Sampling versus optimization in very high dimensional parameter spaces

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Collaborators

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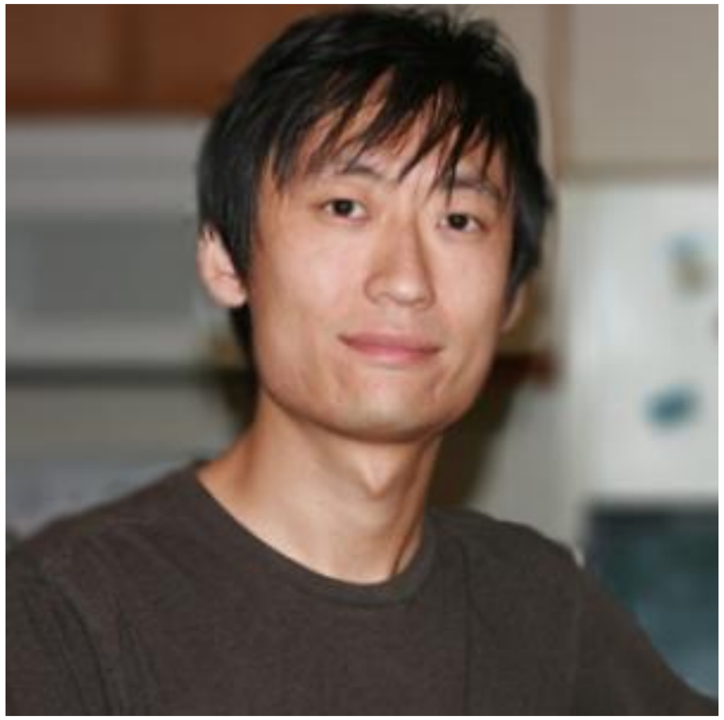

Yu Feng

Chirag Modi

Sampling: Hamiltonian Monte Carlo (HMC)

- Each parameter becomes a “particle” position. Momentum variables are introduced. Particles follow Hamiltonian dynamics. U = -ln(posterior).

- Huge advantage over random walk: Information in the derivatives is used to walk “in the right direction”.

- Acceptance rate = 1 **theoretically**.

- For each iteration need to integrate equations of motion numerically using staggered leapfrog (or similar) methods. Typically ~10 numerical integration steps are taken per iteration.

- Method of choice for sampling high dimensional parameter spaces.

- **Tuning**: masses, integration steps, integration time.

Optimization: BFGS

Quasi-Newton method.

Needs the first, but not second derivatives.

At each iteration the inverse Hessian is estimated from previous iterations (never stored explicitly). A direction of move is deduced, followed by line search.

Line search: Moré-Theunte 1992

L-BFGS: Limited memory BFGS. Store and use only a few previous iterations. Works almost as well as BFGS!

Linear Model

data → $\mathbf{d} = \mathbf{R}\mathbf{s} + \mathbf{n}$ (↑ signal, ↖ noise)

$$\mathbf{S} = \left\langle \mathbf{s}\mathbf{s}^\dagger \right\rangle \quad \mathbf{N} = \left\langle \mathbf{n}\mathbf{n}^\dagger \right\rangle$$

$$\mathbf{C} \equiv \left\langle \mathbf{d}\mathbf{d}^\dagger \right\rangle = \mathbf{R}\mathbf{S}\mathbf{R}^\dagger + \mathbf{N}$$

Binning: $\mathbf{S}_l = \{s_{m_l}\} \ (m_l = 1, \ldots, M_l)$

$$\mathbf{Q}_l = \mathbf{R}\mathbf{\Pi}_l\mathbf{R}^\dagger$$

↑ projection matrix

$$\mathbf{R}\mathbf{S}\mathbf{R}^\dagger = \sum_l \Theta_l \mathbf{Q}_l$$

Likelihood: $\mathcal{L}(\mathbf{d}|\mathbf{\Theta}) = (2\pi)^{-N/2} \det(\mathbf{C})^{-1/2} \exp\left(-\frac{1}{2}\mathbf{d}^\dagger\mathbf{C}^{-1}\mathbf{d}\right)$

Minimum variance estimator (**Wiener Filter**): $\hat{\mathbf{s}} = \mathbf{S}\mathbf{R}^\dagger\mathbf{C}^{-1}\mathbf{d}$

For gaussian fields this is the same as the maximum probability estimator!

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Linear Model

Fisher matrix: $$F_{ll'} = -\left\langle \frac{\partial^2 \ln \mathcal{L}(\mathbf{d}|\boldsymbol{\Theta})}{\partial \Theta_l \partial \Theta_{l'}} \right\rangle_{\hat{\boldsymbol{\Theta}}}$$

The inverse is an estimate of the covariance matrix of the parameters:

$$\left\langle \hat{\boldsymbol{\Theta}} \hat{\boldsymbol{\Theta}}^\dagger \right\rangle - \left\langle \hat{\boldsymbol{\Theta}} \right\rangle \left\langle \hat{\boldsymbol{\Theta}}^\dagger \right\rangle = \mathbf{F}^{-1}$$

Calculation: $$F_{ll'} = \frac{1}{2} tr \left(\mathbf{Q}_l \mathbf{C}^{-1} \mathbf{Q}_{l'} \mathbf{C}^{-1} \right)$$

Window: $$W_{ll'} = \frac{F_{ll'}}{\sum_{l'} F_{ll'}}$$

Power spectrum quadratic estimator:

$$\hat{\Theta}_l = \frac{1}{2} \sum_{l'} F^{-1}_{ll'} \left[\mathbf{d}^\dagger \mathbf{C}^{-1} \mathbf{Q}_{l'} \mathbf{C}^{-1} \mathbf{d} - b_{l'} \right]$$

$$b_l = tr \left[\mathbf{N} \mathbf{C}^{-1} \mathbf{Q}_l \mathbf{C}^{-1} \right]$$

$$\left\langle \hat{\Theta}_l \right\rangle = \sum_{l'} W_{ll'} \Theta_{l'}$$

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Estimating Noise Bias and Fisher Matrix

Noise bias: simulate noise: $\mathbf{d}_n$ Pass through optimizer: $\hat{\mathbf{s}}_n$

$$b_l = \mathbf{\Pi}_l \mathbf{S}^{-1} \hat{\mathbf{s}}_n^\dagger \hat{\mathbf{s}}_n \mathbf{S}^{-1} \mathbf{\Pi}_l$$

Fisher matrix: simulate signal: $\mathbf{s}_s$ Pass through optimizer: $\hat{\mathbf{s}}_s$

For each bin l' simulate extra signal in that bin only: $\Delta \mathbf{s}_{l'}$

$\mathbf{s}_{l'} = \mathbf{s}_s + \Delta \mathbf{s}_{l'}$ Pass through optimizer: $\hat{\mathbf{s}}_{l'}$

$$F_{ll'} = \frac{K_{l'}}{2\Theta_l^2} \left\langle \frac{\sum_{k_l} |\Delta \hat{s}_l(k_l)|^2}{\sum_{k_{l'}} |\Delta s_{l'}(k_{l'})|^2} \right\rangle$$

