Differentiable and accelerated spherical transforms

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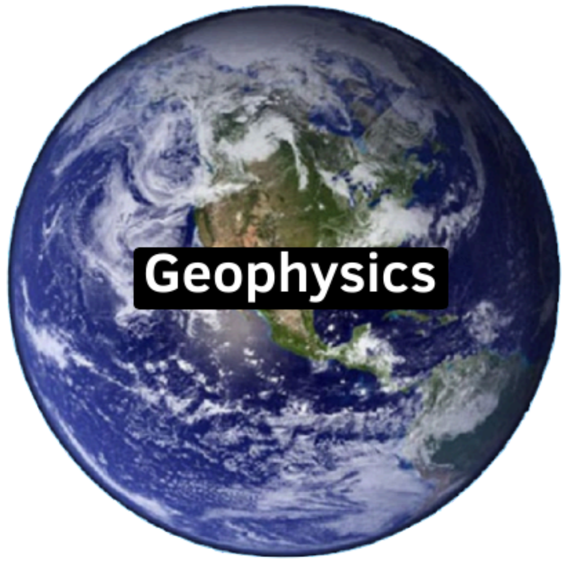
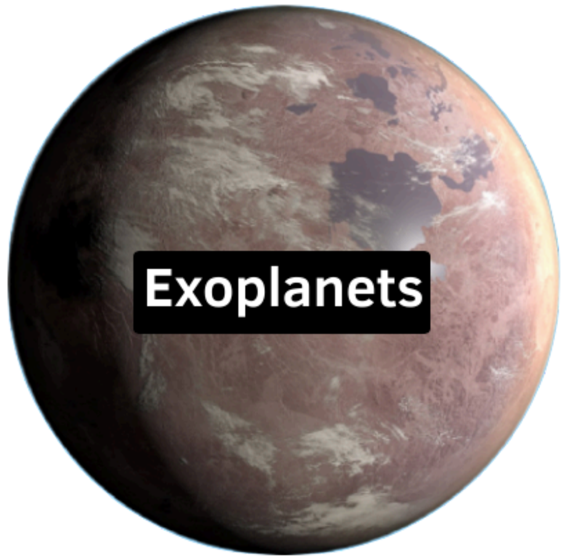
Durham HPC Days, June 2025

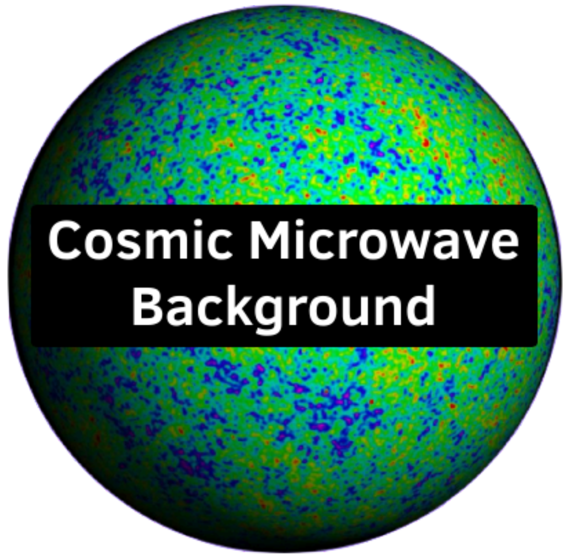
Data observed on the sphere are prevalent

