Advancing materials characterization through physics-guided machine learning

Nina Andrejevic

Maria Goeppert Mayer Fellow

Center for Nanoscale Materials | Argonne National Laboratory

nandrejevic@anl.gov

ALCF AI for Science Series | October 8, 2024

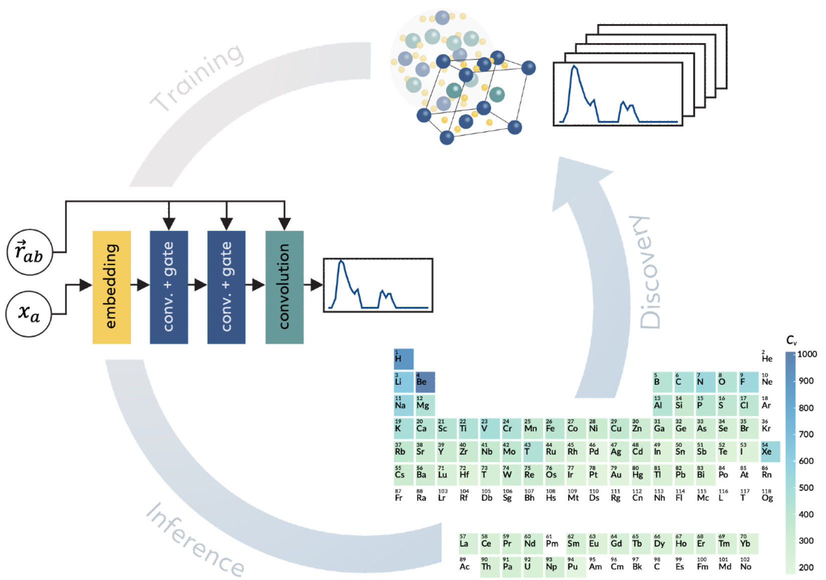
Overview

Data-driven modeling of materials characterization data

Overview

Data-driven modeling of materials characterization data

Accelerated property prediction

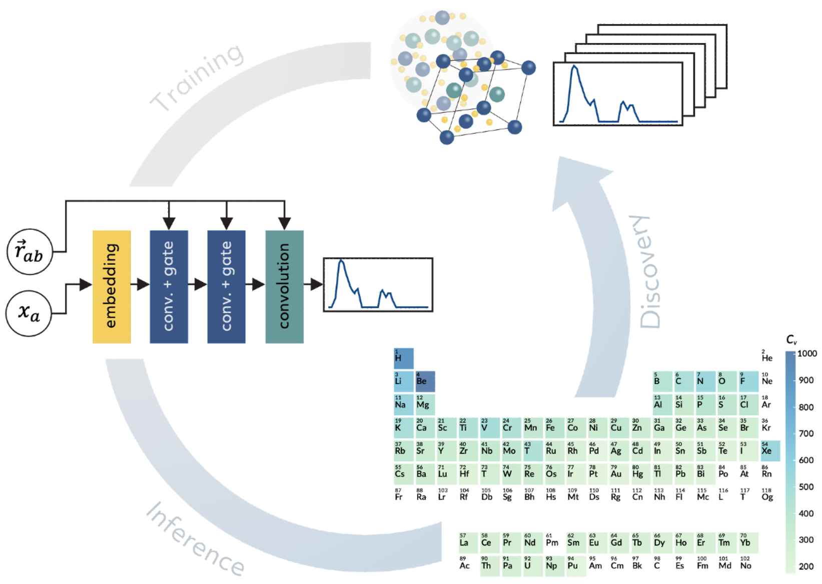


Efficient prediction of materials' vibrational properties with equivariant neural networks

Overview

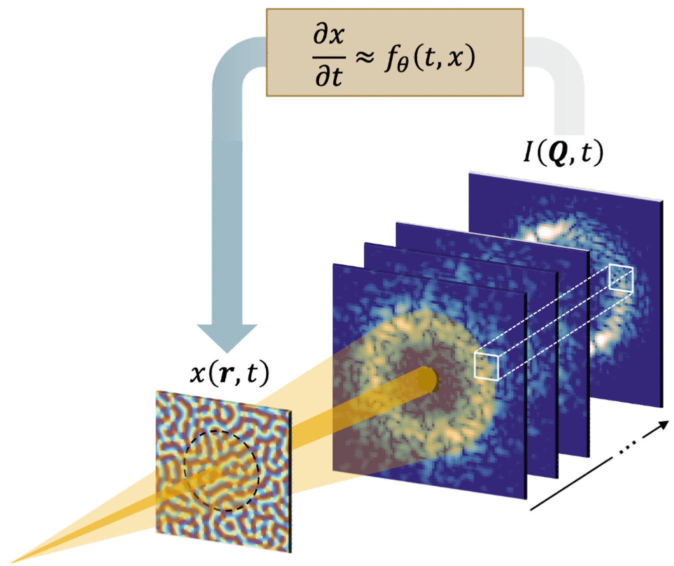
Data-driven modeling of materials characterization data

Accelerated property prediction



Efficient prediction of materials' vibrational properties with equivariant neural networks

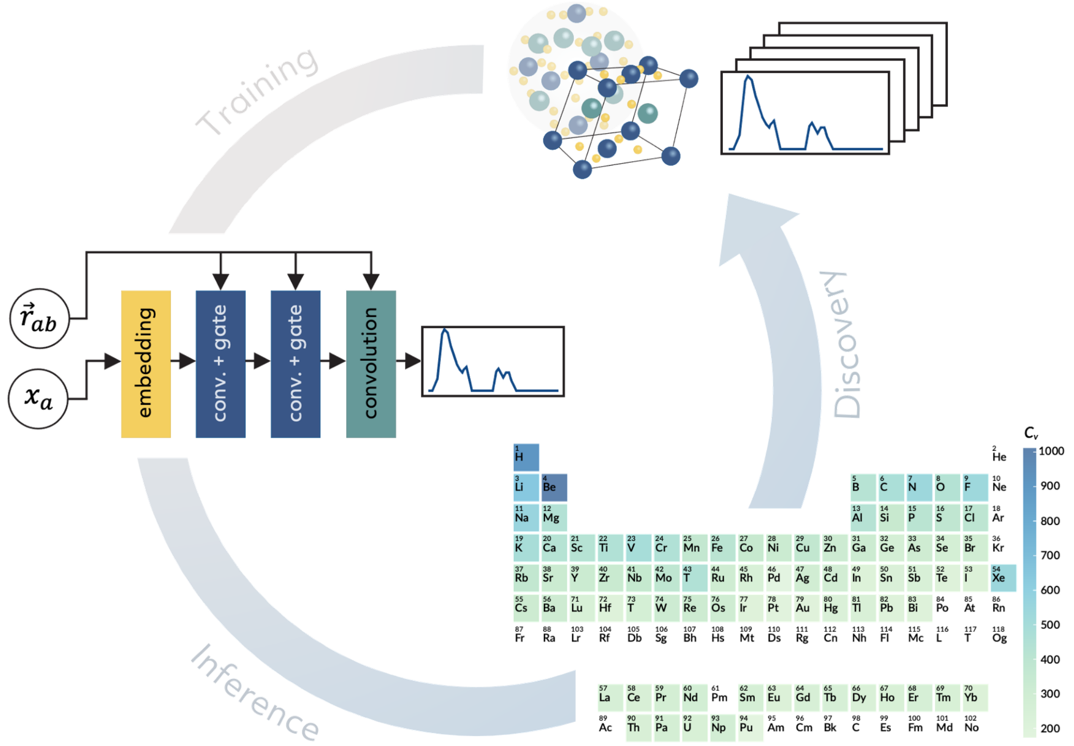
Intelligent data analysis



Data-driven discovery of materials' dynamics from coherent scattering

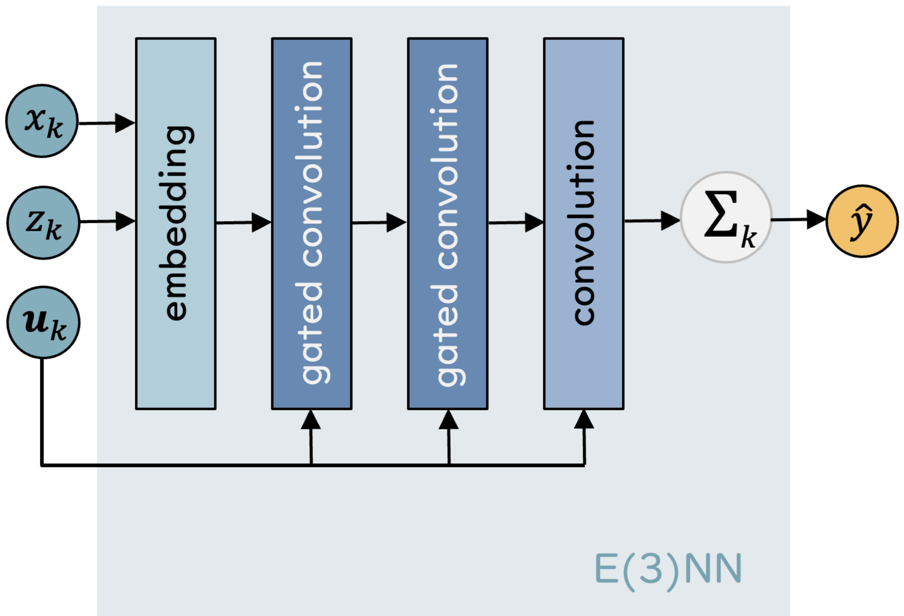
Motivation | Accelerated structure-property prediction