with $\Delta \hat{\mathbf{s}}_{l'} = \hat{\mathbf{s}}_{l'} - \hat{\mathbf{s}}_s$

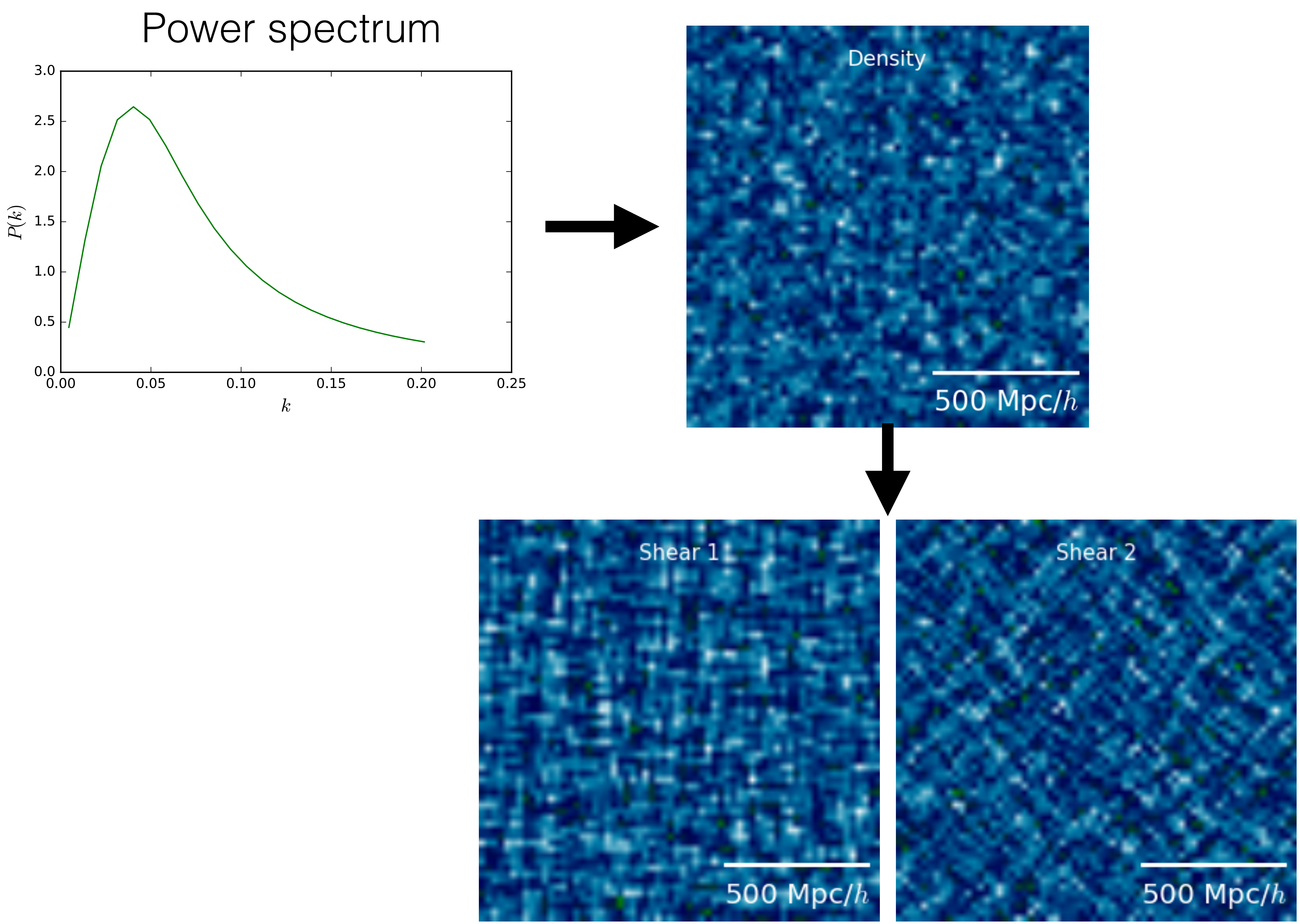
$K_{l'}$ is the number of modes

Power spectrum:

$$\hat{\Theta}_l = \sum_{k_l} \left(|\hat{s}(k_l)|^2 - \langle |\hat{s}_n(k_l)|^2 \rangle \right) \left\langle \frac{\sum_{l'} W_{ll'} K_{l'}^{-1} \sum_{k_{l'}} |s_s(k_{l'})|^2}{\sum_{k_l} |\hat{s}_s(k_l)|^2} \right\rangle$$

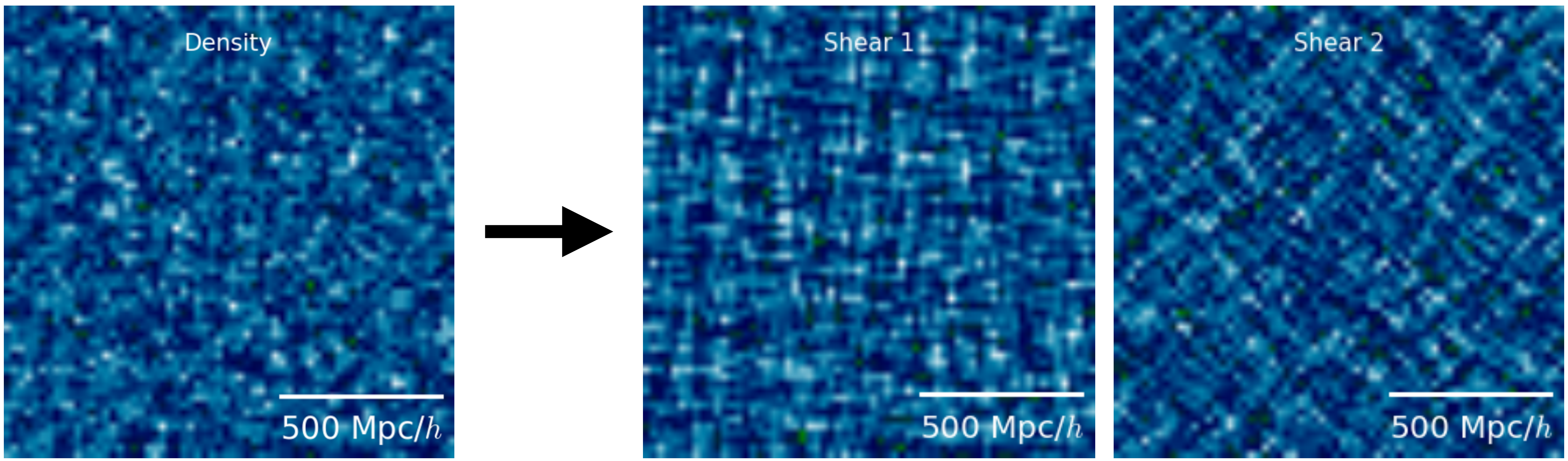
Linear case: Weak Lensing

Toy Example: 64x64 grid



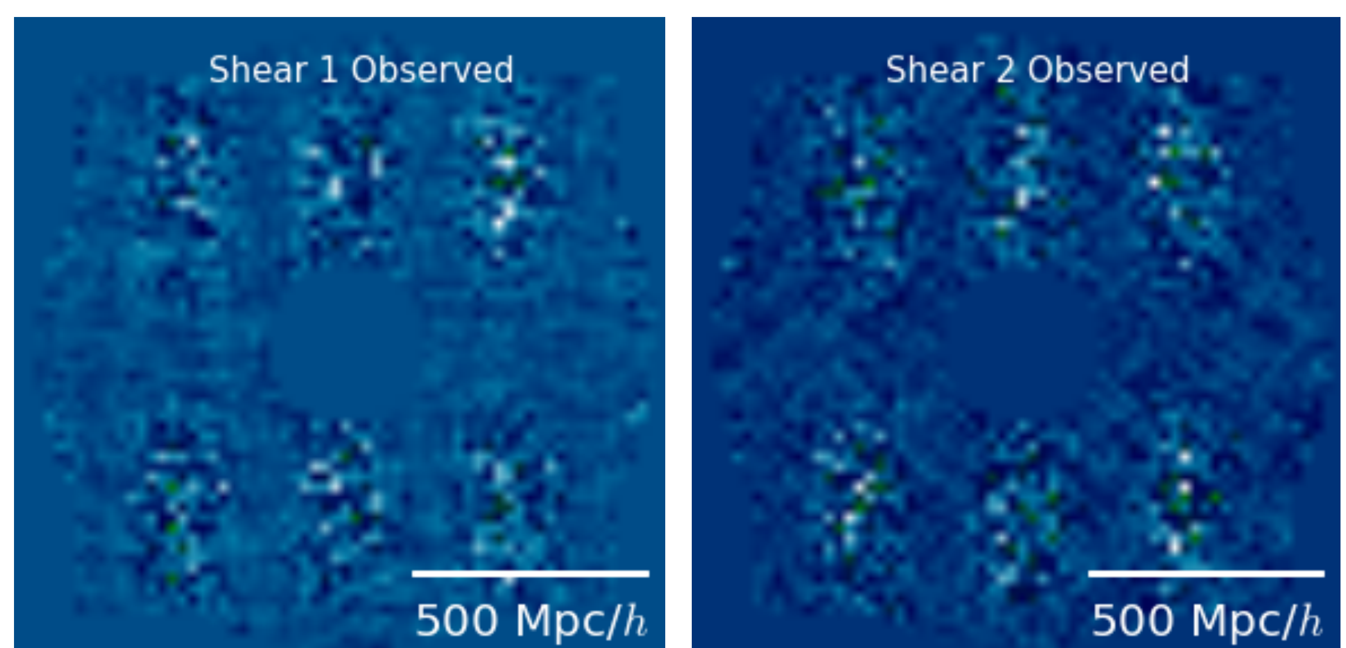
Linear case: Weak Lensing

Toy Example: 64x64 grid



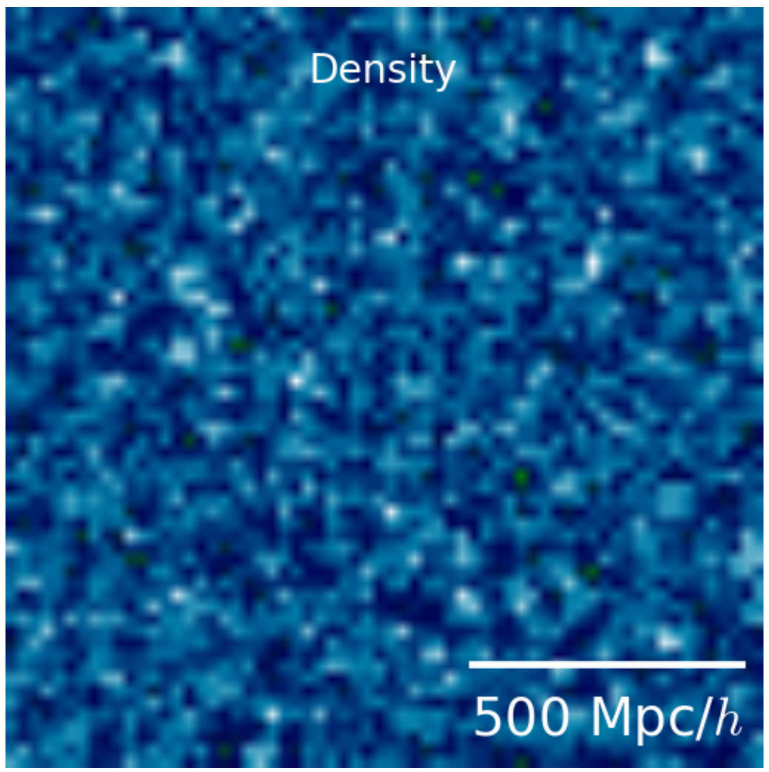
Add noise and mask

Observed data:

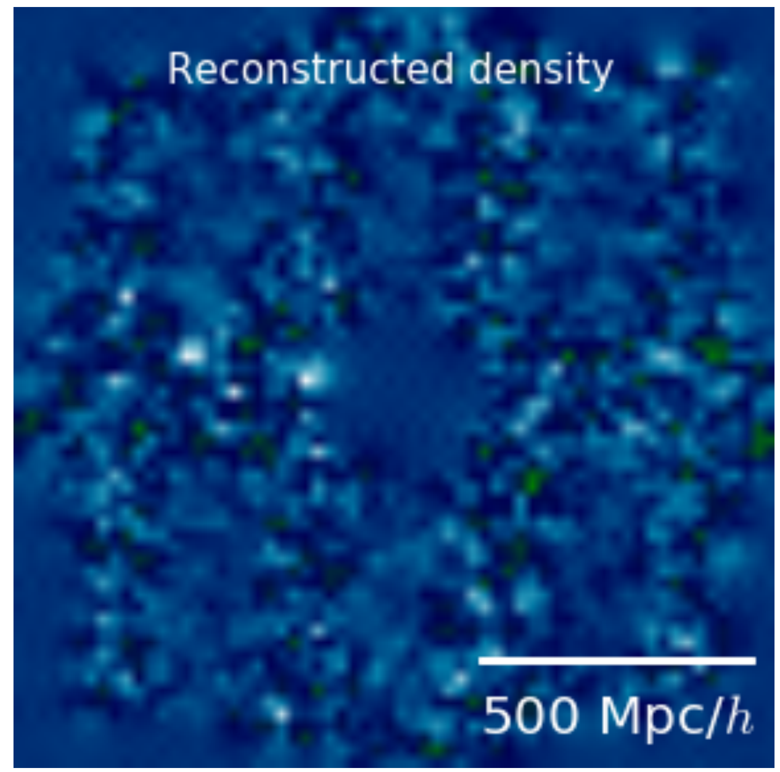


Results

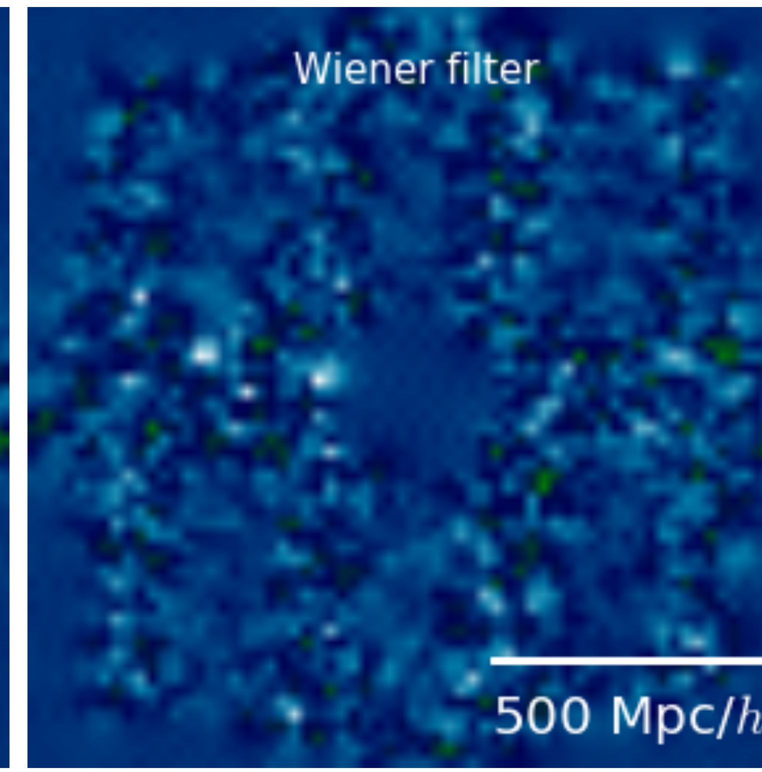
Original

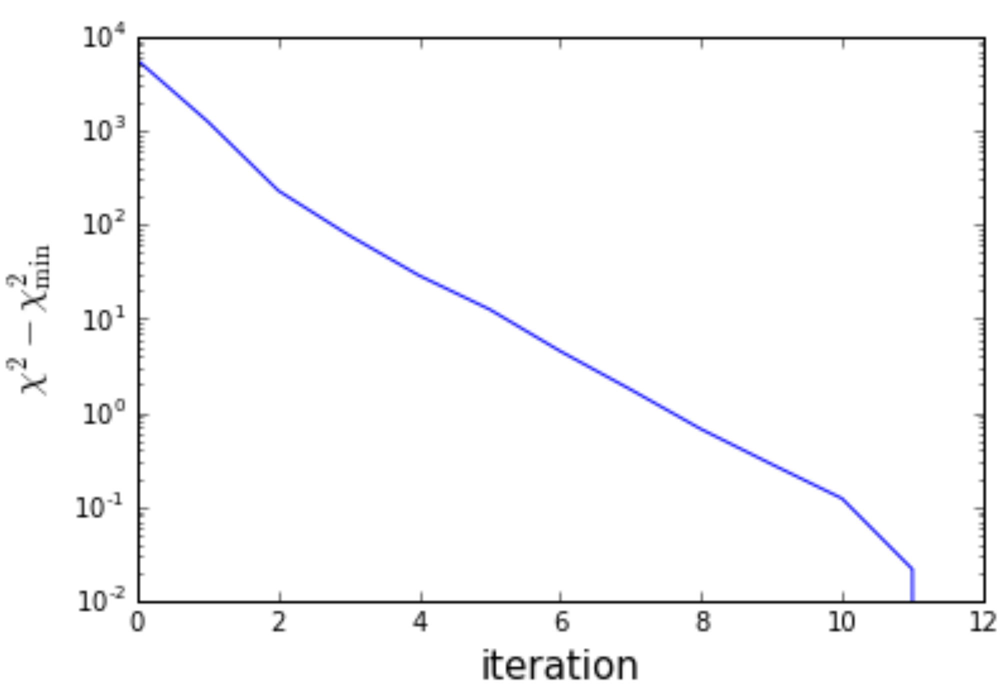


L-BFGS

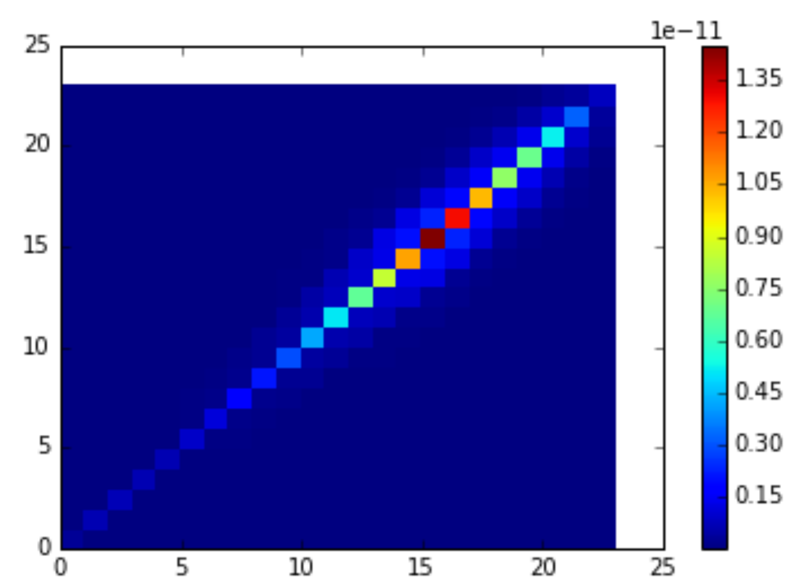


