Parallelizing Gaussian Process Calculations in R

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www.jstatsoft.org/v63/i10
https://github.com/paciorek/bigGP

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A basic Gaussian process (GP) model

$$\begin{aligned} \boldsymbol{Y}|\boldsymbol{g},\boldsymbol{\theta} &\sim N(\boldsymbol{g}, \boldsymbol{C}_y(\boldsymbol{\theta})) \\ \boldsymbol{g}|\boldsymbol{\theta} &\sim N(\boldsymbol{\mu}(\boldsymbol{\theta}), \boldsymbol{C}_g(\boldsymbol{\theta})) \end{aligned}$$

$$f(\boldsymbol{y}) \propto \left| \boldsymbol{C}_y(\boldsymbol{\theta}) + \boldsymbol{C}_g(\boldsymbol{\theta}) \right|^{-\frac{1}{2}} \cdot \exp\left(-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\theta}))^T (\boldsymbol{C}_y(\boldsymbol{\theta}) + \boldsymbol{C}_g(\boldsymbol{\theta}))^{-1} (\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\theta})) \right)$$

Computational goals for GP calculations:
- Likelihood optimization
- Prediction
- Prediction uncertainty
- Simulation (unconditional and conditional on data)

Computational patterns for GP calculations:
- Construct covariance matrices (training and prediction points)
- Cholesky decomposition
- Forward/backsolve
- Matrix multiplication (various forms: matrices, vectors, crossproducts, diagonal matrices, etc.)

Responses to computational considerations

Change the model

- Sparsify the covariance/precision matrix
- Reduce dimensionionality (e.g., basis functions)
- Predict based on subset of data / local models
- Approximate the likelihood

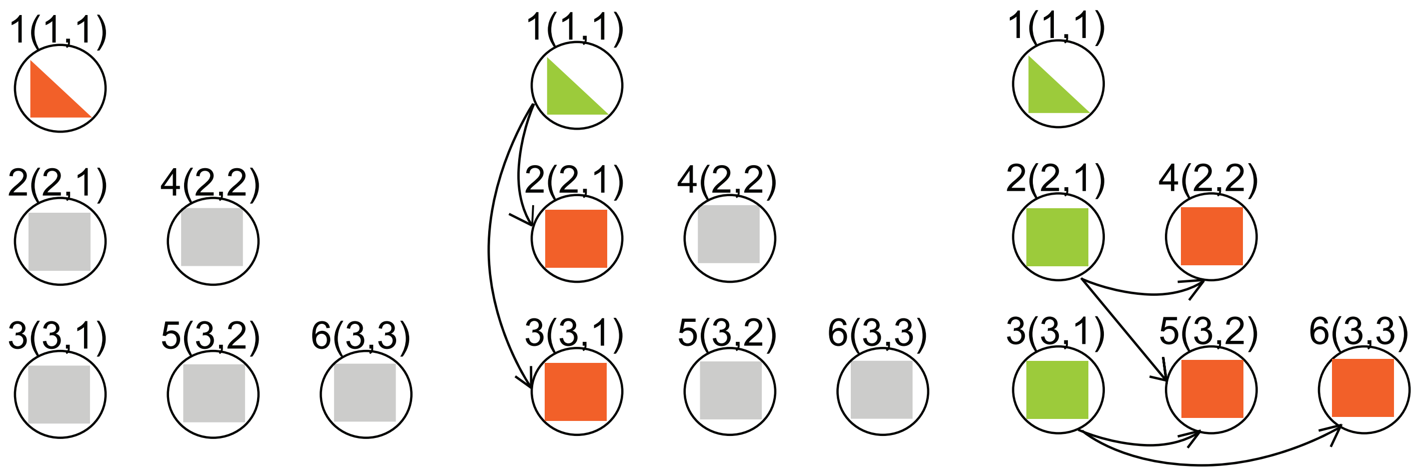
Use a lot of processing power

- Shared memory (multicore architecture)
- GPUs
- Distributed memory (clusters, supercomputers)

