



UNIVERSITY OF  
**GEORGIA**

College of Agricultural &  
Environmental Sciences

# Introduction to BLUPF90 software suite

Daniela Lourenco  
UGA USA

Ignacio Aguilar  
INIA Uruguay

BLUPF90 TEAM – 02/2022

# BLUPF90 software suite

- Collection of software for computations
  - Focus on applications in Breeding and Genetics
- Fortran ≥ 90
- Since 1998/1999 by Ignacy Misztal
- Simple, efficient, and comprehensive
- No GUI (graphical user interface)!!!
- First idea: to solve the MME

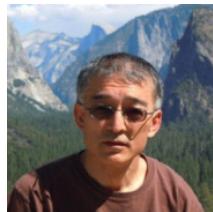
$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{W} \\ \mathbf{W}'\mathbf{X} & \mathbf{W}'\mathbf{W} + \mathbf{A}^{-1} \frac{\sigma_e^2}{\sigma_a^2} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{W}'\mathbf{y}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

- First software: blupf90
- Second idea: variance components estimation
- Developers?

# BLUPF90 software main developers



Ignacy  
Misztal



Shogo  
Tsuruta



Andres  
Legarra



Ignacio  
Aguilar



Yutaka  
Masuda

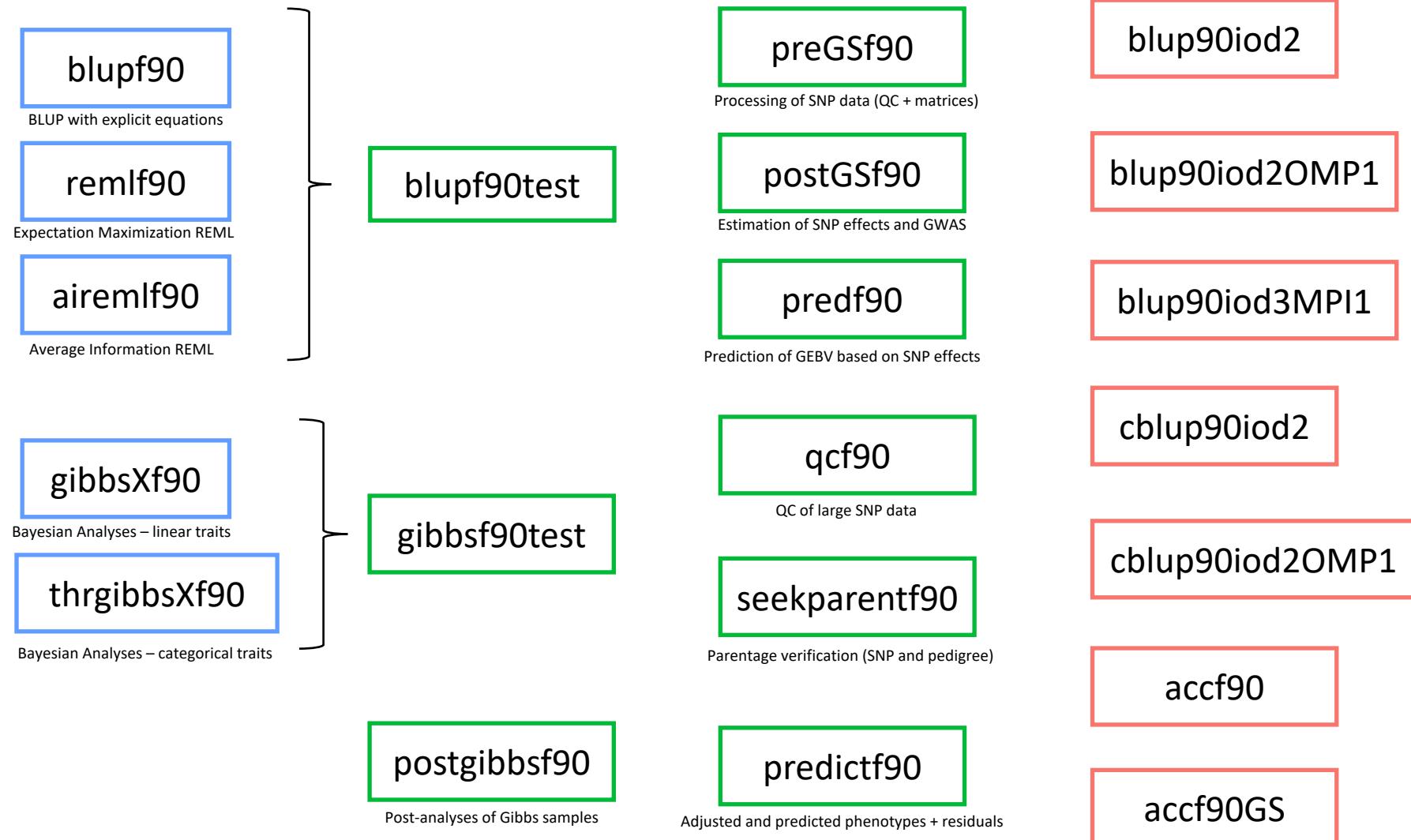
- + Several contributors
- Research turns into code
- Which programs?

