

Generative model and component separation in limited data regime with Scattering Transform

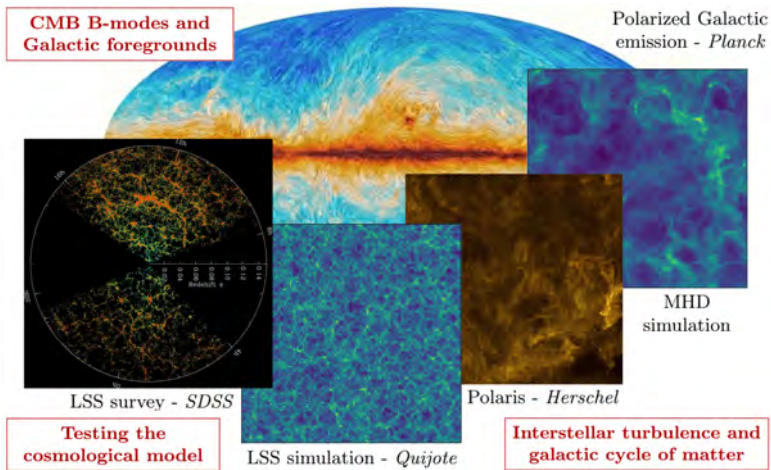
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”Artificial Intelligence for HPC@Exscale” Workshop,
Paris, October 3rd 2024



Outline

- 1 Introduction
- 2 Scattering Transforms and generative models
- 3 Application to component separation



→ Complex spatial/spectral processes ubiquitous in astrophysics
→ Sometimes no model and limited data regime...

Limited data regime in astrophysics

- **A limited amount of intricate observations**
 - ▶ A unique static multi-frequency sky
 - ▶ Mixture of non-stationary components
 - isolated processes can be very rare
 - Depends on angular scale/frequency

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 - ▶ Often no complete physical/numerical models
 - ▶ Simulations are very expensive
 - no or very limited training dataset

Limited data regime in astrophysics

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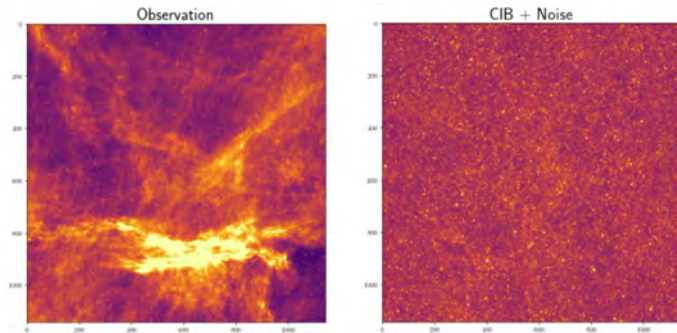
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→ **Work mainly from obs. data and physical knowledge?**
→ **Rely on recent advances in data science?**

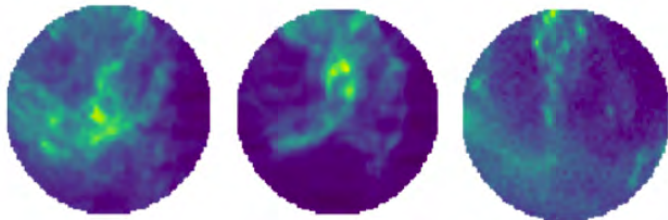
Example I: CIB/Galactic dust emission



- Galactic dust emission and Cosmic Infrared Background (CIB)
 - ▶ Thermal dust emission in the interstellar medium
 - ▶ Cosmic background dominates a smaller scales
 - ▶ CIB isolated observation, no model for Galactic emission

→ Characterize Galactic dust emission on small scales?

Example II: WNM/CNM in HI observations



- **WNM/CNM component separation**

- ▶ Warm (WNM) and Cold (CNM) Neutral Media
- ▶ Two phases with different spectral/spatial properties
- ▶ A few 1000s of unlabeled mixtures in HI (21cm) data

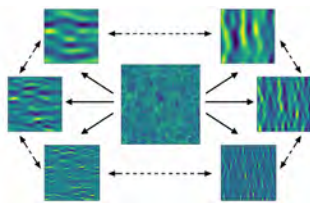
→ Learn phases structures directly from the data?