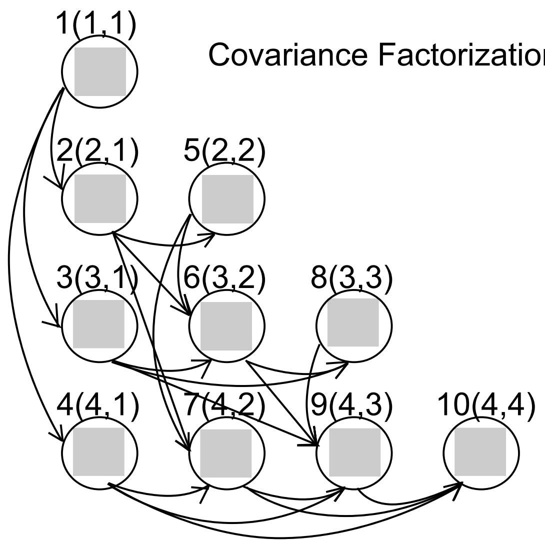
Our approach

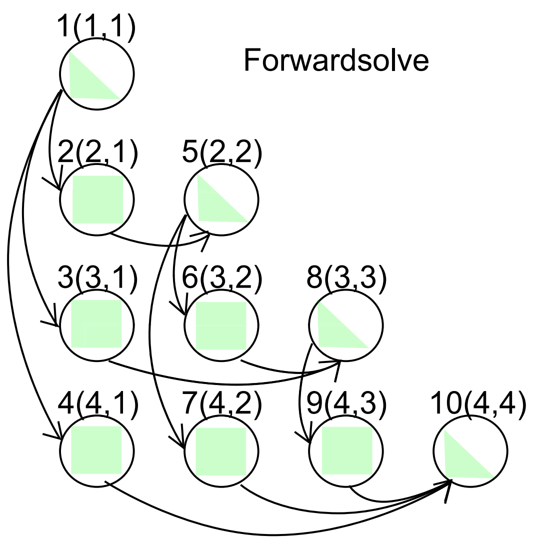
- Use many cores to distribute computation and memory
- Hybrid parallelization = distributed processing (MPI) + threaded computation (OpenMP)
- Original plan to use ScaLapack from R (pbdR now does this)
- bigGP: tailor parallel linear algebra algorithms to Cholesky decomposition (rate-limiting step) and interface to R

Blockwise Cholesky (Crout's algorithm)



⬜ covariance marix   🟩 factored result   🟥 just updated





⬜ covariance marix   🟩◣ factorized result

Computational considerations

Questions

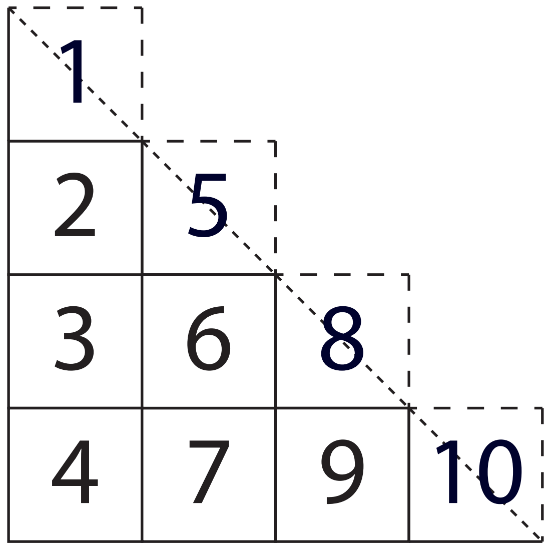
- How many submatrices / how big
- How many submatrices (and which ones) per node or per process
- How many processes per multi-core node / should individual submatrix calculations be threaded

