Scientific AI for Cosmology and Beyond

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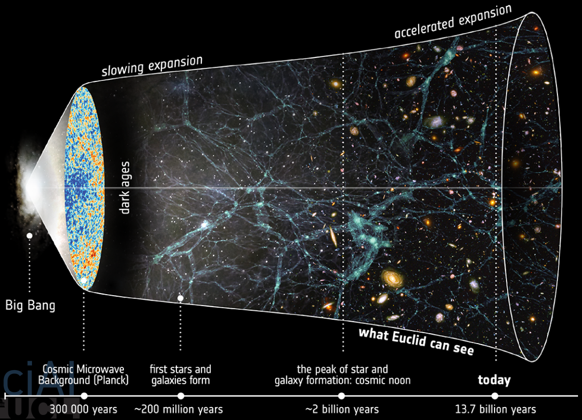
Towards a fundamental understanding of our Universe

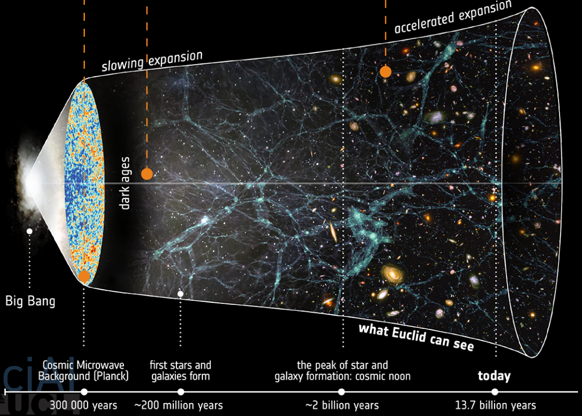


Towards a fundamental understanding of our Universe

What is the origin of structure?

How did luminous large-scale structure form?

What is the nature of dark energy and dark matter?



Towards a fundamental understanding of our Universe

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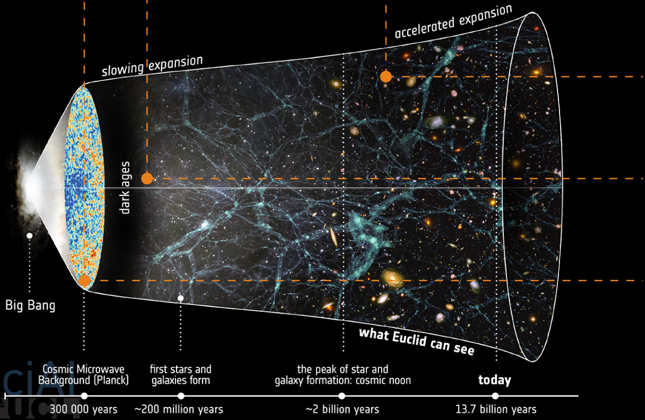
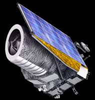