- **Enable high-throughput screening** for discovery of materials with targeted properties
- **Substitute intensive calculations** for inversion of characterization data to atomic structures



- Calculated and experimental data are expensive and scarce
- Incorporate physics to make models more data-efficient

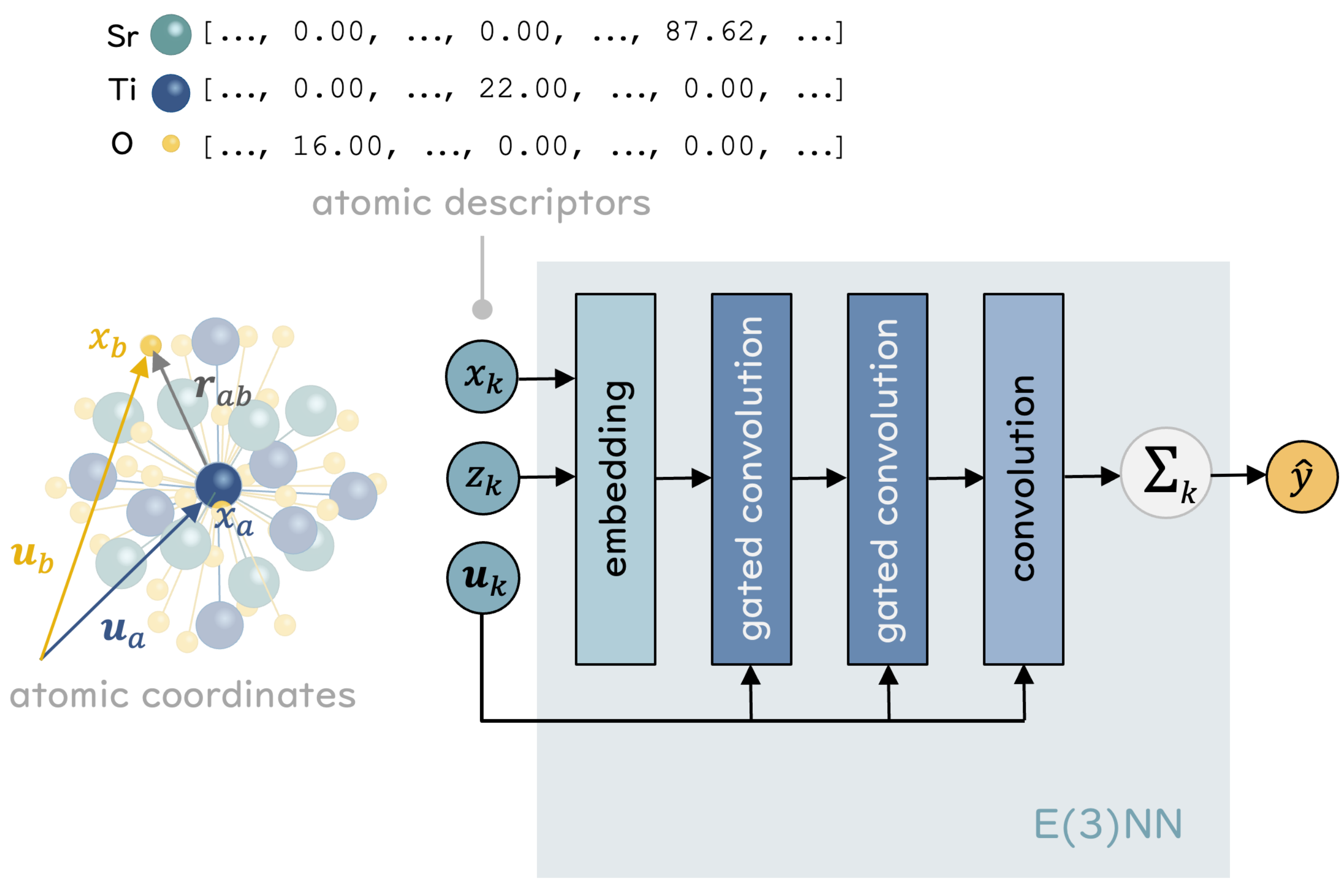
Results | Euclidean neural networks (E(3)NN)



M. Geiger, T. Smidt, et al. Euclidean neural networks: e3nn (2020).

Z. Chen*, N. Andrejevic*, T. Smidt*, et al. *Advanced Science* 8.12 (2021): 2004214. *equally contributing

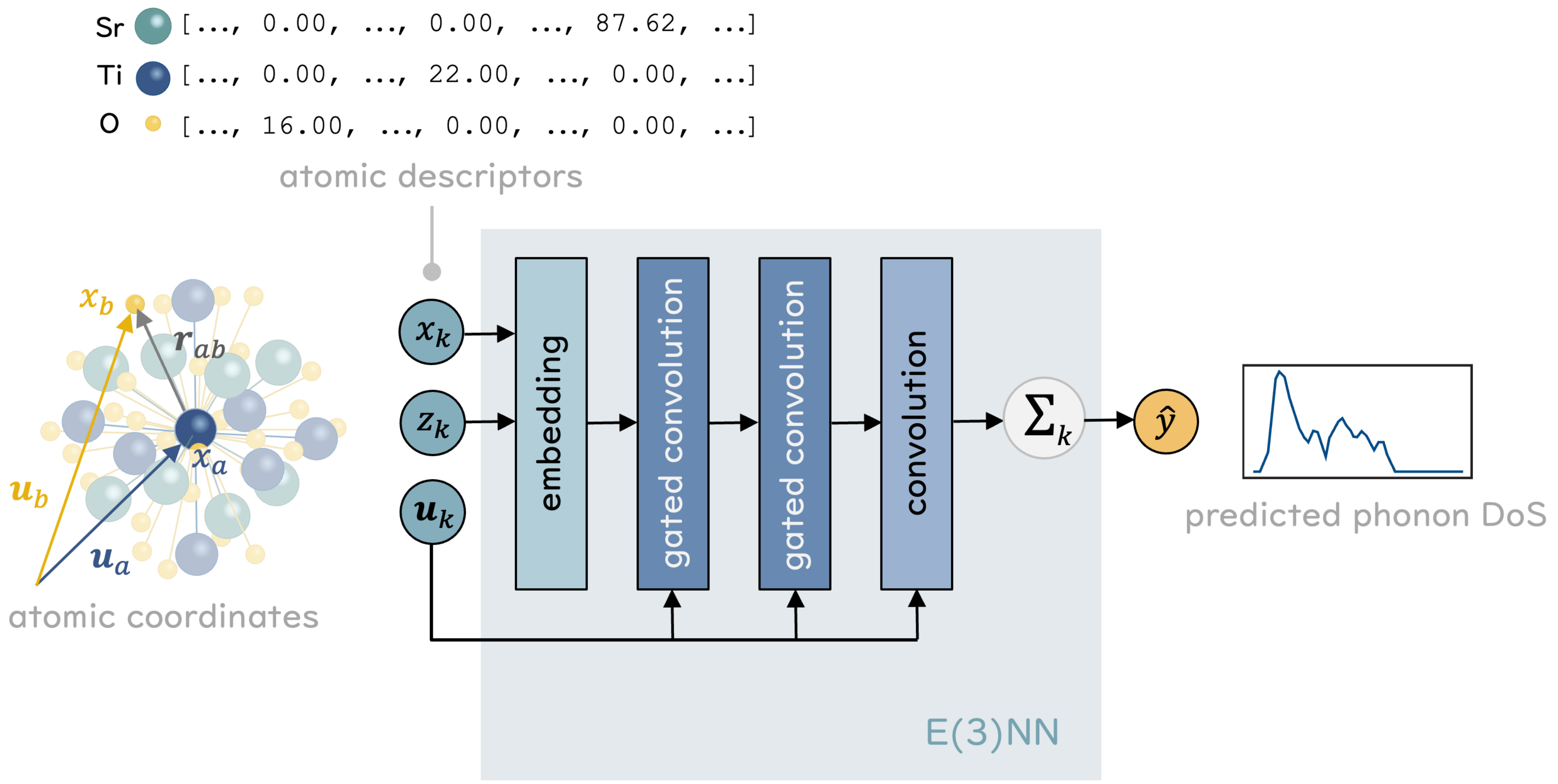
Results | Euclidean neural networks (E(3)NN)