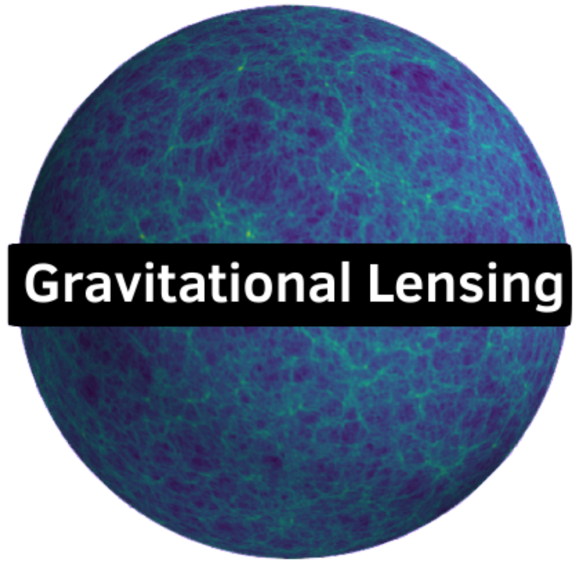
Planetary Science



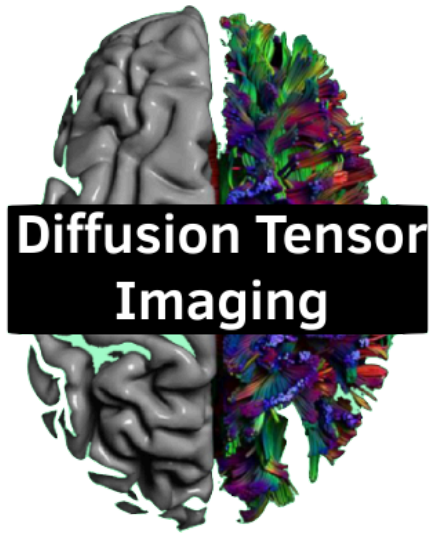


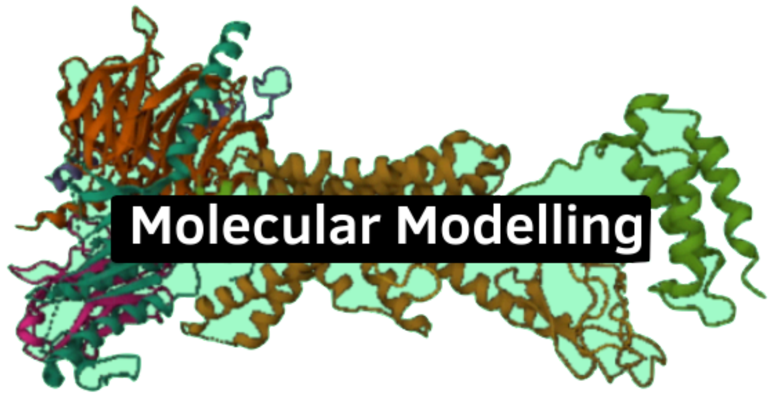
Cosmology





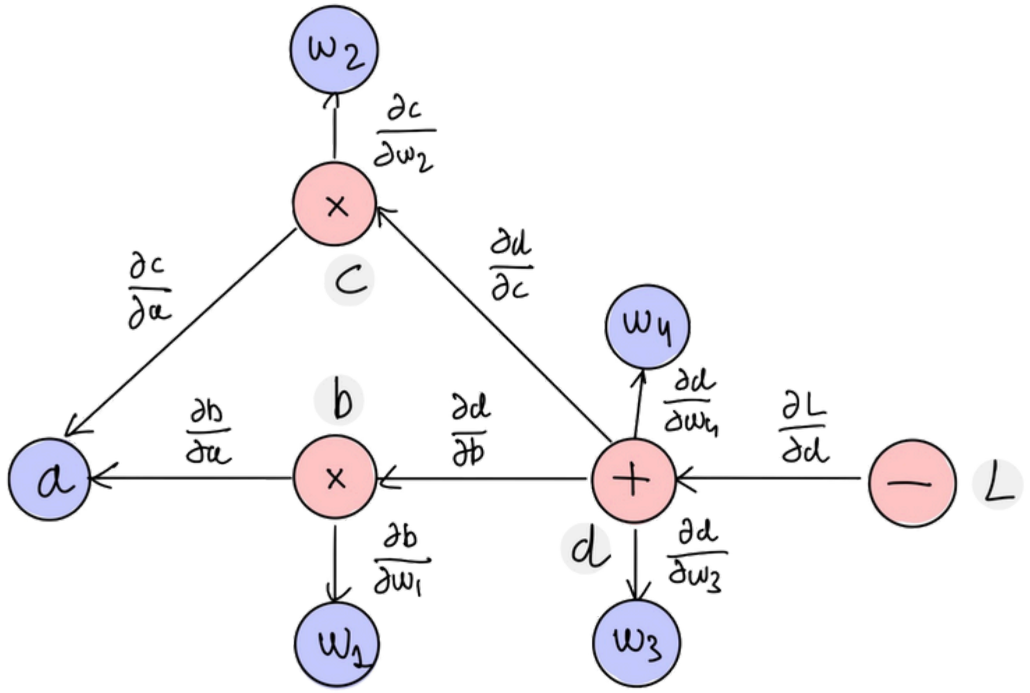
Bioinformatics





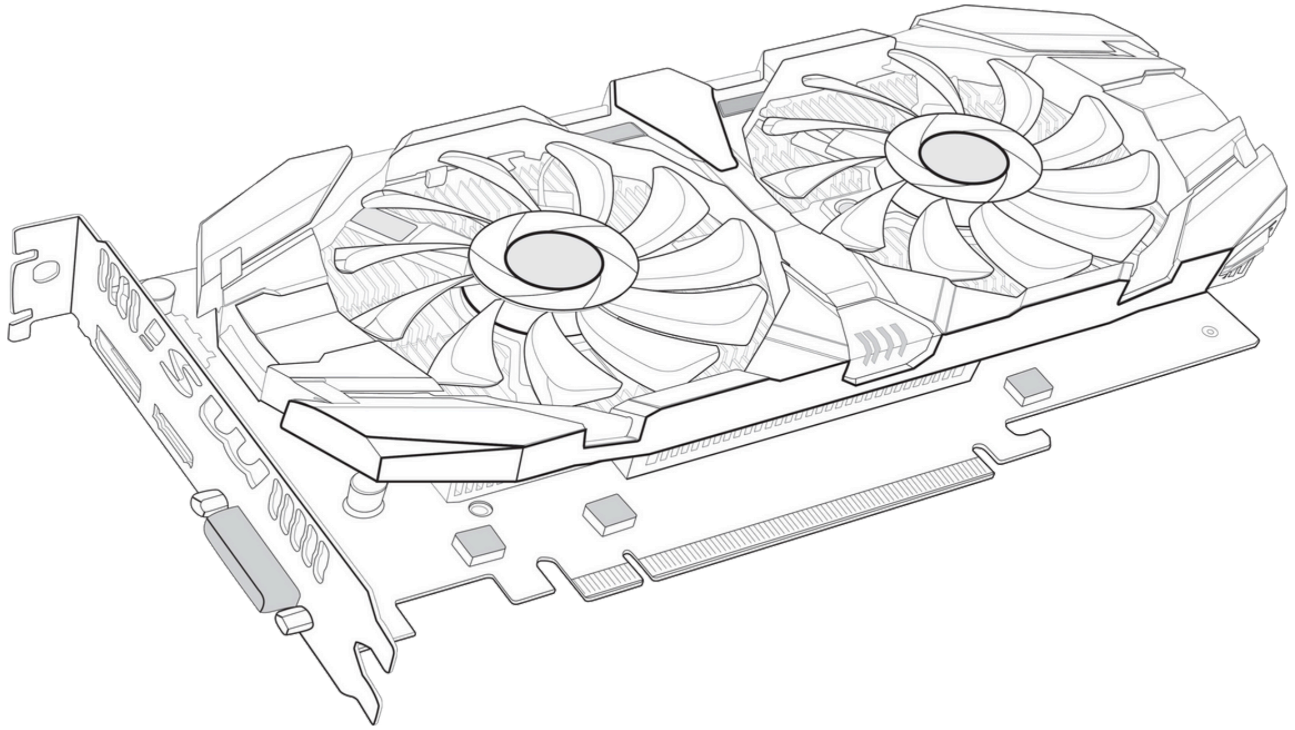
Others

Harnessing modern computing paradigms



Automatic differentiation

- Differential programming
- AI models



GPU acceleration

- Leverage high throughput of modern hardware accelerators

s2x suite of codes

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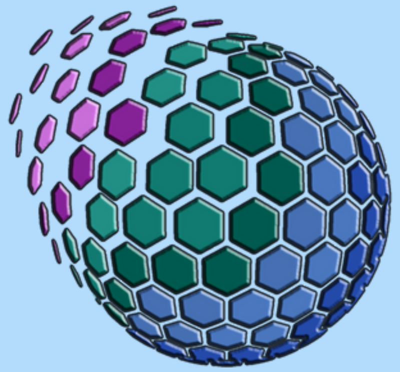
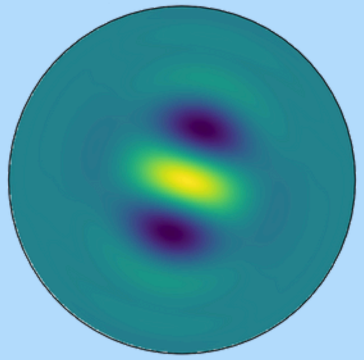


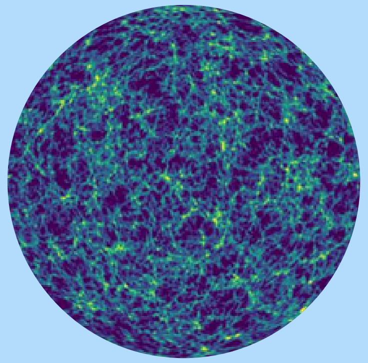
s2fft: Spherical harmonic transforms

https://github.com/astro-informatics/s2fft



s2wav: Spherical wavelet transforms

https://github.com/astro-informatics/s2wav



s2scat: Spherical wavelet scattering transforms

https://github.com/astro-informatics/s2scat

s2ai: Scalable and equivariant spherical AI

https://github.com/astro-informatics/s2ai

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`s2fft`: spherical harmonic and Wigner transforms

Spherical harmonic transform (Fourier transform on the sphere)

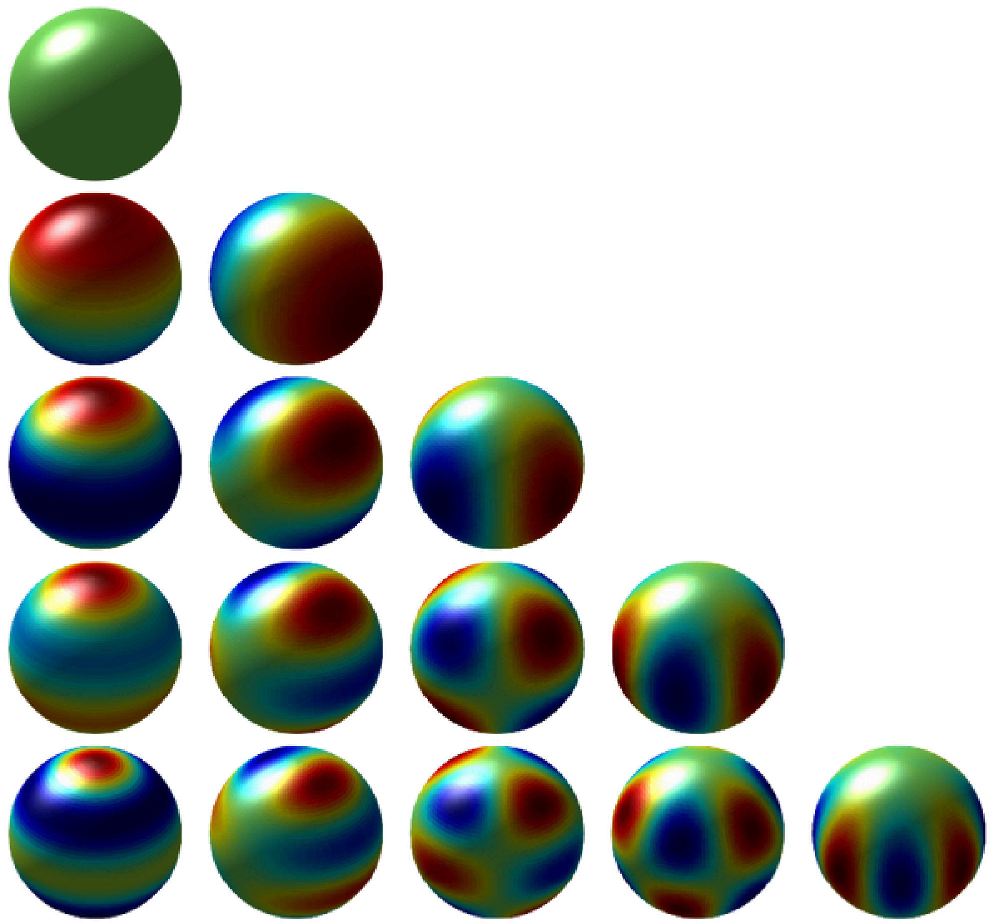
A field $f \in \mathrm{L}^2(\mathbb{S}^2)$ can be decomposed into its harmonic representation by

