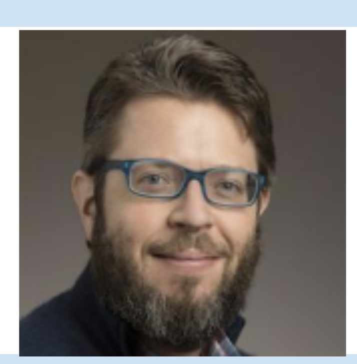
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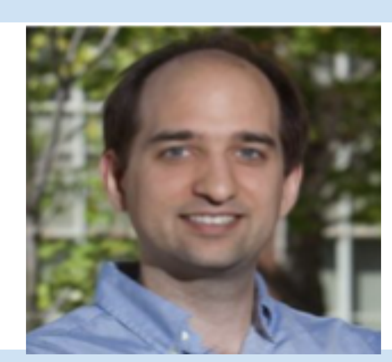
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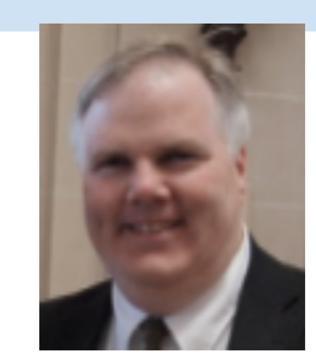
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