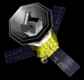


Euclid

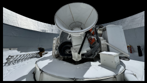
Roman

Rubin-LSST

SKA

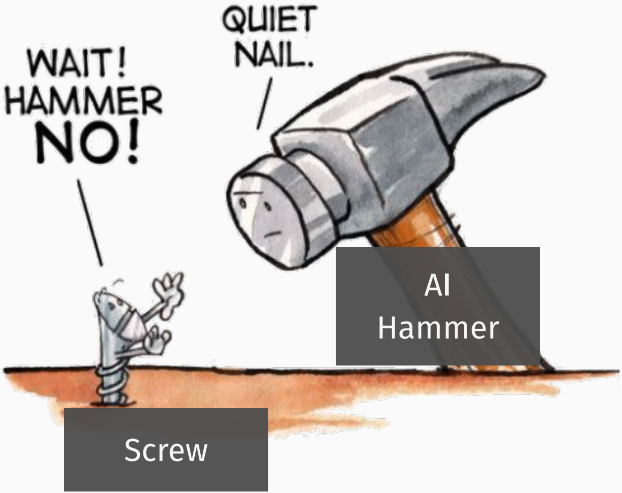


LiteBIRD

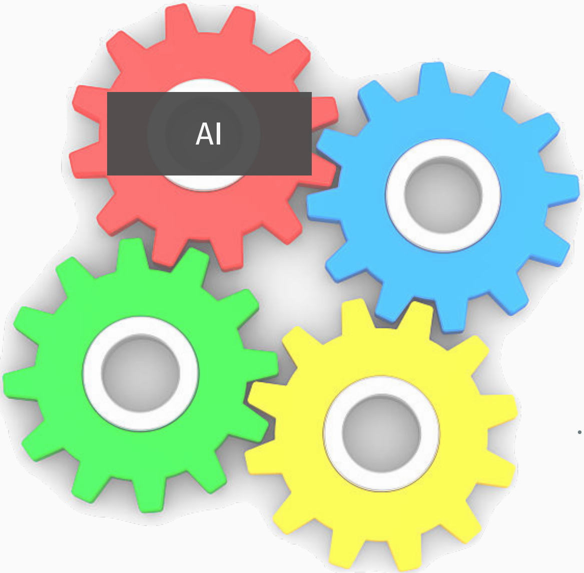


Simons

The AI hammer



The AI cog



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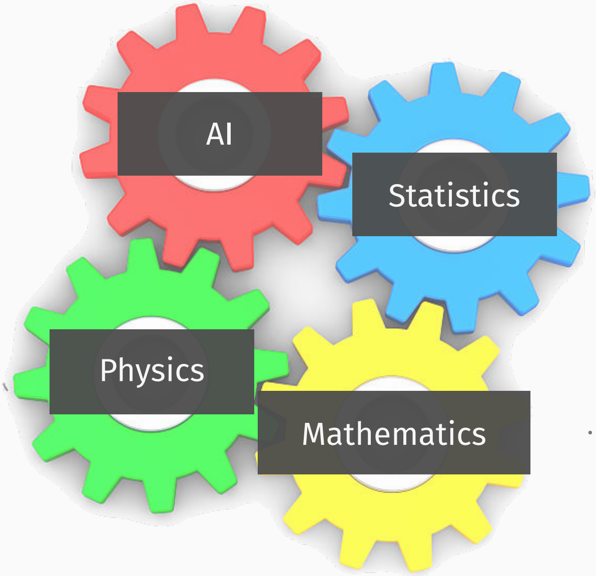
The AI cog



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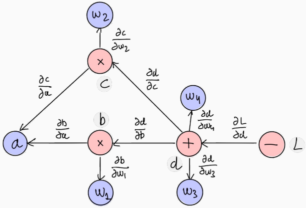
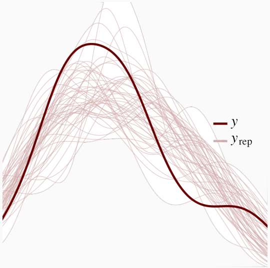
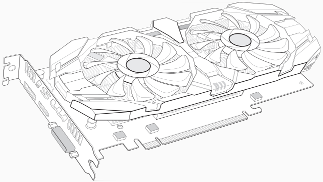
Harnessing modern computing paradigms



