

# Big Data in Cosmology

## Data Intensive Science (DIS) in Cosmology

Jason McEwen

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@jasonmcewen

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*University College London (UCL)*

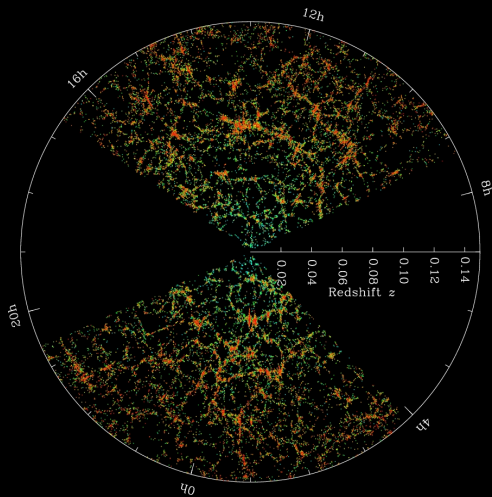
Theory of Big Data Workshop

University College London (UCL), June 2017

# Large-scale structure (LSS) of the Universe

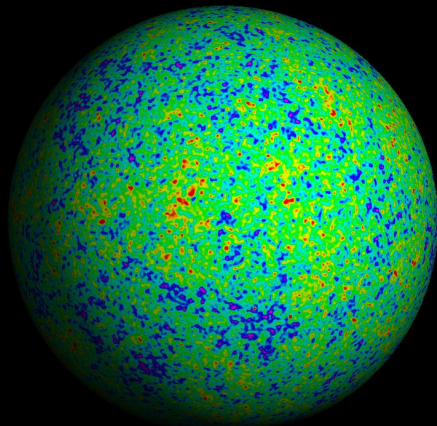


## Observations of galaxies tracing large-scale structure (LSS)



Credit: SDSS

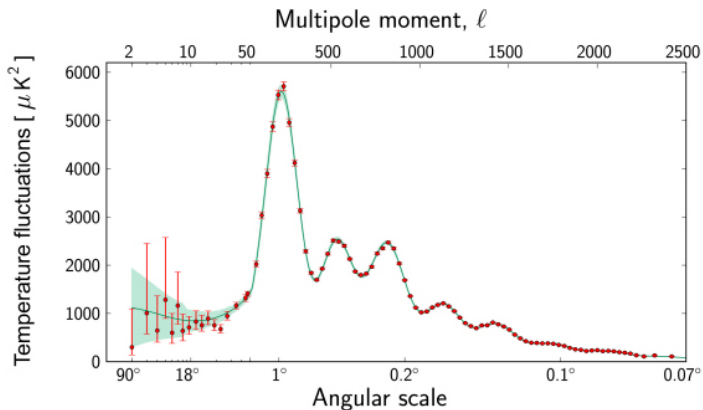
# Observations of cosmic microwave background (CMB)



Credit: WMAP

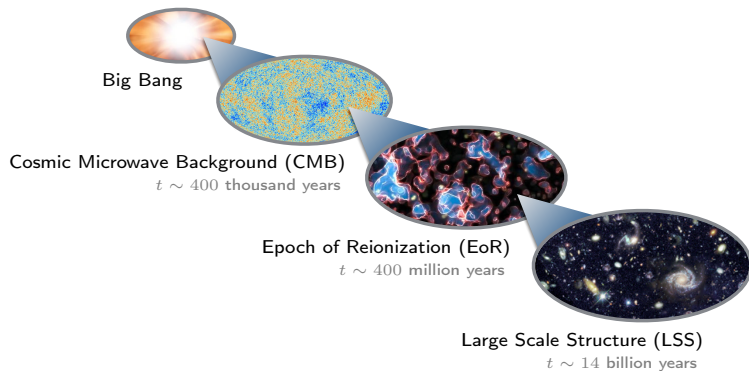
# CMB power spectrum

## Theory and observational data

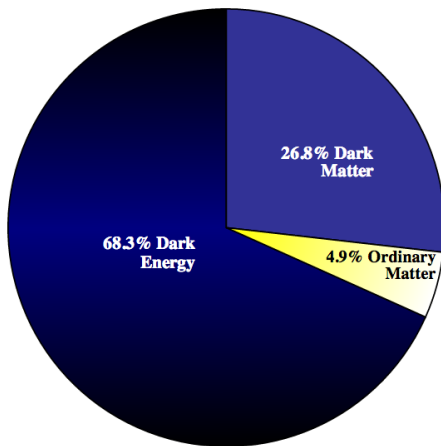


Credit: Planck

# Cosmic evolution of our Universe

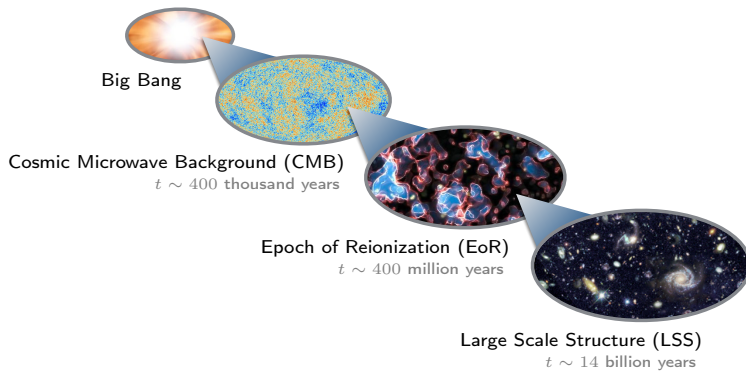


# Content of the Universe

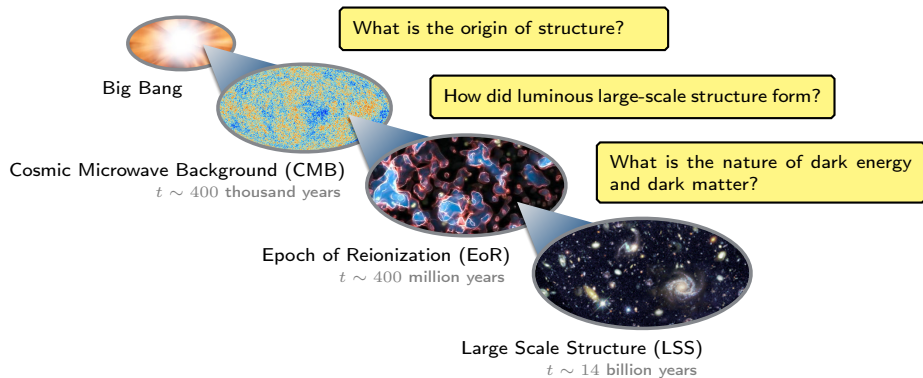


Credit: Planck

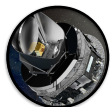
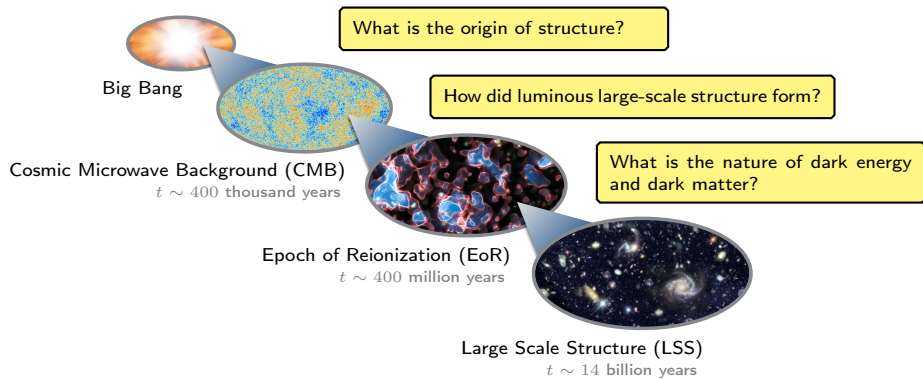
## Unanswered fundamental questions



# Unanswered fundamental questions



# Unanswered fundamental questions



Planck



Gaia



LOFAR



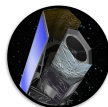
SKA



DES



DESI



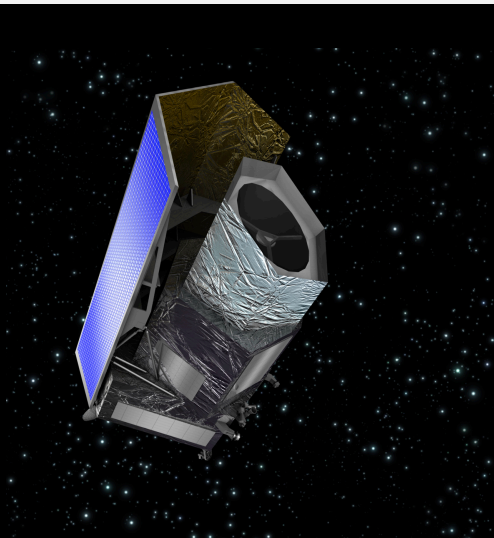
Euclid



LSST



# ESA Euclid satellite

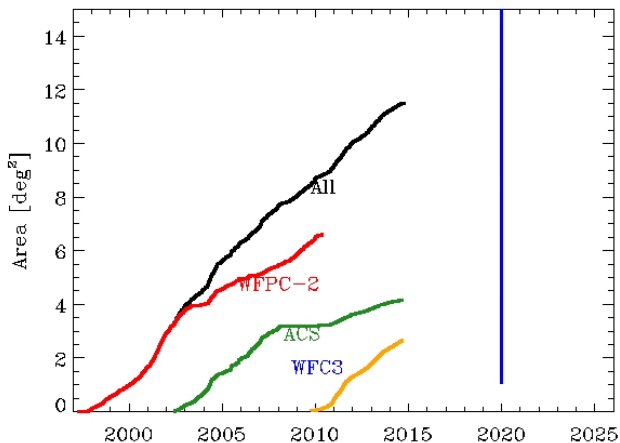


Credit: Euclid



## Euclid sky coverage

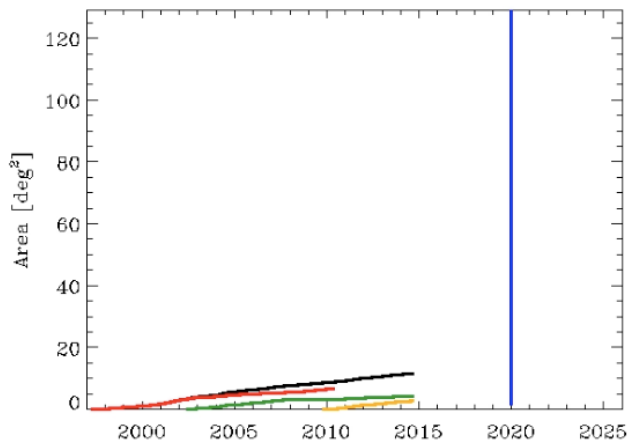
Switch on



Credit: Tom Kitching

## Euclid sky coverage

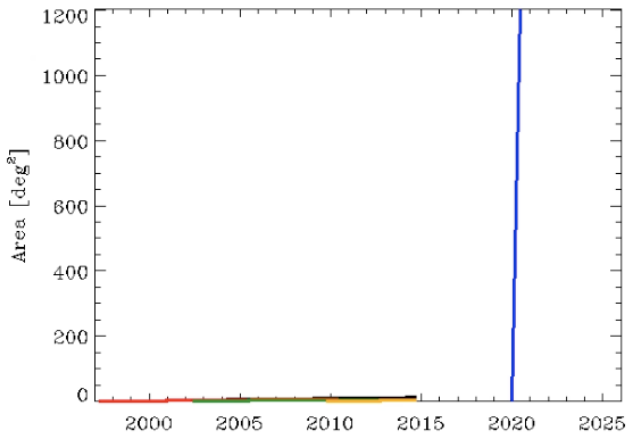
2 weeks



Credit: Tom Kitching

## Euclid sky coverage

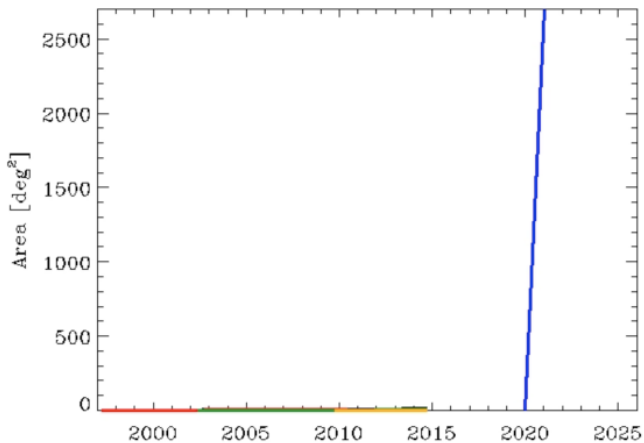
6 months



Credit: Tom Kitching

## Euclid sky coverage

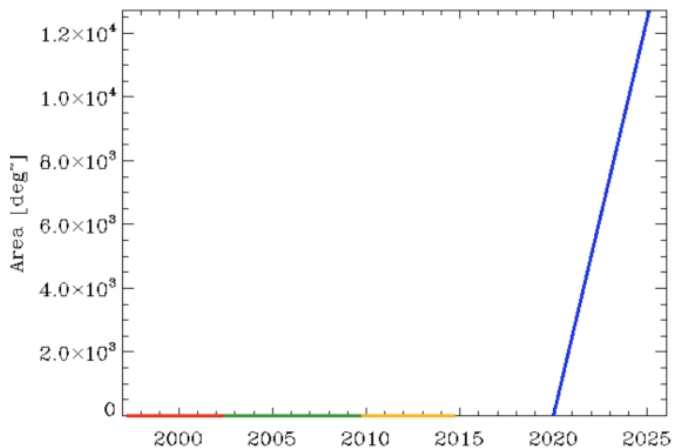
1 year



Credit: Tom Kitching

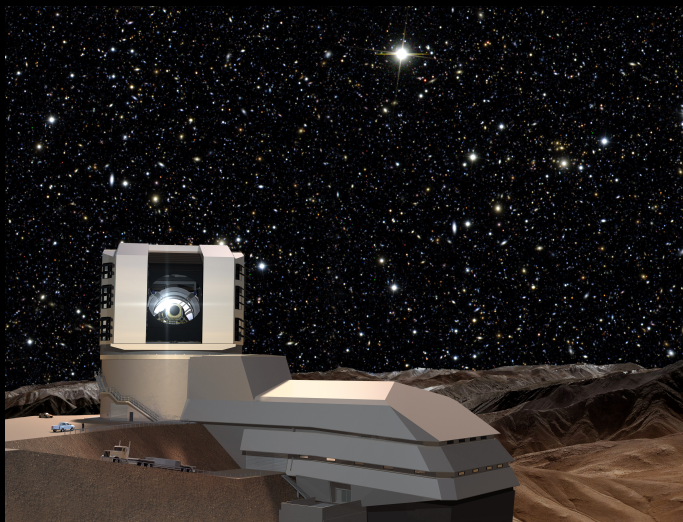
## Euclid sky coverage

5 years



Credit: Tom Kitching

# Large Synoptic Survey Telescope (LSST)



Credit: LSST



# Large Synoptic Survey Telescope (LSST)

## Data Releases:

Number of Data Releases = 11

Date of DR1 release = Date of Operations Start+ 12  
months

Estimated numbers for DR-1 release

Objects = 18 billion

Sources = 350 billion (single epoch)

Forced Sources = 0.75 trillion

Estimated numbers for DR-11

Objects = 37 billion

Sources = 7 trillion (single epoch)

Forced Sources = 30 trillion

Visits observed = 2.75 million

Images collected = 5.5 million

## Alert Production:

Real-time alert latency = 60 seconds

Average number of alerts per night= "about 10 million"

## Data and compute sizes:

Final image collection (DR11) = 0.5 Exabytes

Final database size (DR11) = 15 PB

Final disk storage = 0.4 Exabytes

Peak number of nodes = 1750 nodes

Peak compute power in LSST data centers = 1.8 PFLOPS



# Square Kilometre Array (SKA)



SPDO / Swinburne Astronomy Products

# The SKA poses a considerable big-data challenge

**2x**

The SKA will use enough optical fiber to wrap twice around the Earth!

**10x**

The dishes of the SKA will produce 10 times the global internet traffic.

**100x**

The aperture arrays in the SKA could produce more than 100 times the global internet traffic.

**64GB x 15 MILLION**

The SKA will generate enough raw data to fill 15 million 64GB iPods every day!

**SKA super computer**

The SKA central computer will have the processing power of about one hundred million PCs.

**x 100,000,000 Personal Computers**

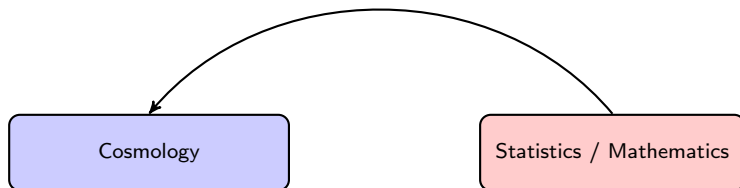
# The SKA poses a considerable big-data challenge



# Cosmostatistics & Cosmoinformatics

## Closing the loop

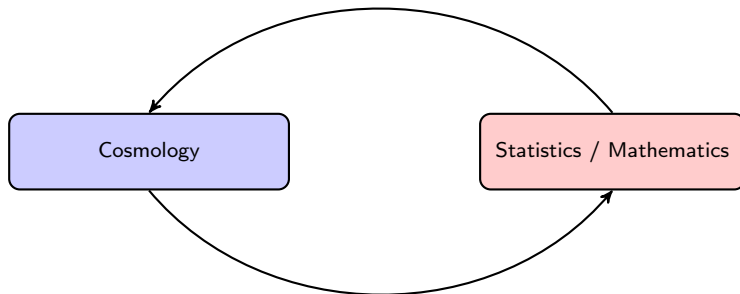
*Extracting weak observational signatures of fundamental physics from complex data-sets requires sensitive, robust and principled analysis techniques.*



# Cosmostatistics & Cosmoinformatics

## Closing the loop

*Extracting weak observational signatures of fundamental physics from complex data-sets requires sensitive, robust and principled analysis techniques.*



*Constructing appropriate analysis techniques requires a deep understanding of cosmological problems and methodological foundations.*

# UCL Centre for Doctoral Training (CDT) in Data Intensive Science (DIS)

- UCL won bid to host **STFC's first CDT**.  
Learn more at our temporary website: <https://www.hep.ucl.ac.uk/cdt-dis/>
- Focused on **Data Intensive Science (DIS)**.
- Aims:
  - Train next generation of leaders in the field of DIS (in both academic and industry).
  - Promote development and application of novel DIS techniques.
  - Promote **knowledge transfer**:
    - between academic fields;
    - between non-academic and academic organisations.
- Unique opportunity to **bring together DIS research** from perspective of **applications, methodologies, and theoretical foundations**.



Science & Technology  
Facilities Council

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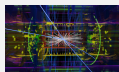
Science & Technology  
Facilities Council



# UCL Centre for Doctoral Training (CDT) in Data Intensive Science (DIS)

Who we are

**Particle Physics**  
Dpt. of Physics and  
Astronomy  
(20 CDT Staff Members)



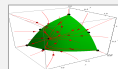
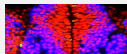
**Astrophysics**  
Dpt. of Physics and  
Astronomy  
(20 CDT Staff Members)

Department of  
**Space and Climate  
Science**  
(20 CDT Staff Members)



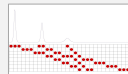
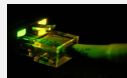
**Atomic & Molecular  
Physics**  
Dpt. of Physics and Astronomy  
(2 CDT Staff Members)

Department of  
**Computer Science**  
(8 CDT Staff Members)



Department of  
**Mathematics**  
(9 CDT Staff Members)

Department of  
**Electrical Engineering**  
(3 CDT Staff Members)



Department of  
**Statistical Science**  
(5 CDT Staff Members)

Aim to **foster closer collaboration** between these areas to aid the development of novel DIS techniques or applications to new areas.

# UCL Centre for Doctoral Training (CDT) in Data Intensive Science (DIS)

Management team

**Centre Co-Directors:** Profs N. Konstantinidis & O. Lahav



**Directors of Research:** Drs J. McEwen & T. Scanlon



**Directors of Training:** Prof. J. Tennyson FRS, & C. Gryce



**Admissions & Graduate Tutor:** Prof. S. Viti



**Partner Liaison & Placements Co-Ordinator:** Dr J. Yates

# UCL Centre for Doctoral Training (CDT) in Data Intensive Science (DIS)

## Industrial partners



- Students will undertake **6 month internships** with partners on a DIS project
- Promote **knowledge transfer** between academic and non-academic organisations.
- We've been approached by more organisations since winning the bid (UKAEA, Asos, GroupM, S&P, Illuminas, ASI, ...).

