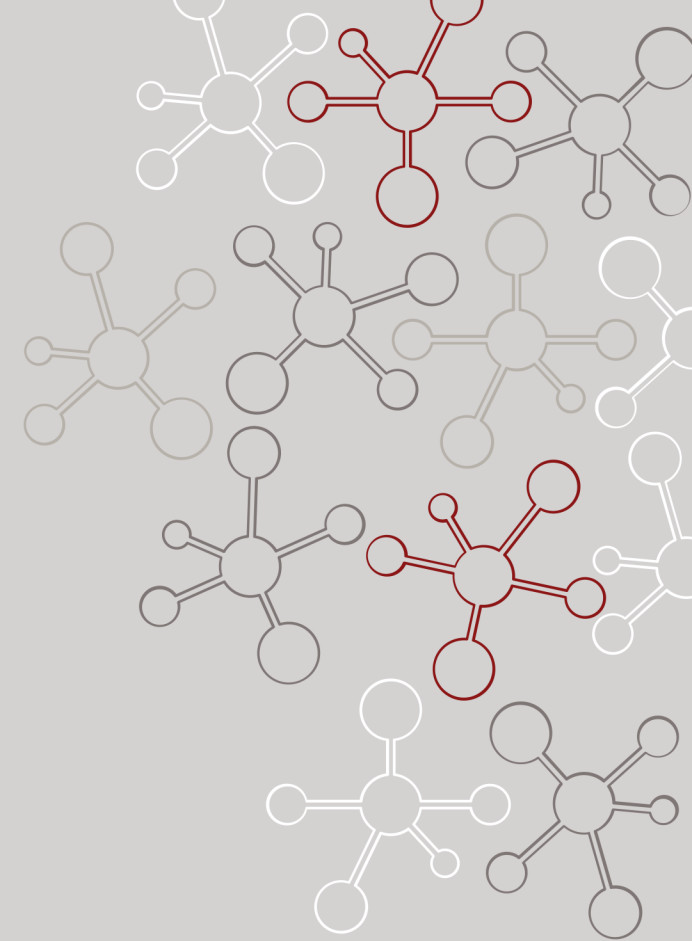


Neural Fields

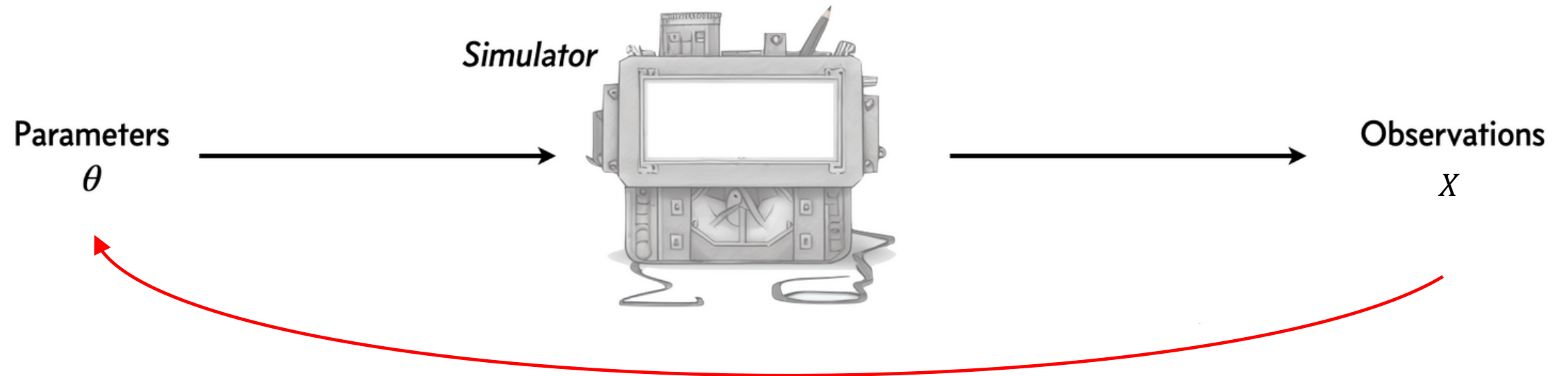
Michael Kagan
SLAC

July 21, 2023



Making use of Simulators

So far, we looked at *Simulation-Based Inference*:



Making use of Simulators

So far, we looked at *Simulation-Based Inference*:

From Lukas Heinrich: learned about *Differentiable Programming*

$$f(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$$

↓ **automatic
differentiation**

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n} \right)$$

$$f(x) \{...\};$$

↓

$$df(x) \{...\};$$

Making use of Simulators

So far, we looked at *Simulation-Based Inference*:

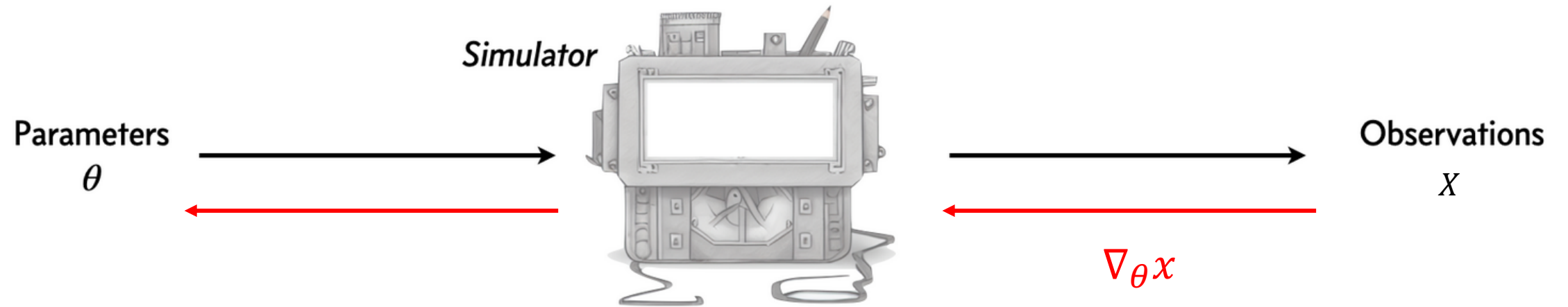
From Lukas Heinrich: learned about *Differentiable Programming*

What can we do with a differentiable simulator?

$$\frac{d}{d\theta} \mathbb{E}[L(x)] = \mathbb{E} \left[\frac{dL}{dx} \frac{dx}{d\theta} \right] = \mathbb{E} \left[\frac{dL}{dx} \frac{d}{d\theta} SIM(\theta) \right]$$

Where $x = SIM(\theta)$

Optimization through simulator



What can we do with a Differentiable Simulator?

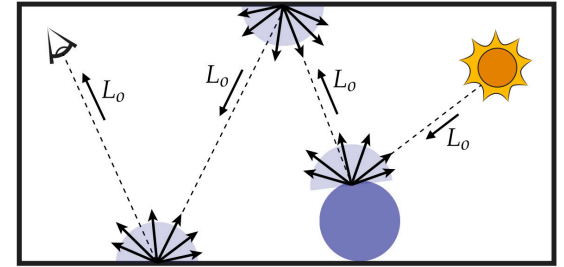


Rendering and Inverse Rendering

Rendering:

From 3D model scene, simulate image on camera at given position and angle

rendering equation



$$L(x, \vec{\omega}_o) = \int_{\mathcal{H}^2} f_r(x, \vec{\omega}_i, \vec{\omega}_o) L(x, -\vec{\omega}_i) \cos \theta d\omega_i$$

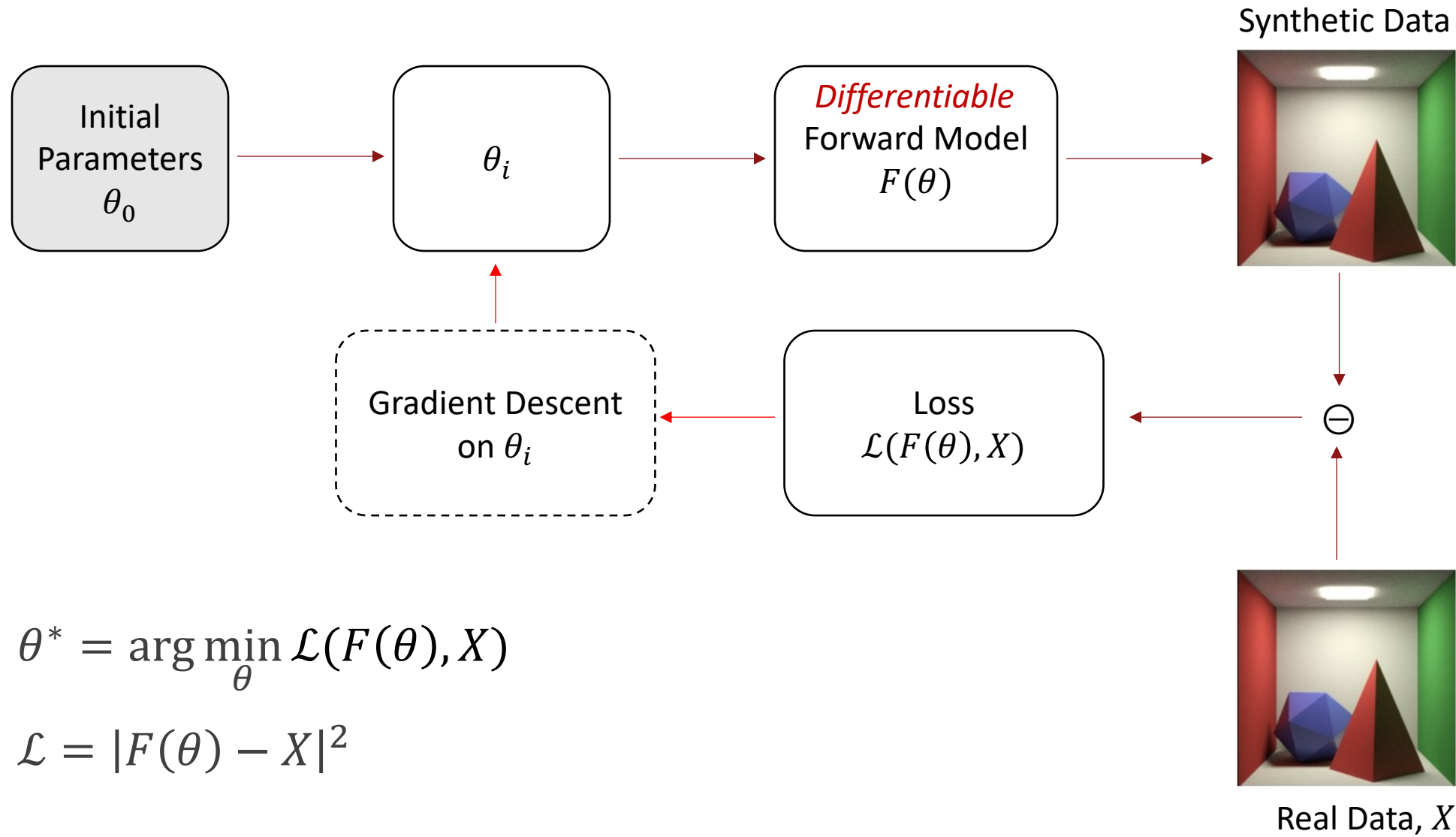
Inverse Rendering:

From multiple 2D images, reconstruct 3D model of scene

Input Images



Analysis-by-Synthesis



Analysis-by-Synthesis

Goal:

Find parameters θ such that the simulator with these parameters, $F(\theta)$, generates synthetic data that matches the observed data

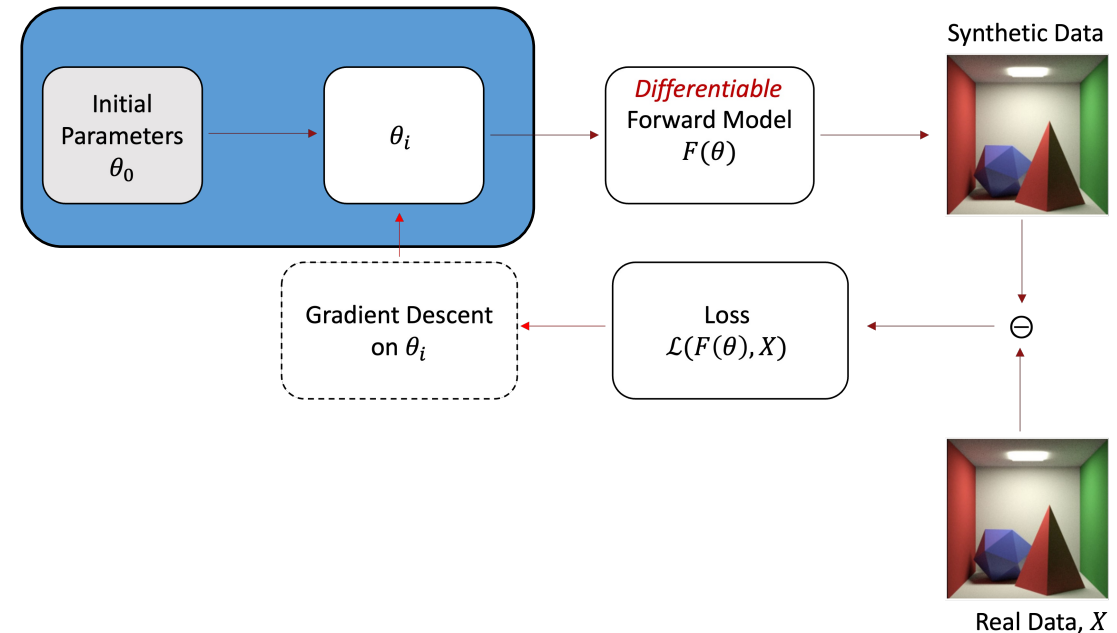
Analysis-by-Synthesis

Goal:

Find parameters θ such that the simulator with these parameters, $F(\theta)$, generates synthetic data that matches the observed data

Basic idea:

- Start with initial guess θ_0



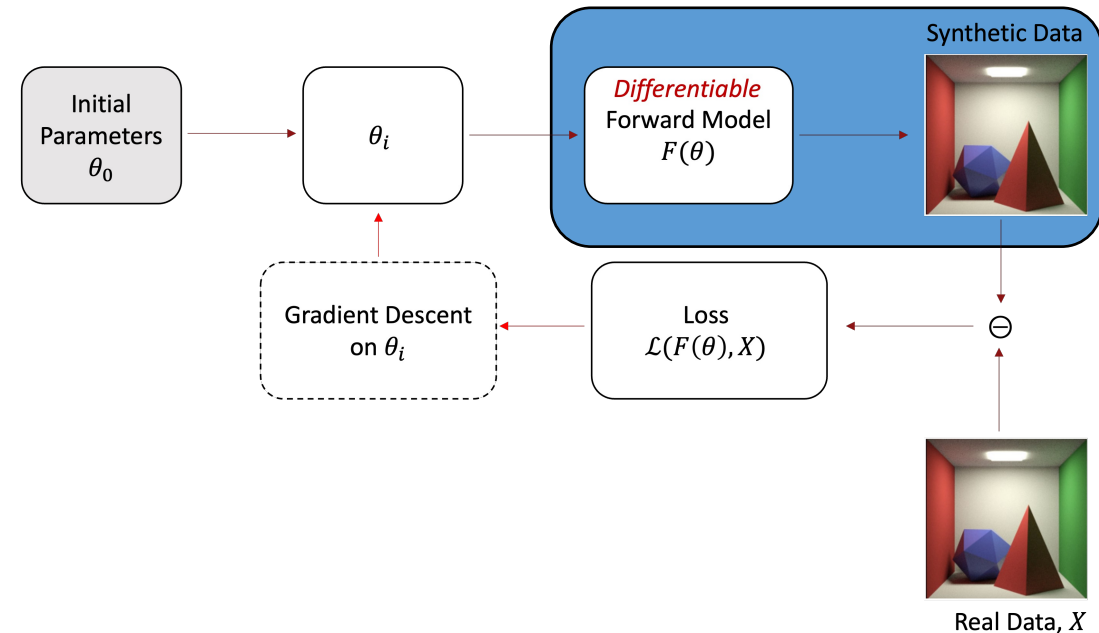
Analysis-by-Synthesis

Goal:

Find parameters θ such that the simulator with these parameters, $F(\theta)$, generates synthetic data that matches the observed data

Basic idea:

- Start with initial guess θ_0
- Given θ_i Generate synthetic data with simulator $F(\theta)$



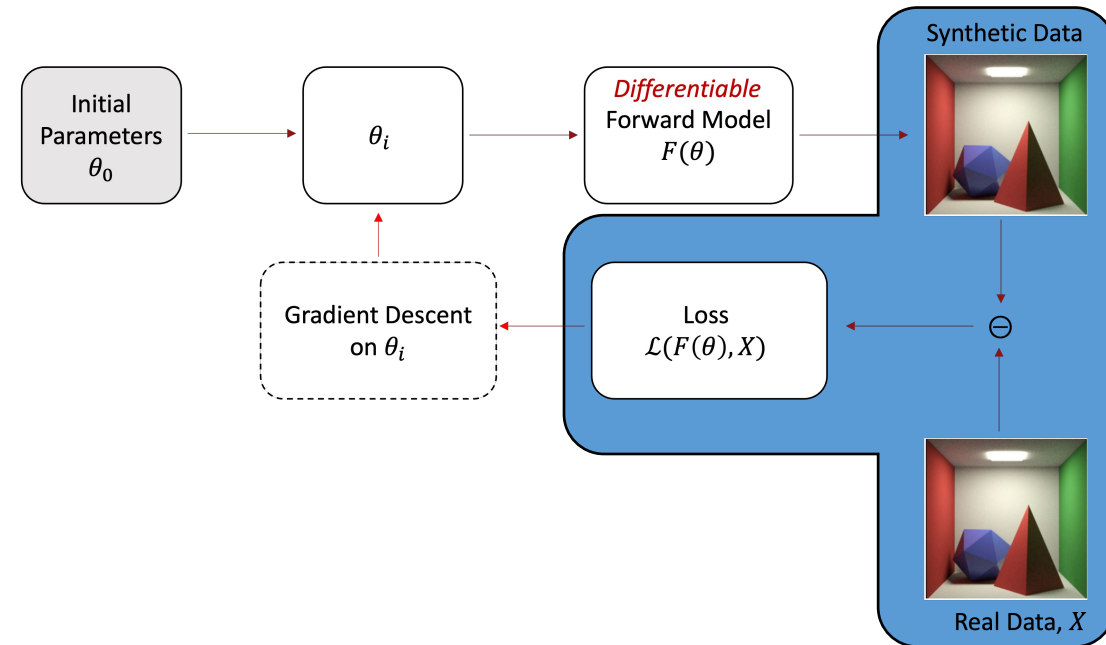
Analysis-by-Synthesis

Goal:

Find parameters θ such that the simulator with these parameters, $F(\theta)$, generates synthetic data that matches the observed data

Basic idea:

- Start with initial guess θ_0
- Given θ_i Generate synthetic data with simulator $F(\theta)$
- Loss function compares synthetic & real data



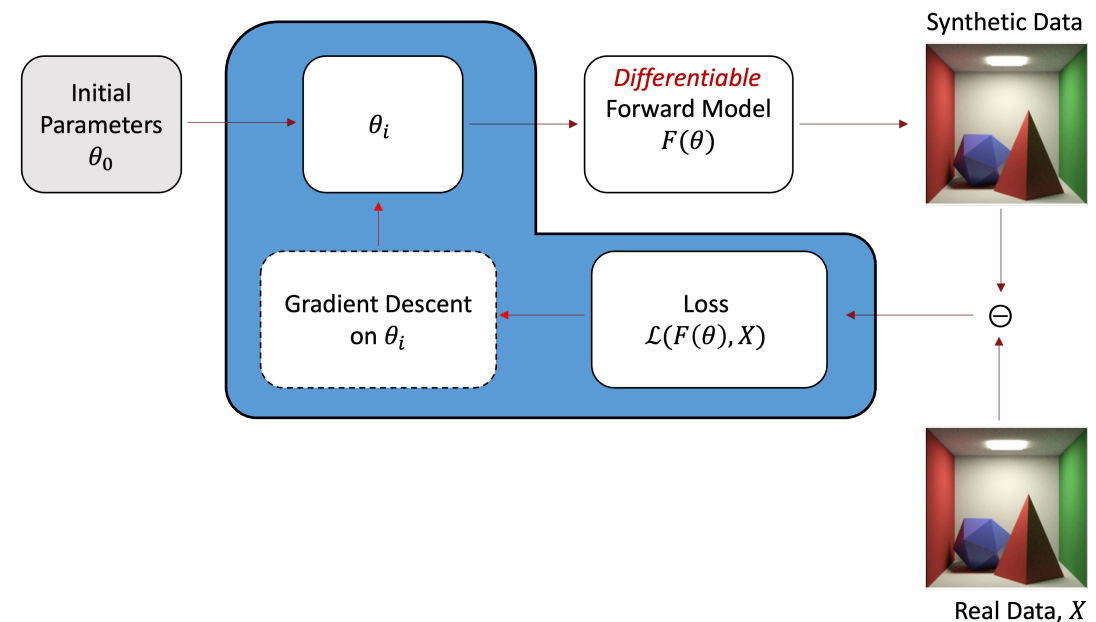
Analysis-by-Synthesis

Goal:

Find parameters θ such that the simulator with these parameters, $F(\theta)$, generates synthetic data that matches the observed data

Basic idea:

- Start with initial guess θ_0
- Given θ_i Generate synthetic data with simulator $F(\theta)$
- Loss function compares synthetic & real data
- Update θ_{i+1} to lower loss



Gradient descent with differentiable simulator: $\theta \leftarrow \theta - \eta \frac{d\mathcal{L}}{dF} \frac{dF(\theta)}{d\theta}$

What's going on here? *Maximum Likelihood Estimation*

If we assume an error model $I = F(\theta) + \epsilon$ where $\epsilon \sim N(0,1)$

Then
$$p(X|\theta) = N(F(\theta), 1)$$

And
$$\mathcal{L} = -\log p(X|\theta) = |F(\theta) - X|^2$$

What's going on here? *Maximum Likelihood Estimation*

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We get a *point estimate* for the MLE θ by solving this optimization

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And
$$\mathcal{L} = -\log p(X|\theta) = |F(\theta) - X|^2$$

We get a *point estimate* for the MLE θ by solving this optimization

Note: In general this is **NOT** an amortized process,

for each observation X , have to solve a different optimization problem

Combining partial measurements

Goal

Input Images



Measurements from different view points



Combine to form 3D model



So Why Analysis-by-Synthesis?

Reconstructing spatio-temporal signals from a set of observations

$$\mathcal{L} = \sum_i |F_i(S(\mathbf{x}, \theta)) - X_i|^2 \quad i \in \text{observations}$$

Ill-posed inverse problems: often not enough X 's to fully constrain system

Often signal $S(\cdot)$ is represented with voxels, meshes, etc... with parameters θ

$F_i \equiv$ simulation of i^{th} observation... e.g. simulate camera i at specific position

So Why Analysis-by-Synthesis?

Reconstructing spatio-temporal signals from a set of observations

$$\mathcal{L} = \sum_i |F_i(NN_{\theta}(\mathbf{x})) - X_i|^2 \quad i \in \text{observations}$$

Ill-posed inverse problems: often not enough X 's to fully constrain system

Analysis-by-Synthesis approach has recently been highly successful for reconstructing a signal parameterized by a neural network,
→ often called a *Neural Field*

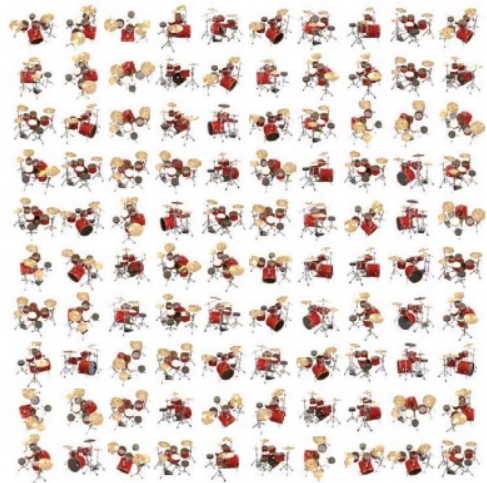
Combining partial measurements

Goal

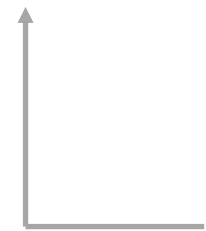
Input Images

Measurements from different view points

Combine to form 3D model



Neural Network Model of 3D system



Definition 1: A *field* is a function which assigns scalar / vector / tensor values for all spatial and / or temporal coordinates*.

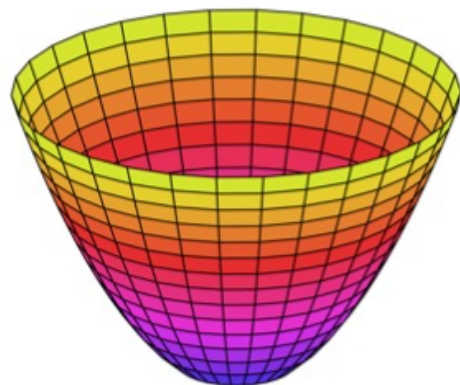
Definition 2: A *neural field* is a field that is parameterized fully or partially by a neural network.