Automatic differentiation



Probabilistic programming



GPU acceleration

Towards scientific AI

Scientific AI

Physical
- Augmentation
- Physical Properties
- Physical Models

Statistical
- Bayesian Inference
- Implicit Inference
- Generative Models

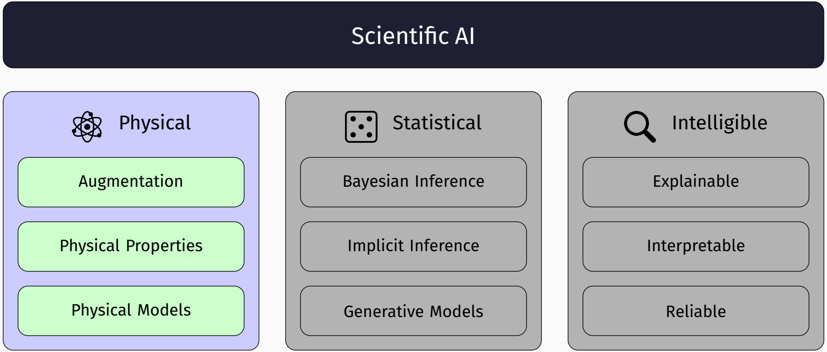
Intelligible
- Explainable
- Interpretable
- Reliable

Physics enhanced AI

Physics Enhanced AI

Embed physical understanding of the world into AI models.

(See review by Karniadakis *et al.* 2021.)



Augmentation

Apply **physical transformations** that data known to satisfy to augment training data $\rightsquigarrow$ AI model **learns physics through training**.

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- Common to augment image data-set with rotations, flips, shifts, scales, contrast, ...

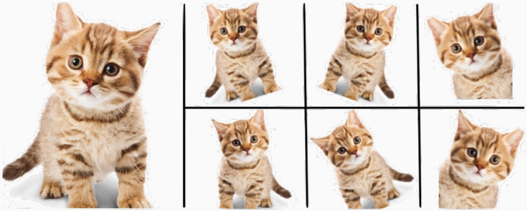
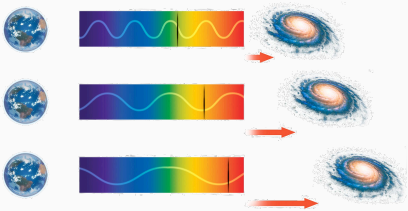


Image augmentation

Apply **physical transformations** that data known to satisfy to augment training data $\rightsquigarrow$ AI model **learns physics through training**.

- Redshift augmentation of supernovae
  (Boone 2019, Alves *et al.* (inc. McEwen) 2022, 2023)



Redshift augmentation

Physical properties: geometries, symmetries, conservation laws

Encode physical properties of the world into AI models (e.g. geometry, symmetries, conservation laws) $\rightsquigarrow$ **Physics embedded in architecture** of AI model.

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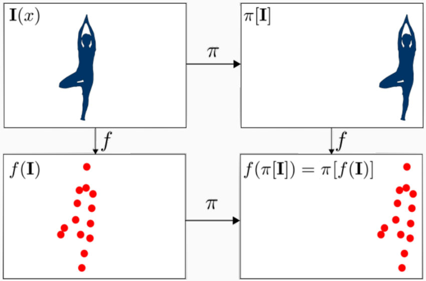
Encode physical properties of the world into AI models (e.g. geometry, symmetries, conservation laws) $\rightsquigarrow$ **Physics embedded in architecture** of AI model.

- Key factor CNNs so successful is due to encoding translational equivariance.

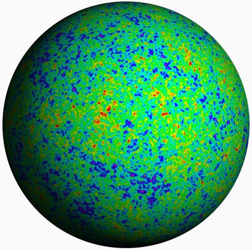


Translational equivariance

Physical properties: geometries, symmetries, conservation laws

Encode physical properties of the world into AI models (e.g. geometry, symmetries, conservation laws) $\rightsquigarrow$ **Physics embedded in architecture** of AI model.

- Geometric deep learning on the sphere (Cobb et al. 2021, McEwen et al. 2022, Ocampo, Price & McEwen 2023)



CMB observed on the celestial sphere

Physical models: PINNS and differentiable physics

Encode physical models of world into AI models:

1. Encode dynamics (differential equations) via loss functions (PINNs).
2. Embed full (differentiable) physical models inside AI model.

$\rightsquigarrow$ Physics learned in training and embedded in model.

