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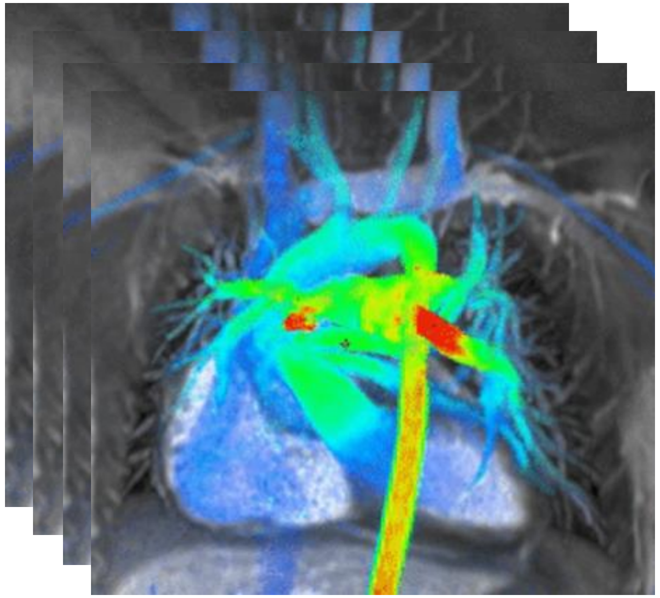
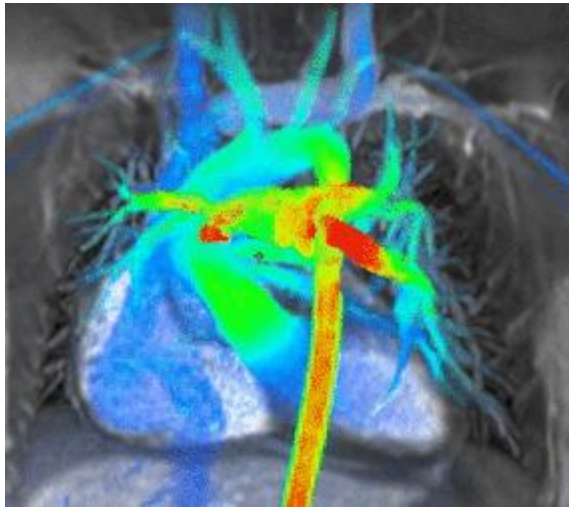
4D-KI Track:
Directed Diffusion of Colloidal Nanoparticles

Background

4D KI Track



Physics Informed Modelling

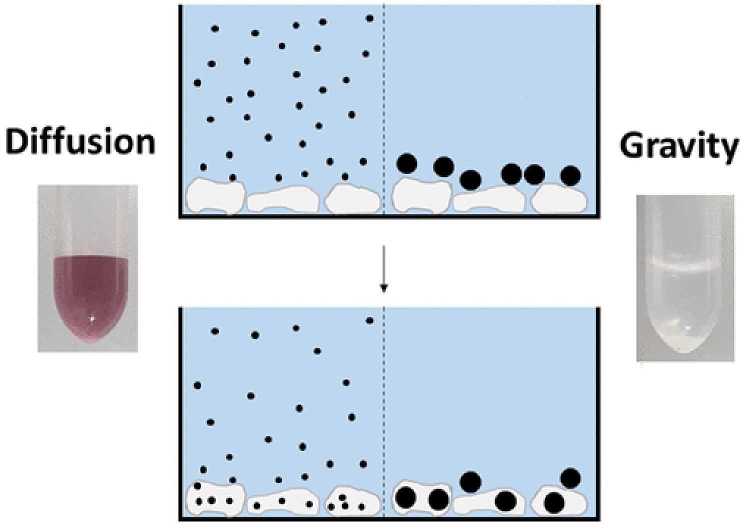


Temporally Sparse Data

Fully 4D Output

Cardiac MRI flow, Vasanawala, commons.wikimedia.org/wiki/File:Cardiac_MRI_flow.gif