*Sometimes over other spaces, like frequency space

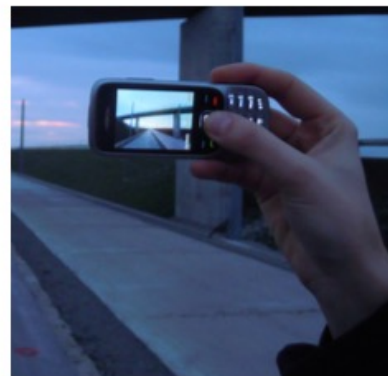
Examples of Neural Fields



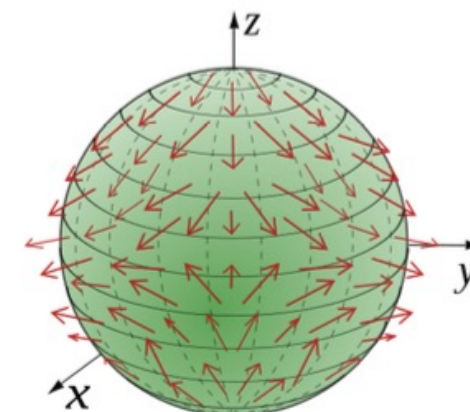
3D Signed Distance Fields
(Implicit Surface)



3D Parabola
(Explicit Surface)

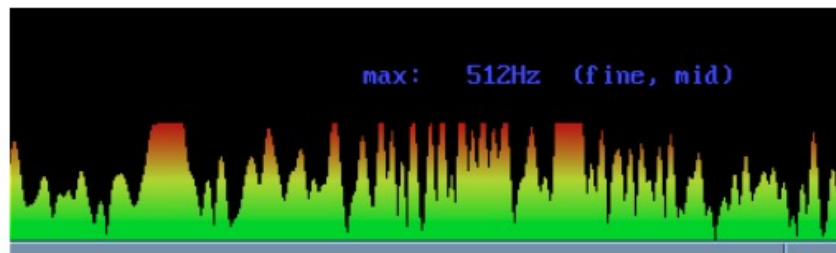


Image



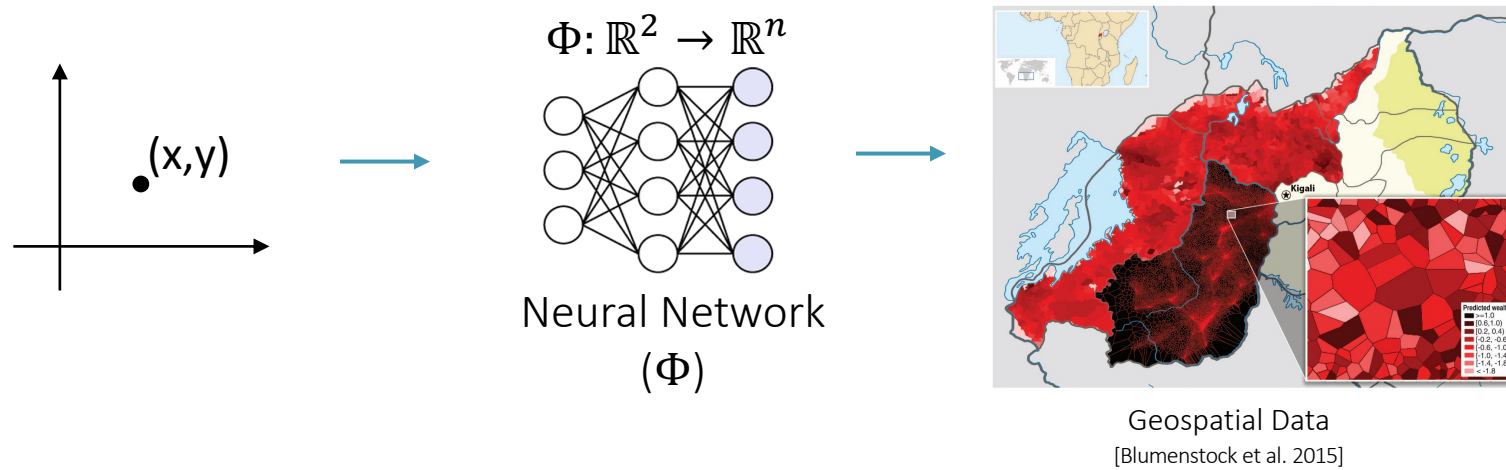
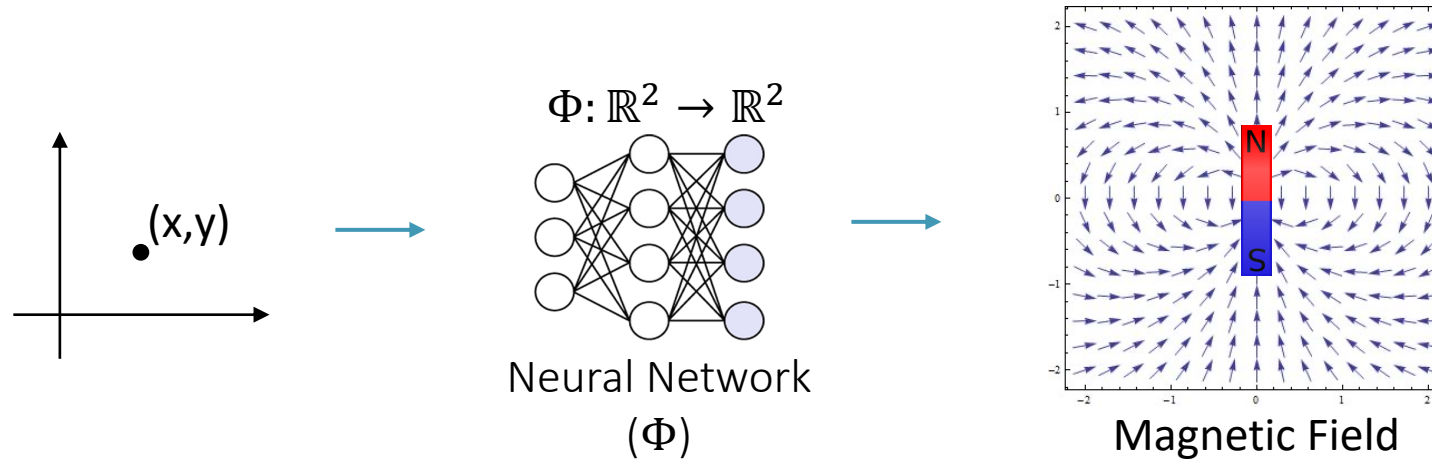
Vector Field

Fields

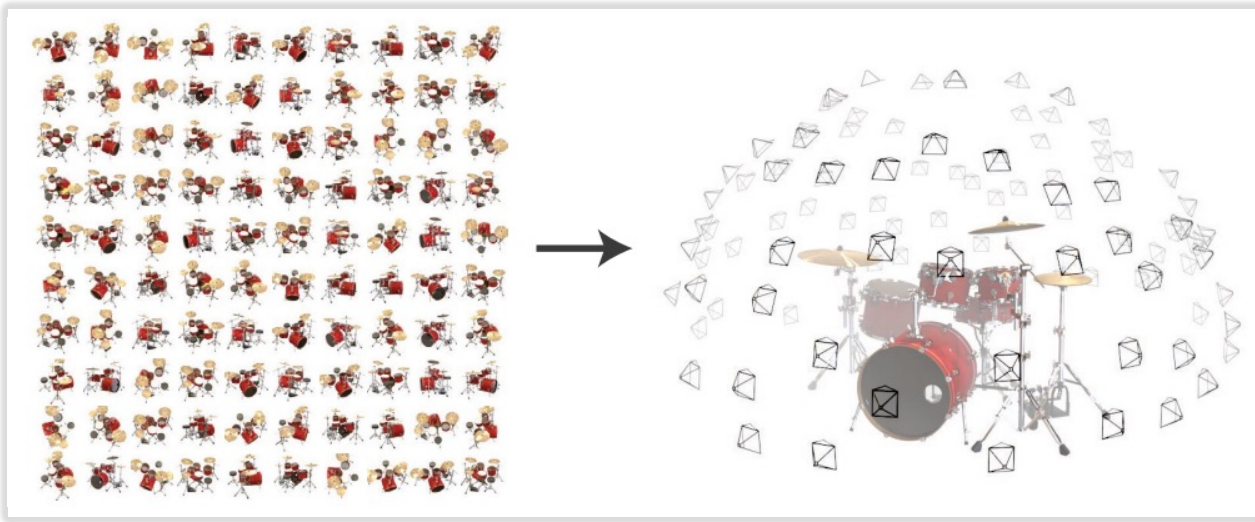


Audio

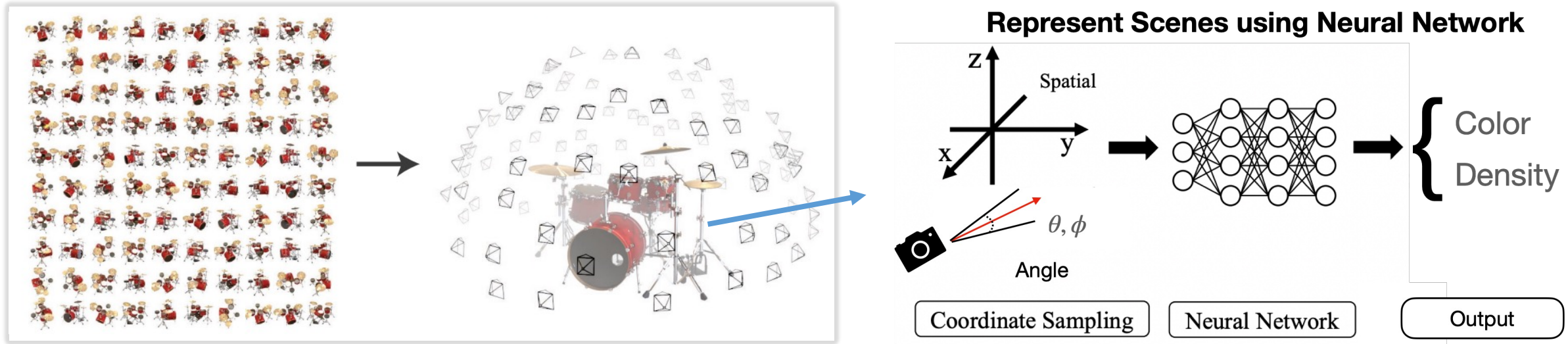
What are Neural Fields?



Neural Radiance Fields (NeRF)



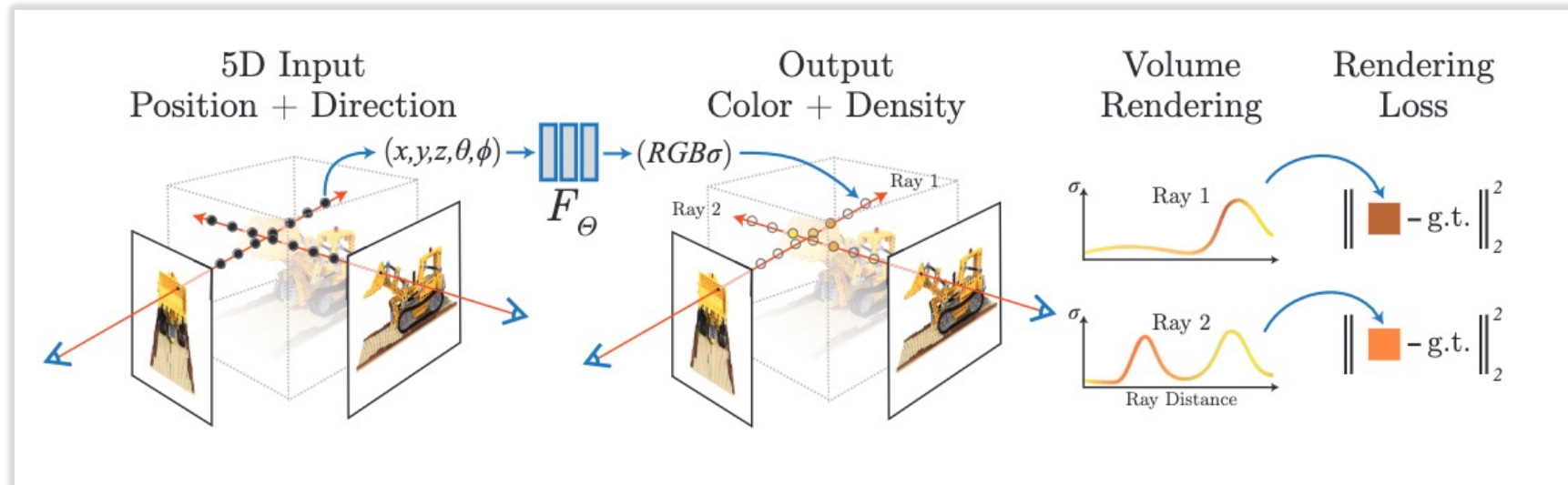
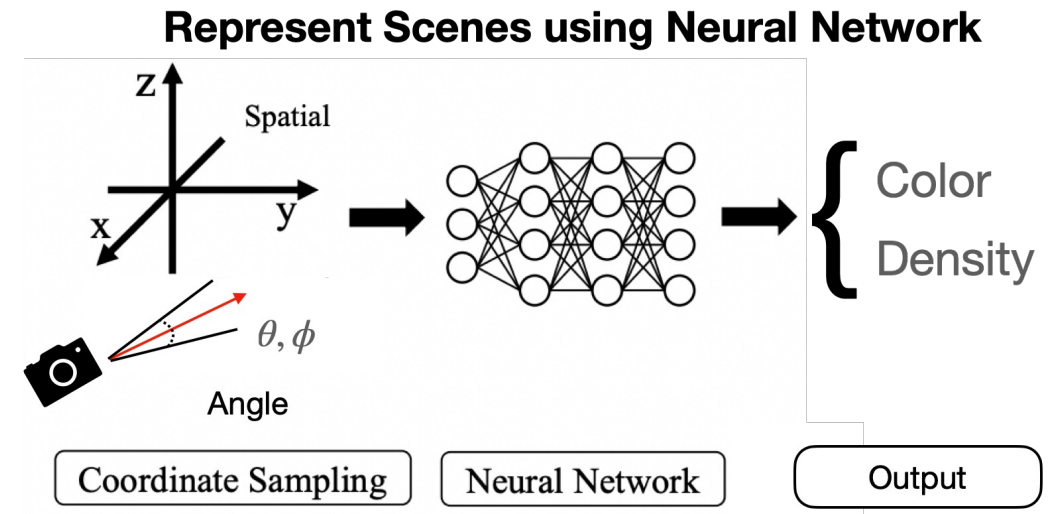
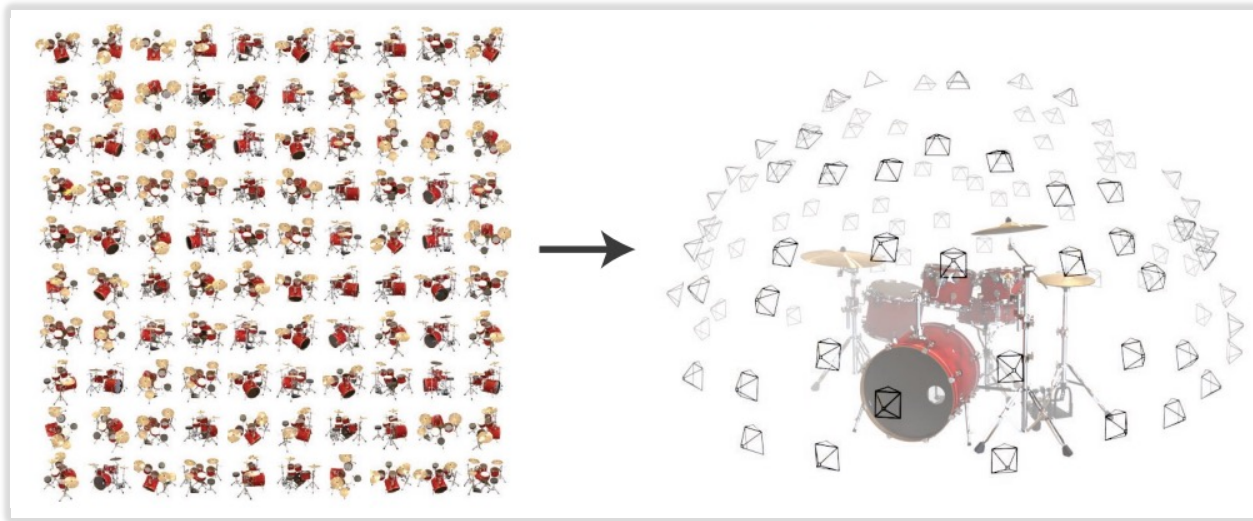
Neural Radiance Fields (NeRF)



Model 3D Object density and color using neural network

Input:
position \rightarrow neural network \rightarrow *Output:*
density & color

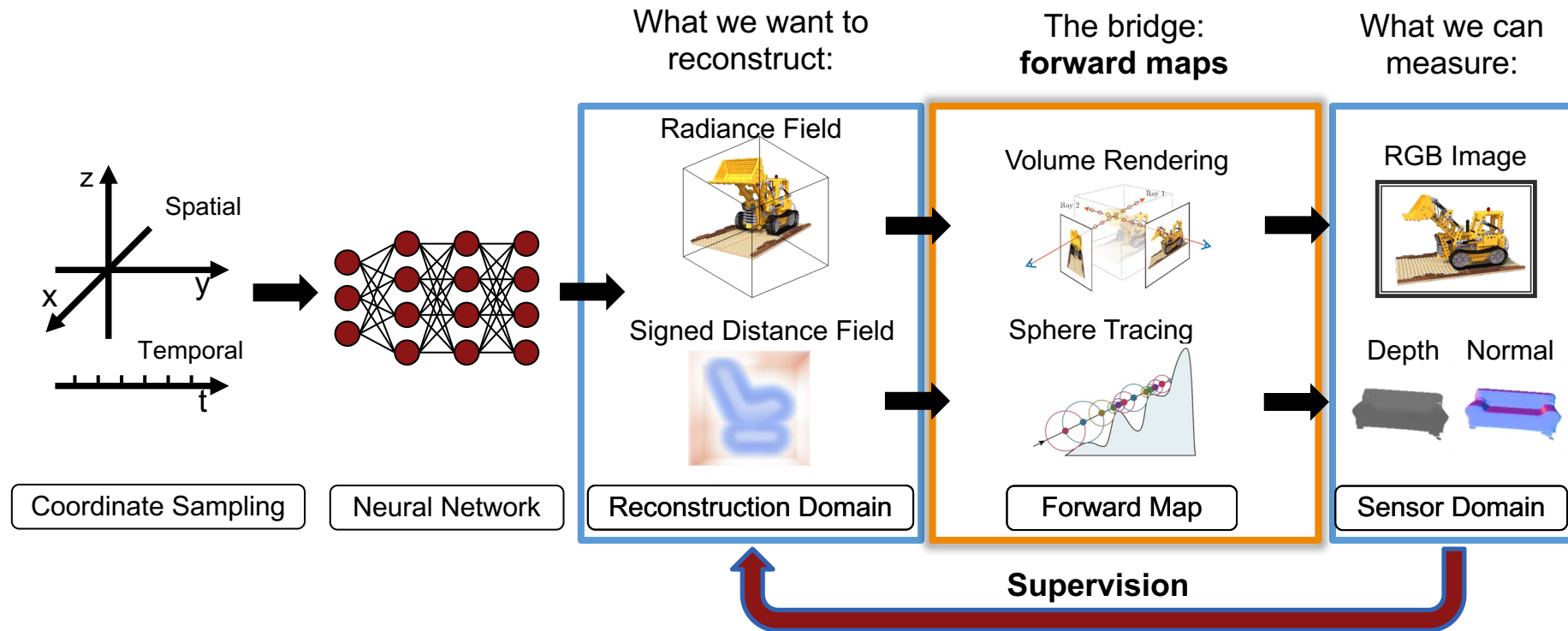
Neural Radiance Fields (NeRF)



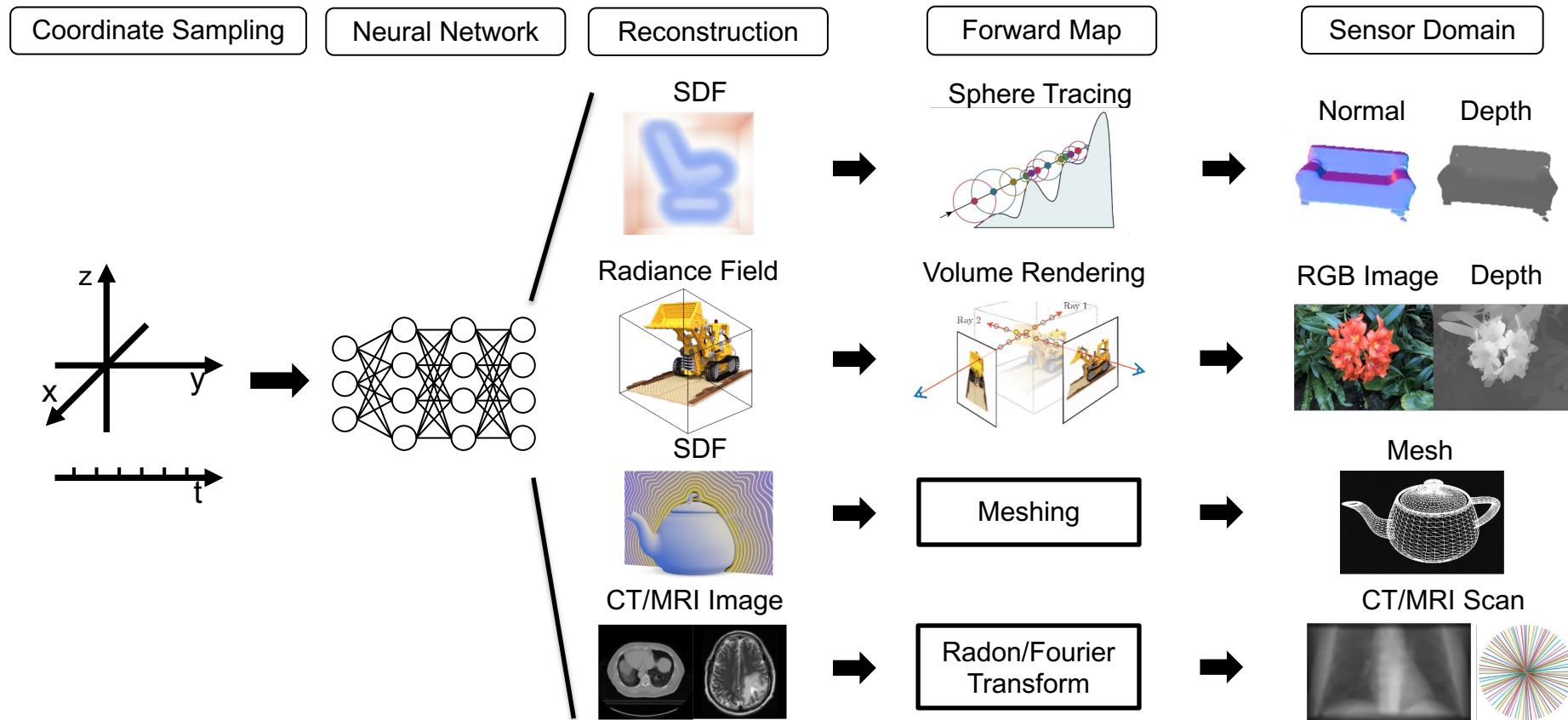
Neural Radiance Fields (NeRF)



Neural Field General Framework



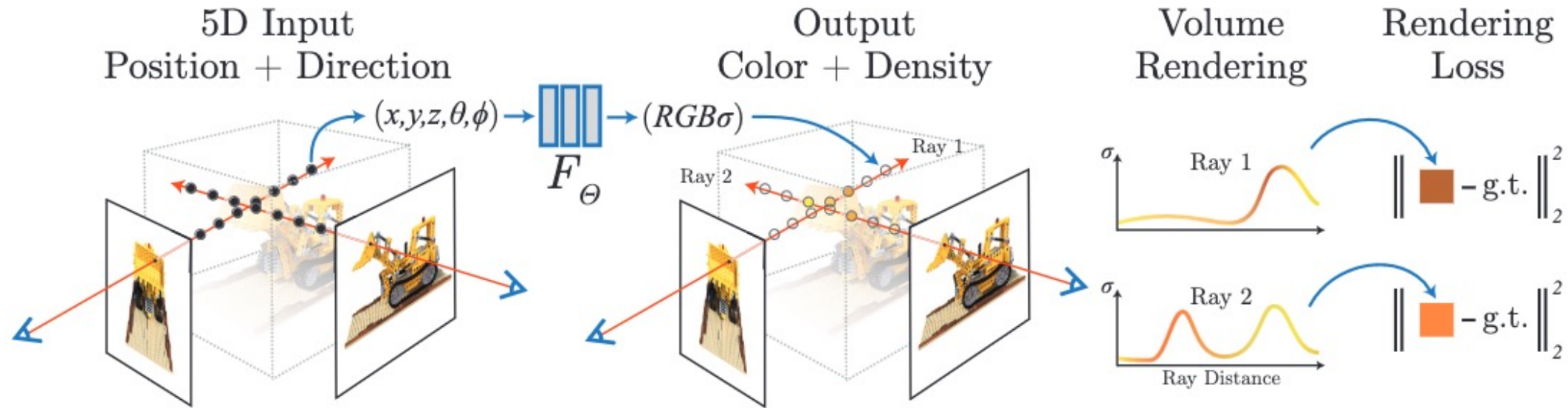
Many Applications



Figures adapted from:
Mildenhall et al. 2020 (NeRF)
Shen et al. 2021 (NeRP)

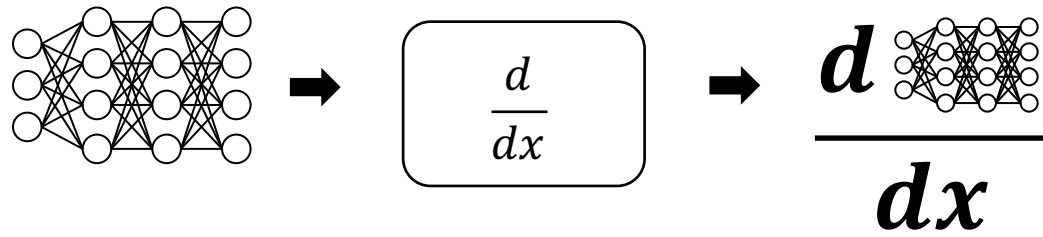
Forward Map: Differentiable Rendering

30



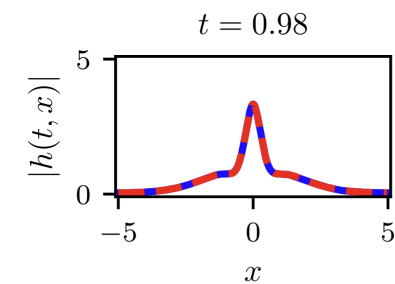
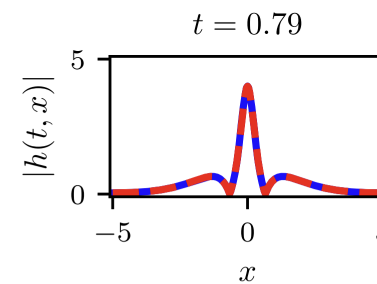
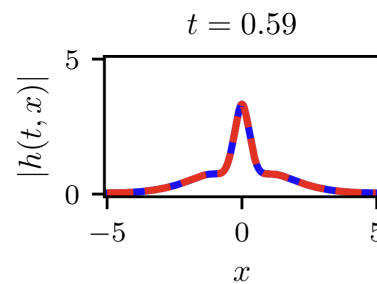
$$C(\mathbf{r}) = \int_{t_n}^{t_f} T(t) \sigma(\mathbf{r}(t)) \mathbf{c}(\mathbf{r}(t), \mathbf{d}) dt, \text{ where } T(t) = \exp\left(-\int_{t_n}^t \sigma(\mathbf{r}(s)) ds\right)$$

Neural Fields + Differential Equations: Physics-Informed Neural Networks (PINN)