# Outline

- 1 Bayesian inference
- 2 Computational harmonic analysis
- 3 Machine learning
- 4 Inverse problems

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# Bayesian inference for parameter estimation

## Case study: CMB

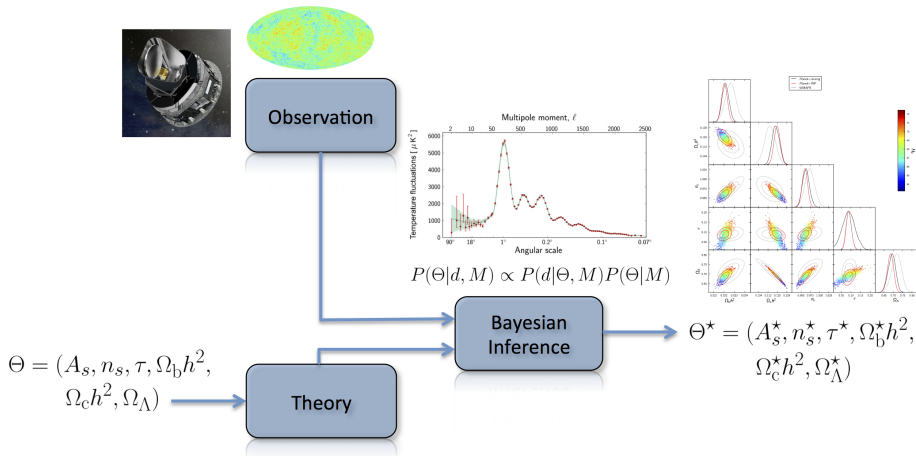
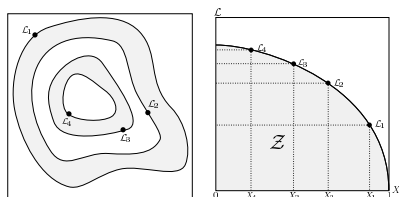


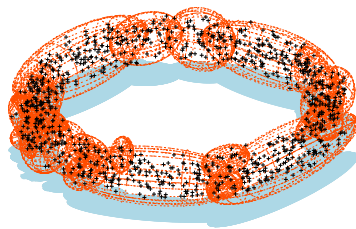
Figure: CMB Bayesian inference pipeline.

# Bayesian inference for model selection

- **Nested sampling** (Skilling 2005).
- **MultiNest**: multi-modal ellipsoidal sampling (Feroz & Hobson 2007; Feroz, Hobson & Bridges 2008).
- **PolyChord**: multi-modal whitened slice sampling (Handley, Hobson & Lasenby 2015).



(a) Nested sampling



(b) Ellipsoidal sampling

**Figure:** Computing the marginalised likelihood (Bayesian evidence) [Credit: Feroz *et al.* 2008].

# Bayesian hierarchical models

## Weak gravitational lensing

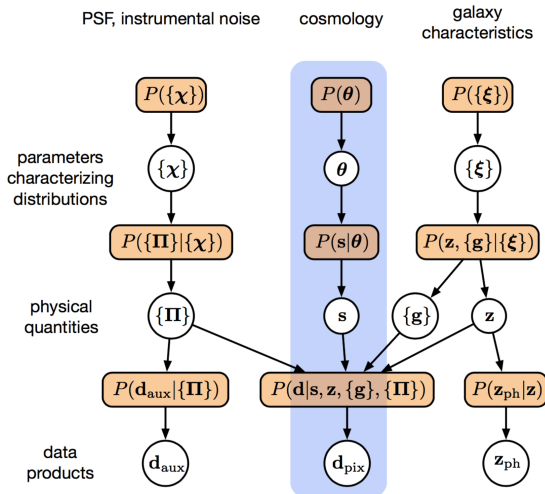


Figure: HBM for weak gravitational lensing (Alsing *et al.* 2015)

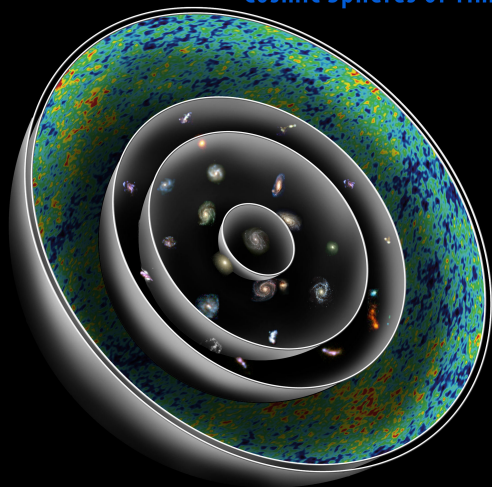


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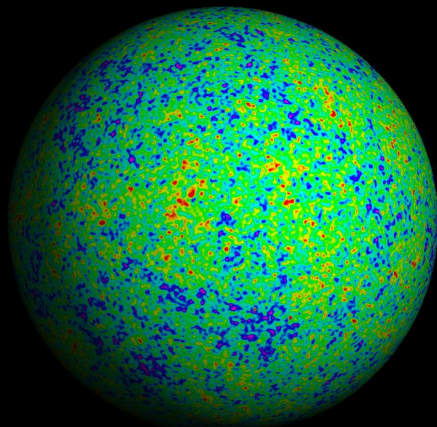
# Observations made on the celestial sphere

## Cosmic Spheres of Time



© 2006 Abrams and Primack, Inc.

# Cosmic microwave background (CMB) on the celestial sphere



Credit: WMAP

# Wavelets on the sphere

- Spin scale-discretised wavelet transform given by projection onto each wavelet (McEwen *et al.* 2015; McEwen 2015; McEwen *et al.* 2013; Wiaux, McEwen *et al.* 2008):

$$W^s \Psi^j(\rho) = \underbrace{\langle s f, \mathcal{R}_\rho s \Psi^j \rangle}_{\text{projection}} = \int_{\mathbb{S}^2} d\Omega(\theta, \varphi) s f(\theta, \varphi) (\mathcal{R}_\rho s \Psi^j)^*(\theta, \varphi).$$

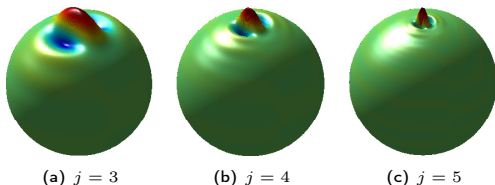


Figure: Wavelets on sphere

- Original function may be recovered exactly in practice from wavelet coefficients:

$$s f(\omega) = \underbrace{\sum_{j=0}^J}_{\text{finite sum}} \underbrace{\int_{\text{SO}(3)} d\varrho(\rho) W^s \Psi^j(\rho) (\mathcal{R}_\rho s \Psi^j)(\omega)}_{\text{wavelet contribution}}.$$

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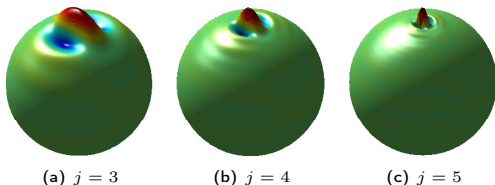


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# Wavelets on the sphere

## Localisation of Gaussian random fields

### Wavelet localisation (McEwen *et al.* 2016)

Directional scale-discretised wavelets  $\Psi \in L^2(\mathbb{S}^2)$ , defined on the sphere  $\mathbb{S}^2$  and centred on the North pole, satisfy the **localisation bound**:

$$|\Psi^{(j)}(\theta, \varphi)| \leq \frac{C_1^{(j)}}{(1 + C_2^{(j)} \theta)^\xi}$$

(there exist strictly positive constants  $C_1^{(j)}, C_2^{(j)} \in \mathbb{R}_*^+$  for any  $\xi \in \mathbb{R}_*^+$ ).

### Wavelet asymptotic uncorrelation (McEwen *et al.* 2016)

For Gaussian random fields on the sphere, directional scale-discretised wavelet coefficients are **asymptotically uncorrelated**. The directional wavelet correlation satisfies the bound:

$$\Xi^{(jj')}(\rho_1, \rho_2) \leq \frac{C_1^{(j)}}{(1 + C_2^{(j)} \beta)^\xi},$$

where  $\beta \in [0, \pi)$  is an angular separation between Euler angles  $\rho_1$  and  $\rho_2$  (there exist strictly positive constants  $C_1^{(j)}, C_2^{(j)} \in \mathbb{R}_*^+$  for any  $\xi \in \mathbb{R}_*^+$ ,  $\xi \geq 2M$ , where  $M$  is the azimuthal band-limit of the wavelet and  $|j - j'| < 2$ ).

# Wavelets on the sphere

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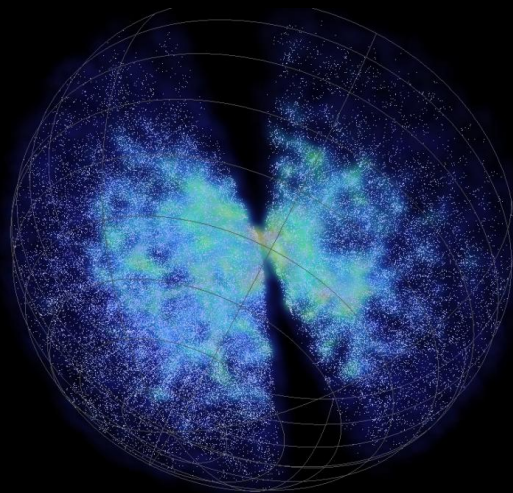
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# Galaxy distribution tracing large-scale structure (LSS) on the 3D ball



Credit: SDSS



# Wavelets on the ball

## Fourier-LAGuerre wavelets (flaglets)

- Fourier-Laguerre wavelet (flaglet) transform is given by the projection onto each wavelet (Leistedt & McEwen 2012):

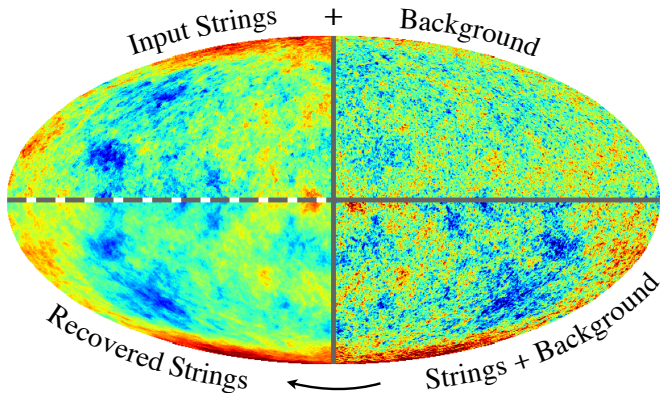
$$W^{s\Psi^{jj'}}(r, \rho) = \underbrace{\langle s f, \mathcal{T}_{(r, \rho)} s \Psi^{jj'} \rangle}_{\text{projection}} = \int_{\mathbb{B}^3} d^3 \mathbf{r} s f(\mathbf{r}) (\mathcal{T}_{(r, \rho)} s \Psi^{jj'})^*(\mathbf{r}).$$

- Original function may be recovered exactly in practice from wavelet coefficients:

$$s f(\mathbf{r}) = \underbrace{\sum_{j j'}}_{\text{finite sum}} \underbrace{\int_{\text{SO}(3)} d\varrho(\rho) \int_{\mathbb{R}^+} dr W^{s\Psi^{jj'}}(r, \rho) (\mathcal{T}_{(r, \rho)} s \Psi^{jj'})}_{\text{wavelet contribution}}(\mathbf{r}).$$

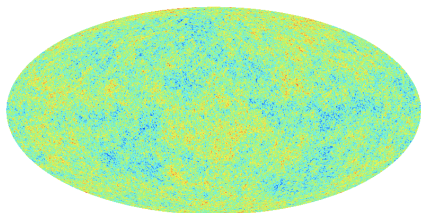
- Opens up wavelet analyses of galaxy distribution tracing the large-scale structure (LSS).

# Cosmic strings Problem

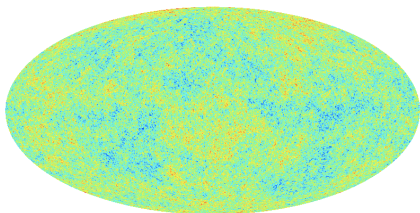


# Cosmic strings

Typical amplitude



(a) CMB

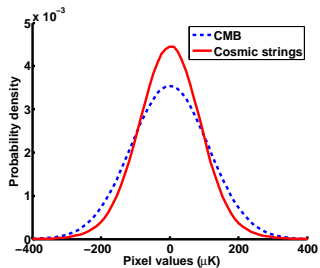


(b) CMB with embedded string contribution

Figure: CMB simulation with string contribution embedded ( $G\mu = 5 \times 10^{-7}$ ).

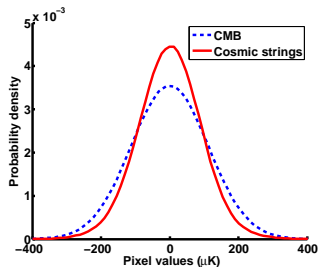
# Cosmic strings

## Wavelet representation

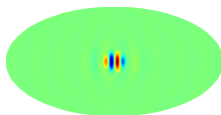


# Cosmic strings

## Wavelet representation

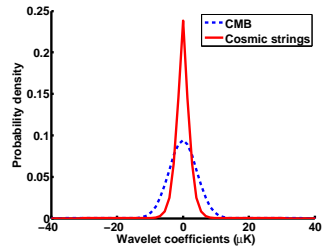
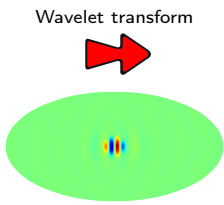
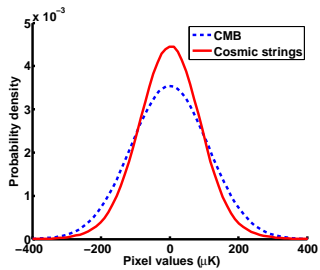


Wavelet transform



# Cosmic strings

## Wavelet representation



# Cosmic strings

## Hierarchical Bayesian model

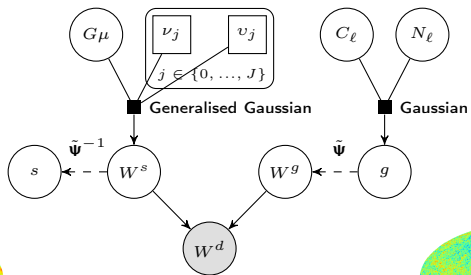


Figure: Hierarchical Bayesian model (McEwen *et al.* 2016)

# Cosmic strings

## Bayesian inference

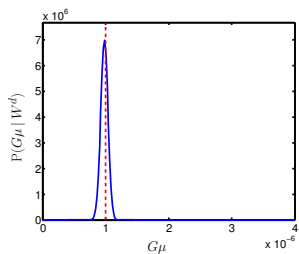


Figure: Posterior

Table: Bayes factors

$G\mu$ truth $/ 10^{-7}$	Bayes factor [ $\log_e$ ]
10.0	51.4
7.00	12.5
5.00	1.19
3.00	-3.87



# Cosmic strings

## Bayesian inference

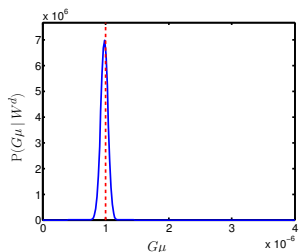
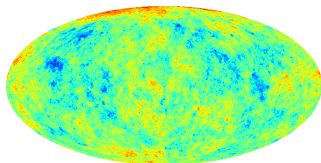


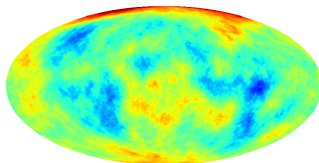
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$G\mu$ truth $/ 10^{-7}$	Bayes factor [ $\log_e$ ]
10.0	51.4
7.00	12.5
5.00	1.19
3.00	-3.87



(a) Ground truth



(b) Recovered

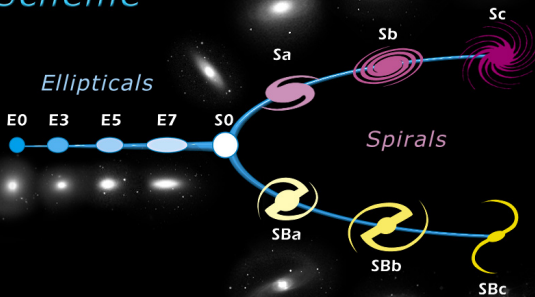
Figure: String map

# Outline

- 1 Bayesian inference
- 2 Computational harmonic analysis
- 3 Machine learning**
- 4 Inverse problems

# Galaxy morphology classification

## Edwin Hubble's Classification Scheme



Credit: Wikipedia

## Galaxy morphology classification

- Galaxy classification with **neural networks** pioneered by Lahav in 1990s (Lahav, Naim *et al.* 1995; Banerji, Lahav *et al.* 2009).
- Galaxy Zoo to **crowdsource** galaxy classification → **~50 million classifications / year**.
- For upcoming surveys with **~1.5 billion galaxies**, would take **30 years!**

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f t r

## Few have witnessed what you're about to see

Experience a privileged glimpse of the distant universe as observed by the SDSS, CTIO and VST.

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To understand how galaxies formed we need your help to classify them according to their shapes. If you're quick, you may even be the first person to see the galaxies you're asked to classify.

[Begin Classifying](#)

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# Galaxy morphology classification

- Use Galaxy Zoo classification as training data (Lahav, Olhede, *et al.*, ongoing).

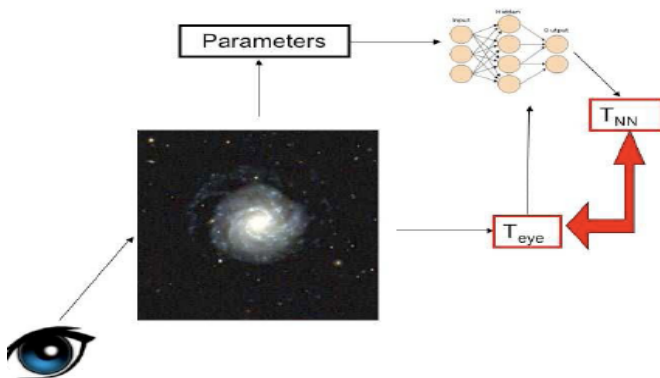


Figure: Crowdsourcing and machine learning for galaxy classification [Credit: Lahav]

## Photometric redshift estimation

- Photometric redshift estimation with [neural networks](#) pioneered by Lahav in 2000s (Collister & Lahav 2004; Sadeh, Abdalla & Lahav 2016).

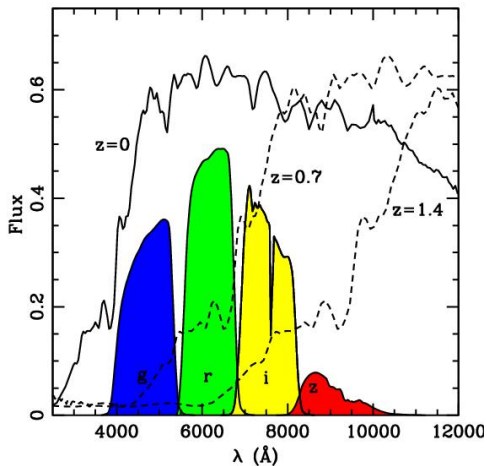


Figure: Photometric redshift estimation [Credit: Lahav]



# Artist impression of Supernova explosion

Thermonuclear explosion or core collapse



# Supernova classification

## Spectroscopic classification

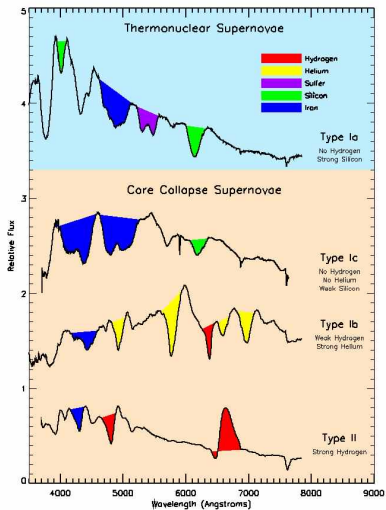


Figure: Spectroscopic observations

# Supernova classification

## Photometric classification

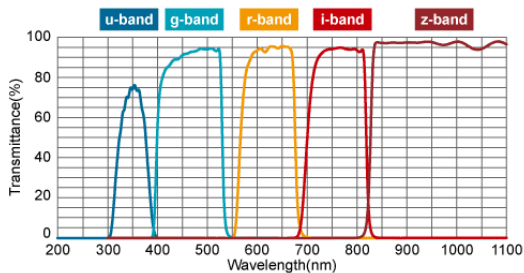
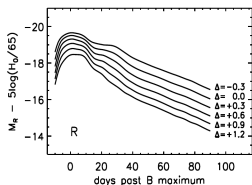


Figure: Photometric observations.