Nanoparticle Diffusion



diffusion + gravity → directed diffusion

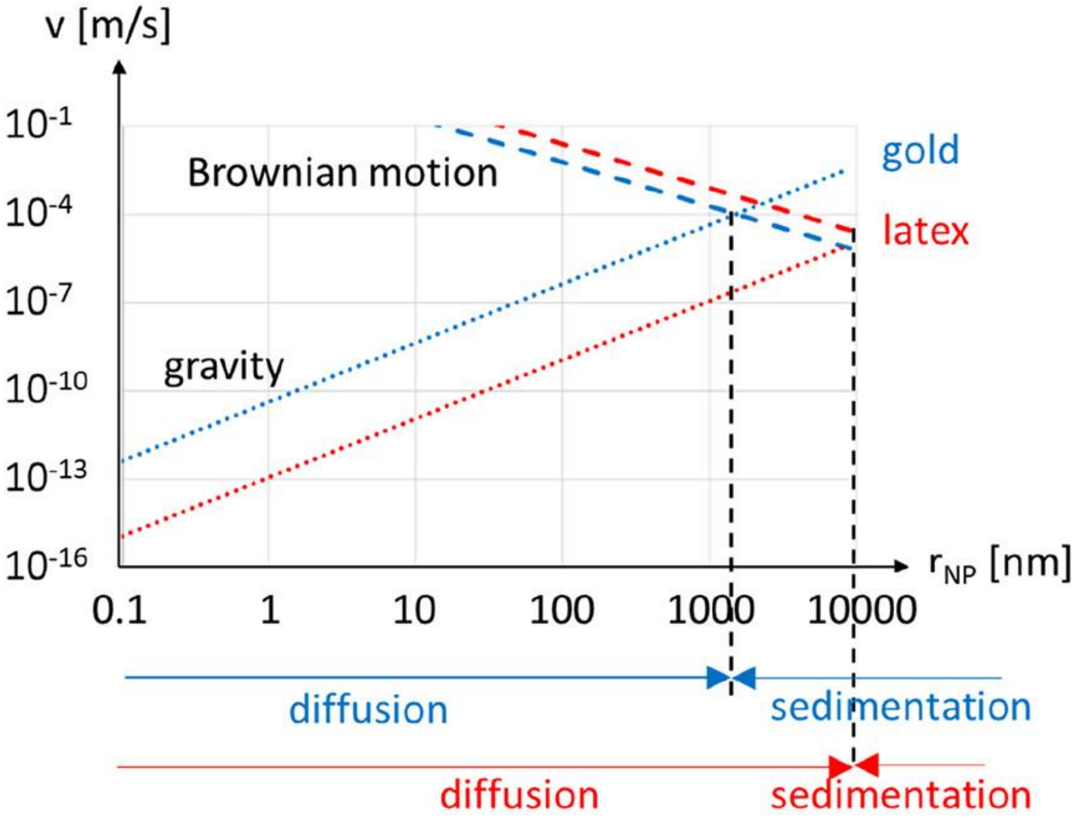
⇒ good initial model system for biological processes

Quantative Particle-Cell Interaction, Feliu et al, Langmuir
Sedimentation of Colloidal Nanoparticles in Solution, Midelet et al, Particle Journal

Previous work

- Feliu et al (2017) give analytical estimate of critical particle size for sedimentation
- Results do not match experiments

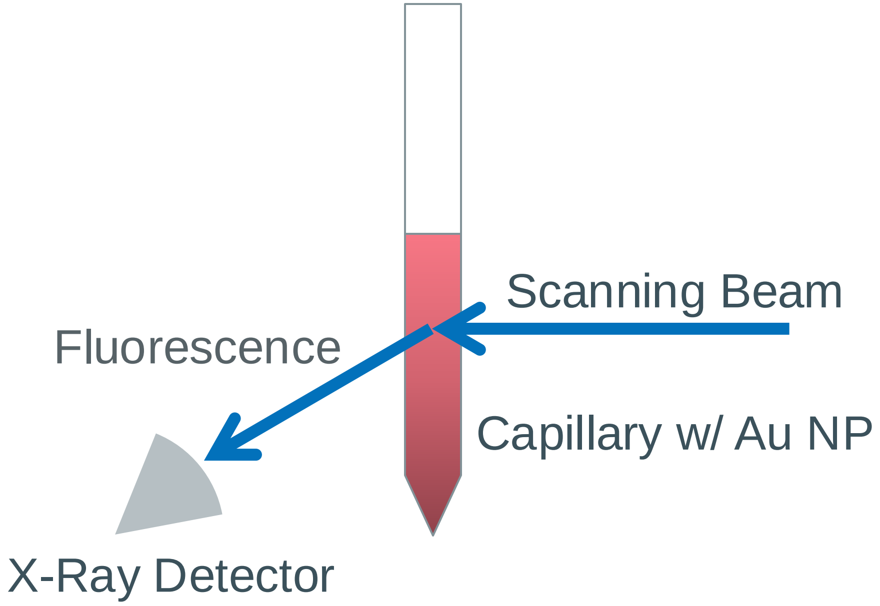
➡ Need to solve describing partial differential equation numerically