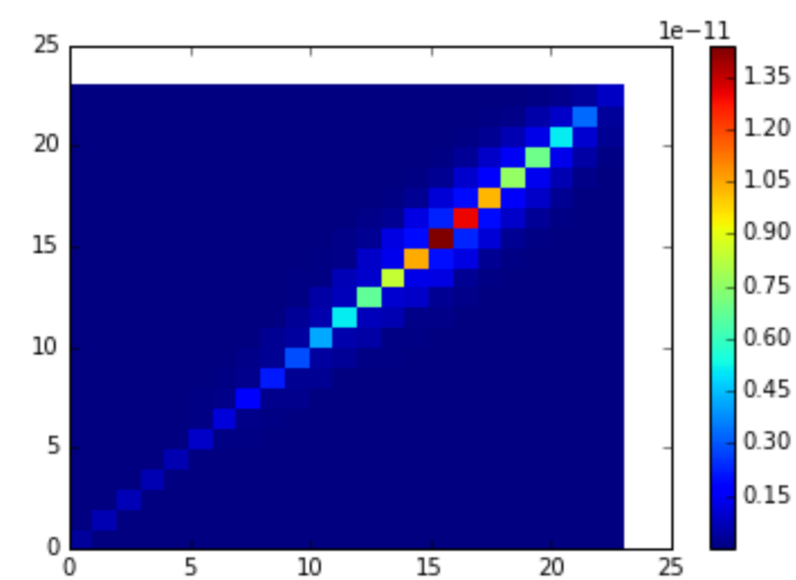
Linear Algebra





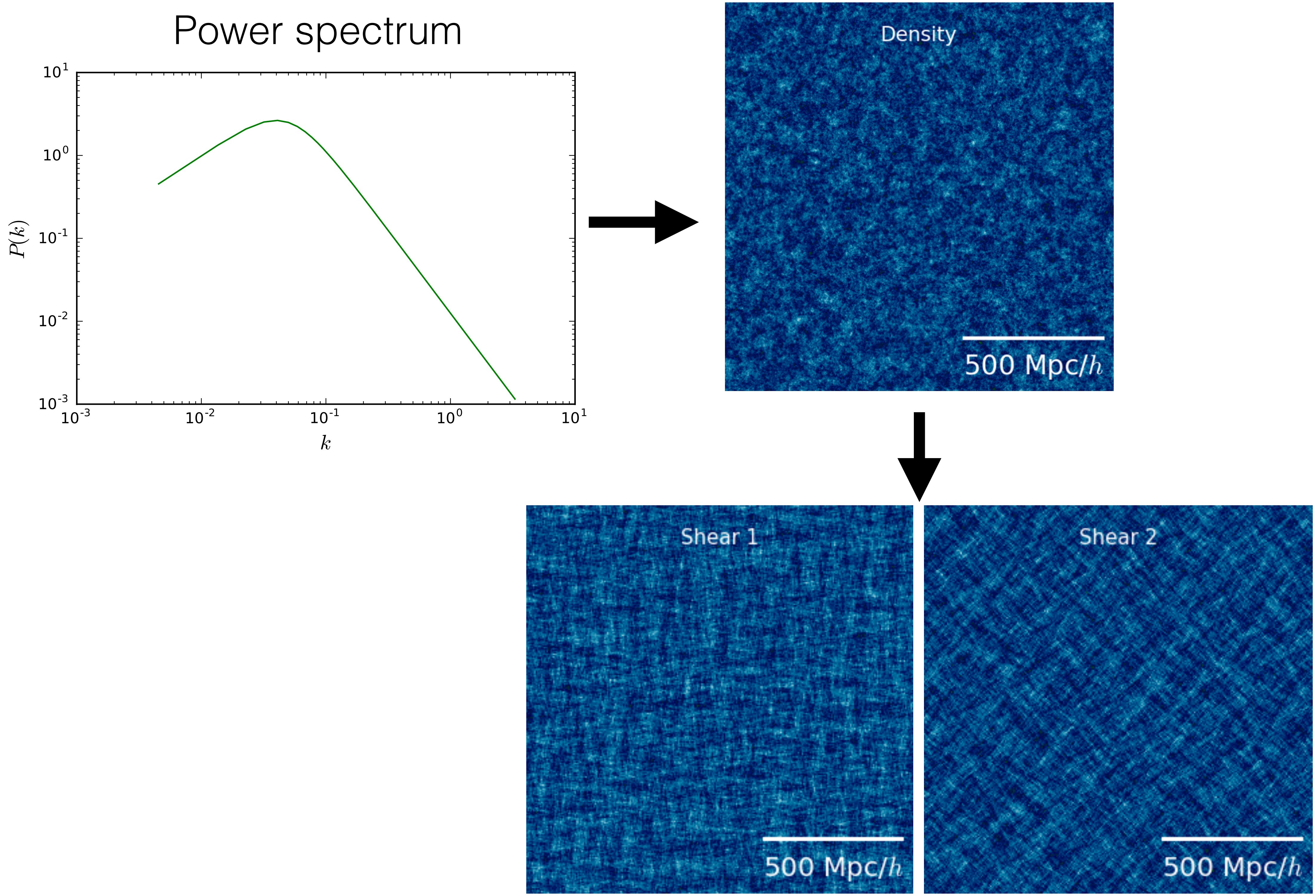
Fisher matrix:





Linear case: Weak Lensing

1024x1024 grid: ~million parameters



