
UNIVERSITY OF
GEORGIA
College of Agricultural &
Environmental Sciences
*Animal Breeding and*
*Genetics Group*

# Introduction to BLUPF90 software suite

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BLUPF90 TEAM – 03/2023

# BLUPF90 software suite

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

## The State of Fortran

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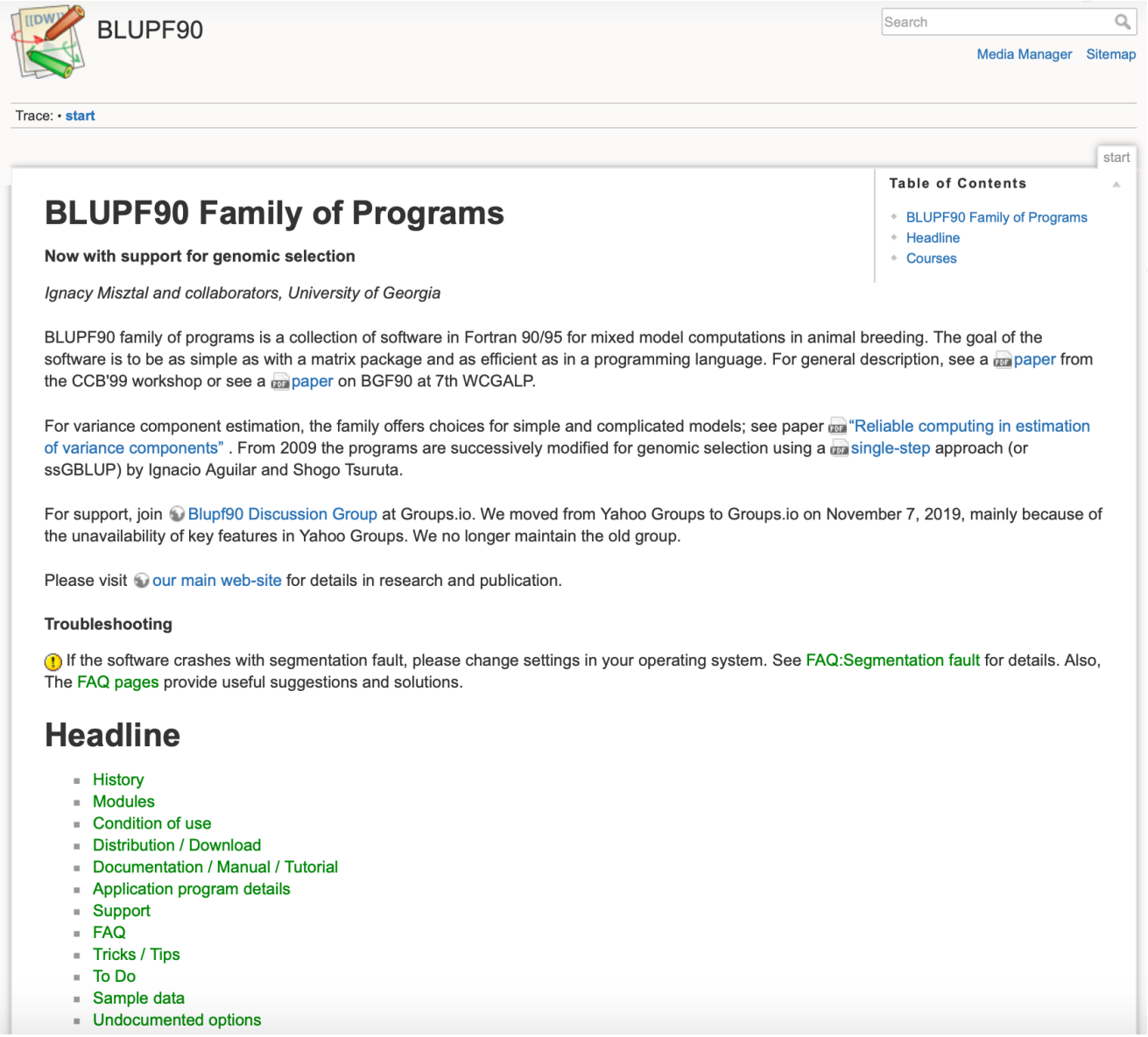
***Abstract*—A community of developers has formed to modernize the Fortran ecosystem. In this article, we describe the high-level features of Fortran that continue to make it a good choice for scientists and engineers in the 21st century. Ongoing efforts include the development of a Fortran standard 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.**

# BLUPF90 software suite


BLUPF90

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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
  - Fortran ≥ 90
  - Computations in AB & G
- Since 1997/1998 by Ignacy Misztal
- Several developers + collaborators
- Simple, efficient, and comprehensive
  - Very general models