M. Geiger, T. Smidt, et al. Euclidean neural networks: e3nn (2020).

Z. Chen*, N. Andrejevic*, T. Smidt*, et al. *Advanced Science* 8.12 (2021): 2004214. *equally contributing

Results | Euclidean neural networks (E(3)NN)



M. Geiger, T. Smidt, et al. Euclidean neural networks: e3nn (2020).
Z. Chen*, N. Andrejevic*, T. Smidt*, et al. *Advanced Science* 8.12 (2021): 2004214. *equally contributing

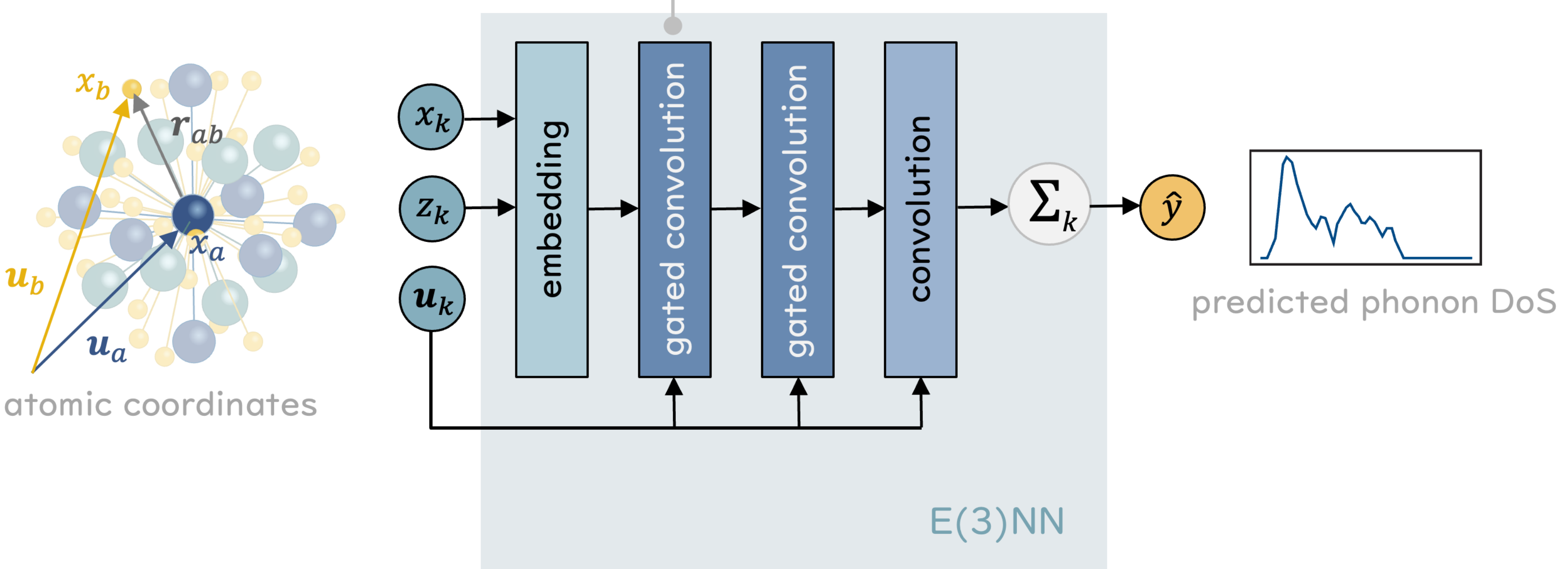
Results | Euclidean neural networks (E(3)NN)

- E(3) equivariant convolution operations: Constrain function optimization space, enabling data-efficient learning without data augmentation

$$x'_a = \frac{1}{\sqrt{z}} \sum_{b \in \partial(a)} x_b \otimes_{w(|\vec{r}_{ab}|)} Y(\vec{r}_{ab}/|\vec{r}_{ab}|)$$

learned radial function

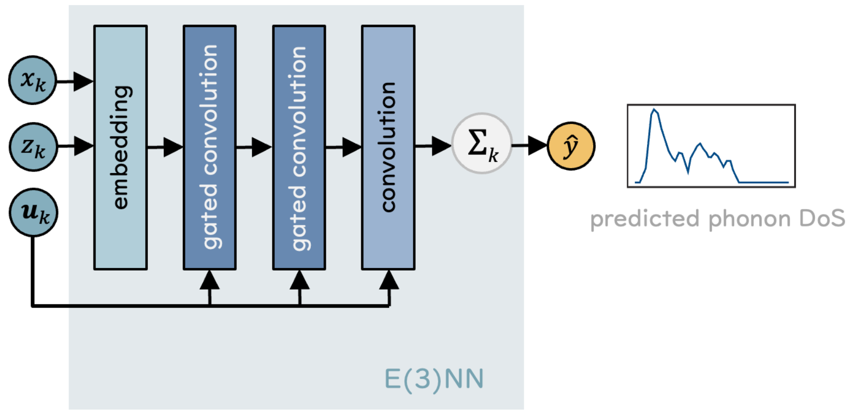
spherical harmonic



M. Geiger, T. Smidt, et al. Euclidean neural networks: e3nn (2020).

Z. Chen*, N. Andrejevic*, T. Smidt*, et al. *Advanced Science* 8.12 (2021): 2004214. *equally contributing

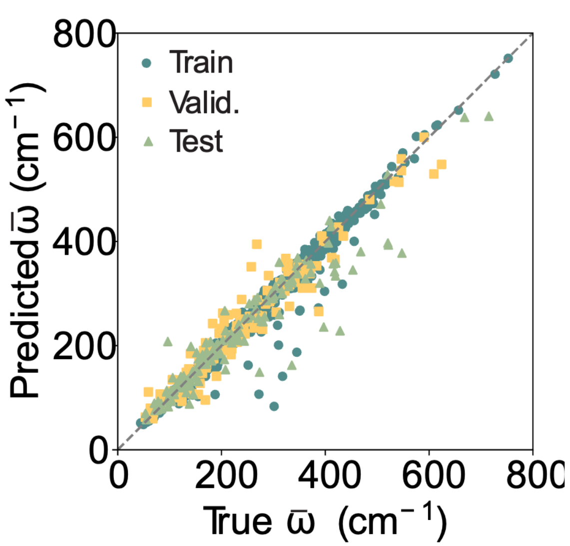
Results | Euclidean neural networks (E(3)NN)

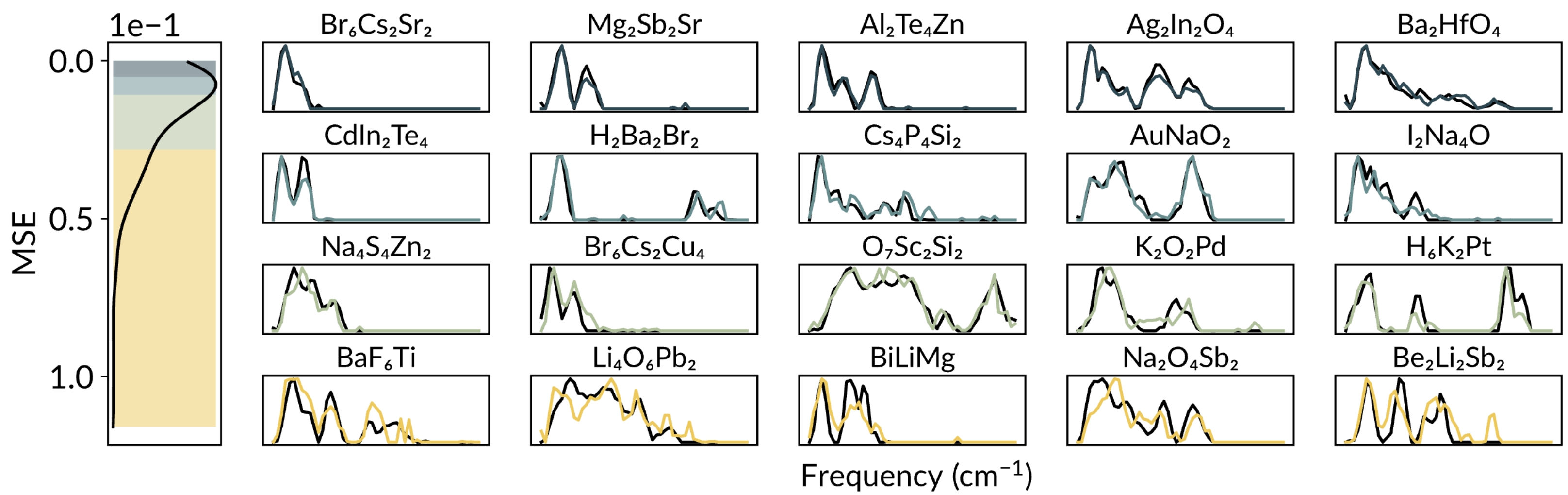


- Chemically- and structurally-diverse dataset (~1,200) of ab initio DoS sampled at 50 points up to 1,000 cm^{-1}

