Everyday Multithreading

Parallel computing for genomic evaluations in *R*

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Introduction

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- High Dimensional livestock data sets
- New computational challenges
- Paradigm shift in breeding programs **and** computing
- From sparse to dense MME (or mixtures)
- High storage, memory and computing demands

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- **Solution**: Making use of available hardware resources by parallel computing

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- In general: First single-threaded optimization then parallelization

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But: Can be extended and multi-threaded through C/C++/Fortran shared libraries

General Implementation

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1. *R* as the basic environment for data preparation and supply
2. Linking C++ to R: *Rcpp* (Eddelbuettel and Francois, 2011)
3. Linear Algebra: *Eigen* $\rightarrow$ Vectorization! (Guennebaud et al., 2010)
4. Eigen + Rcpp + Sparse-Matrix support: *RcppEigen* (Bates and Eddelbuettel, 2013)
5. Parallelization: *OpenMP*

Parallel Computing in *cpgen*

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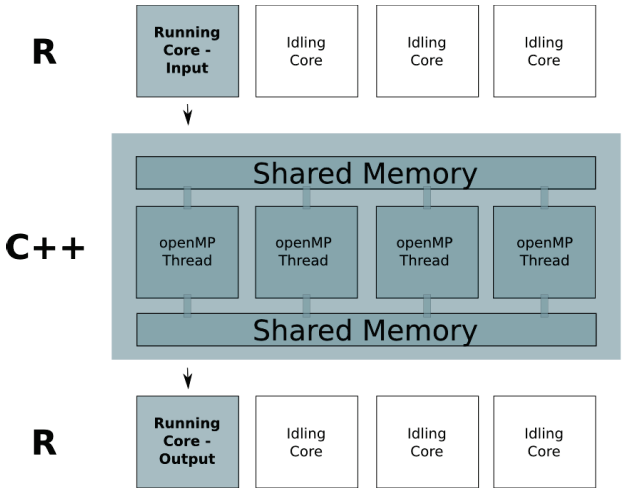

Functionality

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1. Single-Site Gibbs Sampler for Mixed Models with arbitrary number of random effects (sparse or dense design matrices)
2. Genomic Prediction Module: Different Methods, Cross Validation
3. GWAS Module: *EMMAX* - highly efficient and very flexible single marker GWAS
4. Tools: Genomic additive and dominance relationships, Crossproducts, Covariance Matrices, ...

Gibbs Sampler

Runs models of the following form:

$$\mathbf{y} = \mathbf{Xb} + \mathbf{Z}_1\mathbf{u}_1 + \mathbf{Z}_2\mathbf{u}_2 + \mathbf{Z}_3\mathbf{u}_3 + ... + \mathbf{Z}_n\mathbf{u}_n + \mathbf{e}$$

- For all u_k: $MVN(\mathbf{0}, \mathbf{I}\sigma^2_{u_k})$
- If u_k is assumed to follow some $MVN(\mathbf{0}, \mathbf{G}_k\sigma^2_k)$:

Design matrix must be constructed as: $\mathbf{Z}_k = \mathbf{Z}_k\mathbf{G}^{1/2}$, yielding independent effect in $\mathbf{u}_k$ (Waldmann et al., 2008).

Genomic BLUP

GBLUP can be accomplished very efficiently (Kang et al., 2008):

$$\mathbf{y} = \mathbf{Xb} + \mathbf{a} + \mathbf{e} \quad \text{with: } \mathbf{a} \sim MVN(\mathbf{0}, \mathbf{G}\sigma_a^2)$$

By finding the decomposition: $\mathbf{G} = \mathbf{UDU}'$ and premultiplying the model equation by $\mathbf{U}'$ we get:

$$\mathbf{U}'\mathbf{y} = \mathbf{U}'\mathbf{Xb} + \mathbf{U}'\mathbf{a} + \mathbf{U}'\mathbf{e}$$

with:

$$\begin{aligned} Var(\mathbf{U}'\mathbf{y}) &= \mathbf{U}'\mathbf{GU}\sigma_a^2 + \mathbf{U}'\mathbf{U}\sigma_e^2 \\ &= \mathbf{U}'\mathbf{UDU}'\mathbf{U}\sigma_a^2 + \mathbf{I}\sigma_e^2 \\ &= \mathbf{D}\sigma_a^2 + \mathbf{I}\sigma_e^2 \end{aligned}$$