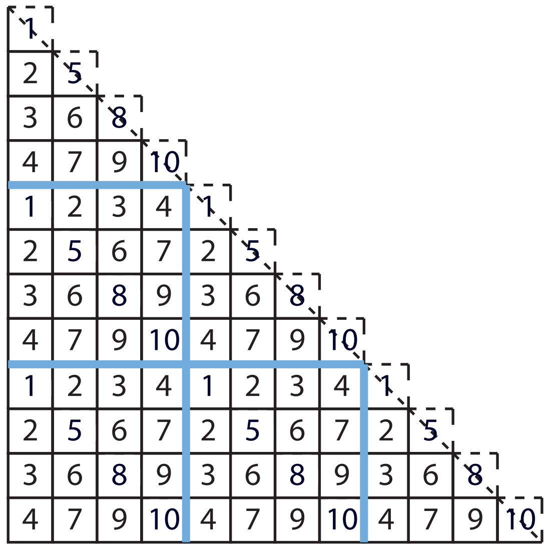
Basic tradeoffs

- Efficient local computation (increase block size up to point that submatrix doesn't fit in cache)
- Load-balancing (want all processors active)
- Reduce communication (pass less information between processes)

Computational approach

Suppose we have P=10 processes and D=4 blocks. We could have one submatrix per process (left with blocking factor B=4 and h=1) or multiple submatrices per process (right with replication factor h=3 and blocking factor of B=hD=12)





Computational approach

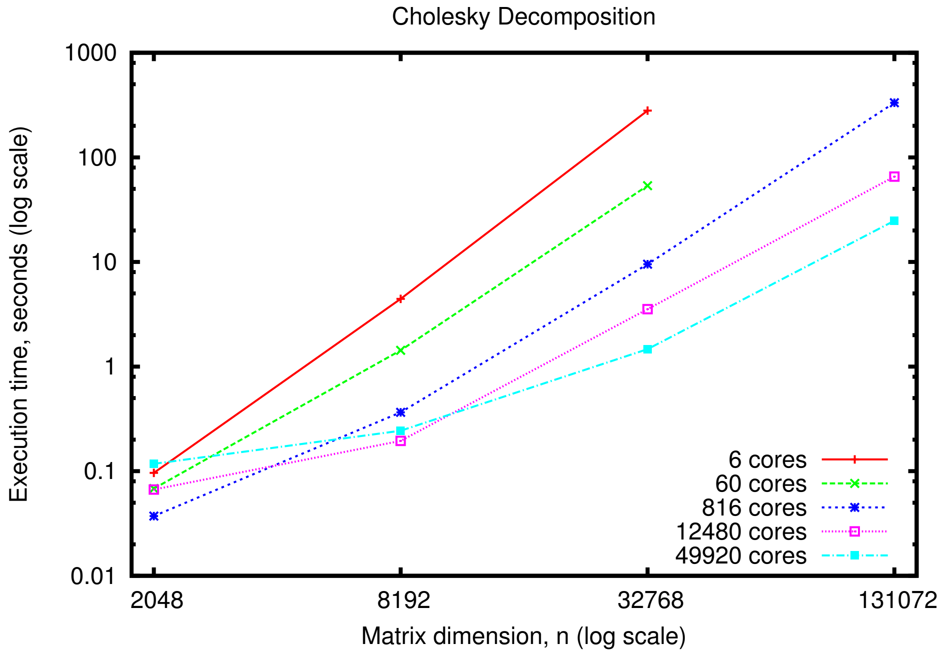
Answers:

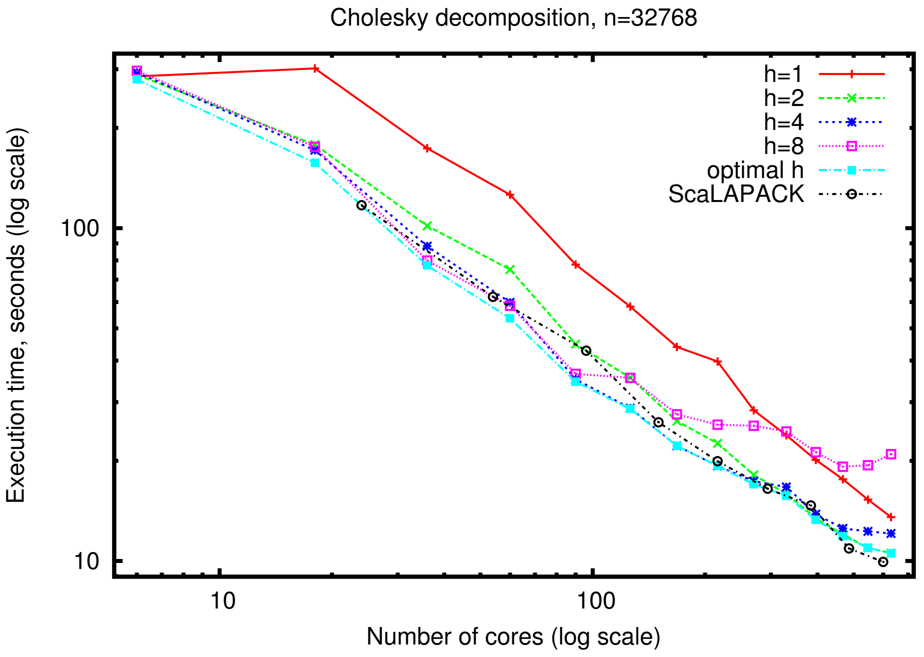
- How many blocks (submatrices) / how big:
  Your choice but 1000x1000 may be good; submatrix size is ~ n/hD where P=D(D+1)/2
- How many submatrices (and which ones) per node or per process:
  Your choice of h. We allocate submatrices to processes for you.
- How many processes per node / should individual block calculations be threaded:
  One process per node with threading, but might define a "node" as a subset of processors on cluster machine – e.g. divide 24 cores into 4 6-core "nodes"

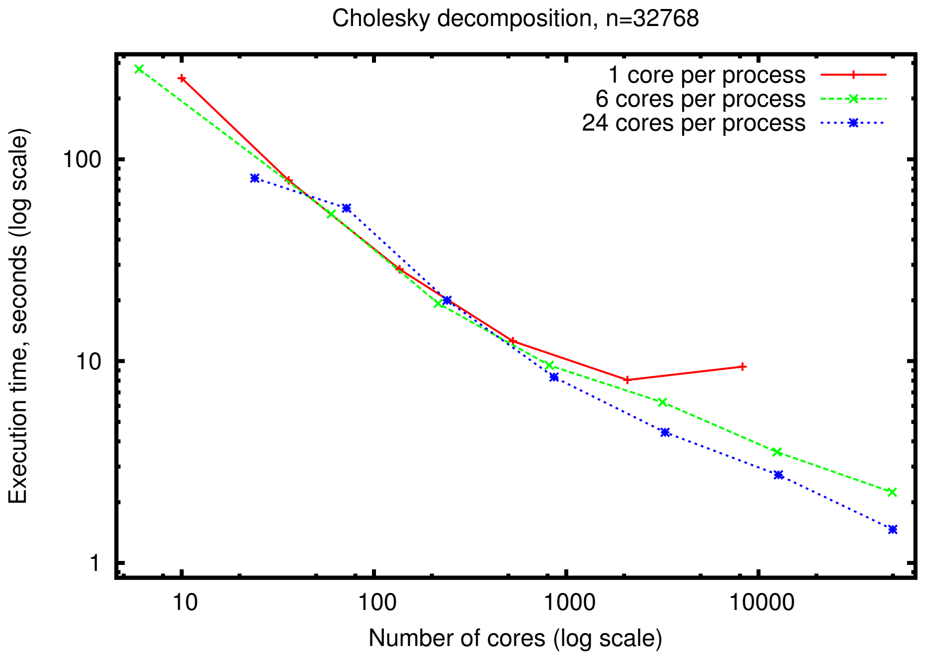
Comments

- Our allocation of which submatrices are grouped on a process improves load-balancing
- Using multiple submatrices per process and one process per "node" reduces communication
- Flexible choice of #submatrices per process allows tailoring of submatrix size to cache
- Flexible number of cores per process (cores on a virtual node) allows hybrid parallelization that balances threading vs. additional virtual nodes

