Introduction to BLUPF90 software suite

UNIVERSITY OF GEORGIA

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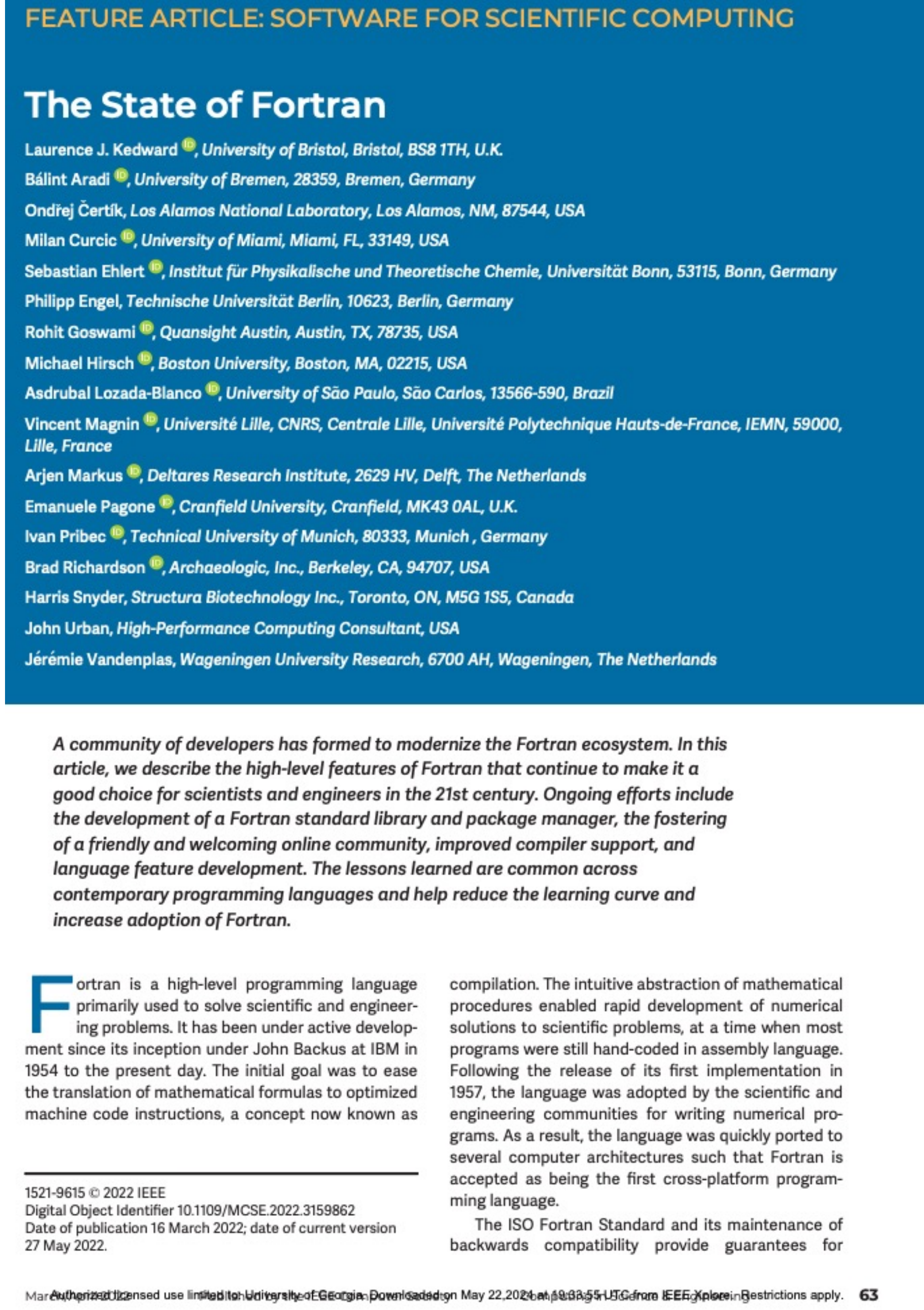
BLUPF90 TEAM – 05/2024

ANIMAL BREEDING AND GENETICS GROUP
SUMMER COURSE 2024

BLUPF90 software suite

- Collection of software
  - Fortran ≥ 90
    - Fortran = Formula Translation System
    - Fortran = Formula Translator
    - First compiler in 1957 by IBM



FEATURE ARTICLE: SOFTWARE FOR SCIENTIFIC COMPUTING

The State of Fortran

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John Urban, High-Performance Computing Consultant, USA
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A community of developers has formed to modernize the Fortran ecosystem. In this article, we describe the high-level features of Fortran that continue to make it a good choice for scientists and engineers in the 21st century. Ongoing efforts include the development of a Fortran standard library and package manager, the fostering of a friendly and welcoming online community, improved compiler support, and language feature development. The lessons learned are common across contemporary programming languages and help reduce the learning curve and increase adoption of Fortran.

Fortran is a high-level programming language primarily used to solve scientific and engineering problems. It has been under active development since its inception under John Backus at IBM in 1954 to the present day. The initial goal was to ease the translation of mathematical formulas to optimized machine code instructions, a concept now known as compilation. The intuitive abstraction of mathematical procedures enabled rapid development of numerical solutions to scientific problems, at a time when most programs were still hand-coded in assembly language. Following the release of its first implementation in 1957, the language was adopted by the scientific and engineering communities for writing numerical programs. As a result, the language was quickly ported to several computer architectures such that Fortran is accepted as being the first cross-platform programming language.

The ISO Fortran Standard and its maintenance of backwards compatibility provide guarantees for

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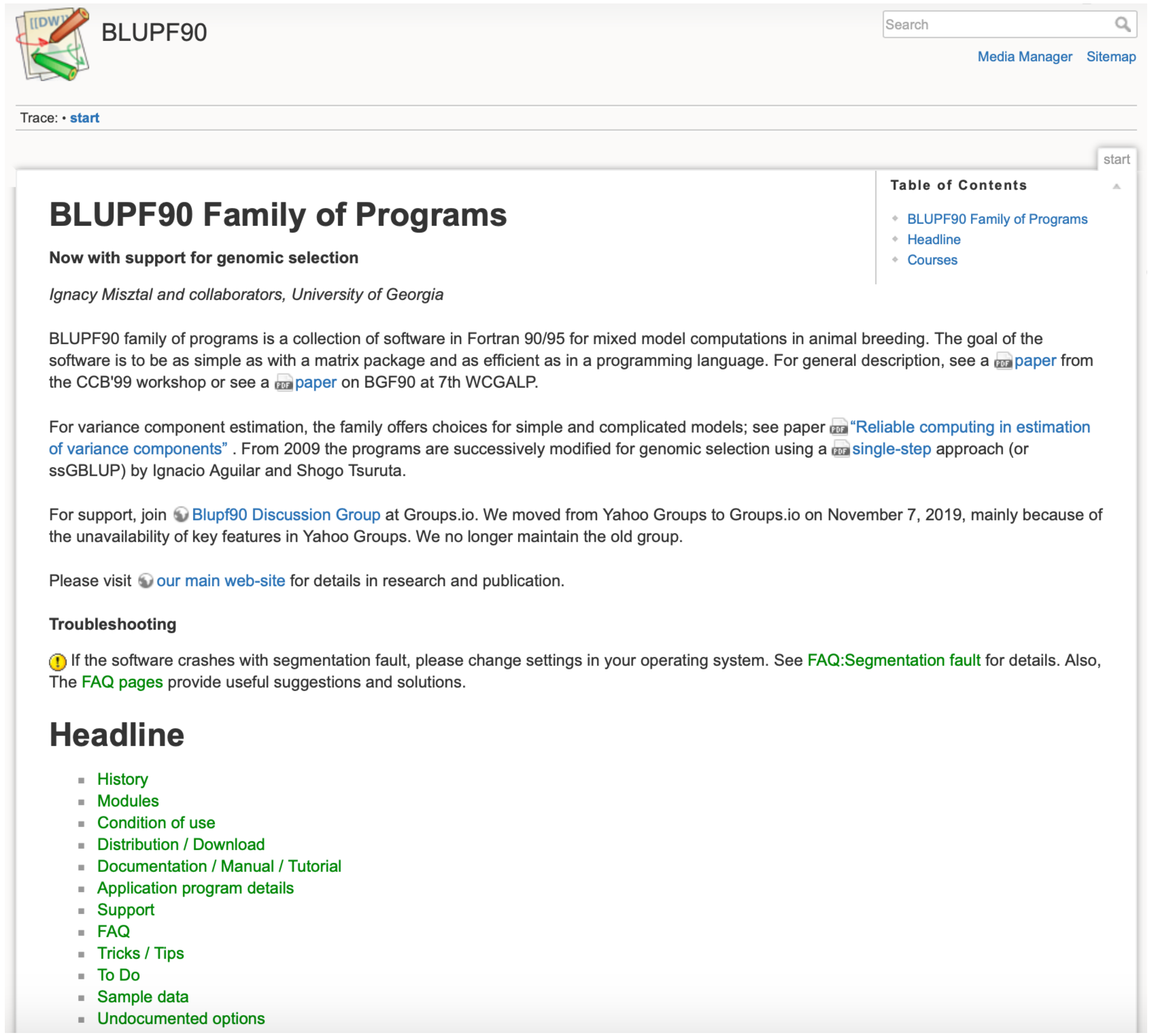
BLUPF90 software suite



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BLUPF90 Family of Programs

Now with support for genomic selection

Ignacy Misztal and collaborators, University of Georgia

BLUPF90 family of programs is a collection of software in Fortran 90/95 for mixed model computations in animal breeding. The goal of the software is to be as simple as with a matrix package and as efficient as in a programming language. For general description, see a paper from the CCB'99 workshop or see a paper on BGF90 at 7th WCGALP.

For variance component estimation, the family offers choices for simple and complicated models; see paper "Reliable computing in estimation of variance components" . From 2009 the programs are successively modified for genomic selection using a single-step approach (or ssGBLUP) by Ignacio Aguilar and Shogo Tsuruta.

For support, join Blupf90 Discussion Group at Groups.io. We moved from Yahoo Groups to Groups.io on November 7, 2019, mainly because of the unavailability of key features in Yahoo Groups. We no longer maintain the old group.

Please visit our main web-site for details in research and publication.

Troubleshooting

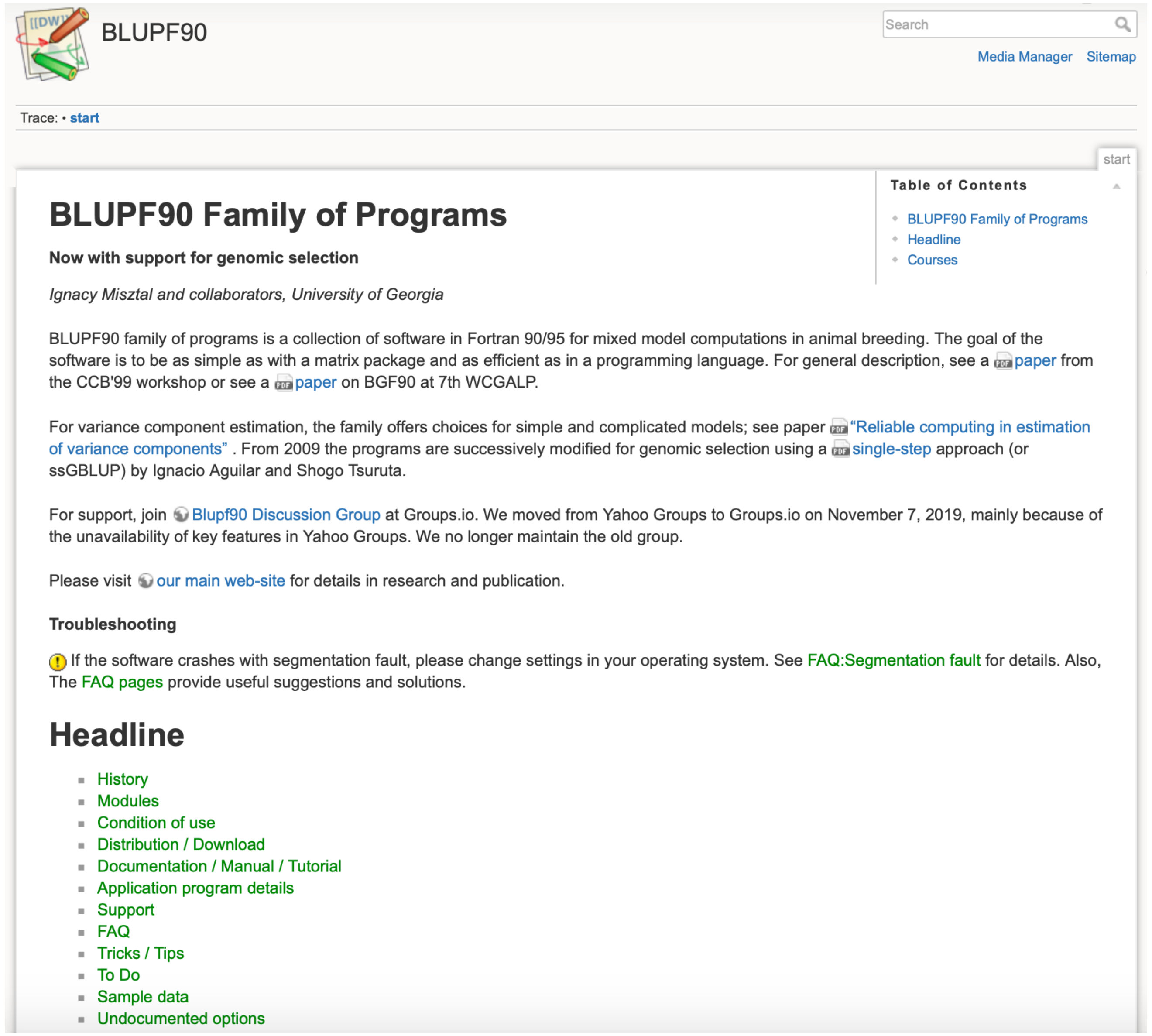
If the software crashes with segmentation fault, please change settings in your operating system. See FAQ:Segmentation fault for details. Also, The FAQ pages provide useful suggestions and solutions.

Headline

- History
- Modules
- Condition of use
- Distribution / Download
- Documentation / Manual / Tutorial
- Application program details
- Support
- FAQ
- Tricks / Tips
- To Do
- Sample data
- Undocumented options

- Collection of software written in Fortran
  - Computations in AB & G
- Since 1997/1998 by Ignacy Misztal
- Several developers + collaborators
- Simple, efficient, and comprehensive
  - Very general models

BLUPF90 software suite


BLUPF90

Search

Media Manager Sitemap

Trace: • start

start

BLUPF90 Family of Programs

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- No GUI (graphical user interface)!!!
- First idea: to solve the MME

$$\begin{bmatrix} \mathbf{X'X} & \mathbf{X'W} \\ \mathbf{W'X} & \mathbf{W'W}+\mathbf{A}^{-1}\dfrac{\sigma_e^2}{\sigma_a^2} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X'y} \\ \mathbf{W'y} \end{bmatrix}$$

- First software: blupf90

- Second idea: VCE

$$\begin{bmatrix} \mathbf{X'X} & \mathbf{X'W} \\ \mathbf{W'X} & \mathbf{W'W}+\mathbf{A}^{-1}\dfrac{\sigma_e^2}{\sigma_a^2} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X'y} \\ \mathbf{W'y} \end{bmatrix}$$

- Software: remlf90, airemlf90 , gibbsf90

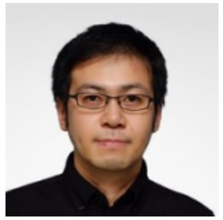
BLUPF90 software main developers

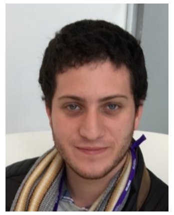
Ignacy Misztal

Shogo Tsuruta

Andres Legarra

Ignacio Aguilar


Yutaka Masuda


Matias Bermann

You??

- + Several contributors
- Research turns into code

- Which programs?