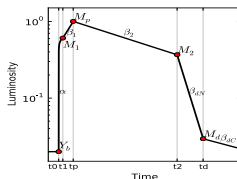
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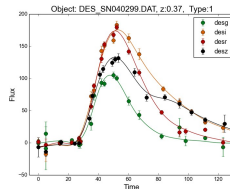
- Photometric Supernova classification by machine learning (Lochner, McEwen, Peiris, Lahav & Winter 2016)
- Go beyond single techniques to **study classes**.



(a) Templates



(b) Generic parameterisations



(c) Wavelets (non-parametric)

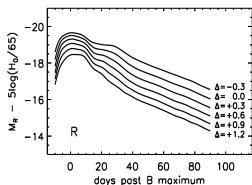
Figure: Feature selection classes (in order of increasing model independence)

- Integrate physics into machine learning (scale and dilation invariance).

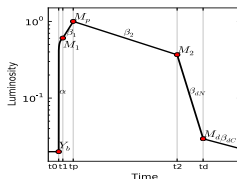
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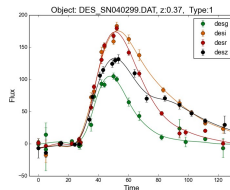
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# Supernova classification

## Representativeness of training data

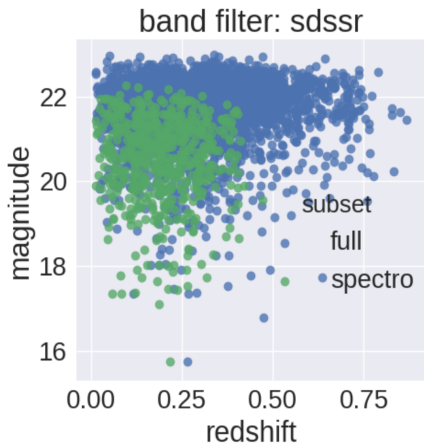


Figure: Training (green) vs test (blue) data

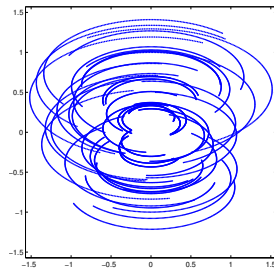
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# Radio interferometric telescopes acquire "Fourier" measurements



"Fourier"  
Measurements





## Radio interferometric inverse problem

- Consider the **ill-posed inverse problem** of radio interferometric imaging:

$$\mathbf{y} = \Phi \mathbf{x} + \mathbf{n},$$

where  $\mathbf{y}$  are the measured visibilities,  $\Phi$  is the linear measurement operator,  $\mathbf{x}$  is the underlying image and  $\mathbf{n}$  is instrumental noise.

- Measurement operator, e.g.  $\Phi = \mathbf{GFA}$ , may incorporate:
  - primary beam  $\mathbf{A}$  of the telescope;
  - Fourier transform  $\mathbf{F}$ ;
  - convolutional de-gridding  $\mathbf{G}$  to interpolate to continuous  $uv$ -coordinates;
  - direction-dependent effects (DDEs)...

Interferometric imaging: recover an image from noisy and incomplete Fourier measurements.

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# Sparse regularisation

## Synthesis and analysis frameworks

- Sparse **synthesis** regularisation problem:

$$\mathbf{x}_{\text{synthesis}} = \Psi \times \arg \min_{\alpha} \left[ \|\mathbf{y} - \Phi \Psi \alpha\|_2^2 + \lambda \|\alpha\|_1 \right]$$

Synthesis framework

where consider sparsifying (e.g. wavelet) representation of image:  $\mathbf{x} = \Psi \alpha$  .

- Sparse **analysis** regularisation problem (Elad *et al.* 2007, Nam *et al.* 2012):

$$\mathbf{x}_{\text{analysis}} = \arg \min_{\mathbf{x}} \left[ \|\mathbf{y} - \Phi \mathbf{x}\|_2^2 + \lambda \|\Psi^\dagger \mathbf{x}\|_1 \right]$$

Analysis framework

- For **orthogonal bases** the two approaches are **identical** but otherwise very different.
- Sparsity averaging reweighted analysis (**SARA**)  
(Carrillo, McEwen & Wiaux 2012; Carrillo, McEwen, Van De Ville, Thiran & Wiaux 2013).

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## Public open-source codes

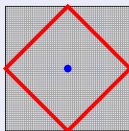
## PURIFY code

<http://basp-group.github.io/purify/>*Next-generation radio interferometric imaging*

Carrillo, McEwen, Wiaux, Pratley, d'Avezac

**PURIFY** is an open-source code that provides functionality to perform radio interferometric imaging, leveraging recent developments in the field of compressive sensing and convex optimisation.

## SOPT code

<http://basp-group.github.io/sopt/>*Sparse OPTimisation*

Carrillo, McEwen, Wiaux, Kartik, d'Avezac, Pratley, Perez-Suarez

**SOPT** is an open-source code that provides functionality to perform sparse optimisation using state-of-the-art convex optimisation algorithms.

## Imaging observations from the VLA and ATCA with PURIFY



(a) NRAO Very Large Array (VLA)



(b) Australia Telescope Compact Array (ATCA)

Figure: Radio interferometric telescopes considered



## PURIFY reconstruction

VLA observation of 3C129

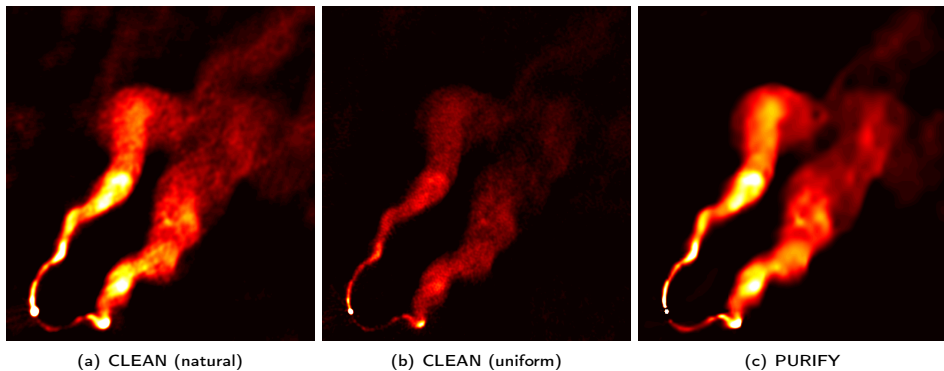
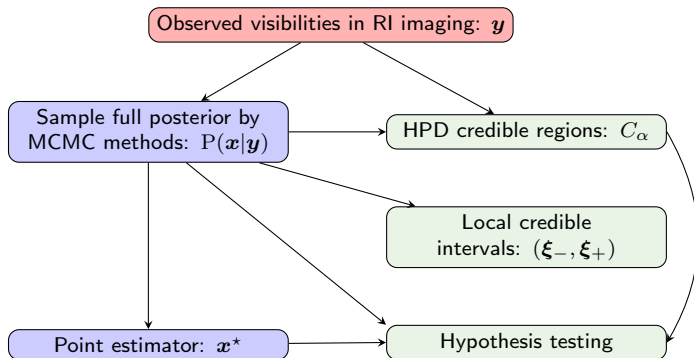


Figure: 3C129 recovered images (Pratley, McEwen, et al. 2016)

## Proximal MCMC sampling and uncertainty quantification

- See poster by [Xiaohao Cai](#)  
(Cai, Pereyra & McEwen, 2017a, in prep.; Cai, Pereyra & McEwen, 2017b, in prep.)



# Sampling the full posterior distribution

## Markov Chain Monte Carlo (MCMC)

- Sample full posterior distribution  $P(\mathbf{x} | \mathbf{y})$ .
- MCMC methods for high-dimensional problems (like interferometric imaging):
  - Gibbs sampling (sample from conditional distributions)
  - Hamiltonian MC (HMC) sampling (exploit gradients)
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Require MCMC approach to support sparse priors, which shown to be highly effective.

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# MCMC sampling with gradients

## Langevin dynamics

- Consider posteriors of the following form (and more compact notation):

$$P(\mathbf{x} | \mathbf{y}) = \underbrace{\pi(\mathbf{x})}_{\text{Posterior}} \propto \exp\left(-\underbrace{g(\mathbf{x})}_{\text{Smooth}}\right)$$

- If  $g(\mathbf{x})$  differentiable can adopt MALA (Langevin dynamics) or HMC (Hamiltonian dynamics) MCMC methods.
- MALA based on Langevin diffusion process  $\mathcal{L}(t)$ , with  $\pi$  as stationary distribution:

$$d\mathcal{L}(t) = \frac{1}{2} \nabla \log \pi(\mathcal{L}(t)) dt + d\mathcal{W}(t), \quad \mathcal{L}(0) = l_0$$

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- Need gradients so **cannot support sparse priors**.

# Proximity operators

## A brief aside

- Define **proximity operator**:

$$\text{prox}_g^\lambda(\mathbf{x}) = \arg \min_{\mathbf{u}} \left[ g(\mathbf{u}) + \|\mathbf{u} - \mathbf{x}\|^2 / 2\lambda \right]$$

- Generalisation of **projection operator**:

$$\mathcal{P}_{\mathcal{C}}(\mathbf{x}) = \arg \min_{\mathbf{u}} \left[ \iota_{\mathcal{C}}(\mathbf{u}) + \|\mathbf{u} - \mathbf{x}\|^2 / 2 \right],$$

where  $\iota_{\mathcal{C}}(\mathbf{u}) = \infty$  if  $\mathbf{u} \notin \mathcal{C}$  and zero otherwise.

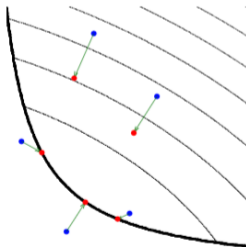


Figure: Illustration of proximity operator [Credit: Parikh & Boyd (2013)]

# Proximal MALA

## MCMC sampling

### Proximal Metropolis adjusted Langevin algorithm (P-MALA)

Pereyra (2016a)

- Consider log-convex posteriors:  $P(\mathbf{x} | \mathbf{y}) = \pi(\mathbf{x}) \propto \exp(-\underbrace{g(\mathbf{x})}_{\text{Convex}})$ .
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- Euler discretisation and apply Moreau approximation to  $\pi$ :

$$l^{(m+1)} = l^{(m)} + \frac{\delta}{2} \underbrace{\nabla \log \pi(l^{(m)})}_{\text{Moreau approximation}} + \sqrt{\delta} w^{(m)}.$$

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# Proximal MALA

## Computing proximity operators for the analysis case

- Recall posterior:  $\pi(\mathbf{x}) \propto \exp(-g(\mathbf{x}))$ .

- Let  $\bar{g}(\mathbf{x}) = \bar{f}_1(\mathbf{x}) + \bar{f}_2(\mathbf{x})$ , where  $\bar{f}_1(\mathbf{x}) = \mu \|\Psi^\dagger \mathbf{x}\|_1$  and  $\bar{f}_2(\mathbf{x}) = \|\mathbf{y} - \Phi \mathbf{x}\|_2^2 / 2\sigma^2$ .

Prior

Likelihood

- Must solve an optimisation problem for each iteration!

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) = \underset{\mathbf{u} \in \mathbb{R}^N}{\text{argmin}} \left\{ \mu \|\Psi^\dagger \mathbf{u}\|_1 + \frac{\|\mathbf{y} - \Phi \mathbf{u}\|_2^2}{2\sigma^2} + \frac{\|\mathbf{u} - \mathbf{x}\|_2^2}{\delta} \right\}.$$

- Taylor expansion at point  $\mathbf{x}$ :  $\|\mathbf{y} - \Phi \mathbf{u}\|_2^2 \approx \|\mathbf{y} - \Phi \mathbf{x}\|_2^2 + 2(\mathbf{u} - \mathbf{x})^\top \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y})$ .
- Then proximity operator approximated by

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) \approx \text{prox}_{\bar{f}_1}^{\delta/2} \left( \mathbf{x} - \delta \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y}) / 2\sigma^2 \right).$$

Single forward-backward iteration

- Analytic approximation:

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) \approx \bar{\mathbf{v}} + \Psi \left( \text{soft}_{\mu\delta/2}(\Psi^\dagger \bar{\mathbf{v}}) - \Psi^\dagger \bar{\mathbf{v}} \right), \text{ where } \bar{\mathbf{v}} = \mathbf{x} - \delta \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y}) / 2\sigma^2.$$

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$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) \approx \text{prox}_{\bar{f}_1}^{\delta/2} \left( \mathbf{x} - \delta \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y}) / 2\sigma^2 \right).$$

Single forward-backward iteration

- Analytic approximation:

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) \approx \bar{\mathbf{v}} + \Psi \left( \text{soft}_{\mu\delta/2}(\Psi^\dagger \bar{\mathbf{v}}) - \Psi^\dagger \bar{\mathbf{v}} \right), \text{ where } \bar{\mathbf{v}} = \mathbf{x} - \delta \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y}) / 2\sigma^2.$$



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Prior Likelihood

- Must solve an optimisation problem for each iteration!

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) = \underset{\mathbf{u} \in \mathbb{R}^N}{\text{argmin}} \left\{ \mu \|\Psi^\dagger \mathbf{u}\|_1 + \frac{\|\mathbf{y} - \Phi \mathbf{u}\|_2^2}{2\sigma^2} + \frac{\|\mathbf{u} - \mathbf{x}\|_2^2}{\delta} \right\}.$$

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## MYULA

## MCMC sampling

## Moreau-Yosida unadjusted Langevin algorithm (MYULA)

Durmus, Moulines &amp; Pereyra (2016)

- Consider log-convex posteriors:  $P(\mathbf{x} | \mathbf{y}) = \pi(\mathbf{x}) \propto \exp(-g(\mathbf{x}))$ , where

$$g(\mathbf{x}) = \boxed{f_1(\mathbf{x})}^{\text{Convex}} + \boxed{f_2(\mathbf{x})}^{\text{Smooth}}.$$

- Langevin diffusion process  $\mathcal{L}(t)$ , with  $\pi$  as stationary distribution ( $\mathcal{W}$  Brownian motion):

$$d\mathcal{L}(t) = \frac{1}{2} \nabla \log \pi(\mathcal{L}(t)) dt + d\mathcal{W}(t), \quad \mathcal{L}(0) = l_0.$$

- Euler discretisation and apply Moreau-Yosida approximation to  $f_1$ :

$$l^{(m+1)} = l^{(m)} + \frac{\delta}{2} \boxed{\nabla \log \pi(l^{(m)})} + \sqrt{\delta} w^{(m)}.$$

$$\nabla \log \pi(\mathbf{x}) \approx (\text{prox}_{f_1}^\lambda(\mathbf{x}) - \mathbf{x})/\lambda - \nabla f_2(\mathbf{x})$$

- No Metropolis-Hastings accept-reject step. Converges geometrically fast, where bias can be made arbitrarily small. To achieve precision target  $\epsilon$  requires:
  - Worst case: order  $N^5 \log^2(\epsilon^{-1}) \epsilon^{-2}$  iterations.
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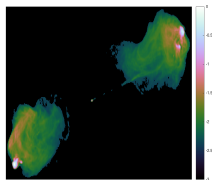
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# Numerical experiments

## MYULA with analysis model

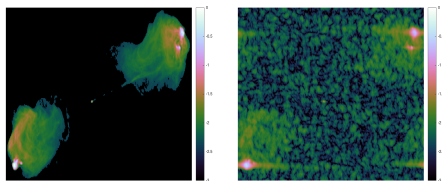


(a) Ground truth

Figure: Cygnus A

# Numerical experiments

## MYULA with analysis model



(a) Ground truth

(b) Dirty image

Figure: Cygnus A

# Numerical experiments

## MYULA with analysis model

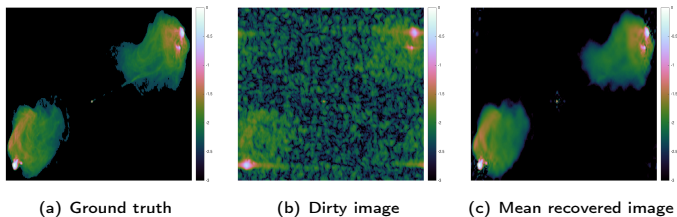


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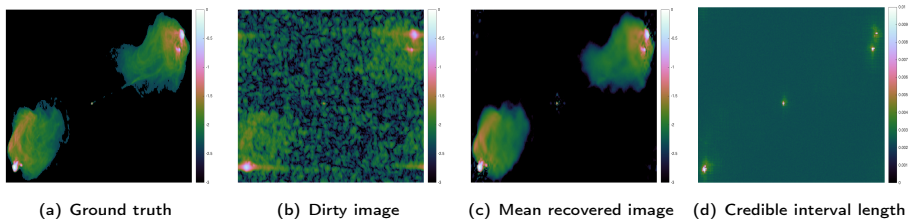


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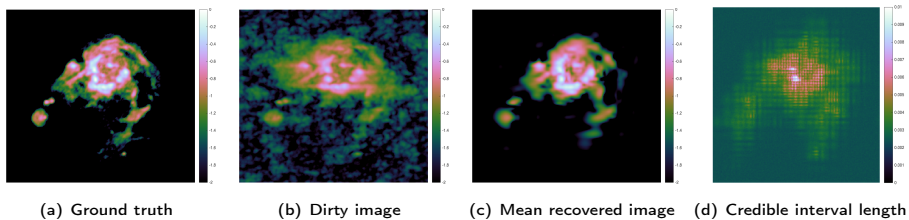


Figure: HII region of M31

# Numerical experiments

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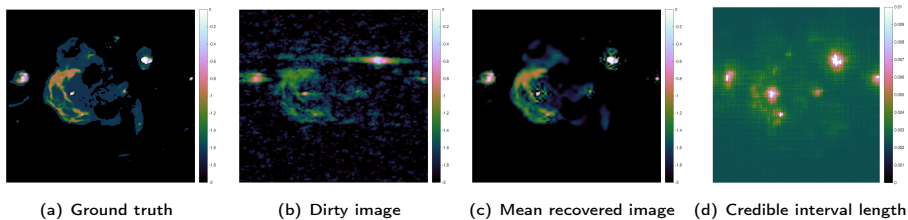


Figure: W28 Supernova remnant

# Numerical experiments

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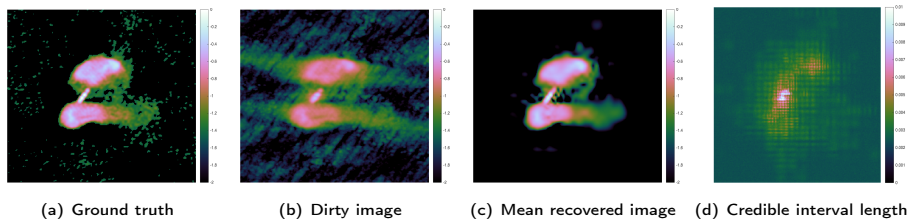
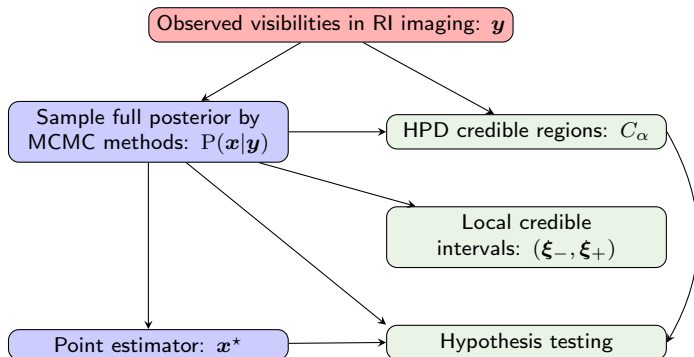


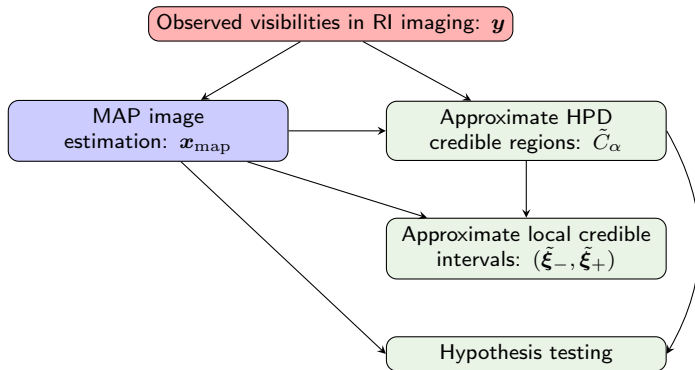
Figure: 3C288

## Proximal MCMC sampling and uncertainty quantification





## MAP estimation and uncertainty quantification



## Approximate Bayesian credible regions for MAP estimation

- Combine **uncertainty quantification** with **fast sparse regularisation** to scale to big-data.
- Recall  $C_\alpha$  denotes the **highest posterior density (HPD) Bayesian credible region** with confidence level  $(1 - \alpha)\%$  defined by posterior isosurface:  $C_\alpha = \{\mathbf{x} : g(\mathbf{x}) \leq \gamma_\alpha\}$ .
- Analytic approximation of  $\gamma_\alpha$ :

$$\tilde{\gamma}_\alpha = g(\mathbf{x}^*) + N(\tau_\alpha + 1)$$

where  $\tau_\alpha = \sqrt{16 \log(3/\alpha)/N}$  and  $\alpha \in (4\exp(-N/3), 1)$  (Pereyra 2016b). Follows by recent results from information theory, related to a concentration property of log-concave random vectors.