# BLUPF90 software main developers

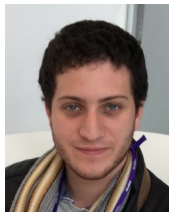
Ignacy Misztal

Shogo Tsuruta

Andres Legarra

Ignacio Aguilar

Yutaka Masuda



Matias Bermann

- + 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

# nce.ads.uga.edu/wiki

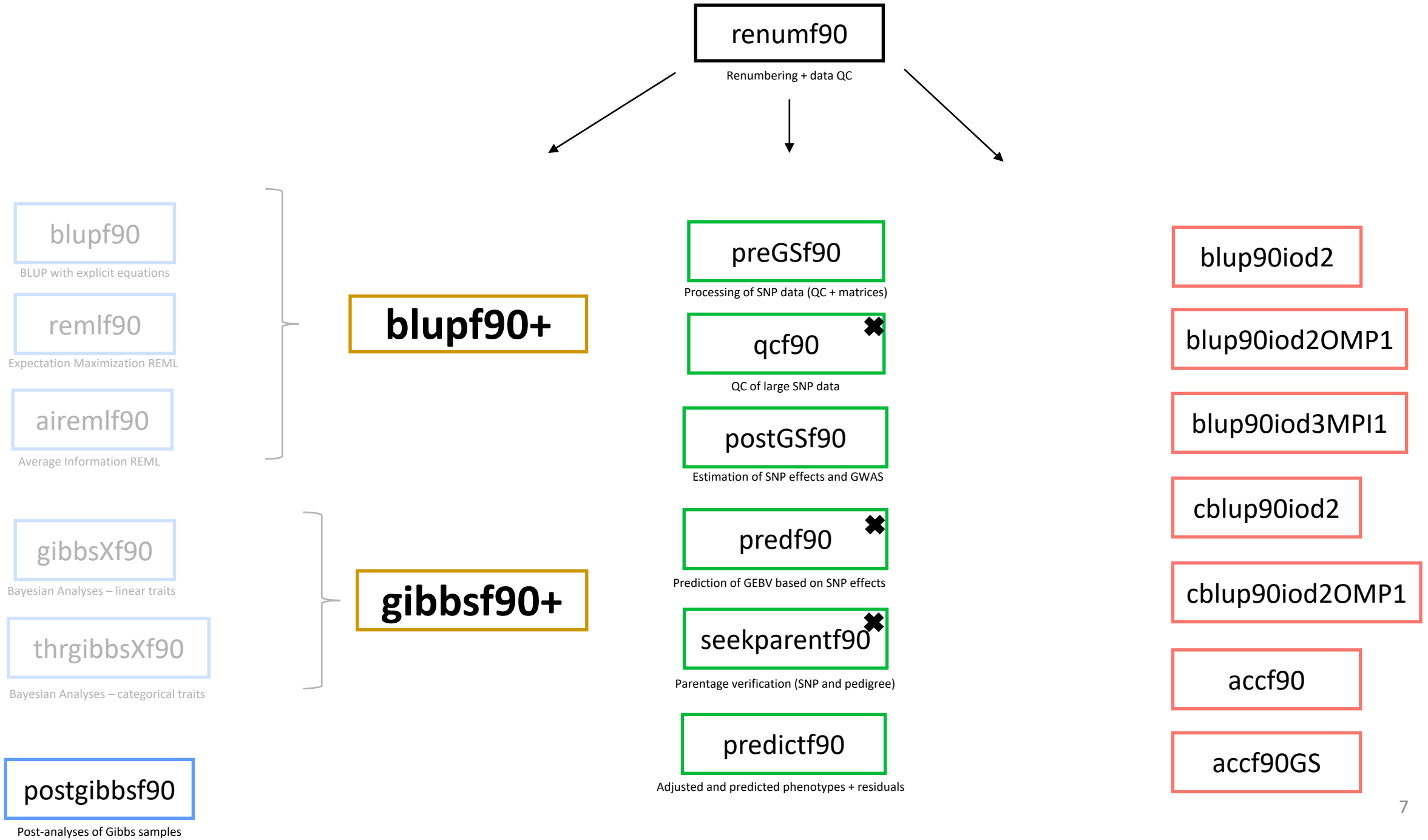
## Programs

**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


renumf90
Renumbering + data QC
blupf90
BLUP with explicit equations
remlf90
Expectation Maximization REML
airemlf90
Average Information REML
blupf90+
gibbsXf90
Bayesian Analyses – linear traits
thrgibbsXf90
Bayesian Analyses – categorical traits
gibbsf90+
postgibbsf90
Post-analyses of Gibbs samples
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 + residuals
blup90iod2
blup90iod2OMP1
blup90iod3MPI1
cblup90iod2
cblup90iod2OMP1
accf90
accf90GS

# RENUMF90

The **renumbering software** for the BLUPF90 suite

# RENUMF90

- **Renumbers data and pedigree**
- **Creates a parameter file for BLUPF90 family**
  - **Parameter file can be modified by the users for new models**
- **Traces back pedigree for individuals in the data**
- **Performs comprehensive pedigree checks**
- **Provides data statistics**
- **Creates an Xref file for genotyped individuals**
- **Computes inbreeding by default in v ≥ 1.157**

# RENUMF90

- **Supports**
  - virtually any dataset
  - multiple traits
  - different models (effects) per trait
  - alphanumeric and numeric fields
  - unknown parent groups
  - covariates for random regression models

# RENUMF90 – Input files

- **Data file and pedigree file as flat files**
  - Columns separated by at least one SPACE
  - No TABS !!!! (current version checks for it)
  - Input files cannot contain character #
  - Missing sire/dams must have code 0
  - code 00 is treated as a known animal

