

# Estimation of multiscale fields representing anthropogenic CO<sub>2</sub> emissions from sparse observations

J. Ray<sup>1</sup>, B. van BloemenWaanders<sup>2</sup> and S. A. McKenna<sup>2</sup>  
*jairay [at] sandia [dot] gov*

<sup>1</sup>Sandia National Laboratories, Livermore, CA

<sup>2</sup>Sandia National Laboratories, Albuquerque, NM

Acknowledgements: The work was funded by the LDRD program in Sandia National Labs

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.



# Problem statement

---

- **Aim:** Develop a technique to estimate anthropogenic CO<sub>2</sub> emissions from sparse observations
- **Motivations:**
  - An alternative to estimating CO<sub>2</sub> emission using bottom-up (economic model) techniques
  - Can provide independent verification in case of CO<sub>2</sub> abatement treaties
- **How is it done?**
  - Measure CO<sub>2</sub> concentrations in flasks at measurement sites; also column-averaged satellite measurements
  - Use an atmospheric transport model to invert for source locations



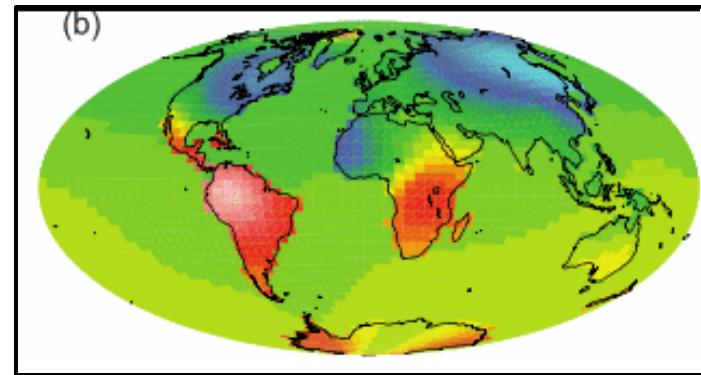
# Technical challenges

---

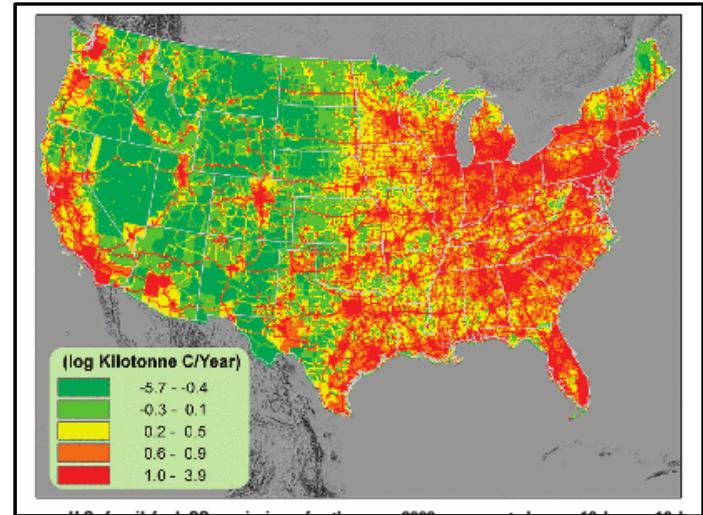
- Atmospheric transport model - largest source of uncertainty
- Limited measurements - second-largest contribution to uncertainty
- Spatial models for anthropogenic CO<sub>2</sub>
  - Non-stationary distribution in space
  - No spatial models exist to date – but need one is emissions are to be estimated from sparse observations
  - Impact of choice of spatial model on emission estimates?
- Discriminating between anthropogenic and biogenic CO<sub>2</sub> (biogenic is 10x larger)
  - But anthropogenic and biogenic CO<sub>2</sub> are different (and known) proportions of <sup>12</sup>CO<sub>2</sub> and <sup>14</sup>CO<sub>2</sub>

# Differences in spatial characteristics

- Biogenic CO<sub>2</sub> fluxes:
  - Smoothly variable in space
  - Modeled using multivariate Gaussian
  - Separate correlation lengths over land and oceans
- Anthropogenic (fossil fuel) emissions
  - Currently, only bottom-up estimates exist
  - A few databases – Vulcan (US-only, 2002); EDGAR (world)
  - Gaussian process will probably not work
    - What non-stationary covariance model to use?



Biogenic emissions: Mueller et al, *JGR*, 2008



Anthropogenic emissions: Gurney et al, *EST*, 2009



# Outline of the talk

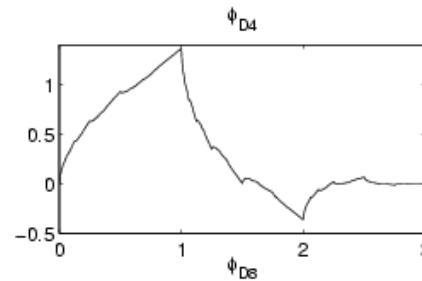
---

- Choosing a spatial model
  - Our hypothesis: *wavelets*
  - Study spatial and temporal characteristic of CO<sub>2</sub> emissions
    - Use Vulcan as source of emissions
    - Search for a good wavelet model - and what makes it good
- Demonstrate the spatial model in an OSS (observing system simulation)
  - Estimate CO<sub>2</sub> emissions from synthetic CO<sub>2</sub> observations
  - Using Ensemble Kalman Filters
    - Can handle large number of unknowns; estimates uncertainty in them
  - Using sparsity-enforcing methods used in compressive-sensing
    - If a parameter makes no difference to outputs, identifies and zeros it out