  G. Petretto, et al. *Scientific data* 5 (2018): 180065

- Recover key spectral features even among lowest-performing examples



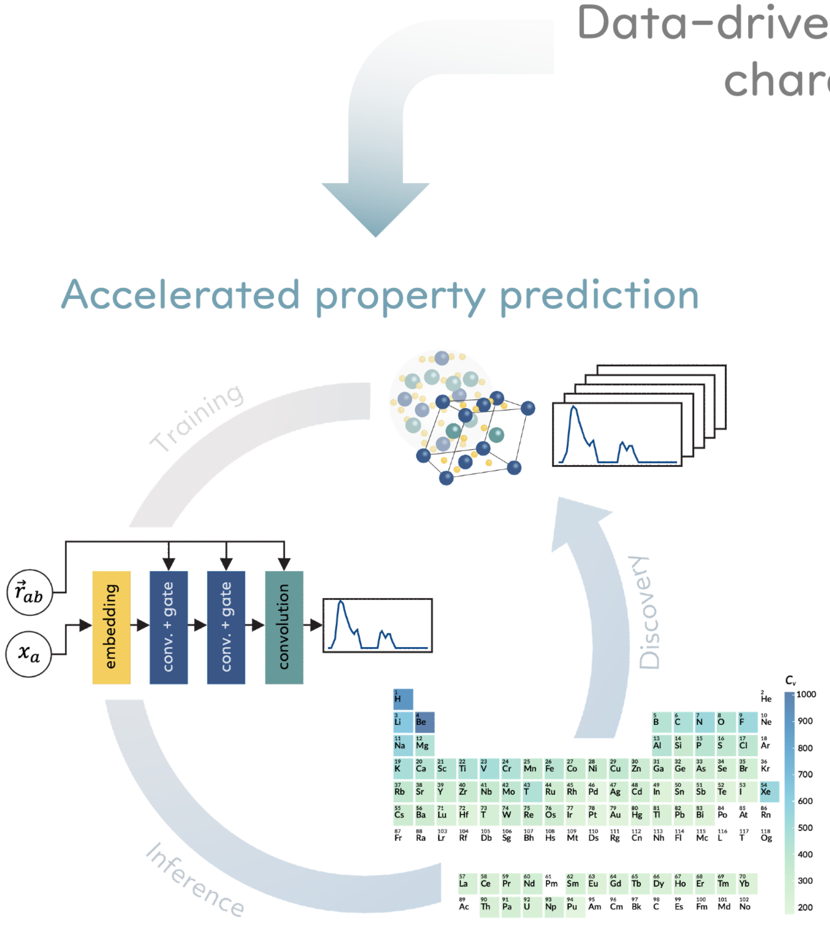


Z. Chen*, N. Andrejevic*, T. Smidt*, et al. *Advanced Science* 8.12 (2021): 2004214. *equally contributing

Overview

Data-driven modeling of materials characterization data

Accelerated property prediction



Efficient prediction of materials' vibrational properties with equivariant neural networks

Train neural networks that generalize to unseen crystal structures and compositions to predict a materials property that is expensive to calculate or measure

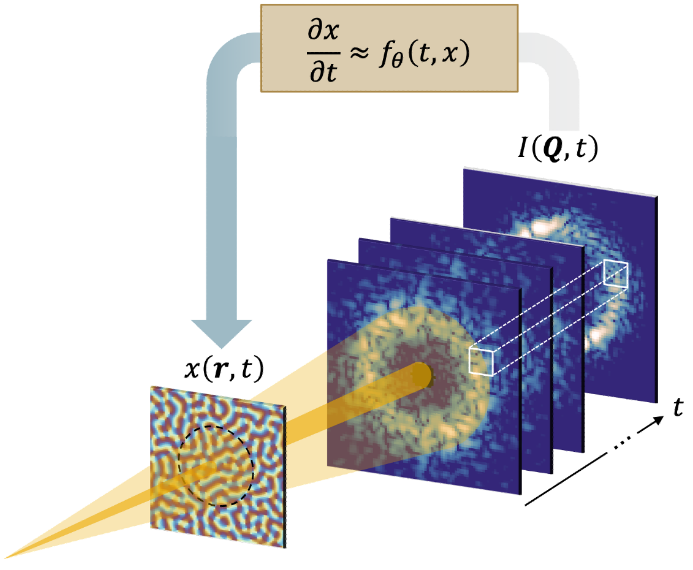
Overview

Data-driven modeling of materials characterization data

Accelerated property prediction

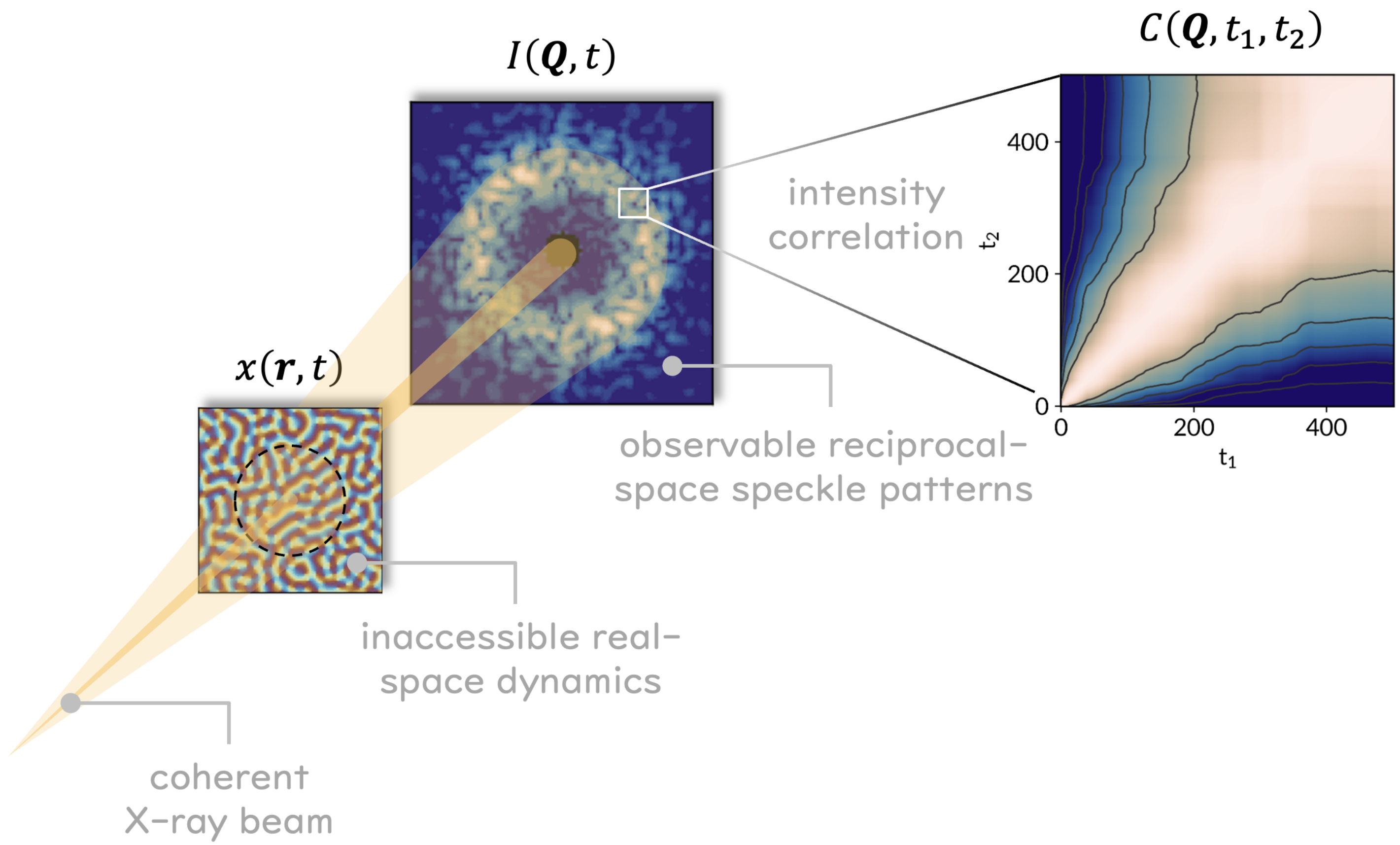
Efficient prediction of materials' vibrational properties with equivariant neural networks