# RENUMF90 – Output files

- **Creates files to be used by BLUPF90 family**
  - renf90.inb - file with inbreeding
  - renf90.tables - cross reference file with renumbered and original effects
  - renf90.fields - description of the effects in each field of renf90.dat

  - renf90.dat - renumbered data
  - renaddxx.ped - renumbered pedigree + statistics
  - renf90.par - new parameter file

# RENUMF90 parameter file

## MANDATORY

| Keyword | possible value | description |
|---|---|---|
| DATAFILE | character | The name of data file to be processed |
| TRAITS | integer | Position for phenotype (trait) in the data file |
| FIELDS_PASSED TO OUTPUT | integer | Position for the columns in the original data that will be passed to the renumbered data without changes<br>Keep empty if not needed |
| WEIGHT(S) | integer | The position(s) for weight in the data file<br>Keep empty if not needed |
| RESIDUAL_VARIANCE | real value(s) | Residual (co)variance |
| EFFECT | (next slide …) | Description of an effect<br>Repeatable – 1 for each effect in the model |

# RENUMF90 parameter file

## Effects

| Keyword | Possible value | effect type | form |
|---|---|---|---|
| EFFECT | integer (column where the effect is) | cross | alpha |
| | | | numer |
| | | cov | |

| Keyword (only for covariables) | Possible value | form |
|---|---|---|
| NESTED | integer (column where the effect is) | alpha |
| | | numer |

# RENUMF90 parameter file

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

```
DATAFILE
data1.txt
TRAITS
5
FIELDS_PASSED TO OUTPUT
2
WEIGHT(S)

RESIDUAL_VARIANCE
1.0
EFFECT        #1st effect - farm
2 cross alpha
EFFECT        #2nd effect - sex
3 cross numer
EFFECT        #3rd effect - age
4 cov
```

*Fixed linear model*

data1.txt

| ID | farm | sex | age | phen |
|---|---|---|---|---|
| ID006 | A | 1 | 1.0 | 3.0 |
| ID009 | A | 2 | 1.0 | 2.0 |
| ID012 | A | 1 | 2.0 | 4.0 |
| ID007 | B | 2 | 2.0 | 6.0 |
| ID010 | B | 1 | 1.0 | 3.0 |
| ID013 | B | 2 | 2.0 | 6.0 |
| ID008 | C | 1 | 2.0 | 6.0 |
| ID011 | C | 2 | 1.0 | 6.0 |
| ID014 | C | 1 | 1.0 | 8.0 |
| ID015 | C | 2 | 2.0 | 4.0 |

# RENUMF90 parameter file

## Random Effects

| Keyword after EFFECT | possible value | description |
|---|---|---|
| RANDOM | diagonal | Non-correlated |
| | animal | Correlation structure among animals |

| Keyword | possible value | description |
|---|---|---|
| OPTIONAL | pe | Permanent environmental |
| | mat | Maternal |
| | mpe | Permanent environmental maternal (only if mat is used) |

# RENUMF90 parameter file

## Random effects file section

| Keyword after RANDOM (animal only) | possible value | description |
|---|---|---|
| FILE | character | Name of the pedigree file<br>for animal models only |

| Keyword after FILE<br>(for RANDOM animal only) | possible value | description |
|---|---|---|
| FILE_POS | integer | Specifies positions in the pedigree for<br>ani sire dam alternate_dam yob<br>Default: 1 2 3 0 0<br>*If maternal effect alternate_dam* |

| Keyword<br>(for RANDOM animal only) | possible value | description |
|---|---|---|
| SNP_FILE | character | Optional: If genomic info is to be used<br>Name of the SNP file<br>Format: ID 0111222111555152222 |

# RENUMF90 parameter file

## Pedigree options

| **Keyword**<br>**(for RANDOM animal only)** | **possible value** | **description** |
|---|---|---|
| PED_DEPTH | Integer | Optional<br>Specifies the depth of pedigree search<br>Default = 3<br>All pedigree = 0 |

# RENUMF90 parameter file

## Unknown Parent Group options

| **Keyword**<br>**(for RANDOM animal only)** | **possible value** | **description** |
|---|---|---|
| UPG_TYPE | | Optional |
| | yob<br>1990 1992 … | UPG assigned based on yob |
| | in_pedigrees | Missing parent receives -x<br>x is the UPG number |
| | group_unisex | UPG based on the information in pedigree<br>Ex. UPG by breed<br>**FILE_POS**<br>1 2 3 0 0 4 #the 6th field indicates which column the UPG code is in the pedigree |
| | group_sex | Separate UPG code for unknown sire and dam<br>**FILE_POS**<br>1 2 3 0 0 4 5 #the 6th and 7th fields indicate which columns the UPG codes are in the pedigree |

# RENUMF90 parameter file

## Inbreeding option

| **Keyword**<br>**(for RANDOM animal only)** | **possible value** | **description** |
|---|---|---|
| INBREEDING | | Default in RENUMF90 ≥ v1.157 |
| | pedigree | Calculates inbreeding code and saves it in the renumbered pedigree file<br>(Default in RENUMF90 ≥ v1.157) |
| | File <name> | Reads inbreeding from an external file<br>format: original_ID  inbreeding (0 to 1) |
| | self x | Calculates inbreeding with selfing<br>x is the column in the pedigree file with the number of selfing generations |
| | no-inbreeding | Turn inbreeding calculation off in RENUMF90 ≥ v1.157 |