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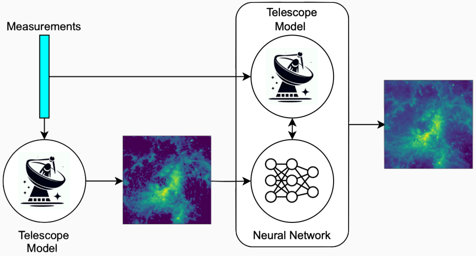
⇝ **Physics learned in training and embedded in model.**

- Differentiable physical models
  - Instrument models (Mars *et al.* McEwen 2023, 2024, Liaudat *et al.* McEwen 2024)
  - Physical models (Piras *et al.* McEwen 2024, Spurio Mancini *et al.* McEwen 2024, Whitney *et al.* McEwen in prep.)



Hybrid physics-enhanced AI model
(Mars *et al.* McEwen 2023, 2024)

Physical models: PINNS and differentiable physics

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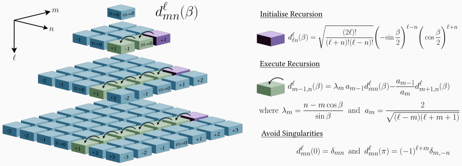
$\rightsquigarrow$ **Physics learned in training and embedded in model.**

- Differentiable mathematical methods
  - Fourier transforms
  - Spherical harmonic transforms (**`s2fft`**; Price & McEwen 2023)
  - Spherical wavelet transforms (**`s2wav`**; Price *et al.* McEwen 2024)
  - Spherical scattering transforms (**`s2scat`**; Mousset *et al.* McEwen 2024)



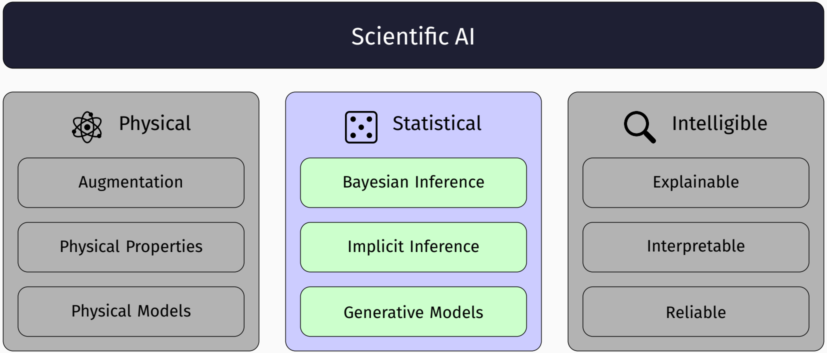
Differentiable and GPU-friendly recursions (Price & McEwen 2023)

Statistical AI

Statistical AI

Embed a statistical representation of data, models and/or outputs.

(See Murray 2022.)



AI techniques can be integrated into Bayesian frameworks to **enhance accuracy and computational efficiency**, making some approaches accessible that were previously intractable.

Bayesian inference

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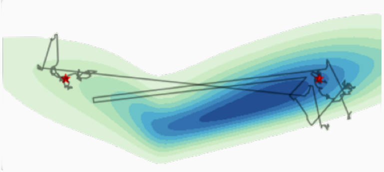
- Enhanced MCMC for parameter estimation (Grabrie *et al.* 2022, Karamanis *et al.* 2022).

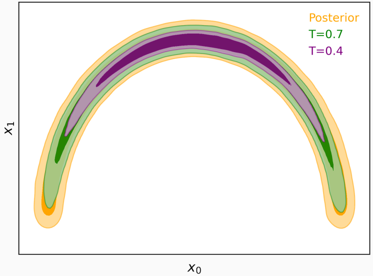


Learned proposal distributions

Bayesian inference

AI techniques can be integrated into Bayesian frameworks to **enhance accuracy and computational efficiency**, making some approaches accessible that were previously intractable.

