

# GPUs and the computational efficiency of Gaussian process based models

Colin Rundel

Duke University

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- 1 Background
- 2 Migratory Bird Spatial Assignment Model
- 3 Speciated PM<sub>2.5</sub> Modeling
- 4 GPUs and Low Rank Approximations

# The problem with GPs ...

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# A simple guide to computational complexity

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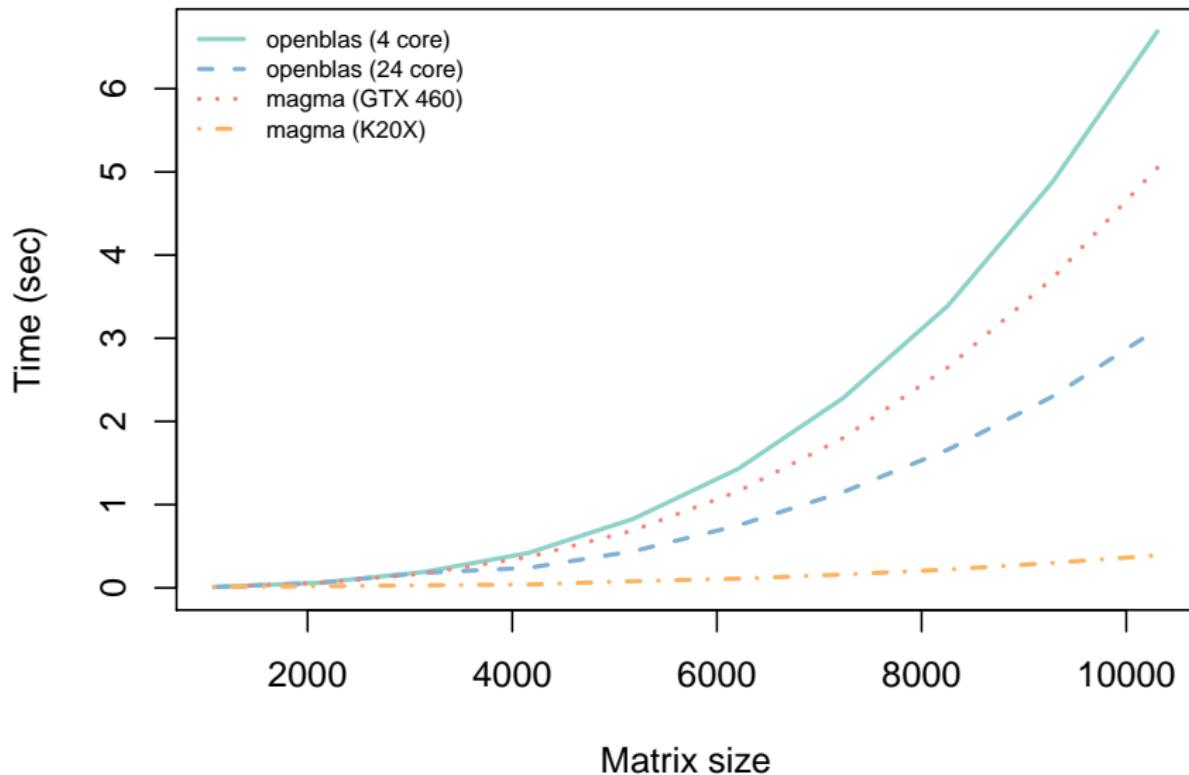
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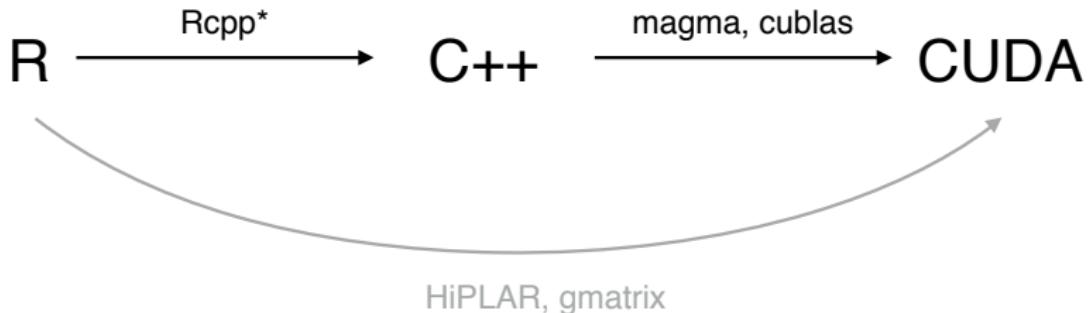
Quadratic complexity? - Pray

Cubic complexity? - Give up

# Improving Cholesky



# Tools and Optimization



Regardless of tools or workflow, measuring / profiling performance is critical.

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## Background

Using intrinsic markers (genetic and isotopic signals) for the purpose of inferring migratory connectivity.

- Existing methods are too coarse for most applications
- Large amounts of data are available ( >150,000 feather samples from >500 species)
- Genetic assignment methods are based on Wasser, et al. (2004)
- Isotopic assignment methods are based on Wunder, et al. (2005)

# Data - DNA microsatellites and $\delta^2\text{H}$

Hermit Thrush (*Catharus guttatus*)

- 138 individuals
- 14 locations
- 6 loci
- 9-27 alleles / locus



Wilson's Warbler (*Wilsonia pusilla*)

- 163 individuals
- 8 locations
- 9 loci
- 15-31 alleles / locus



# Allele Frequency Model

For the allele  $i$ , from locus  $l$ , at location  $k$

$$\mathbf{y}_{\cdot lk} | \Theta \sim \text{Mult}(\sum_i y_{ilk}, \mathbf{f}_{lk})$$

$$f_{ilk} = \frac{\exp(\Theta_{ilk})}{\sum_i \exp(\Theta_{ilk})}$$

$$\Theta_{il} | \alpha, \mu \sim \mathcal{N}(\mu_{il}, \Sigma)$$

$$\{\Sigma\}_{ij} = \alpha_0 \exp\left(-(\{d\}_{ij}/\alpha_1)^{\alpha_2}\right) + \alpha_3 \mathbb{1}_{i=j}$$

# Genetic Assignment Model

Assignment model using Hardy-Weinberg equilibrium allowing for genotyping ( $\delta$ ) and single amplification ( $\gamma$ ) errors.