$$f(\theta, \phi) = \sum_{\ell,m} f_{\ell m} Y_{\ell m}(\theta, \phi),$$

where the spherical harmonic coefficients are given by the usual projection onto the basis functions:

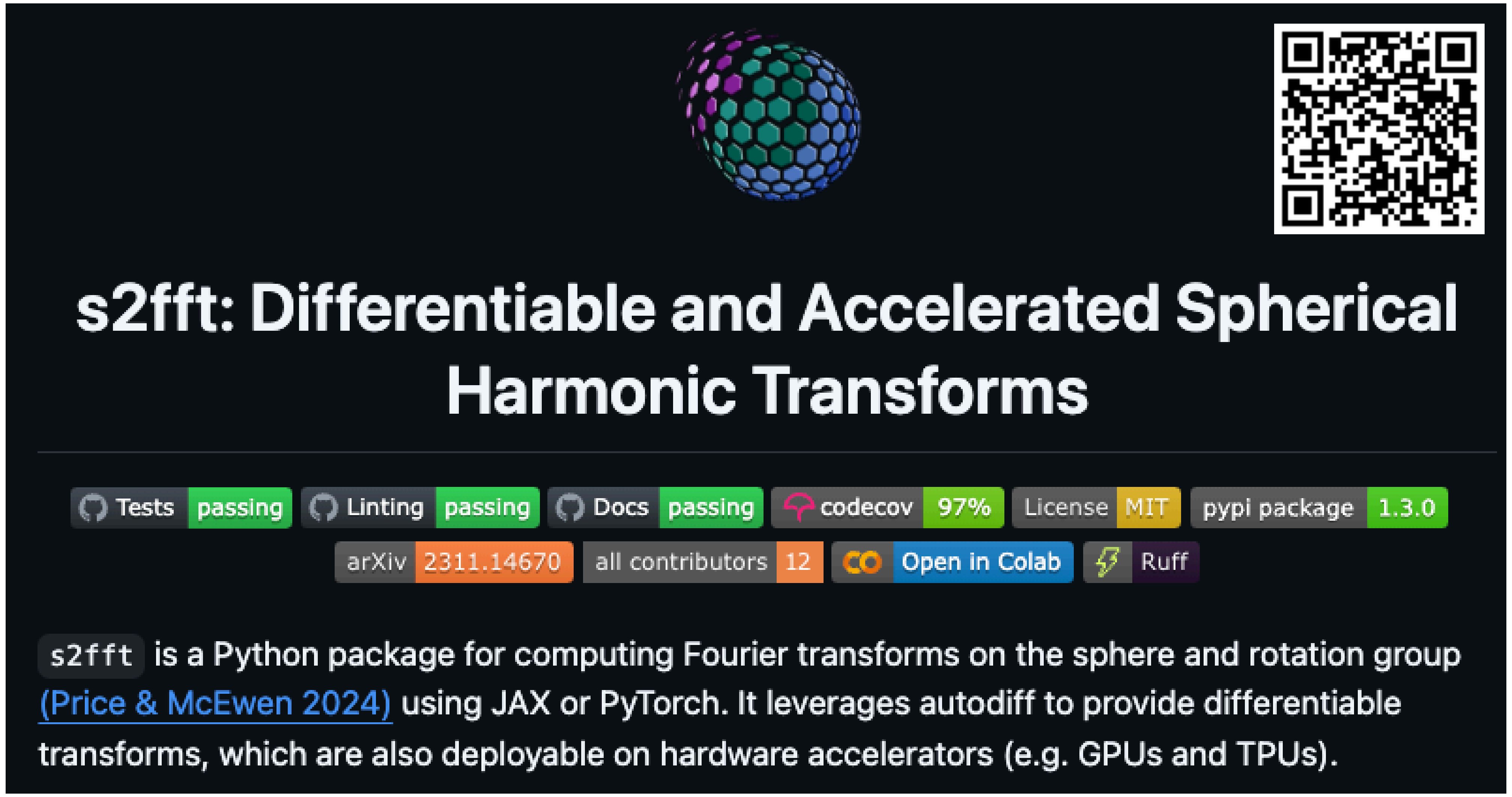
$$f_{\ell m} = \int_{\mathbb{S}^2} f(\theta, \phi) Y^*_{\ell m}(\theta, \phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi.$$

Driscoll & Healy (1995), ..., McEwen & Wiaux (2011), Price & McEwen (2024)



Spherical harmonics

s2fft: spherical harmonic and Wigner transforms



s2fft: Differentiable and Accelerated Spherical Harmonic Transforms

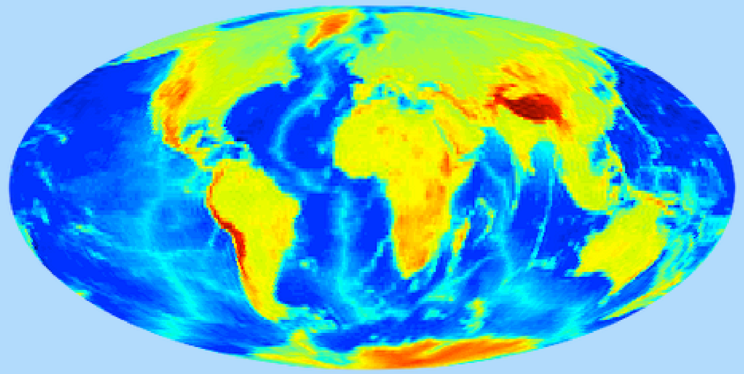
Tests passing | Linting passing | Docs passing | codecov 97% | License MIT | pypi package 1.3.0 | arXiv 2311.14670 | all contributors 12 | Open in Colab | Ruff

`s2fft` is a Python package for computing Fourier transforms on the sphere and rotation group (Price & McEwen 2024) using JAX or PyTorch. It leverages autodiff to provide differentiable transforms, which are also deployable on hardware accelerators (e.g. GPUs and TPUs).

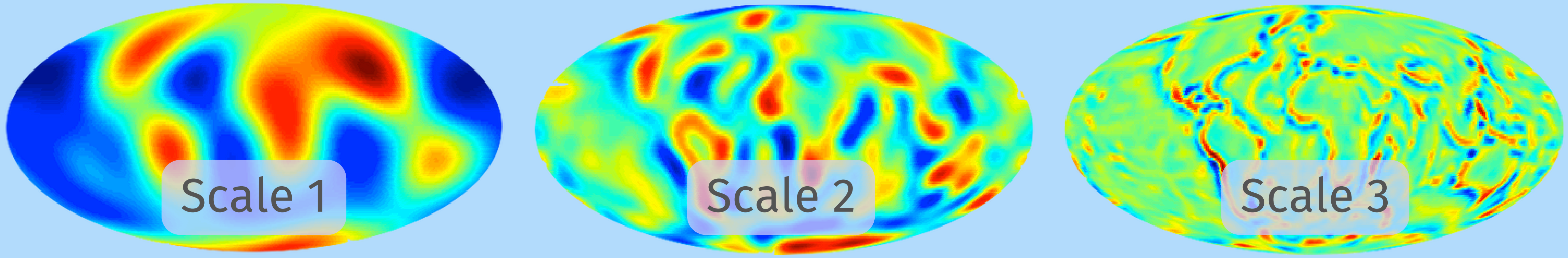
https://github.com/astro-informatics/s2fft

s2wav : wavelet transforms on the sphere

Wavelets capture signal content localised in both scale and space.