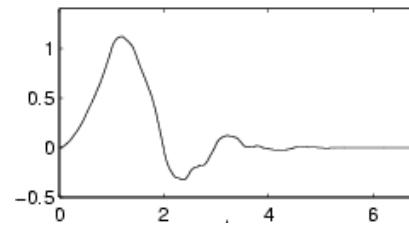
# How does one represent emissions with wavelets?

- Propose  $E(x) = \sum_{s,l} w_{s,l} \phi_{s,l}(x)$ 
  - $\phi_{s,l}(x)$  is a wavelet basis;  $s, l$  are its *scale* and *location* indices
  - $w_{s,l}$  are weights
- So what are wavelets?
  - Basis set with compact support
  - Belong to different families
  - Within a family, can have different orders (high order ~ smoother)
  - One chooses a family and an order, to expand  $E(x)$
  - The expansion consists of varying
    - $s$ , to get different frequency content
    - $l$ , to shift in space (location)

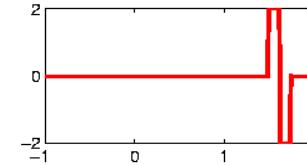
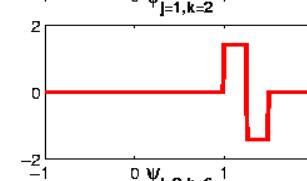
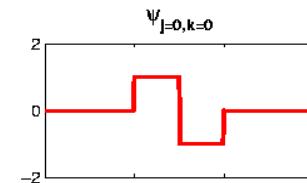
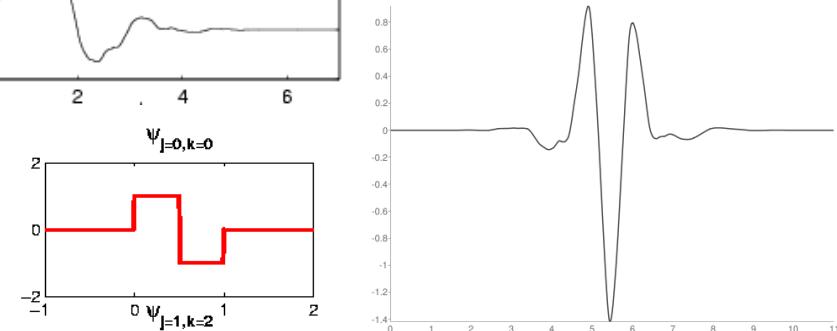
Haars at different scales and locations