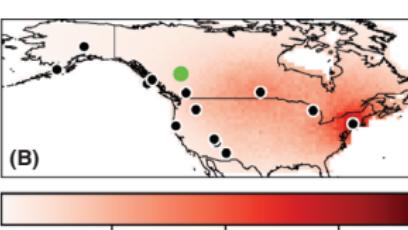
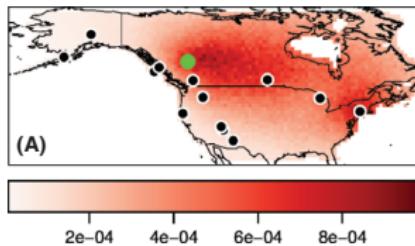
$$P(S_G | \mathbf{f}, k) = \prod_I P(i_I, j_I | \mathbf{f}, k)$$

$$P(i_I, j_I | \mathbf{f}, k) = \begin{cases} \gamma P(i_I | \mathbf{f}, k) + (1 - \gamma) P(i_I | \tilde{\mathbf{f}}, k)^2 & \text{if } i = j \\ (1 - \gamma) P(i_I | \mathbf{f}, k) P(j_I | \mathbf{f}, k) & \text{if } i \neq j \end{cases}$$

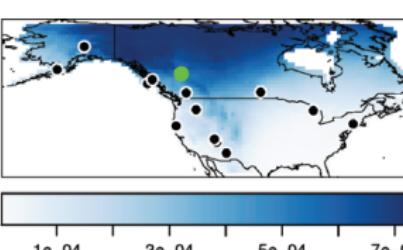
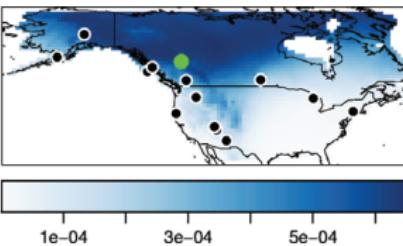
$$P(i_I | \mathbf{f}, k) = (1 - \delta) f_{lik} + \delta / m_I$$

# Combined Model

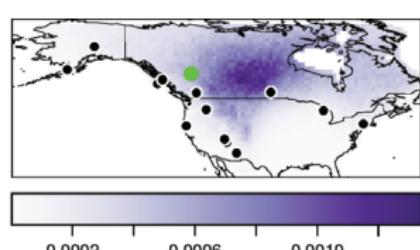
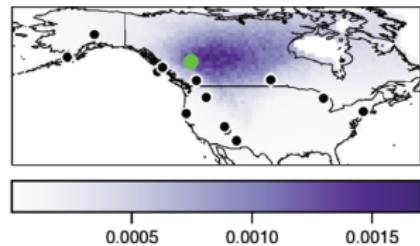
Genetic



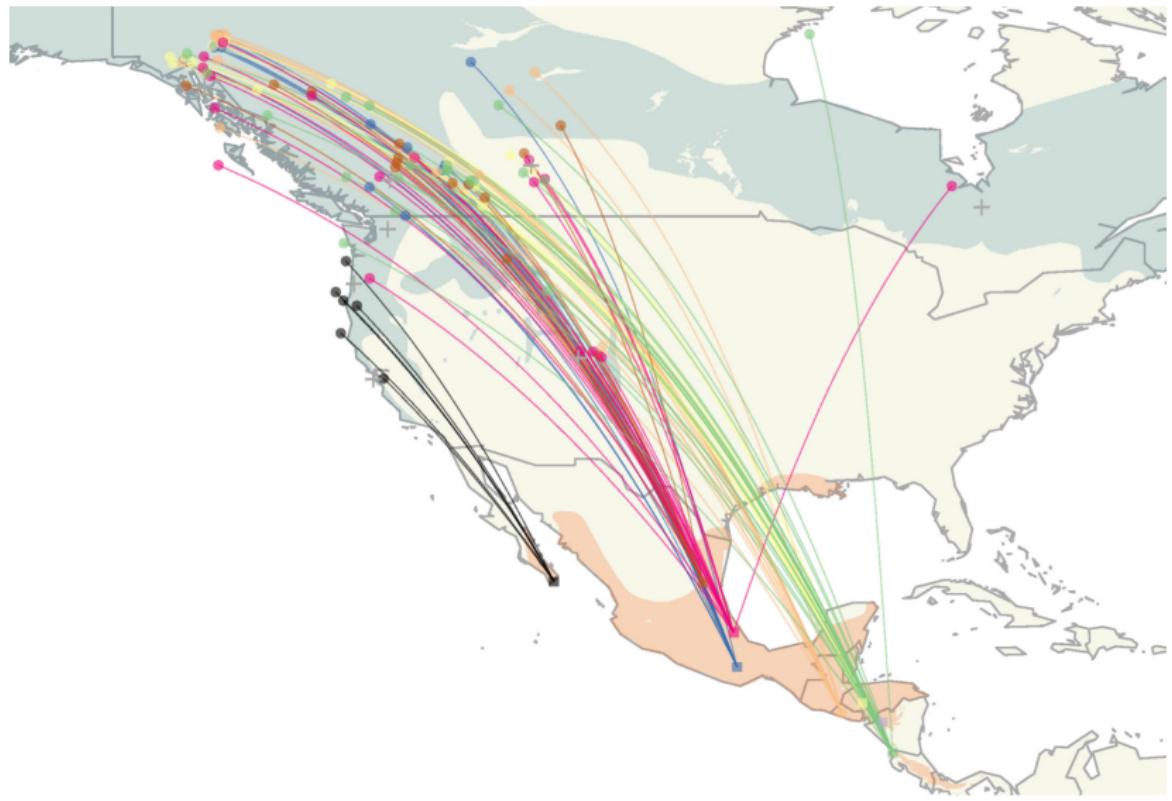
Isotopic



Combined



# Migratory Connectivity



# Implementation

Model fitting is done via MCMC (MH within Gibbs)

- Original implementation in pure C++ with minimal dependencies (Wasser, et al. (2004))
- Rewritten using R / C++ via Rcpp(Armadillo)
  - Code closer to matrix notation (and R)
  - Transparent use of high performance LAPACK implementations
  - R Package - isoscatR - <https://github.com/rundel/isoscatR>
- Model fitting performance is quite good
  - 300,000 iterations in  $\sim 5.5$  minutes
- Bottleneck in drawing posterior predictive samples
  - 1,000 iterations in  $\sim 30$  minutes