- Define **approximate HPD regions** by  $\tilde{C}_\alpha = \{\mathbf{x} : g(\mathbf{x}) \leq \tilde{\gamma}_\alpha\}$ .
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## Local Bayesian credible intervals for MAP estimation

## Local Bayesian credible intervals for sparse reconstruction

(Cai, Pereyra &amp; McEwen, in prep.)

Let  $\Omega$  define the area (or pixel) over which to compute the credible interval  $(\tilde{\xi}_-, \tilde{\xi}_+)$  and  $\zeta$  be an index vector describing  $\Omega$  (i.e.  $\zeta_i = 1$  if  $i \in \Omega$  and 0 otherwise).

Given  $\tilde{\gamma}_\alpha$  and  $\mathbf{x}^*$ , compute the credible interval by

$$\begin{aligned}\tilde{\xi}_- &= \min_{\xi} \{ \xi \mid g_{\mathbf{y}}(\mathbf{x}') \leq \tilde{\gamma}_\alpha, \forall \xi \in [-\infty, +\infty) \}, \\ \tilde{\xi}_+ &= \max_{\xi} \{ \xi \mid g_{\mathbf{y}}(\mathbf{x}') \leq \tilde{\gamma}_\alpha, \forall \xi \in [-\infty, +\infty) \},\end{aligned}$$

where

$$\mathbf{x}' = \mathbf{x}^*(\mathcal{I} - \zeta) + \xi\zeta.$$

## Numerical experiments

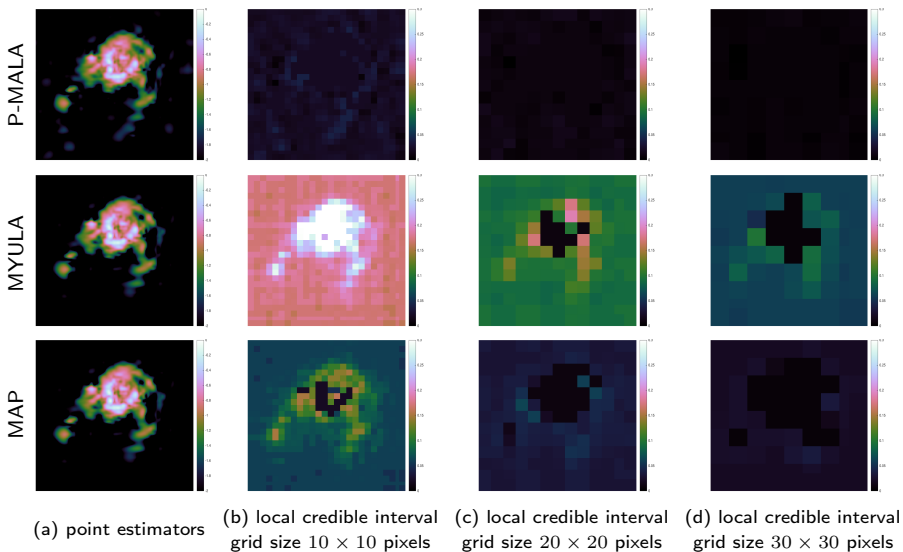


Figure: Local credible interval computation for M31 for the analysis model.

## Numerical experiments

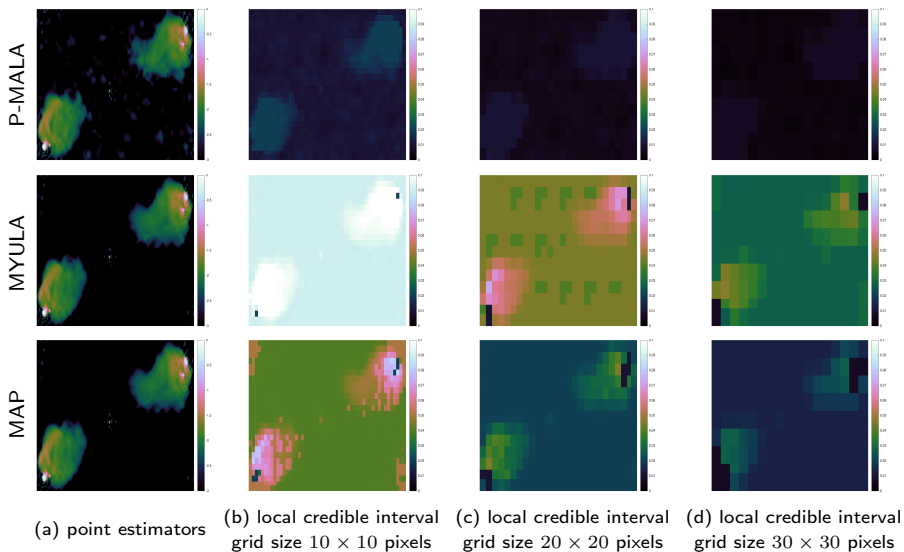


Figure: Local credible interval computation for Cygnus A for the analysis model.



## Numerical experiments

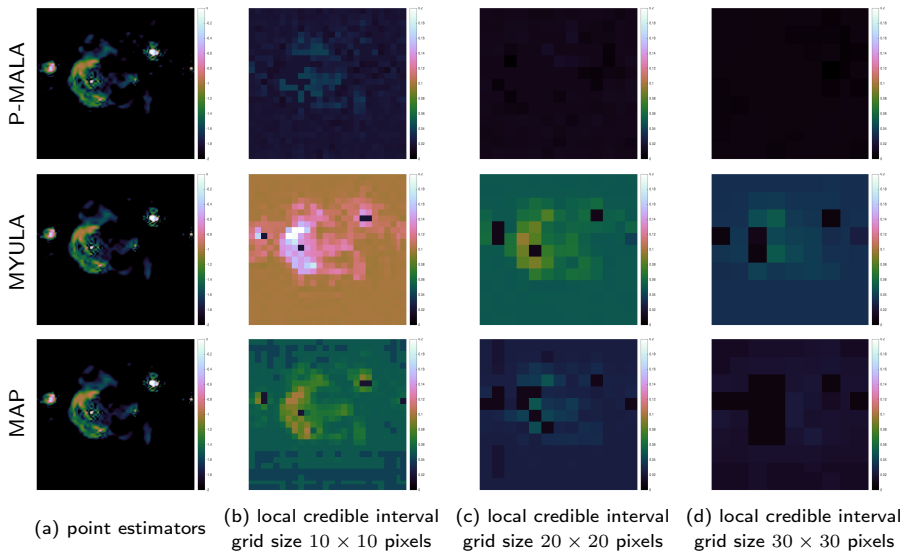


Figure: Local credible interval computation for W28 for the analysis model.

## Numerical experiments

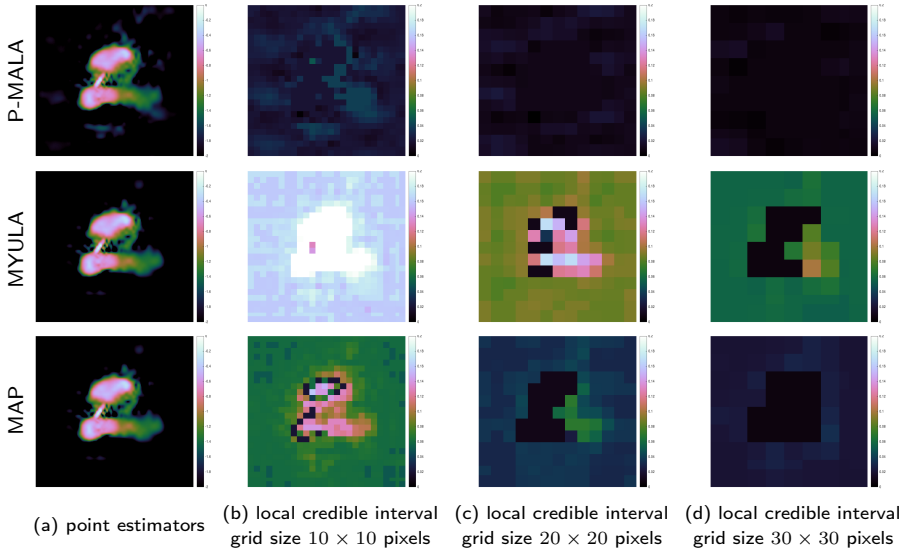


Figure: Local credible interval computation for 3C288 for the analysis model.

## Numerical experiments

## Computation time

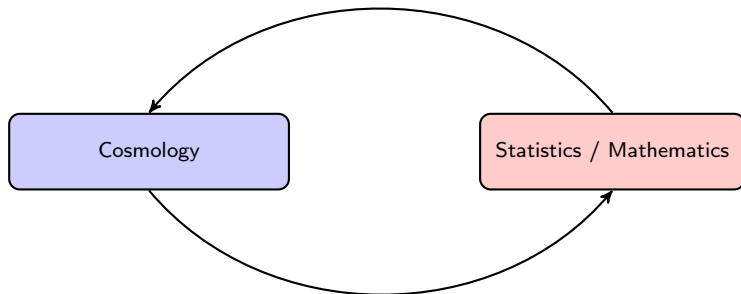
Table: CPU time in minutes for Proximal MCMC sampling and MAP estimation

Image	Method	CPU time	
		Analysis	Synthesis
Cygnus A	P-MALA	2274	1762
	MYULA	1056	942
	MAP	.07	.04
M31	P-MALA	1307	944
	MYULA	618	581
	MAP	.03	.02
W28	P-MALA	1122	879
	MYULA	646	598
	MAP	.06	.04
3C288	P-MALA	1144	881
	MYULA	607	538
	MAP	.03	.02

## Summary

### Closing the DIS loop

*Extracting weak observational signatures of fundamental physics from complex data-sets requires sensitive, robust and principled analysis techniques.*



*Constructing appropriate analysis techniques requires a deep understanding of cosmological problems and methodological foundations.*

# Extra Slides

Wavelets on the sphere

Wavelets on the ball

E/B separation

Cosmic strings

Analysis vs synthesis

Bayesian interpretations

Distribution and parallelisation

PURIFY reconstructions

Proximal MCMC

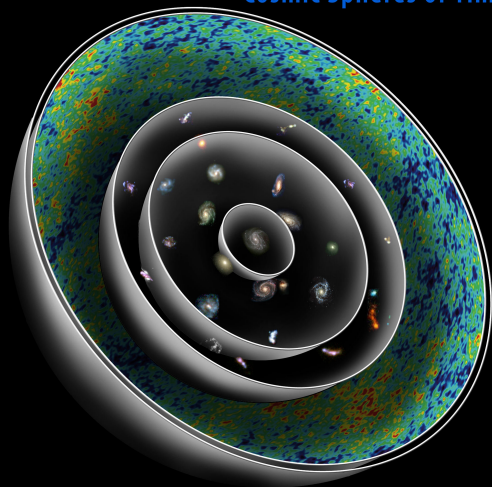
Hypothesis testing

# Extra Slides

## Wavelets on the sphere

# Observations made on the celestial sphere

## Cosmic Spheres of Time



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# Wavelets on the sphere

How can we construct sparsifying transforms?

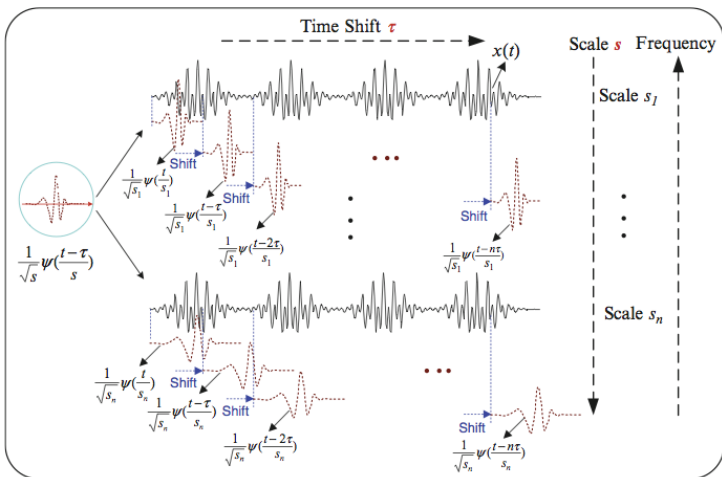


Figure: Wavelet scaling and shifting [Credit: Gao & Yan (2010)]



# Wavelets on the sphere

## Dilation and translation

- Construct **wavelet atoms** from affine transformations (dilation, translation) on the sphere of a mother wavelet.
- The natural **extension of translations to the sphere are rotations**. Rotation of a function  $f$  on the sphere is defined by

$$[\mathcal{R}(\rho)f](\omega) = f(\mathcal{R}_\rho^{-1}\omega), \quad \omega = (\theta, \varphi) \in \mathbb{S}^2, \quad \rho = (\alpha, \beta, \gamma) \in \text{SO}(3).$$

- How define dilation on the sphere?

- Stereographic projection**

Antoine & Vandergheynst (1999), Wiaux *et al.* (2005)

- Harmonic dilation wavelets**

McEwen *et al.* (2006), Sanz *et al.* (2006)

- Isotropic undecimated wavelets**

Starck *et al.* (2005), Starck *et al.* (2009)

- Needlets**

Narcowich *et al.* (2006), Baldi *et al.* (2009), Marinucci *et al.* (2008), Geller *et al.* (2008)

- Scale-discretised wavelets**

Wiaux, McEwen *et al.* (2008), McEwen *et al.* (2003), McEwen *et al.* (2015)

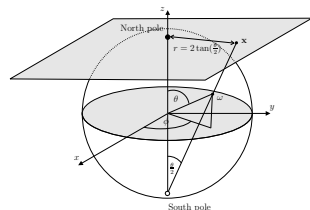


Figure: Stereographic projection

# Wavelets on the sphere

## Spin scale-discretised wavelet construction

- Spin scale-discretised wavelet  ${}_s\Psi^j$  constructed in separable form in harmonic space:

$${}_s\Psi_{\ell m}^j = \kappa^j(\ell) \zeta_{\ell m}.$$

- Admissible wavelets constructed to satisfy a resolution of the identity:

$$|{}_s\Phi_{\ell 0}|^2 + \sum_{j=0}^J \sum_{m=-\ell}^{\ell} \underbrace{|{}_s\Psi_{\ell m}^j|^2}_{\text{wavelet}} = 1, \quad \forall \ell.$$

scaling function

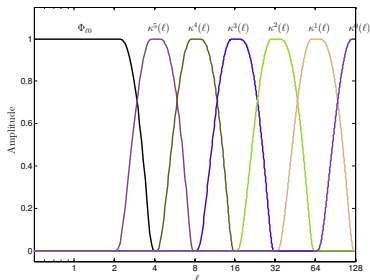


Figure: Harmonic tiling on the sphere.

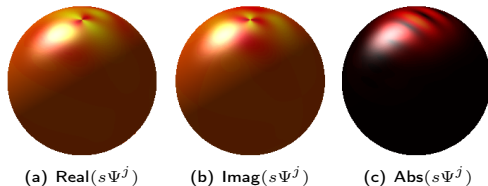


Figure: Spin scale-discretised wavelets on the sphere.

# Wavelets on the sphere

## Fast algorithms, variations, and applications

- **Fast algorithms critical** to scale to large observational data-sets (McEwen *et al.* 2015; McEwen *et al.* 2013; Leistedt, McEwen *et al.* 2013; McEwen *et al.* 2007).
- Variety of types:
  - Spin (McEwen *et al.* 2015)
  - Directional (McEwen *et al.* 2015; Wiaux, McEwen *et al.* 2008)
  - Curvelets (Chan, Leistedt, Kitching & McEwen 2016)
  - Ridgelets (McEwen 2016)
  - Steerable (McEwen *et al.* 2015; Wiaux, McEwen *et al.* 2008)
  - Morphological components (McEwen *et al.* 2008)
- Wavelets ideally suited to cosmological analysis:
  - Physical processes are often manifest on particular physical scales but spatially localised.
  - Localised covariance structure of both theory and data.
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  - Prevalent CMB analysis technique.

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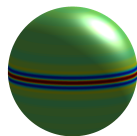


Figure: Ridgelet

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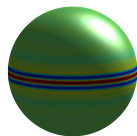


Figure: Ridgelet

# Extra Slides

## Wavelets on the ball

# Wavelets on the ball (flaglets)

## Translation and convolution on the radial line

- Construct translation and convolution on radial line by analogy with infinite line.
- For the standard orthogonal basis  $\phi_\omega(x) = \exp^{i\omega x}$  translation of the basis functions defined by shift of coordinates:

$$(\mathcal{T}_u^{\mathbb{R}} \phi_\omega)(x) \equiv \phi_\omega(x - u) = \phi_\omega^*(u) \phi_\omega(x) .$$

- Define **translation** of the spherical Laguerre basis functions on the radial line by analogy:

$$(\mathcal{T}_s K_p)(r) \equiv K_p(s) K_p(r) .$$

- **Convolution** on the radial line defined by

$$(f \star h)(r) \equiv \langle f, \mathcal{T}_r h \rangle_{\mathbb{R}^+} = \int_{\mathbb{R}^+} ds s^2 f(s) (\mathcal{T}_r h)(s),$$

- In harmonic space, radial convolution is given by the product

$$(f \star h)_p = \langle f \star h, K_p \rangle_{\mathbb{R}^+} = f_p h_p .$$

# Wavelets on the ball (flaglets)

## Translation and convolution on the radial line

- Translation on the radial line corresponds to convolution with the Dirac delta:

$$(f \star \delta_s)(r) = \sum_{p=0}^{\infty} f_p K_p(s) K_p(r) = (\mathcal{T}_s f)(r) .$$

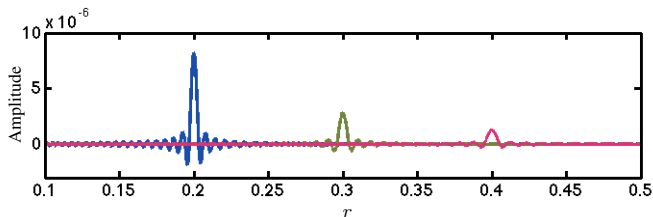


Figure: Band limited translated Dirac delta functions



# Wavelets on the ball (flaglets)

## Fourier-Laguerre translation and convolution

- **Translation operator on the ball** defined by combining the angular and radial translation operators, giving

$$\mathcal{T}_{\mathbf{r}} \equiv \mathcal{T}_{\mathbf{r}} \mathcal{R}_{(\theta, \varphi)}.$$

- **Convolution on the ball** of  $f \in L^2(\mathbb{B}^3)$  with an axisymmetric kernel  $h \in L^2(\mathbb{B}^3)$  is defined by

$$(f \star h)(\mathbf{r}) \equiv \langle f, \mathcal{T}_{\mathbf{r}} h \rangle_{\mathbb{B}^3} = \int_{\mathbb{B}^3} d^3 \mathbf{s} f(\mathbf{s}) (\mathcal{T}_{\mathbf{r}} h)^*(\mathbf{s}),$$

where  $\mathbf{s} \in \mathbb{B}^3$ .