Linear case: Weak Lensing

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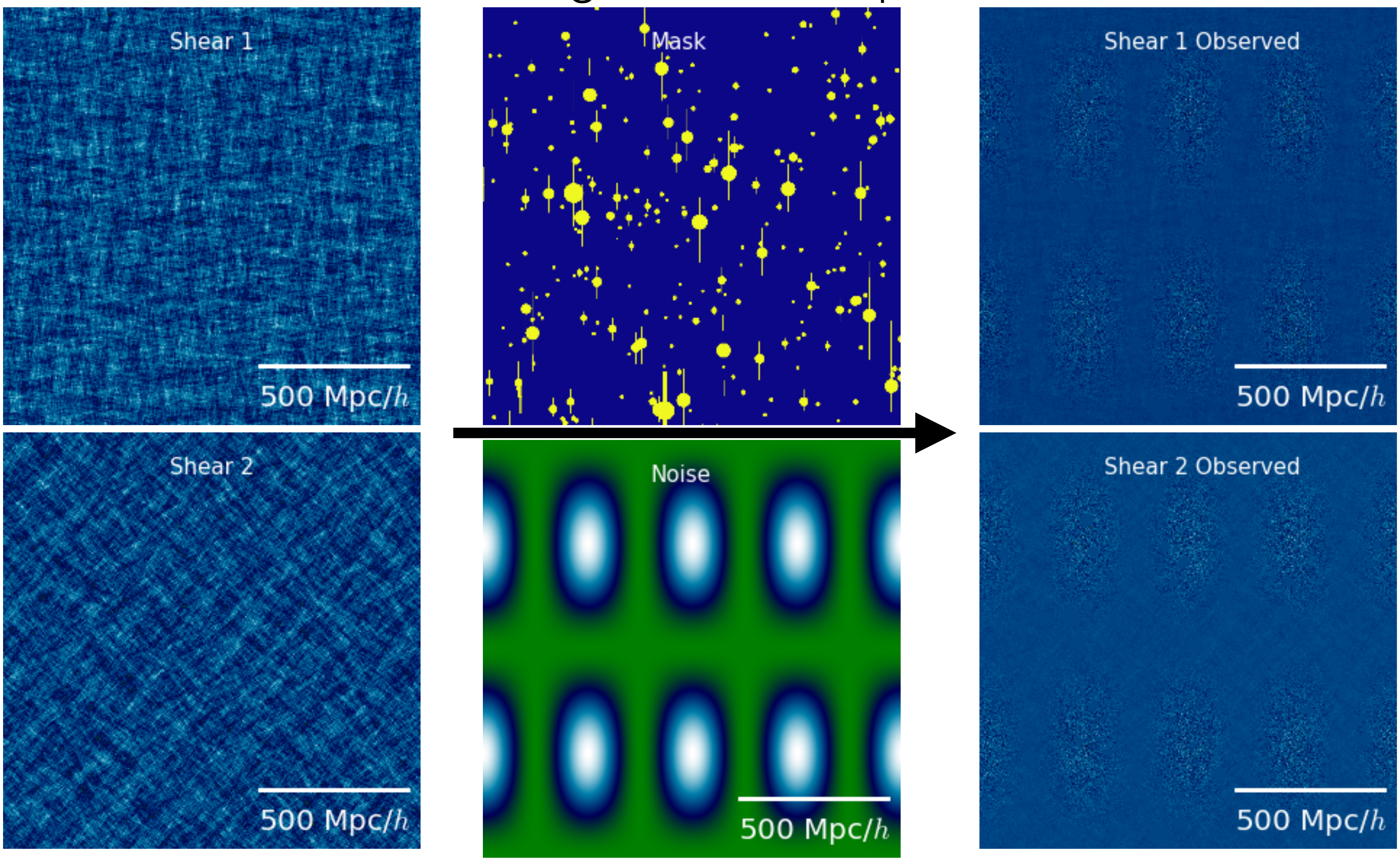
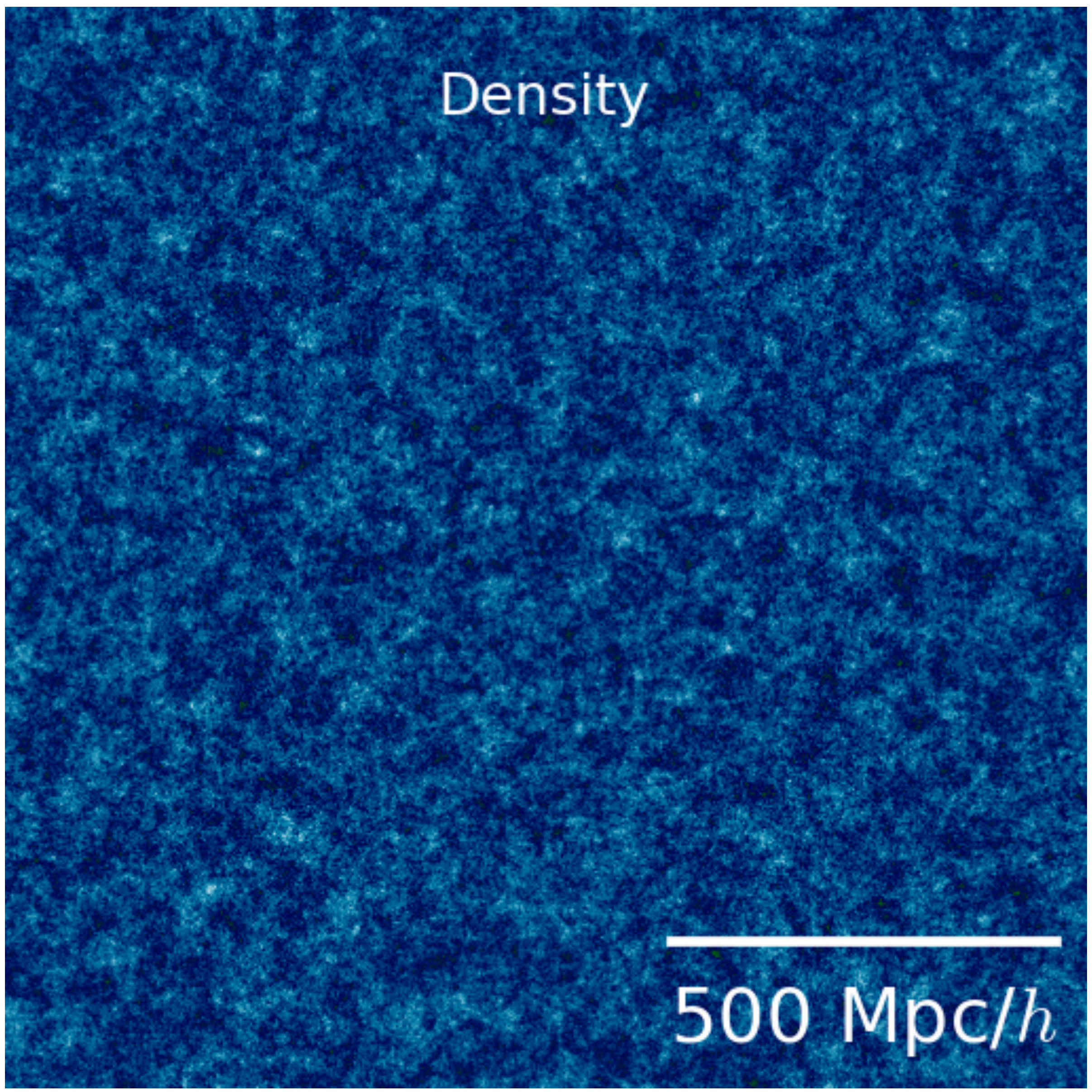
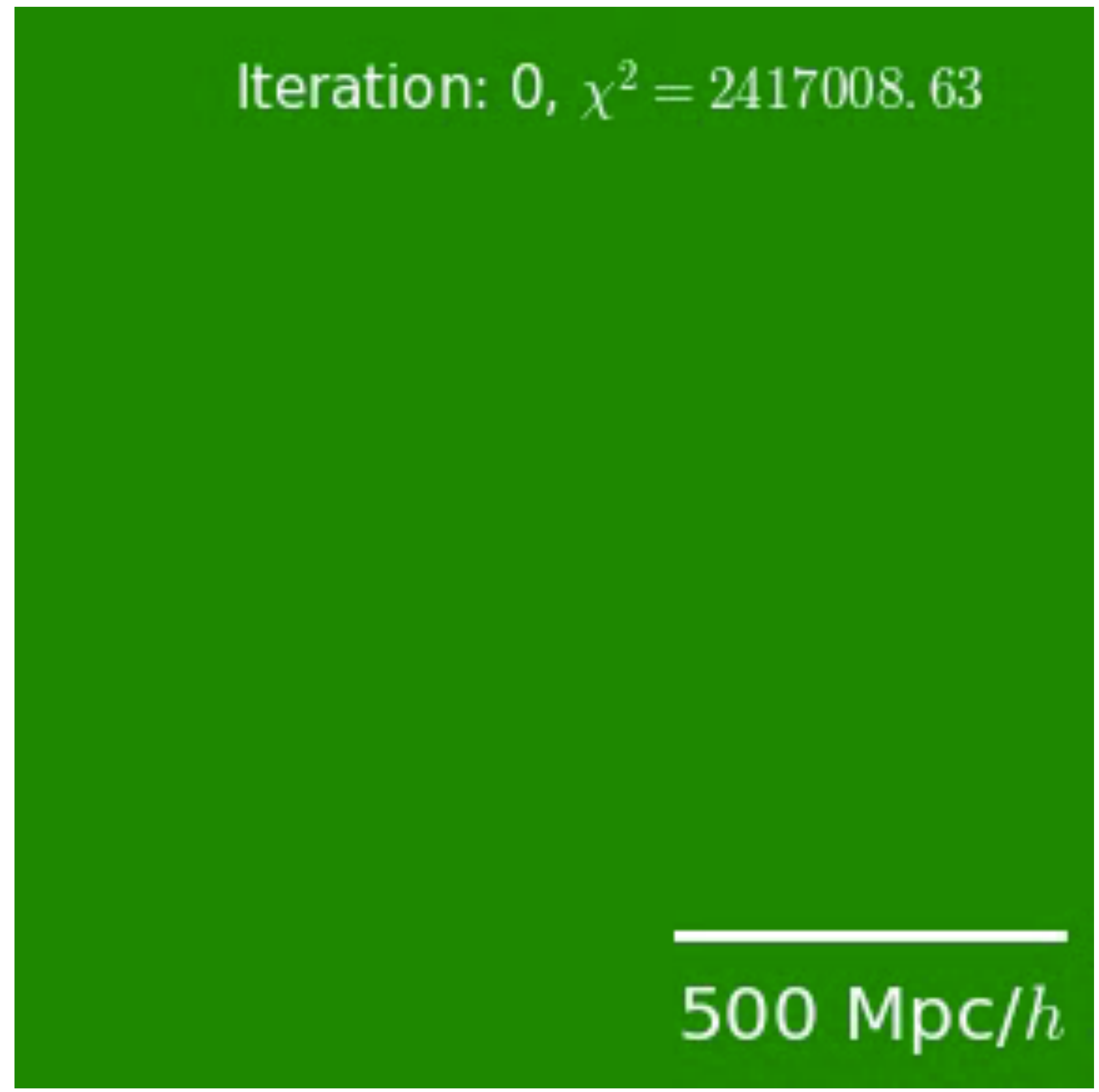