# Prediction details

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To do so we sample from:

$$\Theta_p | \Theta_m \sim \mathcal{N}(\mu_p + \Sigma_{pm} \Sigma_m^{-1} (\Theta_m - \mu_m), \Sigma_p - \Sigma_{pm} \Sigma_m^{-1} \Sigma_{mp})$$

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## Algorithm steps

- ① Calculate  $\Sigma_{pm}$ ,  $\Sigma_p$ , and  $\Sigma_p - \Sigma_{pm}\Sigma_m^{-1}\Sigma_{mp}$
- ② Calculate  $\text{Chol}(\Sigma_p - \Sigma_{pm}\Sigma_m^{-1}\Sigma_{mp})$
- ③ Sample from MVN
- ④ Calculate allele frequencies

## Posterior predictive sampling timings

Step	CPU (secs)	CPU+GPU (secs)	Rel. Performance
1. Covariances	1.080	0.046	23.0
2. Cholesky	0.467	0.208	2.3
3. Sample	0.049	0.052	0.9
4. Allele Freq	0.129	0.127	1.0
Total	1.732	0.465	3.7

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$\times$  CV runs  $\begin{bmatrix} 166 \text{ for Hermit Thrush} \\ 179 \text{ for Wilson's Warbler} \end{bmatrix}$

# Lessons

- Relatively small changes in one function resulted in 3 - 4x improvement
  - Cross validation results in two days instead of a week
  - 1-2 weeks of implementation, 1 week of tweaking / testing
  - Started with Cholesky, other optimizations followed

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- Relatively small changes in one function resulted in 3 - 4x improvement
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  - Started with Cholesky, other optimizations followed
- Issues
  - External library dependency makes package development (much) more complicated
  - Additional code verbosity and complexity

# Improving Covariance Calculations

Covariance is assumed to be stationary and isotropic

- Elements of the covariance matrix can be calculated independently
- Small scale “embarrassingly parallel”
- Implementation is straight forward  
(if we don't worry about things like symmetry)

```
__global__ void powered_exponential_cov_kernel(double* dist, double* cov,
                                                const int nm, const double sigma2,
                                                const double phi, const double kappa)
{
    int n_threads = gridDim.x * blockDim.x;
    int pos = blockDim.x * blockIdx.x + threadIdx.x;

    for (int i = pos; i < nm; i += n_threads)
    {
        cov[i] += sigma2 * exp( -pow(dist[i] * phi, kappa) );
    }
}
```

# Building core tools

Common set of (expensive) tasks for GP models

- Covariance calculation
- Cholesky of Cov.
- Inverse of Cov.

Goal is to make performing these tasks on a GPU as painless as possible and allow interoperability with GPU (magma, CUBLAS) and CPU (Armadillo) libraries.

- GPU matrix class
- Modern resource management (RAII, move semantics)
- Simple translation between GPU and CPU memory

R Package - RcppGP - <https://github.com/rundel/RcppGP>

# CPU vs GPU code

```
arma::mat prop_Sigma = arma::exp(-prop_phi * d_CIF);
arma::mat prop_Sigma_U = arma::chol(prop_Sigma);

double prop_Sigma_log_det = 2*arma::accu(arma::log(prop_Sigma_U.diag()));

arma::mat prop_Sigma_U_inv = arma::inv(arma::trimatu(prop_Sigma_U));
arma::mat prop_Sigma_inv = prop_Sigma_U_inv * prop_Sigma_U_inv.t();
```

```
exponential_cov_gpu(d_CIF_gpu.mat, cov_gpu.mat, nr_CIF, nr_CIF, 1.0, prop_phi, 64);
cov_gpu.chol('L',false);

double prop_Sigma_log_det = 2*arma::accu(arma::log(cov_gpu.get_mat().diag()));

cov_gpu.inv_chol('L',true);
arma::mat prop_Sigma_inv = cov_gpu.get_mat();
```

Back

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## Background

Fine particulate matter ( $\text{PM}_{2.5}$ ) is an EPA regulated air pollutant linked to a variety of adverse health effects

- Classified based on particle size ( $< 2.5 \mu\text{m}$  diameter)
- Major species: Sulfate, Nitrate, Ammonium, Soil, Carbon.
- Minor species: trace elements (K, Mg, Ca), heavy metals (Cu, Fe), etc.
- Complex spatio-temporal dependence between species

# Data

## Speciated PM<sub>2.5</sub> Sources

- Chemical Speciation Network (CSN) - 221 stations
- Interagency Monitoring of Protected Visual Environments (IMPROVE) - 172 stations

## Total PM<sub>2.5</sub> Sources

- Federal Reference Method (FRM) - 949 stations

## Model Output

- Community Multi-scale Air Quality (CMAQ) - 12 km grid

## Data Issues

- Monitoring frequency
- Total vs Sum of Species

## Species Model Details

For the 5 major species (Sulfate, Nitrate, Ammonium, Soil, Carbon) and the two networks (CSN, IMPROVE):

$$C_t^i(\mathbf{s}) = Z_t^i(\mathbf{s}) + \epsilon_{C,t}^i(\mathbf{s})$$

$$I_t^i(\mathbf{s}) = Z_t^i(\mathbf{s}) + \epsilon_{I,t}^i(\mathbf{s})$$

where  $Z_t^i(\mathbf{s})$  are the latent “true” concentrations of species  $i$  at time  $t$  and locations  $\mathbf{s}$ , and is given by

$$Z_t^i(\mathbf{s}) = \max(0, \tilde{Z}_t^i(\mathbf{s}))$$

$$\tilde{Z}_t^i(\mathbf{s}) = \beta_{0,t}^i + \beta_{0,t}^i(\mathbf{s}) + \beta_{1,t}^i Q_t^i(B_s)$$

## Total PM<sub>2.5</sub> Model Details

For total PM<sub>2.5</sub> from the three networks (CSN, IMPROVE, FRM):

$$C_t^{tot}(\mathbf{s}) = Z_t^{tot}(\mathbf{s}) + \epsilon_{C,t}^{tot}(\mathbf{s})$$

$$I_t^{tot}(\mathbf{s}) = Z_t^{tot}(\mathbf{s}) + \epsilon_{I,t}^{tot}(\mathbf{s})$$

$$F_t^{tot}(\mathbf{s}) = Z_t^{tot}(\mathbf{s}) + \epsilon_{F,t}^{tot}(\mathbf{s})$$

where  $Z_t^{tot}(\mathbf{s})$  are the latent “true” concentration of total PM<sub>2.5</sub> at time  $t$  and locations  $\mathbf{s}$ , which is given by the sum of the major species and the “other” species concentrations.