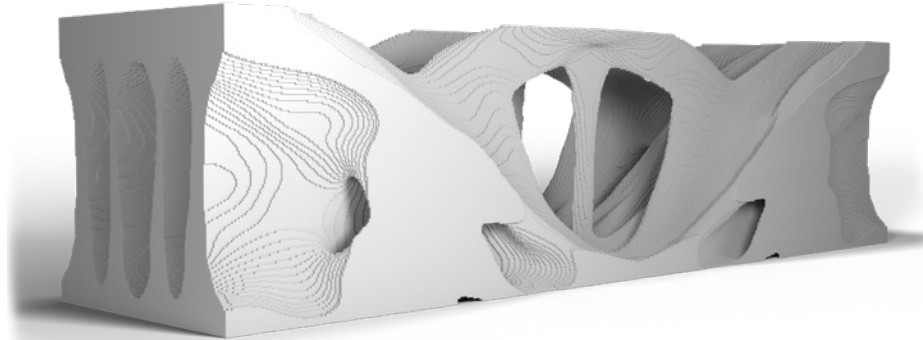
Schrödinger's Equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$$

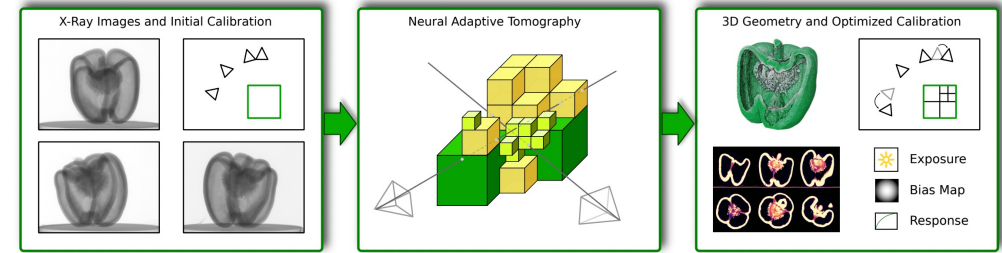


— Exact - - - Prediction

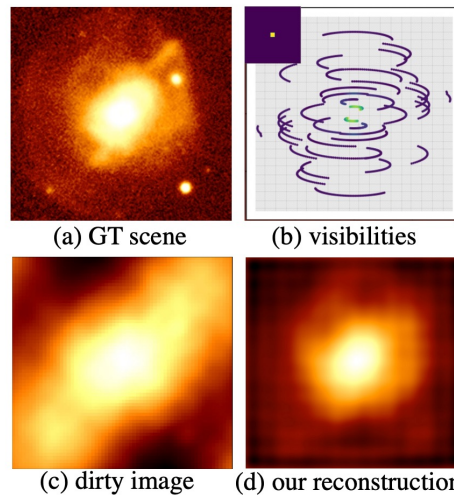
Neural Fields in Science and Engineering



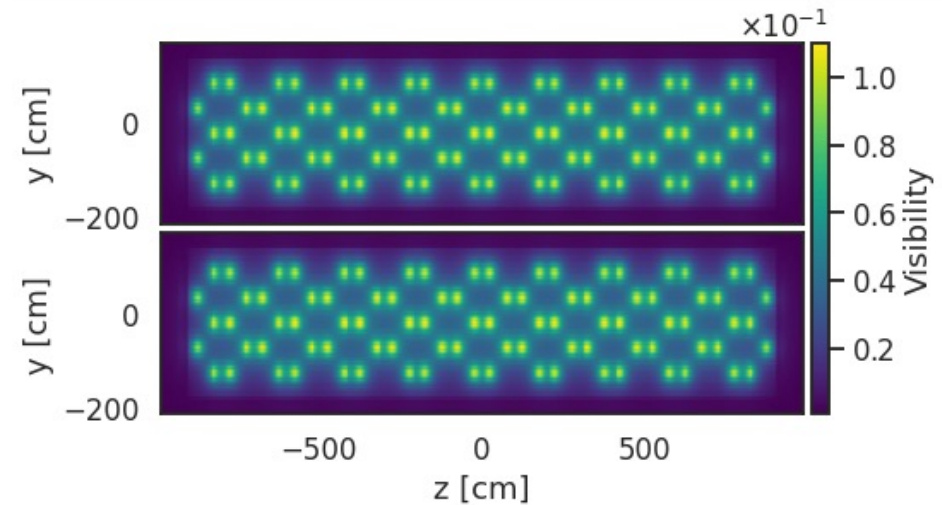
Topology Optimization [[Doosti et al. 2021](#)]



Tomographic Reconstruction [[Ruckert et al. 2022](#)]



Astronomical Interferometry [[Wu et al. 2021](#)]

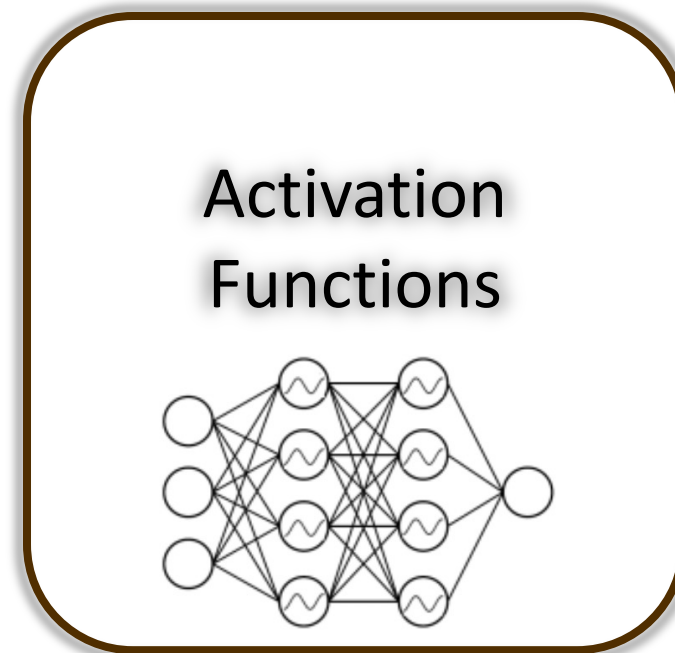
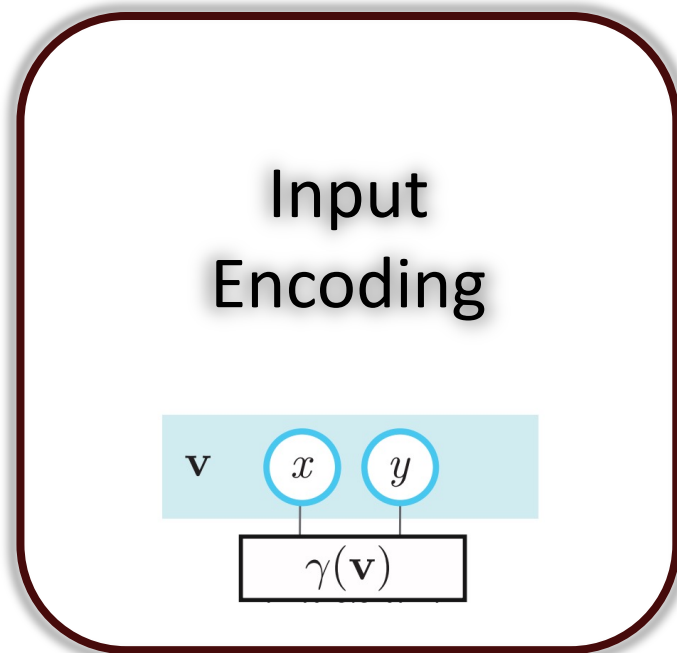


Neutrino Detectors [2211.01505](#)

Model Structures

Many of the neural networks in are relatively simple MLPs, well placed within the synthesis pipeline.

A few novel(-ish) features, especially for modeling spatio-temporal data



On the Spectral Bias of Neural Networks

Nasim Rahaman^{*1,2} Aristide Baratin^{*1} Devansh Arpit¹ Felix Draxler² Min Lin¹ Fred A. Hamprecht²
Yoshua Bengio¹ Aaron Courville¹

Abstract

Neural networks are known to be a class of highly expressive functions able to fit even random input-output mappings with 100% accuracy. In this work we present properties of neural networks that complement this aspect of expressivity. By using tools from Fourier analysis, we highlight a learning bias of deep networks towards low frequency functions – i.e. functions that vary globally without local fluctuations – which manifests itself as a frequency-dependent learning speed. Intuitively, this property is in line with the observation that over-parameterized networks prioritize learning simple patterns that generalize across data samples. We also investigate the role of the shape of the data manifold by presenting empirical and theoretical evidence that, somewhat counter-intuitively, learning higher frequencies gets *easier* with increasing manifold complexity.

1. Introduction

The remarkable success of deep neural networks at generalizing to natural data is at odds with the traditional notions of model complexity and their empirically demonstrated ability to fit arbitrary random data to perfect accuracy (Zhang et al., 2017a; Arpit et al., 2017). This has prompted recent investigations of possible implicit regularization mechanisms inherent in the learning process which induce a bias towards low complexity solutions (Neyshabur et al., 2014; Soudry et al., 2017; Poggio et al., 2018; Neyshabur et al., 2017).

In this work, we take a slightly shifted view on implicit regularization by suggesting that low-complexity functions are *learned faster* during training by gradient descent. We

^{*}Equal contribution ¹Mila, Quebec, Canada ²Image Analysis and Learning Lab, Ruprecht-Karls-Universität Heidelberg, Germany. Correspondence to: Nasim Rahaman <nasim.rahaman@live.com>, Aristide Baratin <aristide.baratin@umontreal.ca>, Devansh Arpit <devansharpit@gmail.com>.

Proceedings of the 36th International Conference on Machine Learning, Long Beach, California, PMLR 97, 2019. Copyright 2019 by the author(s).

expose this bias by taking a closer look at neural networks through the lens of Fourier analysis. While they can approximate arbitrary functions, we find that these networks prioritize learning the low frequency modes, a phenomenon we call the *spectral bias*. This bias manifests itself not just in the process of learning, but also in the parameterization of the model itself: in fact, we show that the lower frequency components of trained networks are more robust to random parameter perturbations. Finally, we also expose and analyze the rather intricate interplay between the spectral bias and the geometry of the data manifold by showing that high frequencies get easier to learn when the data lies on a lower-dimensional manifold of complex shape embedded in the input space of the model. We focus the discussion on networks with rectified linear unit (ReLU) activations, whose continuous piece-wise linear structure enables an analytic treatment.

Contributions¹

1. We exploit the continuous piecewise-linear structure of ReLU networks to evaluate its Fourier spectrum (Section 2).
2. We find empirical evidence of a *spectral bias*: i.e. lower frequencies are learned first. We also show that lower frequencies are more robust to random perturbations of the network parameters (Section 3).
3. We study the role of the shape of the data manifold: we show how complex manifold shapes can facilitate the learning of higher frequencies and develop a theoretical understanding of this behavior (Section 4).

2. Fourier analysis of ReLU networks

2.1. Preliminaries

Throughout the paper we call ‘ReLU network’ a scalar function $f: \mathbb{R}^d \mapsto \mathbb{R}$ defined by a neural network with L hidden layers of widths d_1, \dots, d_L and a single output neuron:

$$f(\mathbf{x}) = \left(T^{(L+1)} \circ \sigma \circ T^{(L)} \circ \dots \circ \sigma \circ T^{(1)} \right) (\mathbf{x}) \quad (1)$$

¹Code: <https://github.com/nasimrahaman/SpectralBias>

“Neural networks are biased to fit lower frequency signals”

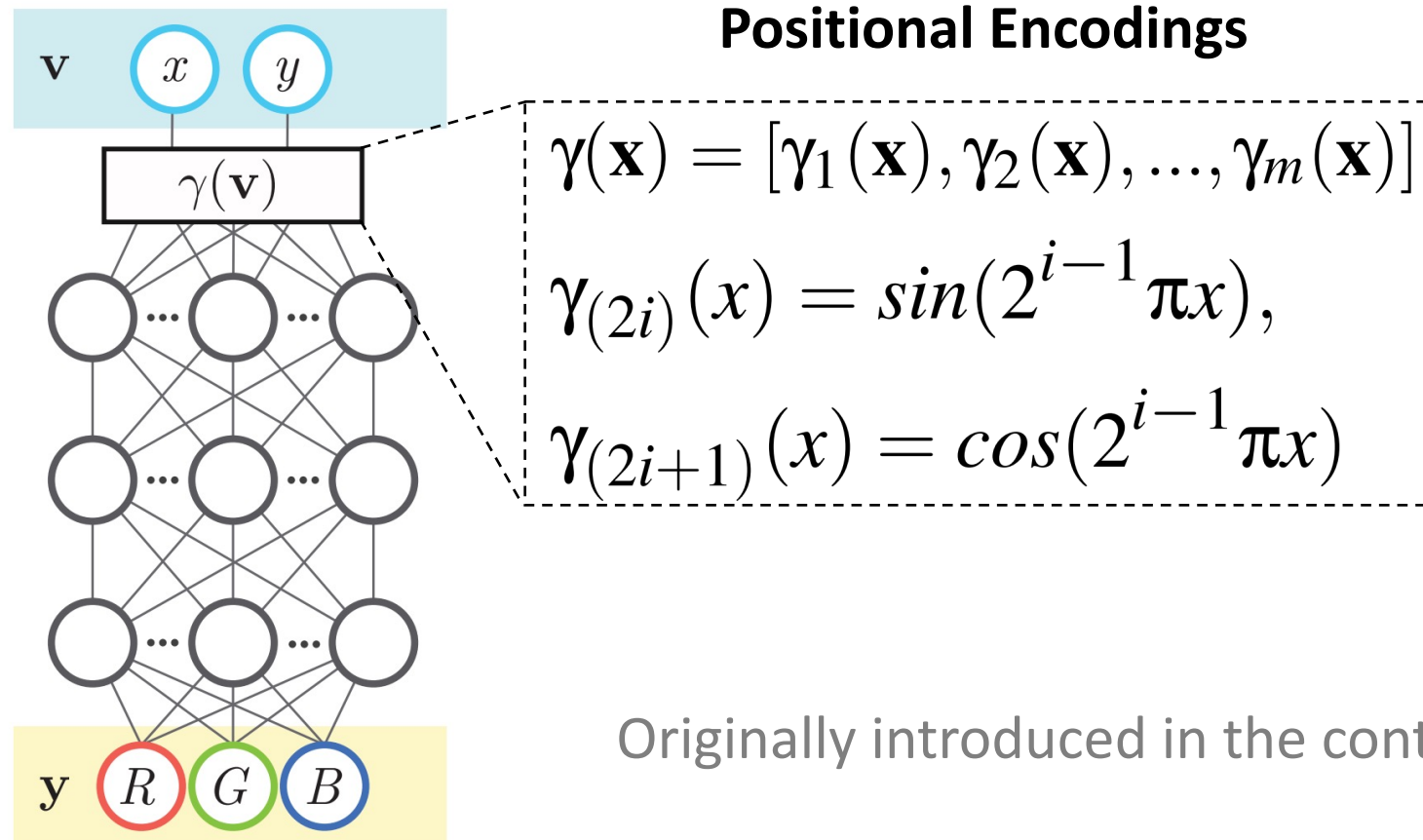


[Baatz et al. 2021]

That’s a problem if we want to learn fine details!

Positional Encoding

Map input value x to a vector of sine & cosine values at different frequencies

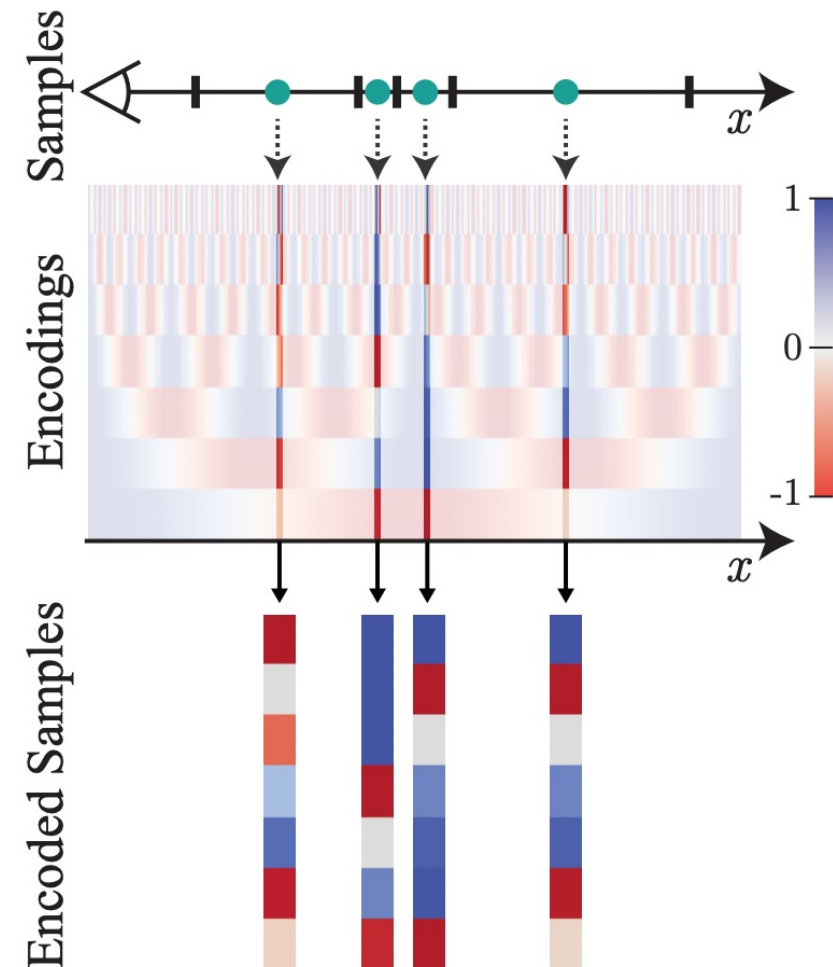


Originally introduced in the context of transformers

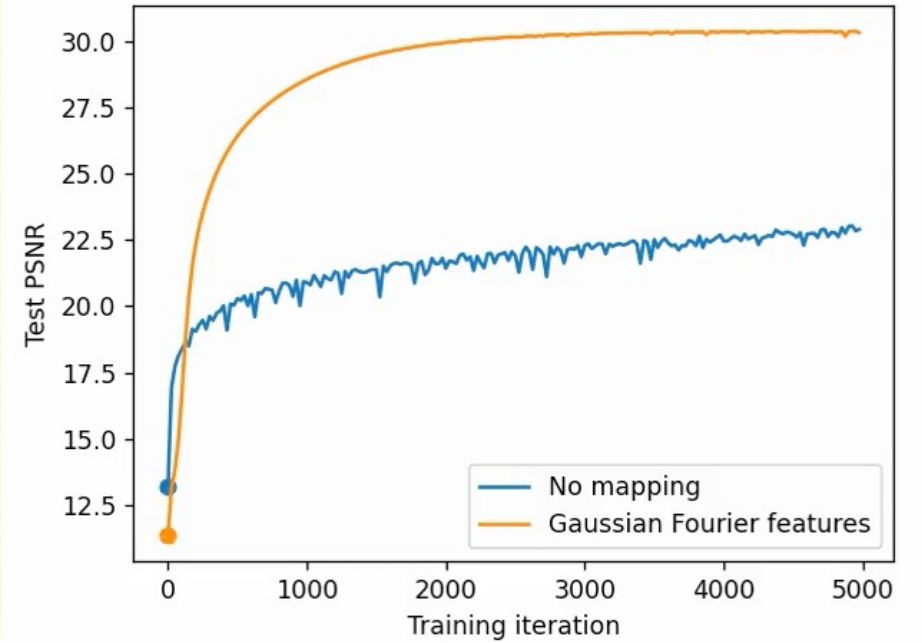
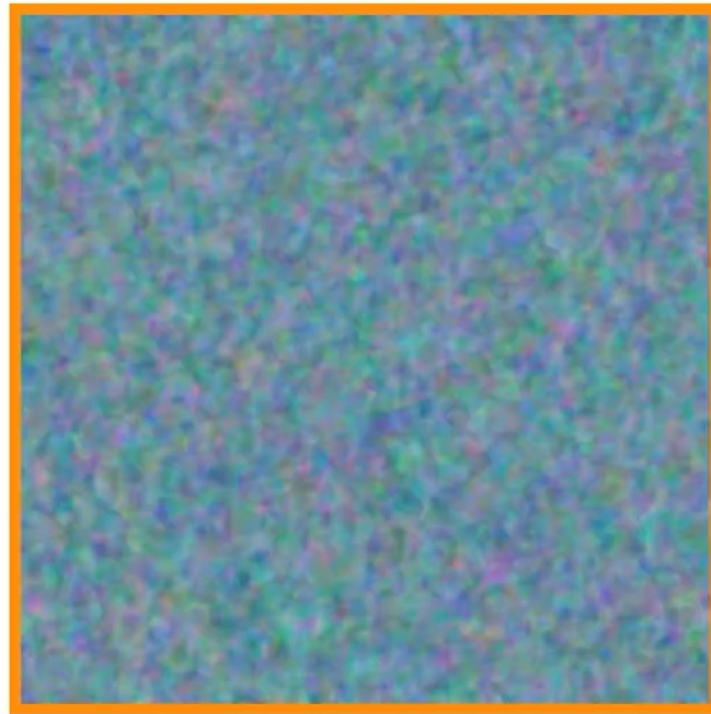
Positional Encoding

Map input value x to a vector of sine & cosine values at different frequencies

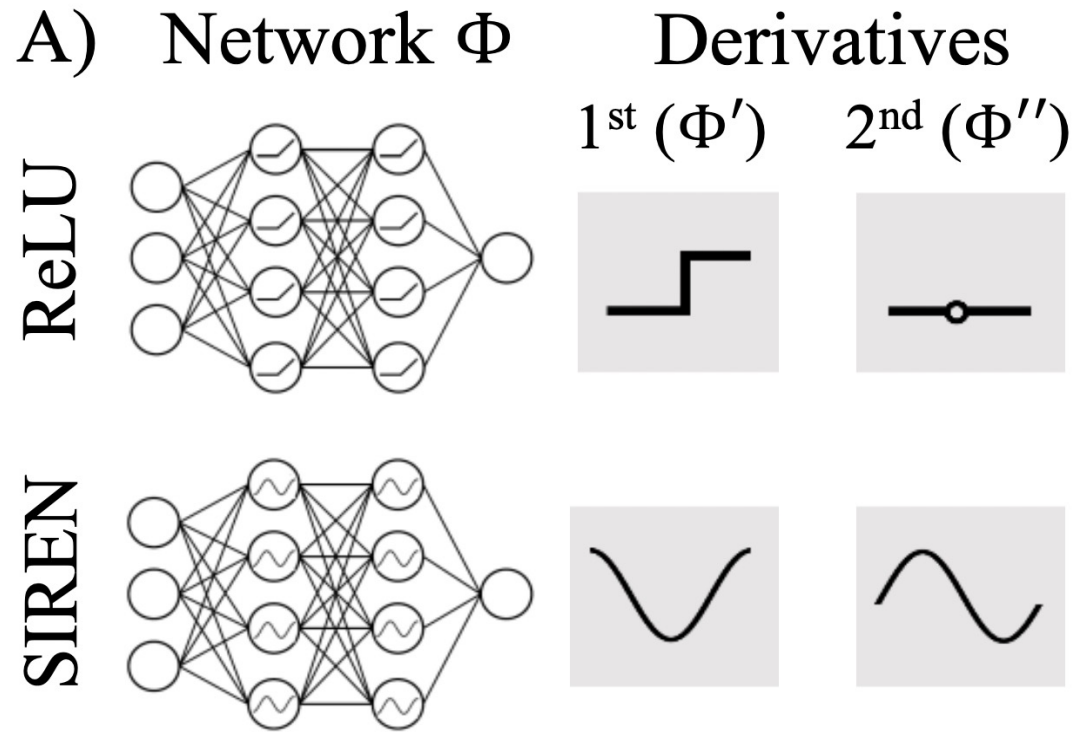
$$\gamma(\mathbf{x}) = [\sin(\mathbf{x}), \cos(\mathbf{x}), \dots, \sin(2^{L-1}\mathbf{x}), \cos(2^{L-1}\mathbf{x})]^T$$



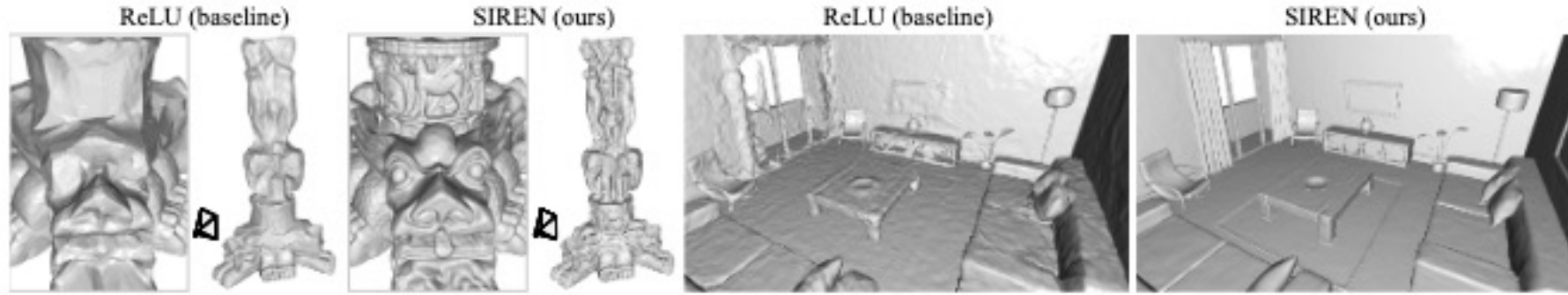
Positional Encoding In Action



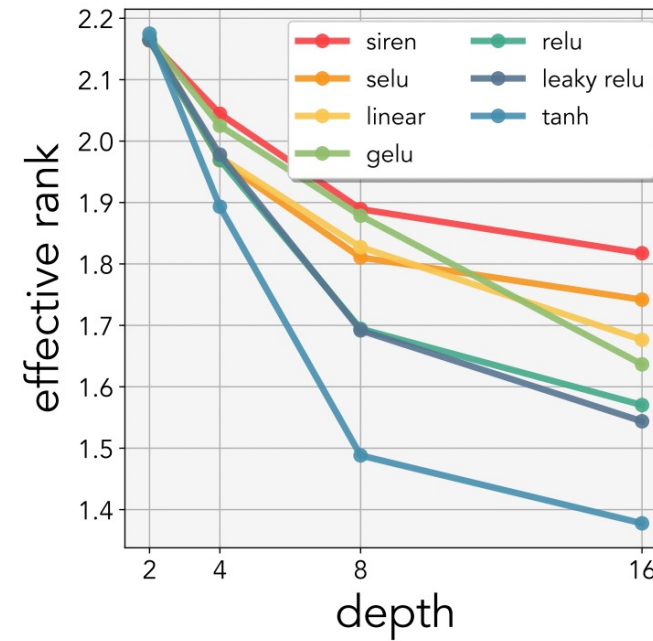
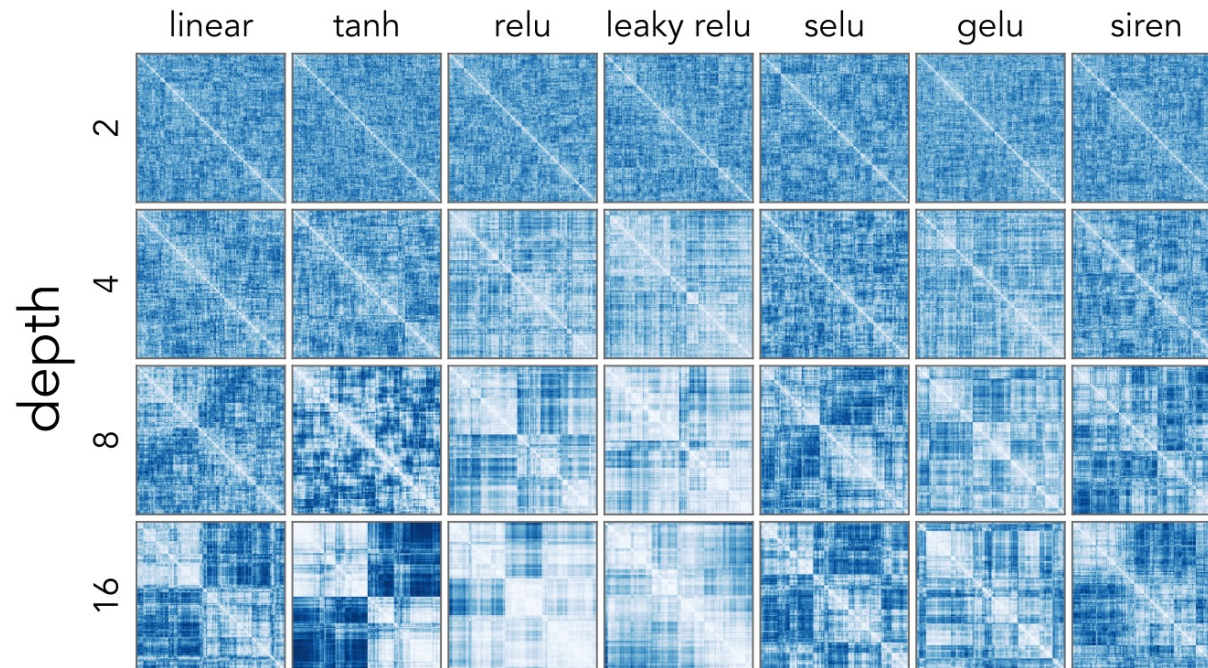
Activation Functions



Activation Functions



[2006.09661](https://arxiv.org/abs/2006.09661)



[2103.10427](https://arxiv.org/abs/2103.10427)

A few points on why neural fields?