- In harmonic space, axisymmetric convolution on the ball may be written

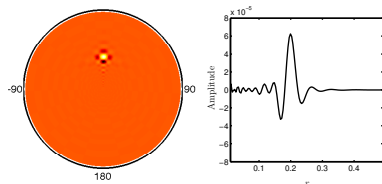
$$(f \star h)_{\ell m p} = \langle f \star h | Z_{\ell m p} \rangle_{\mathbb{B}^3} = \sqrt{\frac{4\pi}{2\ell + 1}} f_{\ell m p} h_{\ell 0 p}^*,$$

with  $f_{\ell m p} = \langle f, Z_{\ell m p} \rangle_{\mathbb{B}^3}$  and  $h_{\ell 0 p} \delta_{m0} = \langle h, Z_{\ell m p} \rangle_{\mathbb{B}^3}$ .

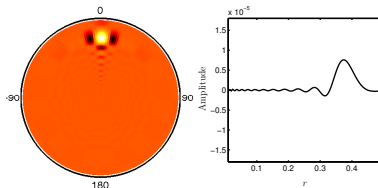
# Wavelets on the ball (flaglets)

## Fourier-Laguerre translation and convolution

- Angular (radial) aperture of localised functions is invariant under radial (angular) translation.



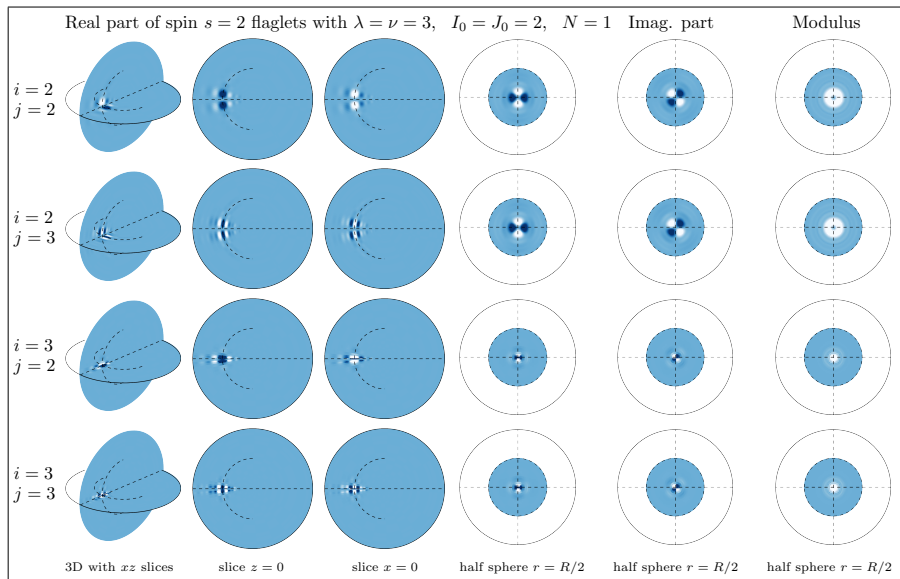
(a) Wavelet kernel translated by  $r = 0.2$



(b) Wavelet kernel translated by  $r = 0.4$

Figure: Slices of an axisymmetric flaglet wavelet kernel plotted on the ball of radius  $R = 0.5$ .

# Wavelets on the ball (flaglets)



# Wavelets on the ball (flaglets)

## Wavelet tiling

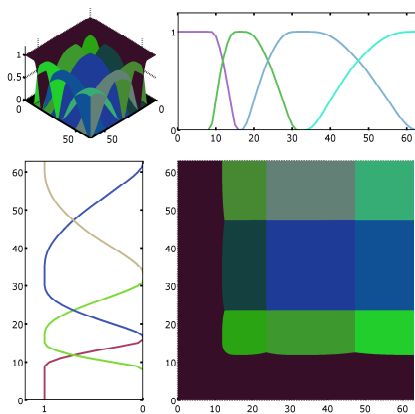


Figure: Tiling of Fourier-Laguerre space.

# Extra Slides

E/B separation

## E/B separation

## Cosmological spin signals

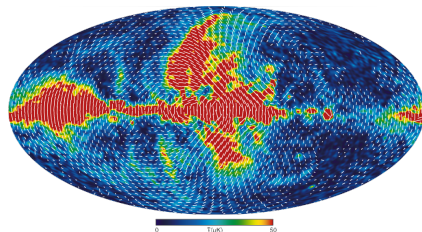
- Observe spin  $\pm 2$  cosmological signals on the celestial sphere, with  $\mathbf{n} = (\theta, \varphi) \in \mathbb{S}^2$ :

$$\pm_2 P(\mathbf{n}) = Q \pm iU$$

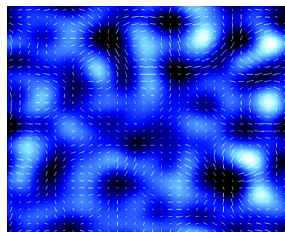
CMB polarization

$$\pm_2 \gamma(\mathbf{n}, r) = \gamma_1 \pm i\gamma_2$$

Cosmic shear



(a) CMB polarization [Credit: WMAP]



(b) Cosmic shear [Credit: Ellis (2010)]

Figure: Cosmological spin signals.

## E/B separation

### Parity even and odd components

- Decompose  $\pm_2 P$  into parity even and parity odd components:

$$\epsilon(\mathbf{n}) = -\frac{1}{2} \left[ \bar{\partial}^2 {}_2P(\mathbf{n}) + \partial^2 {}_{-2}P(\mathbf{n}) \right] \quad \text{E-mode}$$

$$\beta(\mathbf{n}) = \frac{i}{2} \left[ \bar{\partial}^2 {}_2P(\mathbf{n}) - \partial^2 {}_{-2}P(\mathbf{n}) \right] \quad \text{B-mode}$$

where  $\bar{\partial}$  and  $\partial$  are spin lowering and raising (differential) operators, respectively.

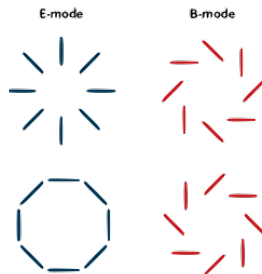


Figure: E-mode (even parity) and B-mode (odd parity) signals [Credit: <http://www.skyandtelescope.com/>].

- Different physical processes exhibit different symmetries.
- Can exploit this property to separate signals arising from different underlying physical mechanisms.

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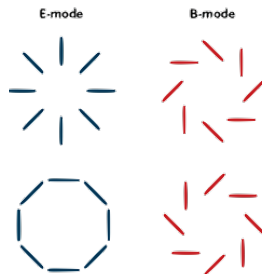


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## E/B separation

## Pure mode wavelet estimator

- On a manifold with boundary (*i.e.* partial sky),  
E/B decomposition not unique.



- Pure mode wavelet estimators (Leistedt, McEwen, Büttner & Peiris 2016):

$$\widehat{W}_\epsilon^0 \Psi^j(\rho) = -\operatorname{Re} \left[ \underbrace{W_{\pm 2 \bar{P}}^{\pm 2} \Upsilon^j(\rho)}_{\text{pseudo}} + \underbrace{2W_{\pm 1 \bar{P}}^{\pm 1} \Upsilon^j(\rho) + W_0^0 \Upsilon^j(\rho)}_{\text{pure correction}} \right],$$

$$\widehat{W}_\beta^0 \Psi^j(\rho) = \mp \operatorname{Im} \left[ \underbrace{W_{\pm 2 \bar{P}}^{\pm 2} \Upsilon^j(\rho)}_{\text{pseudo}} + \underbrace{2W_{\pm 1 \bar{P}}^{\pm 1} \Upsilon^j(\rho) + W_0^0 \Upsilon^j(\rho)}_{\text{pure correction}} \right].$$

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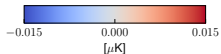
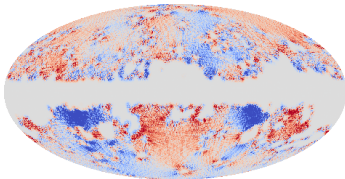
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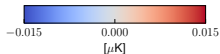
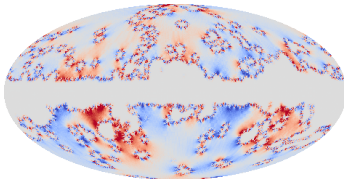
# E/B separation

Results: pseudo harmonic approach

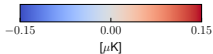
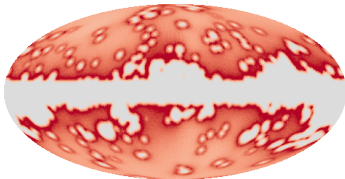
*E* mode error mean (pseudo harmonic recovery)



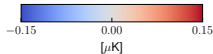
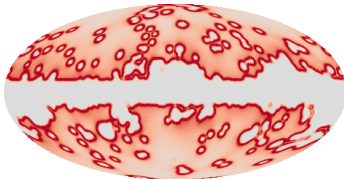
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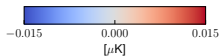
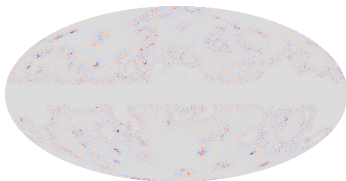
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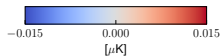
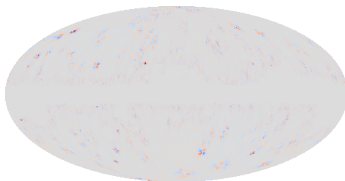
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Results: pure wavelet approach

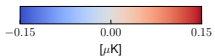
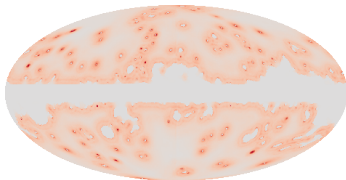
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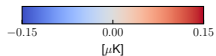
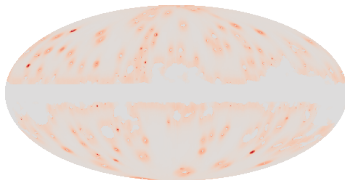
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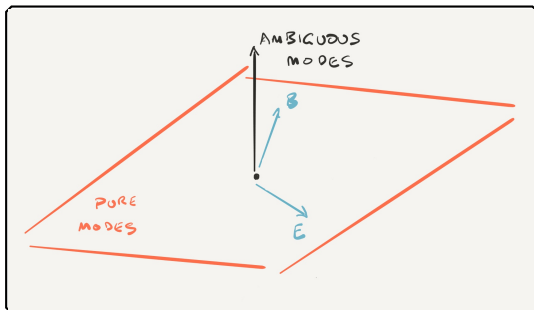
# E/B separation

## Pure and ambiguous modes

- Pure and ambiguous modes

(Lewis et al. 2002, Bunn et al. 2003, Smith 2006, Smith & Zaldarriaga 2007, Grain et al. 2007, Ferté et al. 2013)

- E-modes: vanishing curl
- B-modes: vanishing divergence
- Pure E-modes: orthogonal to all B-modes
- Pure B-modes: orthogonal to all E-modes



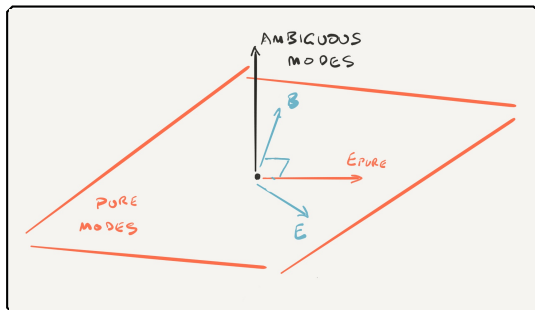
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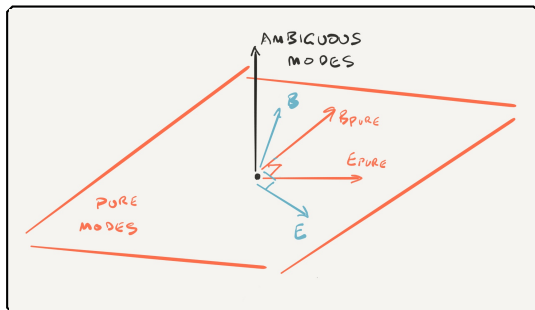
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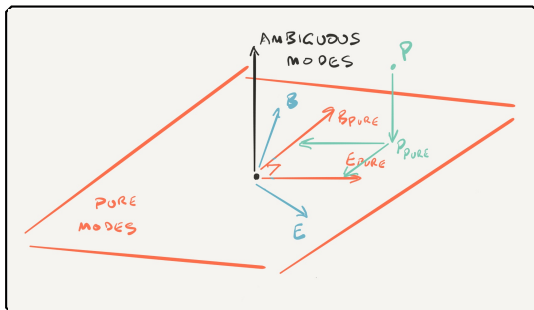
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## E/B separation

## Connections between spin and scalar wavelet coefficients

- Spin wavelet transform of  ${}_{\pm 2}P = Q \pm iU$  (observable):

$$W_{\pm 2P}^{2\Psi^j}(\rho) = \langle {}_{\pm 2}P, \mathcal{R}_\rho {}_{\pm 2}\Psi^j \rangle = \int_{\mathbb{S}^2} d\Omega(\omega) {}_{\pm 2}P(\omega) (\mathcal{R}_\rho {}_{\pm 2}\Psi^j)^*(\omega).$$

spin wavelet transform

- Scalar wavelet transforms of  $E$  and  $B$  (non-observable):

$$W_\epsilon^{0\Psi^j}(\rho) = \langle \epsilon, \mathcal{R}_\rho {}_0\Psi^j \rangle,$$

scalar wavelet transform

$$W_\beta^{0\Psi^j}(\rho) = \langle \beta, \mathcal{R}_\rho {}_0\Psi^j \rangle,$$

scalar wavelet transform

where  ${}_0\Psi^j \equiv \bar{\mathcal{D}}^2 {}_{\pm 2}\Psi^j$ .

- Spin wavelet coefficients of  ${}_{\pm 2}P$  are connected to scalar wavelet coefficients of  $E/B$ :

$$W_\epsilon^{0\Psi^j}(\rho) = -\text{Re} \left[ W_{\pm 2P}^{2\Psi^j}(\rho) \right] \quad \text{and} \quad W_\beta^{0\Psi^j}(\rho) = \mp \text{Im} \left[ W_{\pm 2P}^{2\Psi^j}(\rho) \right].$$

# E/B separation

## Exploiting wavelets

### General approach to recover E/B signals using scale-discretised wavelets

- 1 Compute spin wavelet transform of  $\pm_2 P = Q + iU$ :

$$\pm_2 P(\omega) \xrightarrow[\text{S2LET}]{\text{Spin wavelet transform}} W_{\pm_2 P}^{2\Psi^j}(\rho)$$

- 2 Account for mask in wavelet domain (simultaneous **harmonic and spatial** localisation):

$$W_{\pm_2 P}^{2\Psi^j}(\rho) \xrightarrow{\text{Mitigate mask}} \bar{W}_{\pm_2 P}^{2\Psi^j}(\rho)$$

- 3 Construct E/B maps:

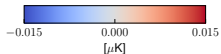
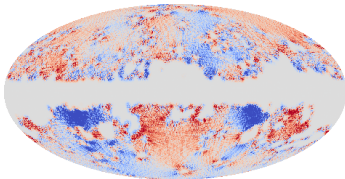
$$(a) W_{\epsilon}^{0\Psi^j}(\rho) = -\text{Re} \left[ \bar{W}_{\pm_2 P}^{2\Psi^j}(\rho) \right] \xrightarrow[\text{S2LET}]{\text{Inverse scalar wavelet transform}} \epsilon(\omega)$$

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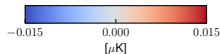
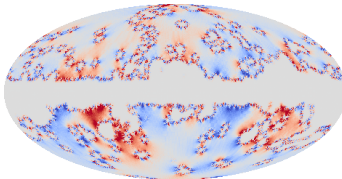
# E/B separation

Results: pseudo harmonic approach

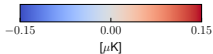
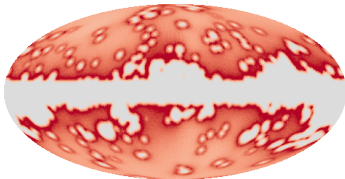
*E* mode error mean (pseudo harmonic recovery)



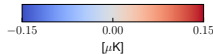
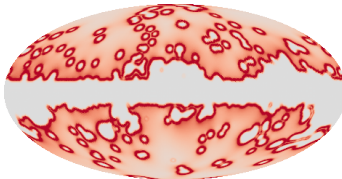
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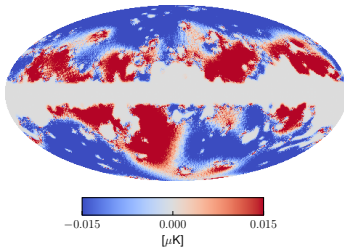
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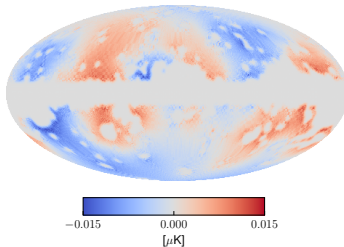
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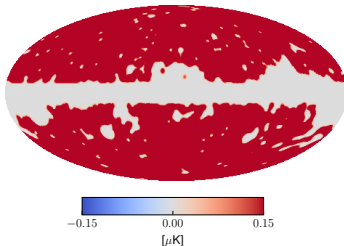
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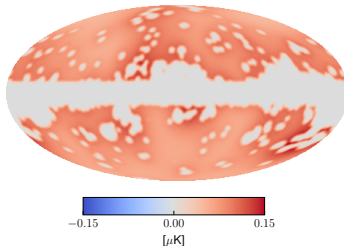
*B* mode error mean (pure harmonic recovery)



*E* mode error std. dev. (pure harmonic recovery)

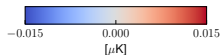
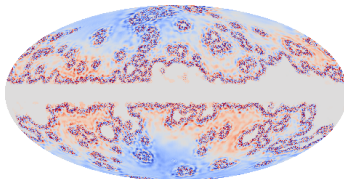
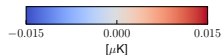
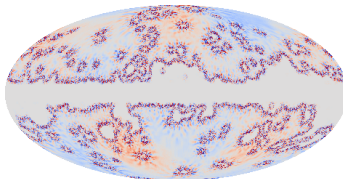
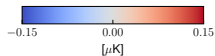
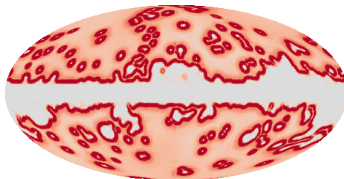
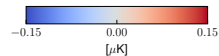
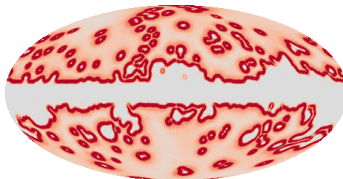


*B* mode error std. dev. (pure harmonic recovery)



## E/B separation

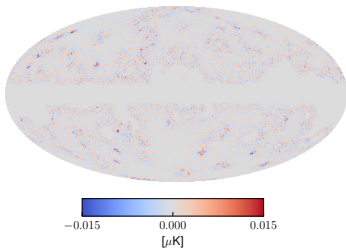
Results: pseudo wavelet approach

*E* mode error mean (pseudo wavelet recovery)*B* mode error mean (pseudo wavelet recovery)*E* mode error std. dev. (pseudo wavelet recovery)*B* mode error std. dev. (pseudo wavelet recovery)

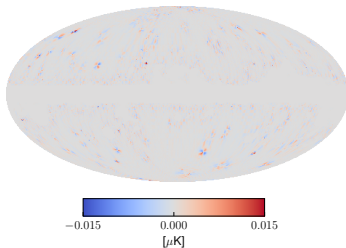
# E/B separation

Results: pure wavelet approach

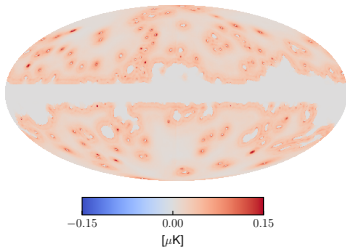
*E* mode error mean (pure wavelet recovery)



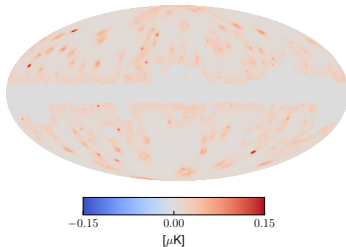
*B* mode error mean (pure wavelet recovery)



*E* mode error std. dev. (pure wavelet recovery)



*B* mode error std. dev. (pure wavelet recovery)



# Extra Slides

## Cosmic strings

## Cosmic strings

## Wavelet space distributions

- Calculate analytically the probability distribution of the CMB in wavelet space:

$$P_j^c(W_{j\rho}^c) = \frac{1}{\sqrt{2\pi(\sigma_j^c)^2}} \exp\left(-\frac{1}{2}\left(\frac{W_{j\rho}^c}{\sigma_j^c}\right)^2\right), \text{ where } (\sigma_j^c)^2 = \langle W_{j\rho}^c W_{j\rho}^{c*} \rangle = \sum_{\ell m} C_\ell |(\Psi_j)_{\ell m}|^2.$$

- Fit a generalised Gaussian distribution (GGD) for the wavelet coefficients of a string training map:

$$P_j^s(W_{j\rho}^s | G\mu) = \frac{\nu_j}{2G\mu\nu_j\Gamma(\nu_j^{-1})} \exp\left(-\left|\frac{W_{j\rho}^s}{G\mu\nu_j}\right|^{\nu_j}\right),$$

with scale parameter  $\nu_j$  and shape parameter  $\nu_j$ .