$$Z_t^{tot}(\mathbf{s}) = \sum_{i=1}^5 Z_t^i(\mathbf{s}) + Z_t^o(\mathbf{s})$$

$$Z_t^o(s) = \max \left( 0, \tilde{Z}_t^o(s) \right) \quad \tilde{Z}_t^o(s) = \beta_{0,t}^o + \beta_{0,t}^o(\mathbf{s}) + \beta_{1,t}^o Q_t^o(B_s)$$

# Spatial Dependence

Spatial dependence enters the model through the  $\beta_{0,t}^i(s)$  parameters for  $i \in \{o, 1, 2, 3, 4, 5\}$ .

$$\beta_{0,t}^i(\mathbf{s}) = \sigma_t^i w_t^i(\mathbf{s})$$

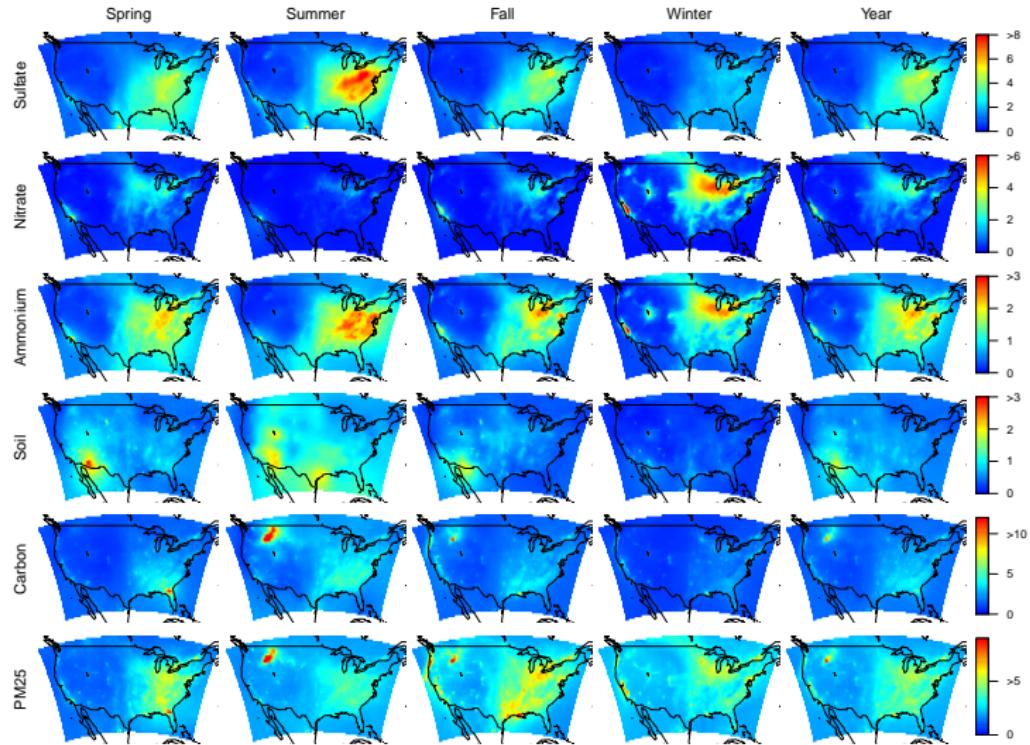
where  $w_t^i(\mathbf{s})$  are zero mean, variance 1, Gaussian processes with exponential correlation given by

$$\text{corr}(w_t^i(\mathbf{s}), w_t^i(\mathbf{s}')) = \exp(-\phi_t^i |\mathbf{s} - \mathbf{s}'|)$$

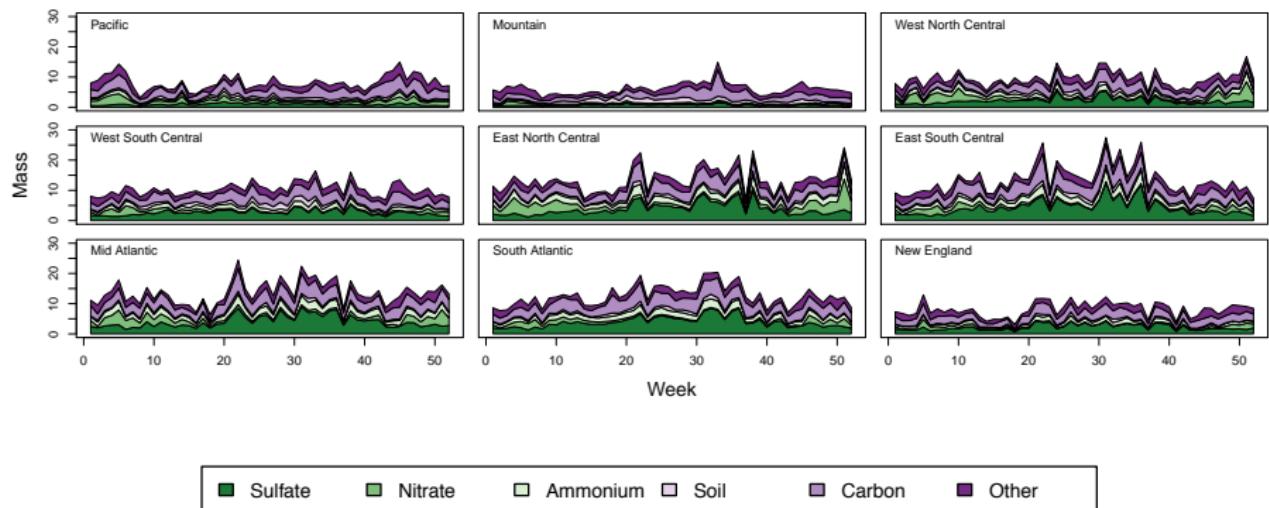
Additional dependence between species is introduced via coregionalization,

$$\begin{pmatrix} \beta_{0,t}^i(\mathbf{s}) \\ \beta_{0,t}^j(\mathbf{s}) \end{pmatrix} = \mathbf{A}_t \begin{pmatrix} w_t^i(\mathbf{s}) \\ w_t^j(\mathbf{s}) \end{pmatrix}.$$