Compact:

Can efficiently summarize signals without dense grids

Combining measurements lets us surpass resolution of any one measurement

Regularization:

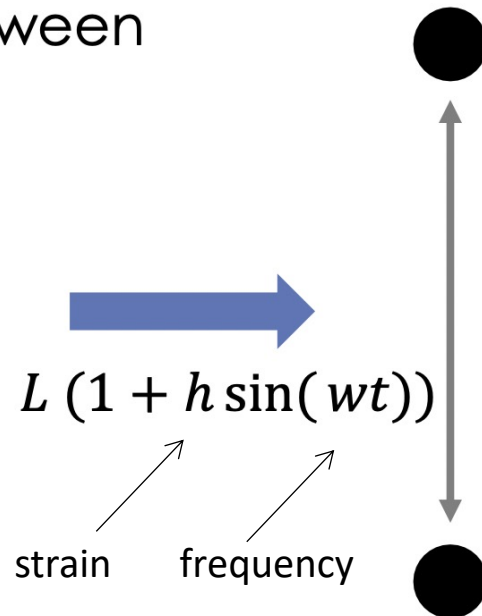
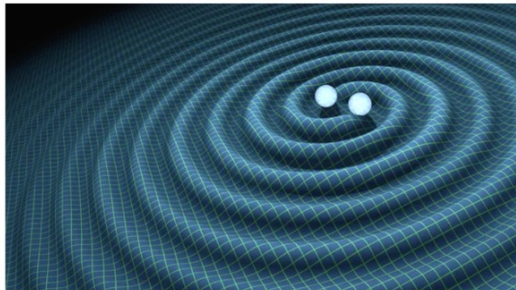
Explicit regularization: in the form of priors: $\min_{\theta} |F(NN_{\theta}(x)) - I|^2 + \Omega(NN(\theta))$

- E.g. total variation, constraining model smoothness $\nabla_x NN_{\theta}(x)$

Implicit regularization: NN imposes implicit priors in the form of architecture choice which determines the set of functions we can fit to data and how we interpolate

Application for MAGIS-100 Experiment

Gravitational waves cause a small modulation in the distance between objects



In MAGIS, atoms play two roles

Inertial References

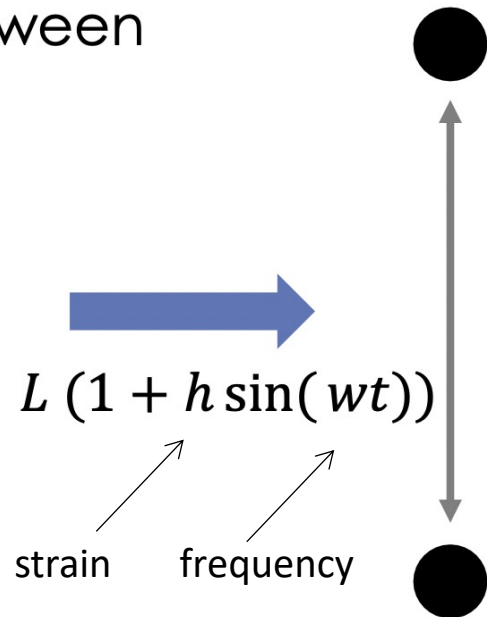
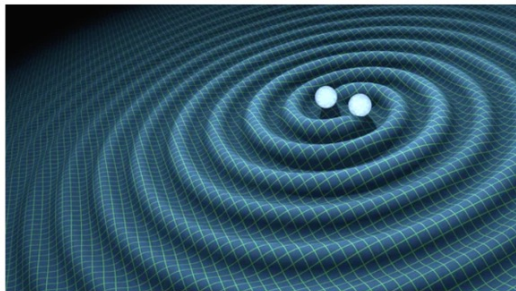
- Freely falling objects, separated by a large baseline
- Must be insensitive to perturbations from non-gravitational forces

Clock

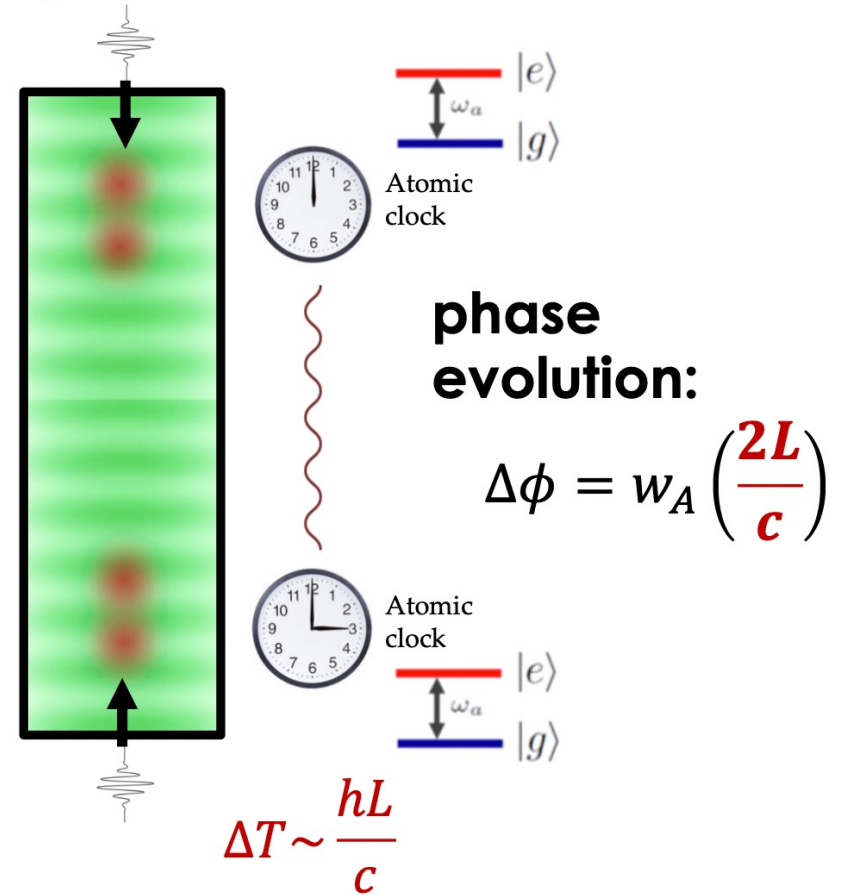
- Monitor separation b/w inertial frames
- Measure time for light to cross baseline

Atomic Sensors

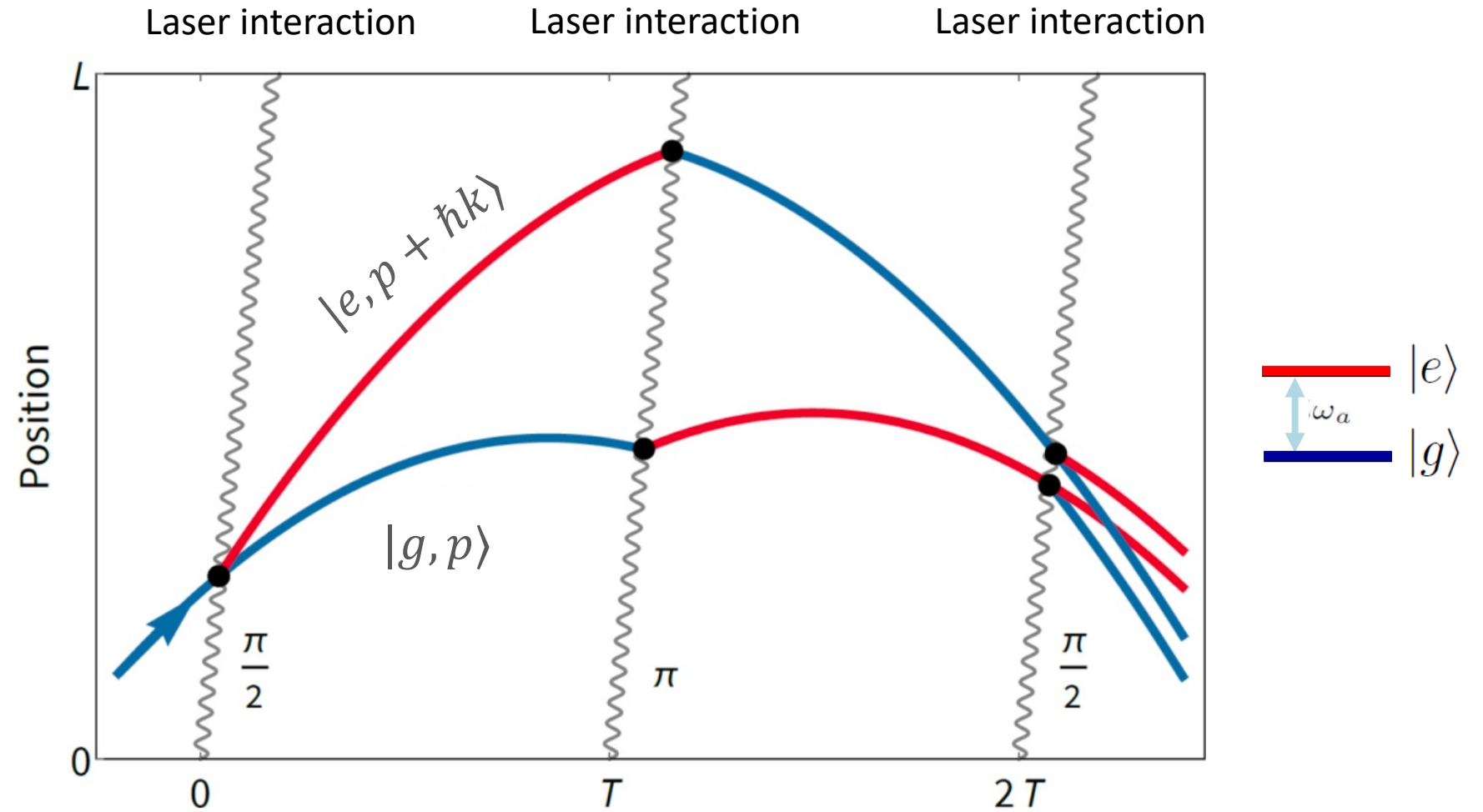
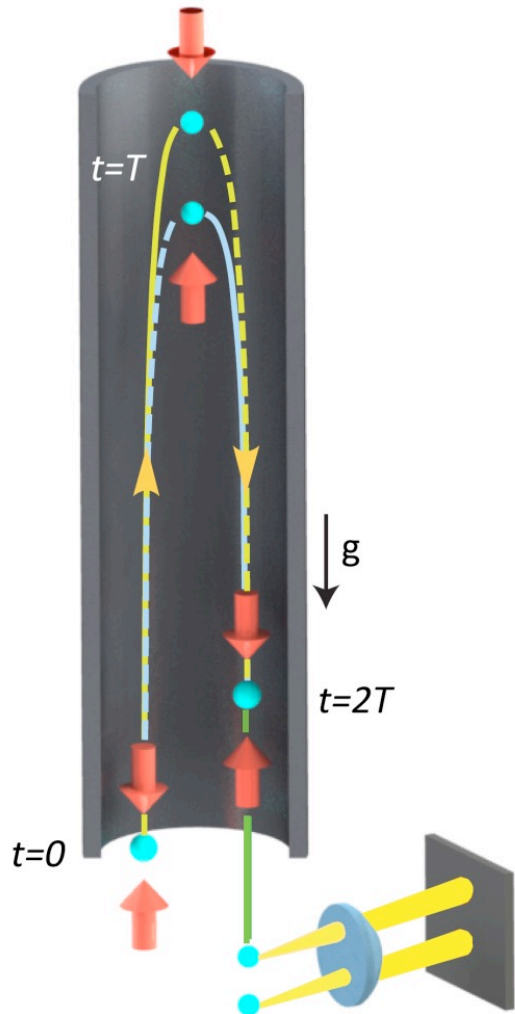
Gravitational waves cause a small modulation in the distance between objects



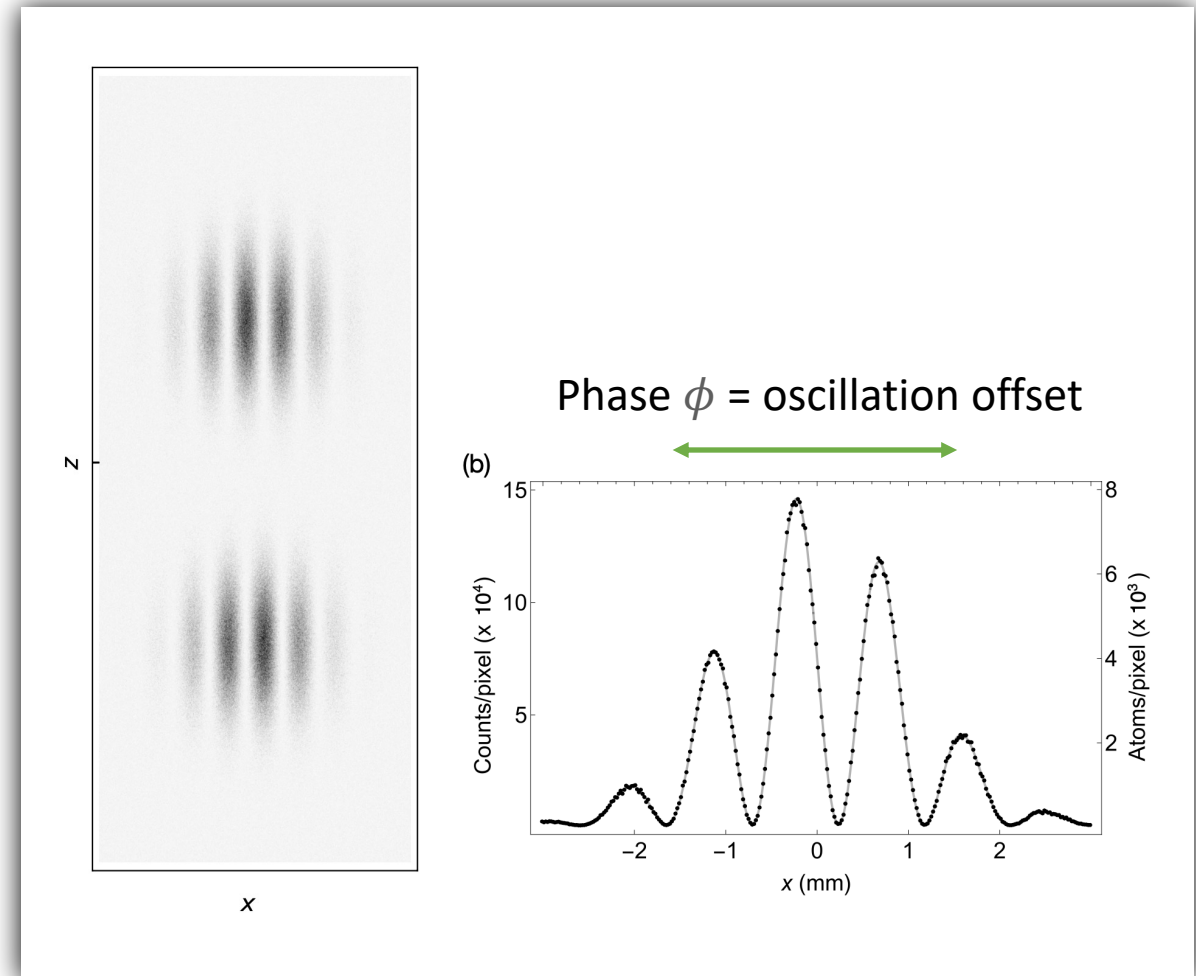
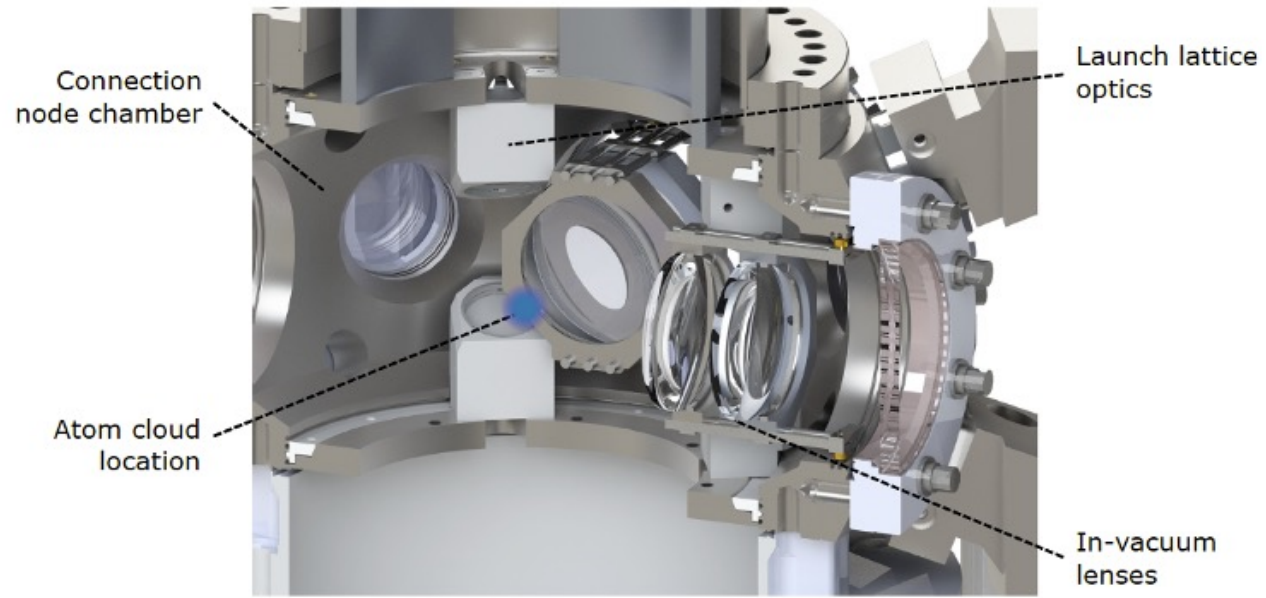
Quantum



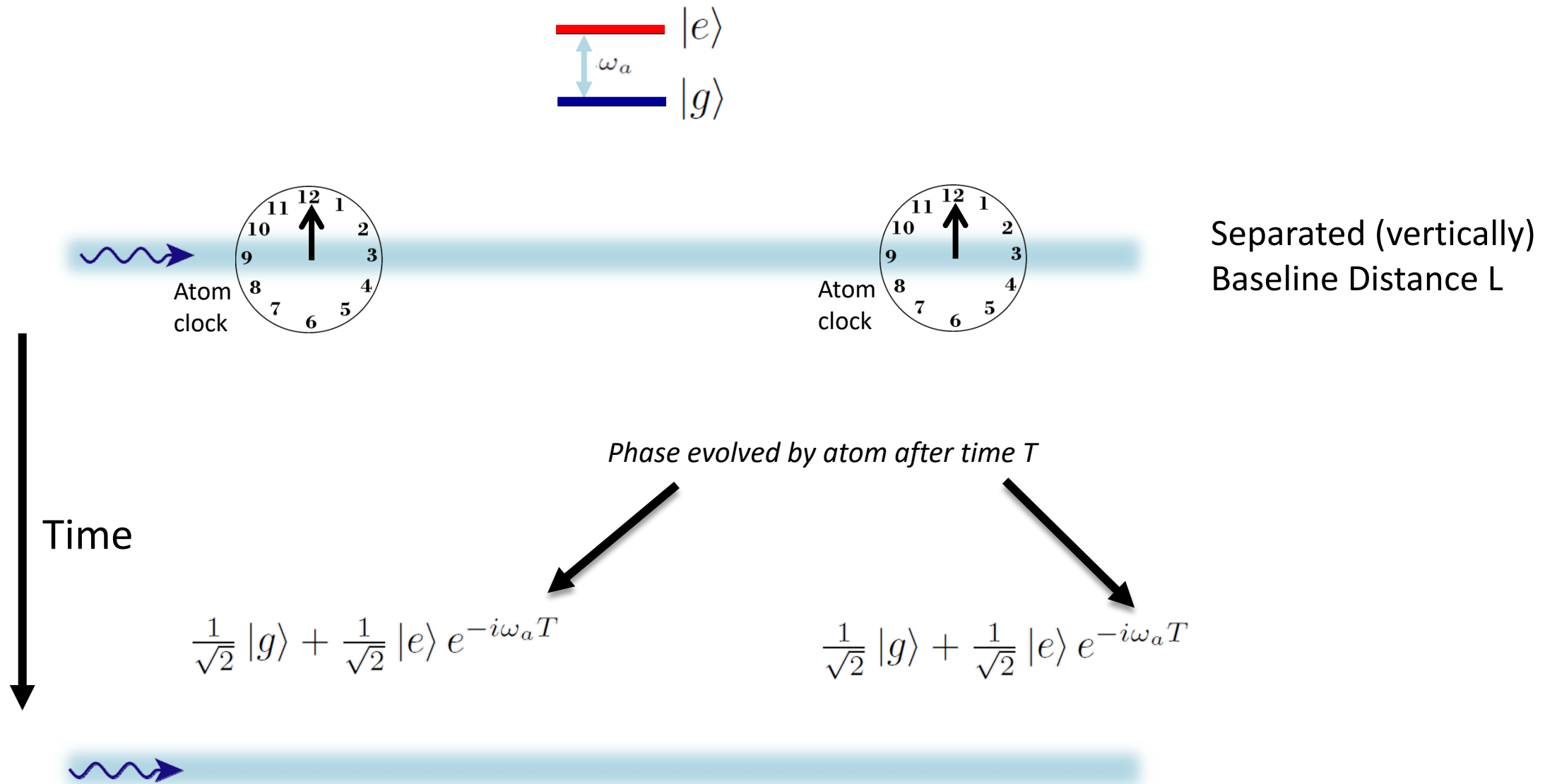
Single Atom Interferometer



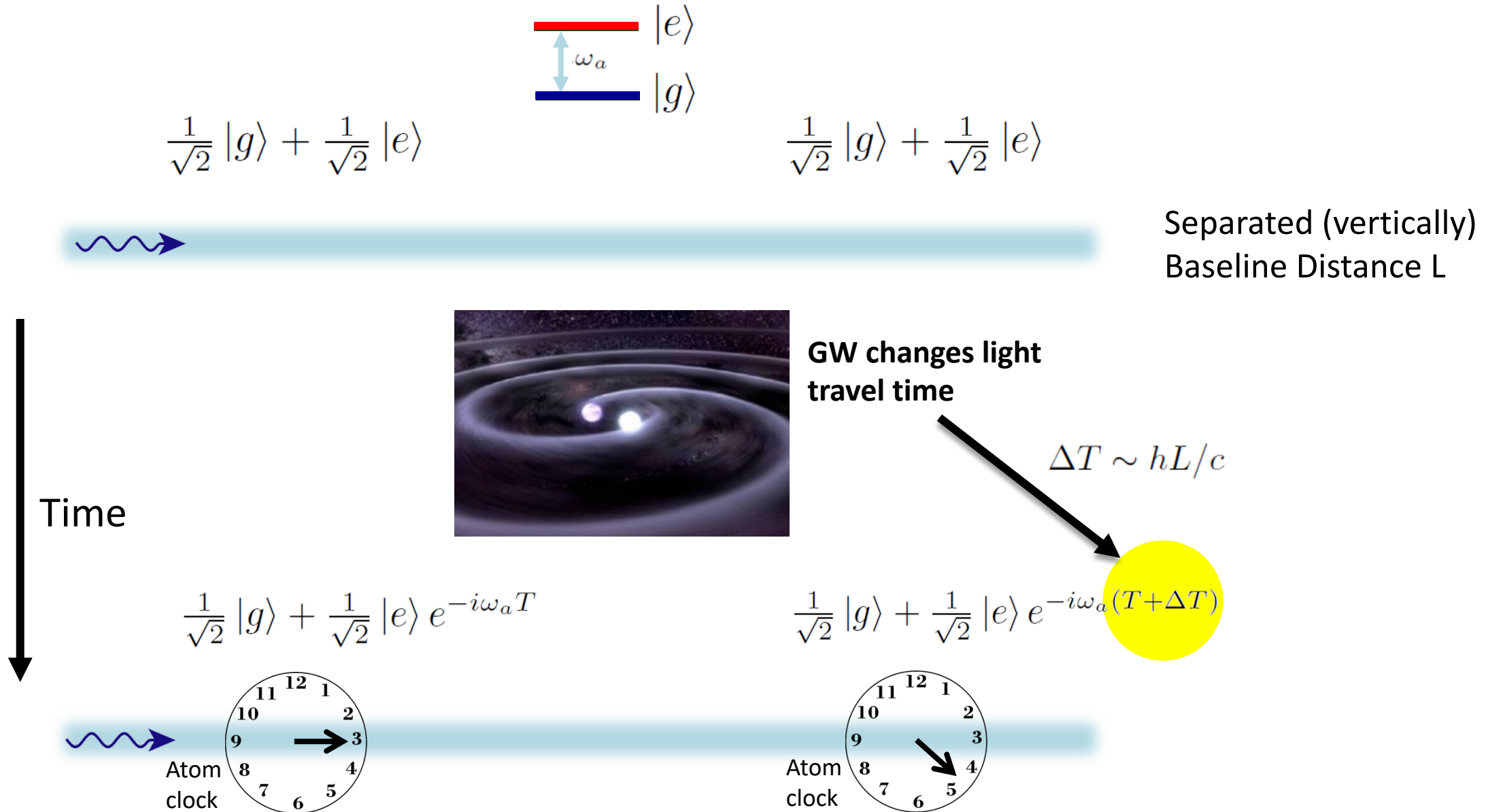
Imagine the Cloud



Simple Example: Two Atomic Clocks



Simple Example: Two Atomic Clocks



Clock Gradiometer

Excited state phase evolution difference:

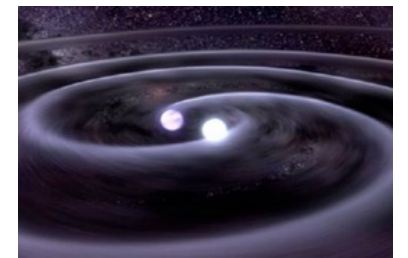
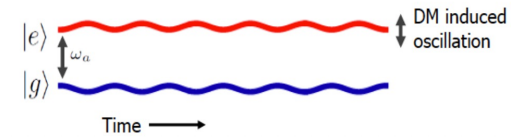
$$\Delta\phi \sim \omega_A (2L/c)$$

Two ways for phase to vary:

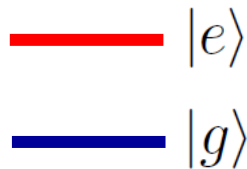
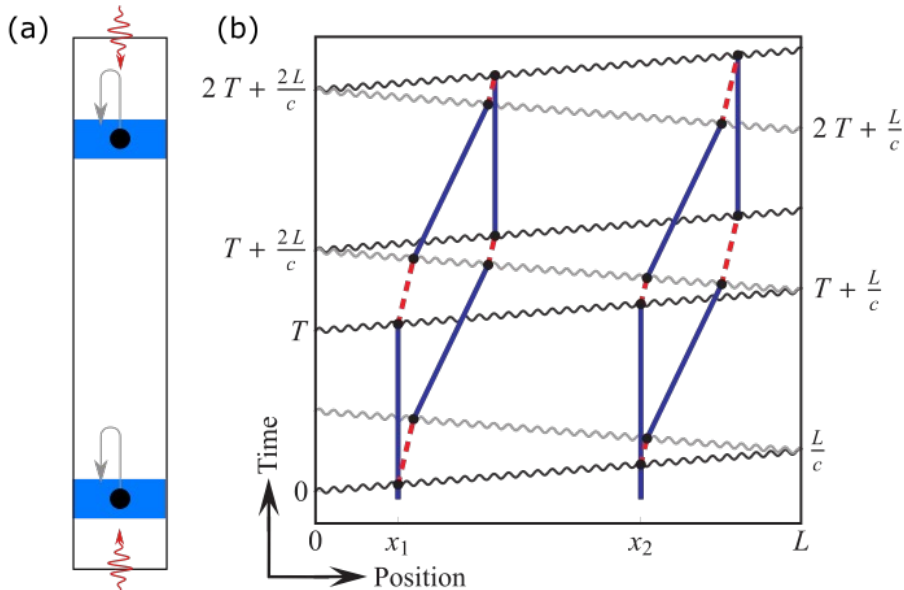
$$\delta\omega_A \quad \text{Dark matter}$$

$$\delta L = hL \quad \text{Gravitational wave}$$

Ultra-light DM coupling causes time-varying atomic energy levels



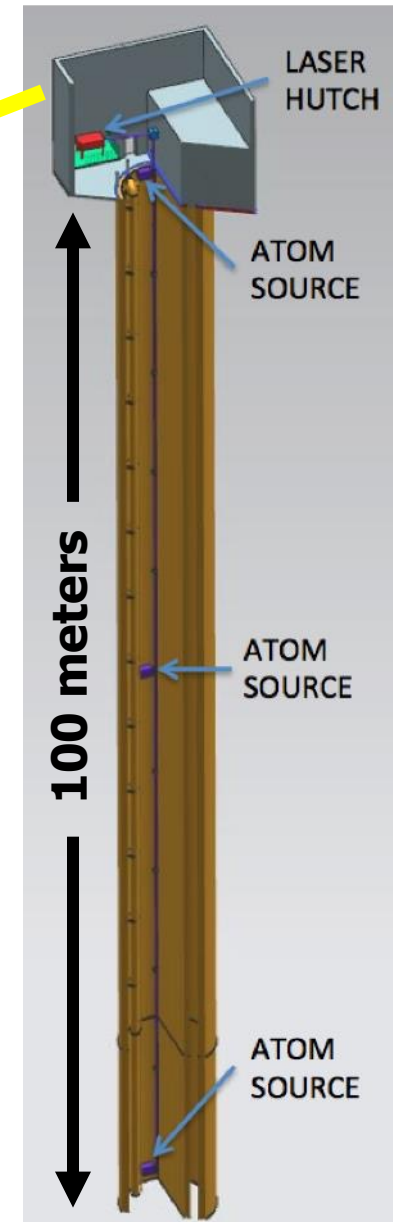
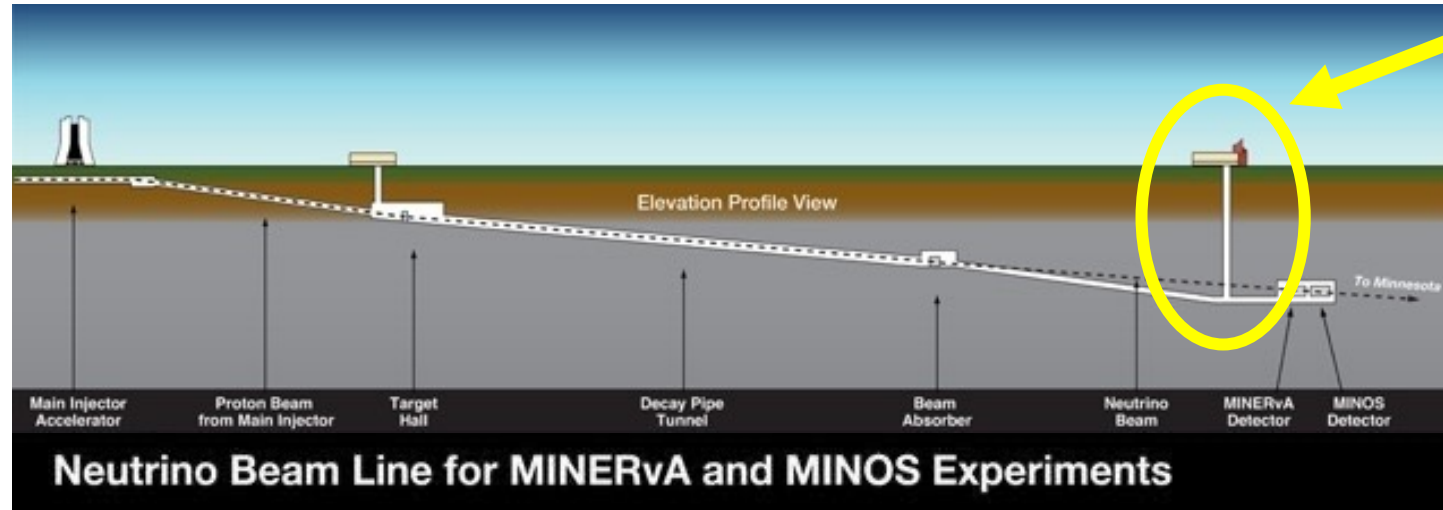
$$L (1 + h \sin(\omega t))$$



Each interferometer measures the change over time T

Laser noise is common-mode suppressed in the gradiometer

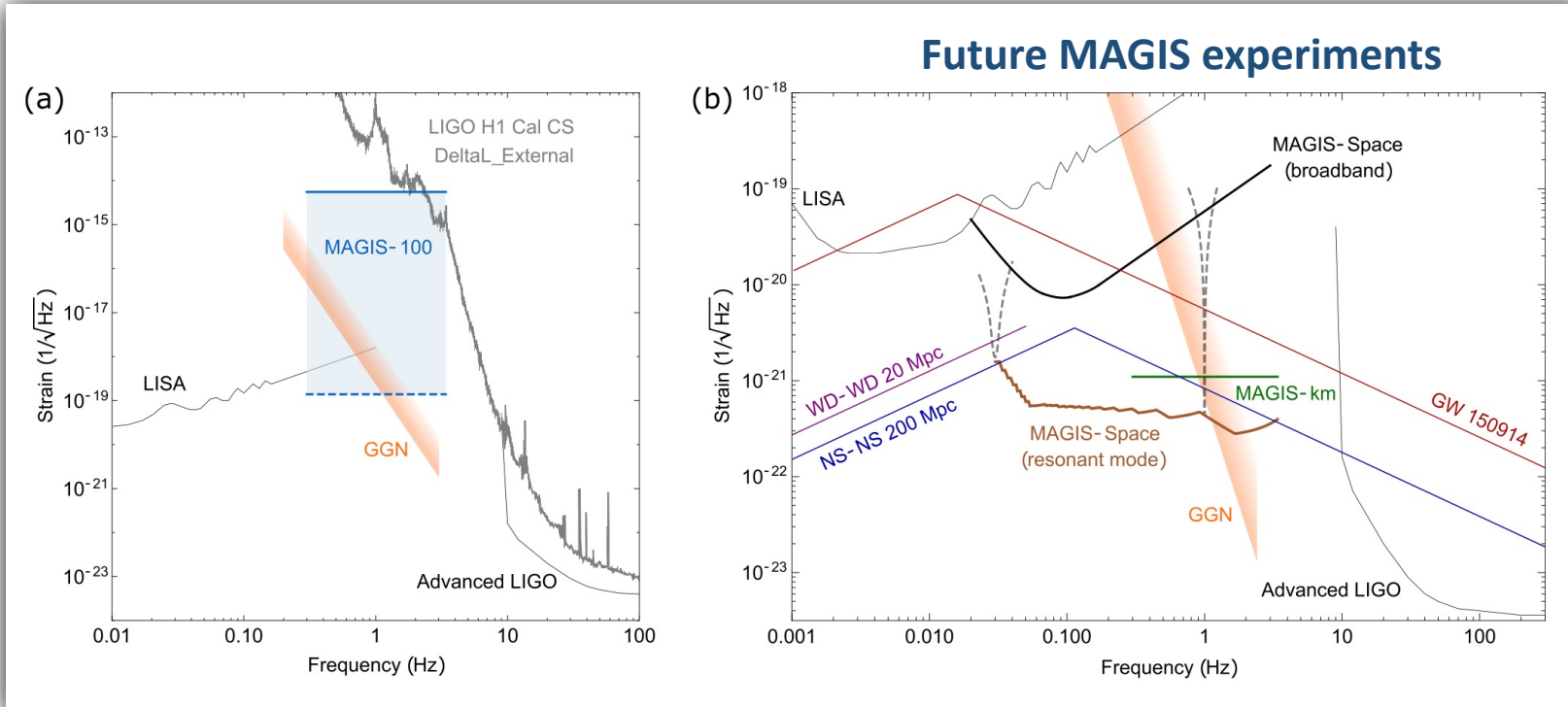
Matter wave Atomic Gradiometer Interferometric Sensor



- 100-meter baseline atom interferometry in existing shaft at Fermilab
- Intermediate step to full-scale (km) detector for gravitational waves
- Clock atom sources (Sr) at three positions to realize a gradiometer
- Probes for ultralight scalar dark matter beyond current limits (Hz range)
- Extreme quantum superposition states: >meter separation, up to 9 s duration

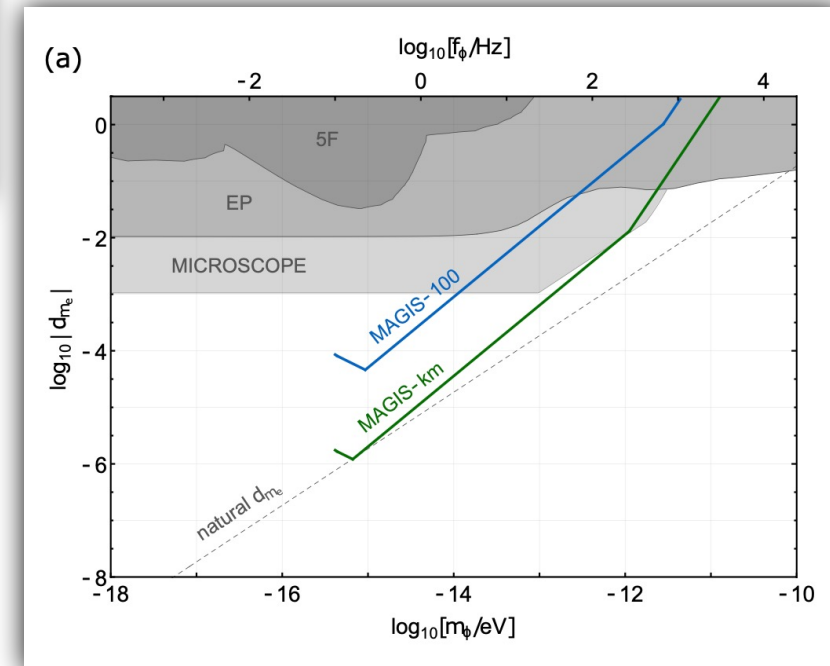


Expected Sensitivity

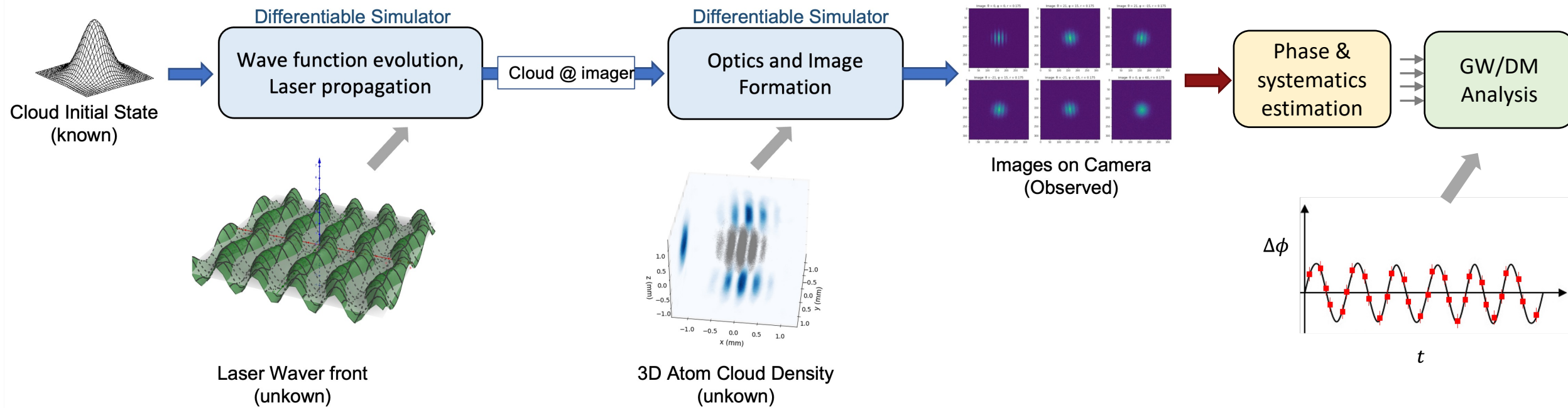


Gravitational Waves

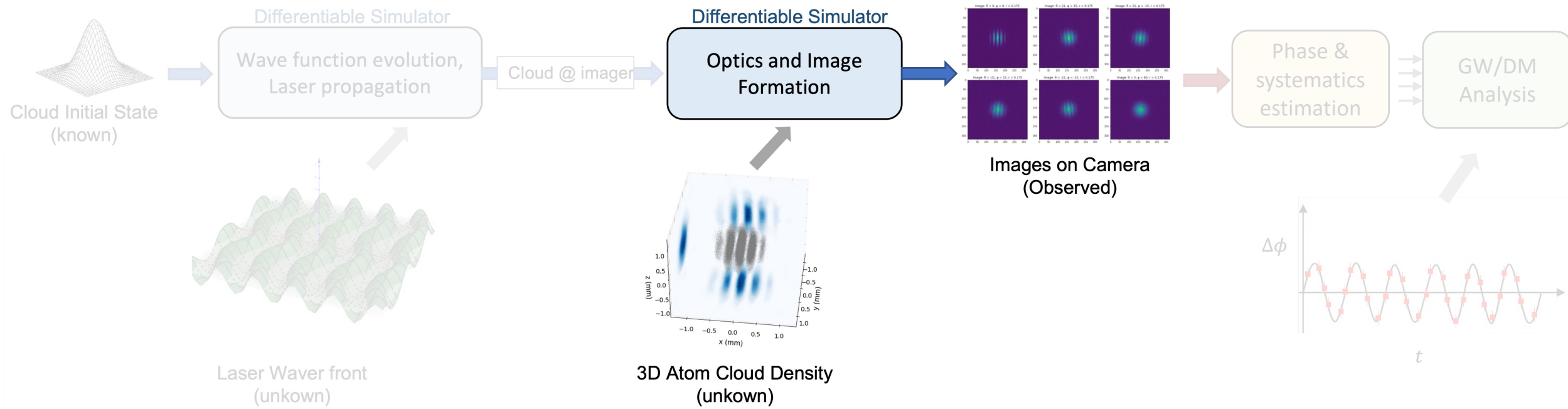
Dark Matter



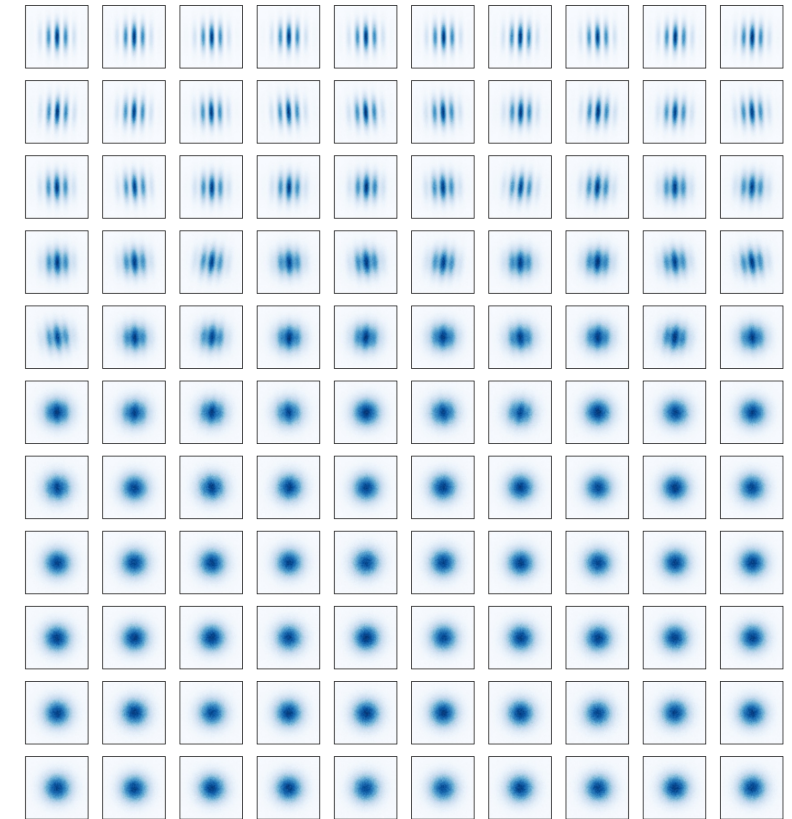
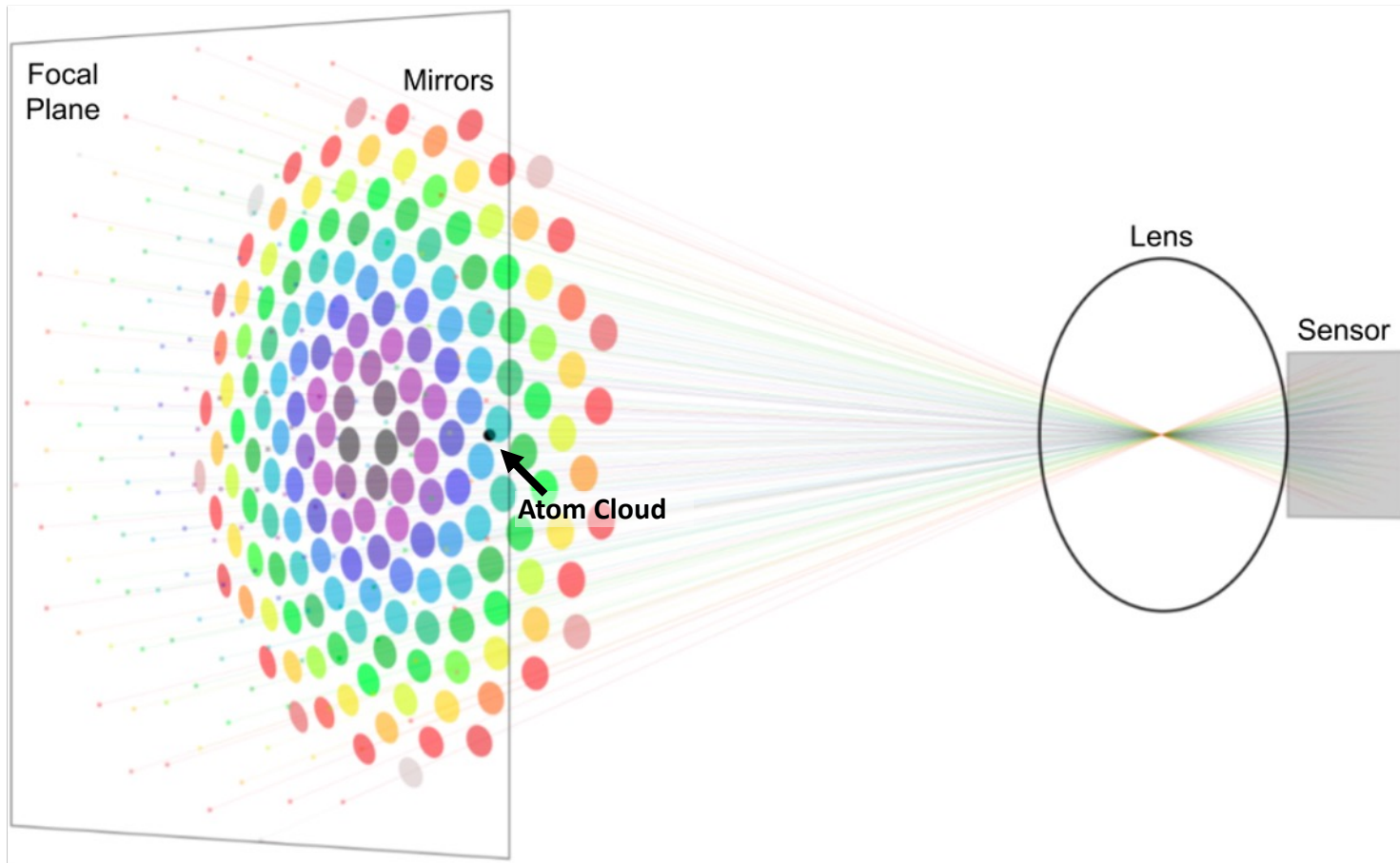
Simulation and Analysis Pipeline