Intelligent data analysis

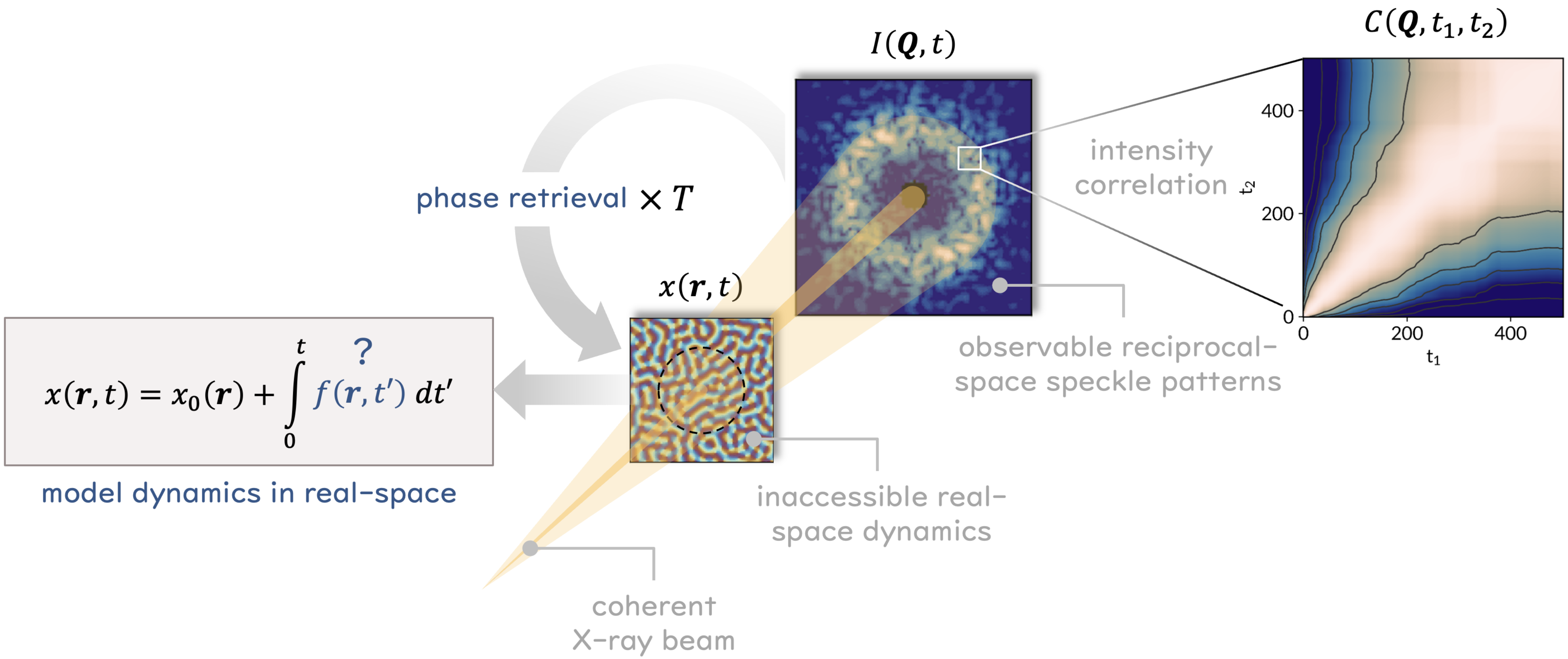


Data-driven discovery of materials' dynamics from coherent scattering

Motivation | Visualizing dynamics with coherent X-rays

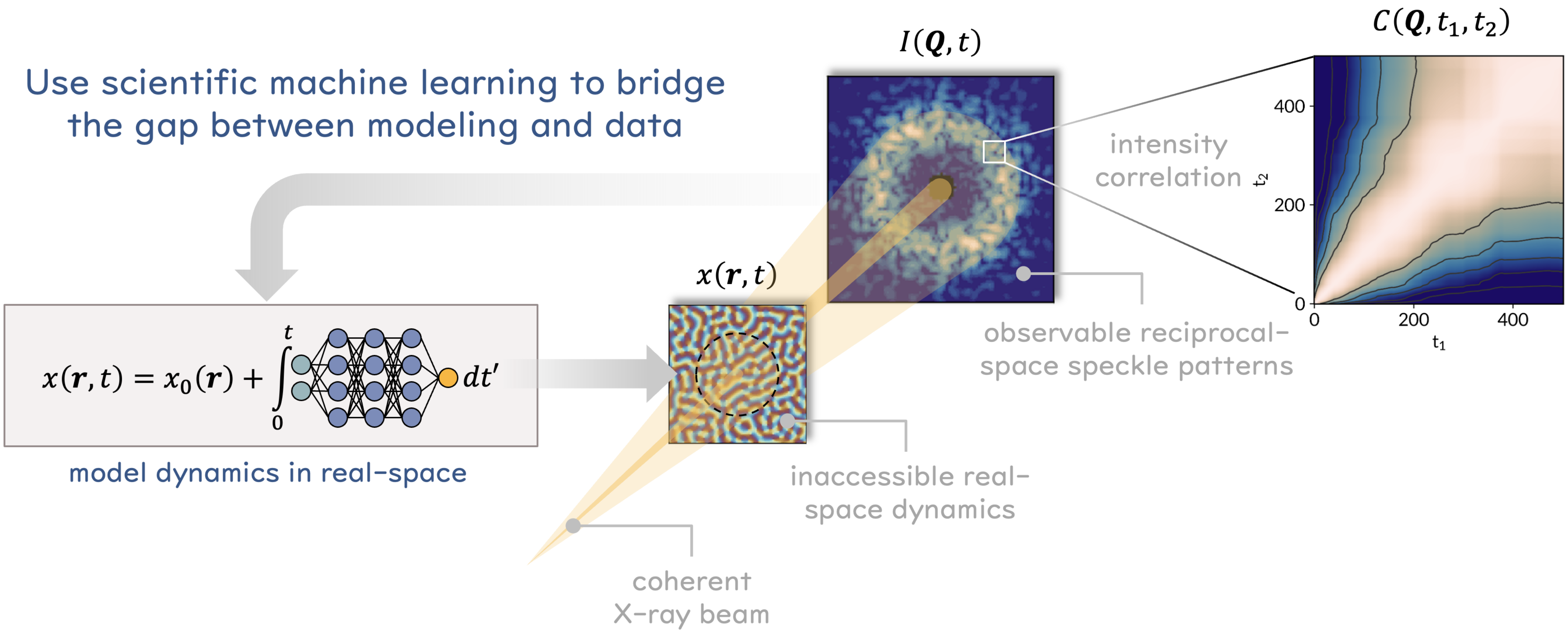


Motivation | Visualizing dynamics with coherent X-rays



Motivation | Visualizing dynamics with coherent X-rays

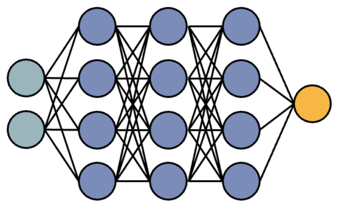
Use scientific machine learning to bridge the gap between modeling and data



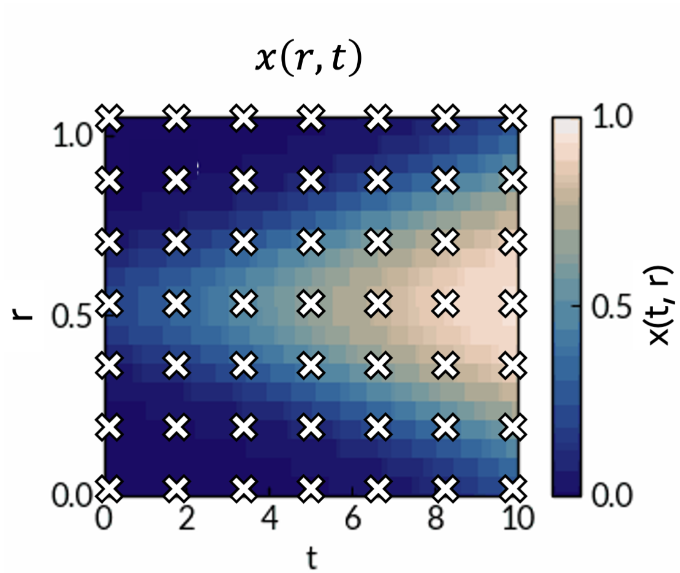
N. Andrejevic, *et al. npj Computational Materials* 10.1 (2024): 225.