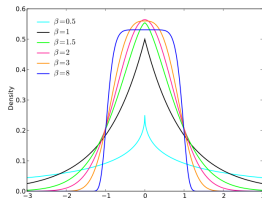


Figure: Generalised Gaussian distribution (GGD).



## Cosmic strings

## Cosmic string distributions in wavelet space

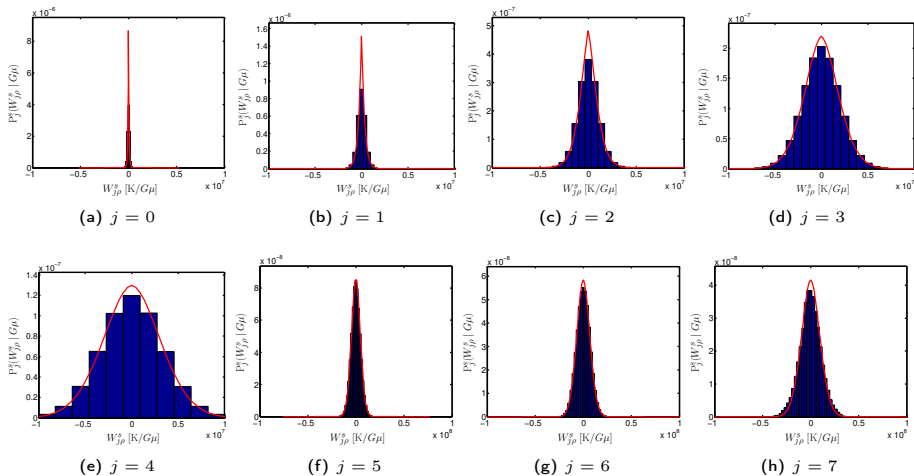
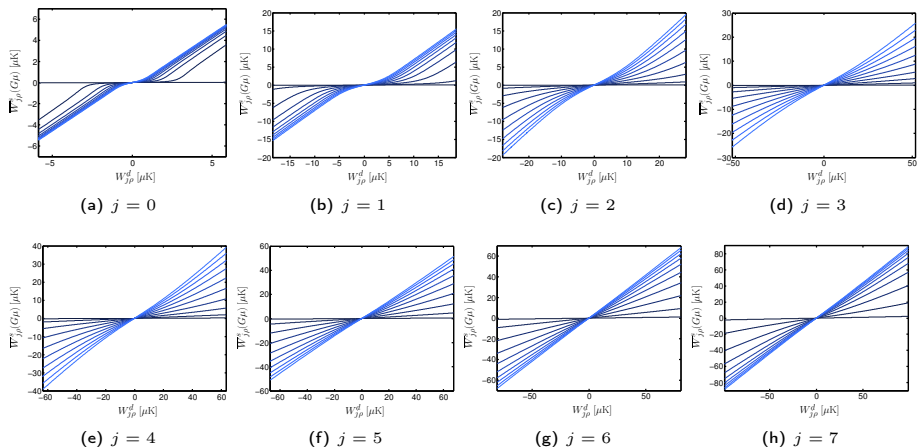


Figure: Distribution of the cosmic string maps in wavelet space for each wavelet scale  $j$ .

## Cosmic strings

## Cosmic string distributions in wavelet space

Figure: Bayesian thresholding functions for each wavelet scale  $j$ .

# Extra Slides

Analysis vs synthesis

# SARA algorithm

- Sparsity averaging reweighted analysis (**SARA**) (Carrillo, McEwen & Wiaux 2012; Carrillo, McEwen, Van De Ville, Thiran & Wiaux 2013).

- Overcomplete dictionary** composed of a concatenation of orthonormal bases:

$$\Psi = [\Psi_1, \Psi_2, \dots, \Psi_q]$$

with following bases: **Dirac** (*i.e.* pixel basis); **Haar wavelets** (promotes gradient sparsity); **Daubechies wavelets** two to eight  $\Rightarrow$  concatenation of 9 bases.

- Promote **average sparsity** by solving the **constrained** reweighted  $\ell_1$  **analysis** problem:

$$\min_{\mathbf{x} \in \mathbb{R}^N} \|\mathbf{W}\Psi^\dagger \mathbf{x}\|_1 \quad \text{subject to} \quad \|\mathbf{y} - \Phi \mathbf{x}\|_2 \leq \epsilon \quad \text{and} \quad \mathbf{x} \geq 0$$

SARA

## Analysis vs synthesis

- Typically sparsity assumption is justified by analysing example signals in terms of atoms of the dictionary.
- Different to synthesising signals from atoms.
- Suggests an **analysis-based** framework (Elad *et al.* 2007, Nam *et al.* 2012):

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} \|\Omega \mathbf{x}\|_1 \text{ subject to } \|\mathbf{y} - \Phi \mathbf{x}\|_2 \leq \epsilon .$$

analysis

- Contrast with **synthesis-based** approach:

$$\mathbf{x}^* = \Psi \cdot \arg \min_{\alpha} \|\alpha\|_1 \text{ subject to } \|\mathbf{y} - \Phi \Psi \alpha\|_2 \leq \epsilon .$$

synthesis

- For **orthogonal bases**  $\Omega = \Psi^\dagger$  and the two approaches are **identical**.

# Analysis vs synthesis

## Comparison

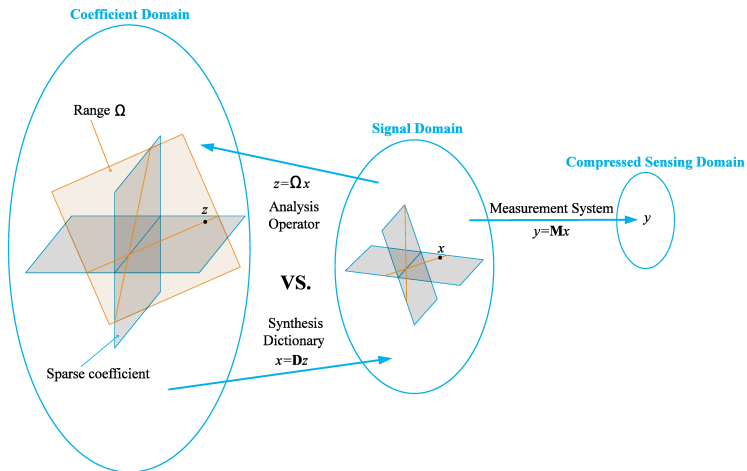


Figure: Analysis- and synthesis-based approaches [Credit: Nam et al. (2012)].

# Analysis vs synthesis

## Comparison

- Synthesis-based approach is more general, while analysis-based approach more restrictive.
- More restrictive analysis-based approach may make it more robust to noise.
- The greater descriptive power of the synthesis-based approach may provide better signal representations (too descriptive?).

# Extra Slides

Bayesian interpretations



## Bayesian interpretations

### One Bayesian interpretation of the synthesis-based approach

- Consider the inverse problem:

$$\mathbf{y} = \Phi\Psi\boldsymbol{\alpha} + \mathbf{n}.$$

- Assume Gaussian noise, yielding the likelihood:

$$P(\mathbf{y} | \boldsymbol{\alpha}) \propto \exp\left(-\frac{\|\mathbf{y} - \Phi\Psi\boldsymbol{\alpha}\|_2^2}{2\sigma^2}\right).$$

- Consider the Laplacian prior:

$$P(\boldsymbol{\alpha}) \propto \exp\left(-\beta\|\boldsymbol{\alpha}\|_1\right).$$

- The **maximum *a-posteriori* (MAP) estimate** (with  $\lambda = 2\beta\sigma^2$ ) is

$$\mathbf{x}_{\text{MAP-synthesis}}^* = \Psi \cdot \arg \max_{\boldsymbol{\alpha}} P(\boldsymbol{\alpha} | \mathbf{y}) = \Psi \cdot \arg \min_{\boldsymbol{\alpha}} \|\mathbf{y} - \Phi\Psi\boldsymbol{\alpha}\|_2^2 + \lambda\|\boldsymbol{\alpha}\|_1.$$

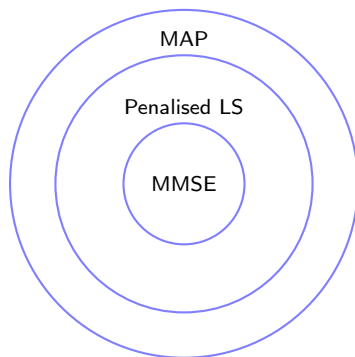
synthesis

- One** possible Bayesian interpretation!
- Signal may be  $\ell_0$ -sparse**, then solving  $\ell_1$  problem finds the correct  $\ell_0$ -sparse solution!

# Bayesian interpretations

## Other Bayesian interpretations of the synthesis-based approach

- Other Bayesian interpretations are also possible (Gribonval 2011).
- Minimum mean square error (MMSE) estimators
  - synthesis-based estimators with appropriate penalty function, *i.e.* penalised least-squares (LS)
  - MAP estimators



## Bayesian interpretations

### One Bayesian interpretation of the analysis-based approach

- Analysis-based MAP estimate is

$$\mathbf{x}_{\text{MAP-analysis}}^* = \Omega^\dagger \cdot \arg \min_{\gamma \in \text{column space } \Omega} \|\mathbf{y} - \Phi \Omega^\dagger \gamma\|_2^2 + \lambda \|\gamma\|_1.$$

analysis

- Different to synthesis-based approach if analysis operator  $\Omega$  is not an orthogonal basis.
- Analysis-based approach **more restrictive** than synthesis-based.
- Similar ideas promoted by Masinger, Hobson & Lasenby (2004) in a Bayesian framework for wavelet MEM (maximum entropy method).

# Extra Slides

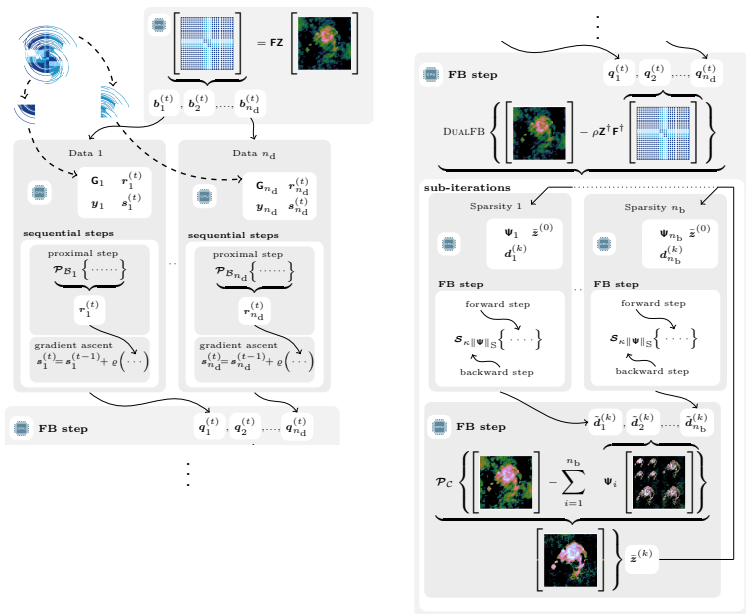
Distributed and parallelised convex optimisation

## Distributed and parallelised convex optimisation

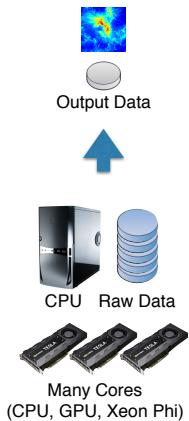
- Solve resulting convex optimisation problems by **proximal splitting**.
- **Block inexact ADMM algorithm** to split data and measurement operator:  
(Carrillo, McEwen & Wiaux 2014; Onose, Carrillo, Repetti, McEwen, *et al.* 2016)

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_{n_d} \end{bmatrix}, \quad \Phi = \begin{bmatrix} \Phi_1 \\ \vdots \\ \Phi_{n_d} \end{bmatrix} = \begin{bmatrix} \mathbf{G}_1 \mathbf{M}_1 \\ \vdots \\ \mathbf{G}_{n_d} \mathbf{M}_{n_d} \end{bmatrix} \mathbf{FZ}.$$

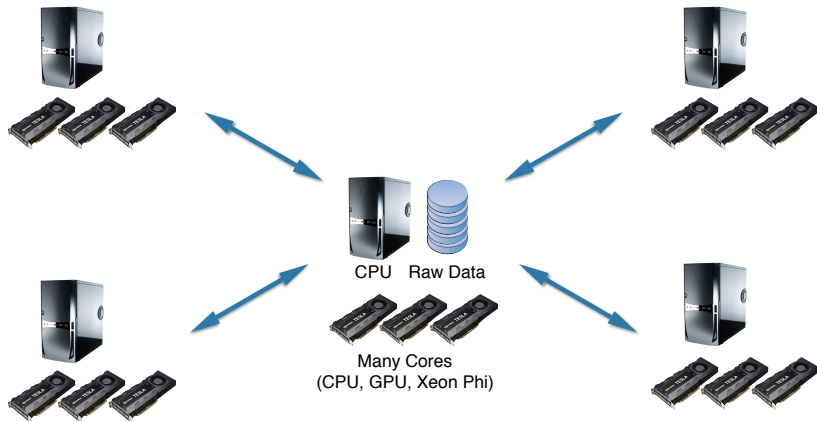
# Distributed and parallelised convex optimisation



# Standard algorithms

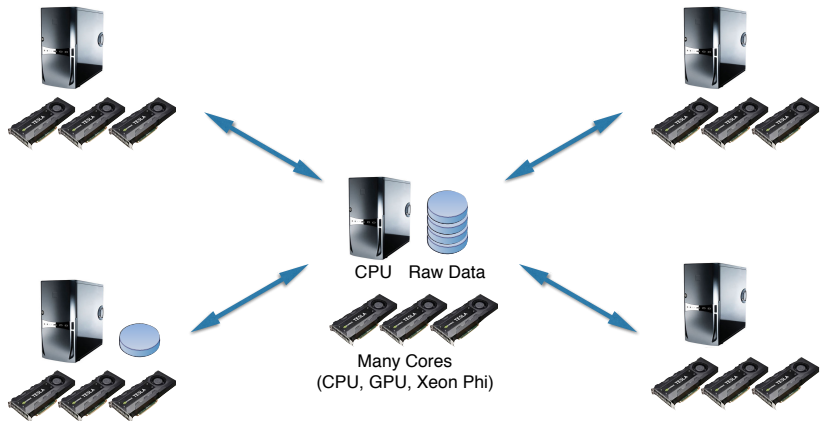


# Highly distributed and parallelised algorithms

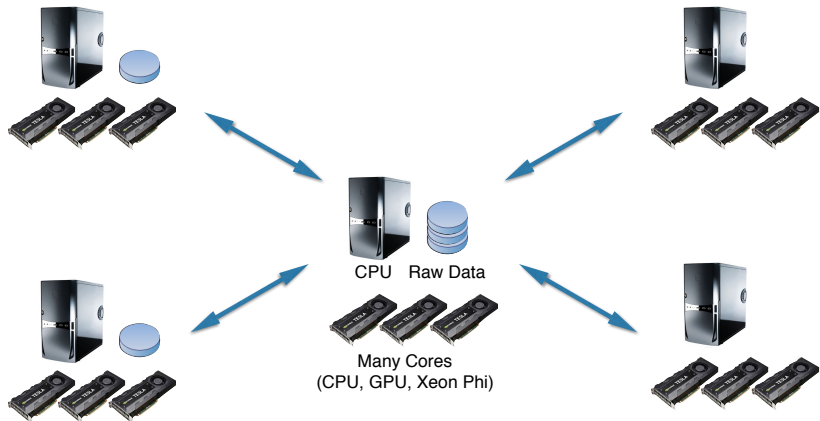




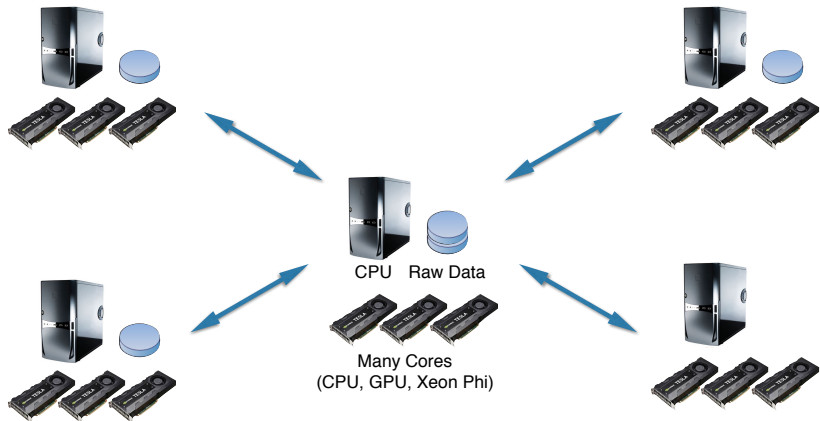
# Highly distributed and parallelised algorithms



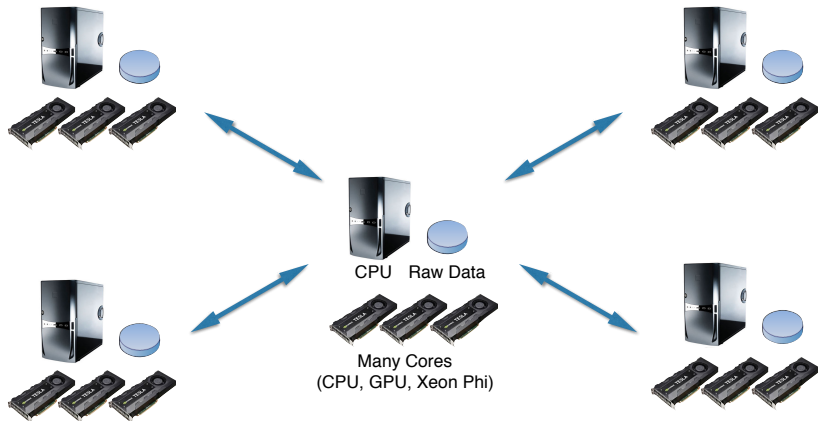
# Highly distributed and parallelised algorithms



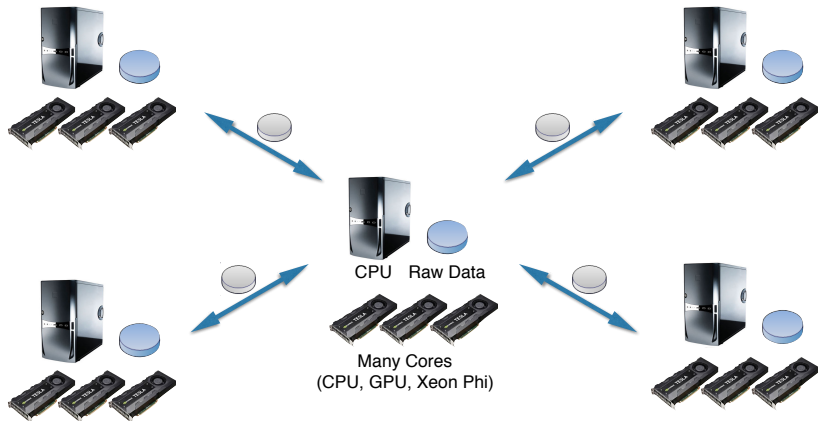
# Highly distributed and parallelised algorithms