Original spherical data



Wavelet coefficients

`s2wav`: wavelet transforms on the sphere

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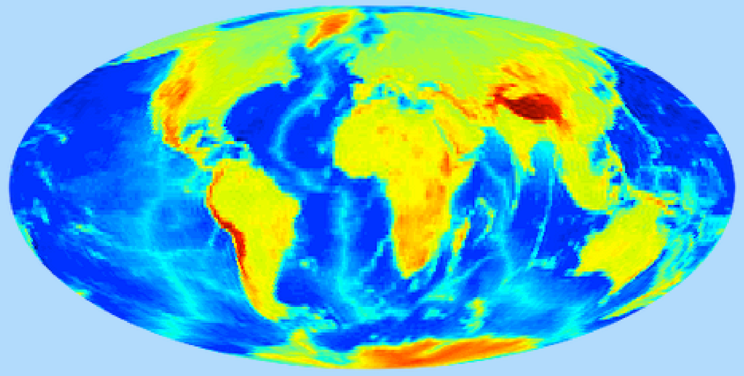

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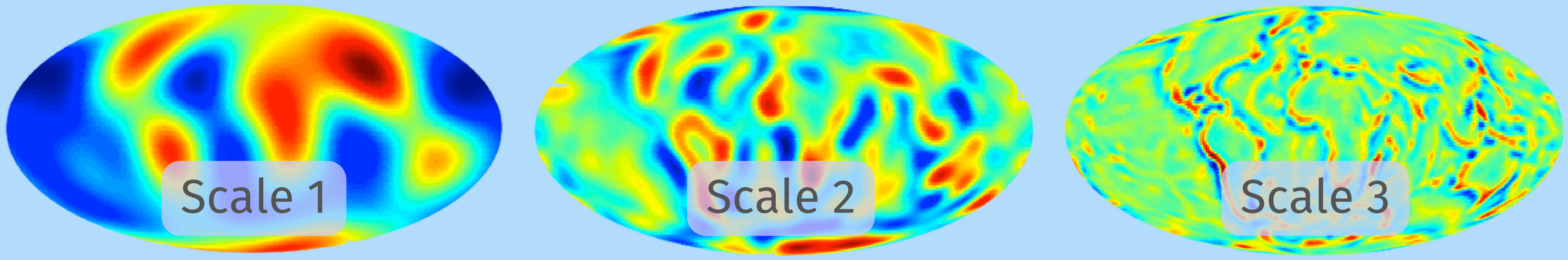


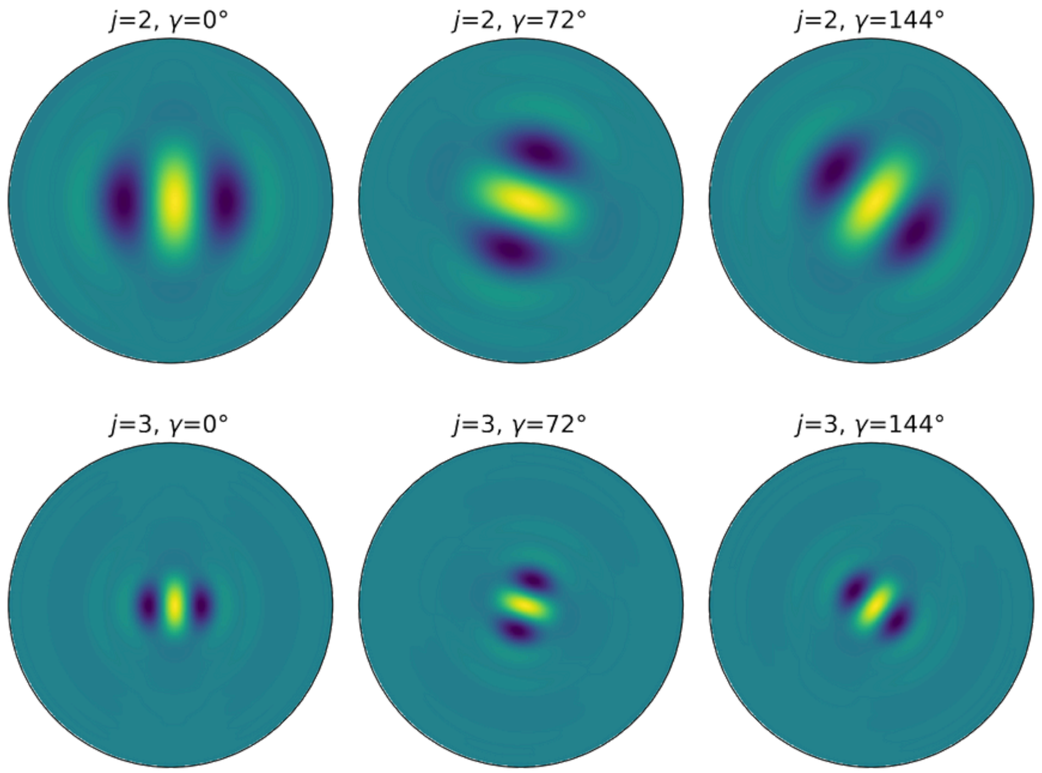
Wavelet coefficients

Spherical wavelet transform

Spherical wavelet transform, with wavelet ψ_j and scaling function φ, given by

$$W_j(\rho) = \underbrace{(f \star \psi_j)}_{\text{Spherical convolution}}(\rho) = \int_{\mathbb{S}^2} f(\theta,\phi)\, \underbrace{(R_\rho \psi_j)}_{\text{Rotated wavelet}}{}^*(\theta,\phi)\, \mathrm{d}\mu(\theta,\phi)$$

Wavelets carefully constructed to satisfy admissibility condition so that field can be reconstructed exactly from its wavelet coefficients.



Spherical wavelets (orthographic)

McEwen et al. (2007), Wiaux, McEwen et al. (2008), McEwen et al. (2013), McEwen et al. (2015), McEwen et al. (2018)

s2wav: wavelet transforms on the sphere

s2wav: Differentiable and Accelerated Wavelet Transforms on the Sphere

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`s2wav` is a python package for computing wavelet transforms on the sphere and rotation group, both in JAX and PyTorch. It leverages autodiff to provide differentiable transforms, which are also deployable on modern hardware accelerators (e.g. GPUs and TPUs), and can be mapped across multiple accelerators.