Methods | Neural (ordinary) differential equations (ODE)

$\frac{dx}{dt} \approx$

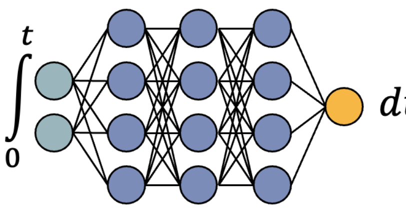


+



→

$\hat{x}(r,t) = x_0(r) + \int_0^t$



dt'

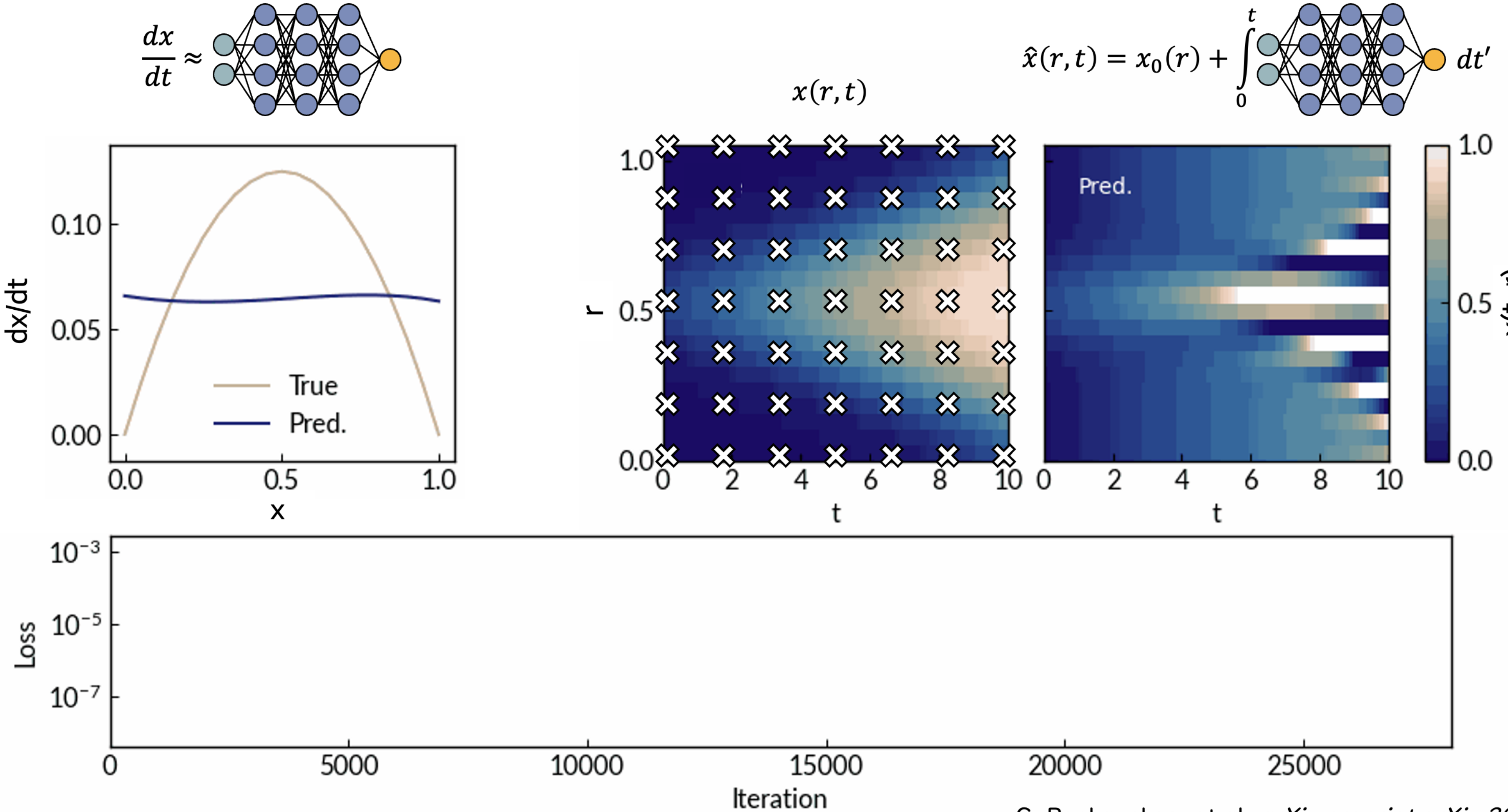
unknown dynamical equation

observations in solution space

numerical integration

C. Rackauckas, et al. *arXiv preprint arXiv:2001.04385* (2020).
R. TQ Chen, et al. *Advances in neural information processing systems* 31 (2018).

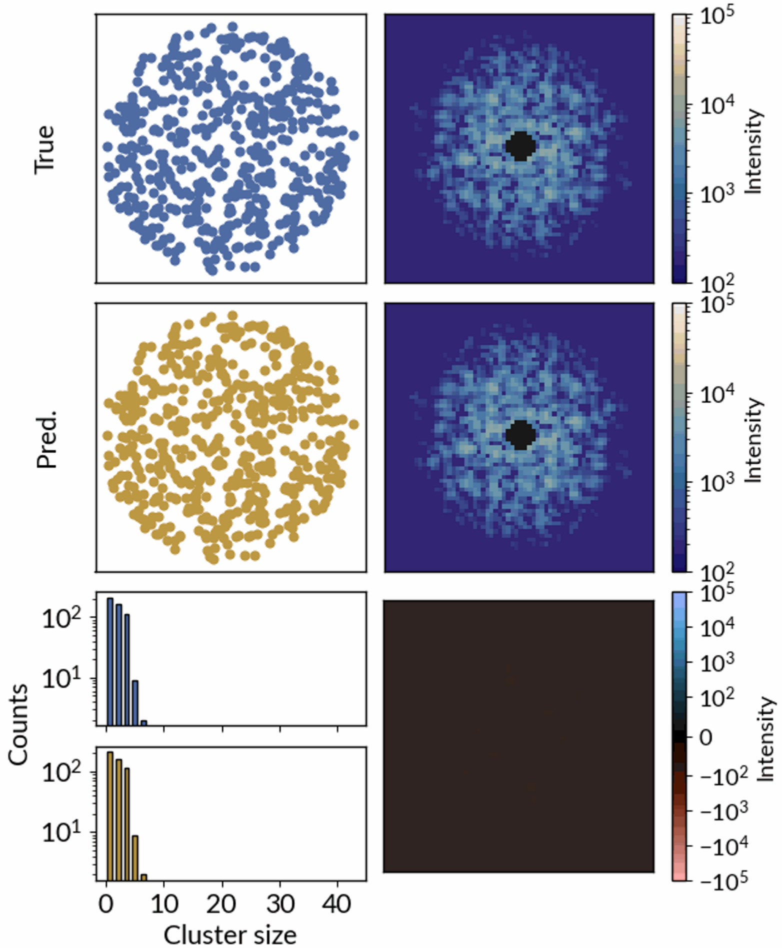
Methods | Neural (ordinary) differential equations (ODE)



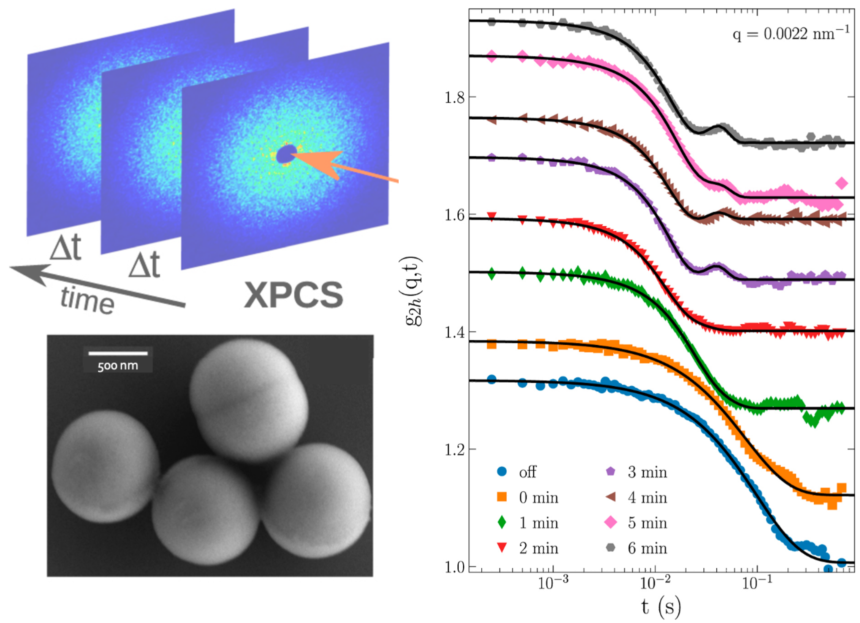
C. Rackauckas, et al. *arXiv preprint arXiv:2001.04385* (2020).
R. TQ Chen, et al. *Advances in neural information processing systems* 31 (2018).