- Enhanced Bayesian model selection (**`harmonic`**; McEwen *et al.* 2021, Polanska *et al.* McEwen 2023, 2024, Piras *et al.* McEwen 2024, Spurio Mancini *et al.* McEwen 2023, 2024).



Learned harmonic mean estimator (**`harmonic`**)

Implicit inference

AI techniques can be used to **learn surrogates of implicit distributions** when they are not tractable or are computationally infeasible.

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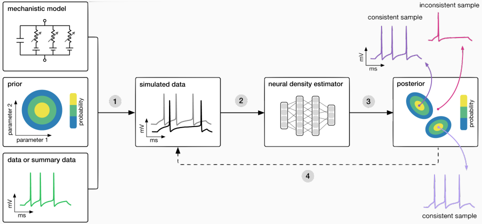
- Simulation-based inference (Cranmer *et al.* 2021).

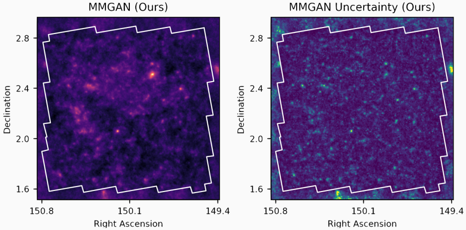


`sbi`

Implicit inference

AI techniques can be used to **learn surrogates of implicit distributions** when they are not tractable or are computationally infeasible.

- Variational inference
  (Whitney *et al.* McEwen 2024).



Mass mapping with uncertainties by variational inference (Whitney *et al.* McEwen 2024)

Generative models

Generative models **learn a prior distribution** from data for sampling and/or evaluating probability densities.

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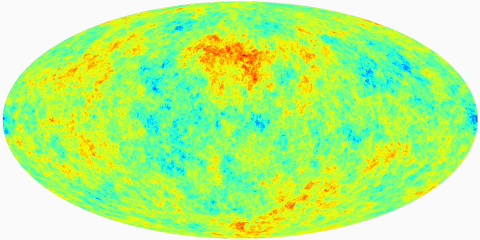
- Emulation: sample from learned prior (Price *et al.* McEwen 2023, Price *et al.* McEwen in prep., Mousset *et al.* McEwen 2024)

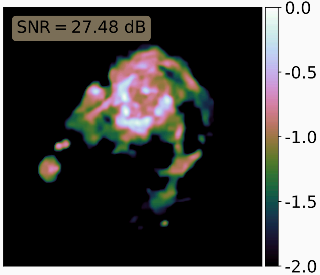


Emulated cosmic string maps (**`stringgen`**, Price *et al.* McEwen 2023, Price *et al.* McEwen in prep.)

Generative models

Generative models **learn a prior distribution** from data for sampling and/or evaluating probability densities.

- Integrate learned priors into analysis
  (McEwen *et al.* 2023, Liaudat *et al.* McEwen 2024)



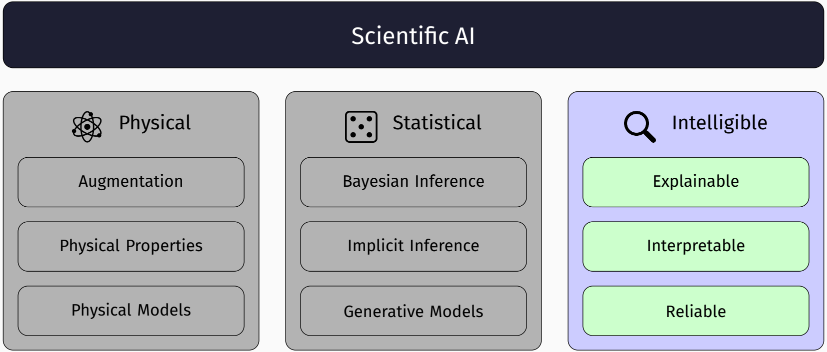
Learn radio galaxy prior
(Liaudat *et al.* McEwen 2024)

Intelligible AI

Intelligible AI

AI methods that are able to be understood by humans and are reliable.