GWAS

- Single marker regression
- Controlling for polygenic background effect through [assumed] covariance structure $\mathbf{V}$ of $\mathbf{y}$ - EMMAX (Kang et al., 2010)
- Obtaining General Least Squares estimates for marker effects:

$$\hat{\beta} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$$

This is equivalent to:

$$\hat{\beta} = (\mathbf{X}^{*\prime}\mathbf{X}^{*})^{-1}\mathbf{X}^{*\prime}\mathbf{y}^{*}, \quad \text{with } \mathbf{X}^{*} = \mathbf{V}^{-1/2}\mathbf{X}, \quad \mathbf{y}^{*} = \mathbf{V}^{-1/2}\mathbf{y}$$

Parallel Computing in *cpgen*

What is parallelized:

1. All crossproduct-like computations
2. Sampling of random effects in Gibbs Sampler (dot product, vector-vector subtraction) $\rightarrow$ Fernando et al., 2014
3. Cross Validation for genomic prediction
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Number of threads being used can be controlled during runtime

2,000 Observations, 50,000 Markers

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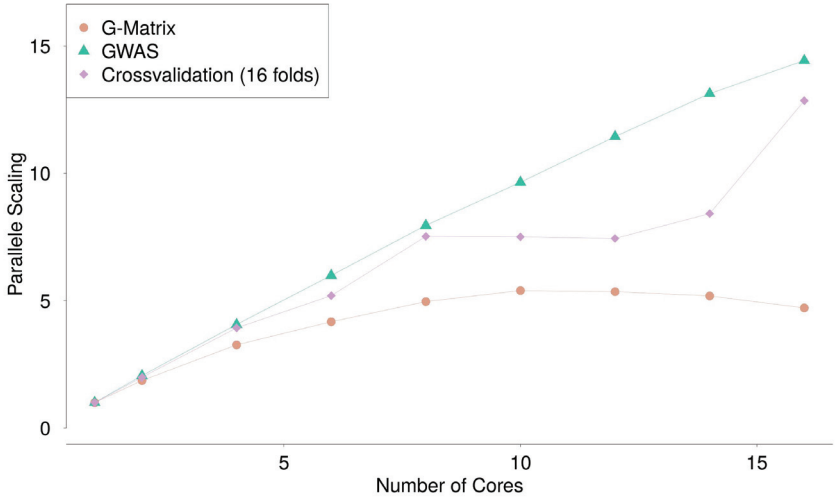

Gibbs Sampler (BRR) - 10,000 Markers

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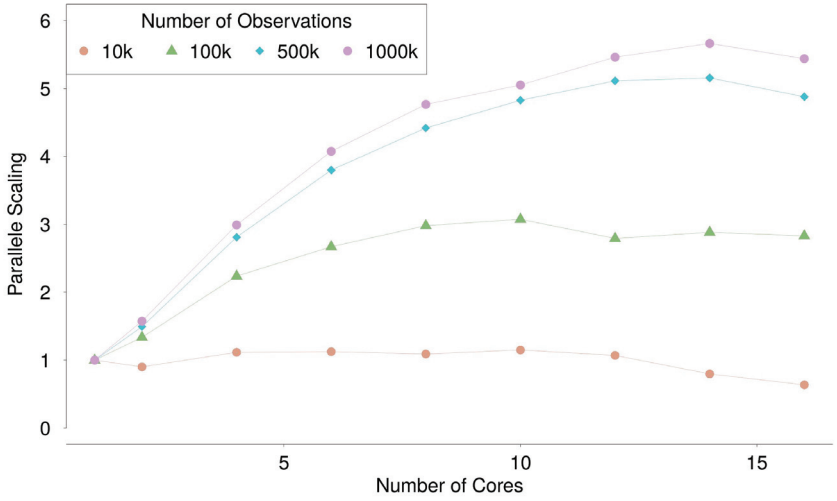

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- We can make use of the computational power present in workstation PCs $\rightarrow$ *Everyday Multithreading*
- **But**: Size of solvable problem is limited by available memory
- With 1 TB of memory, the package could fit a BRR model with 3 million observations and 40k markers

Thank you for the attention

Github `https://github.com/cheuerde/cpgen`
R-Forge `https://r-forge.r-project.org/R/?group_id=1687`

Absolute Timings

10 Cores, 30,000 markers

- BRR: 1 million observations, 30k iterations $\sim$ 100 hours
- GWAS: 10k observations $\sim$ 7 minutes
- G-Matrix: 10k observations $\sim$ 2 minutes