Scaling results





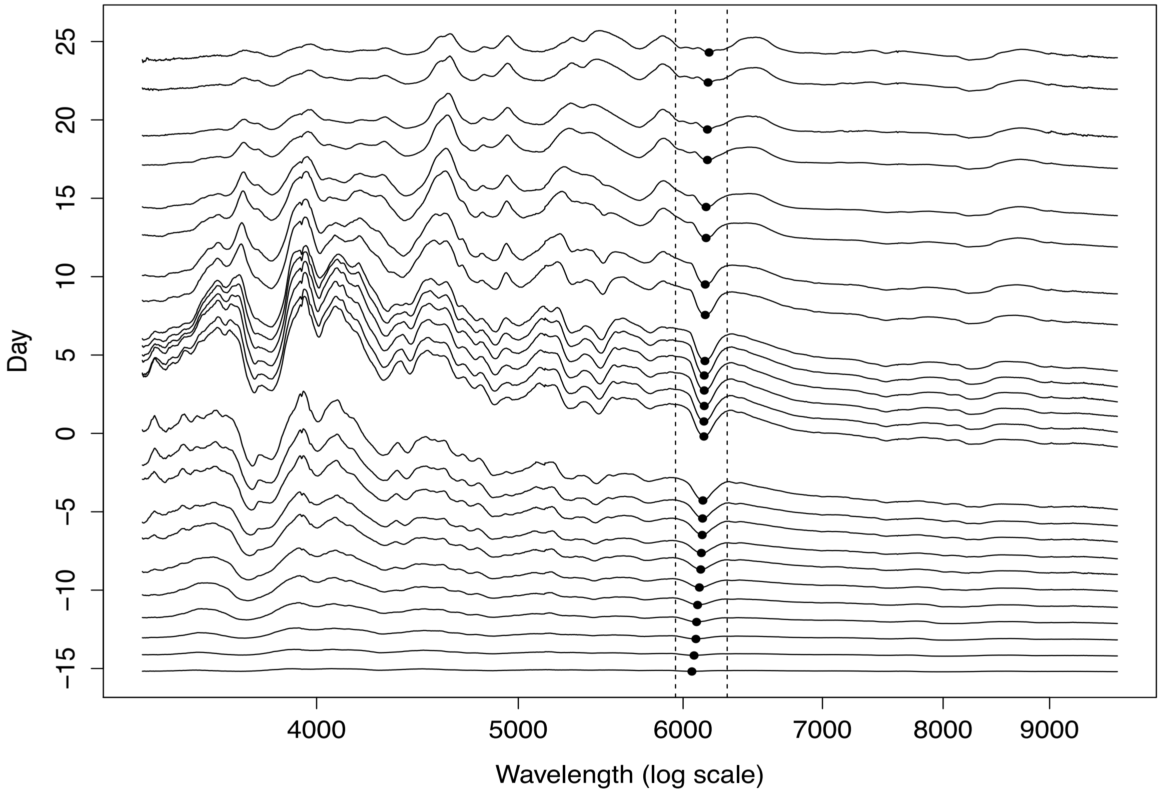


Software design of the *bigGP* package

- Initialization (from R) initializes multiple processes and sets up how submatrices are assigned to processes
- All computations done in a distributed fashion and sequential operations (e.g., Cholesky, then forwardsolve then matrix multiplication) carried out as pipeline
- Core distributed linear algebra operations (Cholesky, forwardsolve, matrix multiplication, etc.) are done via MPI from C
- *bigGP* API controls operations from R
    - Functions for managing objects on worker processes and moving general objects between master and workers
    - Functions for distributing and collecting distributed matrices/vectors between master and workers, hiding details of what is stored where and in what format
    - Wrapper functions that carry out the distributed linear algebra by calling the core C/MPI code
- Specific kriging (likelihood optimization) implementation via *krigeProblem* ReferenceClass and member functions that carry out:
    - Construction of mean and covariance (in distributed fashion) using user-defined functions
    - Calculation of log density
    - Prediction with uncertainty
    - Simulation either conditional or unconditional on data