BLUPF90 software suite

blupf90

BLUP with explicit equations

remlf90

Expectation Maximization REML

airemlf90

Average Information REML

gibbsXf90

Bayesian Analyses – linear traits

thrgibbsXf90

Bayesian Analyses – categorical traits

postgibbsf90

Post-analyses of Gibbs samples

Genomics

preGSf90

Processing of SNP data (QC + matrices)

qcf90 ✖

QC of large SNP data

postGSf90

Estimation of SNP effects and GWAS

predf90 ✖

Prediction of GEBV based on SNP effects

seekparentf90 ✖

Parentage verification (SNP and pedigree)

predictf90

Adjusted and predicted phenotypes

validationf90

Perform validation of predictions

Large-scale

blup90iod2

blup90iod2OMP1

blup90iod3

cblup90iod2

cblup90iod2OMP1

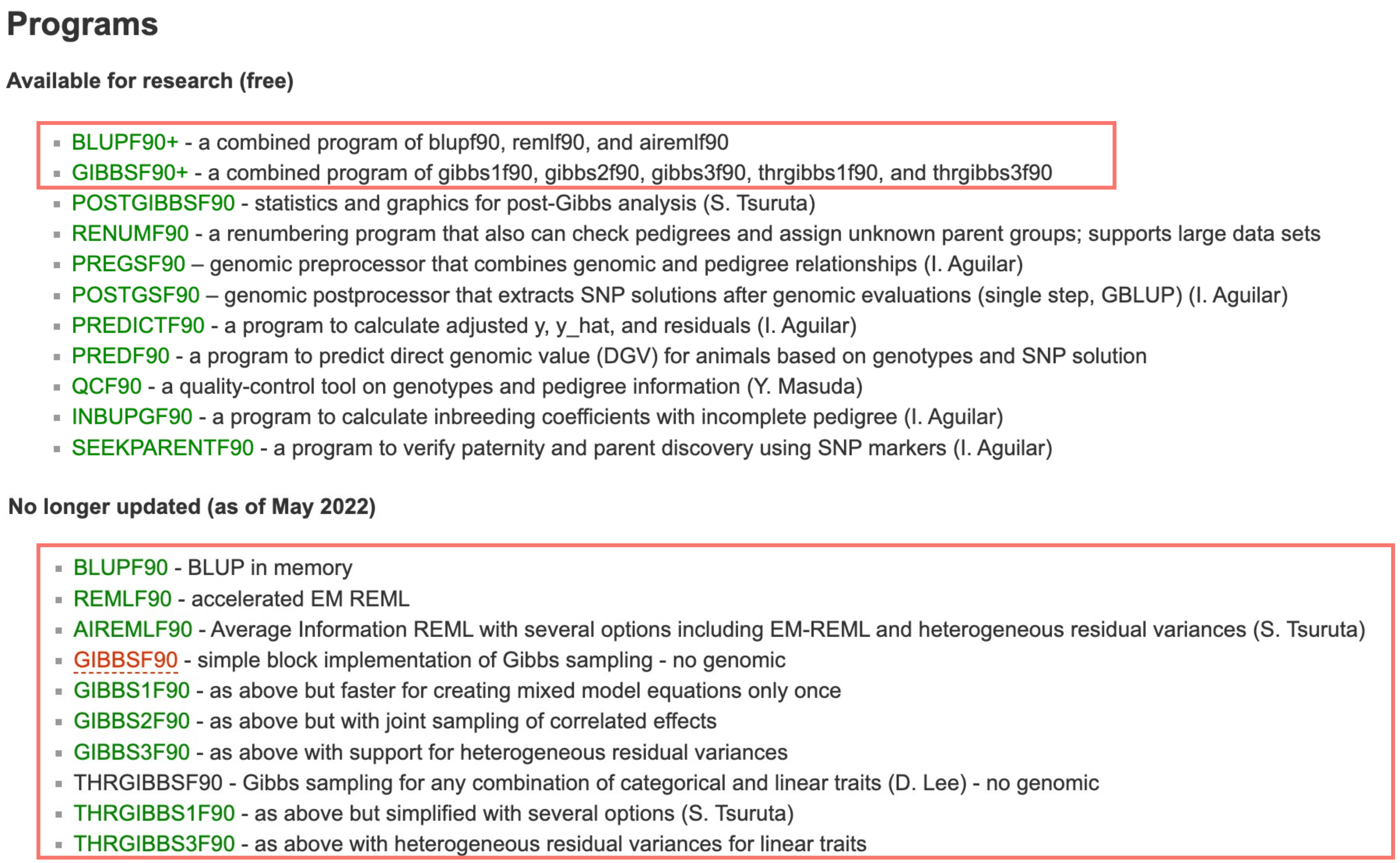
accf90

accf90GS

accf90GS2

accf90GS3

nce.ads.uga.edu/wiki



Programs

Available for research (free)

- BLUPF90+ - a combined program of blupf90, remlf90, and airemlf90
- GIBBSF90+ - a combined program of gibbs1f90, gibbs2f90, gibbs3f90, thrgibbs1f90, and thrgibbs3f90
- POSTGIBBSF90 - statistics and graphics for post-Gibbs analysis (S. Tsuruta)
- RENUMF90 - a renumbering program that also can check pedigrees and assign unknown parent groups; supports large data sets
- PREGSF90 – genomic preprocessor that combines genomic and pedigree relationships (I. Aguilar)
- POSTGSF90 – genomic postprocessor that extracts SNP solutions after genomic evaluations (single step, GBLUP) (I. Aguilar)
- PREDICTF90 - a program to calculate adjusted y, y_hat, and residuals (I. Aguilar)
- PREDF90 - a program to predict direct genomic value (DGV) for animals based on genotypes and SNP solution
- QCF90 - a quality-control tool on genotypes and pedigree information (Y. Masuda)
- INBUPGF90 - a program to calculate inbreeding coefficients with incomplete pedigree (I. Aguilar)
- SEEKPARENTF90 - a program to verify paternity and parent discovery using SNP markers (I. Aguilar)

No longer updated (as of May 2022)

- BLUPF90 - BLUP in memory
- REMLF90 - accelerated EM REML
- AIREMLF90 - Average Information REML with several options including EM-REML and heterogeneous residual variances (S. Tsuruta)
- GIBBSF90 - simple block implementation of Gibbs sampling - no genomic
- GIBBS1F90 - as above but faster for creating mixed model equations only once
- GIBBS2F90 - as above but with joint sampling of correlated effects
- GIBBS3F90 - as above with support for heterogeneous residual variances
- THRGIBBSF90 - Gibbs sampling for any combination of categorical and linear traits (D. Lee) - no genomic
- THRGIBBS1F90 - as above but simplified with several options (S. Tsuruta)
- THRGIBBS3F90 - as above with heterogeneous residual variances for linear traits

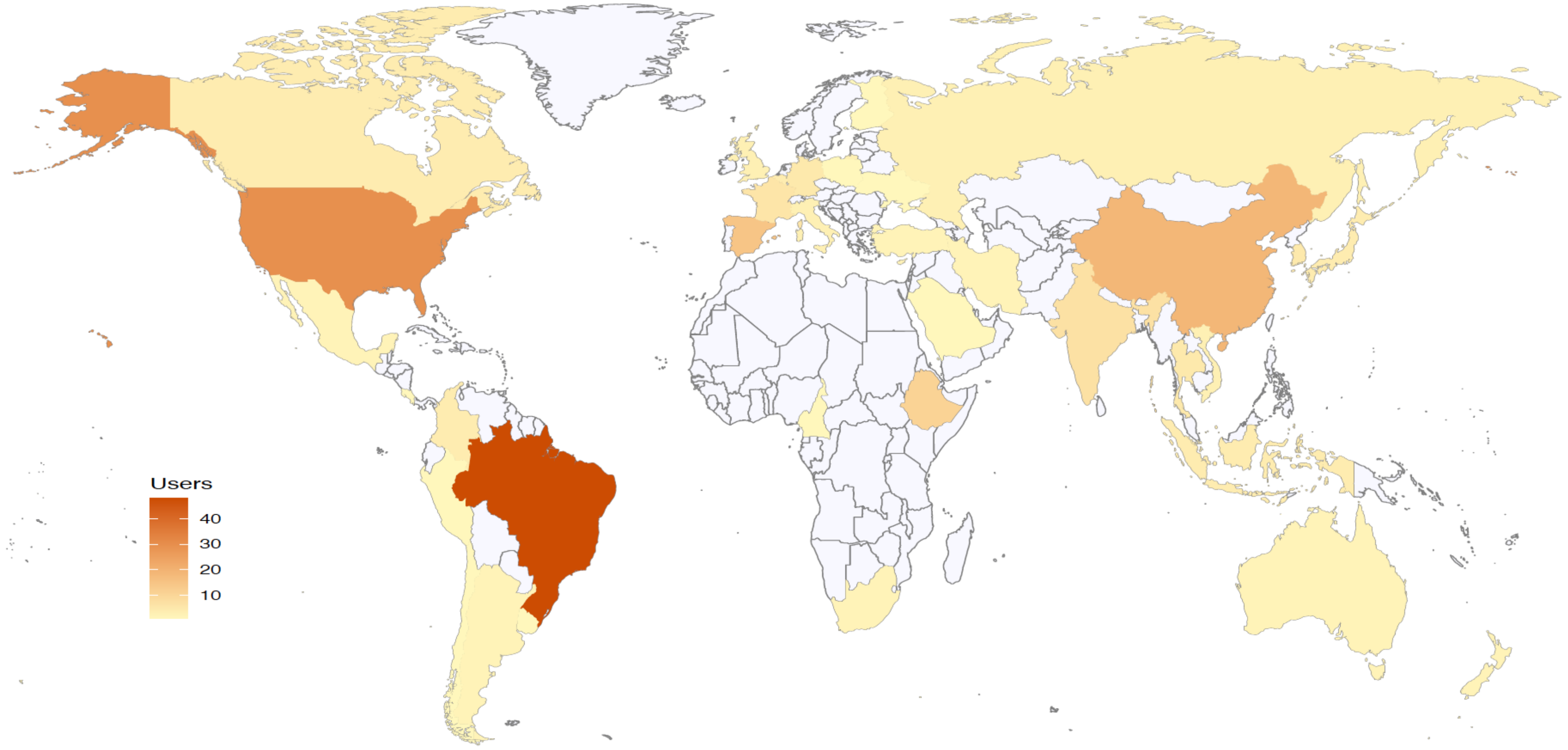
BLUPF90 software suite

March/2024

- 1,684,059 accesses to the nce server
- 1074 true binaries downloads (without duplicates)
- 239 users (IP with at least one binary download)
- BLUPF90+ has the most downloads
- Brazil is the countries with the most users
- Windows is the most used OS

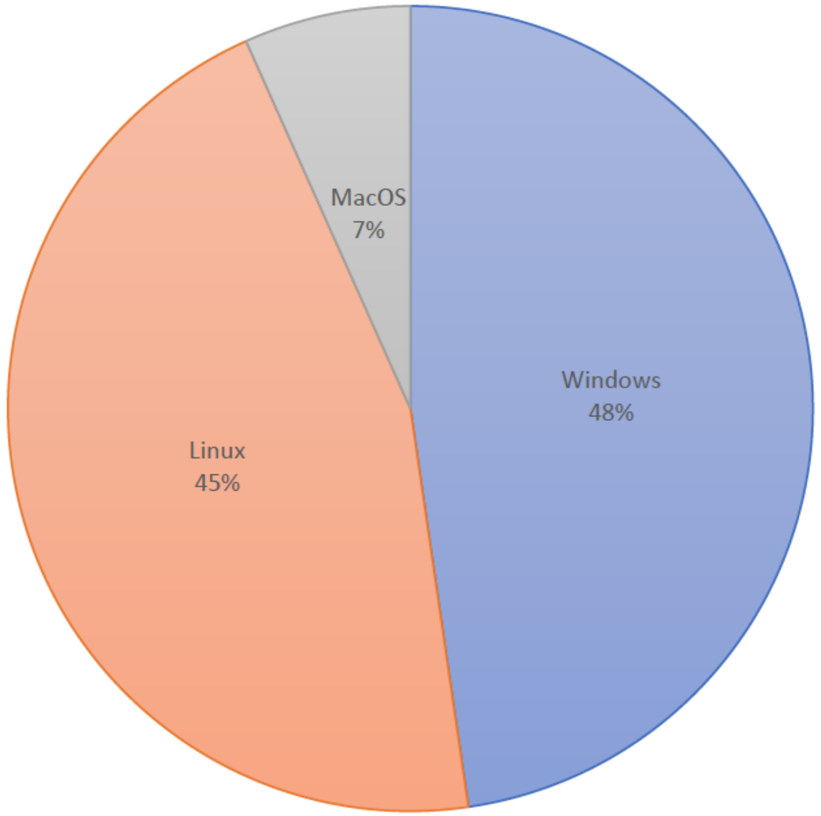
BLUPF90 software suite

Users around the world



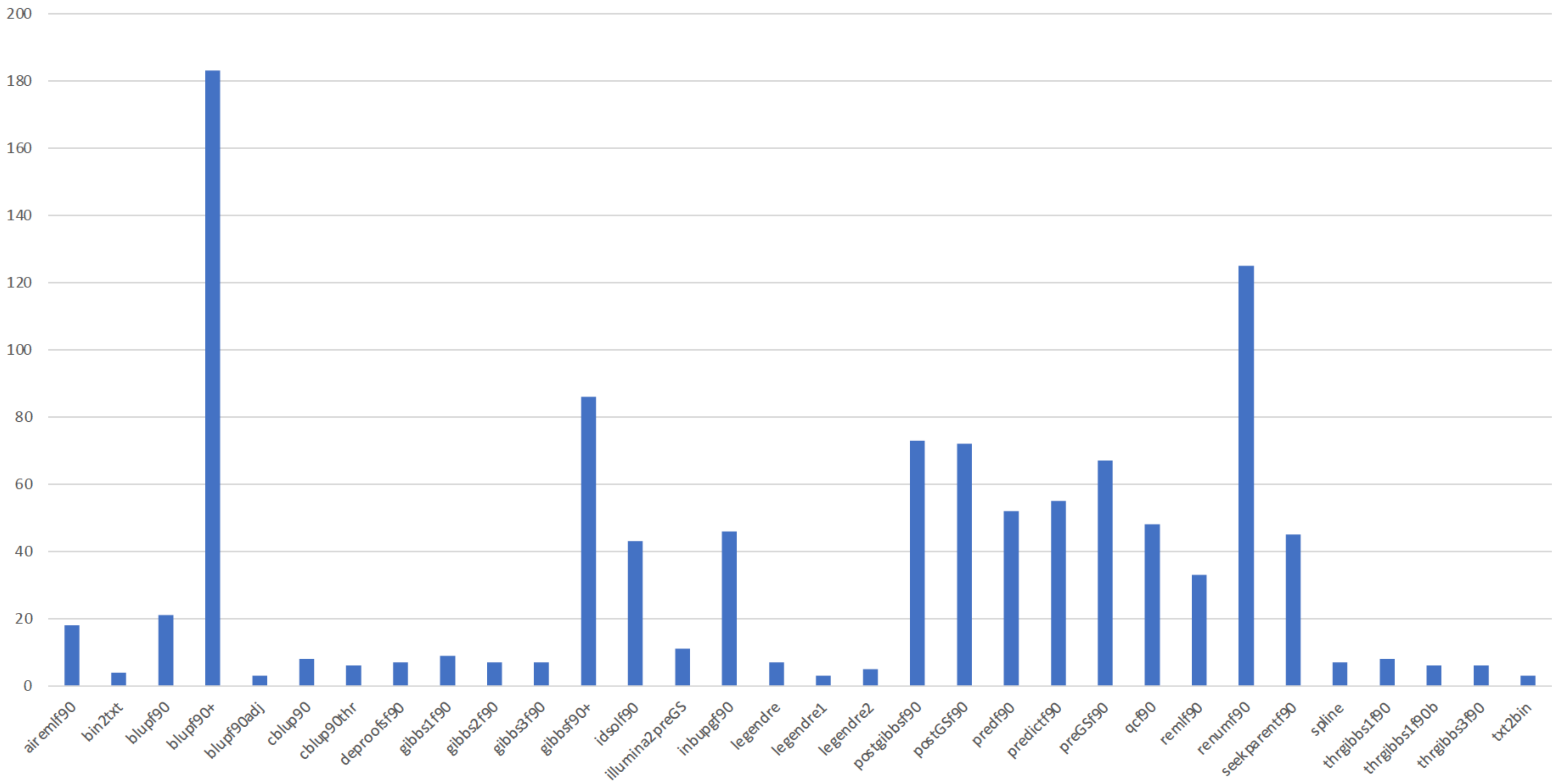
BLUPF90 software suite

Windows	114
Linux	109
MacOS	16
Total	239



BLUPF90 software suite

Program downloads



blupf90+

- `blupf90`: MME solver
- `airemlf90`: variance components using Average Information REML
- `remlf90`: variance components using Expectation Maximization REML

Mixed Model Equations Solver

Variance Components Estimation

$$\begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{W} \\ \mathbf{W}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{W}'\mathbf{R}^{-1}\mathbf{W}+\mathbf{A}^{-1}\otimes\mathbf{G}_0^{-1} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{y} \\ \mathbf{W}'\mathbf{R}^{-1}\mathbf{y} \end{bmatrix}$$

blupf90+

MME Solver

Default

VC Estimation

- AI-REML:

```
OPTION method VCE
```

- EM-REML:

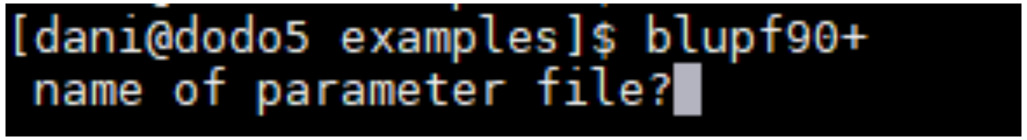
```
OPTION method VCE
OPTION EM-REML
```

blupf90+

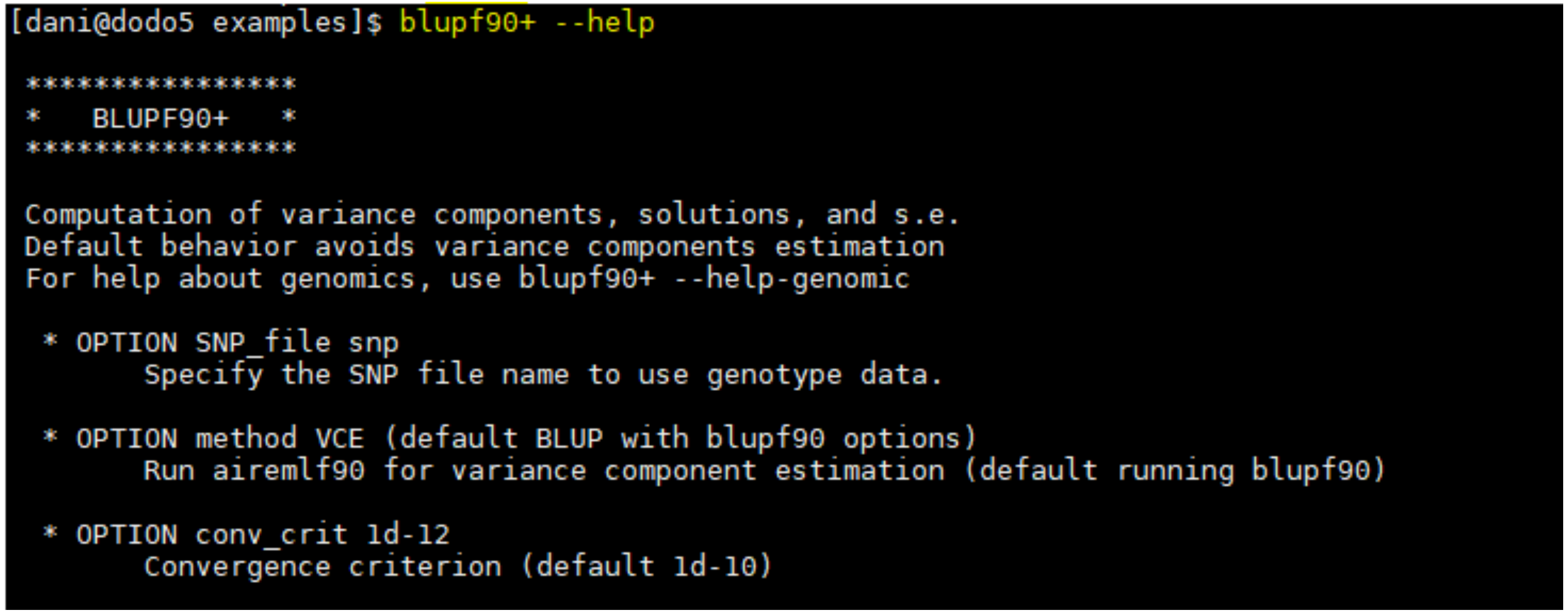
- Supports virtually any model used in AB&G:
  - animal model
  - models with maternal effect
  - MPE
  - PE
  - Random Regression
  - Social interaction
  - Multiple traits
    - up to 70 if no correlated effects
    - up to [70/number of correlated effects]

blupf90+

- How to use:



```
[dani@dodo5 examples]$ blupf90+
 name of parameter file?
```



```
[dani@dodo5 examples]$ blupf90+ --help

 ****************
 *   BLUPF90+   *
 ****************

 Computation of variance components, solutions, and s.e.
 Default behavior avoids variance components estimation
 For help about genomics, use blupf90+ --help-genomic

  * OPTION SNP_file snp
       Specify the SNP file name to use genotype data.

  * OPTION method VCE (default BLUP with blupf90 options)
       Run airemlf90 for variance component estimation (default running blupf90)

  * OPTION conv_crit 1d-12
       Convergence criterion (default 1d-10)
```

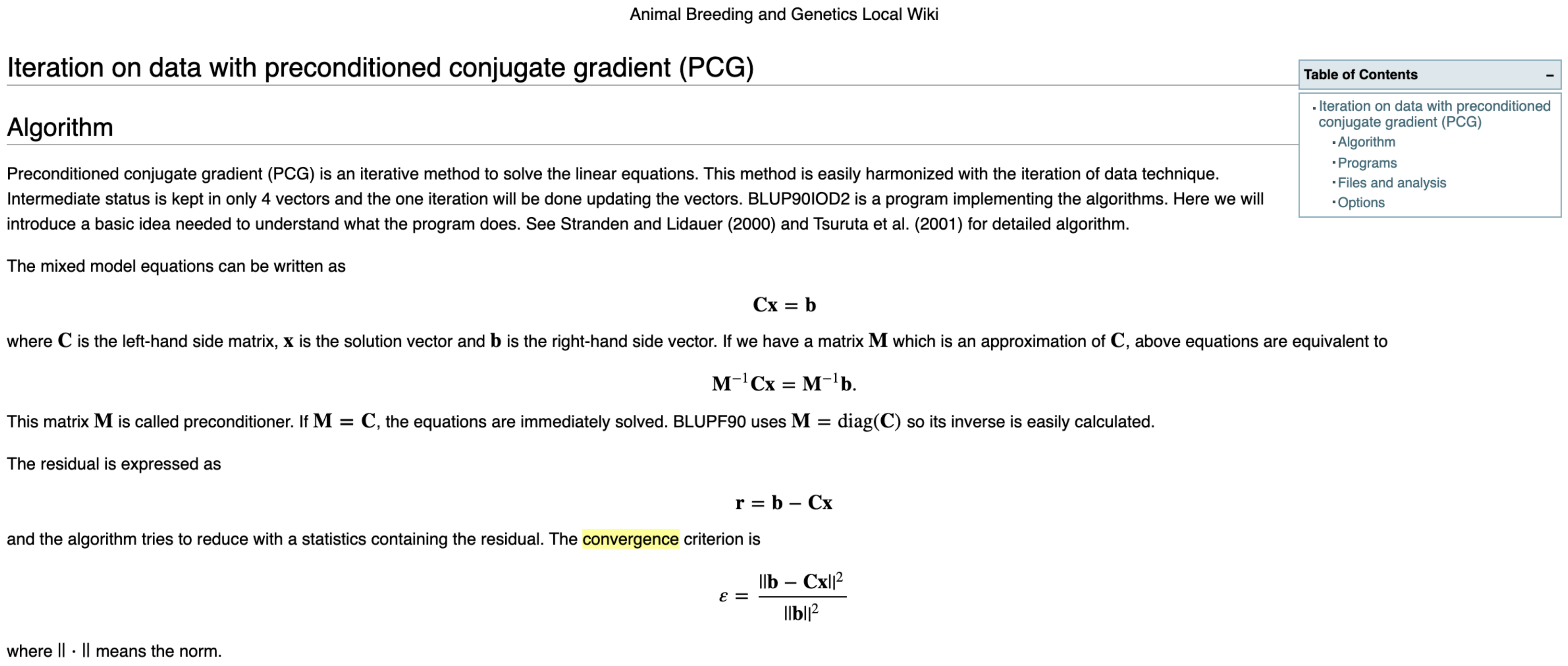
blupf90+

- Input files
  - Free format (minimum one space to separate columns)
  - TAB is not a valid separator
  - Only numbers: integer or real
  - Decimal separators “ . ” not “ , ”
  - One “ . ” is not a missing value as in SAS
  - All effects need to be renumbered from 1 (consecutively)

blupf90+

- Computes generalized solutions by several methods:
  - Preconditioner Conjugate Gradient (PCG)
    - Default Iterative method (fast)
  - Successive over-relaxation (SOR)
    - an iterative method based on Gauss-Seidel
  - Direct solution using sparse Cholesky factorization
    - FSPAK or YAMS (greater memory requirements)
    - Can provide PEV
- Solutions change among methods, but estimable functions should be the same

blupf90+ with PCG



Animal Breeding and Genetics Local Wiki

Iteration on data with preconditioned conjugate gradient (PCG)

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Algorithm

Preconditioned conjugate gradient (PCG) is an iterative method to solve the linear equations. This method is easily harmonized with the iteration of data technique. Intermediate status is kept in only 4 vectors and the one iteration will be done updating the vectors. BLUP90IOD2 is a program implementing the algorithms. Here we will introduce a basic idea needed to understand what the program does. See Stranden and Lidauer (2000) and Tsuruta et al. (2001) for detailed algorithm.

The mixed model equations can be written as

$$\mathbf{Cx} = \mathbf{b}$$

where $\mathbf{C}$ is the left-hand side matrix, $\mathbf{x}$ is the solution vector and $\mathbf{b}$ is the right-hand side vector. If we have a matrix $\mathbf{M}$ which is an approximation of $\mathbf{C}$, above equations are equivalent to

$$\mathbf{M}^{-1}\mathbf{Cx} = \mathbf{M}^{-1}\mathbf{b}.$$

This matrix $\mathbf{M}$ is called preconditioner. If $\mathbf{M} = \mathbf{C}$, the equations are immediately solved. BLUPF90 uses $\mathbf{M} = \mathrm{diag}(\mathbf{C})$ so its inverse is easily calculated.

The residual is expressed as

$$\mathbf{r} = \mathbf{b} - \mathbf{Cx}$$

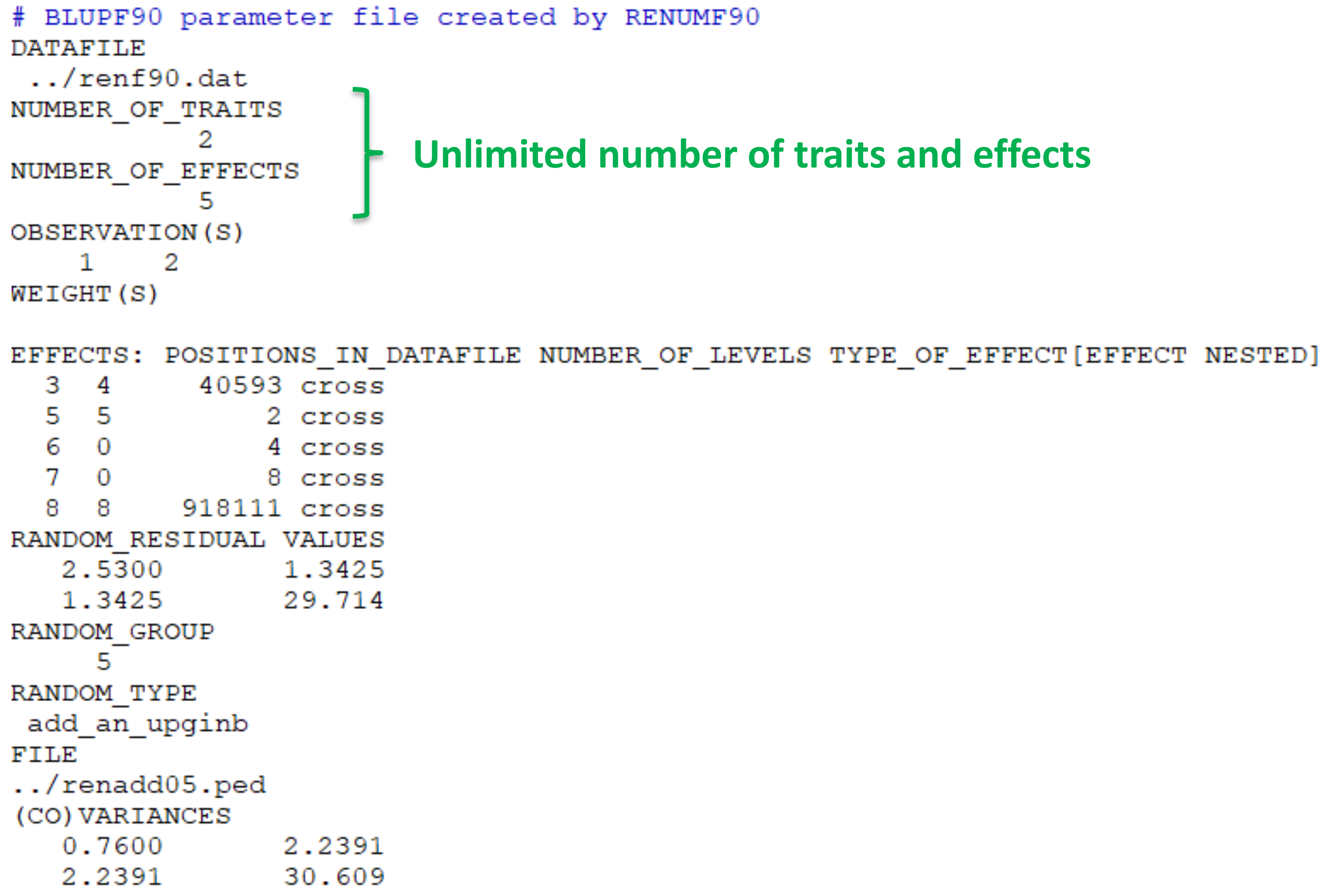
and the algorithm tries to reduce with a statistics containing the residual. The convergence criterion is

$$\varepsilon = \frac{||\mathbf{b} - \mathbf{Cx}||^2}{||\mathbf{b}||^2}$$

where $||\cdot||$ means the norm.

If $\mathbf{M}^{-1}\mathbf{C}$ has a better condition than $\mathbf{C}$, the convergence is reached is faster

Parameter file for blupf90+

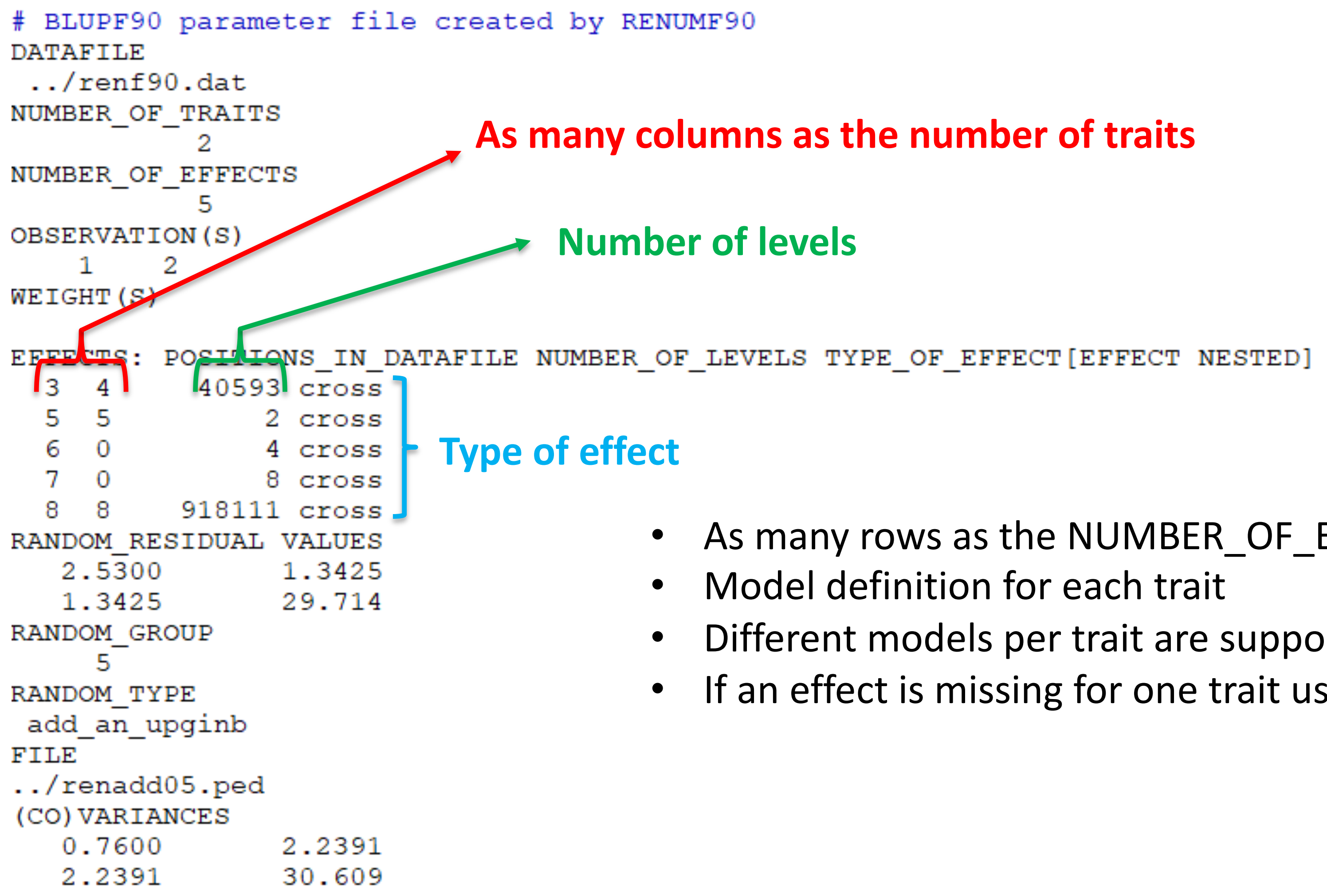


```
# BLUPF90 parameter file created by RENUMF90
DATAFILE
 ../renf90.dat
NUMBER_OF_TRAITS
           2
NUMBER_OF_EFFECTS
           5
OBSERVATION(S)
    1    2
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT[EFFECT NESTED]
  3  4      40593 cross
  5  5          2 cross
  6  0          4 cross
  7  0          8 cross
  8  8     918111 cross
RANDOM_RESIDUAL VALUES
   2.5300       1.3425
   1.3425       29.714
RANDOM_GROUP
     5
RANDOM_TYPE
 add_an_upginb
FILE
../renadd05.ped
(CO)VARIANCES
   0.7600       2.2391
   2.2391       30.609
```