Daubechies, order 4



Daubechies, order 6



Symlet, order 6



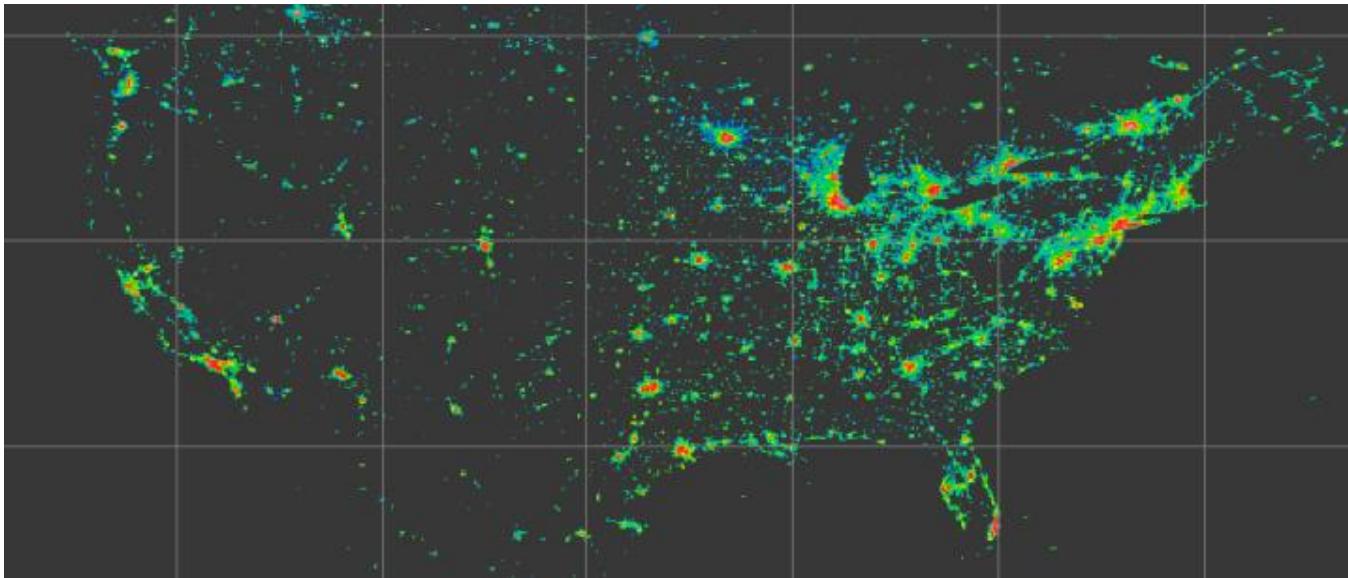
# Posing the problem

---

- An emission field on  $2^N \times 2^N$  pixels
  - Can be decomposed on a wavelet basis,  $N$  deep
  - Each level  $s$  has  $2^s \times 2^s - (2^{s-1} \times 2^{s-1})$  weights
- Emissions
$$E(x) = \sum_{s=1}^N \sum_{i=1}^{2^s} \sum_{j=1}^{2^s} w_{s,i,j} \phi_{s,i,j}(x)$$
- Conjecture
  - $w_{s,i,j}$  are mostly zero (i.e., is sparse)
  - $w_{s,i,j}$  and  $w_{s+1,i,j}$  are correlated – parent-child relationship
- Conjecture checked
  - Using CO<sub>2</sub> emissions from Vulcan (SIAM GeoSc, 2011)
  - Checked Haars, Daubechies of different orders
  - Found that Haar wavelets provided the sparsest representation
  - Reconstruction error was also small

# Dimensionality reduction

---



- Nightlights are a good proxy for FF emissions
  - Except emissions from electricity generation and cement production
  - Nightlights easily observed – DoD's DMSP-OLS
- Use thresholded radiance-calibrated nightlights from 1997-98 to mask out unpopulated regions



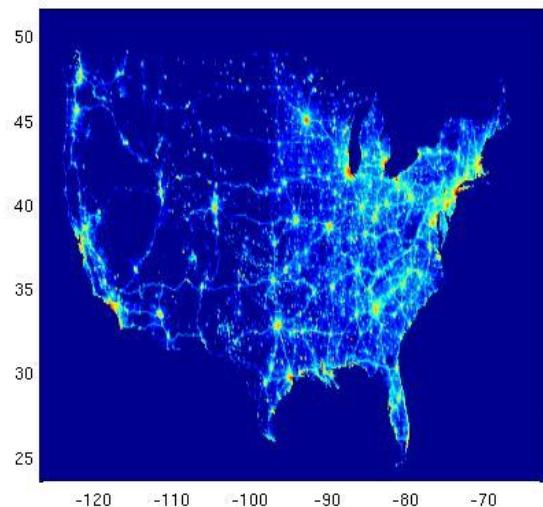
# Random field model using nightlights

---

- Threshold nightlights at radiance  $R_{\min}$ 
  - Removes low-population regions of the US
  - Make a nightlight “mask”
- Mask EDGAR fluxes ( $1^\circ$  resolution; annual average for 2002)
  - Project to a Haar wavelet basis set & retain non-zero wavelet coefficients
- Wavelet-based Random Field model
  - With 635 coefficients (“mid-complexity”)
  - Remove wavelet coefficients at finest level too – 253 parameter model (“low” complexity)
- Errors introduced by this approximation
  - We lost some emissions due to nightlight masking
  - We lost spatial fidelity due to coarsening

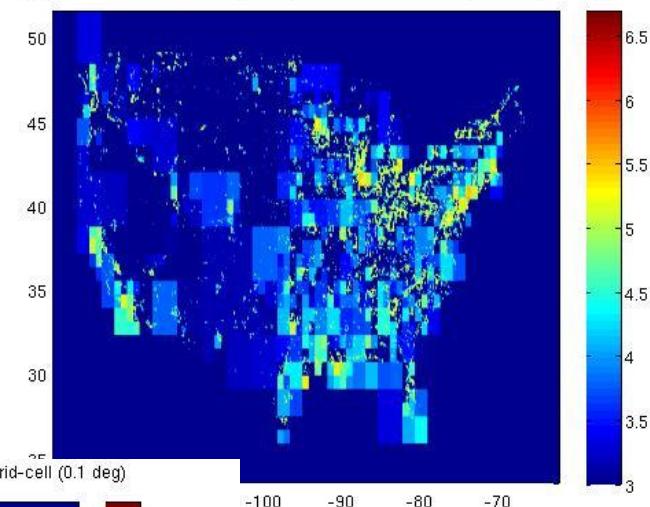
# Emission reconstruction comparison

$\log_{10}(\text{emissions})$  in tonnes/hr/grid-cell (0.1 deg), (-127.5W, 51.5N) (-62.5W, 23.5N)