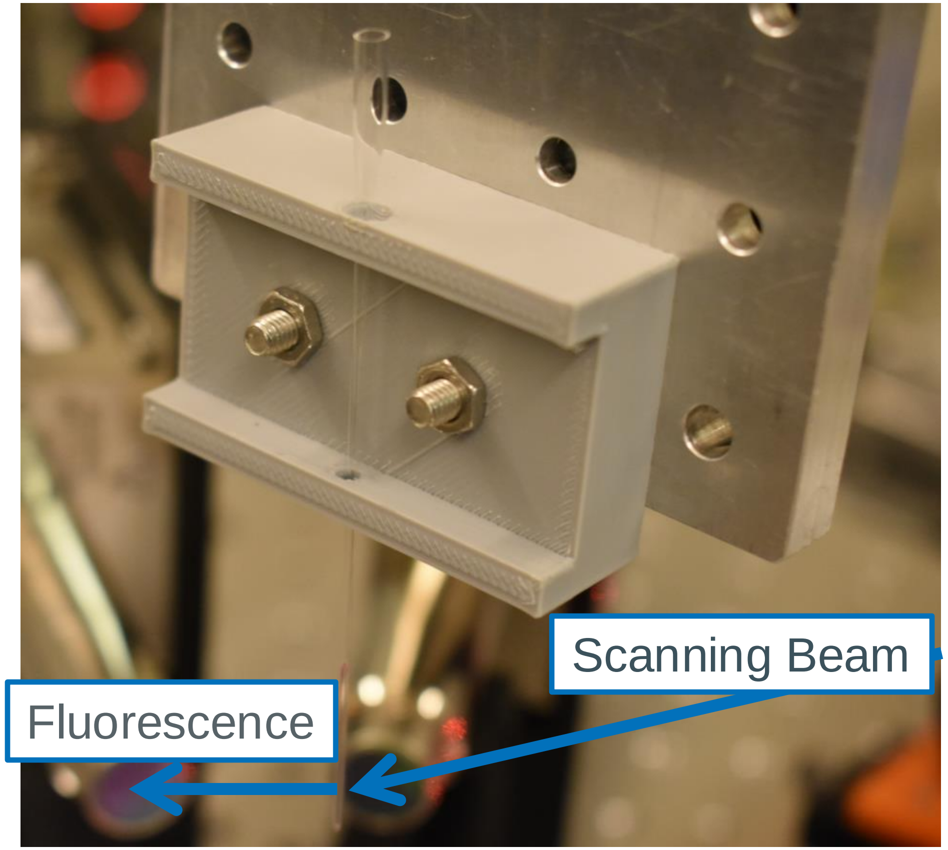


Thanks to:
Juan Barrios (providing samples)
Jannis Haak (measurement)
Florian Ziegler (measurement)

Measurement

Imaging Setup





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Signal Model

- Total Signal proportional to tracer conc.
- Known fluor. energies and cross sections
- Fano noise on energy measurements
- Poisson noise on counts
- Smooth background

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Directed Diffusion Model

- Concentration profile $c(x,t)$ obeys continuity: $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x}$
- Flux J includes sum of diffusive and gravitational term

$$J_{\text{diff}} = -\frac{\lambda}{r_{\text{H}}} \frac{\partial c}{\partial x}$$