# Model results



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# MCMC performance

Parameter	CPU (secs)	CPU+GPU (secs)	Rel. Performance
$\beta_0, \beta_1$	0.00029	0.00030	0.97
$\beta_0(s)$	0.09205	0.09132	1.00
$\sigma^2$	0.00383	0.00385	0.99
$\phi$	0.46084	0.25174	1.83
$\tau_i^2, \tau_{tot}^2$	0.00003	0.00003	1.00
Total	0.55708	0.34729	1.60

## Run times

Total run time for model fitting (50,000 iterations):

- CPU - 7.7 hours  $\times$  52 weeks
- CPU+GPU - 4.8 hours

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                                                 × 3 model variants  
                                                 × 10 for cross validation

# Lessons

- Established infrastructure makes a huge difference in development time
  - 1 hour to go from CPU implementation to CPU+GPU implementation
  - Code shown previously is 2/3 of the changes necessary [Code](#)
- In practice, was easier to run CPU only code across more servers (configuration time / effort)
  - Not possible (or at least easy) for models variants that are not independent in time.
  - There will be ~ 20 desktops with GPUs available in the department (available via Condor)
- Rcpp Attributes offer huge advantages in development and deployment
  - Simplifies external dependencies (locally)
  - Full compatibility is the goal for RcppGP

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# Low rank approximations

For a Gaussian process

$$Y(\mathbf{s}) = \mathbf{x}(\mathbf{s})' \boldsymbol{\beta} + w(\mathbf{s}) + \epsilon, \quad \epsilon \sim N(0, \tau^2 I)$$

$$w(\mathbf{s}) \sim N(0, \mathbf{C}(\mathbf{s})), \quad \mathbf{C}(\mathbf{s}, \mathbf{s}') = \sigma \rho(\mathbf{s}, \mathbf{s}' | \theta)$$

we can approximate  $\mathbf{C}(\mathbf{s})$  with a low rank approximation with the form  $\mathbf{U} \mathbf{S} \mathbf{V}'$  where  $\mathbf{U}$  and  $\mathbf{V}$  are  $n \times k$  and  $\mathbf{S}$  is  $k \times k$ .

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This allows for the use of the Sherman-Morrison-Woodbury formula for the inverse (and determinant),

$$\mathbf{C}(\mathbf{s})^{-1} \approx (\mathbf{A} + \mathbf{U} \mathbf{S} \mathbf{V}')^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1} \mathbf{U} (\mathbf{S}^{-1} + \mathbf{V}' \mathbf{A}^{-1} \mathbf{U})^{-1} \mathbf{V}' \mathbf{A}^{-1}.$$

# Gaussian Predictive Processes

For a rank  $k$  approximation,

- Pick  $k$  knot locations  $\mathbf{s}^*$
- Calculate knot covariance ( $\mathbf{C}(\mathbf{s}^*)$ ) and knot cross-covariance ( $(\mathbf{C}(\mathbf{s}^*))^{-1}$ )
- Approximate full covariance

$$\mathbf{C}(\mathbf{s}) \approx \mathbf{C}(\mathbf{s}, \mathbf{s}^*) \mathbf{C}(\mathbf{s}^*)^{-1} \mathbf{C}(\mathbf{s}^*, \mathbf{s}).$$

- Systematically underestimates variance, inflates  $\tau^2$ .
- Modified predictive process corrects this using

$$\mathbf{C}(\mathbf{s}) \approx \mathbf{C}(\mathbf{s}, \mathbf{s}^*) \mathbf{C}(\mathbf{s}^*)^{-1} \mathbf{C}(\mathbf{s}^*, \mathbf{s}) + \text{diag}\left(\mathbf{C}(\mathbf{s}) - \mathbf{C}(\mathbf{s}, \mathbf{s}^*) \mathbf{C}(\mathbf{s}^*)^{-1} \mathbf{C}(\mathbf{s}^*, \mathbf{s})\right).$$

Banerjee, Gelfand, Finley, Sang (2008)    Finley, Sang, Banerjee, Gelfand (2008)

# Low Rank Approximations via Random Projections

- ① Starting with an  $m \times n$  matrix  $\mathbf{A}$ .
- ② Draw an  $n \times k + p$  Gaussian random matrix  $\Omega$ .
- ③ Form  $\mathbf{Y} = \mathbf{A}\Omega$  and compute its QR factorization  $\mathbf{Y} = \mathbf{Q} \mathbf{R}$
- ④ Form the  $k + p \times n$  matrix  $\mathbf{B} = \mathbf{Q}' \mathbf{A}$ .
- ⑤ Compute the SVD of the small matrix  $\mathbf{B}$ ,  $\mathbf{B} = \hat{\mathbf{U}} \mathbf{S} \mathbf{V}'$ .
- ⑥ Form the matrix  $\mathbf{U} = \mathbf{Q} \hat{\mathbf{U}}$ .

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- ② Draw an  $n \times k + p$  Gaussian random matrix  $\Omega$ .
- ③ Form  $\mathbf{Y} = \mathbf{A}\Omega$  and compute its QR factorization  $\mathbf{Y} = \mathbf{Q} \mathbf{R}$
- ④ Form the  $k + p \times n$  matrix  $\mathbf{B} = \mathbf{Q}' \mathbf{A}$ .
- ⑤ Compute the SVD of the small matrix  $\mathbf{B}$ ,  $\mathbf{B} = \hat{\mathbf{U}} \mathbf{S} \mathbf{V}'$ .
- ⑥ Form the matrix  $\mathbf{U} = \mathbf{Q} \hat{\mathbf{U}}$ .

Resulting approximation has nicely bounded expected error,

$$\mathbb{E} \ \| \mathbf{A} - \mathbf{USV}' \| \leq \left[ 1 + \frac{4\sqrt{k+p}}{p-1} \sqrt{\min(m,n)} \right] \sigma_{k+1}.$$

Halko, Martinsson, Tropp (2011)

# Random Matrix Low Rank Decompositions and GPs

Preceeding algorithm can be modified slightly to take advantage of the positive definite structure of a covariance matrix.