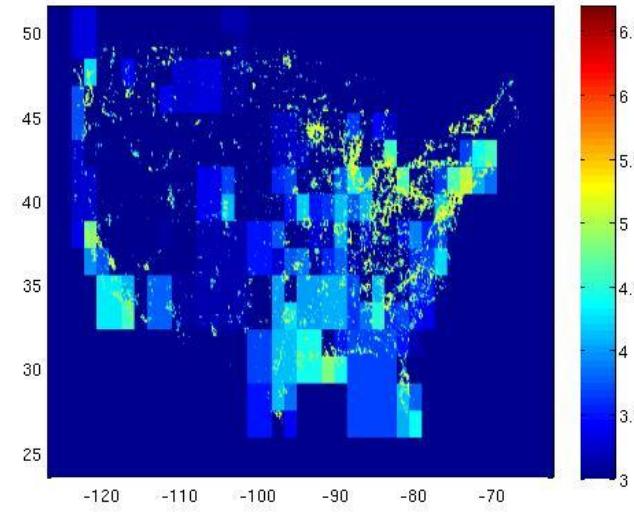


Original from Vulcan database

$\log_{10}(\text{Reconstructed emissions})$  using Haars. tons of CO<sub>2</sub>/hr/grid-cell (0.1 deg)



635 parameter model



253 parameter model

- Lost 10% of total emissions due to masking
- 253 or 635 parameters may be still too many to estimate



# Emission estimation problem

---

- Use the 2 wavelet RF models to fit to synthetic CO<sub>2</sub> concentration data
  - Is the dimensionality of the model high enough?
- Synthetic data generation
  - Choose location of 35 towers (NOAA's network)
  - Use Vulcan emissions, coarsened to 1° resolution, to generate time-dependent CO<sub>2</sub> concentration “observations”
    - Concentration measurements at every 3 hours
  - Atmospheric transport simulated using WRF
- Inverse problem is linear
  - $y = Hx$ , where  $y = \text{CO}_2 \text{ concentrations}$ ;  $x = \text{emissions over } \sim 1 \text{ year}$ 
    - We estimate emissions averaged over 8-day periods (“Period”)
  - $x = \Phi w$ , where  $\Phi = \text{wavelet bases}$ ,  $w = \text{basis weights}$
  - $H$  constructed using WRF and 2008 wind fields

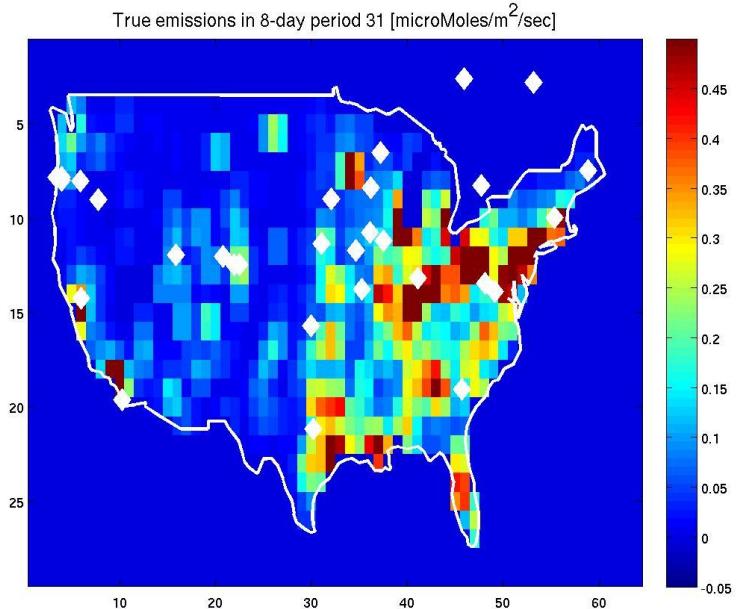


# Sparsity-enforced estimation

---

- The observations may not be sufficient to estimate 253 (or 635) parameters per “Period”
  - Atmospheric transport is diffusive – destroys information
  - If RF model parameters  $w$  cannot be estimated, set to zero
- Fitting procedure
  - Minimize  $\| y - H \Phi w \|_2 + \| w \|_1$
  - Uses a greedy, orthogonal matching pursuit algorithm called StOMP (Donoho & Tsaig, 2006)
- The basic idea is borrowed from compressive sensing
  - $H$  is the “sampling” matrix, but is neither random, nor maximally incoherent with  $\Phi$ , nor does it satisfy Restricted Isometry
  - But will prevent overfitting