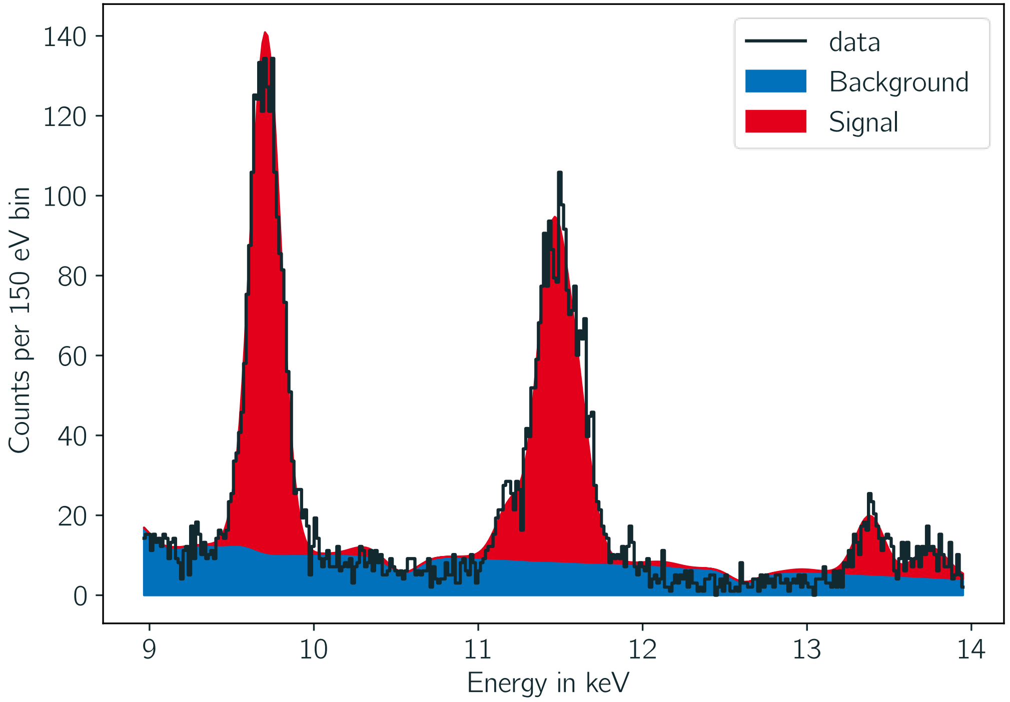
$$J_{\text{grav}} = \mu \frac{r_S^3}{r_H} c$$

r_H - hydrodynamic radius
r_S - solid radius
$c(x,t)$ - concentration field
λ, μ - apriori known constants

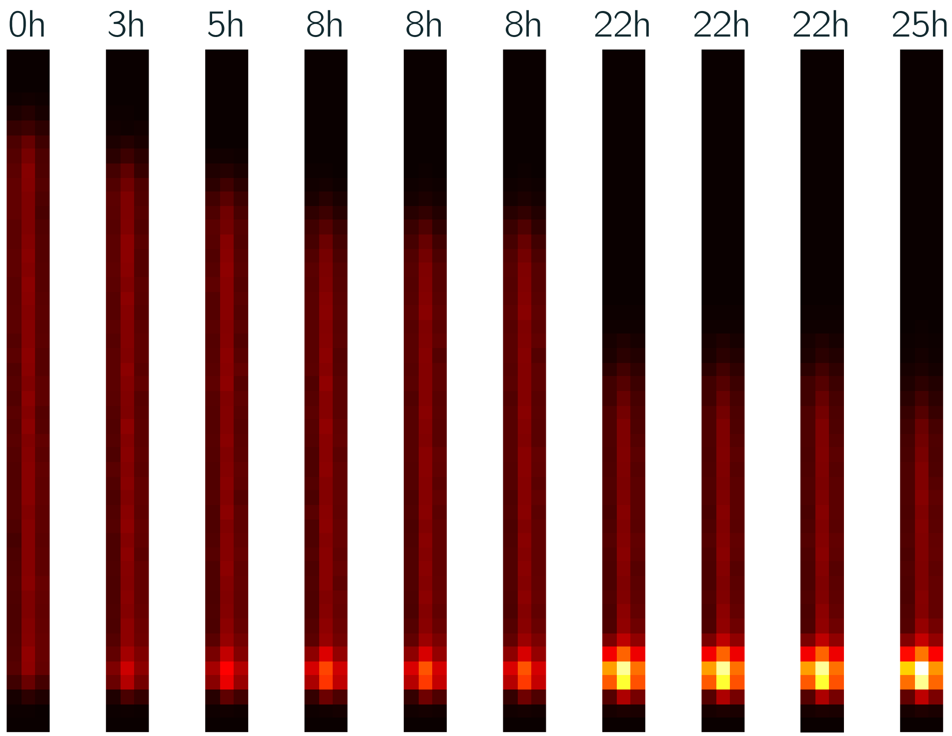
- Two counteracting effects:
  - Diffusion ⟶ homogeneous concentration profile
  - Gravity/Buoyancy ⟶ sedimentation and separation of solvent and solute