# RENUMF90 parameter file

## Random Regression options

| Keyword | possible value | description |
|---|---|---|
| RANDOM_REGRESSION | | Specifies that random regression should be applied to the random effects |
| | data | If covariables are in the data |
| | legendre | Generates legendre polynomials |

| Keyword | possible value | description |
|---|---|---|
| RR_POSITON | Integer | Specifies positions of covariables if RANDOM_REGRESSION type is data<br><br>Specifies the order of the polynomial and the position of the covariable if RANDOM_REGRESSION type is legendre |

# RENUMF90 parameter file

## (CO)VARIANCES for Random effects

| Keyword | possible value | description |
|---|---|---|
| (CO)VARIANCES | real | (co)variance for the animal effect dimension should account for number of traits and random correlated effects |

| | | |
|---|---|---|
| 32.79 | -7.22 | -11.07 |
| -7.22 | 258.06 | 87.66 |
| -11.07 | 87.66 | 194.34 |

# RENUMF90 parameter file

## (CO)VARIANCES structure

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

| | | E1 | | | E2 | | |
|---|---|---|---|---|---|---|---|
| | | T1 | T2 | T3 | T1 | T2 | T3 |
| E1 | T1 | | | | | | |
| | T2 | | | | | | |
| | T3 | | | | | | |
| E2 | T1 | | | | | | |
| | T2 | | | | | | |
| | T3 | | | | | | |

# RENUMF90 parameter file

## (CO)VARIANCES for Random effects

| Keyword | possible value | description |
|---|---|---|
| (CO)VARIANCES | real | (co)variance for non-correlated random effects |

| Keyword | possible value | description |
|---|---|---|
| (CO)VARIANCES_PE | real | (co)variance for the PE effect if present |

| Keyword | possible value | description |
|---|---|---|
| (CO)VARIANCES_MPE | real | (co)variance for the MPE effect if present |

# RENUMF90 parameter file

| Keyword | optional | possible values |
|---|---|---|
| COMBINE | optional | definition of new field as a combination of existing fields |
| DATAFILE | mandatory | name of raw data file |
| TRAITS | mandatory | positions of observations in the raw data file |
| FIELDS_PASSED | mandatory | positions of items in the raw data file to be passed to renf90.dat |
| WEIGHT(S) | mandatory | positions of weights in the raw data file |
| RESIDUAL_VARIANCE | mandatory | residual covariance matrix |
| EFFECT | mandatory | effect description |
| NESTED | optional | positions of nested covariates |
| RANDOM | optional | declaration of random effect |
| OPTIONAL | optional | declaration of MAT, PE, MPE |
| FILE | optional | name of raw pedigree file |
| FILE_POS | optional | positions of animal ID, sire ID, and dam ID |
| SNP_FILE | optional | name of SNP marker file |
| PED_DEPTH | optional | the maximum generation back from animals with phenotype and/or genotype |
| GEN_INT | optional | generation interval to set unknown parent groups (UPG) |
| REC_SEX | optional | check if records are found in specific sex |
| UPG_TYPE | optional | UPG specification |
| INBREEDING | optional | create pedigree file with inbreeding code |
| RANDOM_REGRESSION | optional | put covariates for random regressions |
| RR_POSITION | optional | positions of covariates for random regressions |
| (CO)VARIANCES | optional | covariance components |
| (CO)VARIANCES_PE | optional | covariance components for animal PE effects |
| (CO)VARIANCES_MPE | optional | covariance components for maternal PE effects |
| OPTION | optional | option parameters |

# RENUMF90 parameter file

- If the data and pedigree files have header

```
#Parameter file for renumf90
DATAFILE
data
SKIP_HEADER
1
TRAITS
3
FIELDS_PASSED TO OUTPUT
1 #Line_ID
WEIGHT(S)

RESIDUAL_VARIANCE
1.0
EFFECT
2 cross alpha
EFFECT
1 cross alpha
RANDOM
animal
FILE
ped
SKIP_HEADER
1
(CO)VARIANCES
1.0
OPTION sol se
```

# RENUMF90 parameter file

## Options passed to blupf90

- All lines that begin with the keyword OPTION are passed to parameter file `renf90.par`
  - Unless they are specific to renumf90
- This allows automation of process by using scripts
- For example:
  - `OPTION sol se`
  - `OPTION use_yams`

# RENUMF90 parameter file

**Hints**

- Keyword EFFECT is repeated as many times as effects in the model

- If (CO)VARIANCES for any effect are missing, default matrix with 1.0 in diagonal and 0.1 on off-diagonal will be used

# RENUMF90 parameter file

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

```
DATAFILE
data1.txt
TRAITS
5
FIELDS_PASSED TO OUTPUT
2
WEIGHT(S)

RESIDUAL_VARIANCE
1.0
EFFECT          #1st effect - farm
2 cross alpha
RANDOM
diagonal
(CO)VARIANCES
0.5
EFFECT          #2nd effect - sex
3 cross numer
EFFECT          #3rd effect - age
4 cov
```