https://github.com/astro-informatics/s2wav

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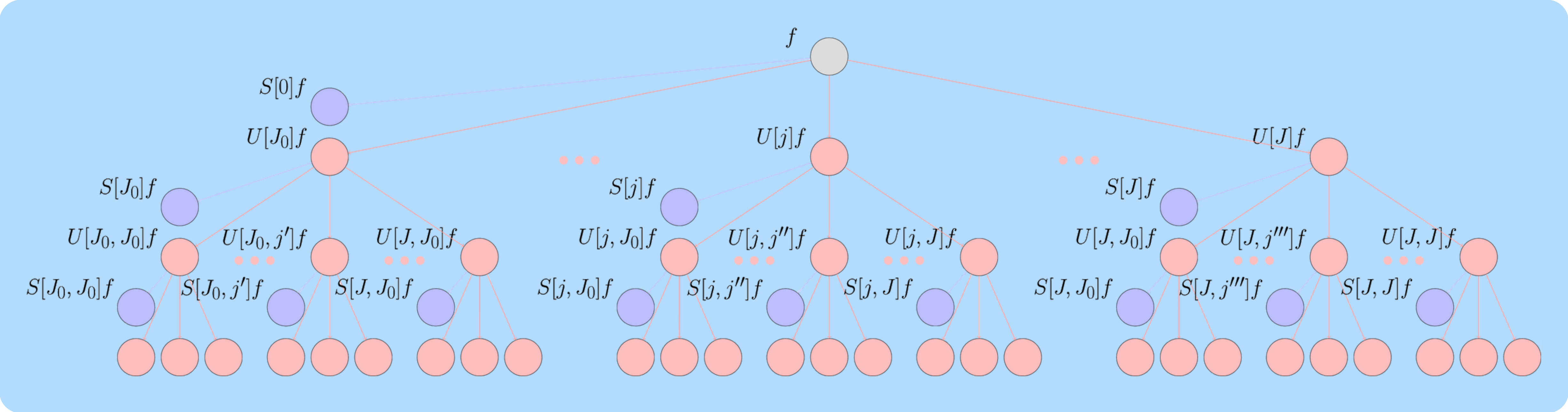
Spherical scattering network

Scattering coefficients for path *p* given by cascade of wavelet transforms with modulus activation function:

$$S[p]f = |||f \star \psi_{j_1}| \star \psi_{j_2}| \ldots \star \psi_{j_d}| \star \varphi.$$

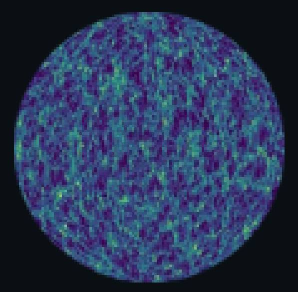
Spherical scatting networks is a collection of scattering transforms for a number of paths.

Mallat (2011), McEwen et al. (2022), Mousset et al. McEwen (2024)



Spherical scattering network

`s2scat`: wavelet scattering transforms on the sphere



s2scat: Differentiable Scattering Covariances on the Sphere

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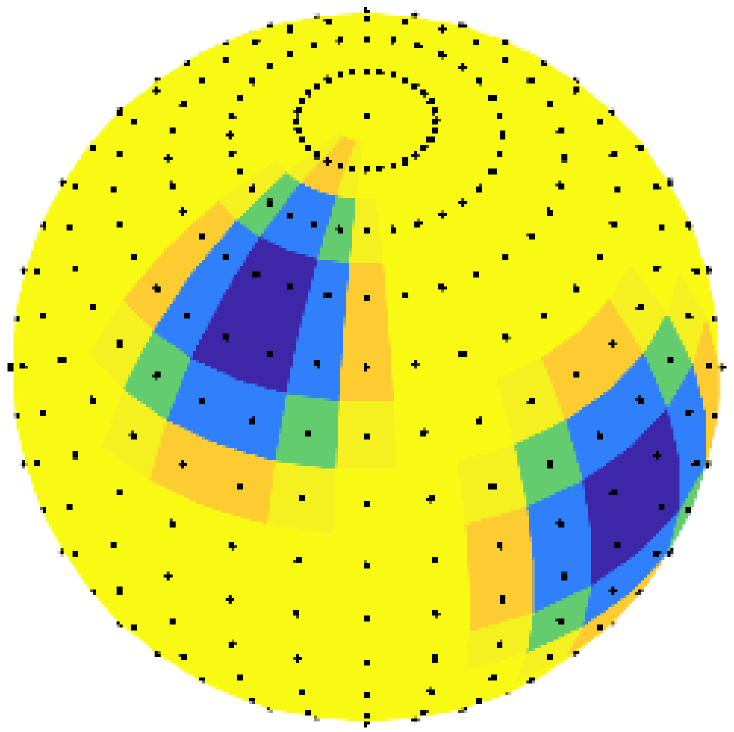
`s2scat` is a Python package for computing scattering covariances on the sphere (Mousset et al. 2024) using JAX. It exploits autodiff to provide differentiable transforms, which are also deployable on hardware accelerators (e.g. GPUs and TPUs), leveraging the differentiable and accelerated spherical harmonic and wavelet transforms implemented in `s2fft` and `s2wav`, respectively. Scattering covariances are useful both for field-level generative modelling of complex non-Gaussian textures and for statistical compression of high dimensional field-level data, a key step of e.g. simulation based inference.

https://github.com/astro-informatics/s2scat

Equivariant and scalable AI for spherical fields.

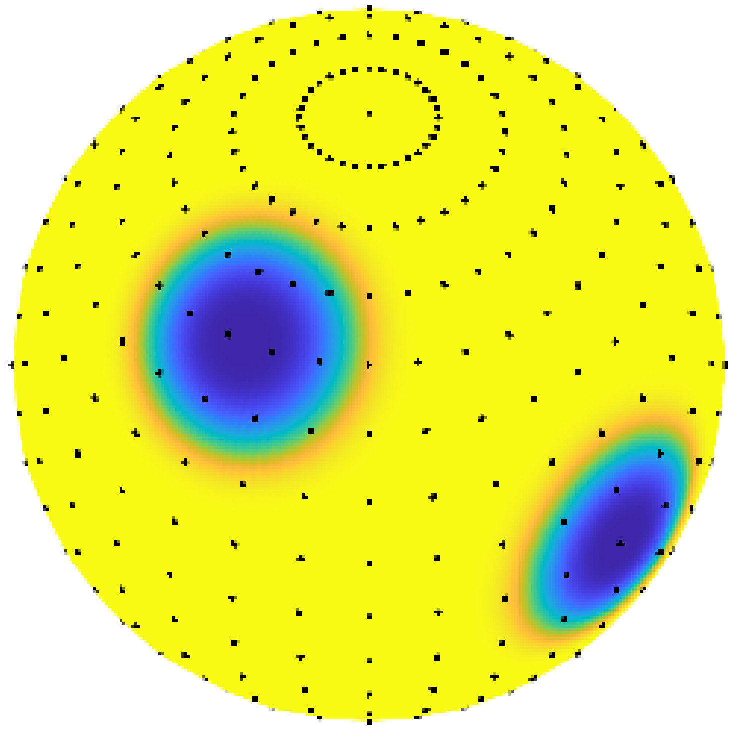
Discrete



✗ Not Equivariant
✓ Scalable

(Jiang et al. 2019, Zhange et al. 2019, Perraudin et al. 2019, Cohen et al. 2019, ...)

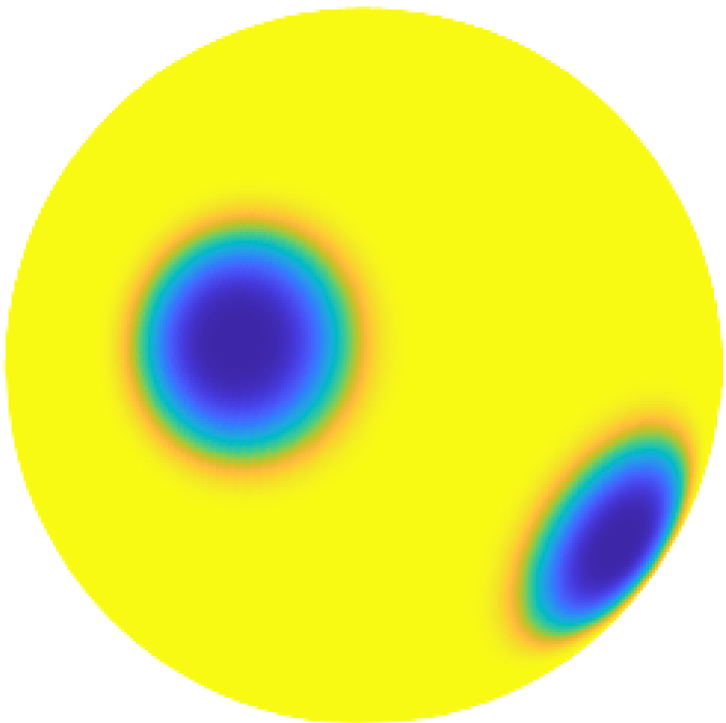
Continuous



✓ Equivariant
✗ Not Scalable

(Cohen et al. 2018, Esteves et al. 2018, Kondor et al. 2018, Cobb et al. McEwen 2021, McEwen et al. 2022, ...)