Unlimited number of traits and effects

Parameter file for blupf90+



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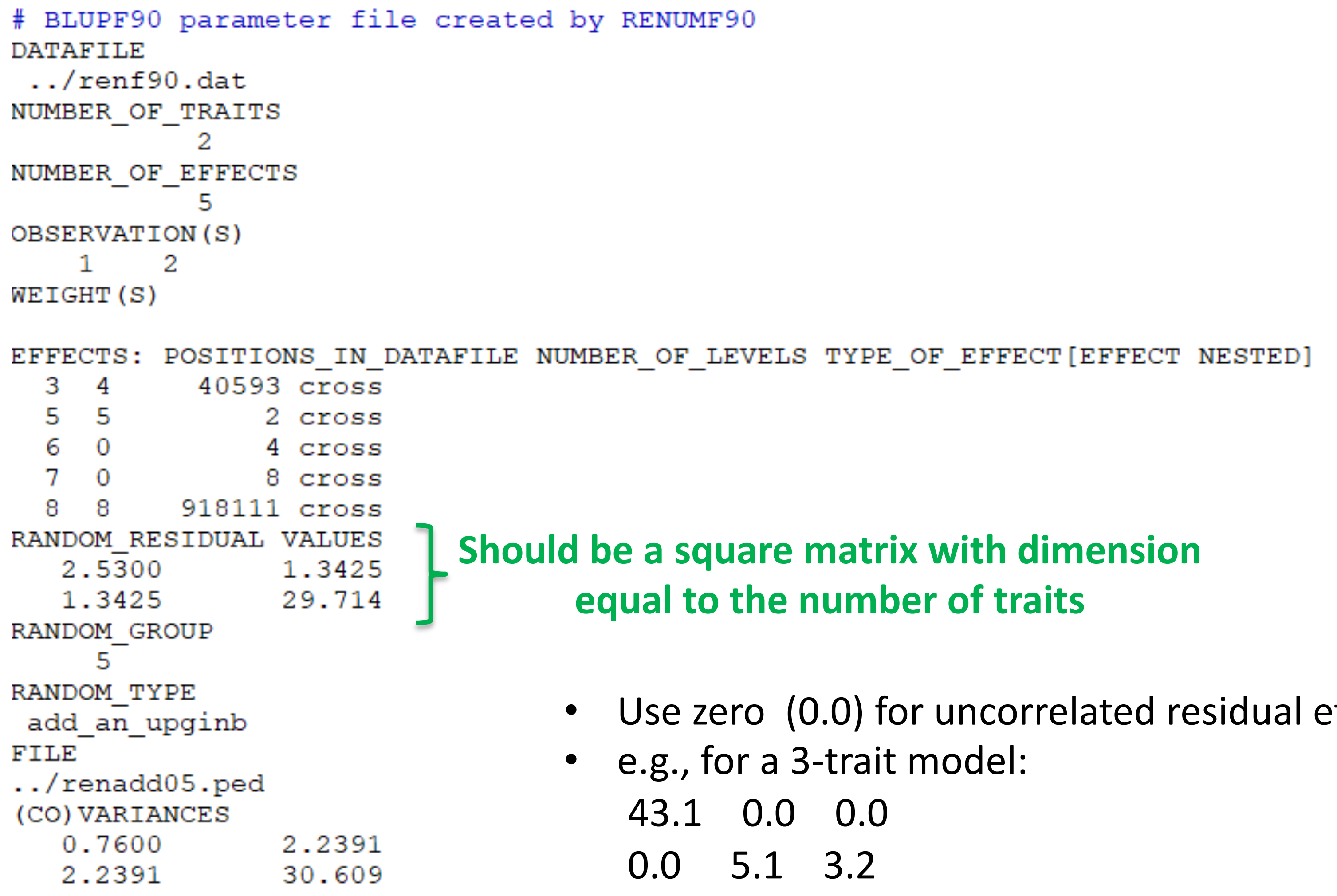
```

- As many rows as the NUMBER_OF_EFFECTS
- Model definition for each trait
- Different models per trait are supported
- If an effect is missing for one trait use 0

Parameter file for blupf90+



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../renadd05.ped
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   2.2391        30.609
```

Should be a square matrix with dimension equal to the number of traits

- Use zero (0.0) for uncorrelated residual effects between traits
- e.g., for a 3-trait model:

```
43.1   0.0   0.0
0.0    5.1   3.2
0.0    3.2   10.3
```

Parameter file for blupf90+

```
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```

Definition of random effects

RANDOM_GROUP
RANDOM_TYPE
FILE
(CO)VARIANCES

Definition of random effects

- RANDOM_GROUP
  - Number of the effect(s) from list of effects
  - Correlated effects should be consecutive e.g., Maternal effects, Random Regression
- RANDOM_TYPE
  - diagonal, add_animal, add_sire, add_an_upg, add_an_upginb, add_an_self, user_file, user_file_i, or par_domin
- FILE
  - Pedigree file, parental dominance, or user file
- (CO)VARIANCES
  - Square matrix with dimension equal to the number_of_traits*number_of_correlated_effects

(CO)VARIANCES

- Assuming 3 traits (T1-T3)

	T1	T2	T3
T1			
T2			
T3			

(CO)VARIANCES

- Assuming 3 traits (T1-T3) and 2 correlated effects (E1-E2)

		Direct			Maternal		
		T1	T2	T3	T1	T2	T3
Direct	T1						
	T2						
	T3						
Maternal	T1						
	T2						
	T3						

RANDOM_TYPE

- *Diagonal*
  - for permanent environmental effects
  - assumes no correlation between levels of the effect

- *add_sire*
  - To create a relationship matrix using sire and maternal grandsire
  - Pedigree file:
    - `individual number, sire number, maternal grandsire number`

- *add_animal*
  - To create a relationship matrix using sire and dam information
  - Pedigree file:
    - `animal number, sire number, dam number`

RANDOM_TYPE

- *add_an_upg*
  - As before but using rules for unknown parent groups
  - Pedigree file:
    - `animal number, sire number, dam number, parent code`
    - missing sire/dam can be replaced by upg number, usually greater than the maximum number of animals
    - Parent code = 3 – # of known parents
      - 1 both parents known
      - 2 one parent known
      - 3 both parents unknown

- *add_an_upginb*
  - As before but using rules for unknown parent groups and inbreeding
  - Pedigree file:
    - `animal number, sire number, dam number, inb/upg code`
    - missing sire/dam can be replaced by upg number, usually greater than maximum number of animals
    - inb/upg code = 4000 / [(1+ms)(1-Fs) + (1+md)(1-Fd)]
    - ms (md) is 0 if sire (dam) is known and 1 otherwise
    - Fs(Fd) inbreeding coefficient of the sire (dam)

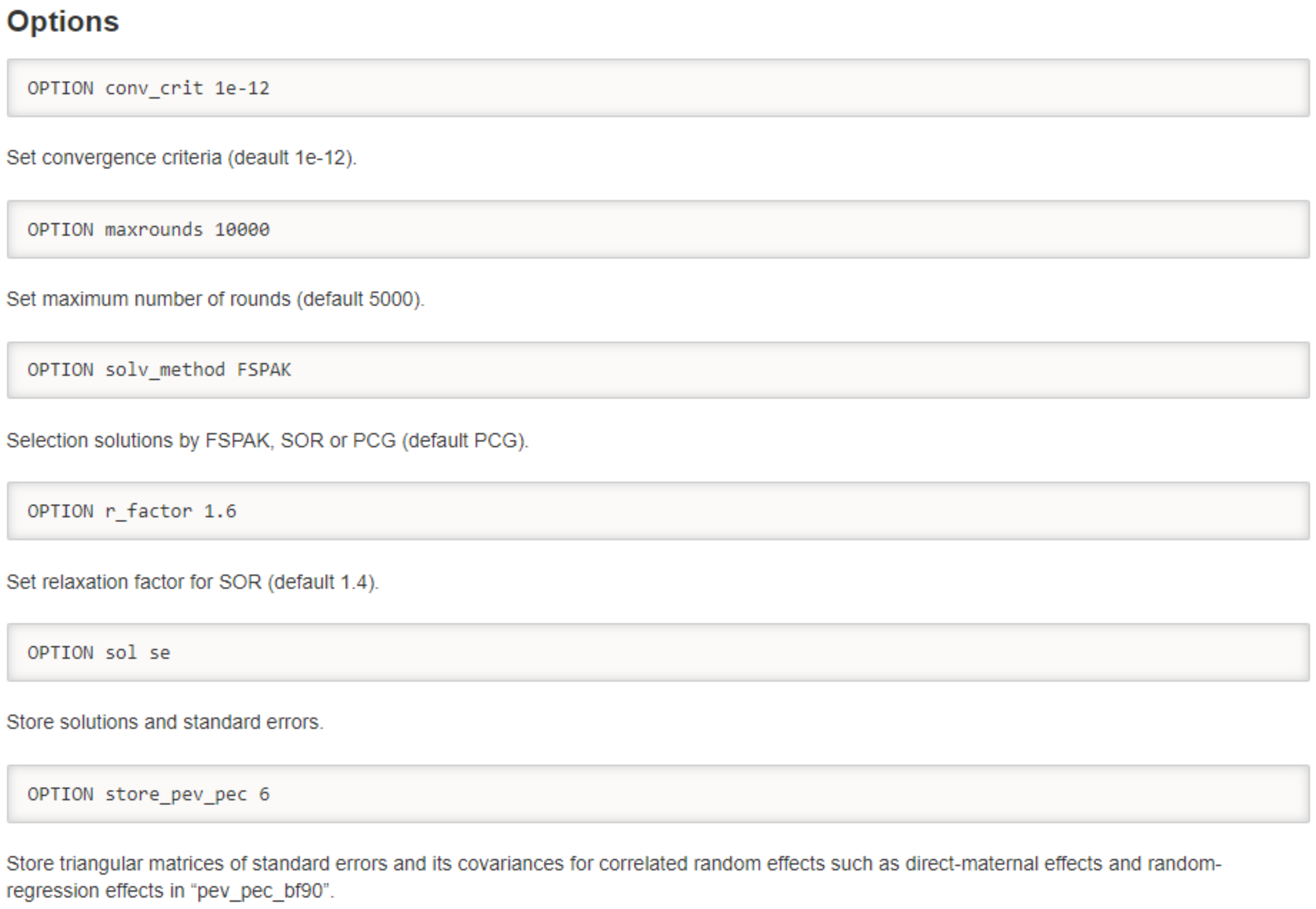
RANDOM_TYPE

- *add_an_meta*
  - *To create a relationship matrix using metafounders rules*
  - Pedigree file:
    - `animal number, sire number, dam number`
    - `needs a gamma file`
- *add_an_self*
  - *To create a relationship matrix when there is selfing*
  - Pedigree file:
    - `individual number, parent 1 number, parent 2, number of selfing generations`
- *user_file*
  - An inverted matrix is read from a file
  - Matrix is stored only upper- or lower-triangular
  - Matrix file:
    - `row, col, value`
- *user_file_i*
  - As before but the matrix will be inverted by the program
- *par_domin*
  - A parental dominance file created by the program RENDOM

OPTIONS for blupf90+

- Program behavior is modified by adding extra options at the end of the par file
- `OPTION option_name x1 x2 …`
- `option_name`: each program has its own options
- `x1 x2:` each option has its own parameters

Options for blupf90+



Options

```
OPTION conv_crit 1e-12
```

Set convergence criteria (deault 1e-12).

```
OPTION maxrounds 10000
```

Set maximum number of rounds (default 5000).

```
OPTION solv_method FSPAK
```

Selection solutions by FSPAK, SOR or PCG (default PCG).

```
OPTION r_factor 1.6
```

Set relaxation factor for SOR (default 1.4).

```
OPTION sol se
```

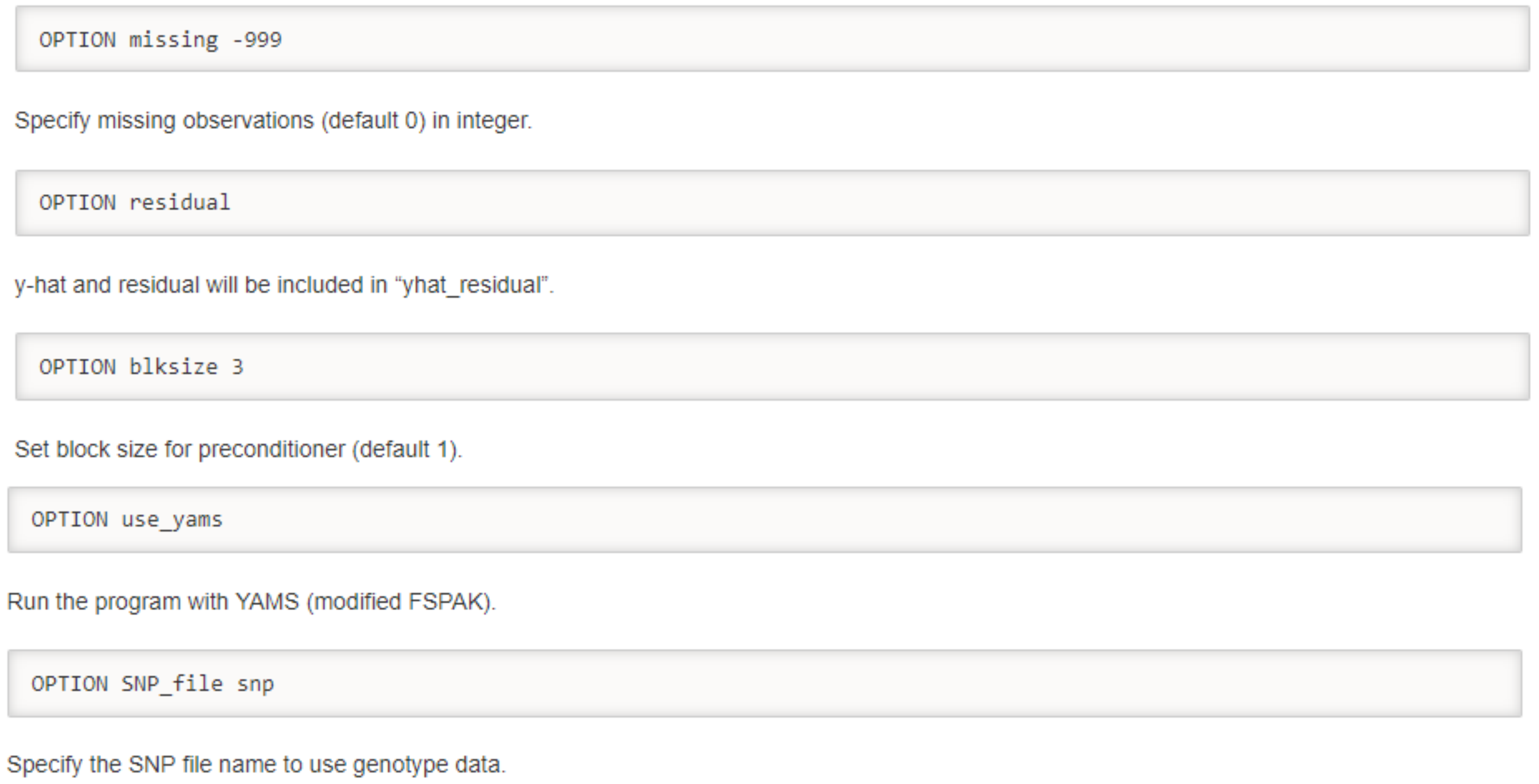
Store solutions and standard errors.

```
OPTION store_pev_pec 6
```

Store triangular matrices of standard errors and its covariances for correlated random effects such as direct-maternal effects and random-regression effects in “pev_pec_bf90”.

Options for blupf90+

Missing data
Not pedigree!



```
OPTION missing -999
```

Specify missing observations (default 0) in integer.

```
OPTION residual
```

y-hat and residual will be included in "yhat_residual".

```
OPTION blksize 3
```

Set block size for preconditioner (default 1).

```
OPTION use_yams
```

Run the program with YAMS (modified FSPAK).

```
OPTION SNP_file snp
```

Specify the SNP file name to use genotype data.

New options for blupf90+

- Storing reliabilities based on PEV

```
OPTION store_accuracy X
```

$\hookrightarrow$ Number of animal effect

$$Rel = 1 - \frac{PEV}{\sigma_u^2(1+f)}$$

  - Adjusts for f (inbreeding) from **A**, **G**, or **H**
  - Turn inbreeding adjustment off
  - `OPTION correct_accuracy_by_inbreeding_direct 0`

- Storing solutions with original ID if renumf90 was used to renumber the data

```
OPTION origID
```

May not work with some programs and options

  - Only *solutions.original* is created

New options for blupf90+

- Storing reliabilities with original ID

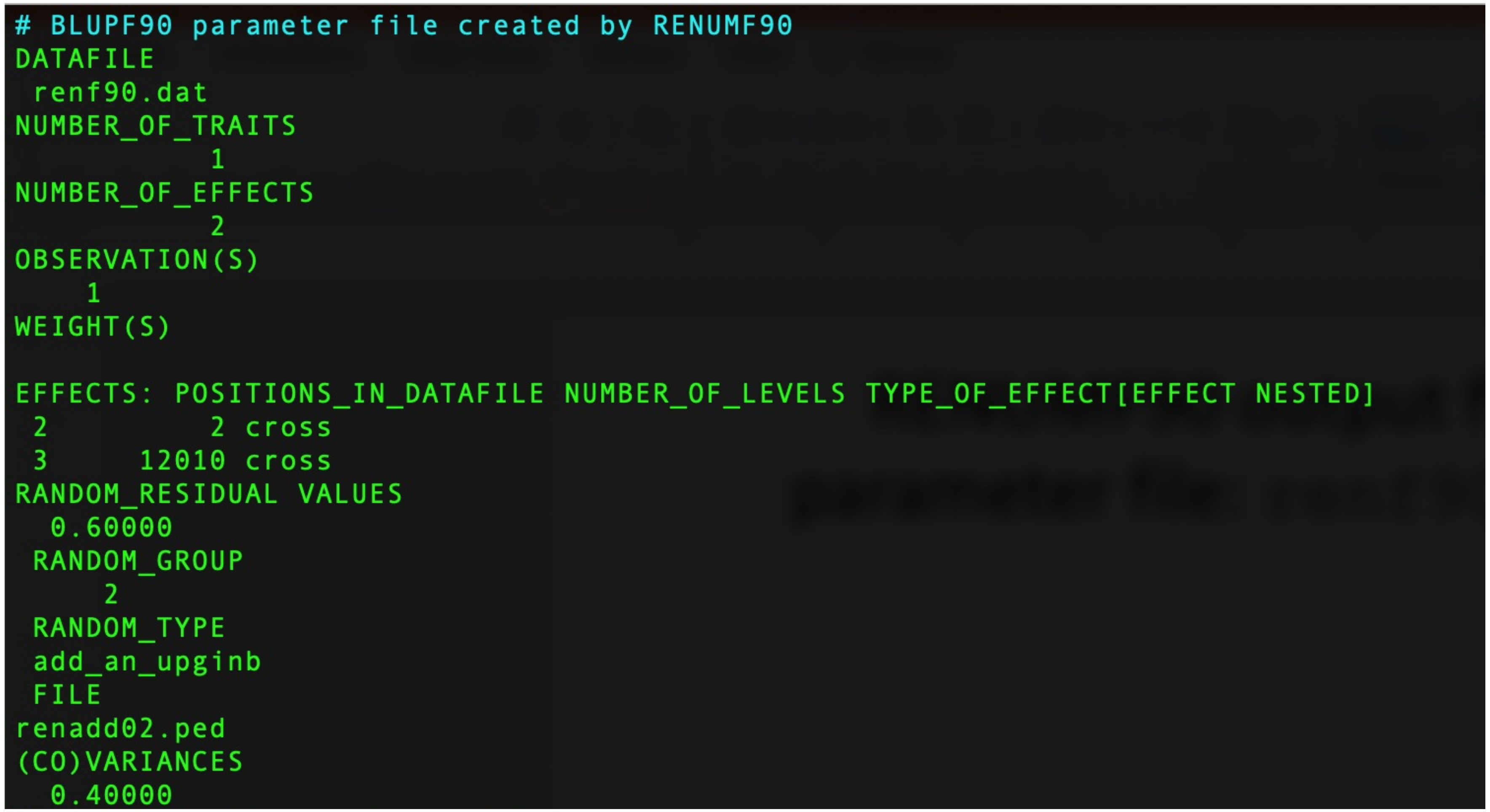
```
OPTION store_accuracy X orig
```

$\llcorner\!\rightarrow$ Number of animal effect

$$Rel = 1 - \frac{PEV}{\sigma_u^2(1+f)}$$

- Storing solutions and rel with original ID if renumf90 was used to renumber the data
    - The option will save *acc_bf90* with renumbered and original ID
    - If want to have *solutions.original* as well, combine with OPTION origID

Common parameter file for blupf90+