(See Weld & Bansal 2018, Ras *et al.* 2020.)



Explainability

Explainable AI techniques may or may not be interpretable themselves but their **outputs can be explained to humans.**

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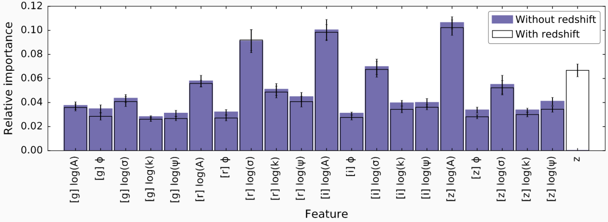
- Feature importances
  (Lochner, McEwen *et al.* 2016)



Supernova feature importances

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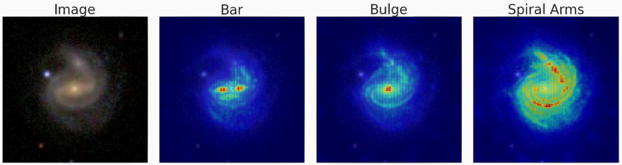
- Saliency maps
  (Bhambra, Joachimi & Lahav 2022)



Galaxy saliency mapping

Interpretability

Interpretable AI models are **white boxes that can be understood by humans**.

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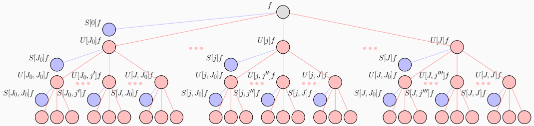
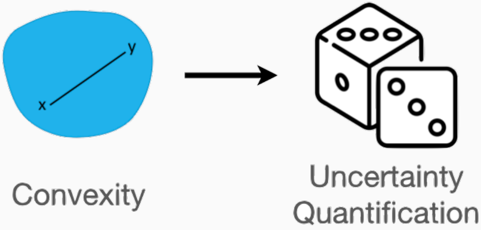
- Designed models such as wavelet scattering networks
  (McEwen *et al.* 2022, Mousset *et al.* McEwen 2024)



Scattering network (McEwen *et al.* 2022)

Interpretable AI models are **white boxes that can be understood by humans**.

- Interpretable constraints on AI models
  (Liaudat *et al.* McEwen 2024)

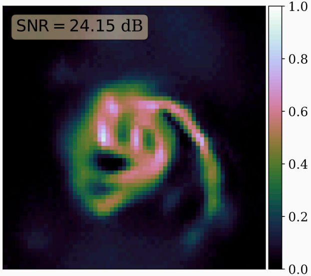


Impose convexity on learned model

Interpretability

Interpretable AI models are **white boxes that can be understood by humans**.

- Deep priors learned from training data (McEwen *et al.* 2023, Liaudat *et al.* McEwen 2024)



Compute Bayesian evidence for model selection (McEwen *et al.* 2023)

Reliability

Reliability and validity **critical for science** to have confidence in results of AI models. Closely coupled with a **meaningful statistical distribution** of outputs.

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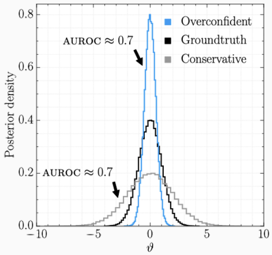
Reliability and validity **critical for science** to have confidence in results of AI models. Closely coupled with a **meaningful statistical distribution** of outputs.

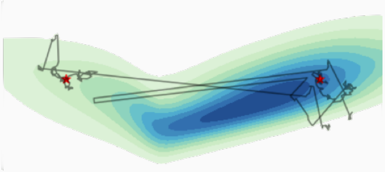
- Validity of statistical distributions (Lueckmann *et al.* 2021, Hermans *et al.* 2022, Cannon *et al.* 2023)



Validity of distribution (Hermans *et al.* 2022)

Reliability and validity **critical for science** to have confidence in results of AI models. Closely coupled with a **meaningful statistical distribution** of outputs.