Reconstruction

Original

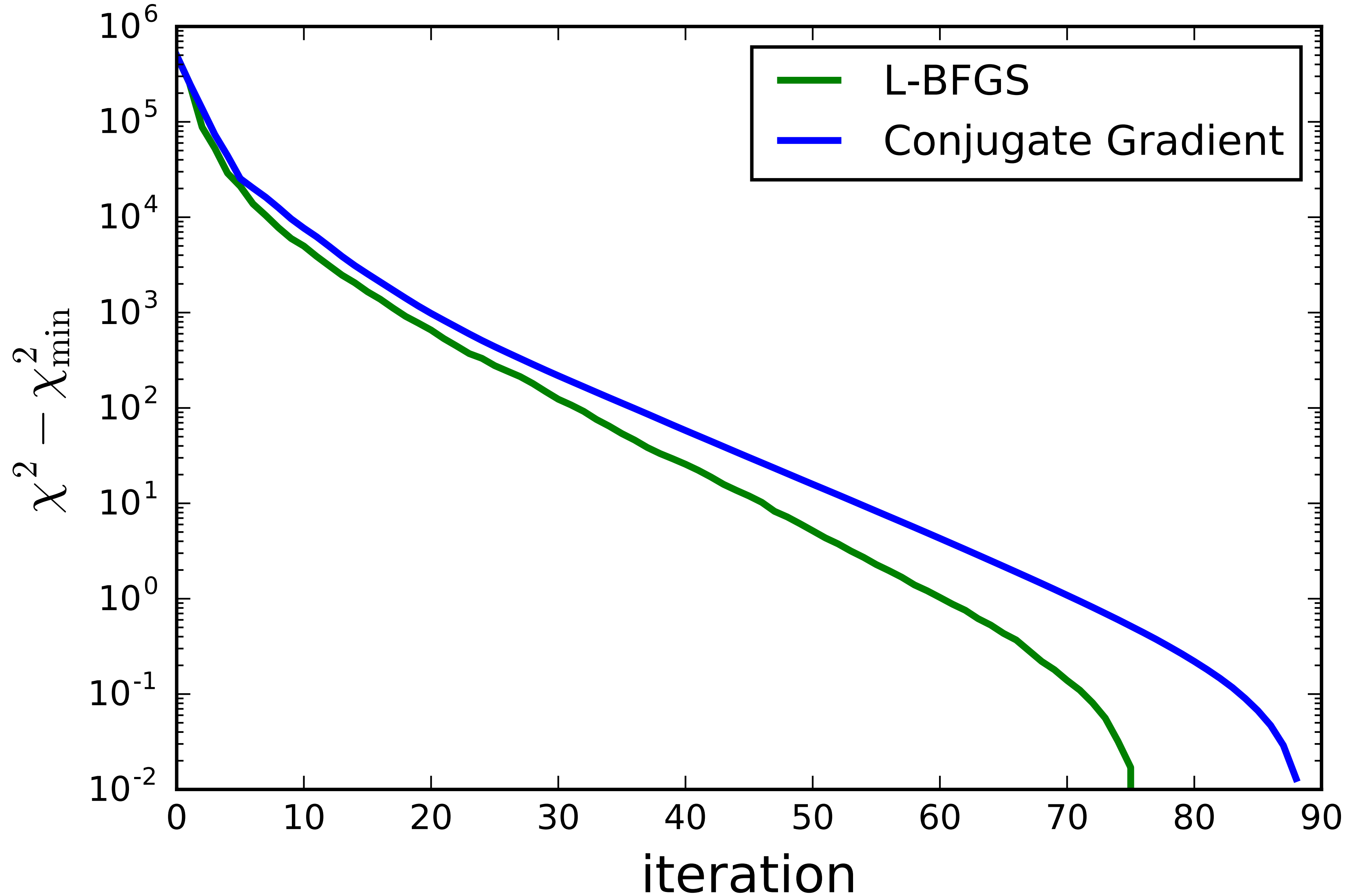


L-BFGS in action

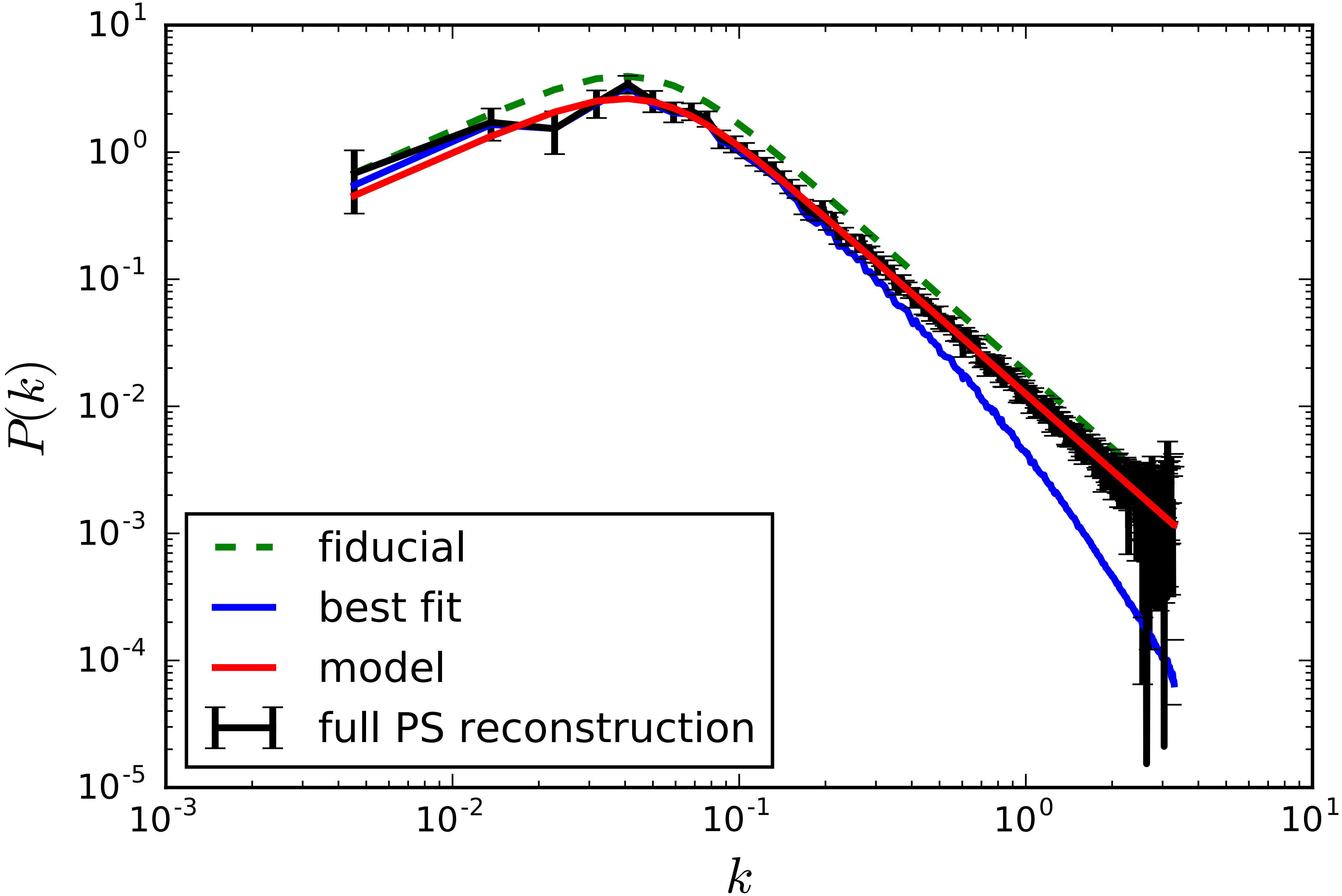


CPU time ~ 1 min.

L-BFGS vs. Conjugate Gradient



Power Spectrum



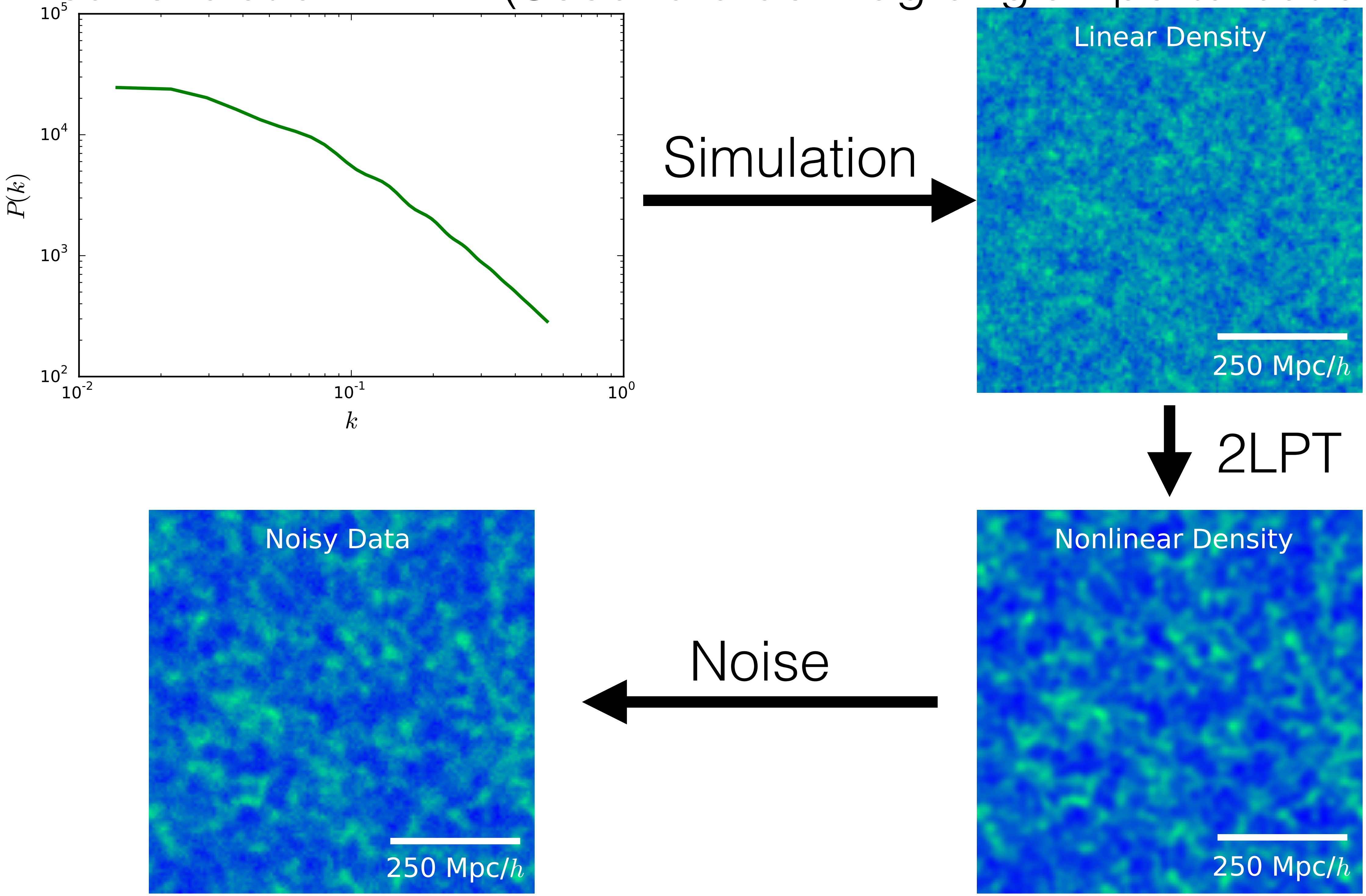
Fiducial power is 50% larger than the true power.

CPU time ~ 1 hour

Nonlinear Case: Large Scale Structure

Grid: 128^3, Box size: $(750\ \mathrm{Mpc/h})^3$

Nonlinear evolution: 2LPT (Second order Lagrangian perturbation theory)