*What if we want to consider farm as random with variance = 0.5?*

data1.txt

| ID | farm | sex | age | phen |
|---|---|---|---|---|
| ID006 | A | 1 | 1.0 | 3.0 |
| ID009 | A | 2 | 1.0 | 2.0 |
| ID012 | A | 1 | 2.0 | 4.0 |
| ID007 | B | 2 | 2.0 | 6.0 |
| ID010 | B | 1 | 1.0 | 3.0 |
| ID013 | B | 2 | 2.0 | 6.0 |
| ID008 | C | 1 | 2.0 | 6.0 |
| ID011 | C | 2 | 1.0 | 6.0 |
| ID014 | C | 1 | 1.0 | 8.0 |
| ID015 | C | 2 | 2.0 | 4.0 |

# RENUMF90 parameter file

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

```
DATAFILE
data1.txt
TRAITS
5
FIELDS_PASSED TO OUTPUT
2
WEIGHT(S)

RESIDUAL_VARIANCE
1.0
EFFECT        #1st effect - farm
2 cross alpha
EFFECT        #2nd effect - sex
3 cross numer
EFFECT        #3rd effect - age
4 cov
EFFECT        #4th effect - animal
1 cross alpha
RANDOM
animal
FILE
ped1.txt
FILE_POS
1 2 3 0 0
(CO)VARIANCES
0.2
```

*What if we want to consider animal effect as random with* $\sigma_u^2 = 0.2$*?*

ped1.txt

| ID | Sire | Dam |
|---|---|---|
| ID006 | ID001 | ID003 |
| ID009 | ID001 | ID004 |
| ID012 | ID001 | ID005 |
| ID007 | ID001 | ID003 |
| ID010 | ID001 | ID004 |
| ID013 | ID002 | ID005 |
| ID008 | ID002 | ID003 |
| ID011 | ID002 | ID004 |
| ID014 | ID002 | ID005 |
| ID015 | ID002 | ID003 |

data1.txt

| ID | farm | sex | age | phen |
|---|---|---|---|---|
| ID006 | A | 1 | 1.0 | 3.0 |
| ID009 | A | 2 | 1.0 | 2.0 |
| ID012 | A | 1 | 2.0 | 4.0 |
| ID007 | B | 2 | 2.0 | 6.0 |
| ID010 | B | 1 | 1.0 | 3.0 |
| ID013 | B | 2 | 2.0 | 6.0 |
| ID008 | C | 1 | 2.0 | 6.0 |
| ID011 | C | 2 | 1.0 | 6.0 |
| ID014 | C | 1 | 1.0 | 8.0 |
| ID015 | C | 2 | 2.0 | 4.0 |

# RENUMF90 output files

Pedigree file: `renaddxx.ped`

Data file: `renf90.dat`

Parameter file: `renf90.par`

Inbreeding file: `renf90.inb`

Renumbering table: `renf90.table`

Fields table: `renf90.fields`

# RENUMF90 output files
# Pedigree file: `renaddxx.ped`

- Structure:
  1. Animal ID (from 1)
  2. Parent 1 ID or UPG number for parent 1
  3. Parent 2 ID or UPG number for parent 2
  4. 3 minus number of known parents
  5. Known or estimated year of birth (0 if not provided)
  6. Number of known parents
     if genotyped: 10+number of known parents
  7. Number of records
  8. Number of progeny as parent 1
  9. Number of progeny as parent 2
  10. Original animal ID

# RENUMF90 output files
# Pedigree file: `renaddxx.ped`

- As inbreeding is default:

  Column 4:

  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 ) is the coefficient of inbreeding of sire (dam)

  Ex: For an animal with both parents known and F=0
  inb/upg code = 2000

# RENUMF90 output files
# Inbreeding file: `renf90.inb`

- renf90.inb will have:

| origID | Inbreeding | newID |
|---|---|---|
| A71342462 | 0.059204 | 6927175 |
| A17194772 | 0.032106 | 29 |
| A13476873 | 0.002958 | 6550405 |
| A1ZEP4813 | 0.000000 | 61 |
| A14347077 | 0.019187 | 6550336 |
| A64547711 | 0.026603 | 12 |
| A71922414 | 0.000000 | 6942899 |
| A17274771 | 0.019961 | 42 |
| A53301967 | 0.000000 | 6550416 |
| A4ZGF7566 | 0.000000 | 167 |
| A3ZZS6645 | 0.000000 | 25 |
| A07818367 | 0.000000 | 7117564 |
| A17354770 | 0.050361 | 55 |
| A53401908 | 0.000000 | 31 |
| A13556872 | 0.063467 | 6550439 |
| A14507075 | 0.071151 | 6550347 |

# RENUMF90 output files
# parameter file: `renf90.par`

```
# 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
OPTION SNP_file genotypes.txt
OPTION map_file gen_map.txt
```

```
DATAFILE
phenotypes.txt
TRAITS
 3
FIELDS_PASSED TO OUTPUT

WEIGHT(S)

RESIDUAL_VARIANCE
0.60
EFFECT
2 cross alpha  #sex
EFFECT
1  cross alpha
RANDOM
animal
FILE
pedigree.txt
FILE_POS
1 2 3 0 0
SNP_FILE
genotypes.txt
PED_DEPTH
4
(CO)VARIANCES
0.40
OPTION map_file gen_map.txt
```