Discrete-Continuous (DISCO)



✓ Equivariant
✓ Scalable

(Ocampo, Price & McEwen 2021)

s2ai: spherical AI

s2ai: Scalable and Equivariant Spherical AI

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Many problems across computer vision and the natural sciences require the analysis of spherical data, for which representations may be learned efficiently by encoding equivariance to rotational symmetries as an inductive bias. `s2ai` provides foundational convolutional layers which encode said equivariance, with the aim to support the development of state-of-the-art machine learning techniques on both the sphere and rotation group.

https://github.com/astro-informatics/s2ai

Generative modelling of cosmological fields

Spherical scattering covariances for generative modelling

Scattering covariance statistics:

1. $S_1[\lambda]\, f = \mathbb{E}\big[\, |f \star \psi_\lambda| \,\big]$
2. $S_2[\lambda]\, f = \mathbb{E}\big[\, |f \star \psi_\lambda|^2 \,\big]$
3. $S_3[\lambda_1, \lambda_2]\, f = \mathrm{Cov}\big[\, f \star \psi_{\lambda_2}, |f \star \psi_{\lambda_1}| \star \psi_{\lambda_2} \,\big]$
4. $S_4[\lambda_1, \lambda_2, \lambda_3]\, f = \mathrm{Cov}\big[\, |f \star \psi_{\lambda_1}| \star \psi_{\lambda_3}, |f \star \psi_{\lambda_2}| \star \psi_{\lambda_3} \,\big]$

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4. $S_4[\lambda_1, \lambda_2, \lambda_3]\, f = \mathrm{Cov}\big[\, |f \star \psi_{\lambda_1}| \star \psi_{\lambda_3}, |f \star \psi_{\lambda_2}| \star \psi_{\lambda_3} \,\big]$

Generative modelling by **matching set of scattering covariance statistics** with a (single) target simulation:

$$\min_f \left\| \mathcal{S}(f) - \mathcal{S}(f_{\text{target}}) \right\|^2$$

↪ Solve by gradient-based optimisation, leverging autodiff
(requires s2fft, s2wav, s2scat)

Generative modelling of cosmic strings

Symmetry breaking **phase transitions** in the early Universe → topological defects.

Cosmic strings well-motivated phenomenon that arise when axial/cylindrical symmetry broken → **line-like discontinuities** in the fabric of the Universe.

Observed transitions string-like topological defects in other media.

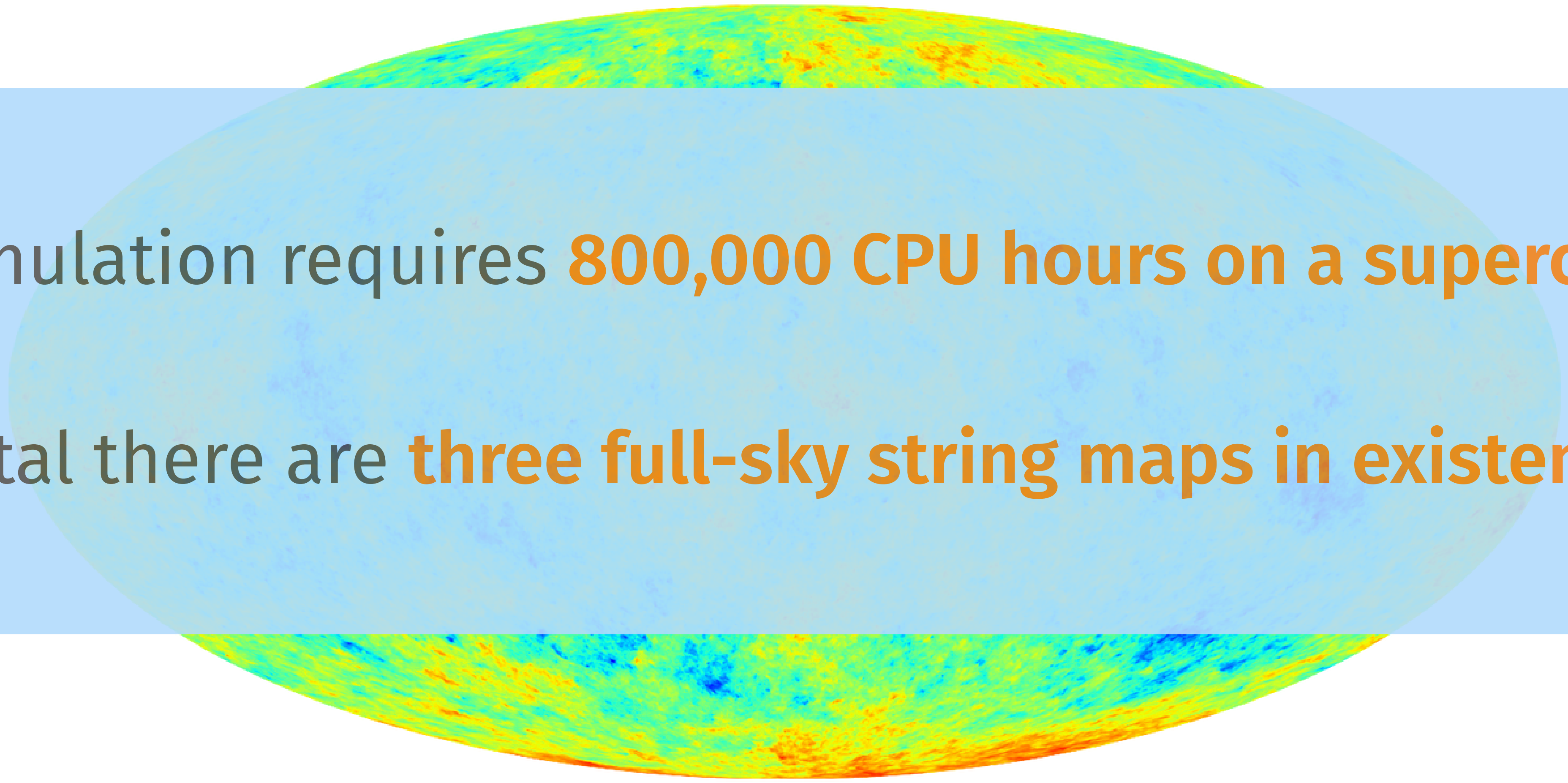
Detection of cosmic strings would open a **new window into the physics of the Universe.**

Optical microscope photograph of liquid crystal following temperature quench (Chuang et al. 1991)

Generative modelling of cosmic strings

Contact between theory and observation via high-resolution simulations (Ringeval et al. 2012).

Need to **simulate full physics**, evolving a network of string through cosmic time and then ray-tracing CMB photons through the string network.



A single simulation requires **800,000 CPU hours on a supercomputer**.

In total there are **three full-sky string maps in existence.**

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Generative modelling of cosmic strings

Instead of simulating full physics, **emulate with a scattering covariance generative model**.

Requires only **single target simulation**.