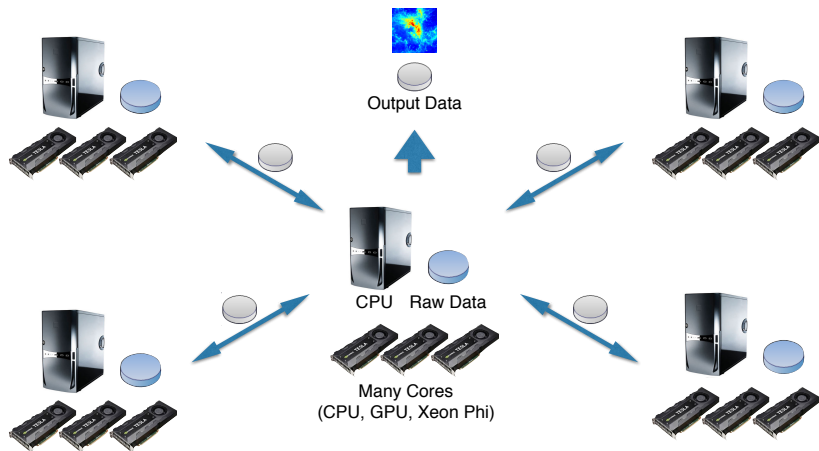
## Highly distributed and parallelised algorithms



## Highly distributed and parallelised algorithms



## Highly distributed and parallelised algorithms



# Extra Slides

PURIFY reconstructions

# PURIFY reconstruction

## VLA observation of 3C129

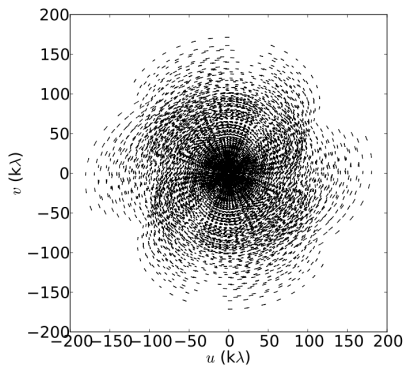


Figure: VLA visibility coverage for 3C129



## PURIFY reconstruction

VLA observation of 3C129

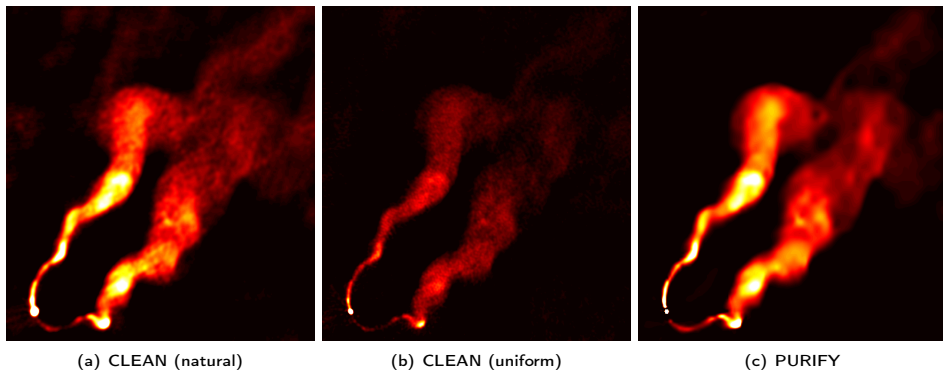
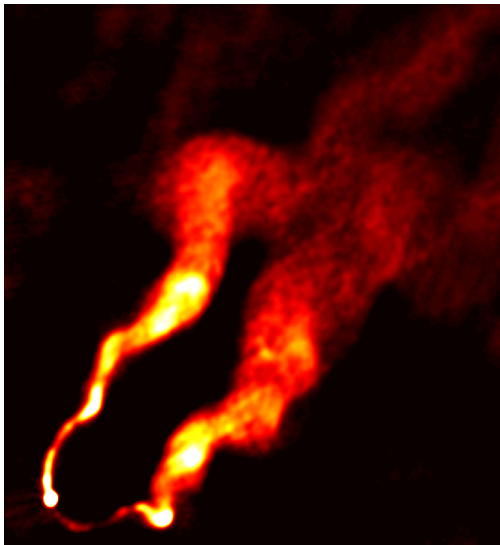


Figure: 3C129 recovered images (Pratley, McEwen, et al. 2016)

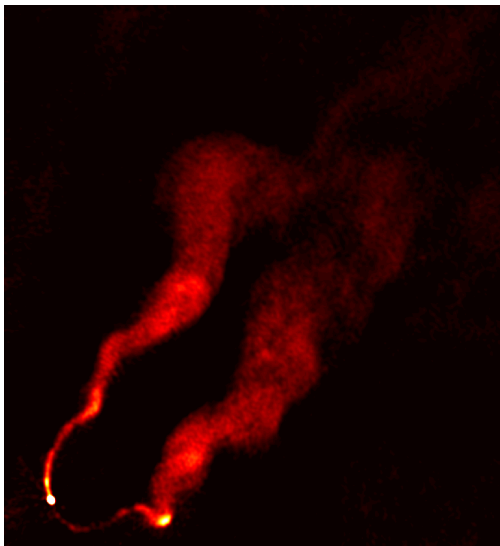
# PURIFY reconstruction

VLA observation of 3C129 imaged by CLEAN (natural)



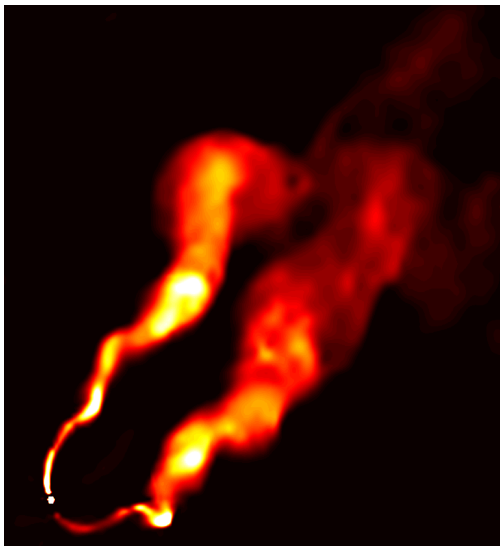
# PURIFY reconstruction

VLA observation of 3C129 images by CLEAN (uniform)



# PURIFY reconstruction

VLA observation of 3C129 images by PURIFY



# PURIFY reconstruction

## VLA observation of 3C129

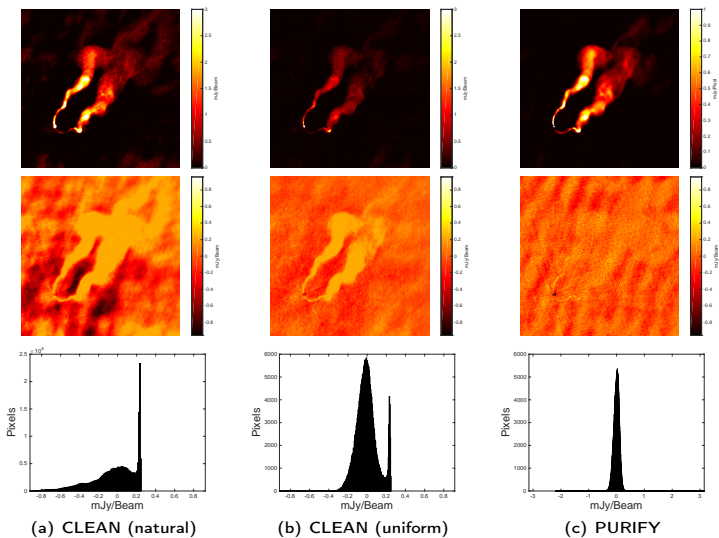


Figure: 3C129 recovered images and residuals (Pratley, McEwen, *et al.* 2016)

# PURIFY reconstruction

## VLA observation of Cygnus A

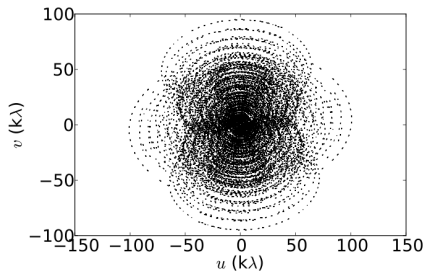


Figure: VLA visibility coverage for Cygnus A

# PURIFY reconstruction

## VLA observation of Cygnus A

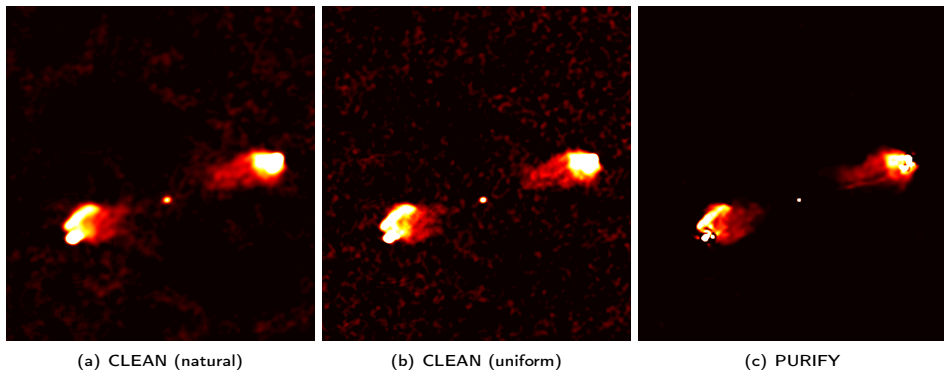
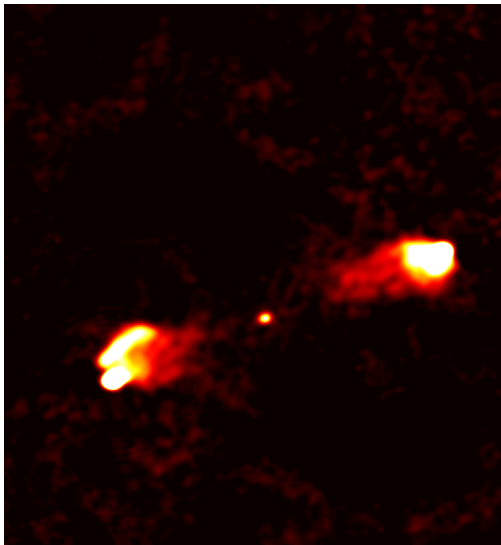


Figure: Cygnus A recovered images (Pratley, McEwen, *et al.* 2016)

# PURIFY reconstruction

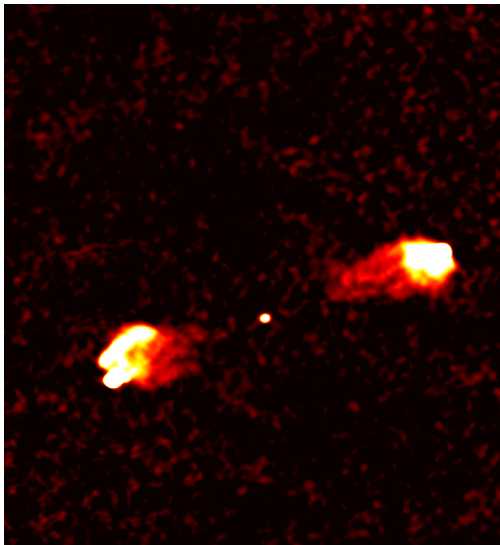
VLA observation of Cygnus A imaged by CLEAN (natural)





# PURIFY reconstruction

VLA observation of Cygnus A images by CLEAN (uniform)



# PURIFY reconstruction

VLA observation of Cygnus A images by PURIFY



# PURIFY reconstruction

## VLA observation of Cygnus A

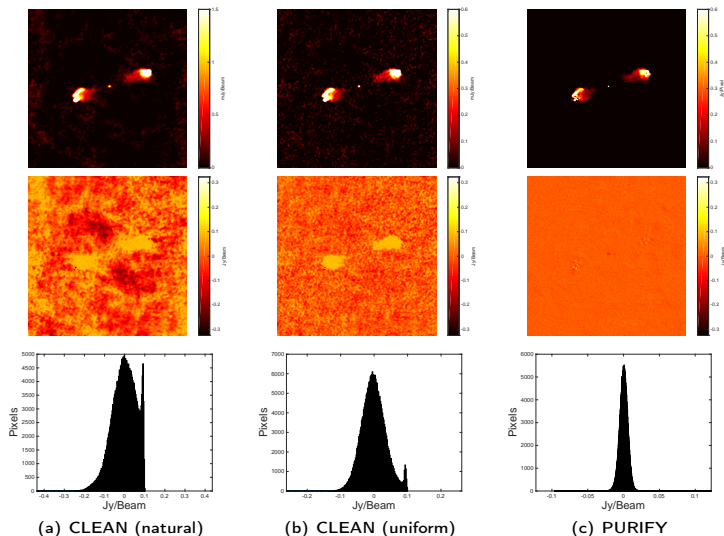


Figure: Cygnus A recovered images and residuals (Pratley, McEwen, *et al.* 2016)

## PURIFY reconstruction

ATCA observation of PKS J0334-39

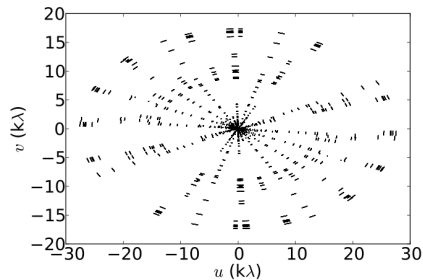


Figure: VLA visibility coverage for PKS J0334-39

## PURIFY reconstruction

ATCA observation of PKS J0334-39

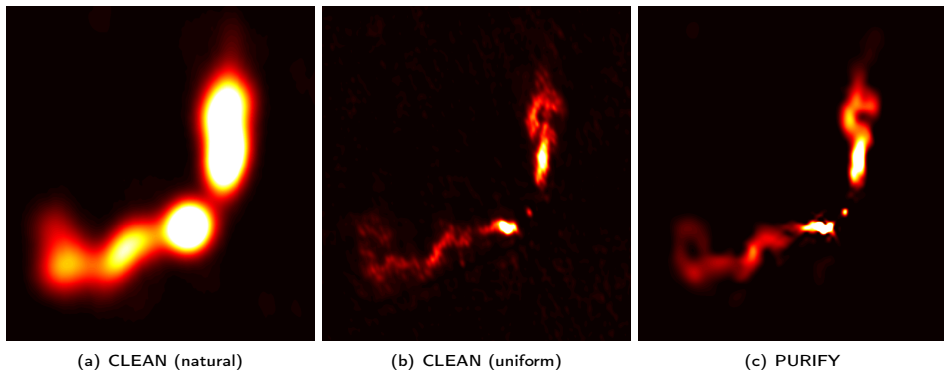
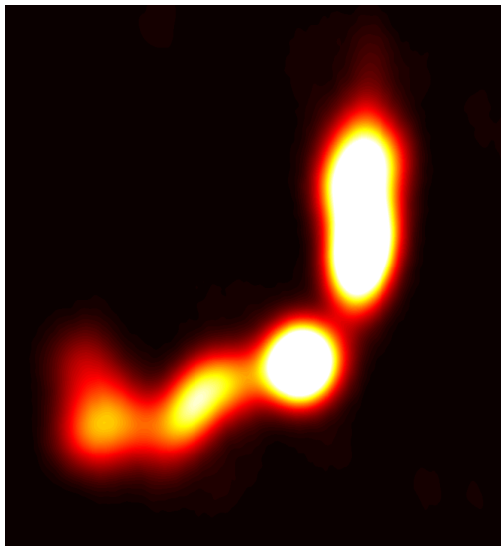


Figure: PKS J0334-39 recovered images (Pratley, McEwen, et al. 2016)

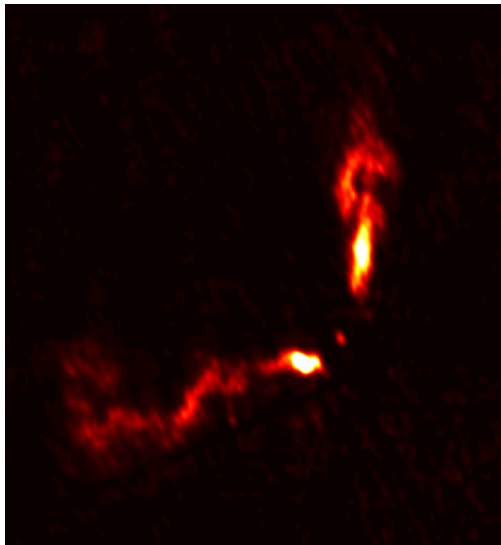
# PURIFY reconstruction

VLA observation of PKS J0334-39 imaged by CLEAN (natural)



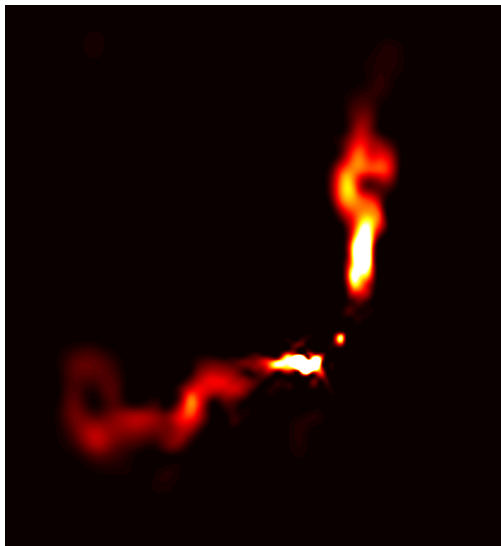
# PURIFY reconstruction

VLA observation of PKS J0334-39 images by CLEAN (uniform)



# PURIFY reconstruction

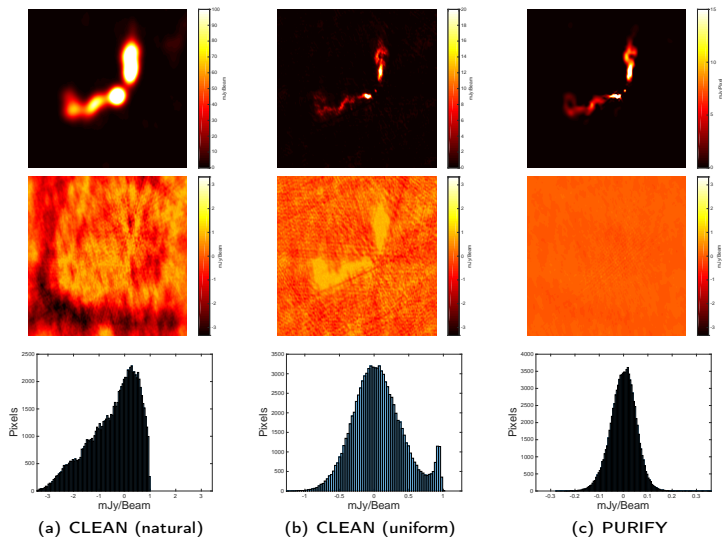
VLA observation of PKS J0334-39 images by PURIFY





## PURIFY reconstruction

ATCA observation of PKS J0334-39

Figure: PKS J0334-39 recovered images and residuals (Pratley, McEwen, *et al.* 2016)