# renumf90 FAQ

1) renumf90 cannot find the data file — Check for typos
2) How to include quadratic covariable? — Column in data file
3) Error when trying to use covariable — 2 cov numer
4) Fixed effects in renf90.dat are different from original — renf90.tables
5) I want to have original IDs in renf90.dat — FIELDS_PASSED TO OUTPUT

# renumf90 FAQ

6) When and how to run renumf90?

a) Objective to compare models

Run renumf90 ONCE with the most complete model

Remove effects from renf90.par

b) Objective to compare non-genomic vs genomic model

Run renumf90 ONCE with SNP file

For non-genomic: Remove option for SNP file from renf90.par

c) Objective to mask phenotypes for some animals for validation

Run renumf90 ONCE with the complete data

Remove animals from renf90.dat

# renumf90 quick trick

- `renumf90 --help`
- `renumf90 --show-template`

```
[dani@dodo2 day13]$ renumf90 --help
 RENUMF90 version 1.158 with zlib

  renumf90 parameter-file [--options ...]

   --version        show version number
   --show-template  show template parameter file
[dani@dodo2 day13]$ renumf90 --show-template
# parameter file for renumf90
DATAFILE

TRAITS

FIELDS_PASSED TO OUTPUT

WEIGHT(S)

RESIDUAL_VARIANCE

EFFECT

#RANDOM
#
#OPTIONAL
#
#FILE
#
#FILE_POS
#
#SNP_FILE
#
#PED_DEPTH
#
#UPG_TYPE
#
#INBREEDING
#
#FIXED_REGRESSION
#
#RANDOM_REGRESSION
#
#RR_POSITION
#
#(CO)VARIANCES
#
#(CO)VARIANCES_PE
#
#(CO)VARIANCES_MPE
#
#OPTION alpha_size 20
#OPTION max_string_readline 800
#OPTION max_field_readline 100
```

# 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 xx
```

xx: # of EM rounds

xx > 0 : switch to aireml
xx < 0 : does not switch if convergence is reached

# 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+

- 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)

- Solutions change among methods, but estimable functions should be the same

- Prediction error variances can be obtained using sparse inverse (FSPAK or YAMS)

# blupf90+ with PCG

Animal Breeding and Genetics Local Wiki

## Iteration on data with preconditioned conjugate gradient (PCG)

### Algorithm

Table of Contents –



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+

```
# 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
```

**As many columns as the number of traits**

**Number of levels**

**Type of effect**

- 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+

```
# 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
```

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

- Use zero (0.0) to indicate 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+

```
# 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
```

**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 a 3 trait (T1-T3) and 2 correlated effects (E1-E2)

| | | E1 | | | E2 | | |
|---|---|---|---|---|---|---|---|
| | | T1 | T2 | T3 | T1 | T2 | T3 |
| E1 | T1 | | | | | | |
| | T2 | | | | | | |
| | T3 | | | | | | |
| E2 | T1 | | | | | | |
| | T2 | | | | | | |
| | T3 | | | | | | |

# RANDOM_TYPE

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

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

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

# RANDOM_TYPE

- *add_an_upg*
  - As before but using rules for unknown parent group
  - Pedigre file:
    - `animal number, sire number, dam number, parent code`
    - missing sire/dam can be replaced by upg number, usually greater than 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 group and inbreeding
  - Pedigre 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_self*
  - *To create a relationship matrix when there is selfing*
  - Pedigre file:
    - `individual number, parent 1 number, parent 2, number of selfing generations`

- *user_file*
  - An inverted matrix is read from 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 program RENDOM

# OPTIONS for blupf90+

- Program behavior can be modified by adding extra options at the end of the par file
- `OPTION option_name x1 x2 …`
- option_name: each program has its definition of options
- The number of optional parameters (x1, x2, …) to control the behavior depends on the option

# 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`

  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`

  - Only *solutions.original* is created

# 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
OPTION SNP_file genotypes.txt
OPTION map_file gen_map.txt
```

# blupf90+

**VC Estimation**

# REML

- blupf90+ has 2 REML algorithms
  - EM-REML: expectation-maximization (EM) algorithm
  - AI-REML: average information (AI) algorithm

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

- Most used method for VCE in AB&G

# EM-REML

- This method requires iterations:

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

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

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 $\mathbf{C}^{uu}$

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

# AI-REML

Vector of variance components

$$\theta_{n+1} = \theta_n - \mathbf{H}^{-1}(\theta_n)\mathbf{d}(\theta_n)$$

Gradient (score vector)

Hessian Matrix

Average-information algorithm uses this matrix as Hessian,

P = Projection or hat matrix

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

**Gradient**

expensive

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

# 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 xx
```

xx: # of EM rounds

xx > 0 : switch to aireml
xx < 0 : does not switch if convergence is reached

Original options for airemlf90 and remlf90 also work!

# Options for blupf90+

```
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 but with a smaller starting value to check the estimate because 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