- ① Starting with an  $n \times n$  covariance matrix  $\mathbf{A}$ .
- ② Draw an  $n \times k + p$  Gaussian random matrix  $\Omega$ .
- ③ Form  $\mathbf{Y} = \mathbf{A}\Omega$  and compute its QR factorization  $\mathbf{Y} = \mathbf{Q}\mathbf{R}$
- ④ Form the  $k + p \times k + p$  matrix  $\mathbf{B} = \mathbf{Q}'\mathbf{A}\mathbf{Q}$ .
- ⑤ Compute the eigen decomposition of the small matrix  $\mathbf{B}$ ,  
$$\mathbf{B} = \hat{\mathbf{U}}\mathbf{S}\hat{\mathbf{U}}'$$
.
- ⑥ Form the matrix  $\mathbf{U} = \mathbf{Q}\hat{\mathbf{U}}$ .

Once again we have a bound on the error,

$$\mathbb{E} \|\mathbf{A} - \mathbf{Q}(\mathbf{Q}'\mathbf{A}\mathbf{Q})\mathbf{Q}'\| = \mathbb{E} \|\mathbf{A} - \mathbf{U}\mathbf{S}\mathbf{U}'\| \lesssim c \cdot \sigma_{k+1}.$$

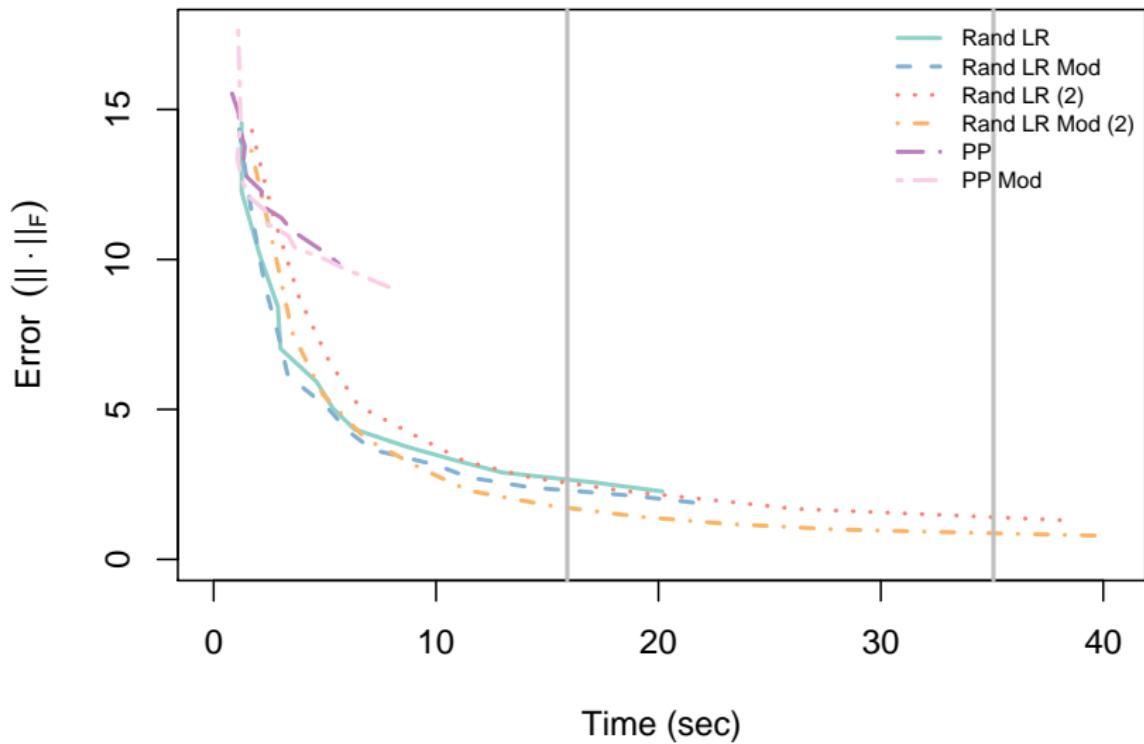
Halko, Martinsson, Tropp (2011), Banerjee, Dunson, Tokdar (2012)

# Low Rank Approximations and GPUs

Both predictive process and random matrix low rank approximations are good candidates for acceleration using GPUs.

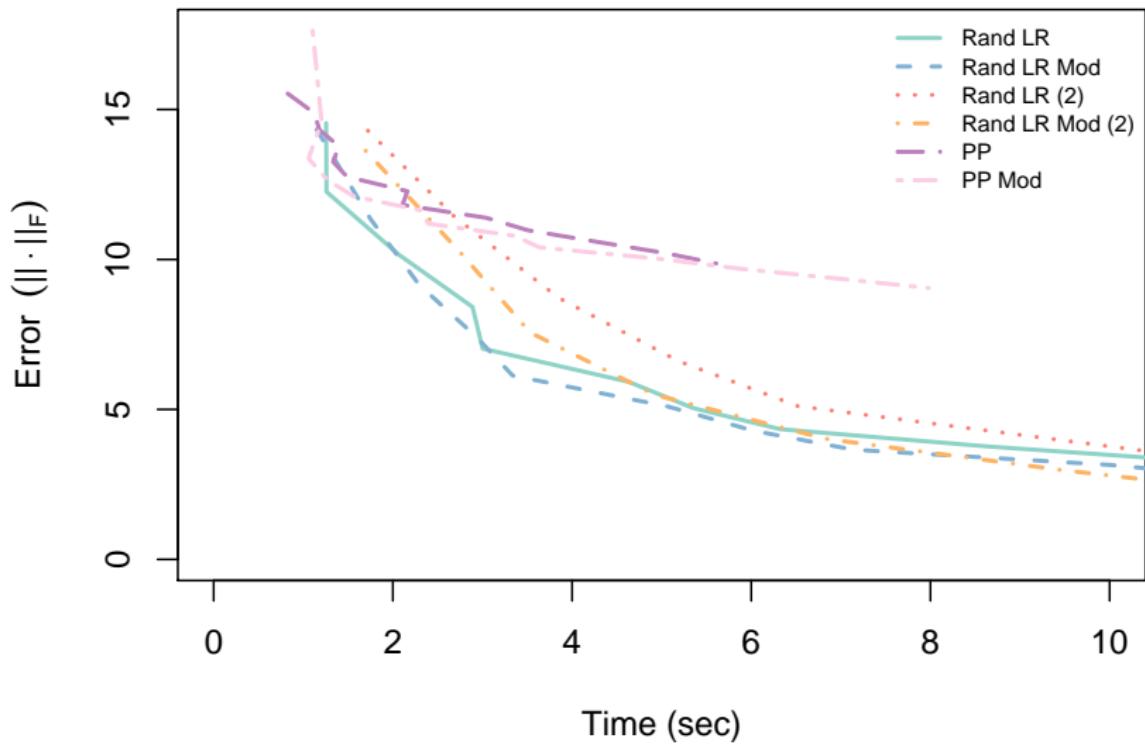
- Both use Sherman-Woodbury-Morrison to calculate the inverse (involves matrix multiplication, addition, and a small matrix inverse).
- Predictive processes involves several covariance matrix calculations (knots and cross-covariance) and a small matrix inverse.
- Random matrix low rank involves a large matrix multiplication ( $\mathbf{A}\Omega$ ) and several small matrix decompositions (QR, eigen).
- Functionality for both approaches included in current version of RcppGP (inv\_lr and inv\_pp).