Astrophysics example

- Analysis by C. Kaufman in collaboration with R. Thomas
- Data are flux from the Type Ia supernova SN2011fe, as a function of wavelength and day
  - n = 67,275
- Interest lies in smoothing the data and estimating the wavelength of minimum flux



Statistical model and code

$$Y_i = Z(t_i\,, w_i) + \alpha_{t_i} + \epsilon_i$$
$$Z \sim GP(\mu(\cdot;\kappa,\lambda), \sigma^2 K(\cdot,\cdot;\rho_t) K(\cdot,\cdot;\rho_w))$$

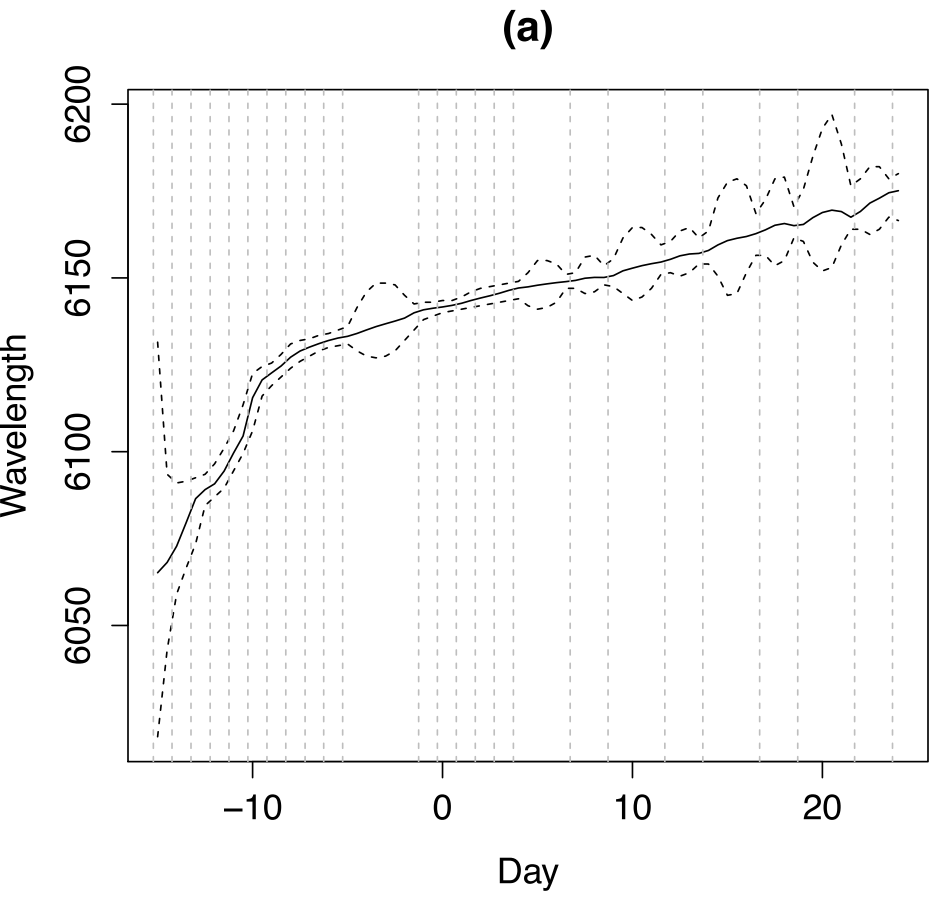
- Random effects, alpha, for each day
- Known, heteroscedastic error variances based on instrumentation
- Covariance of product form in the two dimensions
- Mean function (of time only) based on empirical pattern of variation with wavelength