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Scattering transform (ST) statistics

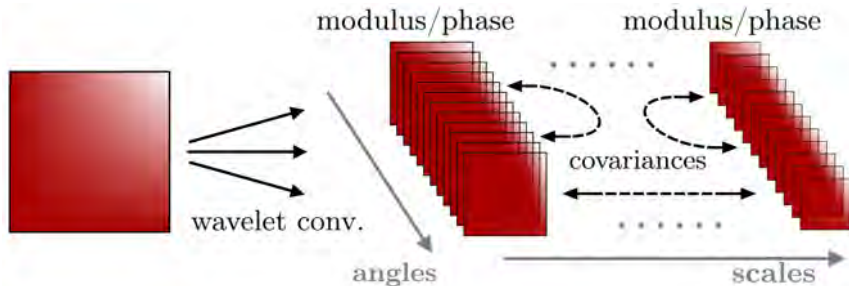
- **Scattering transform statistics (Mallat+, 2010+)**
 - ▶ Initially developed in data science
 - ▶ Inspired from neural networks
 - efficient characterization and reduced variance
 - ▶ Do not need any training stage
 - explicit mathematical form and interpretability



- Wavelet filters separating the different scales
- Coupling between scales with non-linearities

Scattering Transform (ST) statistics

- Computation of ST statistics (*EA+, 20*)



- Shallow network with known filters/non-linearities
- 1 coeff / pair/triplet of scales / type of interaction

Scattering Transform (ST) statistics

- A family of statistics

- ▶ Different generations of statistics
 - Wavelet Scattering Transforms (WST) *(EA+, 19)*
 - Wavelet Phase Harmonics (WPH) *(EA+, 20)*
 - Scattering covariances/spectra *(Cheng+, 23)*
- ▶ All share the same framework

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- Characterization and parameter inference

- ▶ Interstellar medium *(EA+ 19, Regaldo+20, Saydjari+, 20, Lei+, 22)*
- ▶ Weak lensing *(Cheng+, 20, 21)*
- ▶ Large scale structures *(EA+, 20, Eickenberg+, 22, Valogiannis+, 22a, 22b)*
- ▶ 21cm epoch of reionization *(Greig+, 22, Hothi+, 23)*
- ▶ ...

- Very informative (sometimes on par with CNN!)
 - Wide range of applicability (generic, training-less)

Generative models from Scattering transforms

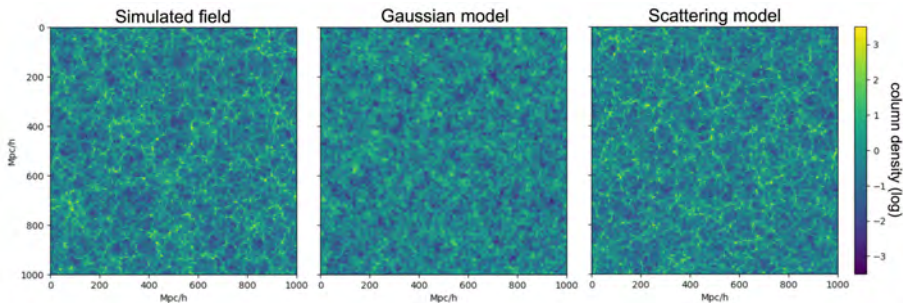
- Generative model from ST statistics (*Bruna, Mallat, 19*)
 - ▶ From the ST statistics $\Phi(s)$ of a map s
 - ▶ Maximum entropy microcanonical model
 - ▶ New approximate samples of a process from examples
 - ▶ Can quantitatively reproduce non-gaussian properties

Generative models from Scattering transforms

- **Generative model from ST statistics** (*Bruna, Mallat, 19*)
 - ▶ From the ST statistics $\Phi(s)$ of a map s
 - ▶ Maximum entropy microcanonical model
 - ▶ New approximate samples of a process from examples
 - ▶ Can quantitatively reproduce non-gaussian properties
- **Practical implementation**
 - ▶ Constraints $\Phi(s)$ from a (set of) data s
 - ▶ Sampled with a gradient-descent algorithm
 - from a white noise realization
 - optimizing \tilde{s} such that $\Phi(\tilde{s}) \simeq \Phi(s)$

Generative models from Scattering transforms

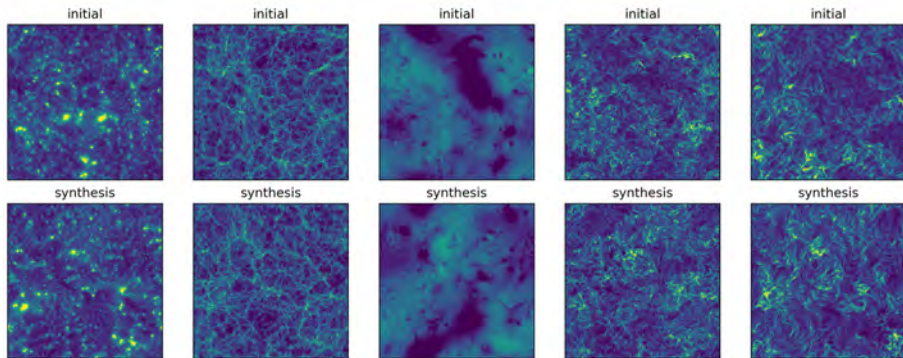
- Quantitative validation of syntheses (*EA+*, 20)
 - ▶ Large scale structures density field, Wavelets Phase Harmonics