Simulation and Analysis Pipeline



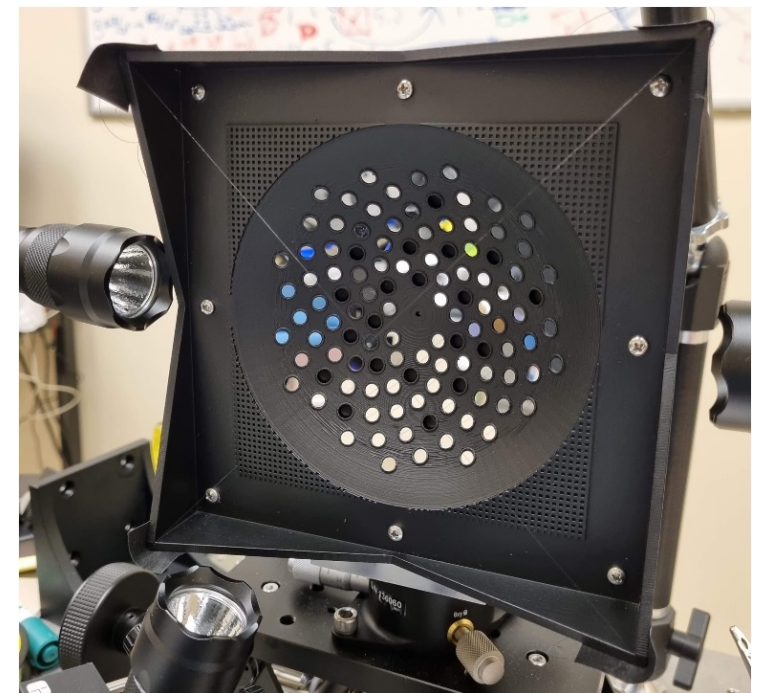
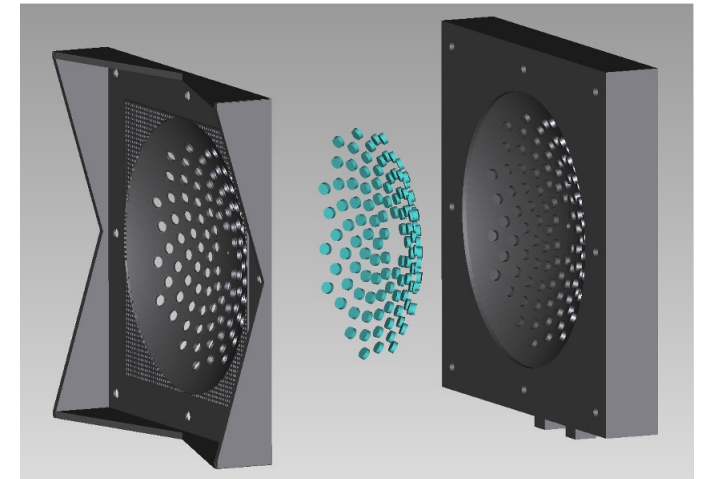
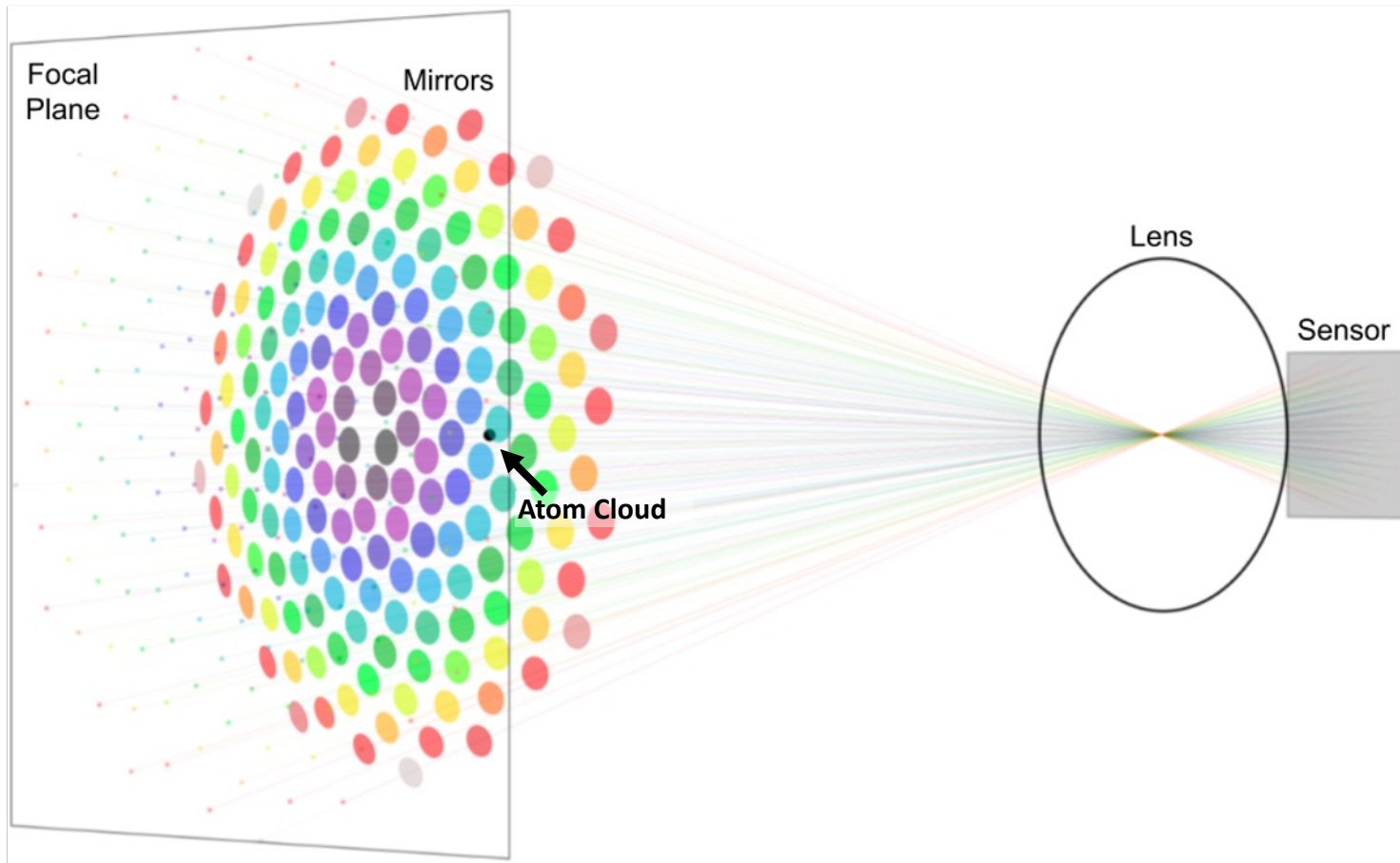
New Single-Shot Multi-View Imaging



Design Goals

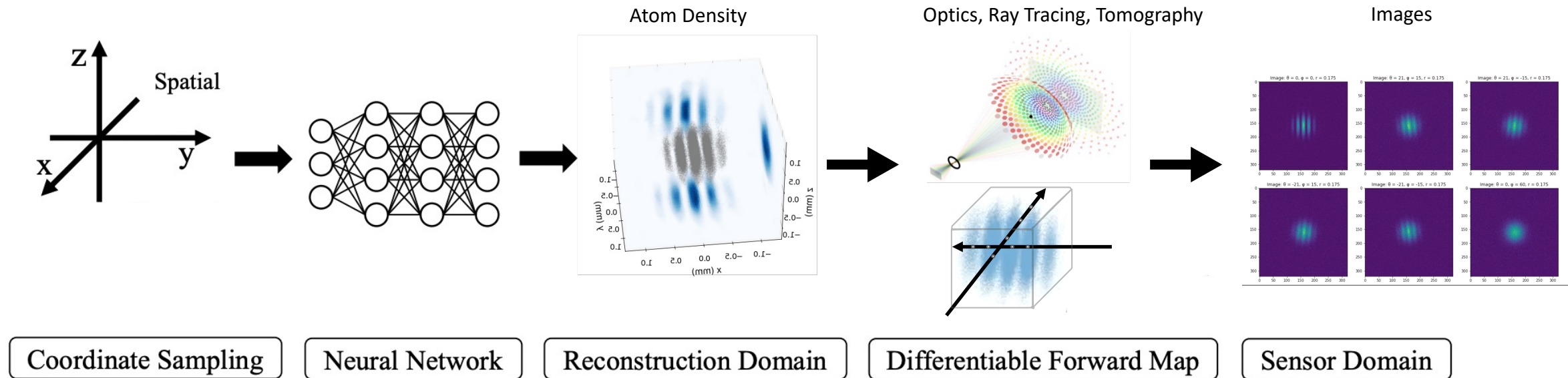
- Increased light detection → improve phase estimation
- Multi-view imaging for 3D reconstruction → improve systematics estimation

New Single-Shot Multi-View Imaging



We built it!

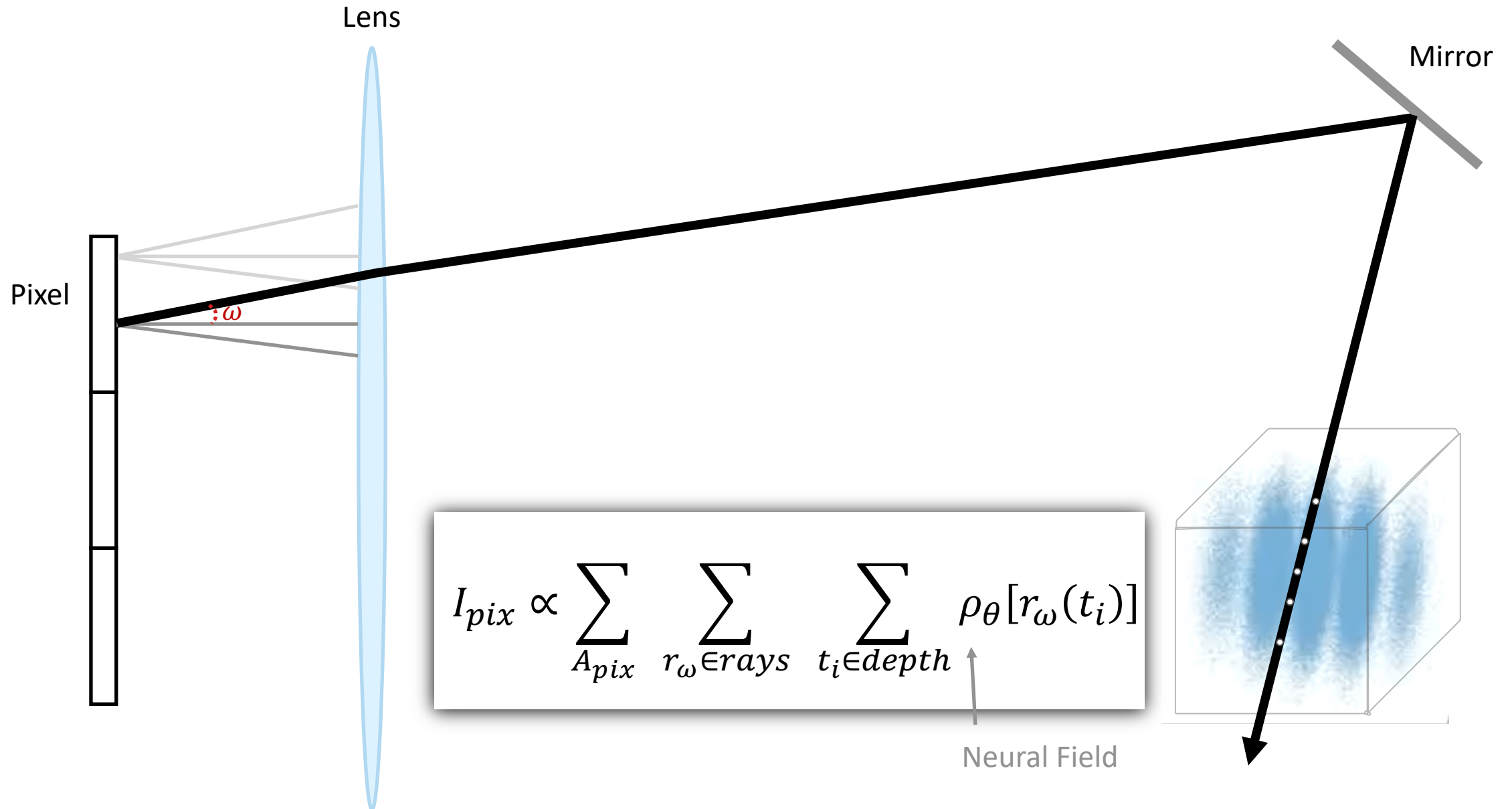
Neural Fields for Atom Cloud Reconstruction



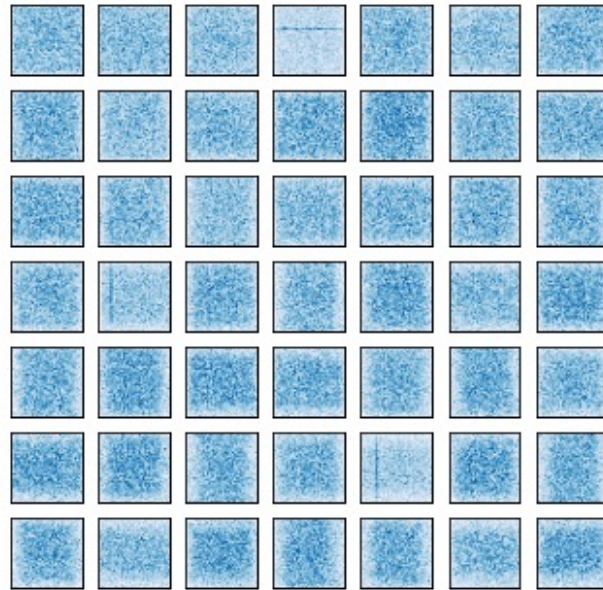
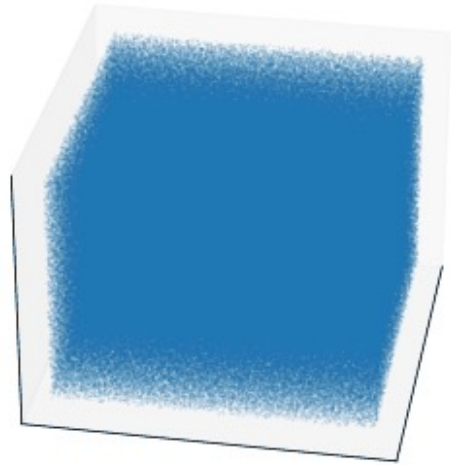
Neural field to model atom cloud density

Forward model: differentiable ray tracing and optics → tomographic imaging

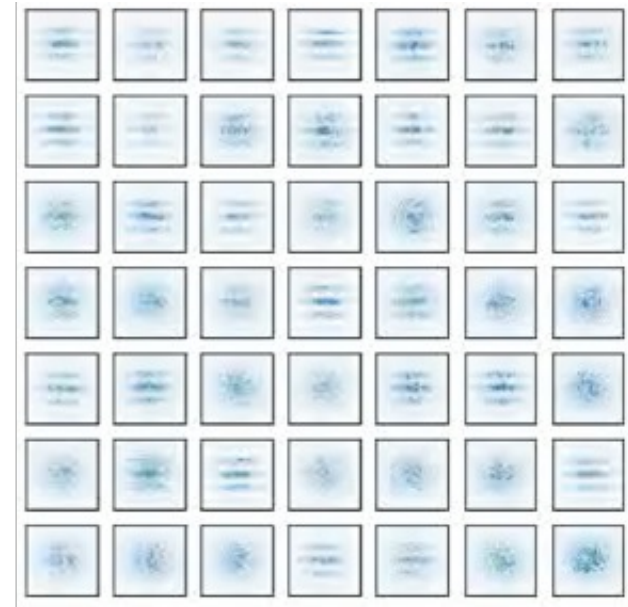
Computing Pixel Intensities



3D Cloud Reconstruction in Simulation

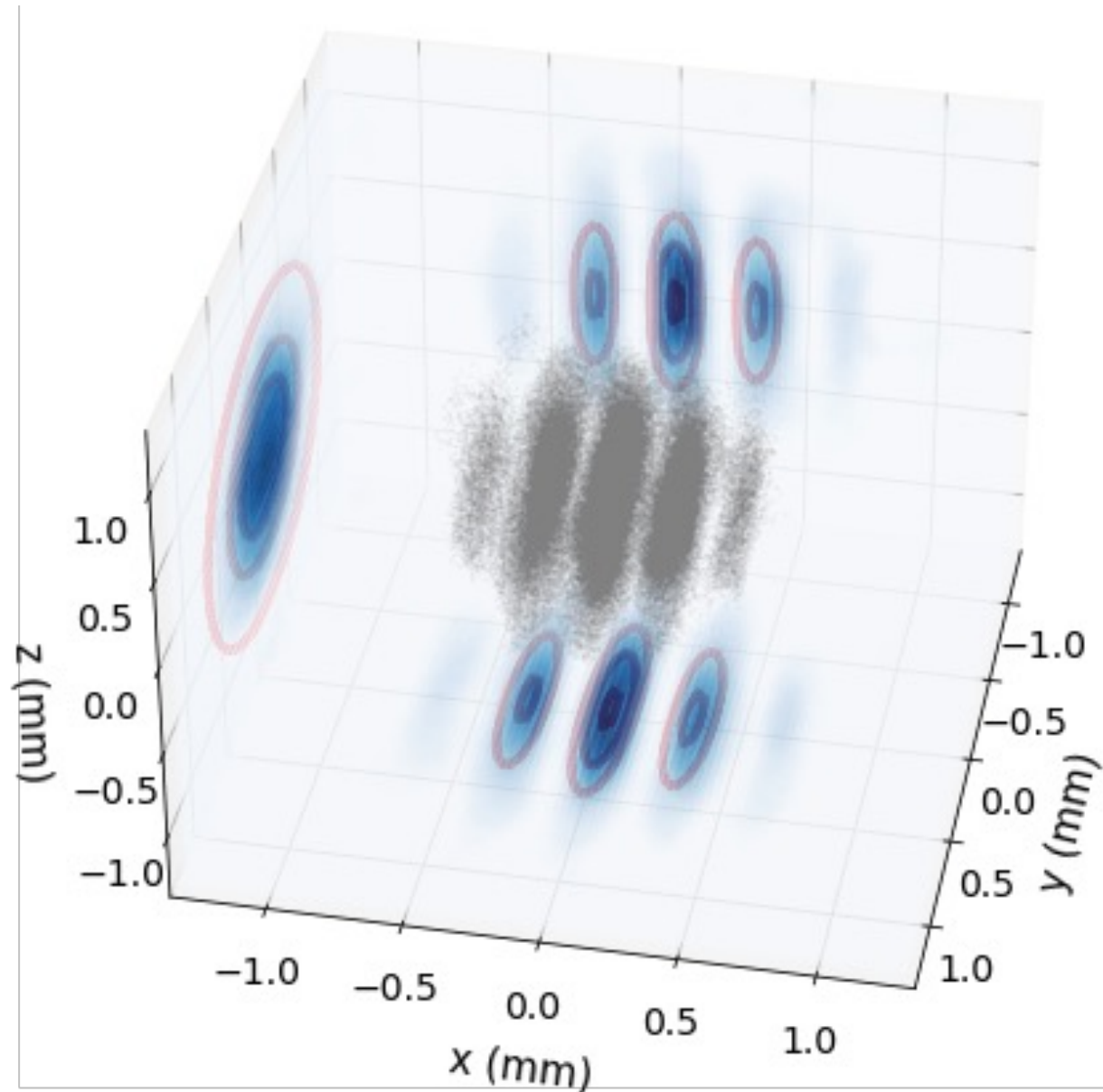


Model



Target: Measured Data

3D Cloud Reconstruction in Simulation



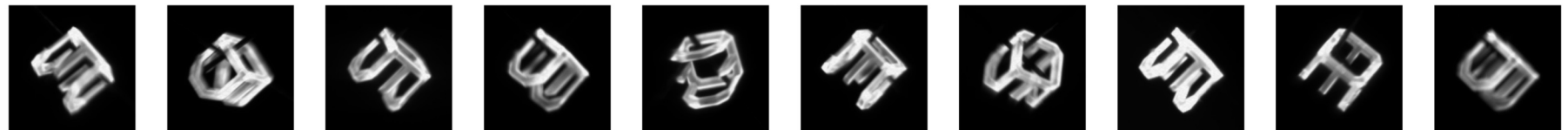
- Learned 3D cloud
- Learned 2D marginal
- Target 2D marginal

Resolution $\sim 60\mu\text{m}$
Computed comparison to
ground truth density with
Fourier Shell Correlation

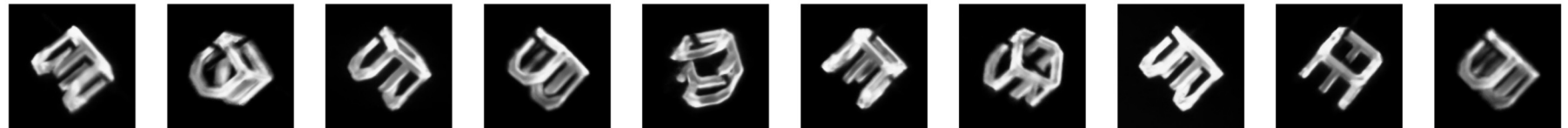
Reconstructing Real Objects



Real Views

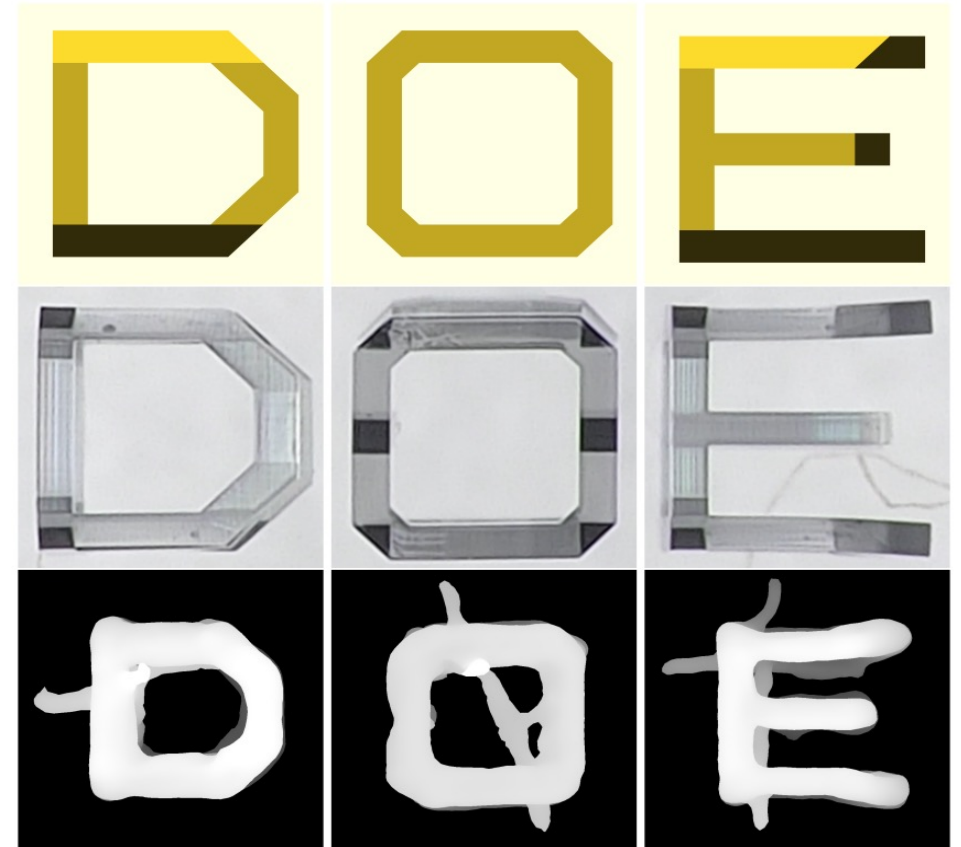
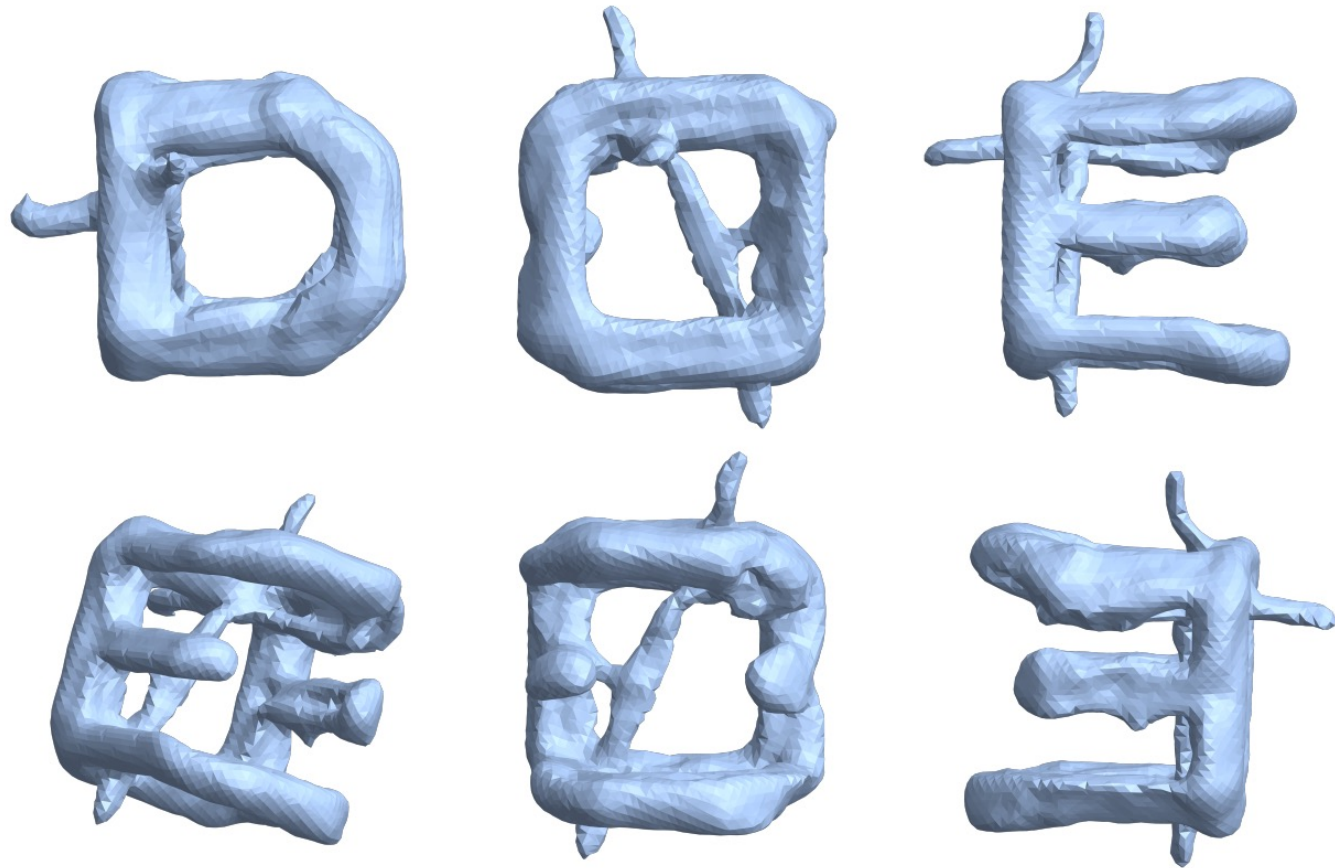


Generated Views



3D Reconstruction Comparisons

Mesh of Reconstructed Surface



CAD

Microscope

Learned Model

Resolution $\sim 70\mu\text{m}$
Computed using split-halves
Fourier Shell Correlation

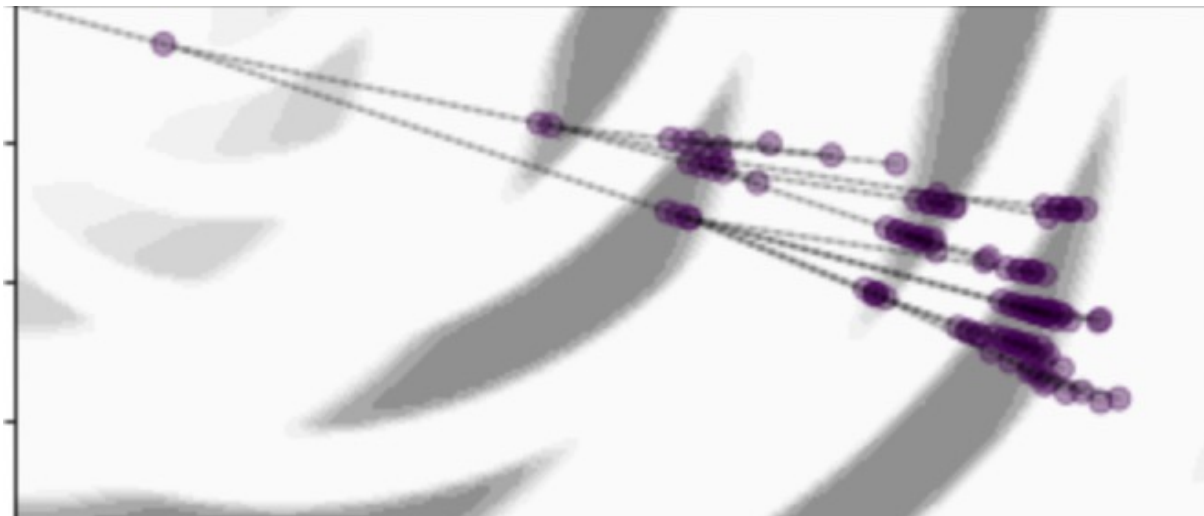
Application for Design Optimization

Detector Design Optimization

As we saw in L. Heinrich's talk:

Goal is to optimize the parameters ϕ of a detector models to minimize a design function $f(\cdot)$ when evaluated on samples of data x

$$\mathbb{E}_{p_{\phi}(x)}[f(x)] = \int dx f(x)p_{\phi}(x)$$

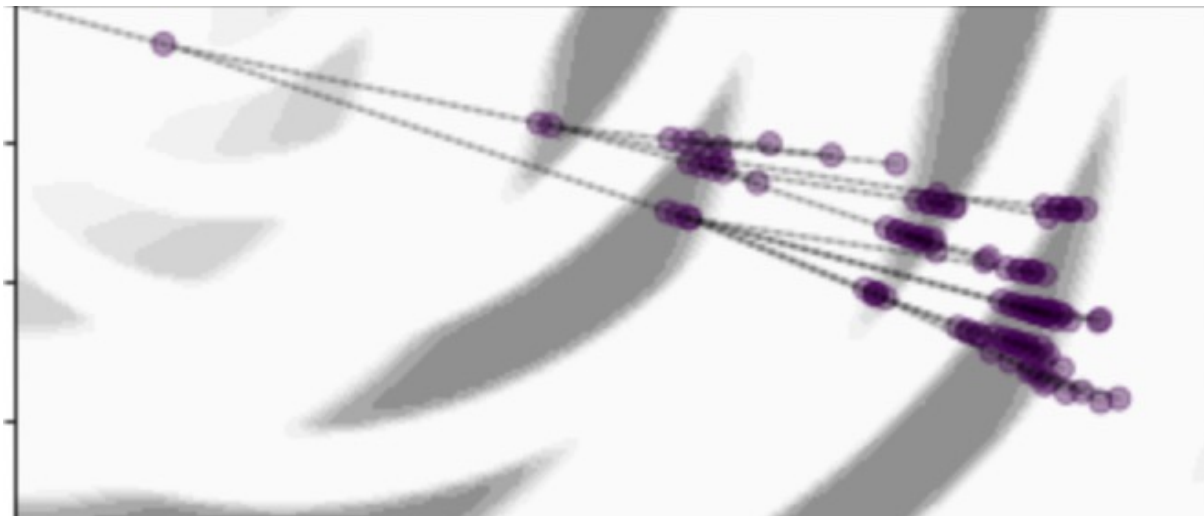


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$$\mathbb{E}_{p_{\phi}(x)}[f(x)] = \int dx f(x)p(\text{interact at } x|\lambda = \text{Detector}_{\phi}(x))$$

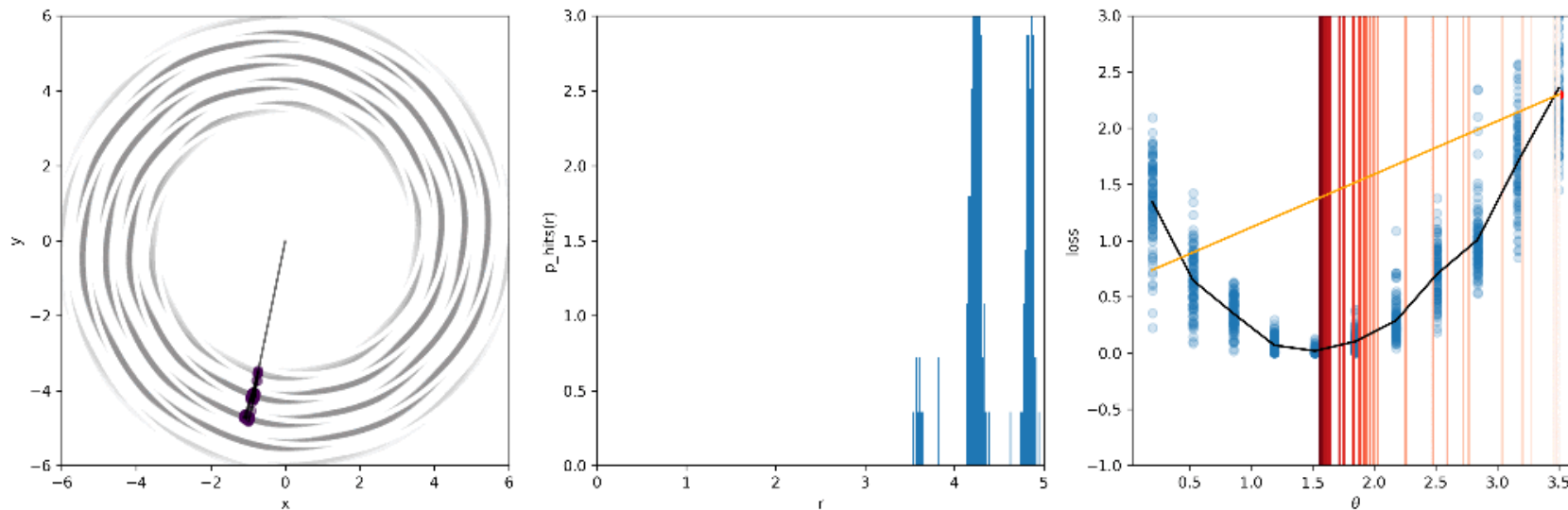


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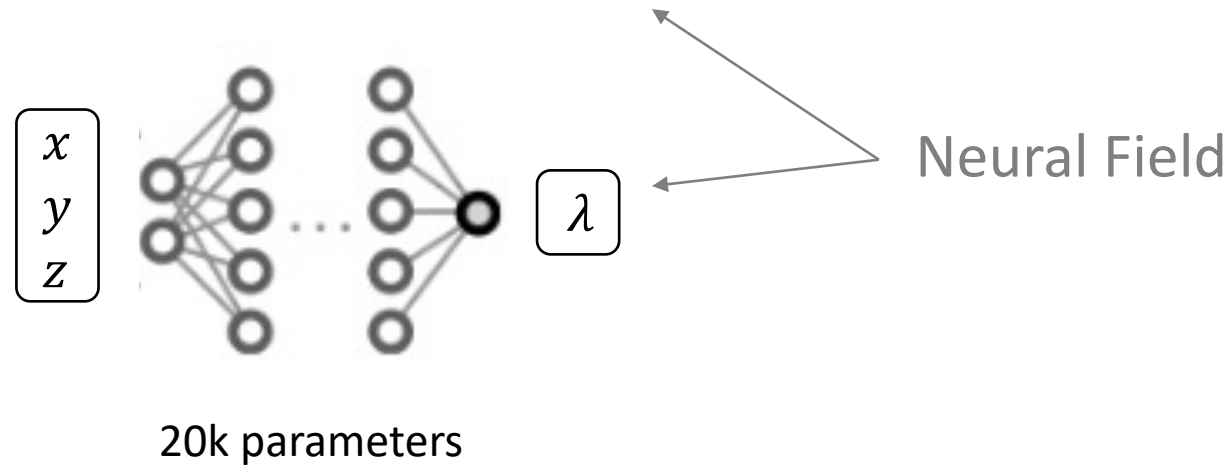
Neural field as a detector

Detector in this example was a very simply toy with 1 parameter

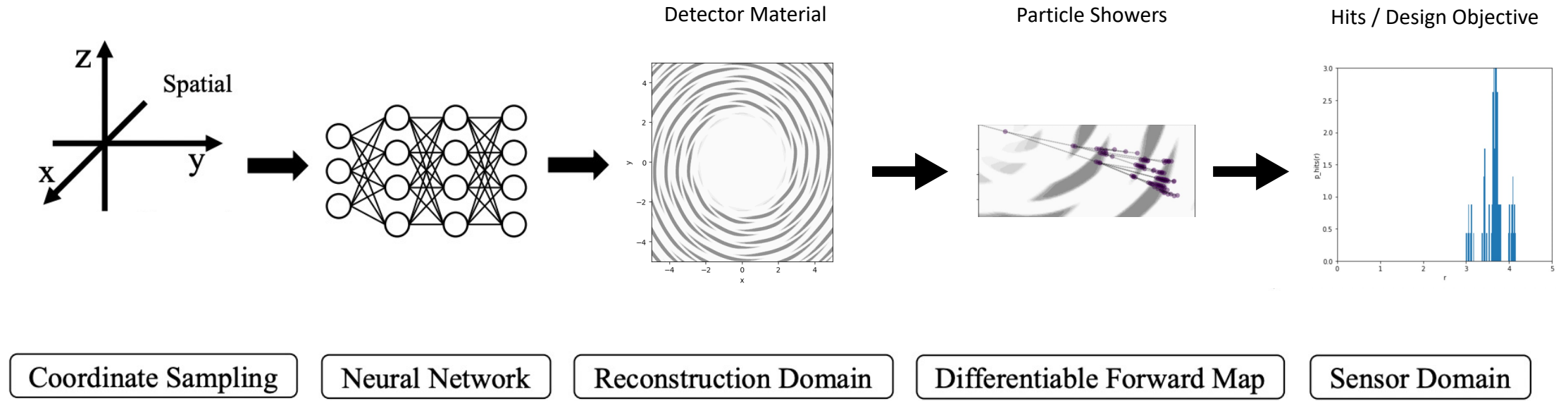
- Predetermined detector structure with varying radius, i.e. $\phi = radius$

Instead, we could try to optimize a detector freeform from scratch

$$p(\text{interact at } x | \lambda = \text{NN}_{\phi}(x))$$



Neural Fields for Detector Design

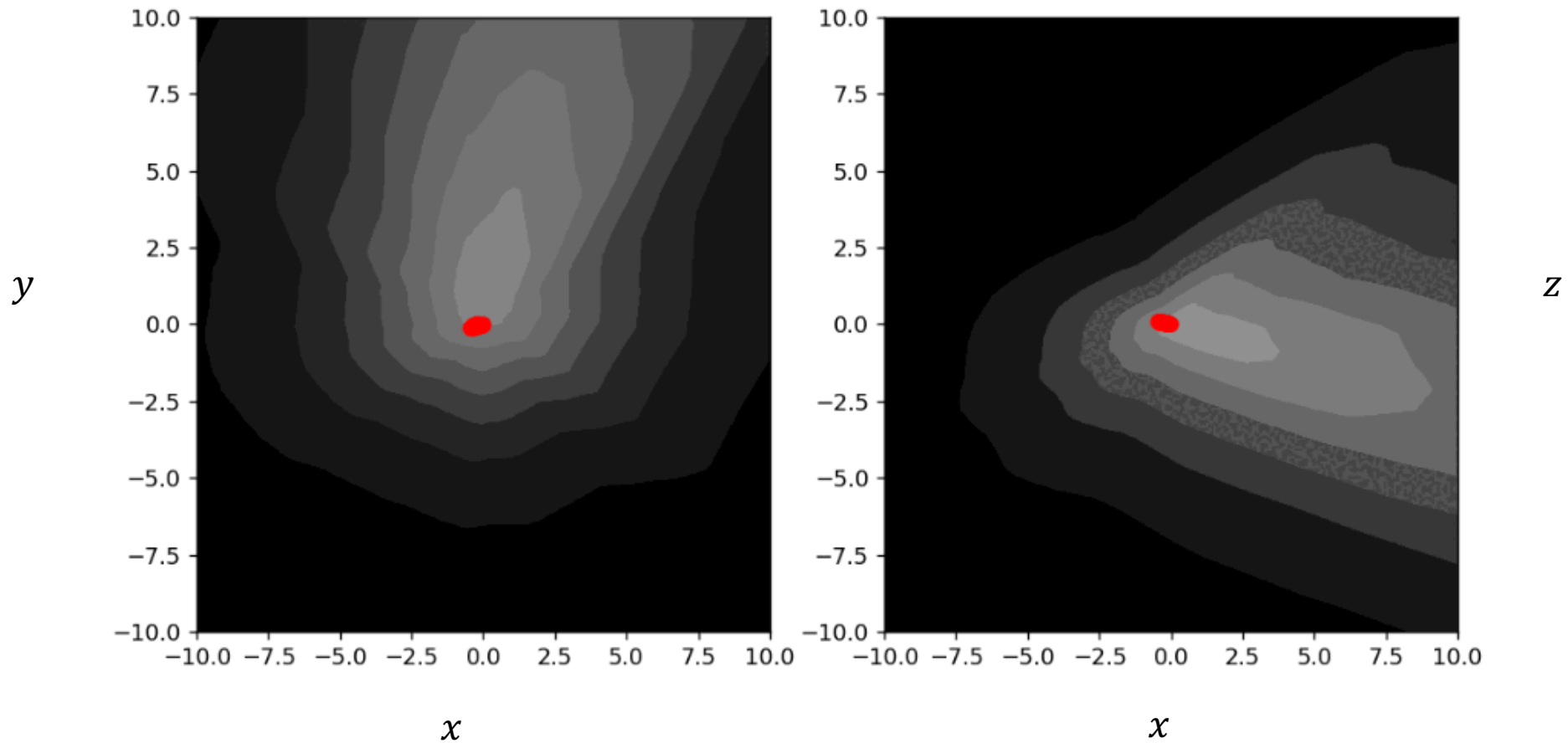


Neural field to model material distribution

Forward model: particle showers

Detector Design Optimization with Neural Field

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Rediscovered “classic” layout:

Learns to contain shower with no material in middle, material outside

A Few Comments Before Wrapping Up

Ongoing work on Neural Fields

Generalization: how to amortize, get beyond per-instance optimization

Uncertainty Quantification: how to get uncertainty on fitted signal for science applications?

Inference: How to extra information, e.g. physical parameter estimates, from a fit neural field?

Generative modeling: How can we generate neural fields instead of generating data in measurement space?

Many open questions, but more progress on some topics (e.g. generalization, generative modeling) which get a lot of focus in graphics community

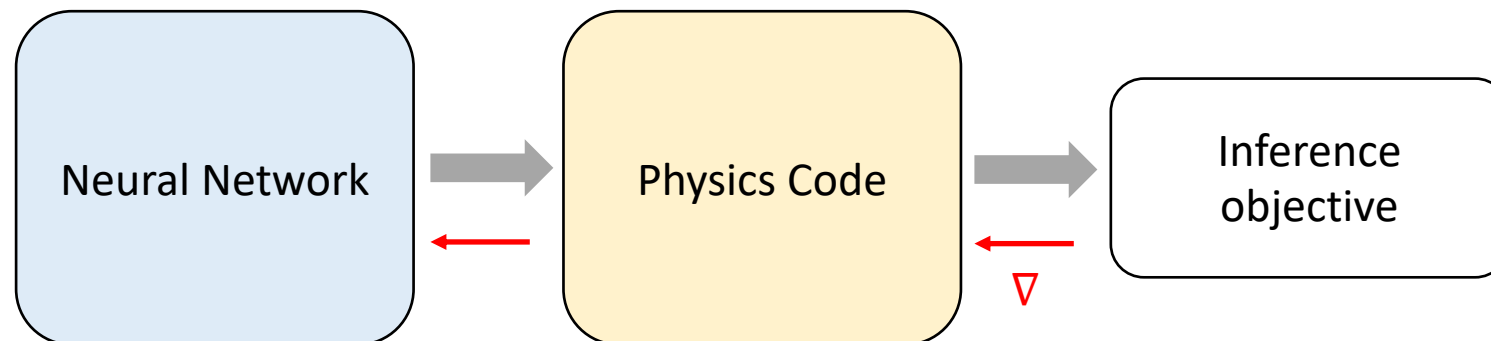
Neural fields are an interesting example of *hybrid Physics-AI systems*

Combines physics knowledge (differentiable simulator) with neural networks to model complex signals

Physics guides learning & ensures we can make physical plausible predictions

Way to add physics inductive bias, in the form of physics code, in NNs

- Where adding symmetries to architectures is like adding structure information, now we can add dynamical information in the form of physics code



Wrapping Up

Neural Fields combine neural networks and differentiable simulators to enable powerful gradient-based optimization of signals

Originally developed in computer graphics, generalizing the concept enable exciting applications in science, from reconstruction to system design

Can be seen as a development of novel *Hybrid Physics+AI Systems* by directly integrating physics code into ML models

Still much to be done! Generalization, Inference on neural fields, generative modeling, uncertainty quantification, ...

Backup

Benefits of Neural Fields

Compact:

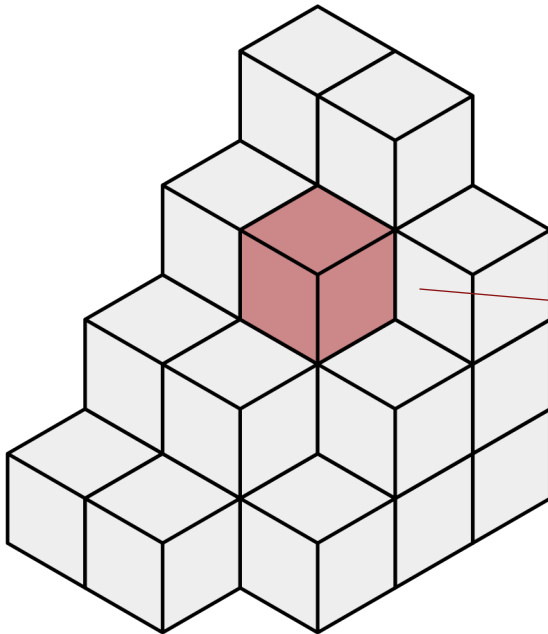


$1024 \times 1024 \times 3 = 3\text{MB}$

Equivalent size neural network
has 750k floating point weights

Why Neural Fields?

Compact:



Even more challenging in 3D

Color, density, distance, ...

Expensive in storage!

Challenges with Neural Fields

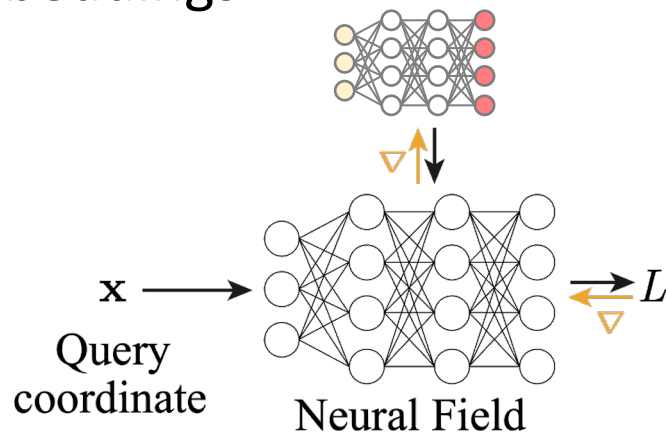
Generalization:

- Basic setup requires per-instance optimization
- Lots of work to share knowledge across reconstructions

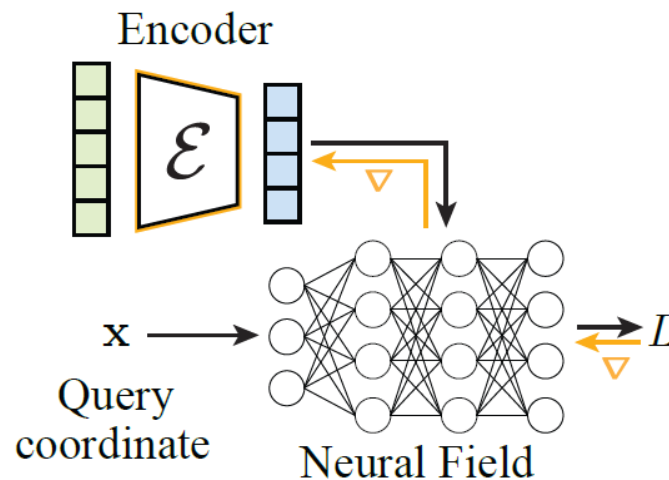
Per-instance Optimization



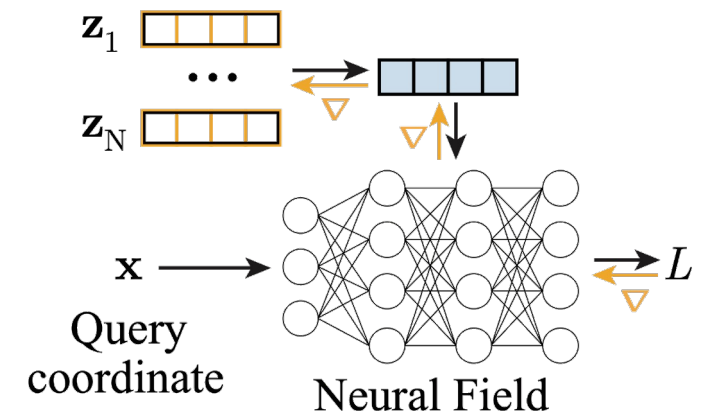
Pre-trained or optimized embeddings



Feature encoding



Auto-decoding



MAGIS-100

Detector Technology: Atom Interferometer

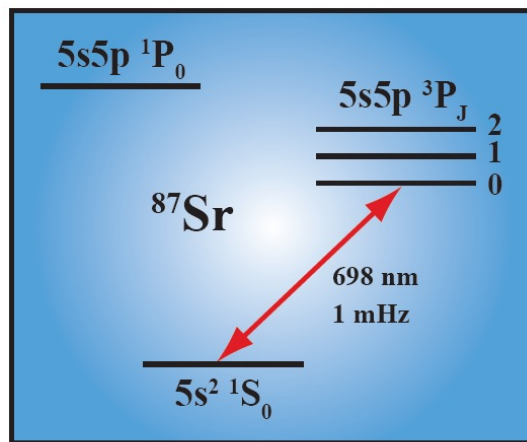
Best clocks in the world now lose <1 second in 10^{18} seconds

MAGIS-100 is based on same physics as Sr optical lattice clock

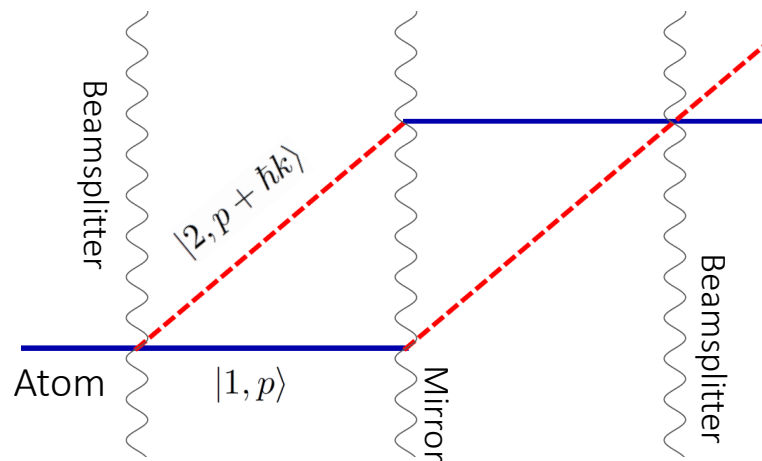
Atom interferometry provides a pristine inertial reference

Compare two (or more) atom ensembles separated by a large baseline

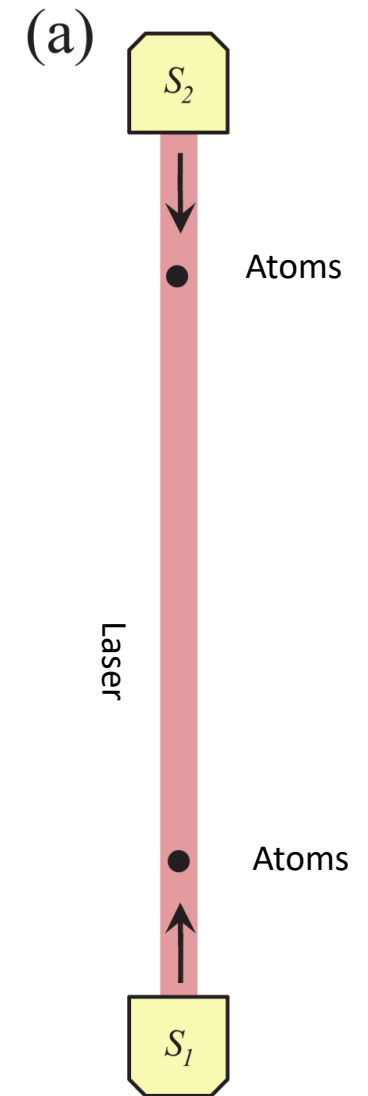
Differential measurement suppresses many sources of common noise and systematic errors



Atomic clock transition



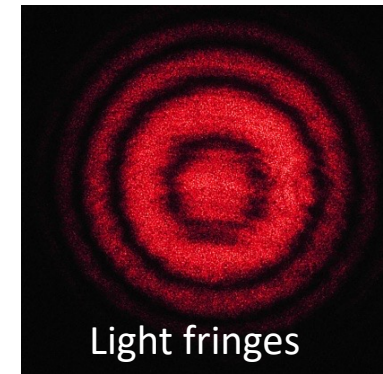
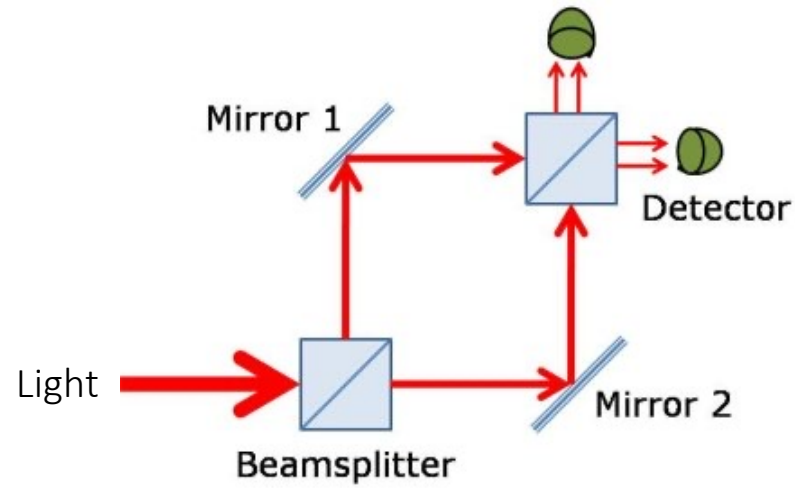
Atom interferometer