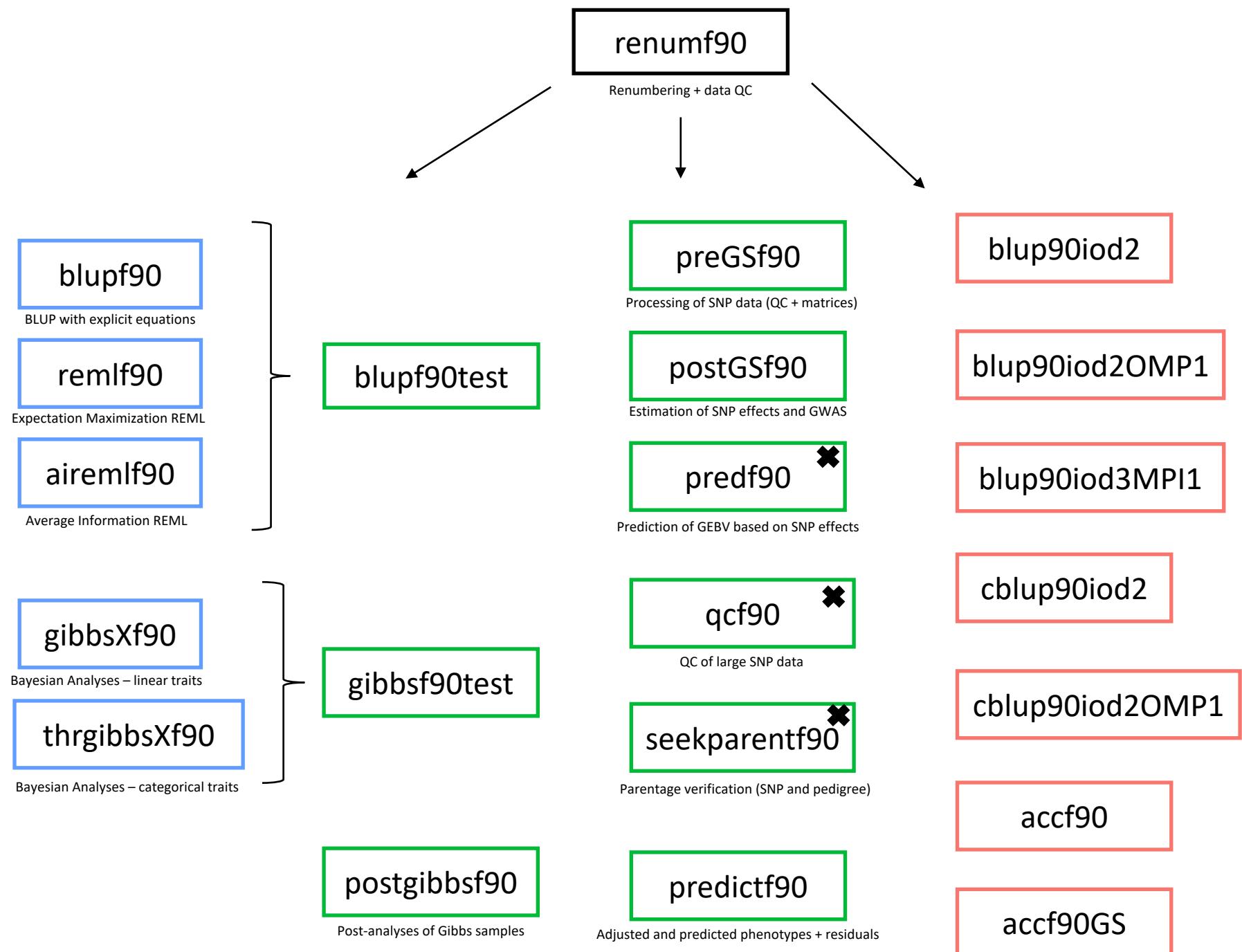
1) Controlled by the same parameter file