# Matrix inverse (fixed rank, strong dependence)



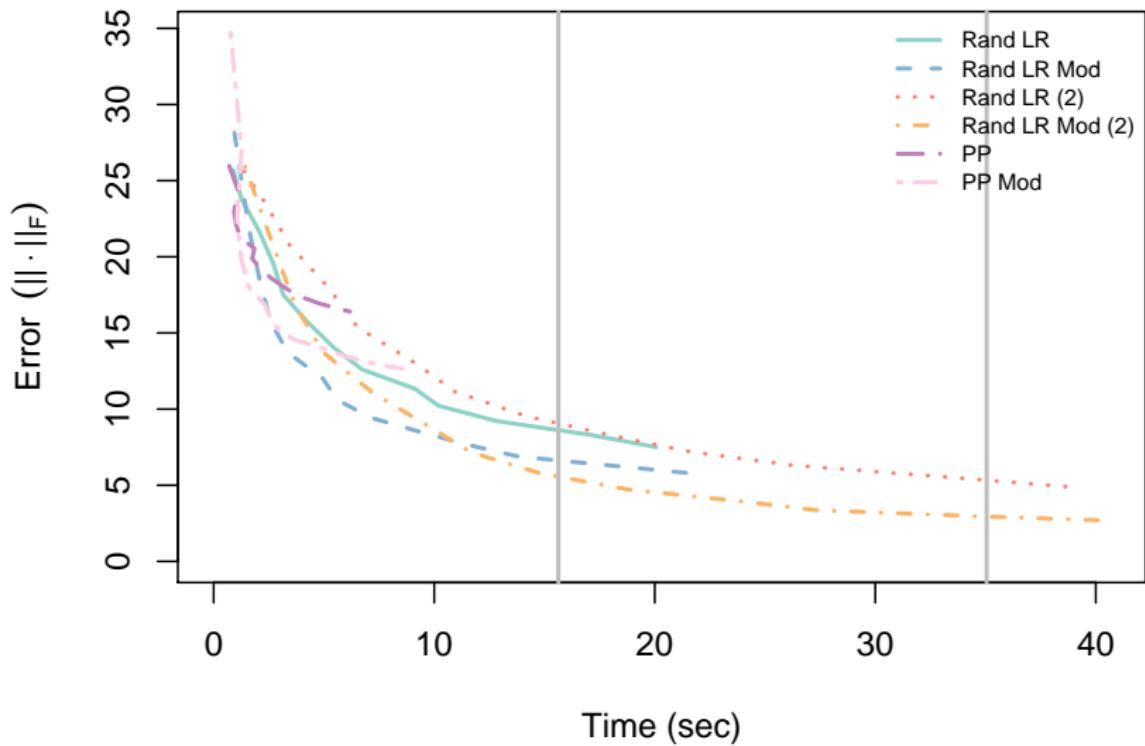
$$n = 15000, \quad k = \{100, \dots, 4900\}$$

# Matrix inverse (fixed rank, strong dependence)



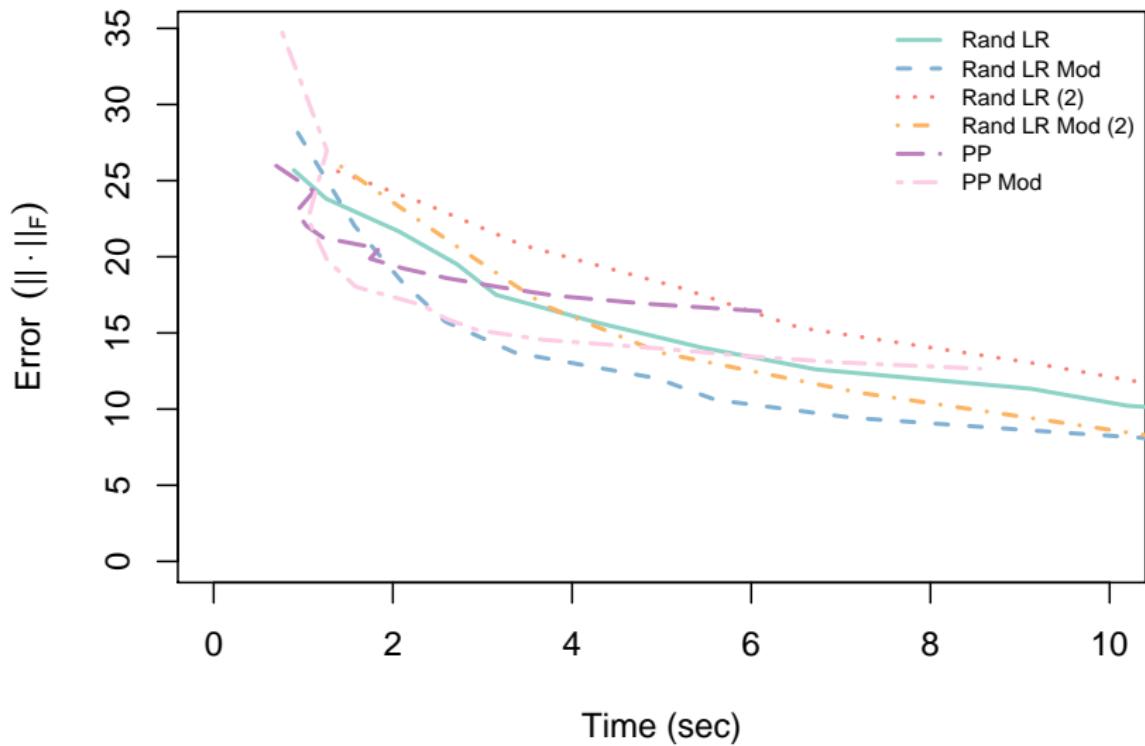
$$n = 15000, \quad k = \{100, \dots, 4900\}$$