# Estimated emissions

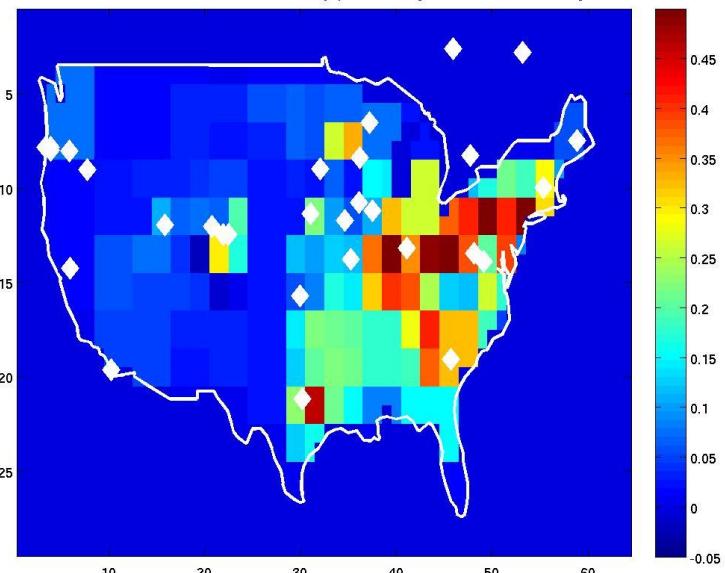


Vulcan emissions; coarsened to 1°

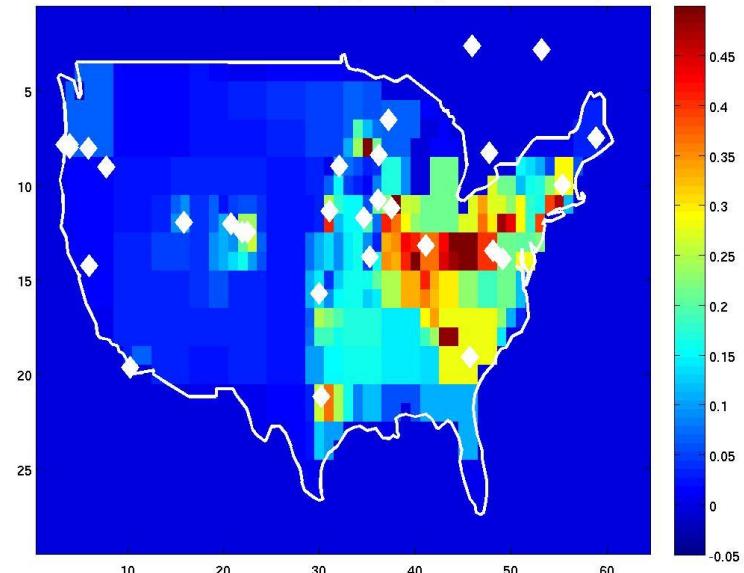
- Reconstructions look similar for Period # 31 (~August 2008)
- Mid-complexity model (635 parameters) has more spatial fidelity
  - Significant, or just artifact?

Reconstruction; mid-complexity RF model

Reconstructed emissions in 8-day period 31 [microMoles/m<sup>2</sup>/sec]

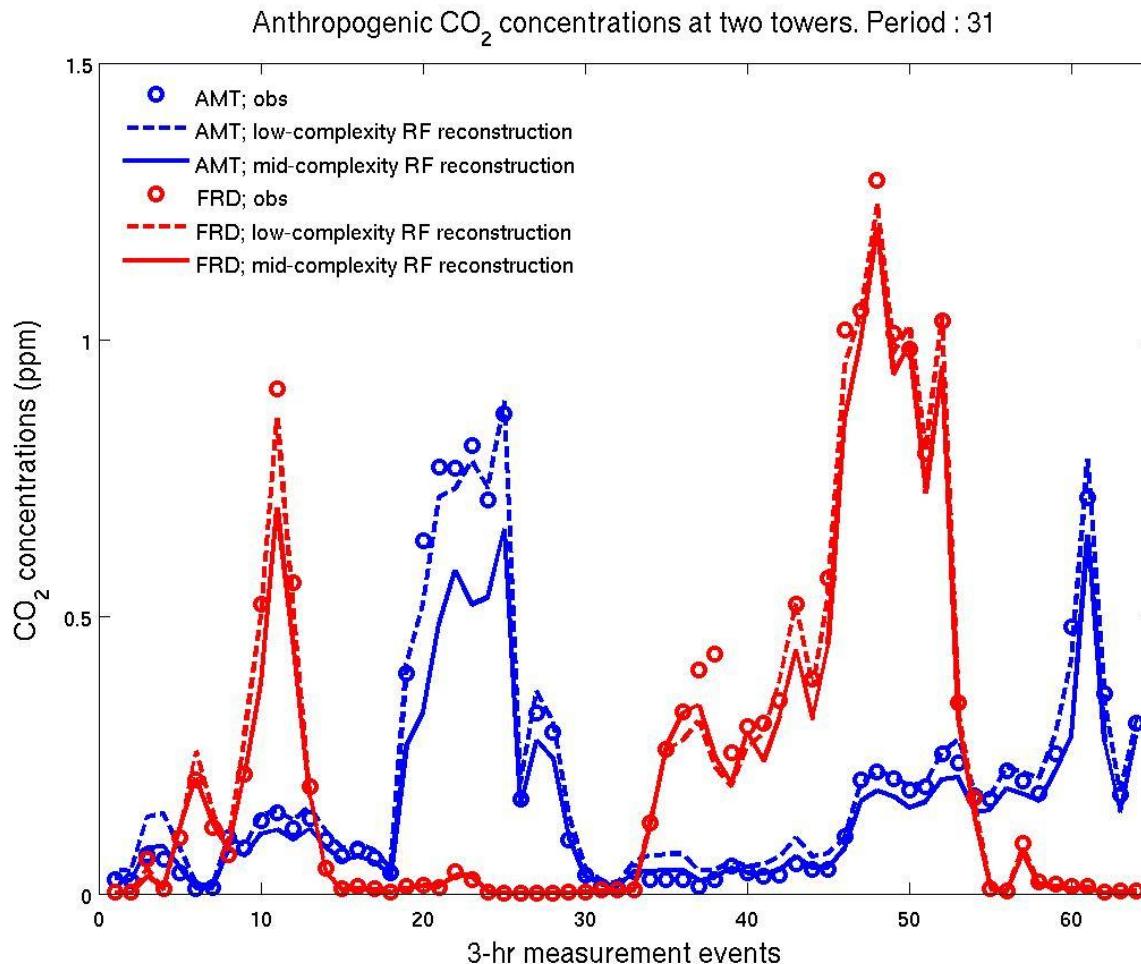


Reconstructed emissions in 8-day period 31 [microMoles/m<sup>2</sup>/sec]