2) Data File for blupf90 family:

a) Only numbers – Integer or real

b) All effects need to be renumbered from 1 to N





# **RENUMF90**

**The renumbering software for the  
BLUPF90 suite**

# RENUMF90

- Renumbers data and pedigree
- Creates a parameter file for BLUPF90 family
- Traces back pedigree for individuals in data file
- Performs comprehensive pedigree checking
- Provides data statistics
- Computes inbreeding
- Creates an Xref file for genotyped individuals

# RENUMF90

- **Supports**
  - virtually any dataset
  - multiple traits
  - different 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
    - if INBREEDING is used
  - renf90.tables
    - cross reference file with renumbered and original effects
  - renf90.fields
    - description of the effects in each field of renf90.dat
  - renf90.dat
    - recoded data
  - renaddxx.ped
    - renumbered pedigree + statistics
  - renf90.par
    - new parameter file

# RENUMF90 parameter file

## MANDATORY

renumf90 --show-template

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 Keep empty if not needed
WEIGHT(S)	integer	The position(s) for weight in the data file Keep empty if not needed
RESIDUAL_VARIANCE	real value(s)	Residual (co)variance
EFFECT	(next slide ...)	Description of an effect Repeatable

# 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:  $y = \text{farm} + \text{sex} + \beta \text{ age} + e$

DATAFILE  
data1.txt

TRAITS

5

FIELDS\_PASSED\_TO\_OUTPUT

2

WEIGHT(S)

RESIDUAL\_VARIANCE

1.0

EFFECT #1<sup>st</sup> effect - farm

2 cross alpha

EFFECT #2<sup>nd</sup> effect - sex

3 cross numer

EFFECT #3<sup>rd</sup> 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 for animal models only

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

Keyword (for RANDOM animal only)	possible value	description
SNP_FILE	character	<b>Optional: If genomic info is to be used</b> Name of the SNP file Format: ID 011122211155152222

# RENUMF90 parameter file

## Pedigree options

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

<b>Keyword</b> (for RANDOM animal only)	<b>possible value</b>	<b>description</b>
GEN_INT	Integer min avg max	<b>Optional</b> Specifies min, avg, max generation interval; if yob is present Average used to predict yob of parents

<b>Keyword</b> (for RANDOM animal only)	<b>possible value</b>	<b>description</b>
REC_SEX	Integer	<b>Optional</b> Specifies which parent has records Checks if records are found in specific sex

# RENUMF90 parameter file

## Unknown Parent Group options

Keyword (for RANDOM animal only)	possible value	description
UPG_TYPE	yob 1990 1992 ...  in_pedigrees  group_unisex	<p>Optional</p> <p>UPG assigned based on yob</p> <p>Missing parent receives -x x is the UPG number</p> <p>UPG based on the information in pedigree Ex. UPG by breed</p> <p><b>FILE_POS</b></p> <p>1 2 3 0 0 4 #the 6th field indicates which column the UPG code is in the pedigree</p>

# RENUMF90 parameter file

## Inbreeding option

Keyword (for RANDOM animal only)	possible value	description
INBREEDING	pedigree file self ×	<p>Optional</p> <p>Calculates inbreeding code and saves it in the renumbered pedigree file</p> <p>Reads inbreeding from an external file format: original_ID inbreeding (0 to 1)</p> <p>Calculates inbreeding with selfing × is the column in the pedigree file with the number of selfing generations</p>

# RENUMF90 parameter file

## Random Regression options

Keyword	possible value	description
RANDOM_REGRESSION	data	Specifies that random regression should be applied to the random* effects  If covariables are in the data

Keyword	possible value	description
RR_POSITON	Integer	Specifies positions of covariables if RANDOM_REGRESSION type is data

# 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

## Creating interaction between effects

Keyword	possible value	description
COMBINE	integer	Should come before DATAFILE <b>COMBINE</b> <b>7 2 3 4</b> Columns 2, 3, 4 are combined into 7 They can be numer or alpha

# 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

## **Options passed to blupf90**

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

# RENUMF90 parameter file

## Extra options

The following options can be added at the end of the parameter file to redefine parameters used to read the input file:

- the default size of character fields (maximum number of characters in a column - 20)

```
OPTION alpha_size nn
```

where *nn* is the new size.

- the size of the record length (maximum number of characters in a line - 800)

```
OPTION max_string_readline nn
```

where *nn* is the new size.

- the maximum number of fields (maximum number of columns in a line - 100)

```
OPTION max_field_readline nn
```

where *nn* is the number of fields.