→ Usual (NG) statistics very well reproduced (up to 1-10 %)

Generative models from Scattering transforms

- Syntheses from a single image (*Cheng+, 24*)
 - ▶ Scattering spectra + physical dimensionality reduction



→ Realistic NG models from a few hundreds coefficients!
→ Well adapted for a large number of physical fields

Generative models from Scattering transforms

- ST generative models
 - ▶ Low-dimensional: few 100s to low 1000s
 - ▶ For regular "physical" fields
 - ▶ Extended to various fields
 - Higher dimensions (3D+)
 - On the sphere (*Mousset+, 24*)
 - Multi-channel (*Régaldo+, 22*)

Generative models from Scattering transforms

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- **Needs related to NumPEx**

- ▶ Versatile and scalable ST computations:
 - Adaptable Wavelet transforms
 - Fourier Transform (for modulus)
- ▶ Sampling algorithms (other than gradient descent ?)
 - Efficiently tracing the gradients
 - Incl. mean-field approach? (*Häggbom+, 24*)

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Statistical component separation

- Framework of the problem
 - ▶ We observe a mixture $d = s + c$
→ d data, s signal of interest, c contamination
 - ▶ Use knowledge of c to recover s
 - ▶ No model for s ...

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- Using ST generative models

- ▶ Assume S is described by p_μ ST models
 - Parametrized by μ such that $E_{s \sim p_\mu}[\phi(x)] = \mu$
- ▶ Estimate (part of) the $p(\mu|d)$ posterior

→ Statistical component separation
→ Allows to get a posterior model of s

Statistical component separation

- Bayesian approach of the problem

- ▶ Parameter space: μ
- ▶ Data space: $\phi(d)$
- ▶ Forward model: $f(s) = d$ converted in ST space

$$\mu \xrightarrow{p_\mu(s)} s \xrightarrow{f(s)=s+c} d \xrightarrow{ST} \phi(d)$$

Statistical component separation

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- Estimating the posterior

- ▶ Forward $f(\mu) = \phi(d)$ samplable in ST space
- ▶ Broad $p(\mu)$ prior can be defined around $\phi(d)$
- ⇒ Well posed Bayesian problem

Statistical component separation

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- Sample/data space dim ~ 500 without structure
- Forward is still expensive (a few seconds on a GPU)

Solution with a gradient descent approach

- Generative model from available sample

- ▶ Estimate $\phi(s)$ from sample s
- ▶ Generate maps \tilde{s} such that

$$\Phi(\tilde{s}) \simeq \Phi(s)$$

- ▶ Sampled with gradient descent from white noise

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- **Indirect observation with know contamination**

- ▶ $d = s_0 + c_0$, assume we have $p(c)$
- ▶ Find map(s) \tilde{s} such that

$$\langle \Phi(\tilde{s} + c_i) \rangle_i \simeq \Phi(d)$$

- ▶ Gradient descent from d (for instance)

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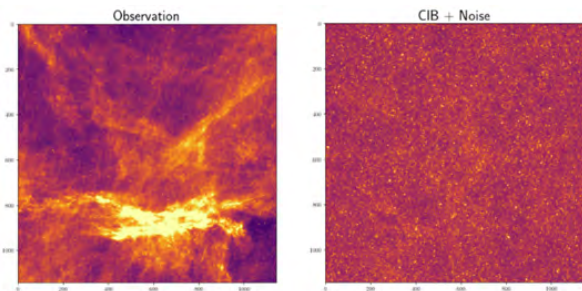
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→ Framework for component separation
→ Can include various other statistical constraints

Solution with a gradient descent approach

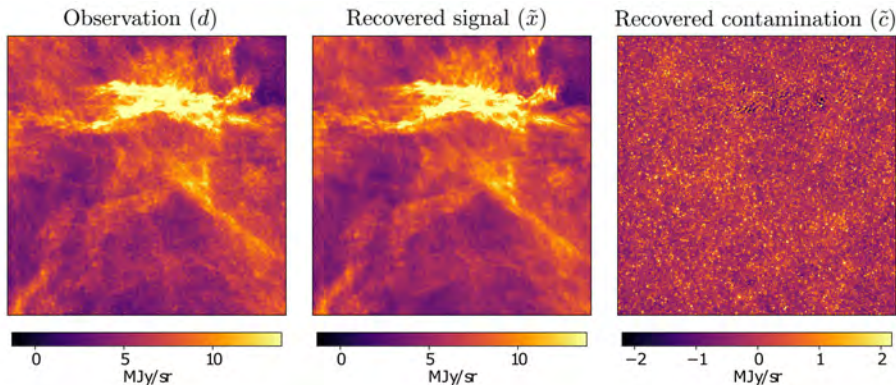


- Dust emission/Cosmic Infrared Background (Auclair+, 24)