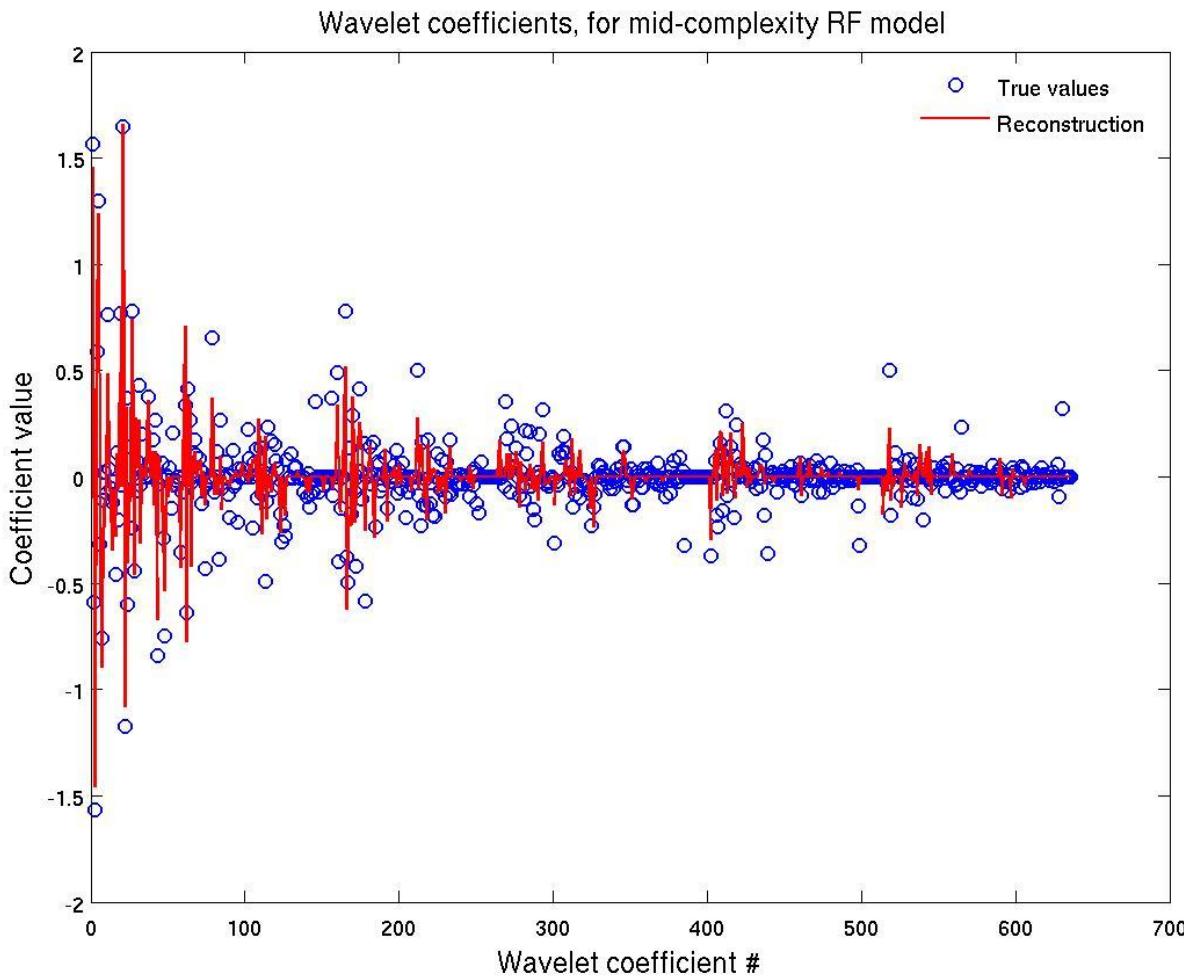
Reconstruction; low-complexity RF model

# Predictive capacity



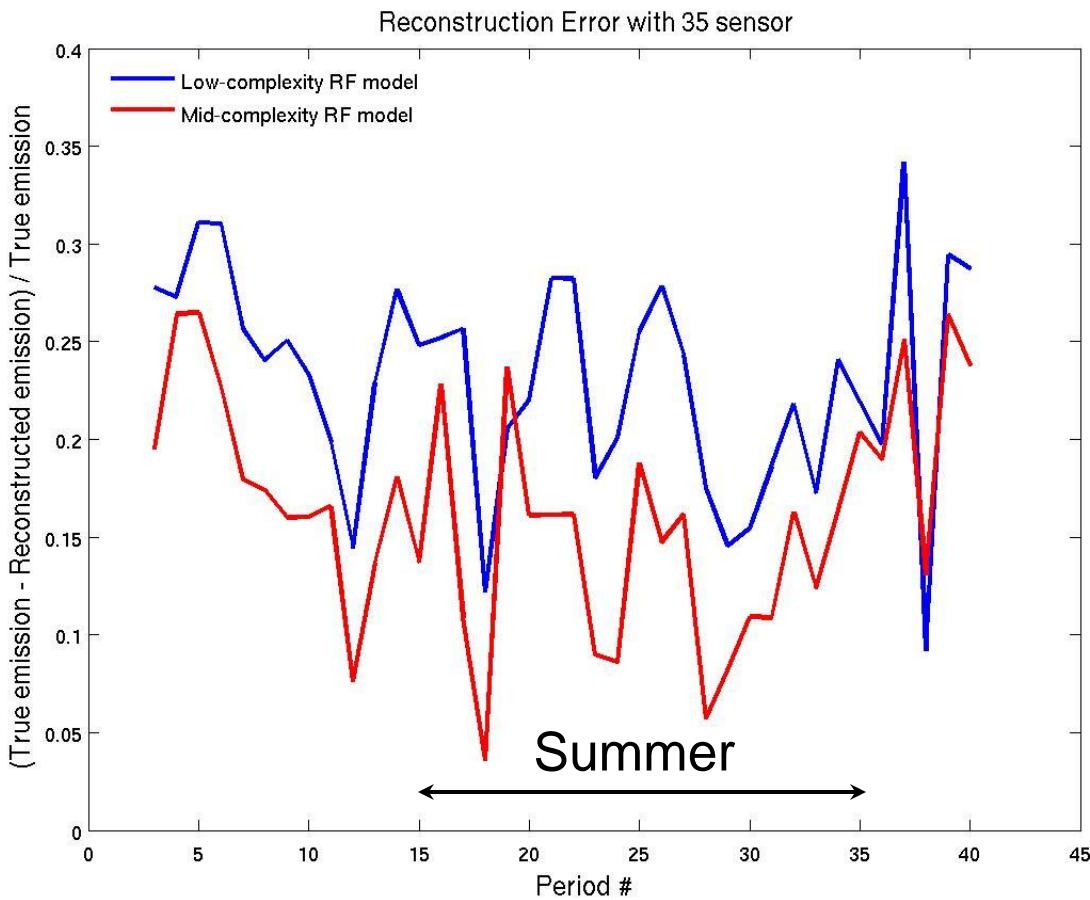
- Predicted CO<sub>2</sub> concentrations at 2 towers
  - Basically, not much difference between 2 RF models
- Results shown for Period 31

# Did sparsification work?



- In the mid-complexity model (635 parameters), about 57% of the parameters are set to zero
- In the low-complexity, about 30%
- **Lesson learnt:** Our RF models are still too high-dimensional
  - But perhaps we're not over-fitting

# Accuracy of reconstruction



- The mid-complexity RF model has lower errors
  - But the errors are uncomfortably high
- Requirements
  - Need UQ of parameters
  - Need finer spatial resolution, but
    - With sparsity enforcement
- More sensors would be nice



# Estimating emission

---

- **Aim:** Estimate emissions, given time-variant CO<sub>2</sub> concentrations
  - Use a wavelet-based RF model
  - Quantify uncertainty in estimates
  - Use EnKF (scalable; also captures uncertainty in estimates)
- **Basically:**
  - Can wavelet-based RF models be used in estimation with UQ?
  - How large are the uncertainties if no model-reduction is done (CS or a priori)
- **Data** – CO<sub>2</sub> concentrations at sensor locations
  - Generated synthetically, using a transport model
  - Domain: Lower 48 states of USA (51.5N, -127.5W) to (23.5N, 62.5W)



# Modeling and numerical details

---

- **Transport model:** Simple advection-diffusion

$$\frac{\partial c}{\partial t} - D\Delta c + v\nabla c = f \quad \in \omega \times (0, T)$$
$$\nabla c = 0 \quad \in \Gamma \times (0, T)$$

- $c$  = concentration
- $v$  = velocity,
- $f$  = CO<sub>2</sub> source
- $D$  = diffusion coefficient.