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

# gibbsf90+

**Linear**

Default

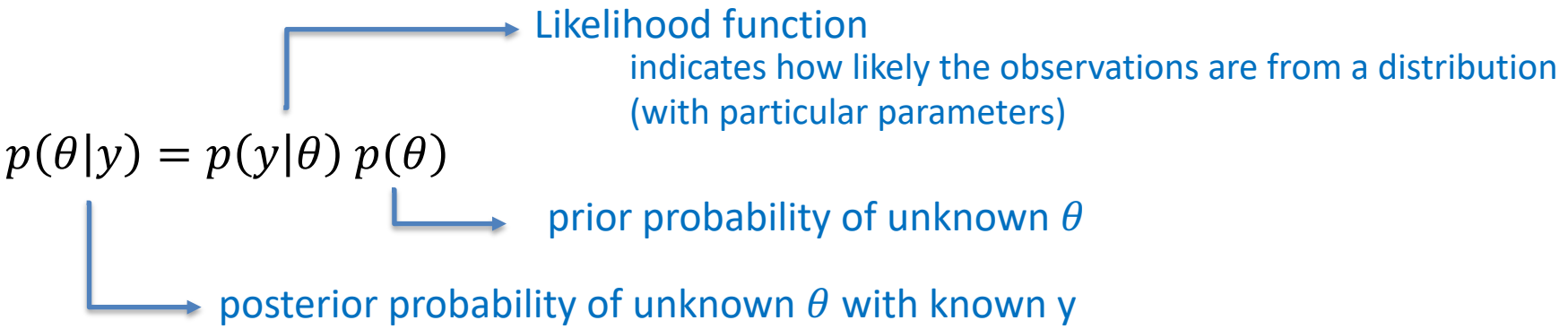
**Threshold (-Linear)**

```
OPTION cat 0 2 5
```

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

# gibbsf90+

Bayes Theorem




- 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

```
# 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
}
```

# gibbsf90+

- Name of parameter file?

  gibbs1.par
- Number of samples and length of burn-in?

  samples=10,000 to 100,000; burn-in=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 |

******** P[illegible]io

Lower and upper bounds of Mean ± 1.96PSD

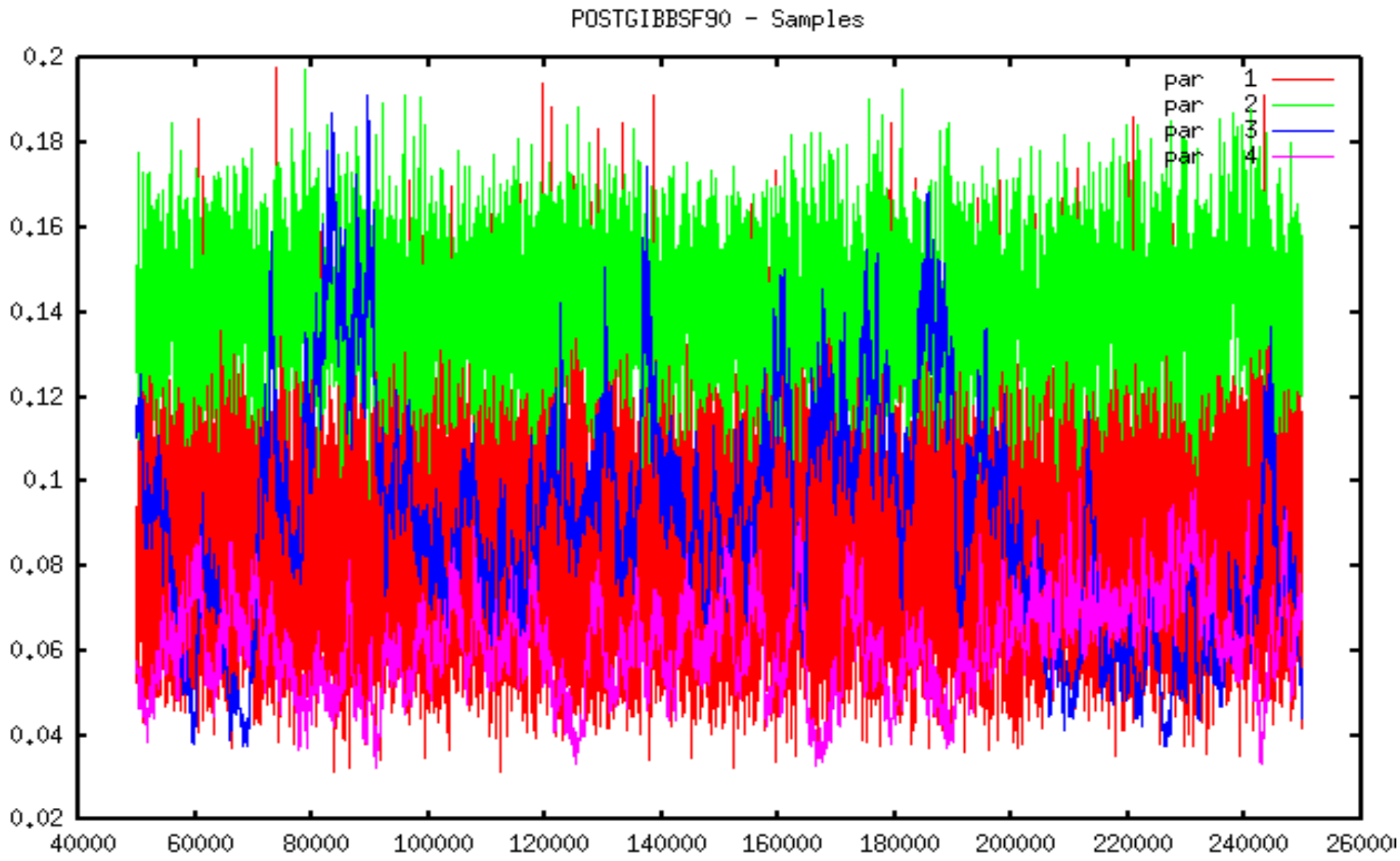
ratio between first half and second half of the samples ; should be < 1.0