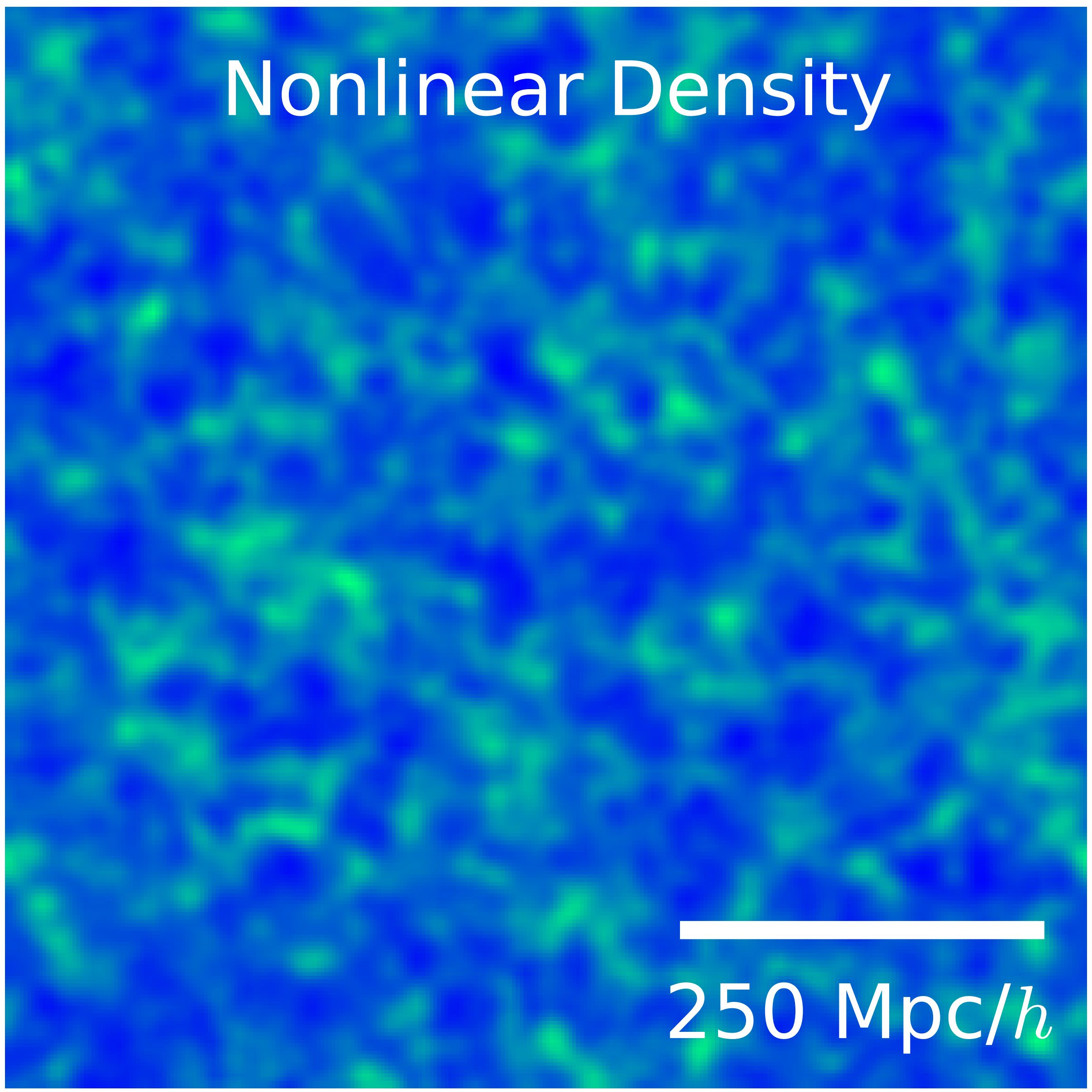


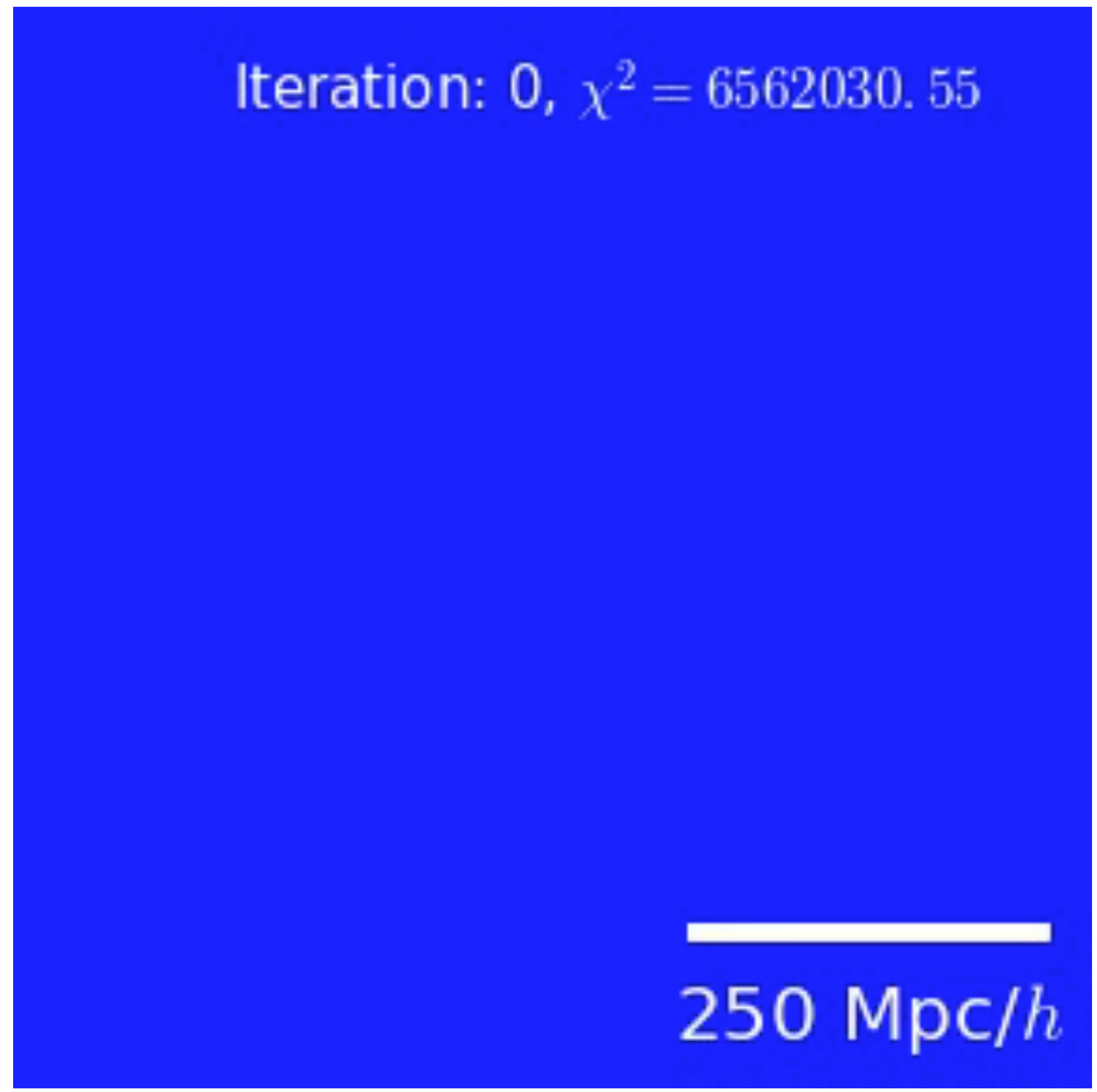
Code used: **fastPM** (Yu Feng, Man-Yat Chu, Uros Seljak, *1603.00476*)