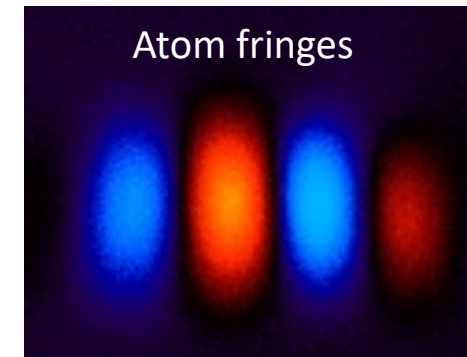
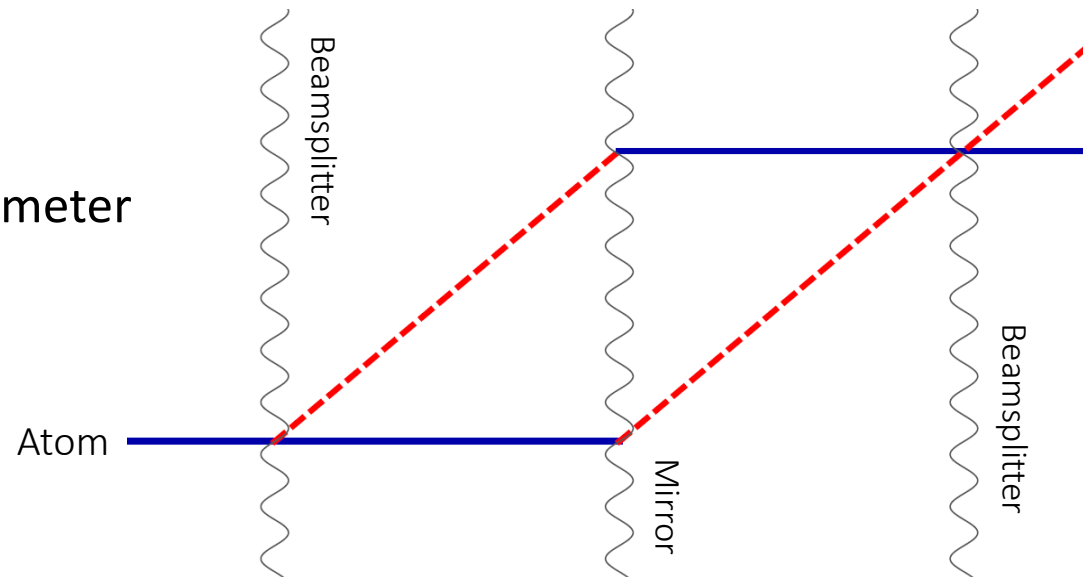
Gradiometer

Atom Interference

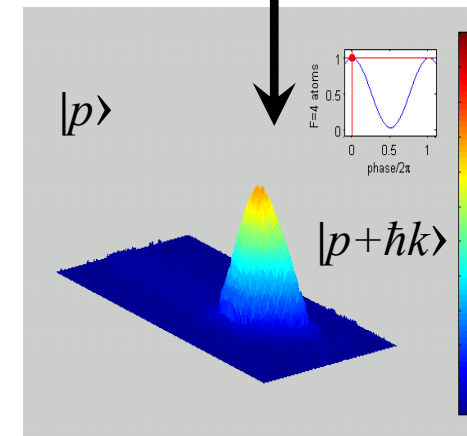
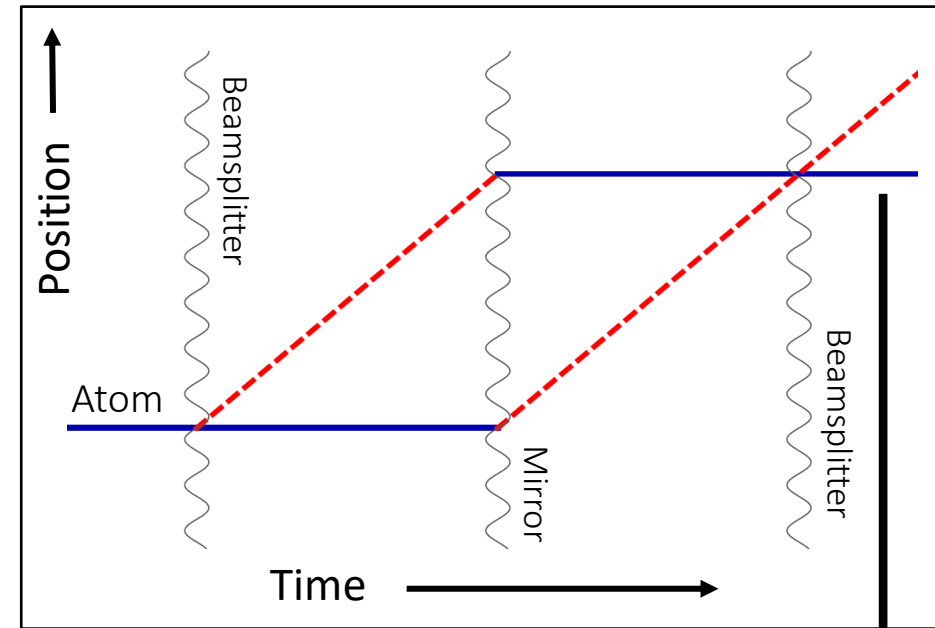
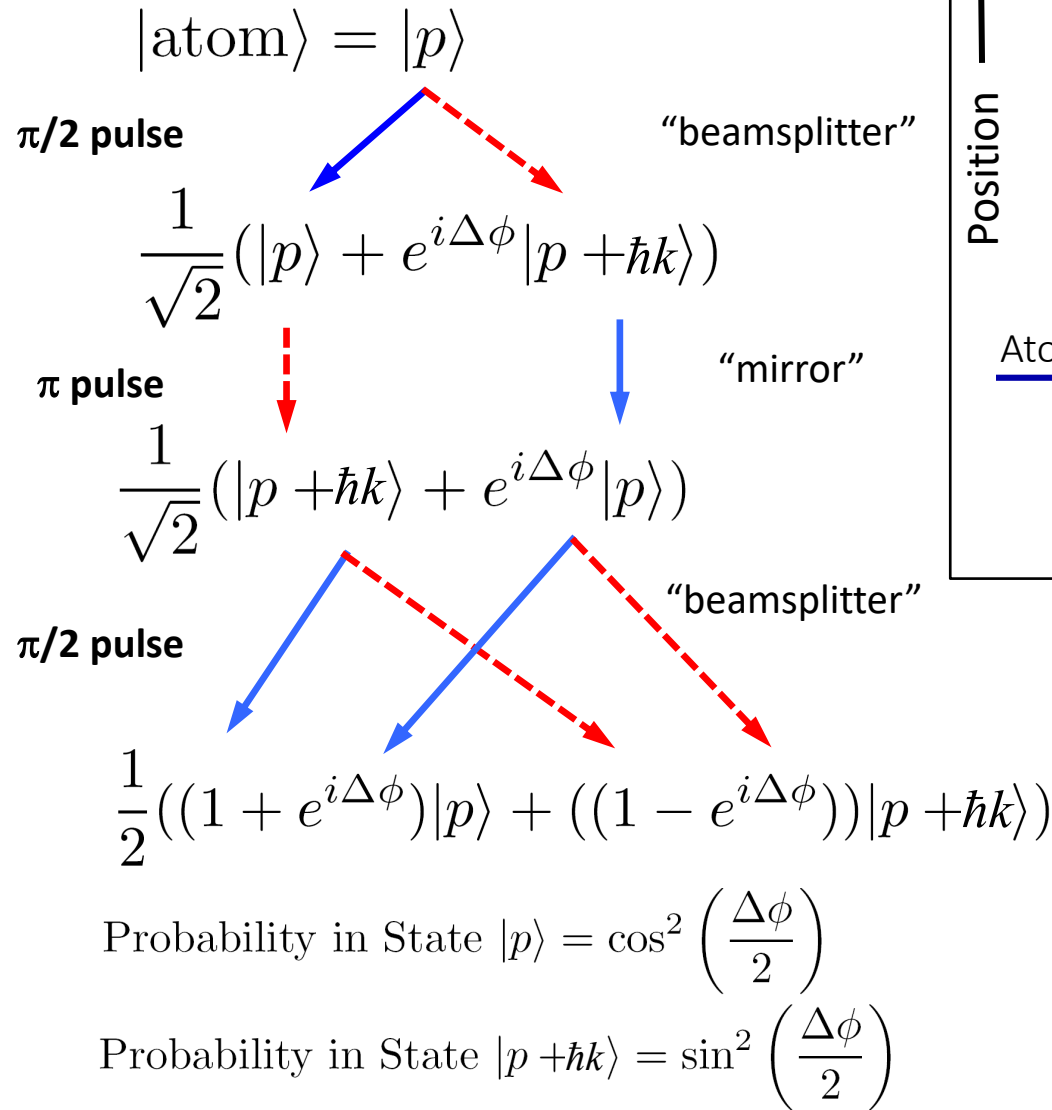
Light interferometer



Atom interferometer



Light pulse atom interferometry



Clock Gradiometer

Clock:

measure light travel time

Accelerometer:

atoms excellent inertial test masses

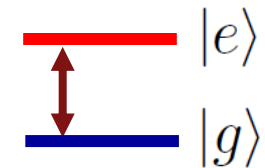
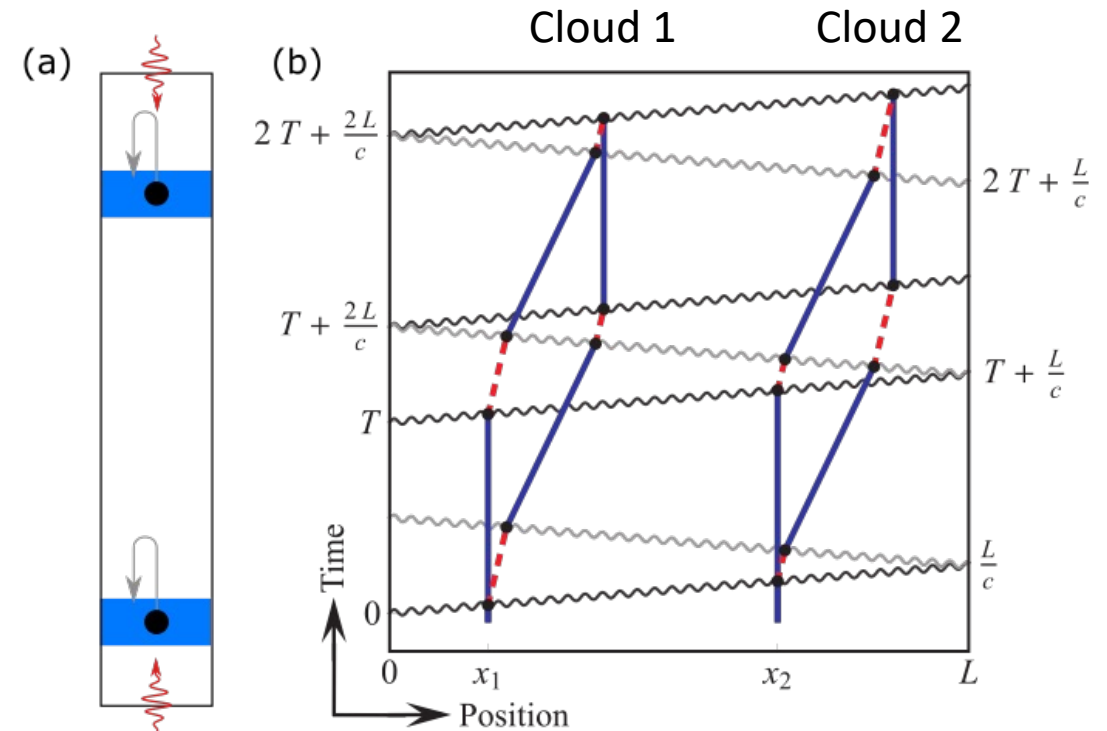
→ follow geodesics

Gradiometer:

Differential accelerometer

→ remove laser noise w/ single baseline

Measure differential acceleration by comparing the light travel times



GW / DM Analysis Principle

Launch sequence repetition rate ~ 1 Hz

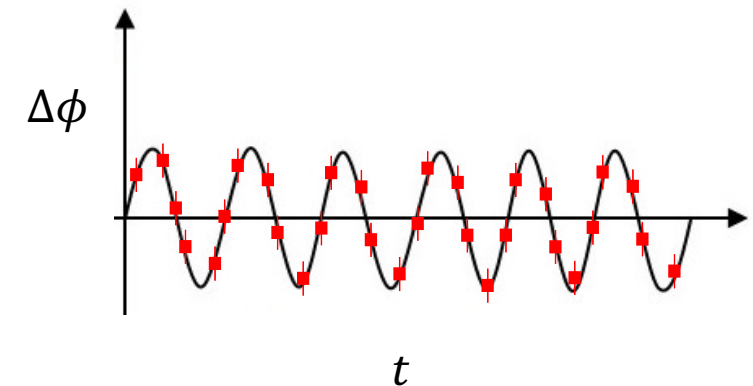
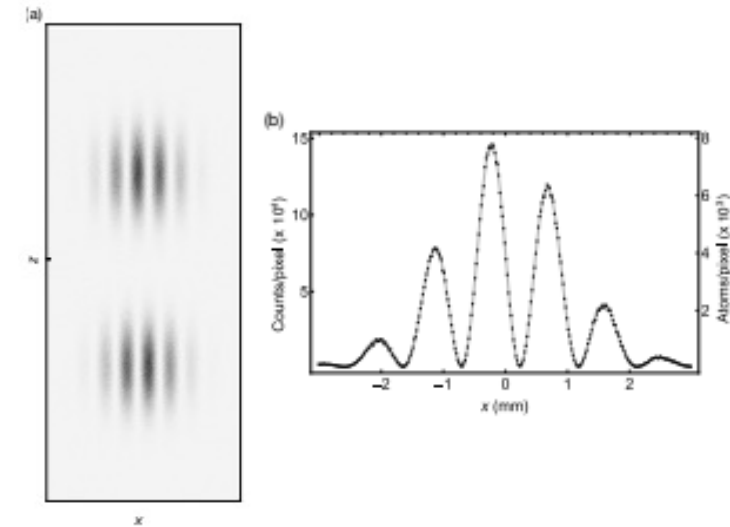
Image clouds (fluorescent imaging) at end of sequence

Extract phase from interference pattern per launch

Look for signals of time-varying phase difference

In this Mid-band frequency range

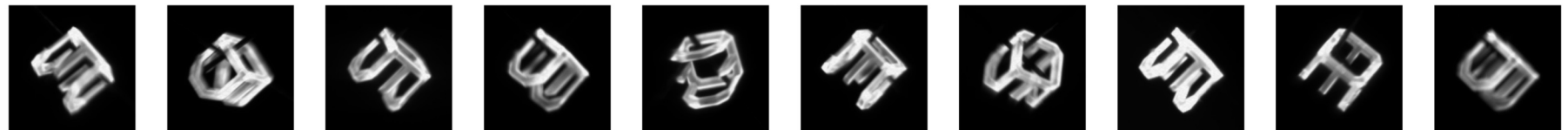
- GW signals can persist for months
- Can have multiple overlapping signals
- Measurements at different times of year can help signal localization



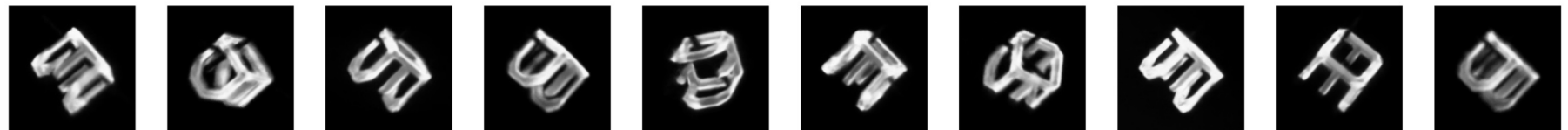
Rendering Views



Real Views



Generated Views



Many systematic effects can be sources of noise in phase measurements

- Especially laser wavefront variations – i.e. laser phase varying spatially

Goal: 3D Cloud Reconstruction

Why:

- Increased light detection
- Model spatially varying systematic effects

How: Single-Shot Multi-View Imaging System

Challenge: How to reconstruct the cloud in 3D?

- Tomographic imaging with complex geometry

Table 3. Summary of key experimental parameters and target values of MAGIS-100 (initial) (see Table 2). Spectral densities are taken to be in the $\sim 0.1 - 3$ Hz frequency band of interest. Note that the cloud kinematics can either be stabilized to below the target values or measured each shot at the target uncertainty.

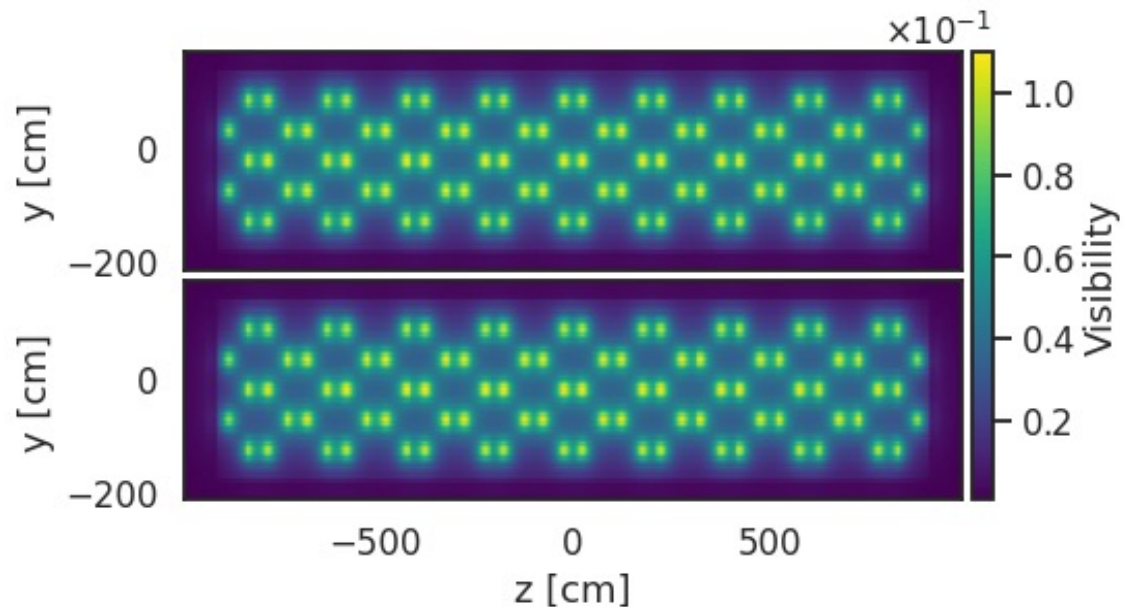
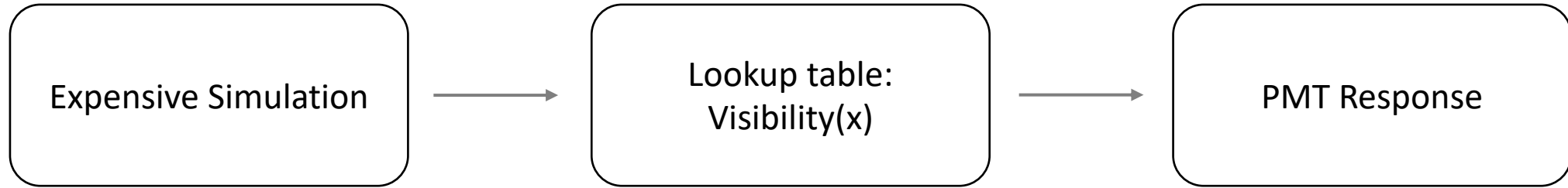
Parameter	Target Value	Primary Driving Factors
LMT atom optics	$n = 100$	Increase sensitivity to science signals
Phase resolution	$10^{-3} \text{ rad}/\sqrt{\text{Hz}}$	Increase sensitivity to science signals
Frequency noise/drift	$< 10 \text{ Hz}$	Increase pulse transfer efficiency (Section 4.3)
Per shot position uncertainty	$10 \mu\text{m}/\sqrt{\text{Hz}}$	Coupling to wavefront aberrations (Section 5.2)
Per shot velocity uncertainty	$10 \mu\text{m}/\text{s}/\sqrt{\text{Hz}}$	Coupling to wavefront aberrations (Section 5.2)
Laser wavefront variation	5 mrad^*	Coupling to cloud kinematic and laser pointing jitter (Section 5.2 and Section 5.4)
Laser intensity stabilization	$0.1\%/\sqrt{\text{Hz}}$	AC Stark shifts (Section 5.5)
Laser pointing stability	$30 \text{ nrad}/\sqrt{\text{Hz}}$	Coupling to wavefront aberrations (Section 5.4)
Magnetic field uniformity	1 mG (rms)	Clock frequency shifts

* at transverse length scales $\lesssim 3 \text{ mm}$

Application for Dune

DUNE Photon Response

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Photon simulation involves modeling optical visibility

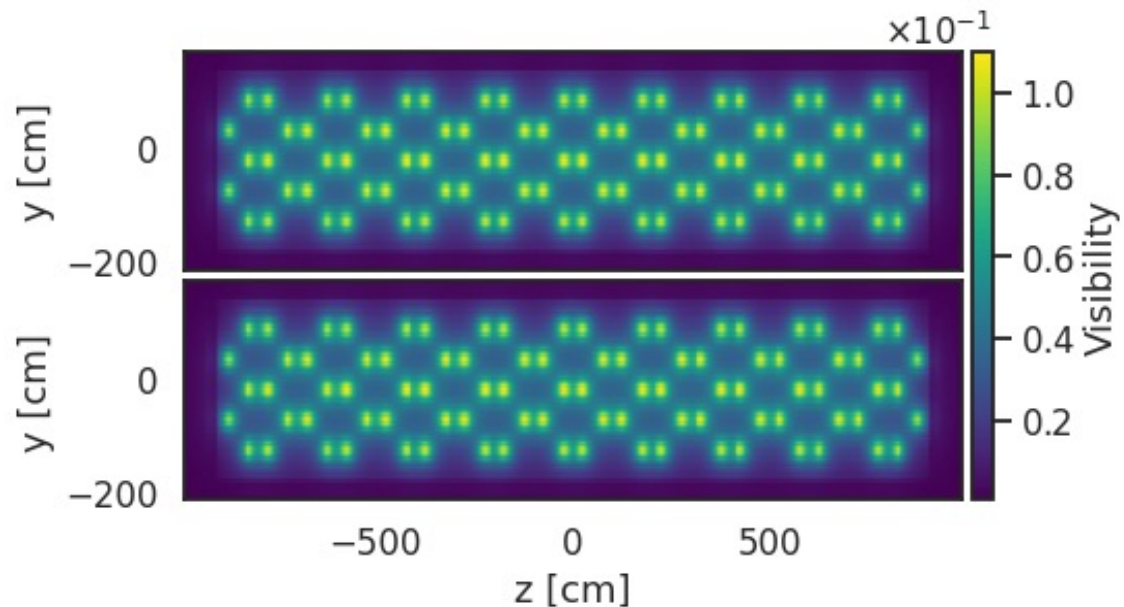
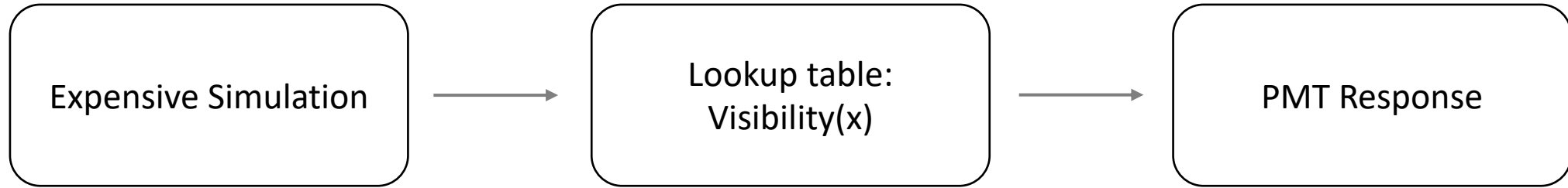
- Probability of observing a photon produced at a given point per PMT

Typically, expensive simulation done to produce grid of points (voxels)

Very large grid \rightarrow large memory consumption, not easily tunable to data

DUNE Photon Response

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Lookup table
↓
Neural Network
([SIREN](#))

Train neural network to represent lookup table

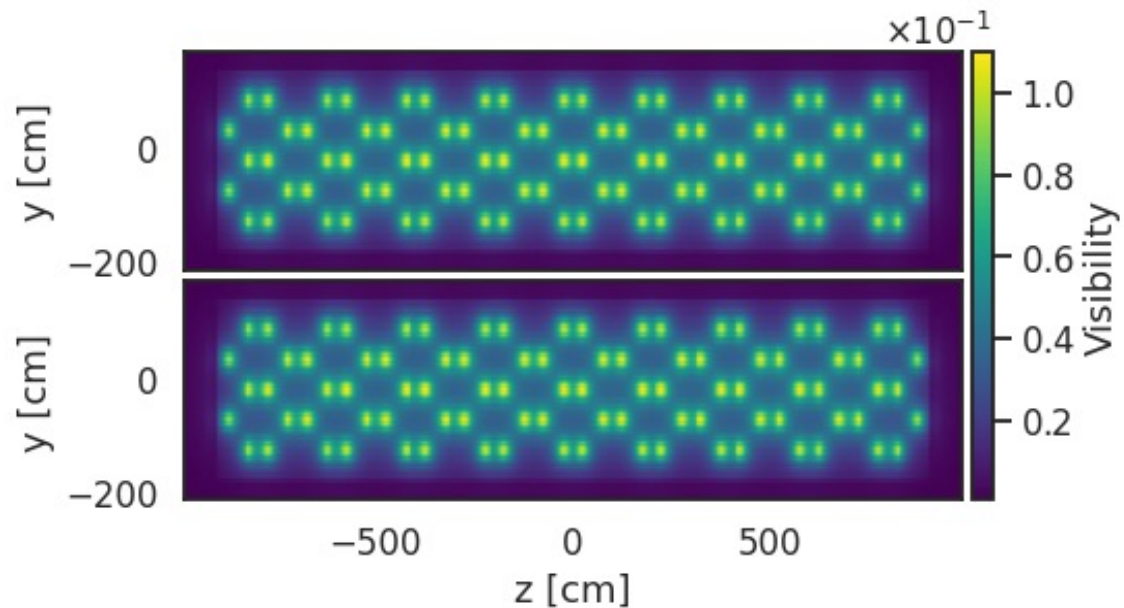
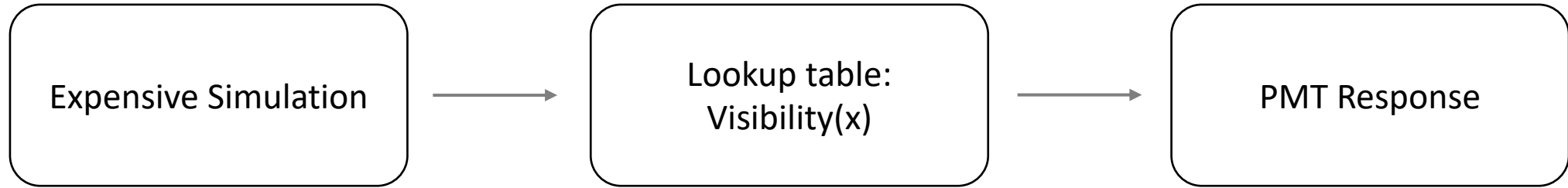
Voxels \rightarrow network weights

- More memory efficient

Network easily trainable

- Tune representation on measured data

DUNE Photon Response



Lookup table
↓
Neural Network (SIREN)