| 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

```
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
```

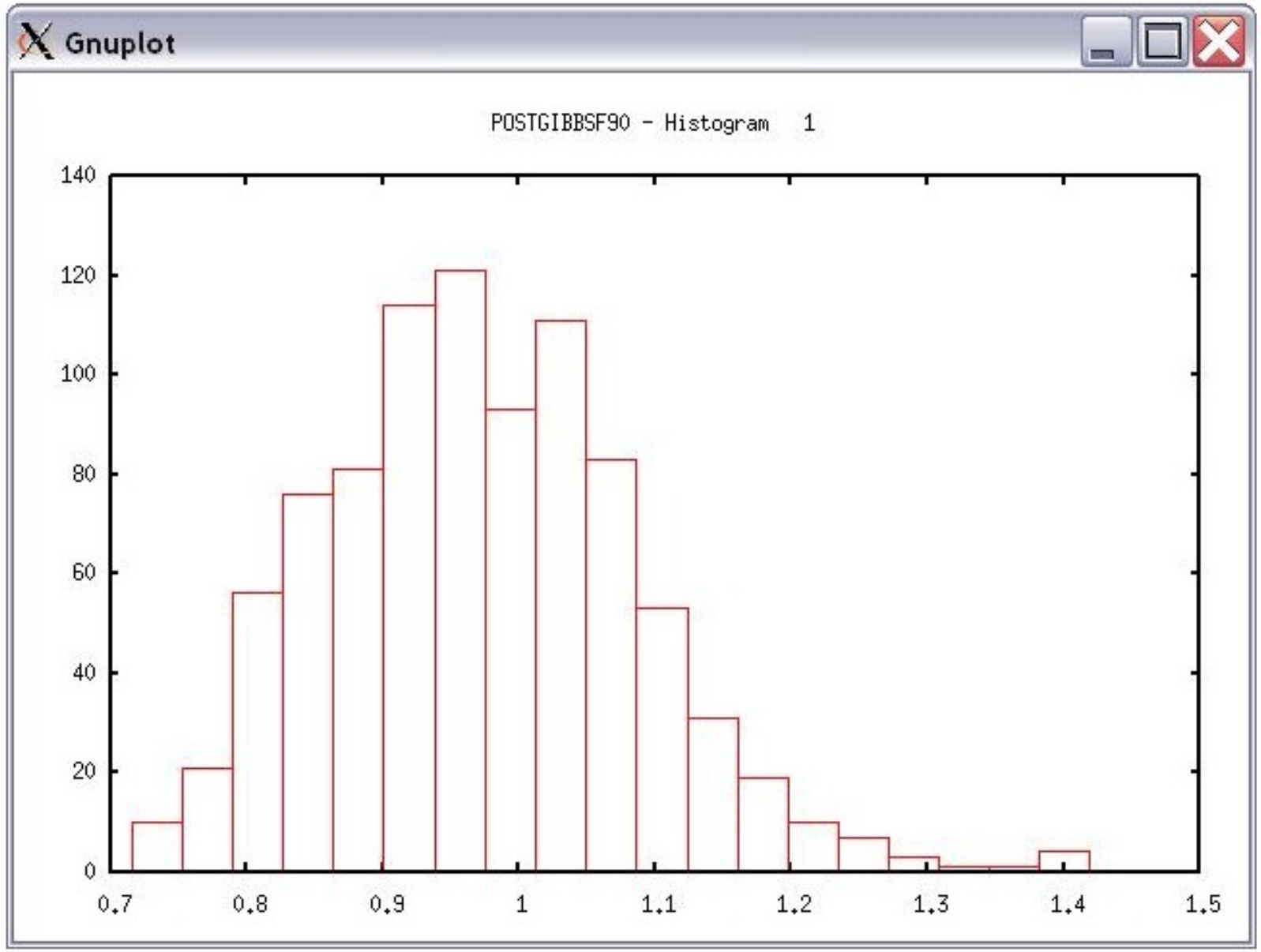
# postgibbsf90



# 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

**renumf90**

```
renumf90 renum.par | tee renum.log
```

**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
```

# Add Windows PATH Environment Variable

- Settings
- Control panel
- Search for advanced
- View advanced system settings
- Environmental variables
- System variables -> select **Path** ->  [Edit…]
- ;C:\blupf90 (this is the path to the directory where programs are)
- Open a new terminal