Results | Computational case studies

Cluster formation in self-organizing particles



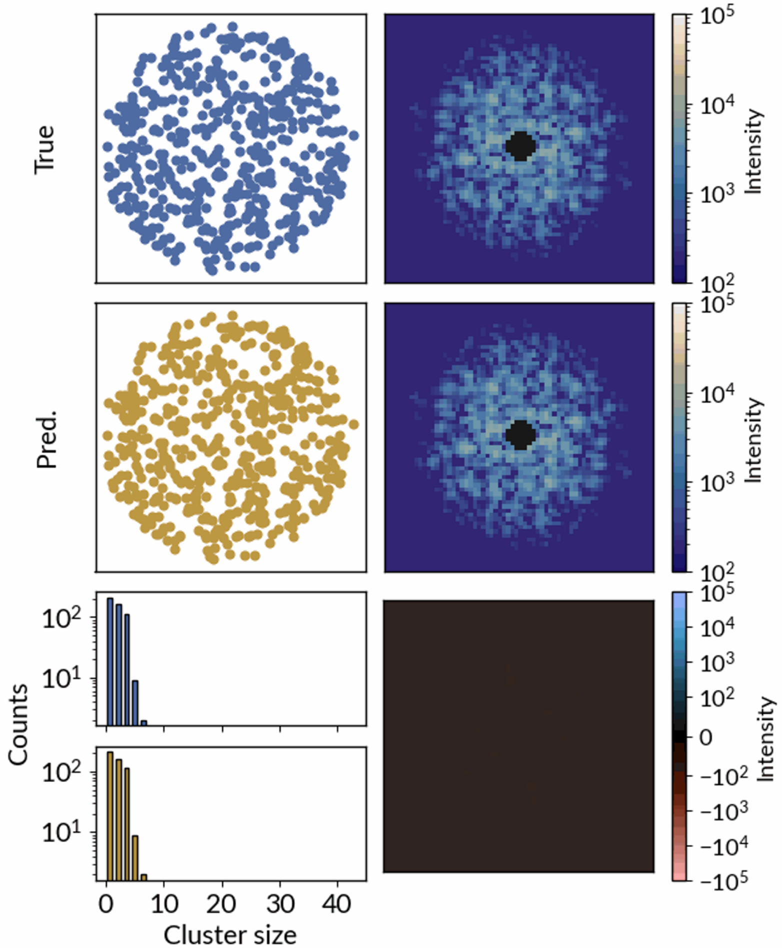
emergent dynamics of light-induced active colloids probed by XPCS



T. Zinn, et al. *New Journal of Physics* 24.9 (2022): 093007.

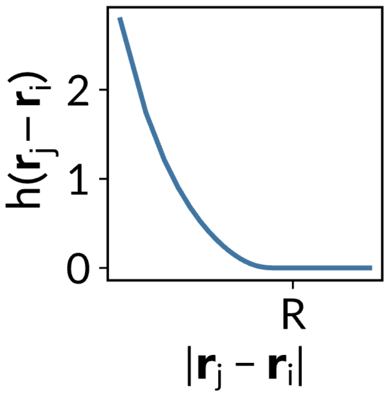
Results | Computational case studies

Cluster formation in self-organizing particles



$$\frac{d\boldsymbol{r}_i}{dt} = \sum_{j \in \mathcal{N}_R(i)} h(\boldsymbol{r}_j - \boldsymbol{r}_i)\left(1 - h(\boldsymbol{r}_j - \boldsymbol{r}_i)\right)(\boldsymbol{r}_j - \boldsymbol{r}_i)$$

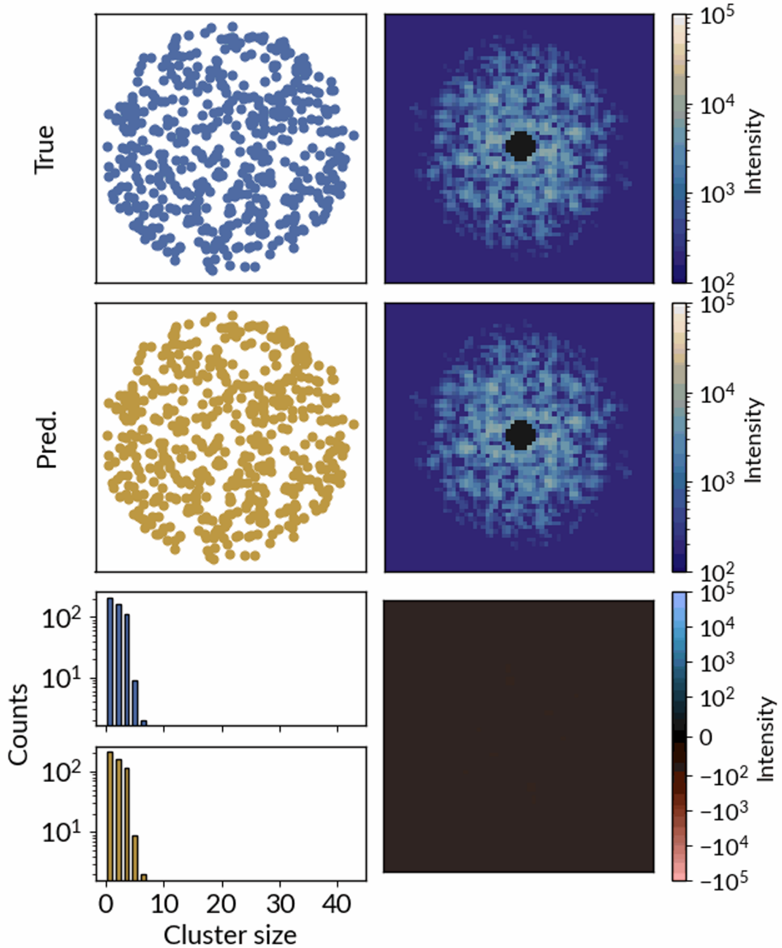
evolution of particle positions $\boldsymbol{r}_i$



K. P. O'Keeffe, *Nature communications* 8.1 (2017): 1504.

Results | Computational case studies

Cluster formation in self-organizing particles



$$\frac{d\boldsymbol{r}_i}{dt} = \sum_{j \in \mathcal{N}_R(i)} h(\boldsymbol{r}_j - \boldsymbol{r}_i)\left(1 - h(\boldsymbol{r}_j - \boldsymbol{r}_i)\right)(\boldsymbol{r}_j - \boldsymbol{r}_i)$$

evolution of particle positions $\boldsymbol{r}_i$

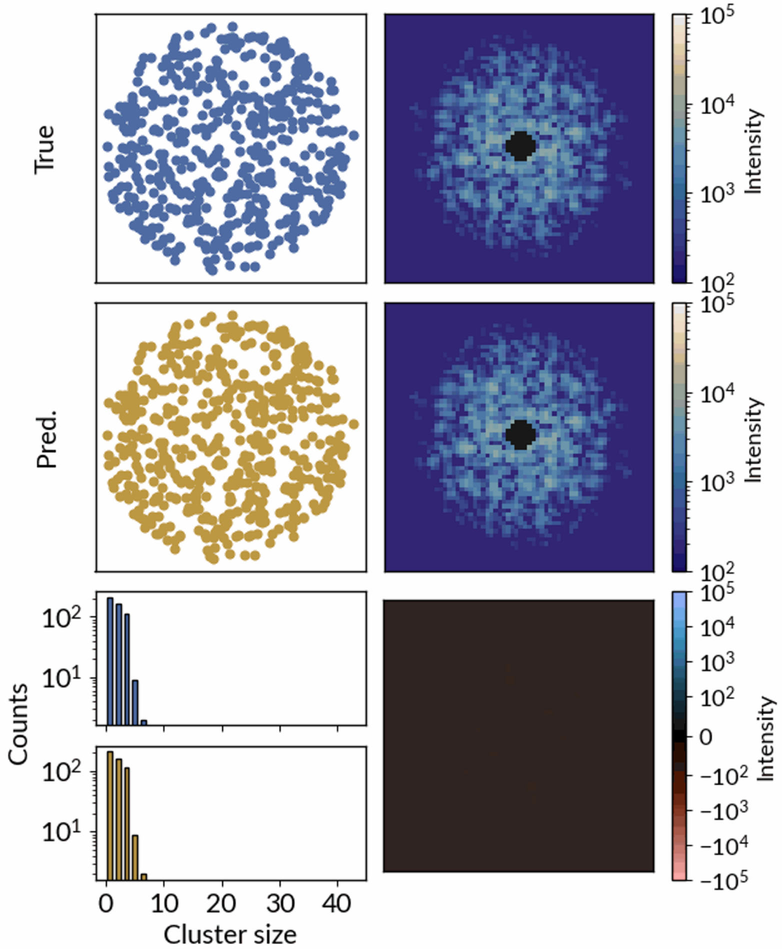
$$\frac{d\boldsymbol{r}_i}{dt} = \sum_{j \in \mathcal{N}_R(i)} f_{NN}(\boldsymbol{r}_j - \boldsymbol{r}_i; \boldsymbol{\theta})\left(1 - f_{NN}(\boldsymbol{r}_j - \boldsymbol{r}_i; \boldsymbol{\theta})\right)(\boldsymbol{r}_j - \boldsymbol{r}_i)$$