Tracer Quantification

Example of Single Point Spectrum



Scan Maps at Various Times



Physics Informed Modelling

Physics Informed Neural Networks

- Neural Networks trained to solve supervised learning task while respecting physical laws

$$\frac{\partial c}{\partial t} + \mathcal{N}_\nu[c] = 0,\ x \in \Omega,\ t \in [0, T]$$

$c(x,t)$ - unknown solution
$\Omega \subset \mathbb{R}^D$ - spatial domain
$\mathcal{N}_\nu$ - differential operator
ν - potentially unknown parameters

Measurement data $\{x_i, t_i, c_i\}_{i=1}^{N_{\text{data}}}$

Collocation points $\{x_j, t_j\}_{j=1}^{N_{\text{col}}}$

- Neural Network which outputs estimate

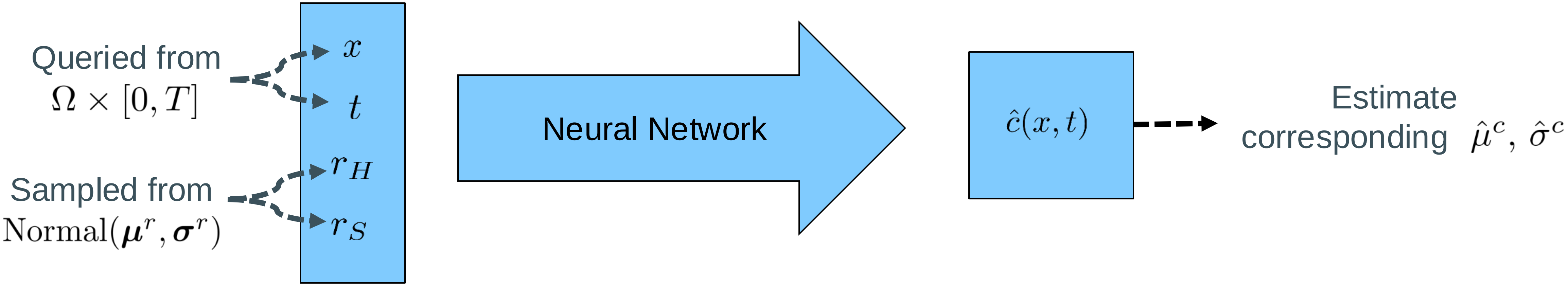
$$\hat{c}(x,t) = \text{NN}_\nu(x,t)$$

- Loss weighted sum of data term and PDE residual

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \alpha \mathcal{L}_{\text{PDE}}$$