# 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:  $y = \text{farm} + \text{sex} + \beta \text{ age} + e$

```
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?*

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:**  $y = \text{farm} + \text{sex} + \beta \text{ age} + \text{animal} + e$

```
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
0.5
```

*What if we want to consider  
animal effect as random?*

ped1.txt

data1.txt

ID	Sire	Dam	ID	farm	sex	age	phen
ID006	ID001	ID003	ID006	A	1	1.0	3.0
ID009	ID001	ID004	ID009	A	2	1.0	2.0
ID012	ID001	ID005	ID012	A	1	2.0	4.0
ID007	ID001	ID003	ID007	B	2	2.0	6.0
ID010	ID001	ID004	ID010	B	1	1.0	3.0
ID013	ID002	ID005	ID013	B	2	2.0	6.0
ID008	ID002	ID003	ID008	C	1	2.0	6.0
ID011	ID002	ID004	ID011	C	2	1.0	6.0
ID014	ID002	ID005	ID014	C	1	1.0	8.0
ID015	ID002	ID003	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

- If option for inbreeding is used:

Column 4:

$$\text{inb/upg code} = 4000 / [(1+ms)(1-Fs) + (1+md)(1-Fd)]$$

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

$$\text{inb/upg code} = 2000$$

# RENUMF90 output files

## Inbreeding file: renf90.inb

- If the keyword INBREEDING is used, 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

## renumbering tables: renf90.tables

- For each cross-classified effects
  - Original ID, count, consecutive number
- Useful
  - To translate solutions from BLUPF90 program into original alphanumeric values
  - Check counts of records by level

# RENUMF90 output files

## fields tables: renf90.fields

- File with description of the effects in each field of renf90.dat

field	variable	origfield	group	column	random	effect	file
1	trait	3	0	0	*	cov	*
2	renumbered	2	1	1	*	cross	*
3	renumbered	1	2	1	animal	cross	renadd02.ped

# 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]
    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
0
INBREEDING
pedigree
(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) I want to have original IDs in renf90.dat [FIELDS\\_PASSED TO OUTPUT](#)
- 5) Fixed effects in renf90.dat are different from original [renf90.tables](#)

# 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



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# blupf90

Mixed Model Equations Solver

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

# 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)
- The solution values change among methods but estimable functions should be the same
- Prediction error variances can be obtained using sparse inverse (FSPAK or YAMS)

# Blupf90 - PCG

Animal Breeding and Genetics Local Wiki

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

### Table of Contents

- Iteration on data with preconditioned conjugate gradient (PCG)
  - Algorithm
  - Programs
  - Files and analysis
  - Options

### 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 Strandén 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  $\mathbf{M} = \text{diag}(\mathbf{C})$  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

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

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_upginiB
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_upglnb
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  
$$\begin{matrix} 43.1 & 0.0 & 0.0 \\ 0.0 & 5.1 & 3.2 \\ 0.0 & 3.2 & 10.3 \end{matrix}$$

# 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 parameter file
- `OPTION option_name x1 x2 ...`
- `option_name`: each program has its own 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 (default 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.

# Example of parameter file for blupf90

Single trait “USDA-type” animal model

$$y_{ijkl} = hys_i + p_k + hs_{ij} + a_k + e_{ijkl}$$

where

$y_{ijkl}$  - production yield

$hys_i$  - fixed herd year season

$p_k$  - random permanent environment

$hs_{ij}$  - random herd x sire interaction

$a_k$  - random animal

and

$$\text{var}(hs_{ij}) = .05, \text{var}(p_k) = .1, \text{var}(a_k) = .5, \text{var}(e_{ijkl}) = 1$$