approximate unknown potential $h(\boldsymbol{r}_j - \boldsymbol{r}_i)$ using f_{NN} within a graph neural network-type architecture

N. Andrejevic, *et al. npj Computational Materials* 10.1 (2024): 225.

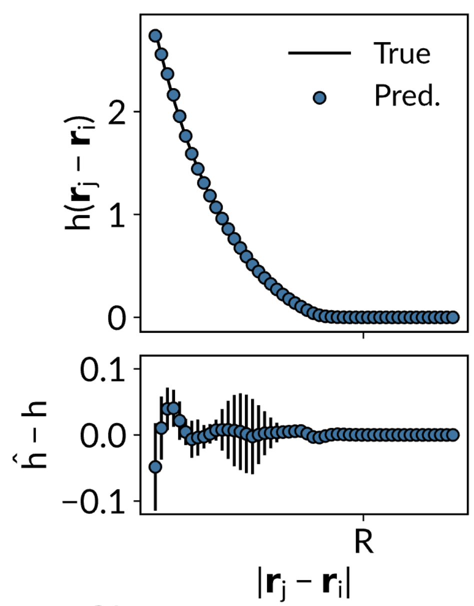
Results | Computational case studies

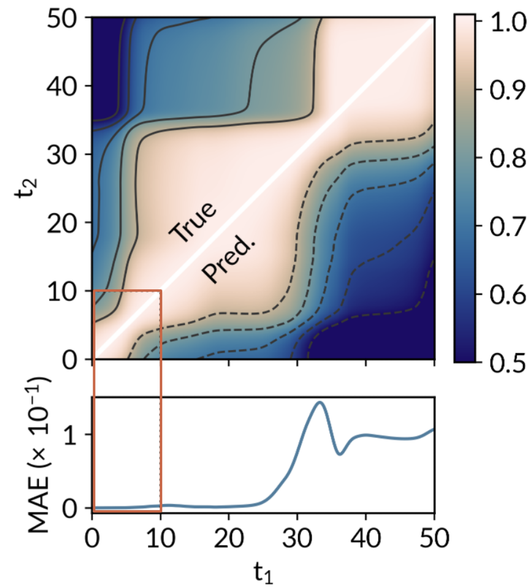
Cluster formation in self-organizing particles



$$\frac{d\boldsymbol{r}_i}{dt} = \sum_{j \in \mathcal{N}_R(i)} f_{NN}(\boldsymbol{r}_j - \boldsymbol{r}_i; \boldsymbol{\theta}) \left(1 - f_{NN}(\boldsymbol{r}_j - \boldsymbol{r}_i; \boldsymbol{\theta})\right) (\boldsymbol{r}_j - \boldsymbol{r}_i)$$

approximate unknown potential $h(\boldsymbol{r}_j - \boldsymbol{r}_i)$ using f_{NN} within a graph neural network-type architecture

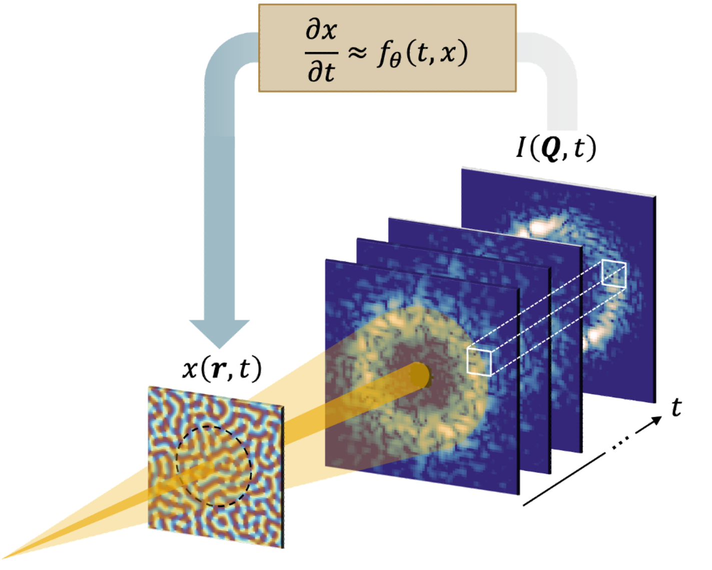




Overview

Data-driven modeling of materials characterization data

Intelligent data analysis

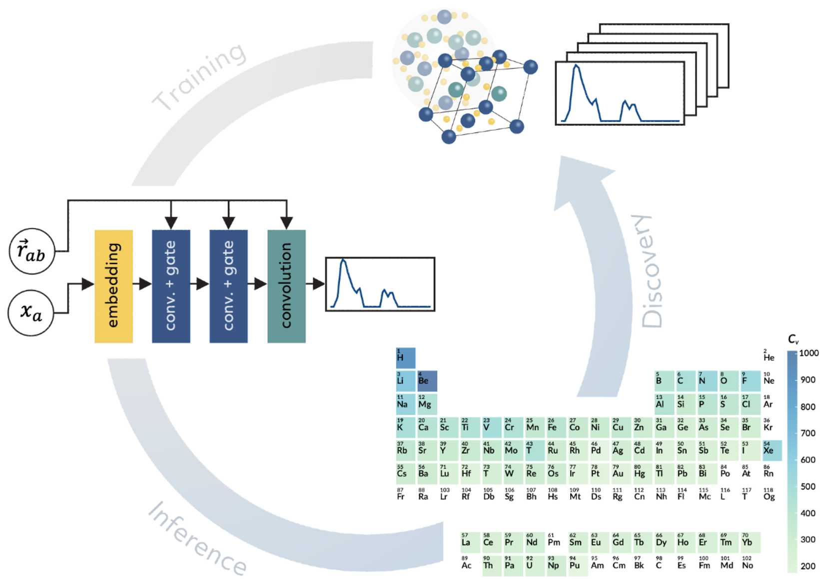


Data-driven discovery of materials' dynamics from coherent scattering

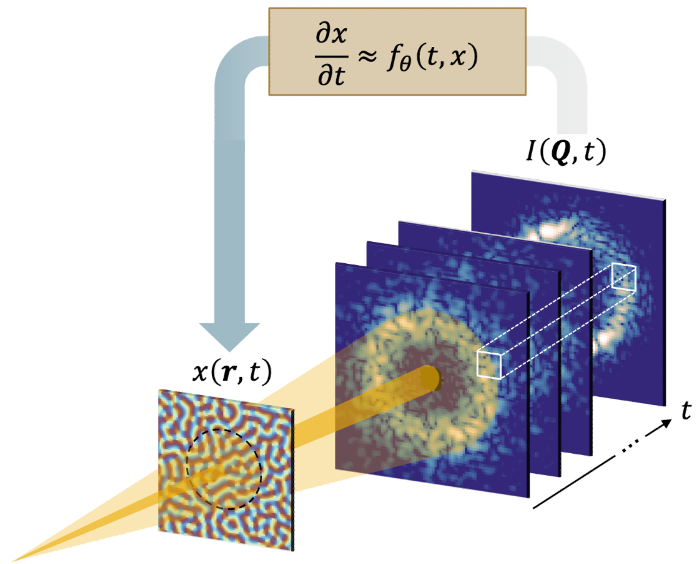
Train neural networks to model dynamics that cannot be directly observed in order to extrapolate materials behavior beyond the duration of experiments or generalize to other initial conditions

Conclusion

Accelerated property prediction



Intelligent data analysis



THANK YOU!

nandrejevic@anl.gov