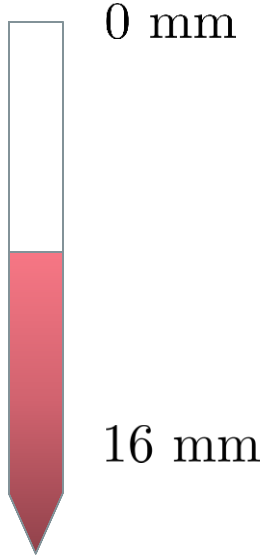
Stochastic Parameters and Output

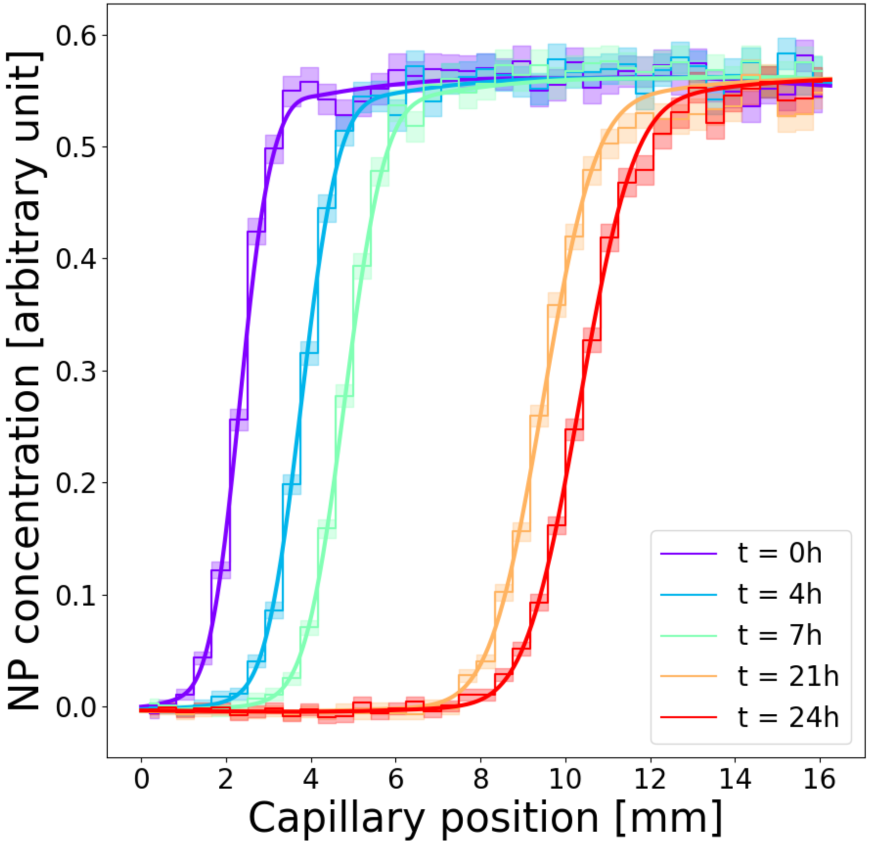
- Estimate unknown solid and hydrodynamic radius, $\mathcal{N}_\nu$ with $\nu = \{r_H, r_S, \lambda, \mu\}$
- Data is subject to Gaussian noise $c_i \sim \text{Normal}(\mu_i^c, \sigma_i^c) \Rightarrow \{x_i, t_i, \mu_i^c, \sigma_i^c\}_{i=1}^{N_{\text{data}}}$
- Radii estimates with uncertainty $(r_H, r_S) \sim \text{Normal}(\boldsymbol{\mu}^r, \boldsymbol{\sigma}^r)$



- Train via Kullback-Leibler divergence $\mathcal{L}_{\text{data}} = \frac{1}{2N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} \left[\frac{(\mu_i^c - \hat{\mu}_i^c)^2}{{\sigma_i^c}^2} + \left(\frac{\hat{\sigma}_i^c}{\sigma_i^c}\right)^2 - \ln\left(\frac{\hat{\sigma}_i^c}{\sigma_i^c}\right)^2 - 1 \right]$

4D Interpolation and Radii Estimates





- Continuous 4D interpolation in $\Omega \times [0, T]$
- $r_S, r_H \approx$ TEM and DLS measurement

$$r_H = 48.1\,\text{nm} \pm 9.0\,\text{nm}$$
$$r_S = 47.7\,\text{nm} \pm 3.0\,\text{nm}$$

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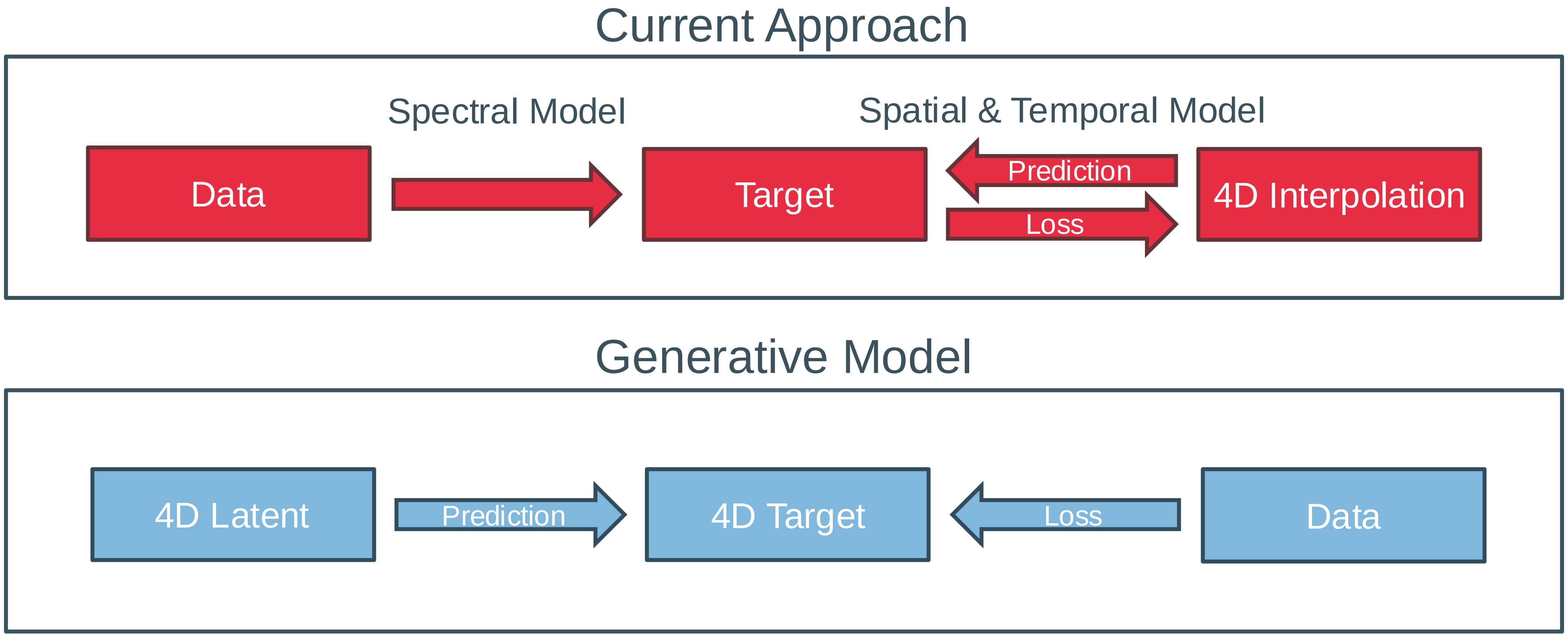
Outlook