Reconstruction

Nonlinear density

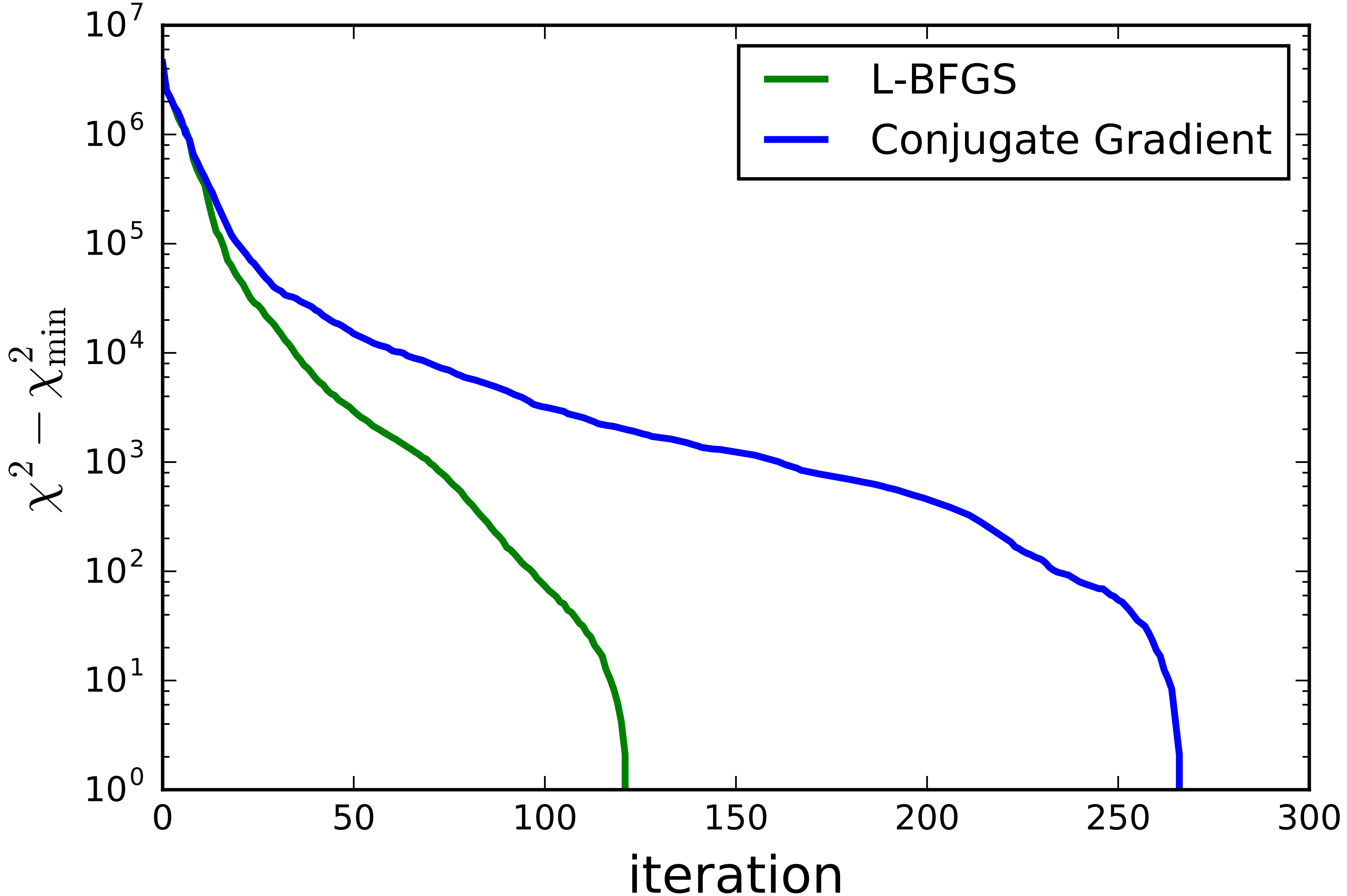
Original	L-BFGS in action



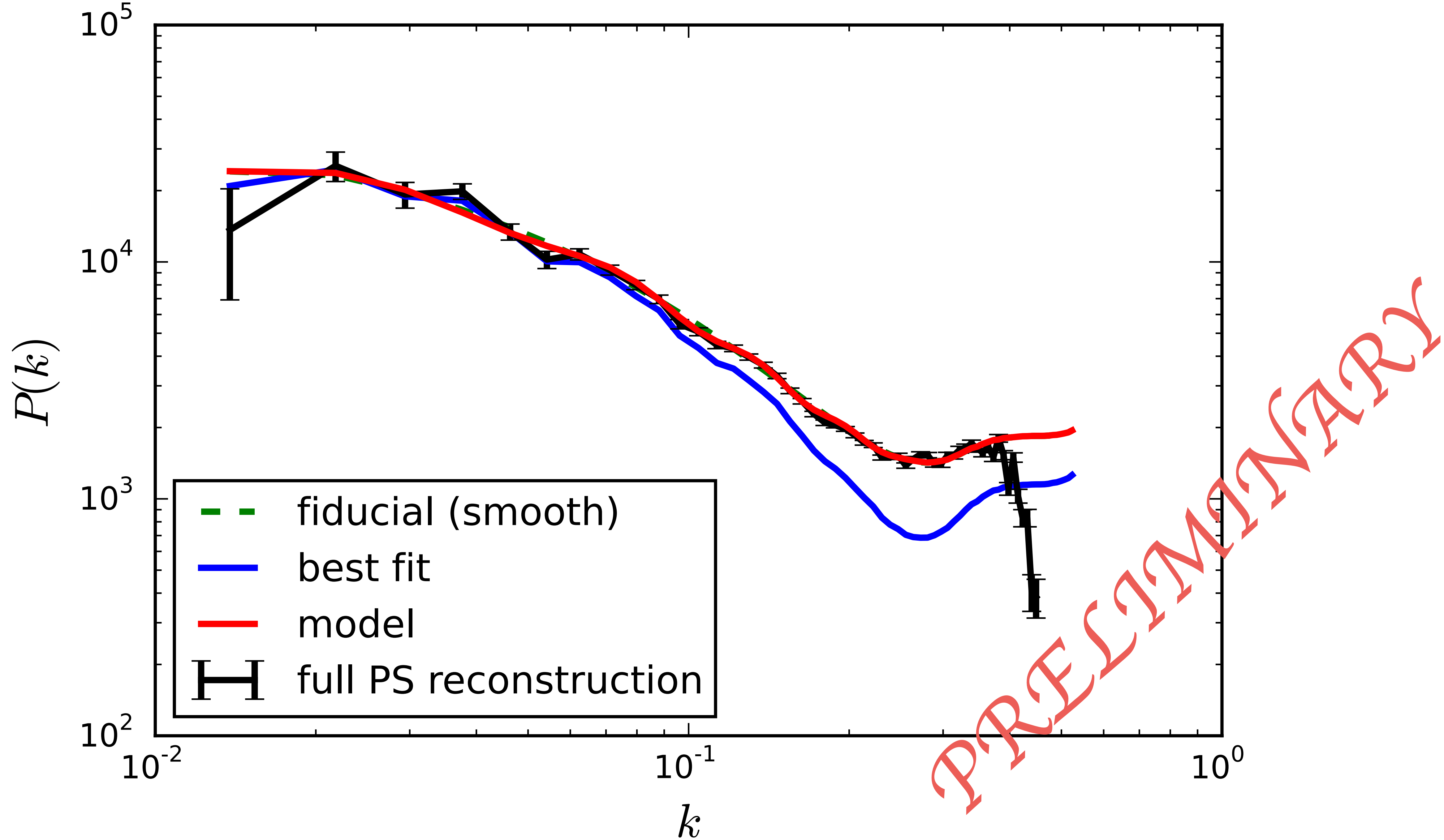


CPU time ~ 1 hour

L-BFGS vs. Conjugate Gradient



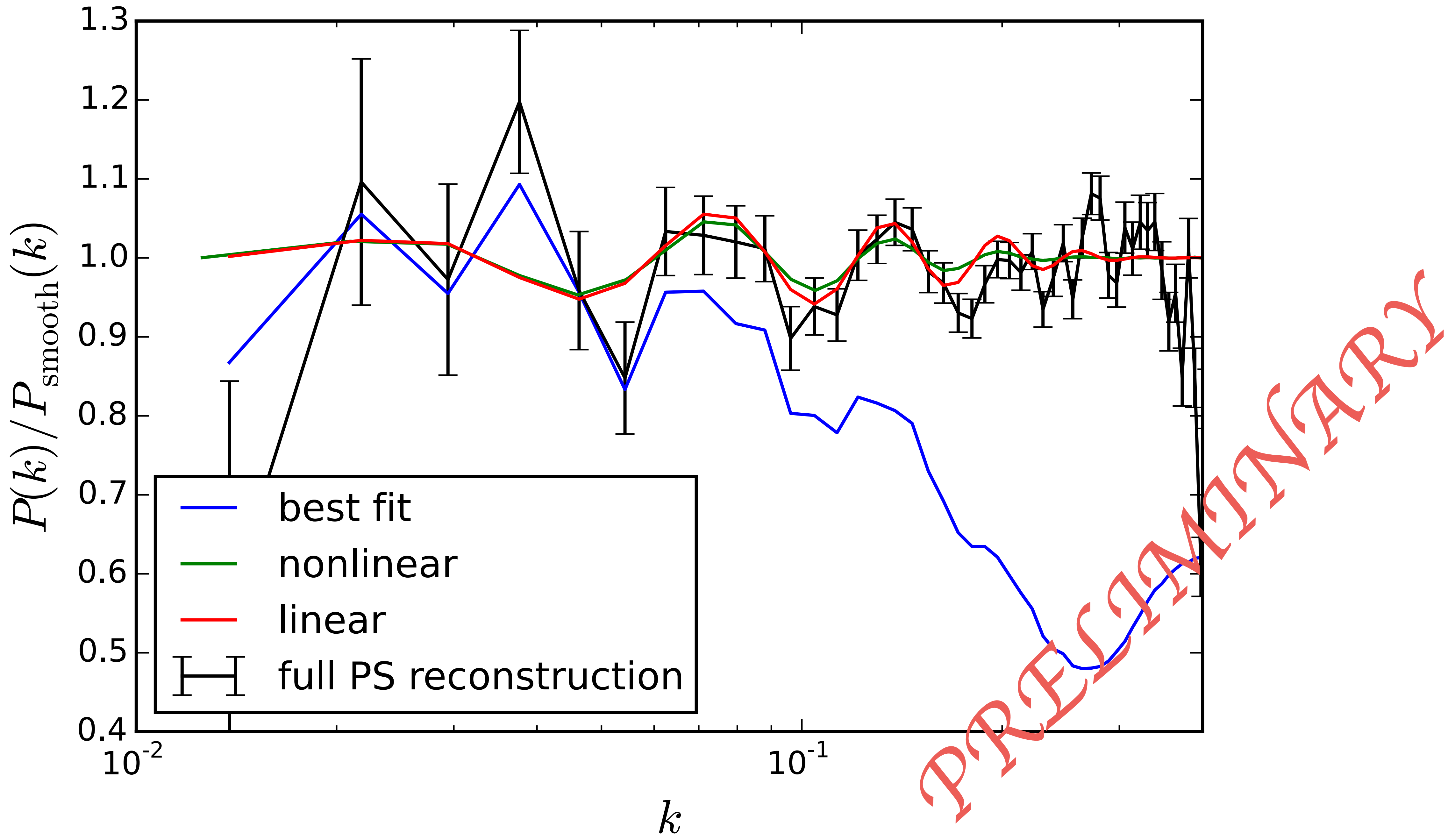
Power Spectrum



Fiducial power has no wiggles. Power spectra are convolved with window.

CPU time ~ 60 hours

Power Spectrum



Showing ratio to fiducial (smooth) power.

CPU time ~ 60 hours

Comparison with HMC

Previously:
HMC: Jasche, Wandelt, *1203.3639,…*
Wang, Mo, Yang, van den Bosch, *1301.1348,…*

- HMC Burnin: ~500 iterations (~5,000 function/derivative calls).
- L-BFGS optimization: ~100 iterations (~100 function/derivative calls).
- HMC correlation length: ~200.
- HMC sample of 10,000: ~100,000 function/derivative calls.
- L-BFGS full fisher matrix/power spectrum estimation: ~5,000 function/derivative calls.

Summary

- L-BFGS is a fast optimizer for very high dimensional parameter spaces.
- Conjugate gradient works almost as well as L-BFGS for the linear case. Not so much for the nonlinear case.
- Our reconstruction method works well for both linear and nonlinear models with ~million parameters at least.
- HMC is at least an order of magnitude more expensive. But if you really need a full sample then HMC is the way to go.
- DO NOT use HMC for minimization!
- Optimizers (L-BFGS, Conjugate gradient) and HMC publicly available (soon) as a part of the **cosmo++** package: cosmopp.com