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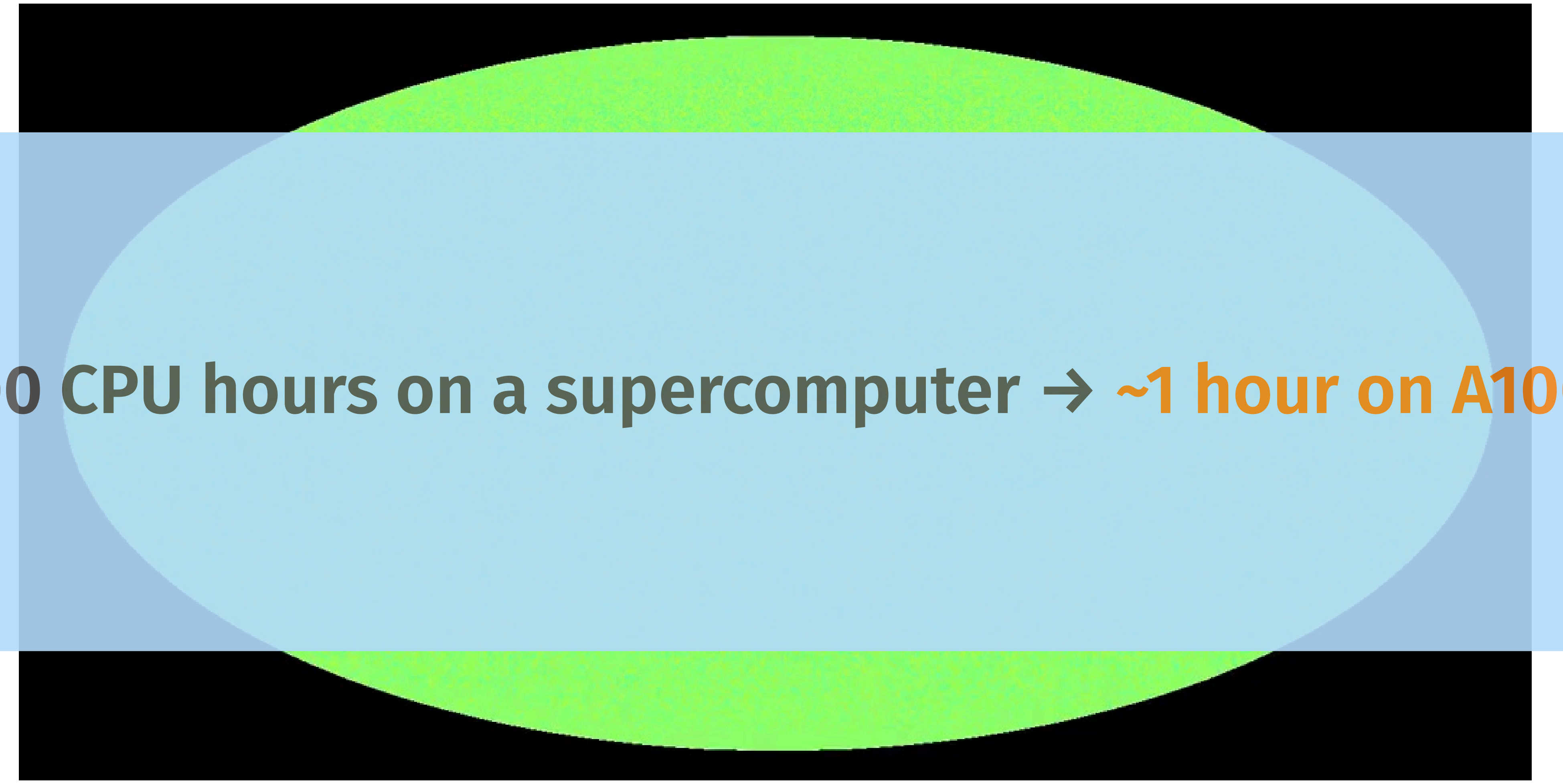

800,000 CPU hours on a supercomputer → ~1 hour on A100 GPU.

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Generative modelling of large-scale structure (LSS)

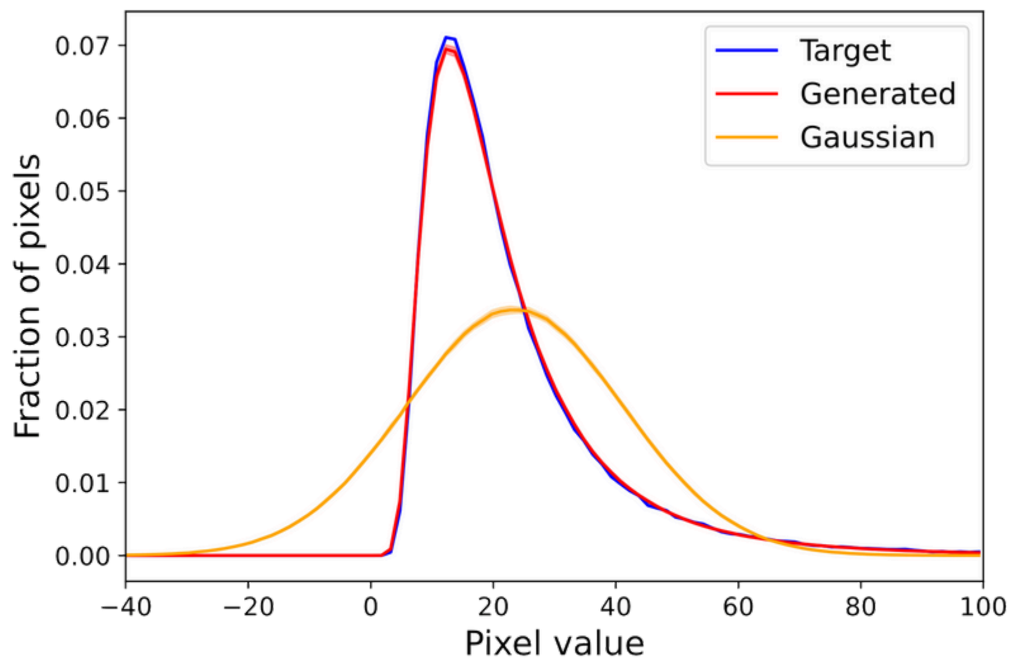
Which field is simulated and which emulated?

Simulations (n-body) can require days of compute on cluster, whereas emulation requires **<1 hour on a single A100 GPU**.

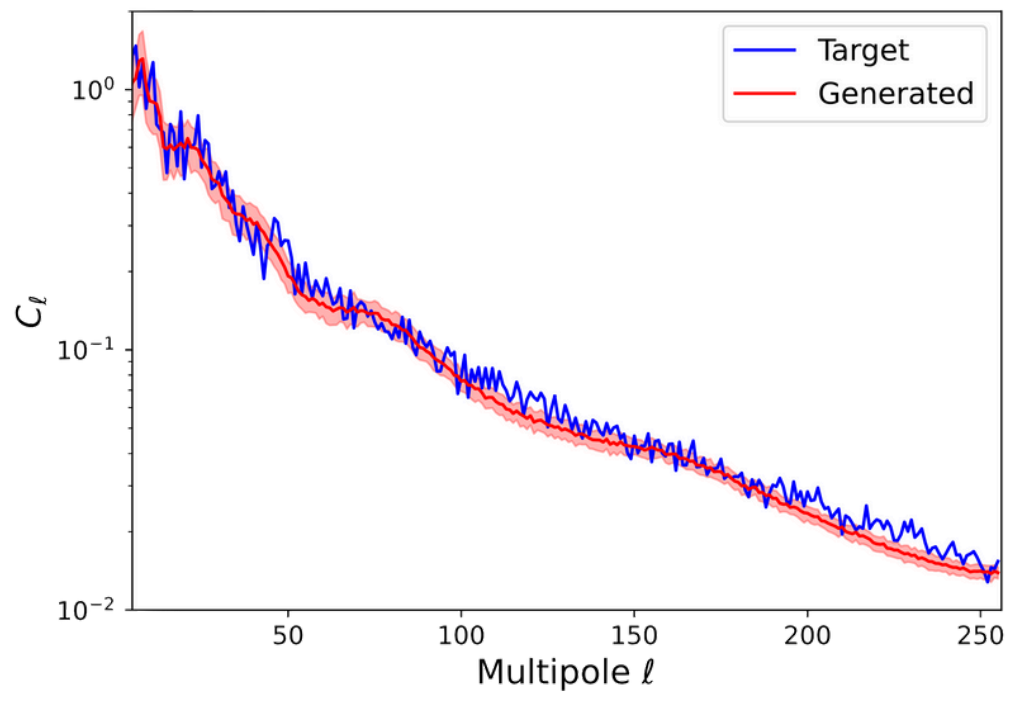
Logarithm (for visualisation) of weak lensing field.