Integration of Steps



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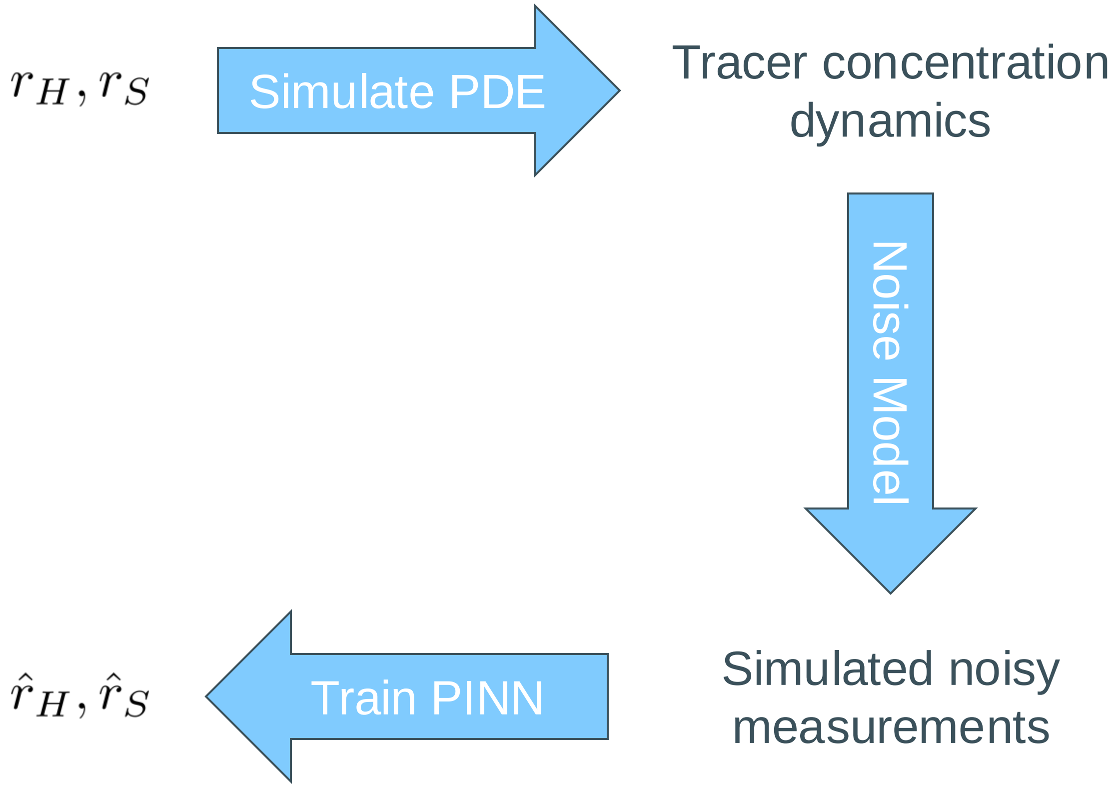
Simulations



What difference $\Delta r_{H/S} = r_{H/S}^{(1)} - r_{H/S}^{(2)}$ can we resolve?