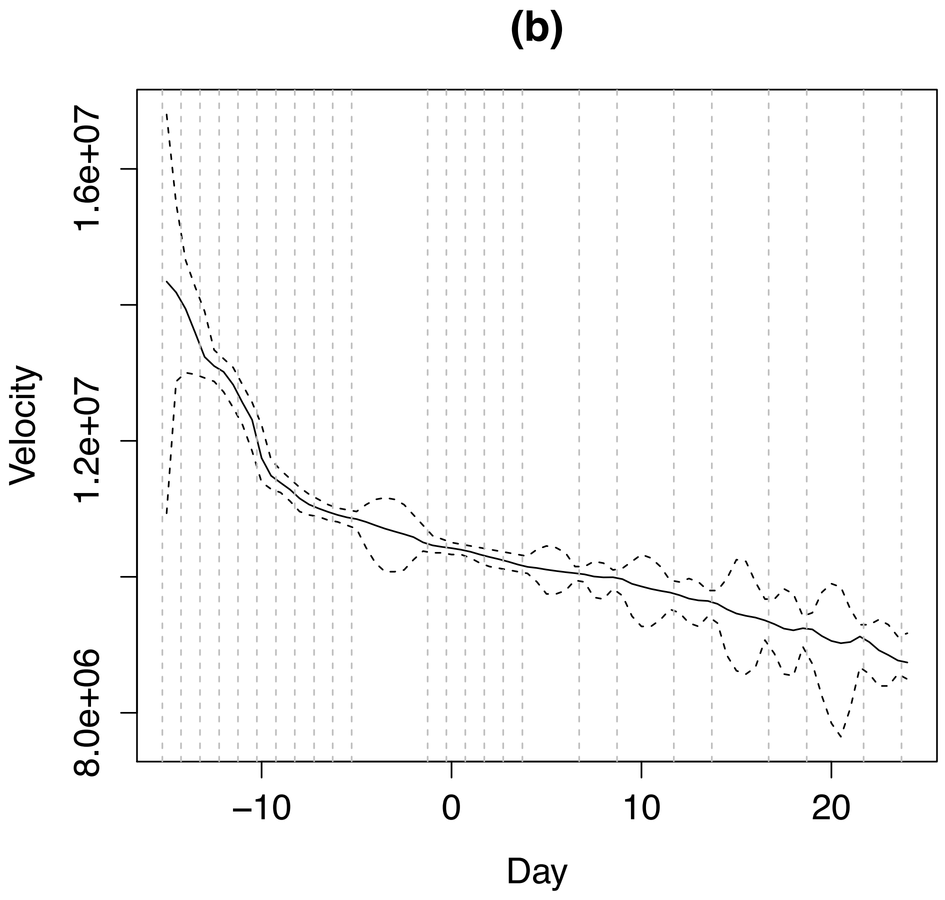
- 465 processes, 6 cores per process, 117 nodes on NERSC's Hopper supercomputer
- R code:

```
R> prob <- krigeProblem$new(‘prob’, numProcesses = 465, meanFunction =
     SN2011fe_meanfunc, predMeanFunction = SN2011fe_predmeanfunc, covFunction
     = SN2011fe_covfun, crossCovFunction = SN2011fe_crosscovfun,
     predCovFunction = SN2011_predcovfun, inputs = c(as.list(SN2011fe),
     as.list(SN2011fe_newdata)), data  = SN2011fe$flux)
R> prob$optimizeLogDens(method = ‘L-BFGS-B’, lower = rep(1e-15, nParams))
R> pred <- prob$predict(ret = TRUE, se.fit = TRUE)
R> realiz <- prob$simulateRealizations(r = 1000, post = TRUE)
```

Results

- Predictions on subdomain on a grid in time and wavelength for 55,379 points
- Numerical issues arise in bigGP (no pivoting) for finer grids (numerically non-positive def.)
- Credible intervals based on 1000 posterior draws, using MLE parameter estimates





- For methodological work on inferring minima, see Lee, Kaufman and Thomas: http://www.stat.berkeley.edu/~cgk/papers/assets/lee2013.pdf

Next steps

- Will try to continue to support bigGP at basic level in spare time
- Current kriging code allows flexible mean and covariance specification, but for a basic model
- Low-level API allows flexible use of linear algebra calls, so others could build more general and flexible models using the API
- pbdR is another option and more general