```
# BLUPF90 parameter file created by RENUMF90
DATAFILE
 renf90.dat
NUMBER_OF_TRAITS
           1
NUMBER_OF_EFFECTS
           2
OBSERVATION(S)
    1
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT[EFFECT NESTED]
 2         2 cross
 3     12010 cross
RANDOM_RESIDUAL VALUES
  0.60000
 RANDOM_GROUP
     2
 RANDOM_TYPE
 add_an_upginb
 FILE
renadd02.ped
(CO)VARIANCES
  0.40000
```

Example

Model: $y = farm + sex + \beta\, age + animal + e$

```
DATAFILE
 data1.txt
NUMBER_OF_TRAITS
           1
NUMBER_OF_EFFECTS
           4
OBSERVATION(S)
    1
WEIGHT(S)


EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT[EFFECT NESTED]
 2         3 cross
 3         2 cross
 4 1 cov
 5        15 cross
RANDOM_RESIDUAL VALUES
   1.0000
 RANDOM_GROUP
     4
 RANDOM_TYPE
 add_animal
 FILE
ped1.txt
(CO)VARIANCES
  0.20000
```

ped1.txt

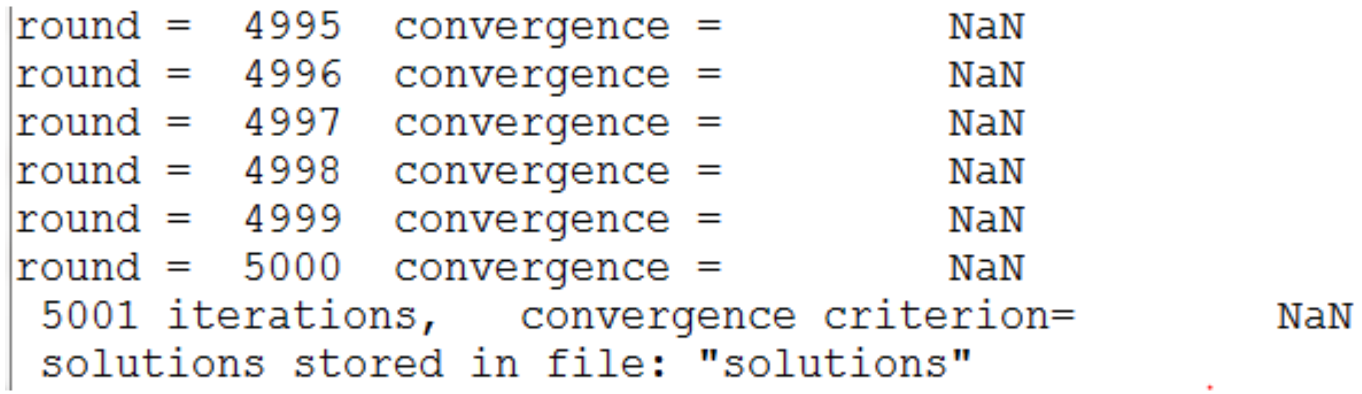
```
Anim  Sire  Dam

1   15 14
14  0   0
2   15 14
11  0   0
3   15 11
4   15 11
5   12 13
12  0   0
6   12 11
7   15 13
13  0   0
8   12 13
9   12 14
15  0   0
10  12 11
```

data1.txt

```
phen farm sex age  Anim

3  1  1  1  6
2  1  2  1  8
4  1  1  2  9
6  2  2  2  10
3  2  1  1  5
6  2  2  2  1
6  3  1  2  3
6  3  2  1  7
8  3  1  1  2
4  3  2  2  4
```

Common problems in blupf90+

- Wrong data file and pedigree name
  - Program may not stop if file name does not exist
  - Check outputs for data file name and number of records and pedigree read



```
round =  4995  convergence =         NaN
round =  4996  convergence =         NaN
round =  4997  convergence =         NaN
round =  4998  convergence =         NaN
round =  4999  convergence =         NaN
round =  5000  convergence =         NaN
 5001 iterations,   convergence criterion=       NaN
 solutions stored in file: "solutions"
```

blupf90+

VC Estimation

EM-REML: expectation-maximization (EM) algorithm

AI-REML: average information (AI) algorithm

REML

- REML = restricted/residual maximum likelihood
  - Patterson and Thompson (1971)

- Most used method for VCE in AB&G

EM-REML

- This method requires iterations:

$$\mathbf{y} = \mathbf{X\beta} + \mathbf{Zu} + \mathbf{e}$$

$$\begin{bmatrix} \mathbf{X'X} & \mathbf{X'Z} \\ \mathbf{Z'X} & \mathbf{Z'Z}+\mathbf{A}^{-1}\dfrac{\sigma_e^2}{\sigma_a^2} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X'y} \\ \mathbf{Z'y} \end{bmatrix}$$

1) set initial variance components

2) compute $\hat{\boldsymbol{\beta}}$ and $\hat{\mathbf{u}}$ via mixed model equations

3) update variance components with the following equations

$$\hat{\sigma}_a^2 = \frac{\hat{\mathbf{u}}'\mathbf{A}^{-1}\hat{\mathbf{u}} + \mathrm{tr}\left(\mathbf{A}^{-1}\mathbf{C}^{uu}\right)}{N_a}$$

$$\hat{\sigma}_e^2 = \frac{\mathbf{y}'(\mathbf{y} - \mathbf{X}\hat{\beta} - \mathbf{Z}\hat{\mathbf{u}})}{N - \mathrm{rank}(\mathbf{X})}$$

Inverse of LHS for animal effect

# animals (rank of A)

4) go to 1 or stop if the parameters do not change anymore

EM-REML

- Simpler equations
    - More complicated equations in multiple-trait models
- Easier to understand
- Very slow convergence (looks stable but may not converge)
- Computationally demanding, especially for **C^uu**

$$\begin{bmatrix}\hat{\boldsymbol{\beta}}\\ \hat{\mathbf{u}}\end{bmatrix} = \begin{bmatrix}\mathbf{X'X} & \mathbf{X'Z}\\ \mathbf{Z'X} & \mathbf{Z'Z}+\mathbf{A}^{-1}\frac{\sigma_e^2}{\sigma_a^2}\end{bmatrix}^{-1}\begin{bmatrix}\mathbf{X'y}\\ \mathbf{Z'y}\end{bmatrix}$$

AI-REML

Vector of variance components

$$\boldsymbol{\theta}_{n+1} = \boldsymbol{\theta}_n - \mathbf{H}^{-1}(\boldsymbol{\theta}_n)\mathbf{d}(\boldsymbol{\theta}_n)$$

Gradient (score vector)

Hessian Matrix

P = Projection
or hat matrix

Average-information algorithm uses this matrix as Hessian,

$$\mathbf{H}(\theta) = \mathcal{I}_A(\theta) = \begin{bmatrix} -\frac{1}{2}\mathbf{y'PZAZ'PZAZ'Py} & -\frac{1}{2}\mathbf{y'PZAZ'PPy} \\ -\frac{1}{2}\mathbf{y'PPZAZ'Py} & -\frac{1}{2}\mathbf{y'PPPy} \end{bmatrix}$$

expensive

Gradient

$$-2\mathrm{d}(\theta) = \begin{bmatrix} \mathrm{tr}(\mathbf{PZAZ'}) - \mathbf{y'PZAZ'Py} \\ \mathrm{tr}(\mathbf{P}) - \mathbf{y'PPy} \end{bmatrix} = \begin{bmatrix} \frac{N_a}{\sigma_a^2} - \frac{\mathrm{tr}(\mathbf{A}^{-1}\mathbf{C}^{uu})}{(\sigma_a^2)^2} - \frac{\hat{\mathbf{u}}'\mathbf{A}^{-1}\hat{\mathbf{u}}}{(\sigma_a^2)^2} \\ \frac{N - \mathrm{rank}(\mathbf{X})}{\sigma_e^2} - \frac{1}{\sigma_e^2}\left[N_a - \frac{\mathrm{tr}(\mathbf{A}^{-1}\mathbf{C}^{uu})}{\sigma_a^2}\right] - \frac{\hat{\mathbf{e}}'\hat{\mathbf{e}}}{(\sigma_e^2)^2} \end{bmatrix}$$

AI-REML

- Computationally demanding
- Much faster than EM-REML
  - Fewer iterations
- Provides estimation of standard errors
- BUT
  - For complex models and poor starting values
    - Slow convergence
    - Parameter estimates out of the parameter space
  - In some cases, initial rounds with EM-REML may help

blupf90+

VC Estimation

- AI-REML:

```
OPTION method VCE
```

- EM-REML:

```
OPTION method VCE
OPTION EM-REML
```

Original options for airemlf90 and remlf90 also work!

OPTION EM-REML

```
OPTION method VCE
```

```
OPTION EM-REML
OPTION EM-REML pure
```

$\longrightarrow$ Runs EM until convergence | shows EM output = remlf90

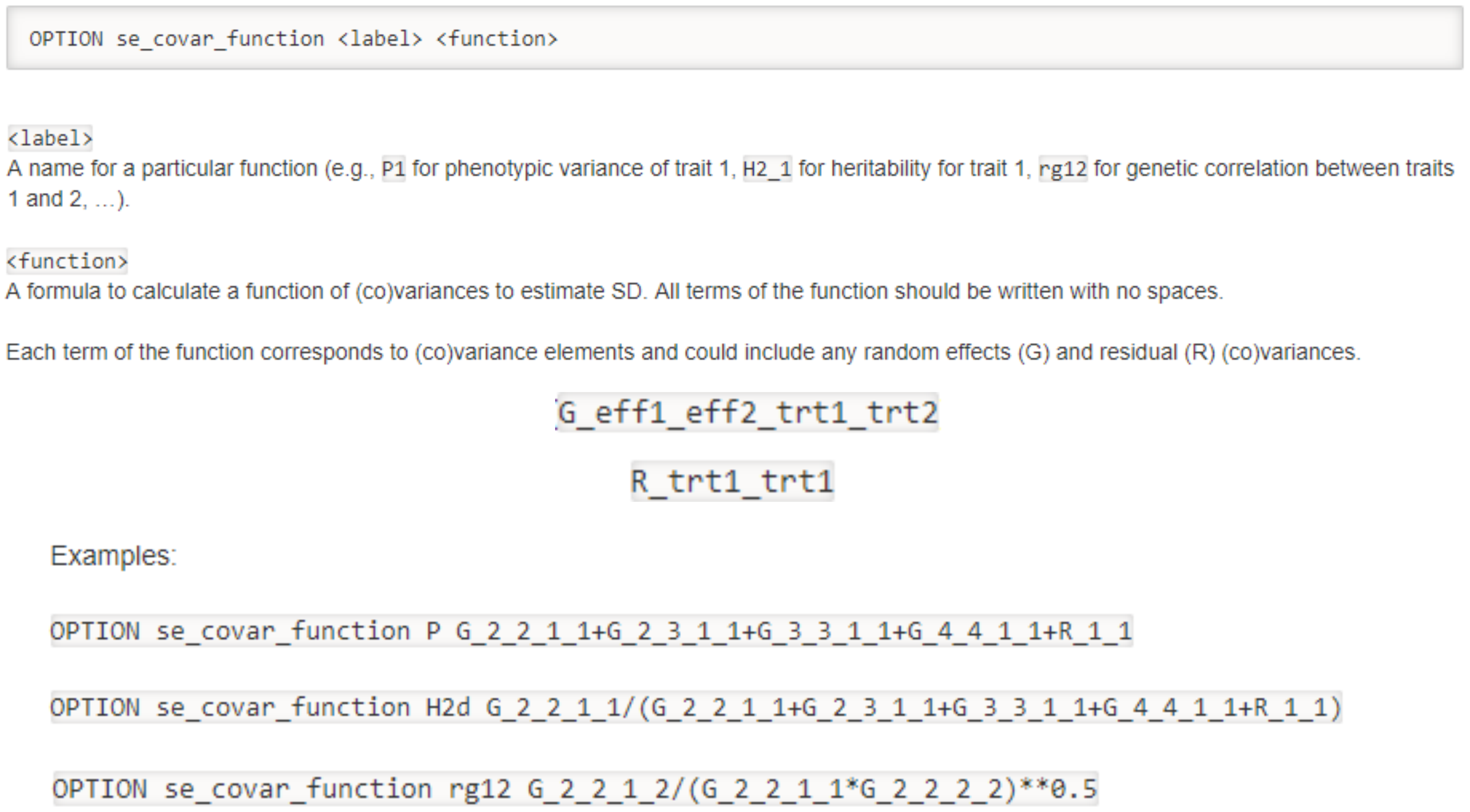
```
OPTION EM-REML n
```

$\longrightarrow$ Runs `n` EM rounds | switches to AI| shows AI output = airemlf90

```
OPTION EM-REML ai
```

$\longrightarrow$ Runs EM until convergence| switches to AI = airemlf90

Options for blupf90+ with VCE



```
OPTION se_covar_function <label> <function>
```

`<label>`
A name for a particular function (e.g., `P1` for phenotypic variance of trait 1, `H2_1` for heritability for trait 1, `rg12` for genetic correlation between traits 1 and 2, ...).

`<function>`
A formula to calculate a function of (co)variances to estimate SD. All terms of the function should be written with no spaces.

Each term of the function corresponds to (co)variance elements and could include any random effects (G) and residual (R) (co)variances.

`G_eff1_eff2_trt1_trt2`

`R_trt1_trt1`

Examples:

```
OPTION se_covar_function P G_2_2_1_1+G_2_3_1_1+G_3_3_1_1+G_4_4_1_1+R_1_1
```

```
OPTION se_covar_function H2d G_2_2_1_1/(G_2_2_1_1+G_2_3_1_1+G_3_3_1_1+G_4_4_1_1+R_1_1)
```

```
OPTION se_covar_function rg12 G_2_2_1_2/(G_2_2_1_1*G_2_2_2_2)**0.5
```

SE for genetic parameters

```
#genetic, permanent, residual
ahat=c(
  0.11478,
  0.13552,
  0.25290,
  )
```

with AI matrix:

```
# inverse of AI matrix (Sampling Variance)
AI=matrix(c(
  0.16799E-05, -0.96486E-06, -0.82566E-08,
 -0.96486E-06,  0.96167E-06, -0.37113E-07,
 -0.82566E-08, -0.37113E-07,  0.10864E-06)
,ncol=3)
```

```
require(MASS)
b=mvrnorm(10000,ahat,AI)
> head(b)
          [,1]      [,2]      [,3]
[1,] 0.1146738 0.1357640 0.2529399
[2,] 0.1163889 0.1342926 0.2528479
[3,] 0.1166155 0.1344342 0.2525161
[4,] 0.1142085 0.1358928 0.2534974
[5,] 0.1136835 0.1361108 0.2530133
[6,] 0.1140485 0.1365707 0.2530573
```

heritability and its standard deviation:

```
h2=b[,1]/(b[,1]+b[,2]+b[,3])
sd(h2)
> 0.002318198
```

Houle and Meyer (2015)   http://artadia.blogspot.com/2016/05/standard-error-of-variance-components.html

SE for genetic parameters

Houle and Meyer (2015):

Large-sample theory shows that maximum-likelihood estimates (including restricted maximum likelihood, REML) asymptotically have a multivariate normal distribution, with covariance matrix derived from the inverse of the information matrix, and mean equal to the estimated ***G****. This suggests that sampling estimates of* ***G*** *from this distribution can be used to assess the variability of estimates of* ***G****, and of functions of* ***G****.*

G = additive genetic variance–covariance matrices

Does blupf90+ for VCE always converge?

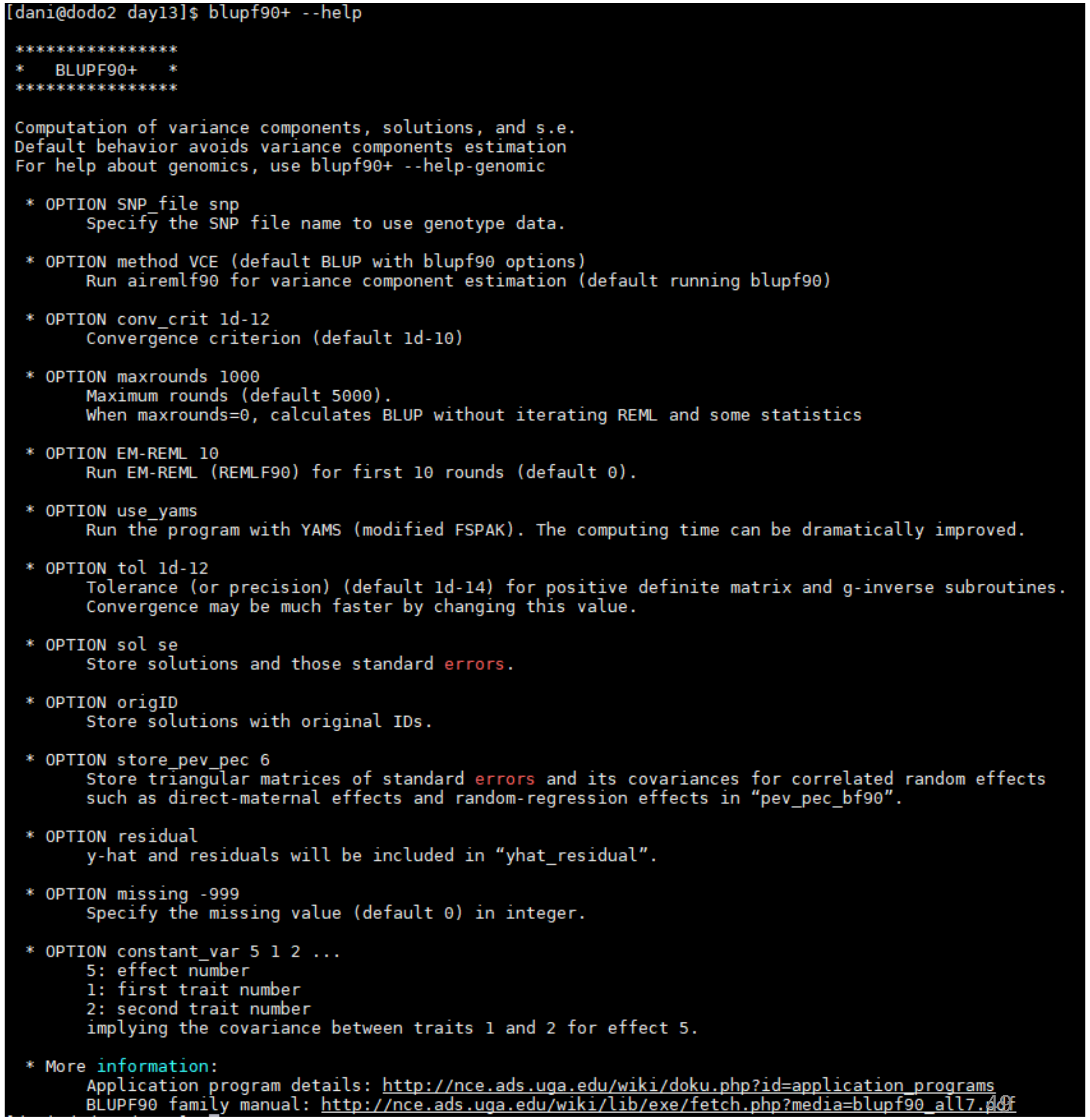
- When the expected variance is very small, or the covariance matrix is close to non-positive definite, try the following starting values:
  - much smaller = 0.00001
  - much bigger = 1000

- If blupf90+ does not converge with AI-REML but converges with EM-REML with the same data set and the same model:
  - run EM-REML again with a smaller starting value to check the estimate as it could be an artifact

  - use OPTION EM-REML inside blupf90+ as an initial point for AI-REML:
    - `OPTION EM-REML xx`

blupf90+ quick trick

- `blupf90+ --help`



```
[dani@dodo2 day13]$ blupf90+ --help

 ****************
 *   BLUPF90+   *
 ****************

 Computation of variance components, solutions, and s.e.
 Default behavior avoids variance components estimation
 For help about genomics, use blupf90+ --help-genomic

  * OPTION SNP_file snp
       Specify the SNP file name to use genotype data.

  * OPTION method VCE (default BLUP with blupf90 options)
       Run airemlf90 for variance component estimation (default running blupf90)

  * OPTION conv_crit 1d-12
       Convergence criterion (default 1d-10)

  * OPTION maxrounds 1000
       Maximum rounds (default 5000).
       When maxrounds=0, calculates BLUP without iterating REML and some statistics

  * OPTION EM-REML 10
       Run EM-REML (REMLF90) for first 10 rounds (default 0).

  * OPTION use_yams
       Run the program with YAMS (modified FSPAK). The computing time can be dramatically improved.

  * OPTION tol 1d-12
       Tolerance (or precision) (default 1d-14) for positive definite matrix and g-inverse subroutines.
       Convergence may be much faster by changing this value.

  * OPTION sol se
       Store solutions and those standard errors.

  * OPTION origID
       Store solutions with original IDs.

  * OPTION store_pev_pec 6
       Store triangular matrices of standard errors and its covariances for correlated random effects
       such as direct-maternal effects and random-regression effects in “pev_pec_bf90”.

  * OPTION residual
       y-hat and residuals will be included in “yhat_residual”.

  * OPTION missing -999
       Specify the missing value (default 0) in integer.

  * OPTION constant_var 5 1 2 ...
       5: effect number
       1: first trait number
       2: second trait number
       implying the covariance between traits 1 and 2 for effect 5.

  * More information:
       Application program details: http://nce.ads.uga.edu/wiki/doku.php?id=application_programs
       BLUPF90 family manual: http://nce.ads.uga.edu/wiki/lib/exe/fetch.php?media=blupf90_all7.pdf
```

`gibbsf90+`

- `gibbs1f90`: stores single trait matrices once – fast for multi-trait models
- `gibbs2f90`: gibbs1f90 with joint sampling of correlated effects – Maternal effects and RRM
- `gibbs3f90`: gibbs2f90 with heterogeneous residual variance
- `thrgibbs1f90`: for linear-threshold models
- `thrgibbs3f90`: thrgibbs1f90 with heterogeneous residual variance

Variance Components Estimation

Mixed Model Equations Solver

$$\begin{bmatrix} \mathbf{X'R^{-1}X} & \mathbf{X'R^{-1}W} \\ \mathbf{W'R^{-1}X} & \mathbf{W'R^{-1}W+A^{-1}\otimes G_0^{-1}} \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{\beta}} \\ \hat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X'R^{-1}y} \\ \mathbf{W'R^{-1}y} \end{bmatrix}$$

gibbsf90+

Linear

Default

Threshold (-Linear)

```
OPTION cat 0 2 5
```

- Categories renumbered from **1**
- Missing records is only **0**

gibbsf90+

Bayes Theorem

Likelihood function

indicates how likely the observations are from a distribution (with particular parameters)

$$p(\theta|y) = p(y|\theta)\, p(\theta)$$

prior probability of unknown θ

posterior probability of unknown θ with known y

- Basic idea of Gibbs Sampling:
- Numerical method to draw samples from a posterior distribution (not always explicitly available)
- Draw samples = generate random numbers following a distribution
- The results are random numbers (not theoretical formulas)
- The posterior distribution will be drawn based on the numerical values (like a histogram)

gibbsf90+

Ingredients for Gibbs sampling

1) Theoretical derivation: conditional posterior distribution for each unknown parameter

2) Software: a random number generator for a particular distribution

```r
# Basic Gibbs sampling for mu (normal) and sigma2 (inverted chi-square)
y <- c(14,16,18)
N <- length(y)
n.samples <- 100
mu <- rep(0,n.samples)
sigma2 <- rep(0,n.samples)

# initial value
mu[1] <- 0
sigma2[1] <- 10

# sampling
for(i in 2:n.samples){
    mu[i] <- rnorm(1, mean=mean(y), sd=sqrt(sigma2[i-1]/N)) # using the most recent sigma2
    df <- N-2
    S <- sum((y-mu[i])^2)
    sigma2[i] <- rinvchisq(1, df=df, scale=S) # using the most recent mu
}
```

Running gibbsf90+

- Name of parameter file?

  gibbs1.par

- Number of samples and length of burn-in?

  100000 0

- Give n to store every n-th sample?

  10

- `gibbsf90+ parfile.par --samples i --burnin j --interval k`

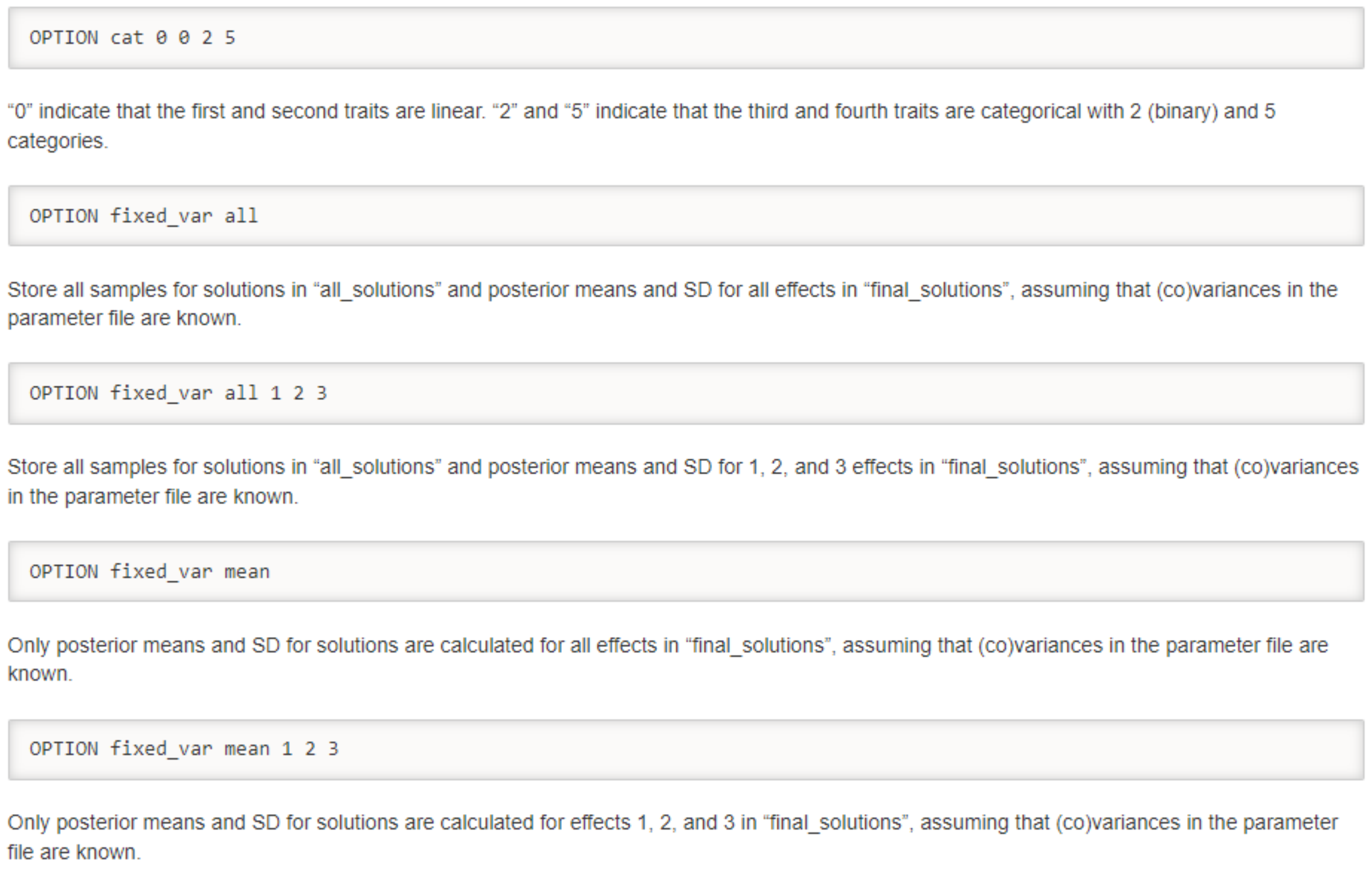
gibbsf90+

- Procedure
  - Run `gibbsf90+` to estimate variance components
  - Run `postgibbsf90` to process the samples and check convergence
  - Run `gibbsf90+` with new variance components to compute EBV (2k to 10k samples)

```
OPTION fixed_var mean X
```

Number of the animal effect

gibbsf90+



```
OPTION cat 0 0 2 5
```

“0” indicate that the first and second traits are linear. “2” and “5” indicate that the third and fourth traits are categorical with 2 (binary) and 5 categories.

```
OPTION fixed_var all
```

Store all samples for solutions in “all_solutions” and posterior means and SD for all effects in “final_solutions”, assuming that (co)variances in the parameter file are known.

```
OPTION fixed_var all 1 2 3
```

Store all samples for solutions in “all_solutions” and posterior means and SD for 1, 2, and 3 effects in “final_solutions”, assuming that (co)variances in the parameter file are known.

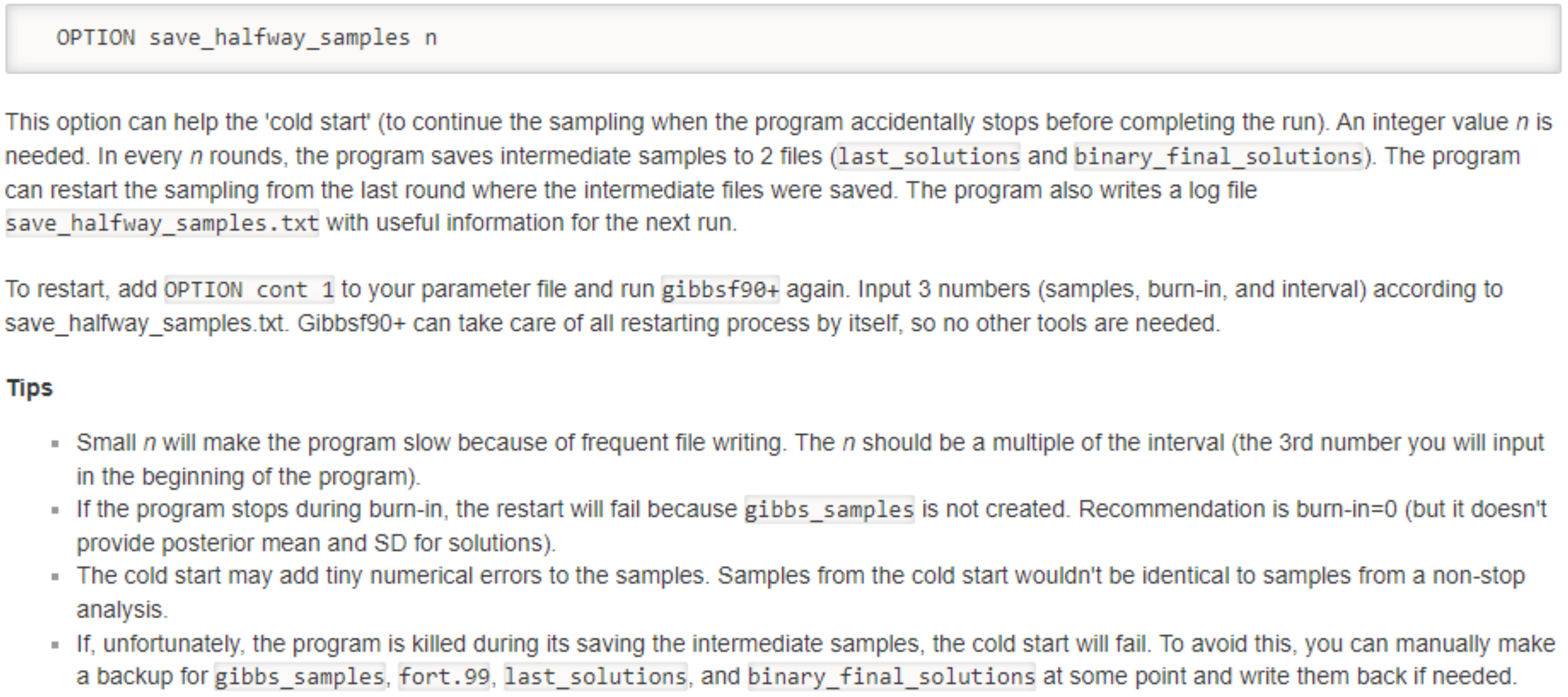
```
OPTION fixed_var mean
```

Only posterior means and SD for solutions are calculated for all effects in “final_solutions”, assuming that (co)variances in the parameter file are known.

```
OPTION fixed_var mean 1 2 3
```

Only posterior means and SD for solutions are calculated for effects 1, 2, and 3 in “final_solutions”, assuming that (co)variances in the parameter file are known.

gibbsf90+



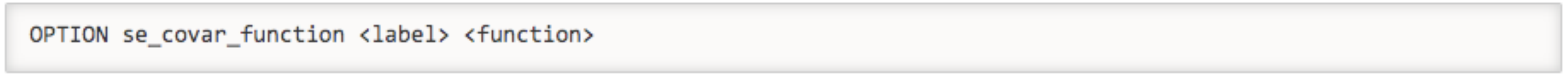
```
OPTION save_halfway_samples n
```

This option can help the 'cold start' (to continue the sampling when the program accidentally stops before completing the run). An integer value *n* is needed. In every *n* rounds, the program saves intermediate samples to 2 files (`last_solutions` and `binary_final_solutions`). The program can restart the sampling from the last round where the intermediate files were saved. The program also writes a log file `save_halfway_samples.txt` with useful information for the next run.

To restart, add `OPTION cont 1` to your parameter file and run `gibbsf90+` again. Input 3 numbers (samples, burn-in, and interval) according to save_halfway_samples.txt. Gibbsf90+ can take care of all restarting process by itself, so no other tools are needed.

Tips

- Small *n* will make the program slow because of frequent file writing. The *n* should be a multiple of the interval (the 3rd number you will input in the beginning of the program).
- If the program stops during burn-in, the restart will fail because `gibbs_samples` is not created. Recommendation is burn-in=0 (but it doesn't provide posterior mean and SD for solutions).
- The cold start may add tiny numerical errors to the samples. Samples from the cold start wouldn't be identical to samples from a non-stop analysis.
- If, unfortunately, the program is killed during its saving the intermediate samples, the cold start will fail. To avoid this, you can manually make a backup for `gibbs_samples`, `fort.99`, `last_solutions`, and `binary_final_solutions` at some point and write them back if needed.