- **Ensemble Kalman filters**

$$u_k = u_{k-1} + K(z_k - Hu_k)$$

$$K = P_k H^T (H P_k H^T + R)^{-1}$$

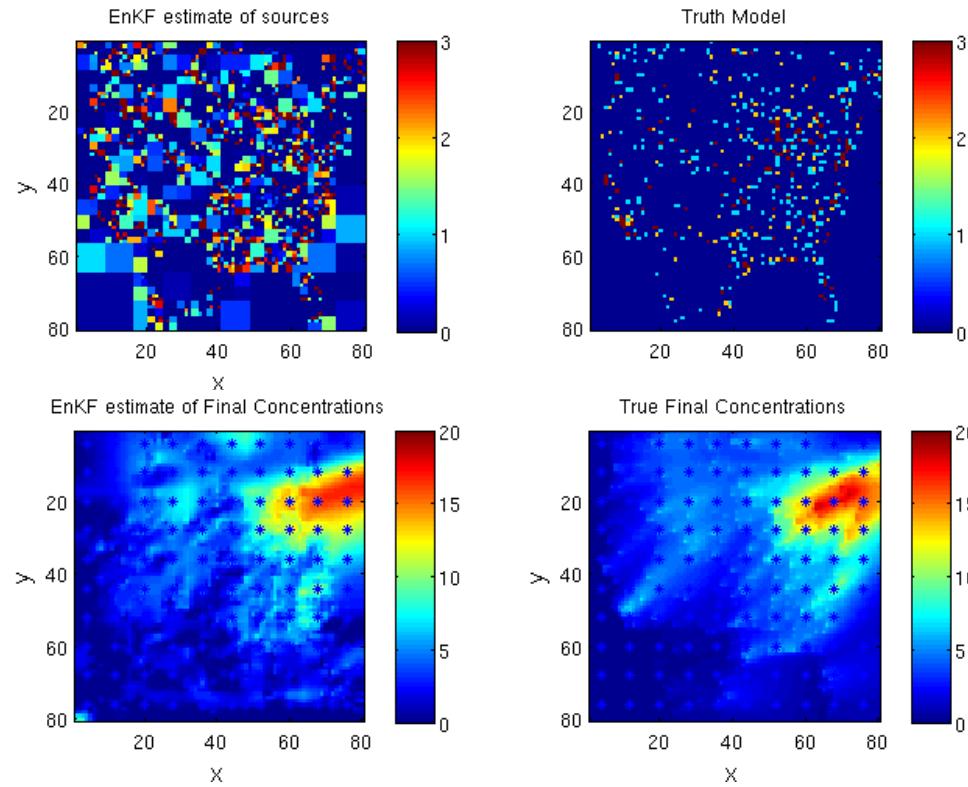
$$P_k = A P_{k-1} A^T + Q$$

- **Spatial models**
  - Used Haars and Debauchies (order = 8)



# Emission estimation (MAP estimates)

---



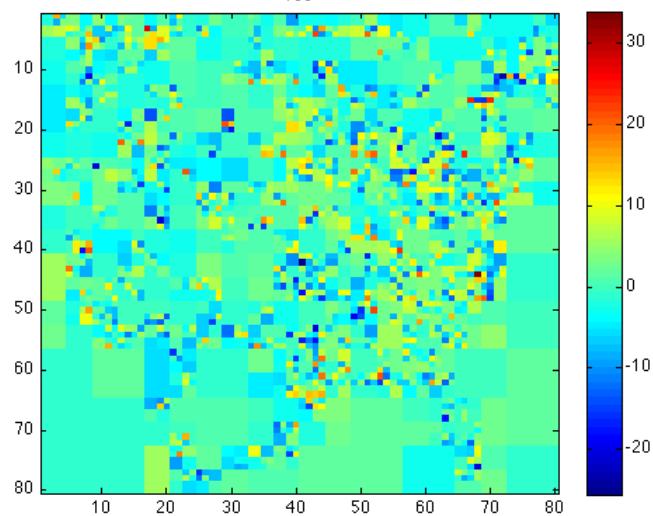
- Emissions with Haars (wavelets on all levels)
- 80x80 grid resolution; sensor grid = 10 x 10



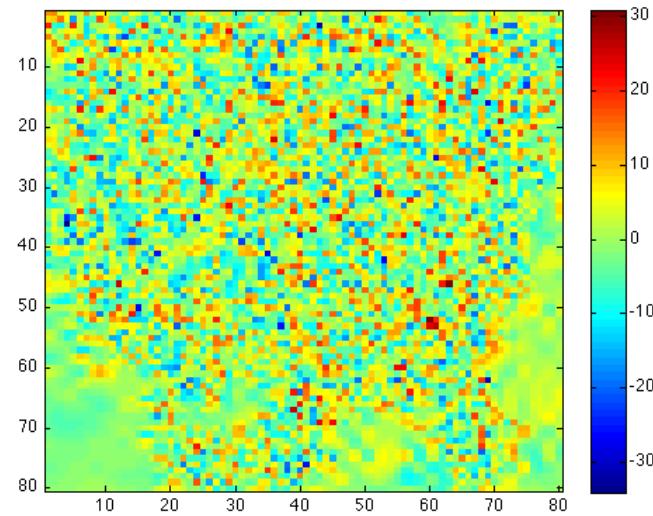
# Emission reconstruction – impact of wavelet model

---

Haar



Daubechies 8



RMSE = 1.44

RMSE = 1.61



# Conclusions

---

- We have created a multiresolution random field (RF) model for CO<sub>2</sub> emissions
- RF model can be fitted to data by enforcing sparsity
  - No uncertainty quantified, by > 50% of the coefficients were identified and inactivated
  - The 35 sensors that we have can estimate anthropogenic emissions if it were an inert tracer
    - 20-30% errors are observed
    - But the sensors were placed for biospheric, not anthropogenic fluxes
    - Unknown when joint anthropogenic and biospheric inversion can be done
- RF model also tested with EnKF, but with simplified transport
  - Both CO<sub>2</sub> concentrations and sources can be estimated

# Questions?