- Integrate into statistical frameworks to inherit theoretical guarantees
  (McEwen *et al.* 2023, Liaudat *et al.* McEwen 2024, McEwen *et al.* 2021, Polanska *et al.* McEwen 2023, 2024, Piras *et al.* McEwen 2024)



Inherit guarantees from overarching statistical frameworks

Reliability

Reliability and validity **critical for science** to have confidence in results of AI models. Closely coupled with a **meaningful statistical distribution** of outputs.

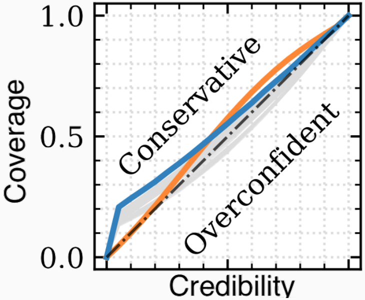
- Design to ensure conservative and avoid mode collapse (Delaunoy *et al.* 2022, Price *et al.* McEwen 2023, Whitney *et al.* McEwen 2024)

Recover probability distribution over full underlying data manifold (Price *et al.* McEwen 2023)

Reliability

Reliability and validity **critical for science** to have confidence in results of AI models. Closely coupled with a **meaningful statistical distribution** of outputs.

- Extensive validation checks:
  - Coverage testing (Lemos *et al.* 2023)
  - Simulation-based calibration checks (Talts *et al.* 2020)
  - Classifier two-sample tests (C2ST) (Lopez-Paz & Oquab 2017)
  - ...



Coverage analysis
(Cannon *et al.* 2023)

Summary

Towards scientific AI

Scientific AI

Physical
- Augmentation
- Physical Properties
- Physical Models

Statistical
- Bayesian Inference
- Implicit Inference
- Generative Models

Intelligible
- Explainable
- Interpretable
- Reliable

Extra Slides

Physics Enhanced AI

Embed physical understanding of the world into AI models.

(See review by Karniadakis *et al.* 2021.)

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Augmentation

Apply **physical transformations** that data known to satisfy to augment training data $\rightsquigarrow$ AI model **learns physics through training**.

▷ Data efficiency suffers: data "used" to learn physics, rather than problem.

▷ Simple and easy to implement.

Physical properties: geometries, symmetries, conservation laws

Encode physical properties of the world into AI models (e.g. geometry, symmetries, conservation laws) $\rightsquigarrow$ **Physics embedded in architecture** of AI model.

- Inductive biases required? Should we just learn from data?
- Highly computationally demanding.

- Improved data-efficiency.
- Inductive biases not necessarily strictly enforced.
- Develop efficient algorithms (e.g. Ocampo, Price & McEwen 2023).

Physical models: PINNS and differentiable physics

Encode physical models of world into AI models:

1. Encode dynamics (differential equations) via loss functions (PINNs).
2. Embed full (differentiable) physical models inside AI model.

$\rightsquigarrow$ **Physics learned in training and embedded in model.**

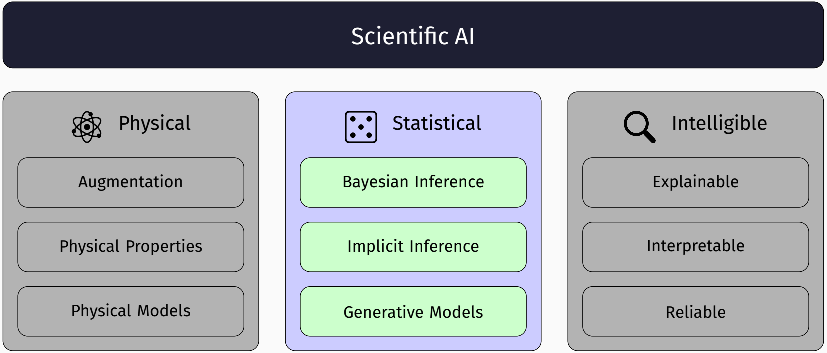
- PINNs only capture limited dynamics via loss.
- Full physical models requires differentiable programming frameworks.