# PURIFY reconstruction

ATCA observation of PKS J0116-473

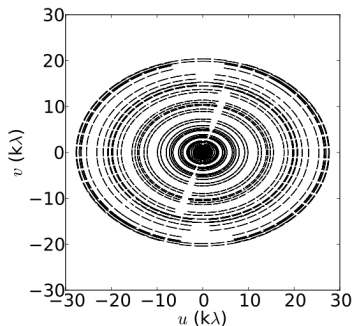


Figure: ATCA visibility coverage for Cygnus A

## PURIFY reconstruction

ATCA observation of PKS J0116-473

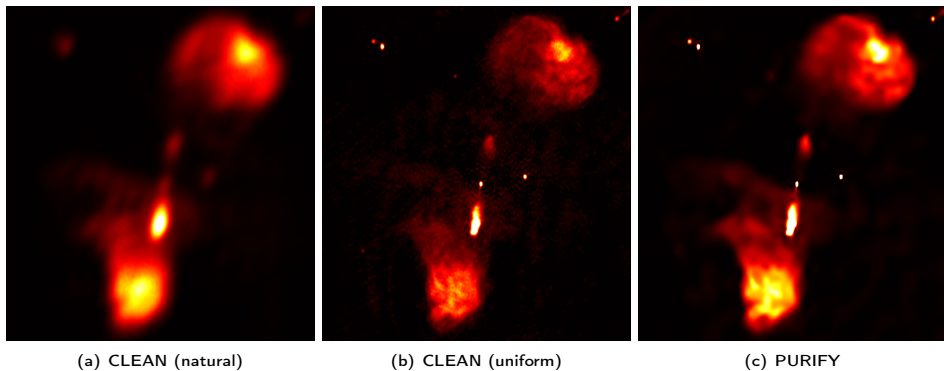
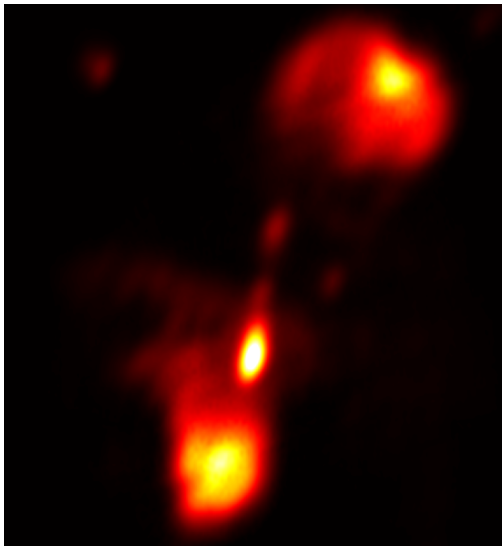


Figure: PKS J0116-473 recovered images (Pratley, McEwen, *et al.* 2016)

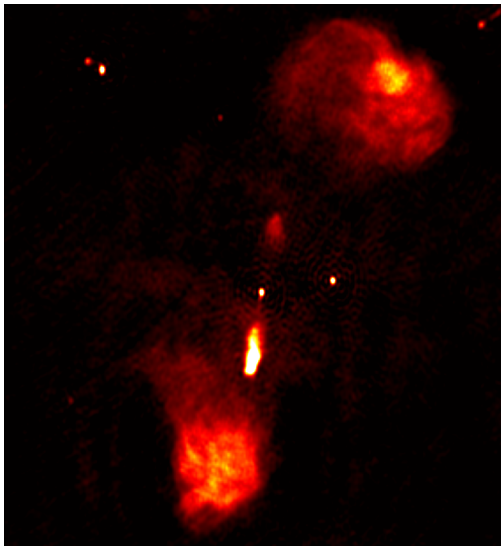
# PURIFY reconstruction

VLA observation of PKS J0116-473 imaged by CLEAN (natural)



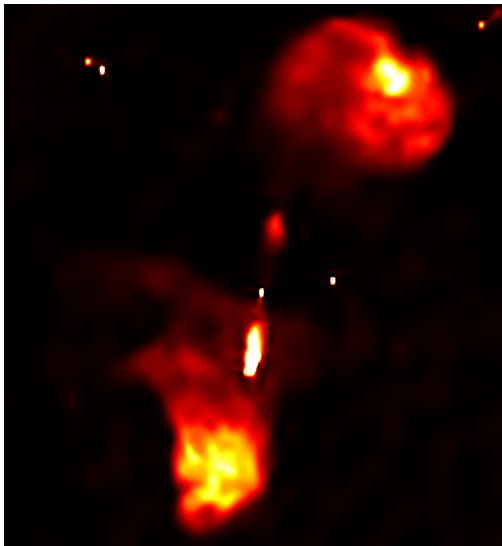
# PURIFY reconstruction

VLA observation of PKS J0116-473 images by CLEAN (uniform)



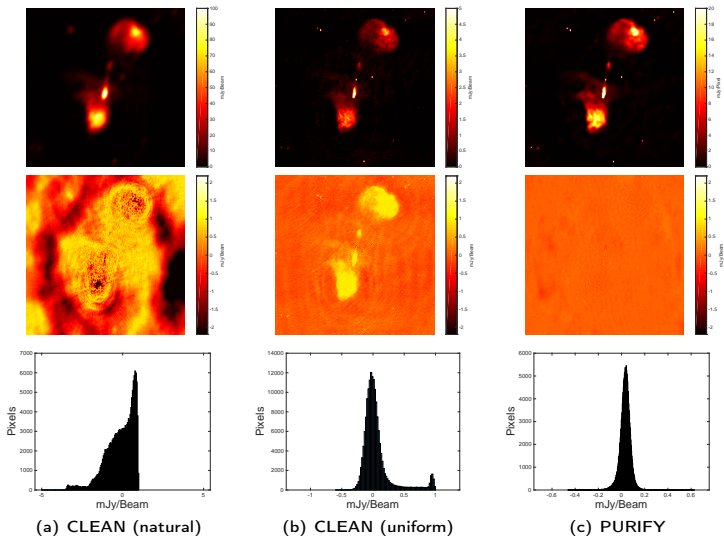
# PURIFY reconstruction

VLA observation of PKS J0116-473 images by PURIFY



## PURIFY reconstruction

ATCA observation of PKS J0116-473

Figure: PKS J0116-473 recovered images and residuals (Pratley, McEwen, *et al.* 2016)

## PURIFY reconstructions

Table: Root-mean-square of residuals of each reconstruction (units in mJy/Beam)

Observation	PURIFY	CLEAN (natural)	CLEAN (uniform)
3C129	0.10	0.23	0.11
Cygnus A	6.1	59	36
PKS J0334-39	0.052	1.00	0.37
PKS J0116-473	0.054	0.88	0.24



# Extra Slides

## Proximal MCMC

# Proximity operators

## A brief aside

- Define **proximity operator**:

$$\text{prox}_g^\lambda(\mathbf{x}) = \arg \min_{\mathbf{u}} \left[ g(\mathbf{u}) + \|\mathbf{u} - \mathbf{x}\|^2 / 2\lambda \right]$$

- Generalisation of **projection operator**:

$$\mathcal{P}_{\mathcal{C}}(\mathbf{x}) = \arg \min_{\mathbf{u}} \left[ \iota_{\mathcal{C}}(\mathbf{u}) + \|\mathbf{u} - \mathbf{x}\|^2 / 2 \right],$$

where  $\iota_{\mathcal{C}}(\mathbf{u}) = \infty$  if  $\mathbf{u} \notin \mathcal{C}$  and zero otherwise.

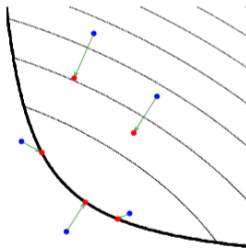


Figure: Illustration of proximity operator [Credit: Parikh & Boyd (2013)]

## Proximal MCMC methods

- Exploit proximal calculus.
- “Replace gradients with sub-gradients”.

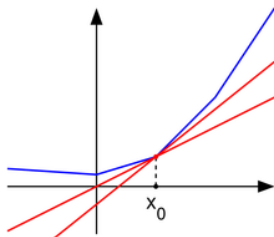


Figure: Illustration of sub-gradients [Credit: Wikipedia (Maksim)]

# Proximal MALA

## Moreau approximation

- Moreau approximation of  $f(\mathbf{x}) \propto \exp(-g(\mathbf{x}))$ :

$$f_{\lambda}^{\text{MA}}(\mathbf{x}) = \sup_{\mathbf{u} \in \mathbb{R}^N} f(\mathbf{u}) \exp\left(-\frac{\|\mathbf{u} - \mathbf{x}\|^2}{2\lambda}\right)$$

- Important properties of  $f_{\lambda}^{\text{MA}}(\mathbf{x})$ :

- As  $\lambda \rightarrow 0$ ,  $f_{\lambda}^{\text{MA}}(\mathbf{x}) \rightarrow f(\mathbf{x})$
- $\nabla \log f_{\lambda}^{\text{MA}}(\mathbf{x}) = (\text{prox}_{\lambda}^g(\mathbf{x}) - \mathbf{x})/\lambda$

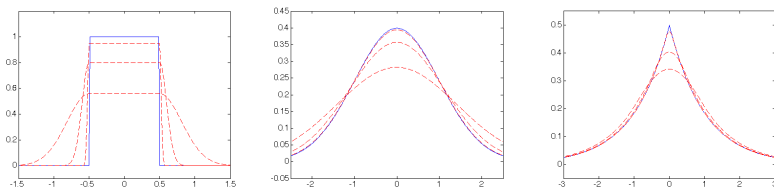


Figure: Illustration of Moreau approximations [Credit: Pereyra 2016a]

# Proximal MALA

## Computing proximity operators for the analysis case

- Recall posterior:  $\pi(\mathbf{x}) \propto \exp(-g(\mathbf{x}))$ .

- Let  $\bar{g}(\mathbf{x}) = \bar{f}_1(\mathbf{x}) + \bar{f}_2(\mathbf{x})$ , where  $\bar{f}_1(\mathbf{x}) = \mu \|\Psi^\dagger \mathbf{x}\|_1$  and  $\bar{f}_2(\mathbf{x}) = \|\mathbf{y} - \Phi \mathbf{x}\|_2^2 / 2\sigma^2$ .  
Prior Likelihood

- Must solve an optimisation problem for each iteration!

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) = \underset{\mathbf{u} \in \mathbb{R}^N}{\text{argmin}} \left\{ \mu \|\Psi^\dagger \mathbf{u}\|_1 + \frac{\|\mathbf{y} - \Phi \mathbf{u}\|_2^2}{2\sigma^2} + \frac{\|\mathbf{u} - \mathbf{x}\|_2^2}{\delta} \right\}.$$

- Taylor expansion at point  $\mathbf{x}$ :  $\|\mathbf{y} - \Phi \mathbf{u}\|_2^2 \approx \|\mathbf{y} - \Phi \mathbf{x}\|_2^2 + 2(\mathbf{u} - \mathbf{x})^\top \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y})$ .
- Then proximity operator approximated by

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) \approx \text{prox}_{\bar{f}_1}^{\delta/2} \left( \mathbf{x} - \delta \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y}) / 2\sigma^2 \right).$$

Single forward-backward iteration

- Analytic approximation:

$$\text{prox}_{\bar{g}}^{\delta/2}(\mathbf{x}) \approx \bar{\mathbf{v}} + \Psi \left( \text{soft}_{\mu\delta/2}(\Psi^\dagger \bar{\mathbf{v}}) - \Psi^\dagger \bar{\mathbf{v}} \right), \text{ where } \bar{\mathbf{v}} = \mathbf{x} - \delta \Phi^\dagger (\Phi \mathbf{x} - \mathbf{y}) / 2\sigma^2.$$

# Proximal MALA

## Computing proximity operators for the synthesis case

- Recall posterior:  $\pi(\mathbf{x}) \propto \exp(-g(\mathbf{x}))$ .
- Let  $\hat{g}(\mathbf{x}(\mathbf{a})) = \hat{f}_1(\mathbf{a}) + \hat{f}_2(\mathbf{a})$ , where  $\hat{f}_1(\mathbf{a}) = \mu \|\mathbf{a}\|_1$  and  $\hat{f}_2(\mathbf{a}) = \|\mathbf{y} - \Phi\Psi\mathbf{a}\|_2^2/2\sigma^2$ .  
 Prior Likelihood
- Must solve an optimisation problem for each iteration!

$$\text{prox}_{\hat{g}}^{\delta/2}(\mathbf{a}) = \underset{\mathbf{u} \in \mathbb{R}^L}{\text{argmin}} \left\{ \mu \|\mathbf{u}\|_1 + \frac{\|\mathbf{y} - \Phi\Psi\mathbf{u}\|_2^2}{2\sigma^2} + \frac{\|\mathbf{u} - \mathbf{a}\|_2^2}{\delta} \right\}.$$

- Taylor expansion at point  $\mathbf{a}$ :  $\|\mathbf{y} - \Phi\Psi\mathbf{u}\|_2^2 \approx \|\mathbf{y} - \Phi\Psi\mathbf{a}\|_2^2 + 2(\mathbf{u} - \mathbf{a})^\top \Psi^\dagger \Phi^\dagger (\Phi\Psi\mathbf{a} - \mathbf{y})$ .
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## MYULA

## Moreau-Yosida approximation

- Moreau-Yosida approximation (Moreau envelope) of  $f$ :

$$f_{\lambda}^{\text{MY}}(\mathbf{x}) = \inf_{\mathbf{u} \in \mathbb{R}^N} f(\mathbf{u}) + \frac{\|\mathbf{u} - \mathbf{x}\|^2}{2\lambda}$$

- Important properties of  $f_{\lambda}^{\text{MY}}(\mathbf{x})$ :

- 1 As  $\lambda \rightarrow 0$ ,  $f_{\lambda}^{\text{MY}}(\mathbf{x}) \rightarrow f(\mathbf{x})$
- 2  $\nabla f_{\lambda}^{\text{MY}}(\mathbf{x}) = (\mathbf{x} - \text{prox}_{f}^{\lambda}(\mathbf{x}))/\lambda$

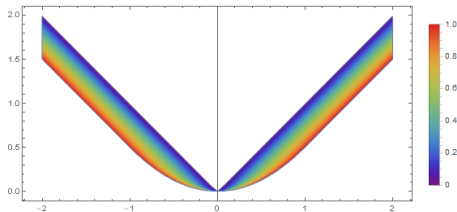


Figure: Illustration of Moreau-Yosida envelope of  $|x|$  for varying  $\lambda$  [Credit: Stack exchange (ubpdqn)]

## MYULA

## Computing proximity operators for the analysis case

- Recall posterior:  $\pi(\mathbf{x}) \propto \exp(-g(\mathbf{x}))$ .
- Let  $\bar{g}(\mathbf{x}) = \bar{f}_1(\mathbf{x}) + \bar{f}_2(\mathbf{x})$ , where  $\bar{f}_1(\mathbf{x}) = \mu \|\Psi^\dagger \mathbf{x}\|_1$  and  $\bar{f}_2(\mathbf{x}) = \|\mathbf{y} - \Phi \mathbf{x}\|_2^2 / 2\sigma^2$ .  

Prior
Likelihood
- Only need to compute proximity operator of  $f_1$ , which can be **computed analytically without any approximation**:

$$\text{prox}_{\bar{f}_1}^{\delta/2}(\mathbf{x}) = \mathbf{x} + \Psi \left( \text{soft}_{\mu\delta/2}(\Psi^\dagger \mathbf{x}) - \Psi^\dagger \mathbf{x} \right).$$



## MYULA

## Computing proximity operators for the synthesis case

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# Extra Slides

## Hypothesis testing

# Hypothesis testing

## Method

- Is structure in an image **physical or an artifact**?
- Perform **hypothesis tests** using Bayesian credible regions (Pereyra 2016b).
- Let  $C_\alpha$  denote the **highest posterior density (HPD) Bayesian credible region** with confidence level  $(1 - \alpha)\%$  defined by posterior isosurface:  $C_\alpha = \{\mathbf{x} : g(\mathbf{x}) \leq \gamma_\alpha\}$ .

### Hypothesis testing of physical structure

- 1 Cut out region containing structure of interest from recovered image  $\mathbf{x}^*$ .
- 2 Inpaint background (noise) into region, yielding surrogate image  $\mathbf{x}'$ .
- 3 Test whether  $\mathbf{x}' \in C_\alpha$ :
  - If  $\mathbf{x}' \notin C_\alpha$  then reject hypothesis that structure is an artifact with confidence  $(1 - \alpha)\%$ , *i.e.* **structure most likely physical**.
  - If  $\mathbf{x}' \in C_\alpha$  uncertainly too high to draw strong conclusions about the physical nature of the structure.

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## Method

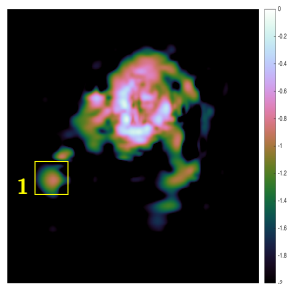
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# Hypothesis testing

## Numerical experiments

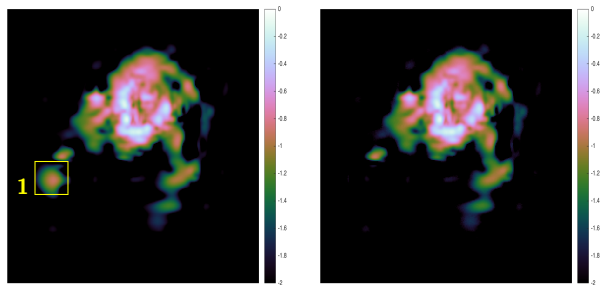


(a) Recovered image

Figure: HII region of M31

# Hypothesis testing

## Numerical experiments



(a) Recovered image

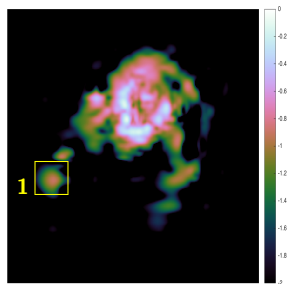
(b) Surrogate with region removed

Figure: HII region of M31

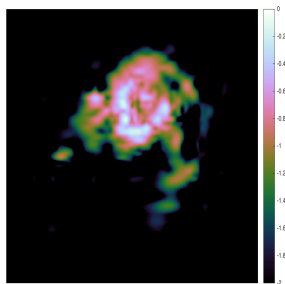


# Hypothesis testing

## Numerical experiments



(a) Recovered image



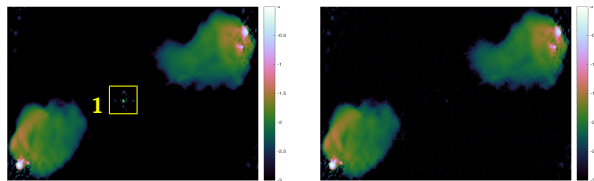
(b) Surrogate with region removed

1. Reject null hypothesis  
⇒ structure physical

Figure: HII region of M31

# Hypothesis testing

## Numerical experiments



(a) Recovered image

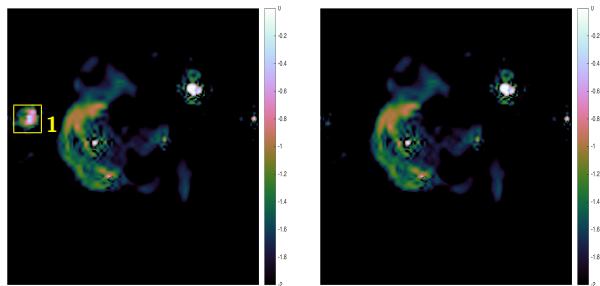
(b) Surrogate with region removed

Figure: Cygnus A

1. Cannot reject null hypothesis  
 $\Rightarrow$  cannot make strong statistical statement about origin of structure

# Hypothesis testing

## Numerical experiments



(a) Recovered image

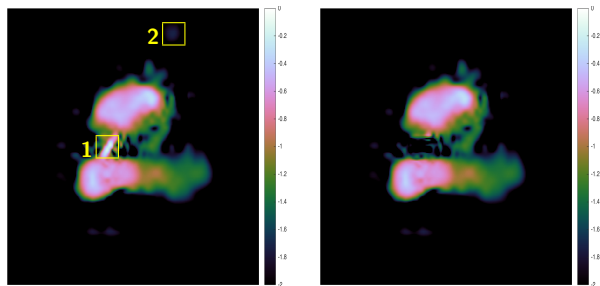
(b) Surrogate with region removed

1. Reject null hypothesis  
 $\Rightarrow$  structure physical

Figure: Supernova remnant W28

# Hypothesis testing

## Numerical experiments



(a) Recovered image

(b) Surrogate with region removed

Figure: 3C288

1. Reject null hypothesis  
 $\Rightarrow$  structure physical
  
2. Cannot reject null hypothesis  
 $\Rightarrow$  cannot make strong statistical statement about origin of structure

# Hypothesis testing

## Comparison of numerical experiments

Table: Comparison of hypothesis tests for different methods for the analysis model.

Image	Test area	Ground truth	Method	Hypothesis test
M31	1	✓	P-MALA	✓
			MYULA	✓
			MAP	✓
Cygnus A	1	✓	P-MALA	✗
			MYULA*	✗
			MAP	✗
W28	1	✓	P-MALA	✓
			MYULA	✓
			MAP	✓
3C288	1	✓	P-MALA	✓
			MYULA	✓
			MAP	✓
	2	✗	P-MALA	✗
			MYULA	✗
			MAP	✗

(\* Can correctly detect physical structure if use median point estimator.)