- ▶ $d = s + c$, s thermal dust emission, c CIB
- ▶ CIB model from separate observation (cosmological \Rightarrow homogeneous)
- ▶ Two constraints, with $\{c_i\}_i$ from ST model

$$\langle \Phi(\tilde{s} + c_i) \rangle_i \simeq \Phi(d), \quad \Phi(\tilde{c}) = \Phi(c)$$

● Recovered components (Auclair+, 24)



- Statistical component separation solely from obs. data!
- Thermal dust is recovered at an unprecedented resolution

Solution with a gradient descent approach

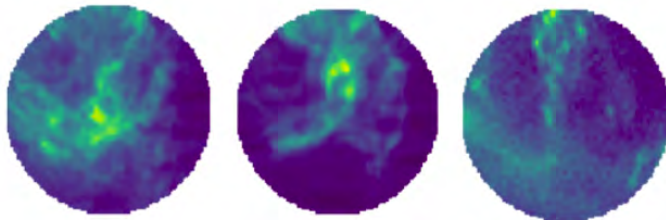
- **Statistical component separation with ST**
 - ▶ Efficient and versatile framework
 - (Régaldou+, 21, Delouis+22, Siahkoohi+23)
 - ▶ Allow joint handling of various constraints
 - 10s of losses in recent works
 - Incl. cross-statistics with ancillary data
 - ▶ Still need to get a proper mathematical framework

Solution with a gradient descent approach

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- **Needs related to NumPEx**
 - ▶ High dimensional optimization
 - Incl. high number of constraints
 - Exploration of "good" solutions
 - ▶ High-dimensional Bayesian inversion
 - Sampling spaces of dim. a few 100s
 - Incl. adaptive learning

Unsupervised separation of HI data



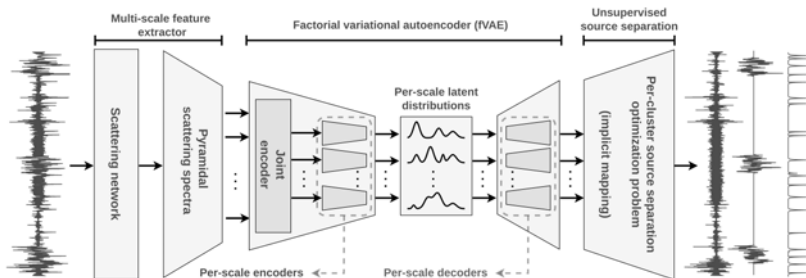
- **Recovering phase structures from the data**

- ▶ A lot of HI observations of CNM/WNM/noise mixture
- ▶ No specific knowledge on each mixture
 - No isolated component observed

→ **Directly learn components ST models from the data?**

Unsupervised separation of HI data

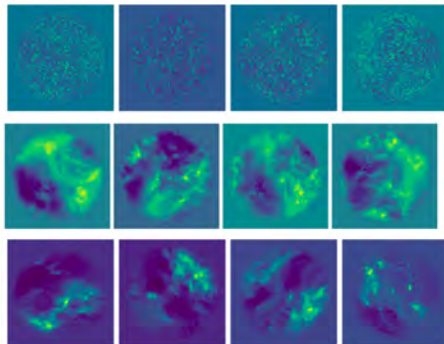
- Variational Auto-Encoder (VAE) in ST space (Siahkoohi+, 23a,b)



→ Unsupervised learning of components in ST space

Unsupervised separation of HI data

- Application to HI data (Lei+, work in progress)
 - ▶ Unsupervised identification of 3 components



- WNM/CNM/noise seem quite well modeled!
- Interfacing ST models with other ML algorithms

Conclusion

- **Scattering Transforms**
 - Non-Gaussian statistics inspired from neural network
 - Efficient low-dim modeling of physical processes
- **New tools for (astro-)physics and beyond**
 - ST models as basis for various inv. problems/comp. sep.
 - First proofs of concepts obtained in component separation
 - Ability to work with a very limited amount of data!
- **Help from NumPEX would be precious**
 - Not always easy to interface with standard algorithms
 - Scale to larger problems from proofs of concept
 - Need to develop HPC expertise as a whole

Thanks for your attention!