# Matrix inverse (fixed rank, weak dependence)



$$n = 15000, \quad k = \{100, \dots, 4900\}$$

# Matrix inverse (fixed rank, weak dependence)



$$n = 15000, \quad k = \{100, \dots, 4900\}$$

## Rand. Matrix Low Rank Decompositions for Prediction

This approach can also be used for prediction, if we want to sample

$$\mathcal{N}(0, \Sigma) \text{ with } \Sigma \approx \mathbf{U} \mathbf{S} \mathbf{U}' = (\mathbf{U} \mathbf{S}^{1/2} \mathbf{U}') (\mathbf{U} \mathbf{S}^{1/2} \mathbf{U}')'$$

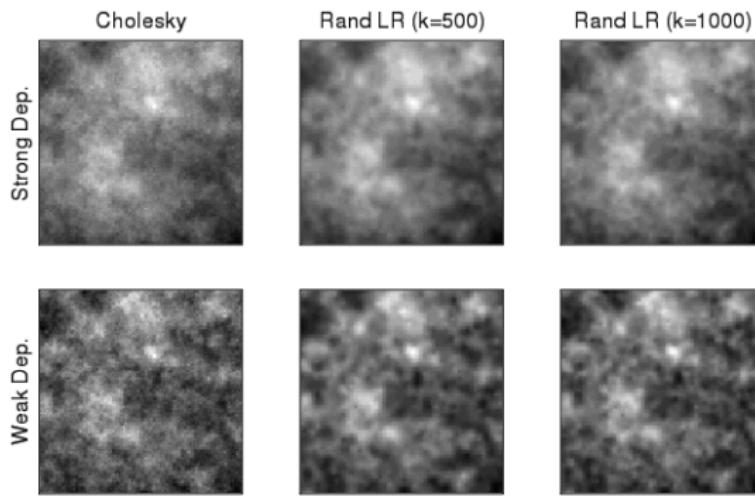
then  $X_{pred} = (\mathbf{U} \mathbf{S}^{1/2} \mathbf{U}') \times \mathbf{Z}$  where  $Z_i \sim \mathcal{N}(0, 1)$ .

# Rand. Matrix Low Rank Decompositions for Prediction

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$$n = 1000, \quad p = 10000$$

Dehdari, Deutsch (2012)

# Future Directions

- Refinement of RcppGP
  - Transition to header only implementation
  - Transparent GPU to CPU failover
  - Support for fixed error (instead of rank) random matrix low rank decomposition
  - Thinking about out-of-memory based approaches
- Future of GPUs, CUDA, and Magma
  - Single vs. Multi-GPU algorithms
  - Mixed precision algorithms
  - NVBLAS
  - Unified memory
  - cuSolver

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UCLA IoES

## Speciated PM<sub>2.5</sub>

- Alan Gelfand - Duke
- Dave Holland - EPA
- Erin Schliep - Duke

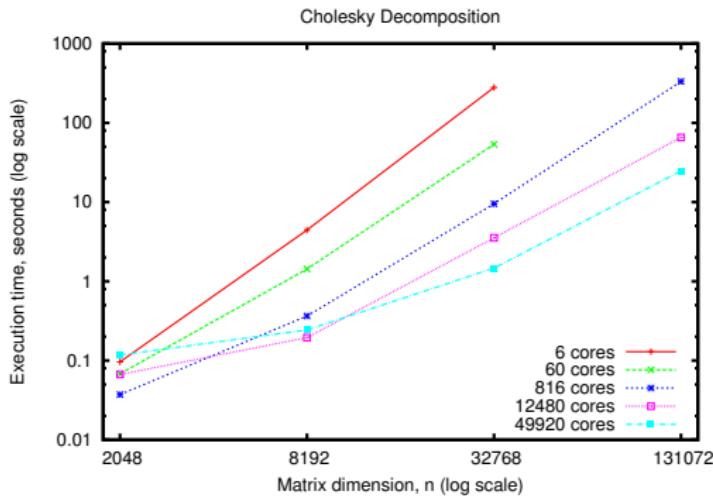
RcppGP    <https://github.com/rundel/RcppGP>  
Talk        <https://github.com/rundel/Presentations>



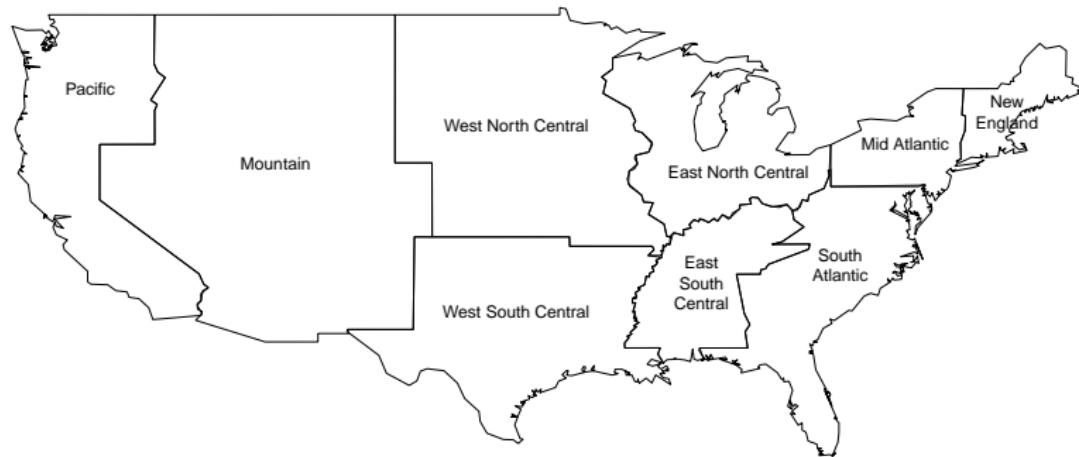
# Another Approach

bigGP is an R package written by Chris Paciorek, et al.

- Specialized implementation of LA operation for GPs
- Designed to run on large super computer clusters
- Uses both shared and distributed memory
- Able to fit models on the order of  $n = 65k$  (32 GB Cov. matrix)



# Regions



Back