Generative modelling of large-scale structure (LSS)

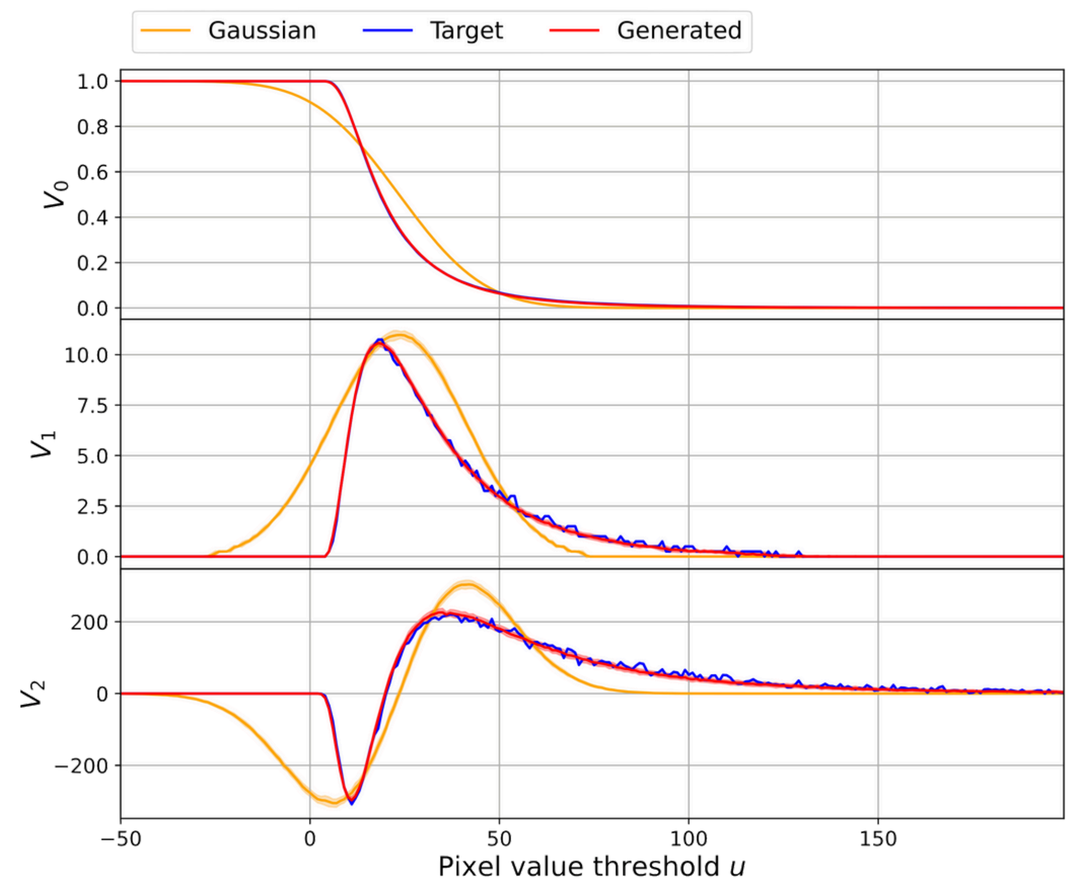
Validation of higher-order statistics.



Pixel distribution



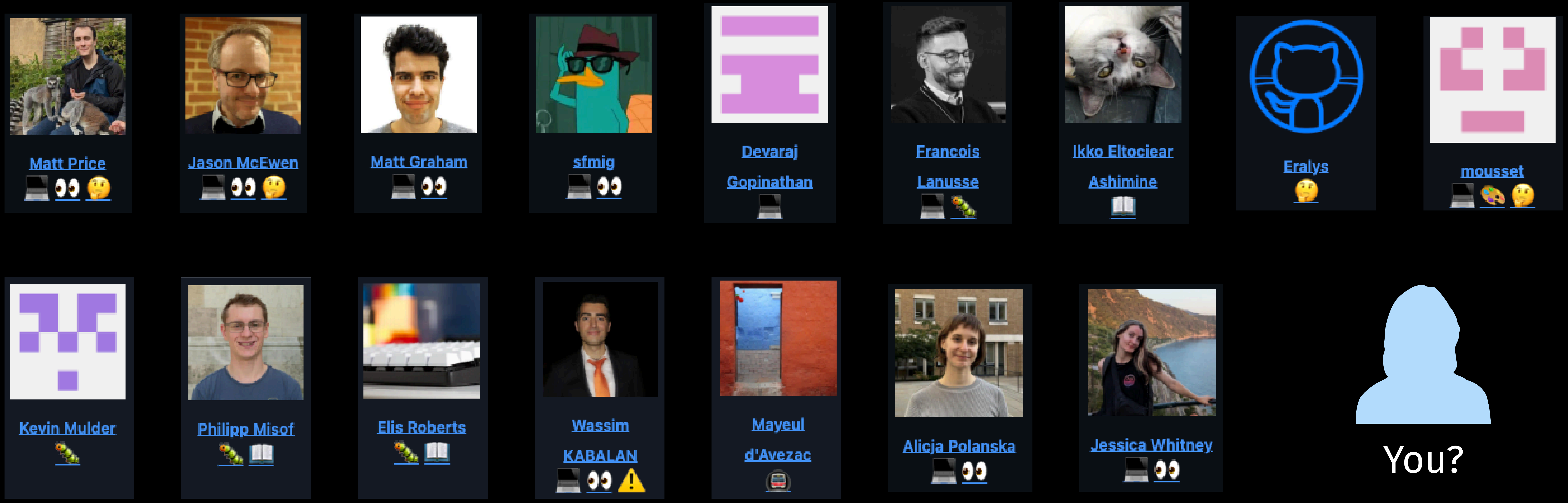
Power spectrum



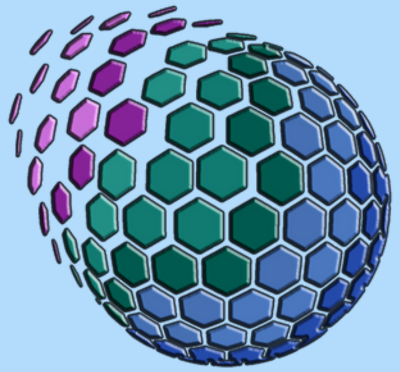
Minkowski functionals

Jason McEwen

All contributors



s2x suite of codes



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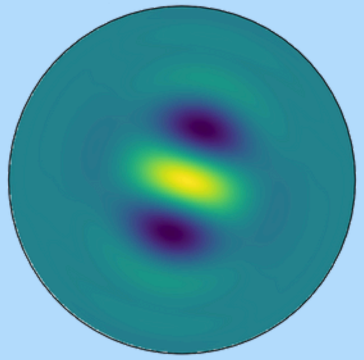

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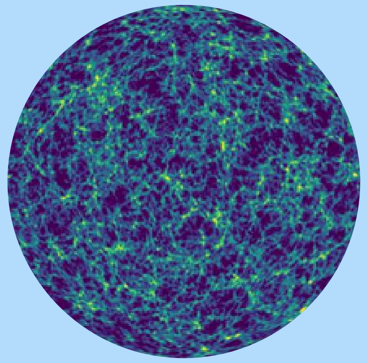

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