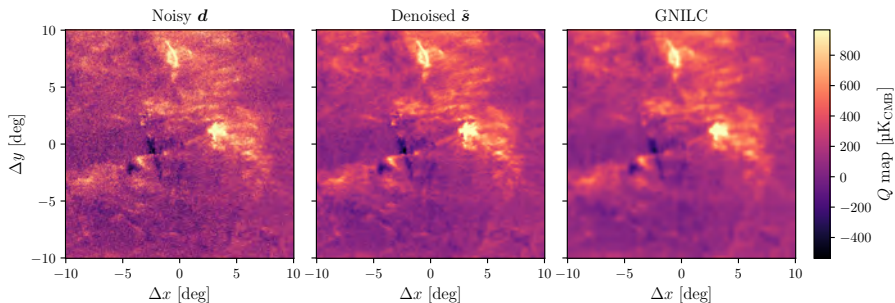
Separation of polarized dust and noise

- Application to dust polarized emission and noise (Regalado+, 21)
 - ▶ $d = s + c$ *Planck* polarization data at 353GHz
 - ▶ s polarized dust emission, c inhomogeneous noise
 - ▶ 300 noise realizations c_i from Planck team
 - ▶ Optimization done from d to keep largest scales

$$\langle \Phi(\tilde{s} + c_i) \rangle_i \simeq \Phi(d)$$

Separation of polarized dust and noise

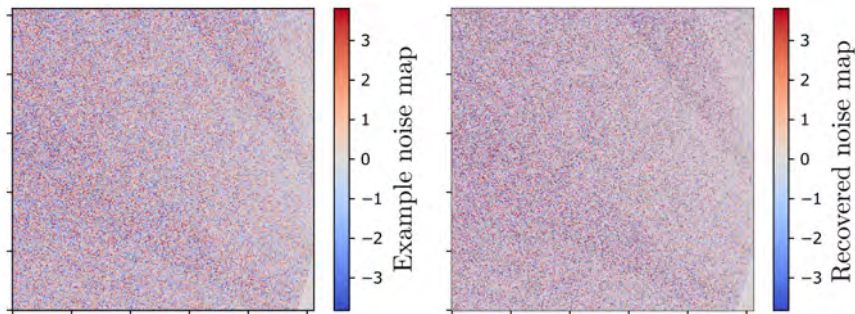
- Application to Chameleon-Musca region (Régaldou+ 21)



→ Transition btw. deterministic and statistical
→ Conceptual validation of the method

Separation of polarized dust and noise

- Recovered contamination (Régaldou+ 21)

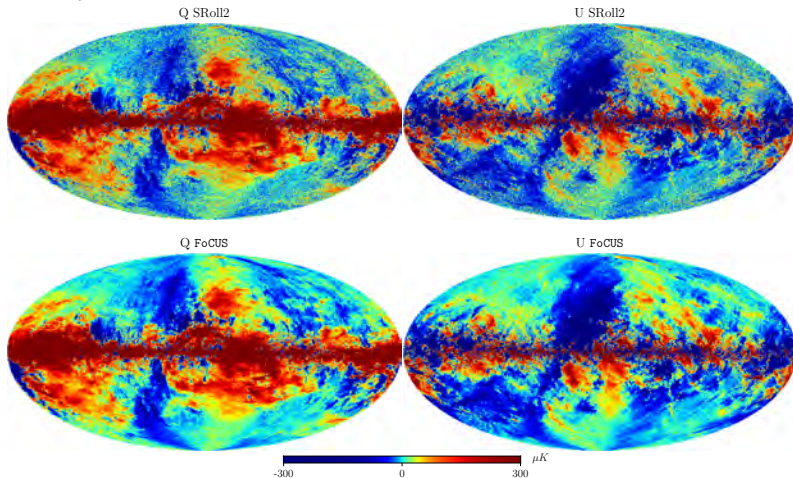


- Statistical separation of components
- Residual structures could also be constrained

Separation of polarized dust and noise

- **Refinements of this work on the whole sky (Delouis+, 22)**
 - ▶ Introduce additional constraints
 - 3 constraints including cross-statistics
 - ▶ Educated normalization of each constraint
 - constraints normalized by variance over $\{c_i\}$
 - ▶ Introduce local constraints for non-stationary
 - 4 selected regions for Galactic heterogeneity

- Full sky results at 353GHz (Delouis+, 22)



- Deterministic up to $SNR \approx 0.1$, statistical up to $SNR \approx 0.01$
- Efficient and versatile framework for statistical comp. separation