- Capture full physics with differentiable models!
- Emulators also provide differentiability.
- Write new differentiable codes (e.g. `s2fft`; Price & McEwen 2023).

Statistical AI

Embed a statistical representation of data, models and/or outputs.

(See Murray 2022.)



AI techniques can be integrated into Bayesian frameworks to **enhance accuracy and computational efficiency**, making some approaches accessible that were previously intractable.

- Learned components (*e.g.* proposals) must satisfy appropriate properties.

- Enforce required properties on learned components.
- Inherit statistical guarantees of overarching Bayesian framework.

Implicit inference

AI techniques can be used to **learn surrogates of implicit distributions** when they are not tractable or are computationally infeasible.

- Availability and representativeness of training data.
- Cost of training.
- Reliability?

- Public datasets/benchmarks (*e.g.* IllustrisTNG, CAMELS, Quijote, CosmoGrid, Gower St).
- Amortized inference (training **not** repeated for new observations).
- Integrate in Bayesian framework to provide some statistical guarantees.
- Statistical validation (hold that thought... see Reliability section).

Generative models

Generative models **learn a prior distribution** from data for sampling and/or evaluating probability densities.

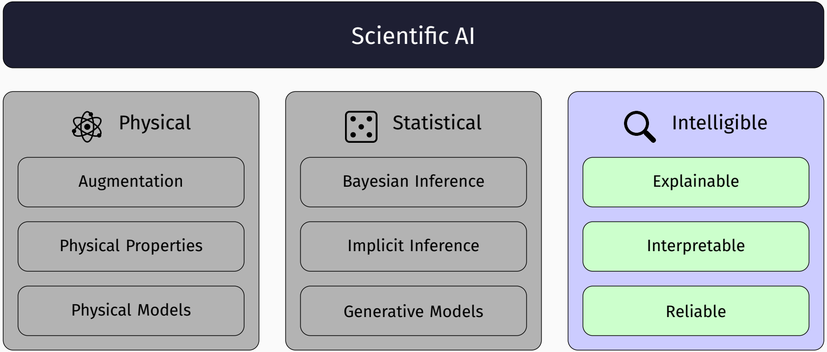
- Availability and representativeness of training data.
- Reliability, *e.g.* diversity of AI models often lacking.

- Public datasets/benchmarks (*e.g.* IllustrisTNG, CAMELS, Quijote, CosmoGrid, Gower St).
- Meta sampling to recover distribution over manifold (*e.g.* Price *et al.* 2023).
- Reliability (hold that thought... see Reliability section).

Intelligible AI

AI methods that are able to be understood by humans and are reliable.

(See Weld & Bansal 2018, Ras *et al.* 2020.)



Explainability

Explainable AI techniques may or may not be interpretable themselves but their **outputs can be explained to humans.**

- Poking the black box.
- Humans still not able to comprehend underlying process.

Interpretability

Interpretable AI models are **white boxes that can be understood by humans**.

- Designed models limit flexibility.

- Benefits of designed models often outweigh (minimal) reduced flexibility.

Reliability

Reliability and validity **critical for science** to have confidence in results of AI models. Closely coupled with a **meaningful statistical distribution** of outputs.

- Uncertainties not aways meaningful.
- Diversity of AI model often lacking.

- Integrate in statistical framework to inherit theoretical guarantees.
- Design to be conservative and avoid mode collapse
  (*e.g.* Price *et al.* McEwen 2023, Whitney *et al.* McEwen 2024).
- Extensive validation tests.
- Well-posed frameworks (*e.g.* physics enhanced, statistical).