```
OPTION se_covar_function <label> <function>
```

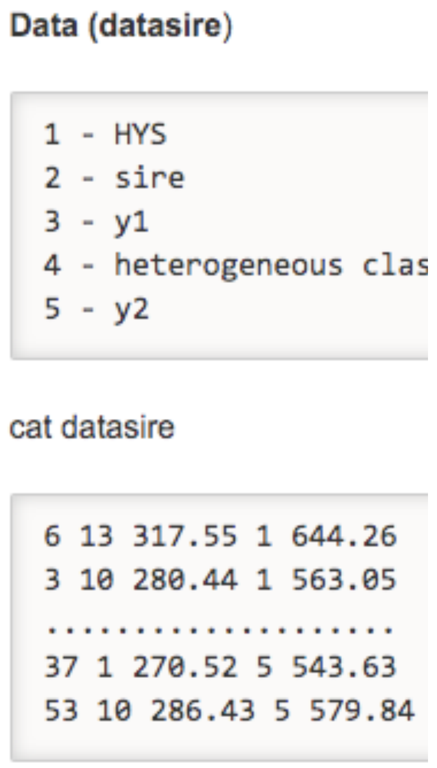
gibbsf90+

```
   OPTION hetres_int col nlev
```

```
OPTION hetres_int 5 10
```

The position “5” to identify the interval in the data file and the number of intervals “10” for heterogeneous residual variances.

gibbsf90+

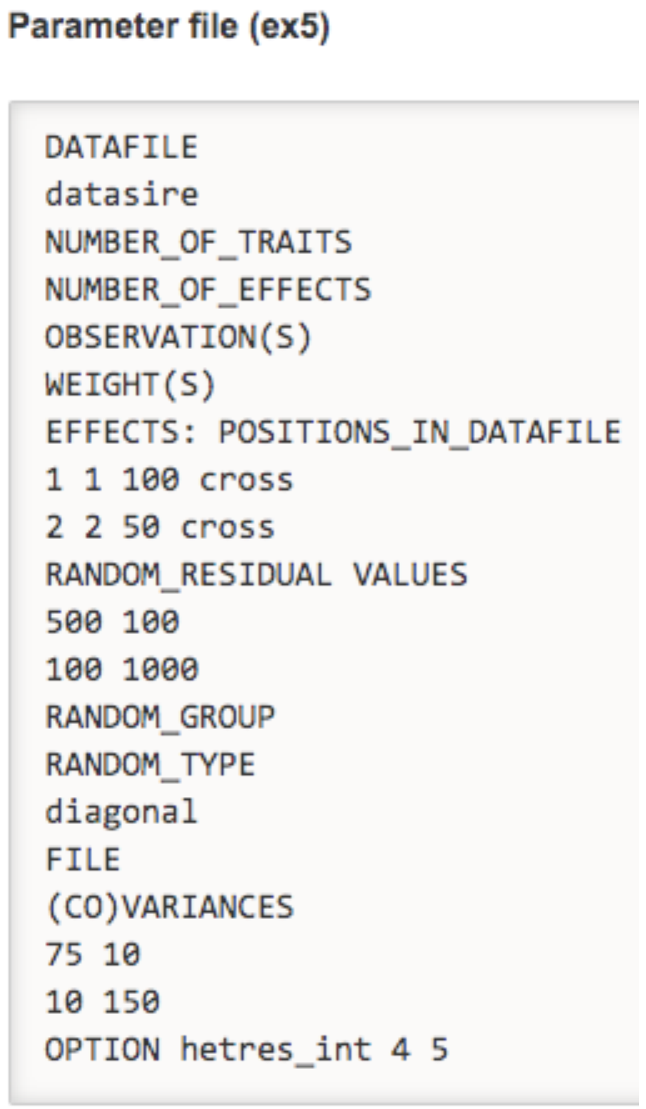


Data (datasire)

```
1 - HYS
2 - sire
3 - y1
4 - heterogeneous clas
5 - y2
```

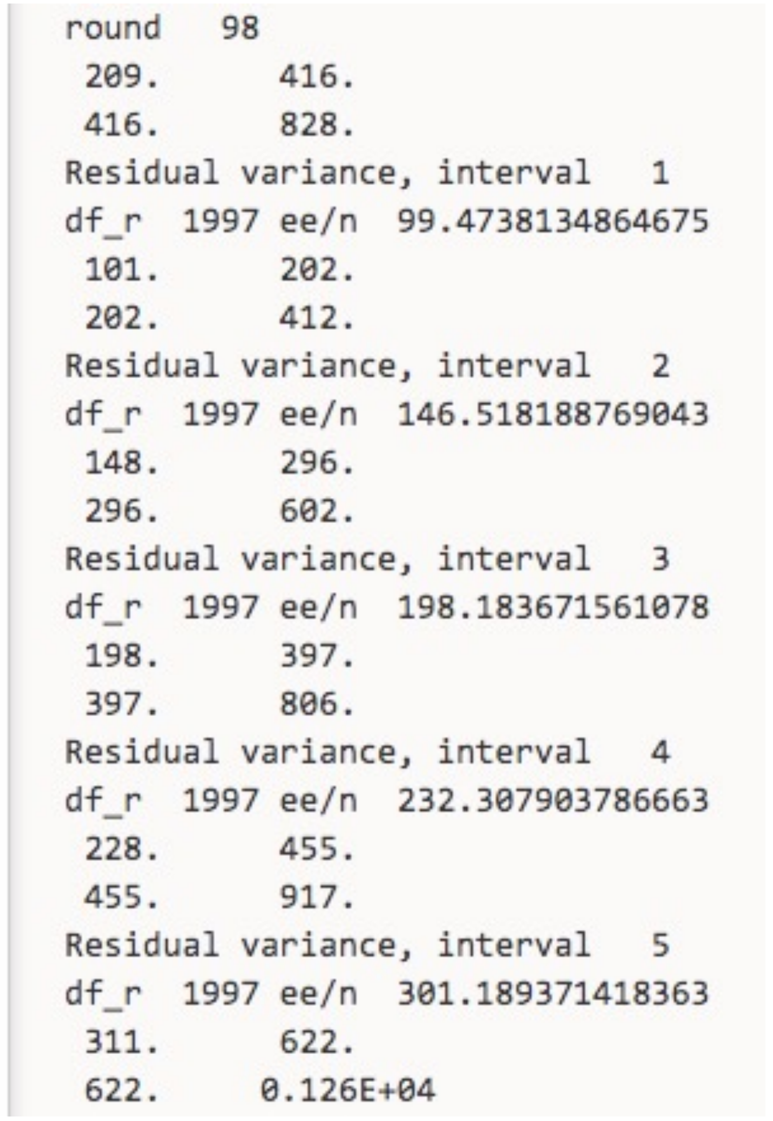
cat datasire

```
6 13 317.55 1 644.26
3 10 280.44 1 563.05
....................
37 1 270.52 5 543.63
53 10 286.43 5 579.84
```



Parameter file (ex5)

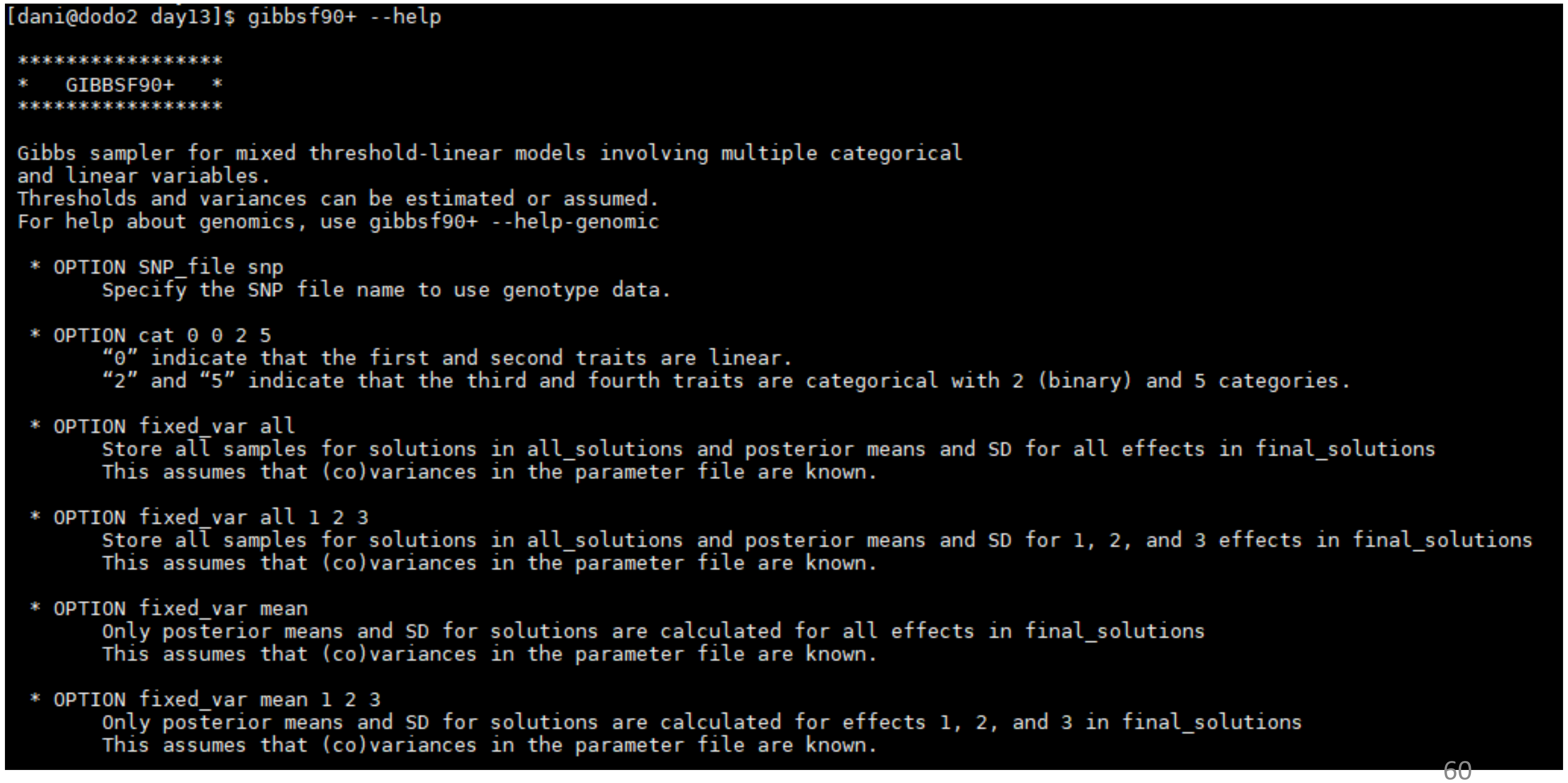
```
DATAFILE
datasire
NUMBER_OF_TRAITS
NUMBER_OF_EFFECTS
OBSERVATION(S)
WEIGHT(S)
EFFECTS: POSITIONS_IN_DATAFILE
1 1 100 cross
2 2 50 cross
RANDOM_RESIDUAL VALUES
500 100
100 1000
RANDOM_GROUP
RANDOM_TYPE
diagonal
FILE
(CO)VARIANCES
75 10
10 150
OPTION hetres_int 4 5
```



```
round    98
 209.       416.
 416.       828.
Residual variance, interval   1
df_r  1997 ee/n  99.4738134864675
 101.       202.
 202.       412.
Residual variance, interval   2
df_r  1997 ee/n  146.518188769043
 148.       296.
 296.       602.
Residual variance, interval   3
df_r  1997 ee/n  198.183671561078
 198.       397.
 397.       806.
Residual variance, interval   4
df_r  1997 ee/n  232.307903786663
 228.       455.
 455.       917.
Residual variance, interval   5
df_r  1997 ee/n  301.189371418363
 311.       622.
 622.     0.126E+04
```

gibbsf90+ quick trick

- `gibbsf90+ --help`



```
[dani@dodo2 day13]$ gibbsf90+ --help

 *****************
 *   GIBBSF90+   *
 *****************

 Gibbs sampler for mixed threshold-linear models involving multiple categorical
 and linear variables.
 Thresholds and variances can be estimated or assumed.
 For help about genomics, use gibbsf90+ --help-genomic

  * OPTION SNP_file snp
       Specify the SNP file name to use genotype data.

  * OPTION cat 0 0 2 5
       “0” indicate that the first and second traits are linear.
       “2” and “5” indicate that the third and fourth traits are categorical with 2 (binary) and 5 categories.

  * OPTION fixed_var all
       Store all samples for solutions in all_solutions and posterior means and SD for all effects in final_solutions
       This assumes that (co)variances in the parameter file are known.

  * OPTION fixed_var all 1 2 3
       Store all samples for solutions in all_solutions and posterior means and SD for 1, 2, and 3 effects in final_solutions
       This assumes that (co)variances in the parameter file are known.

  * OPTION fixed_var mean
       Only posterior means and SD for solutions are calculated for all effects in final_solutions
       This assumes that (co)variances in the parameter file are known.

  * OPTION fixed_var mean 1 2 3
       Only posterior means and SD for solutions are calculated for effects 1, 2, and 3 in final_solutions
       This assumes that (co)variances in the parameter file are known.
```

gibbsf90+ quick trick II

- Optimizing gibbsf90+ when using genomic data

Run renumf90 with the following option:

```
OPTION animal_order genotypes
```

Run gibbsf90+ with the following option:

```
OPTION separate_dense
```

postgibbsf90

- Basic idea of post-Gibbs analysis:

- Summarize and visualize the samples drawn by gibbsf90+
- Confirm if the chain converged
- Find the most probable value = posterior mode as a “point estimate”
- Find the reliability of the estimates = the highest posterior density as a “confidence interval”

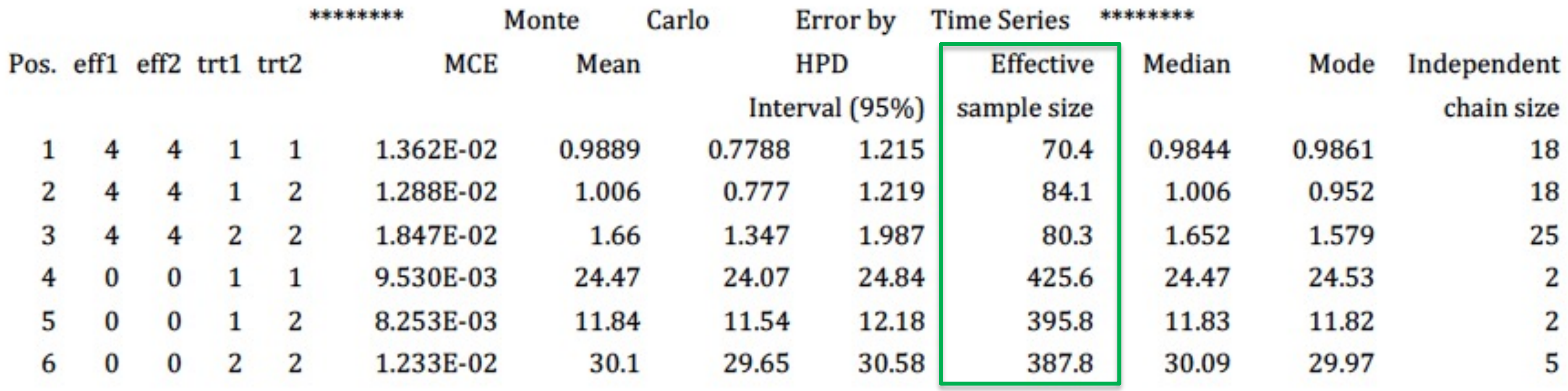
postgibbsf90

- Name of parameter file?
  gibbs1.par
- Burn-in?
  0
- Give n to store every n-th sample? (1 means read all samples)
  10

- input files
  gibbs_samples, fort.99
- output files
  "postgibbs_samples"
    all Gibbs samples for additional post analyses
  "postmean"
    posterior means
  "postsd"
    posterior standard deviations
  "postout"

postgibbsf90

at least > 10 is recommended
> 30 may be better

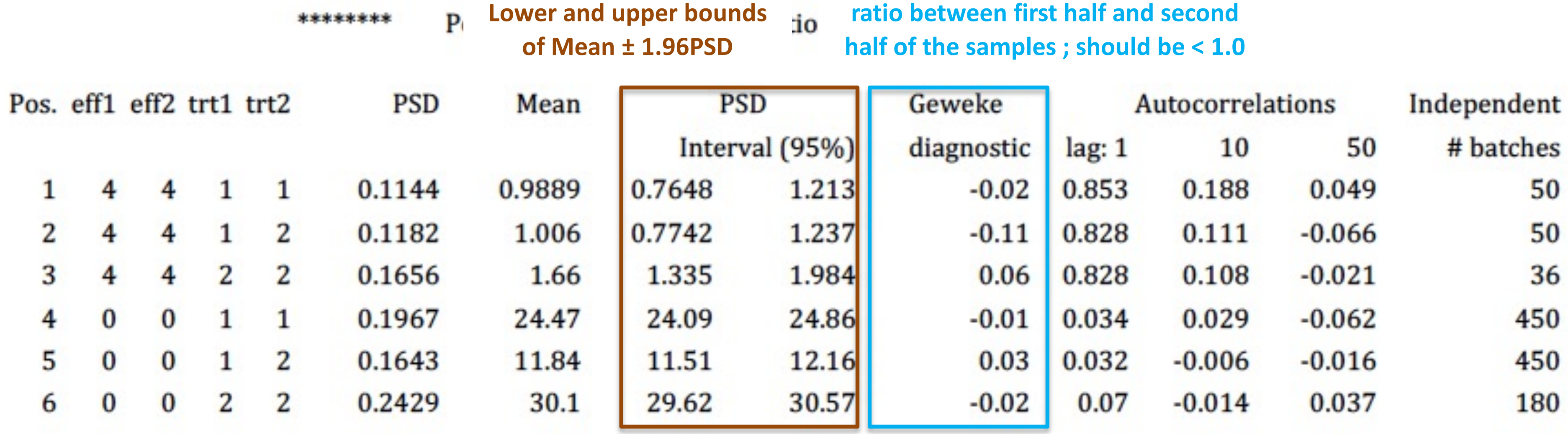


******** Monte Carlo Error by Time Series ********

Pos.	eff1	eff2	trt1	trt2	MCE	Mean	HPD Interval (95%)		Effective sample size	Median	Mode	Independent chain size
1	4	4	1	1	1.362E-02	0.9889	0.7788	1.215	70.4	0.9844	0.9861	18
2	4	4	1	2	1.288E-02	1.006	0.777	1.219	84.1	1.006	0.952	18
3	4	4	2	2	1.847E-02	1.66	1.347	1.987	80.3	1.652	1.579	25
4	0	0	1	1	9.530E-03	24.47	24.07	24.84	425.6	24.47	24.53	2
5	0	0	1	2	8.253E-03	11.84	11.54	12.18	395.8	11.83	11.82	2
6	0	0	2	2	1.233E-02	30.1	29.65	30.58	387.8	30.09	29.97	5

Lower and upper bounds of Mean ± 1.96PSD

ratio between first half and second half of the samples ; should be < 1.0



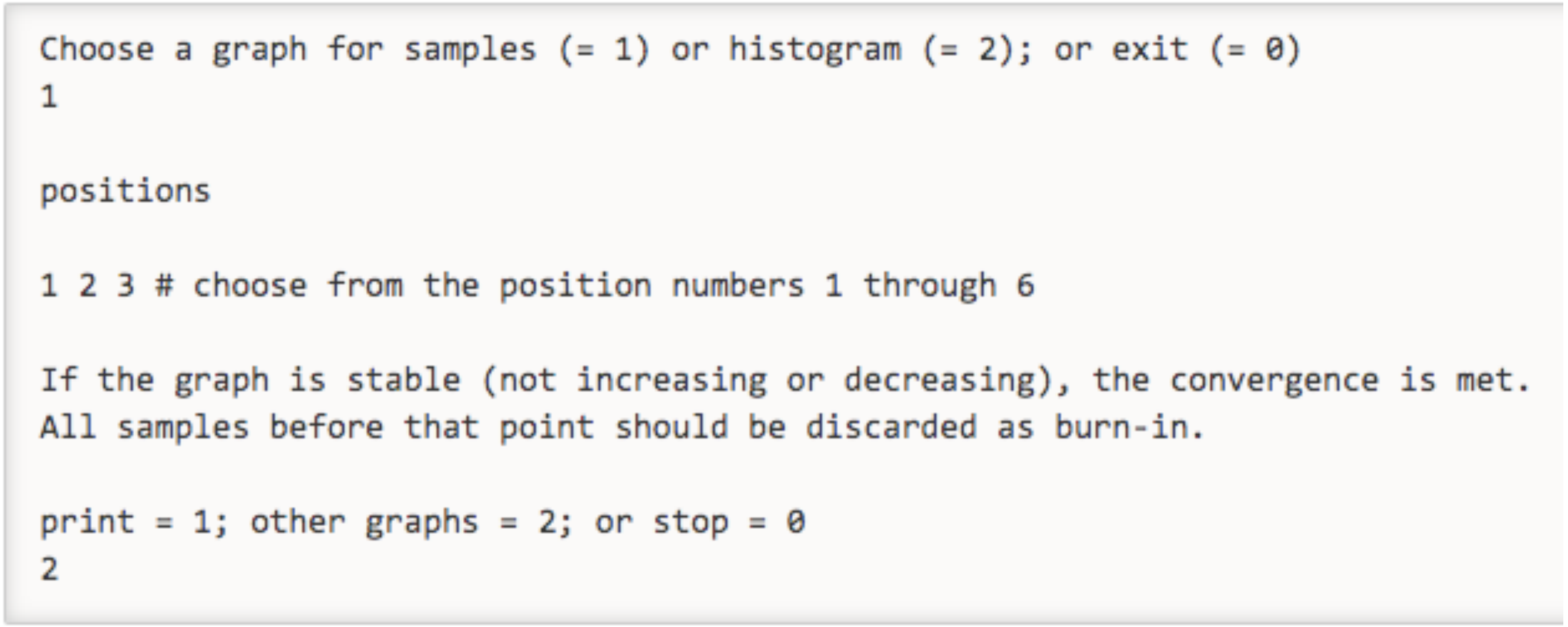
******** P io

Pos.	eff1	eff2	trt1	trt2	PSD	Mean	PSD Interval (95%)		Geweke diagnostic	Autocorrelations lag: 1	10	50	Independent # batches
1	4	4	1	1	0.1144	0.9889	0.7648	1.213	-0.02	0.853	0.188	0.049	50
2	4	4	1	2	0.1182	1.006	0.7742	1.237	-0.11	0.828	0.111	-0.066	50
3	4	4	2	2	0.1656	1.66	1.335	1.984	0.06	0.828	0.108	-0.021	36
4	0	0	1	1	0.1967	24.47	24.09	24.86	-0.01	0.034	0.029	-0.062	450
5	0	0	1	2	0.1643	11.84	11.51	12.16	0.03	0.032	-0.006	-0.016	450
6	0	0	2	2	0.2429	30.1	29.62	30.57	-0.02	0.07	-0.014	0.037	180

postgibbsf90

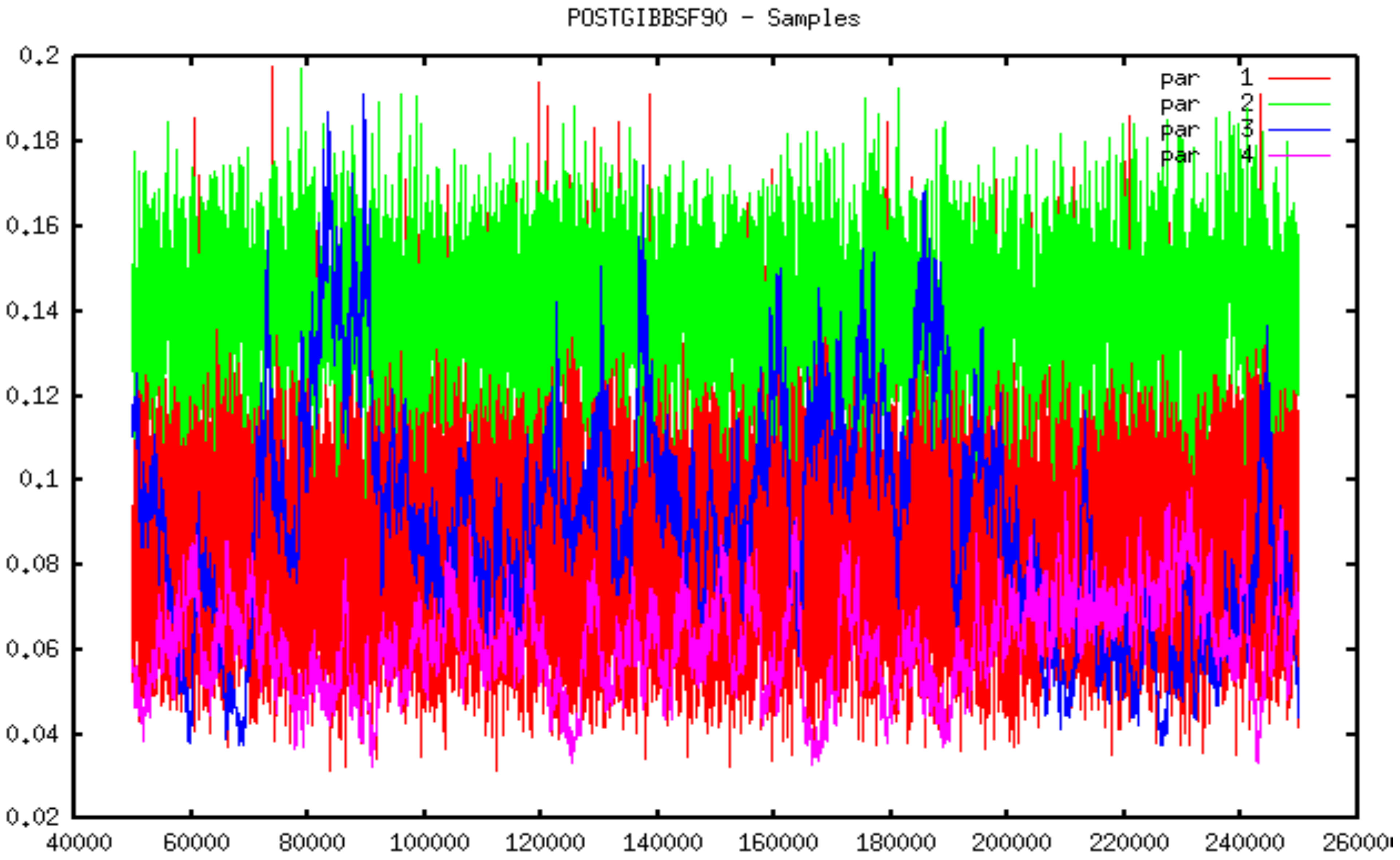
- MCE = Monte Carlo error, corresponding to the ‘’standard error’’ of the posterior mean of a parameter
- Mean = Posterior mean of a parameter
- HPD = High probability density within 95%, close idea to ‘’95% confidence interval’’ in frequentist approach
- Effective sample size = Number of samples after deducting auto-correlation among samples
- Median = Posterior median of a parameter
- Mode = Posterior mode of a parameter; just an approximation
- Independent chain size
- PSD = Posterior standard deviation of a parameter
- Mean = the same as above
- PSD Interval (95%) = Lower and upper bounds of Mean ±1.96PSD
- Geweke diagnostic = Convergence diagnosis; could be converged if this is <1.0
    - (according to the manual, this is almost useless because this is <1.0 in almost all cases)
- Autocorrelations = Lag-correlations with lag 1, 10 and 50; calculated for the saved samples
- Independent # batches = The effective number of blocks after deducting the auto-correlation among samples

postgibbsf90

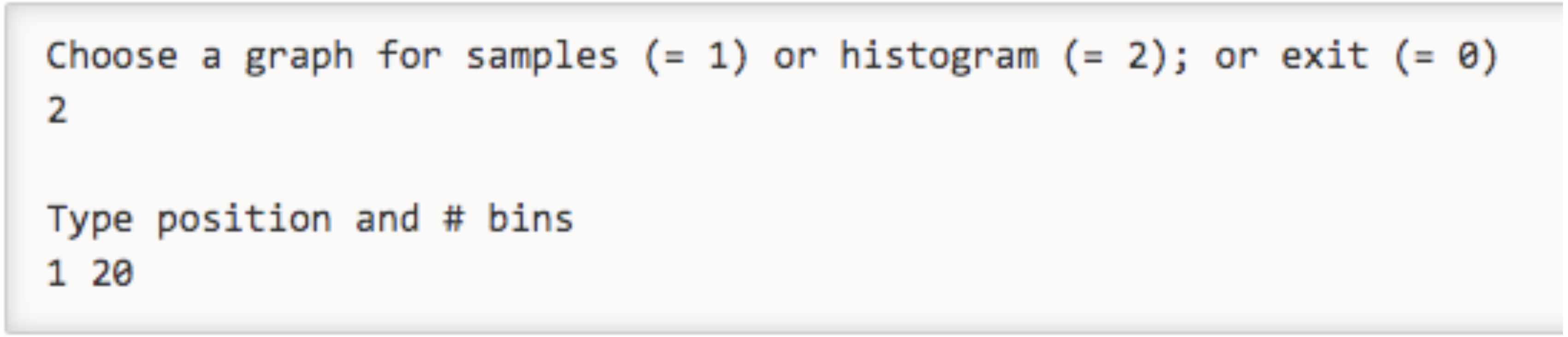


```
Choose a graph for samples (= 1) or histogram (= 2); or exit (= 0)
1

positions

1 2 3 # choose from the position numbers 1 through 6

If the graph is stable (not increasing or decreasing), the convergence is met.
All samples before that point should be discarded as burn-in.

print = 1; other graphs = 2; or stop = 0
2
```

postgibbsf90

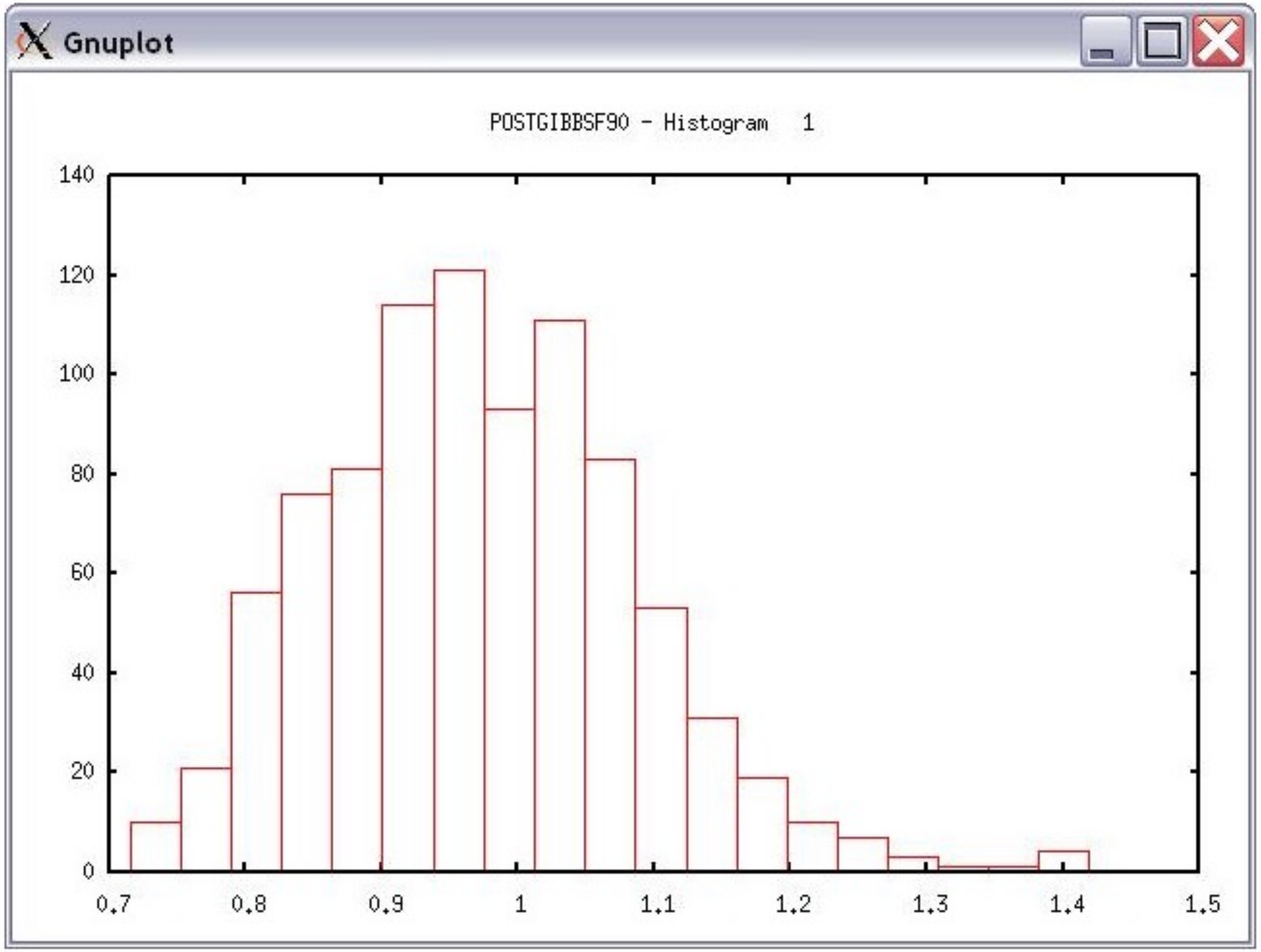


postgibbsf90



```
Choose a graph for samples (= 1) or histogram (= 2); or exit (= 0)
2

Type position and # bins
1 20
```

postgibbsf90



Common problems for BLUPF90 family

- Wrong position or formats for observation and effects
- Misspelling of Keywords
  - Program may stop
- (Co)variance matrices not symmetric, not positive definite
  - Program may not stop
- Large numbers (e.g., 305-day milk yield 10,000 kg)
  - Scale down i.e., 10,000 /1,000 = 10

General output from BLUPF90 family

- Output printed on the screen is not saved to any file!
- Should use redirection or pipes to store output

blupf90+

```
blupf90+ renf90.par | tee blup.log
```

gibbsf90+

```
gibbsf90+ exmr99s1 --samples 1000 --burnin 0 --interval 1 | tee gibbs.log
```

Run in background + Save output

```
$vi gibbs.sh
#type the following commands inside gibbs.sh
      gibbsf90+ <<AA > gibbs.log
      renf90.par
      1000 0
      10
      AA
#save and exit
$bash gibbs.sh &  #can replace bash with sh
```

```
$vi bp.sh
#type the following commands inside bp.sh
      blupf90+ <<AA > blup.log
      renf90.par
      AA
#save and exit
$bash bp.sh &   #can replace bash by sh
```