```
# BLUPF90 parameter file created by RENUMF90
```

```
DATAFILE  
renf90.dat
```

```
NUMBER_OF_TRAITS  
1
```

```
NUMBER_OF_EFFECTS  
4
```

```
OBSERVATION(S)
```

```
1
```

```
WEIGHT(S)
```

```
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS
```

```
2 3 cross
```

```
3 6 cross
```

```
4 4 cross
```

```
5 14 cross
```

```
RANDOM_RESIDUAL_VALUES
```

```
1.0000
```

```
RANDOM_GROUP
```

```
2
```

```
RANDOM_TYPE
```

```
diagonal
```

```
FILE
```

```
(CO)VARIANCES
```

```
0.10000
```

```
RANDOM_GROUP
```

```
3
```

```
RANDOM_TYPE
```

```
diagonal
```

```
FILE
```

```
(CO)VARIANCES
```

```
0.50000E-01
```

```
RANDOM_GROUP
```

```
4
```

```
RANDOM_TYPE
```

```
add_an_upg
```

```
FILE
```

```
renadd04.ped
```

```
(CO)VARIANCES
```

```
0.50000
```

### Model

$$y_{ijkl} = hys_i + p_k + hs_{ij} + a_k + e_{ijkl}$$

where

$y_{ijkl}$  - production yield

$hys_i$  - fixed herd year season

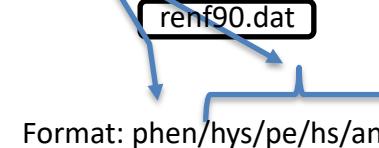
$p_k$  - random permanent environment

$hs_{ij}$  - random herd x sire interaction

$a_k$  - random animal

and

$\text{var}(hs_{ij}) = .05$ ,  $\text{var}(p_k) = .1$ ,  $\text{var}(a_k) = .5$ ,  $\text{var}(e_{ijkl}) = 1$



renadd04.ped

Format: ani/sire/dam/code/.....

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

# Output from blupf90

```
name of parameter file?  
renf90.par  
BLUPF90 ver. 1.66
```

Parameter file:	renf90.par	Parameter file
Data file:	renf90.dat	data file
Number of Traits	1	
Number of Effects	4	
Position of Observations	1	
Position of Weight (1)	0	
Value of Missing Trait/Observation	0	

## EFFECTS

#	type	position	
(2)	levels	[positions for nested]	
1	cross-classified	2	3
2	cross-classified	3	6
3	cross-classified	4	4
4	cross-classified	5	14

Number of levels for each effect

```
read          6 records in  6.1703999E-02 s,  Records read from data file  
nonzeroes  
read          11 additive pedigrees  
finished peds in  6.1760999E-02 s,  Records read from pedigree file  
round =      1 convergence =  0.1435  
round =      2 convergence =  0.3000E-01  
round =      3 convergence =  0.1714E-02  
round =      4 convergence =  0.2914E-03  
round =      5 convergence =  0.1207E-03  
round =      6 convergence =  0.1278E-03  
round =      7 convergence =  0.1085E-03  
round =      8 convergence =  0.1405E-03  
round =      9 convergence =  0.1904E-03  
round =     10 convergence =  0.1119E-03  
round =     11 convergence =  0.1562E-04  
round =     12 convergence =  0.6141E-05  
round =     13 convergence =  0.4609E-05  
round =     14 convergence =  0.1750E-04  
round =     15 convergence =  0.8708E-04  
round =     16 convergence =  0.2800E-03  
round =     17 convergence =  0.1286E-04  
round =     18 convergence =  0.2309E-06  
round =     19 convergence =  0.2566E-08  
round =     20 convergence =  0.1131E-09  
round =     21 convergence =  0.2413E-12  
21 iterations,  convergence criterion= 0.2413E-12  
solutions stored in file: "solutions"
```

Solutions file

# File “solutions”

$$y_{ijkl} = hys_i + p_k + hs_{ij} + a_k + e_{ijkl}$$

where

$y_{ijkl}$  - production yield

$hys_i$  - fixed herd year season

$p_k$  - random permanent environment

$hs_{ij}$  - random herd x sire interaction

$a_k$  - random animal

## Parameter File

```
DATAFILE
renf90.dat
NUMBER_OF_TRAITS
    1
```

```
NUMBER_OF_EFFECTS
    4
```

```
OBSERVATION(S)
    1
```

```
WEIGHT(S)
```

```
EFFECTS: POSITIONS_IN_DATAFILE
```

2	3	cross
3	6	cross
4	4	cross
5	14	cross

trait/effect	level	solution
1	1	0.49585171
1	1	2.52240030
1	1	2.91017217
1	2	-0.00965409
1	2	0.00965406
1	2	-0.01930794
1	2	0.01930787
1	2	0.03861622
1	2	-0.03861599
1	3	-0.00000001
1	3	-0.00965384
1	3	-0.00965406
1	3	0.01930810
1	4	0.64574095
1	4	-0.30035705
1	4	0.61034316
1	4	0.52426082
1	4	0.27486415
1	4	0.39795337
1	4	0.18556405
1	4	-0.90212661
1	4	0.63126003
1	4	-0.17807241
1	4	-0.17807202
1	4	1.25233833
1	4	-1.91741245
1	4	1.51299821

# Common problem 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 FAQ

1) Why solutions are not with original ID?

[ask Ignacy Misztal](#)

2) How to match solutions with original ID?

[Bash scripting](#)

For trait 1 when animal is  
effect number 2

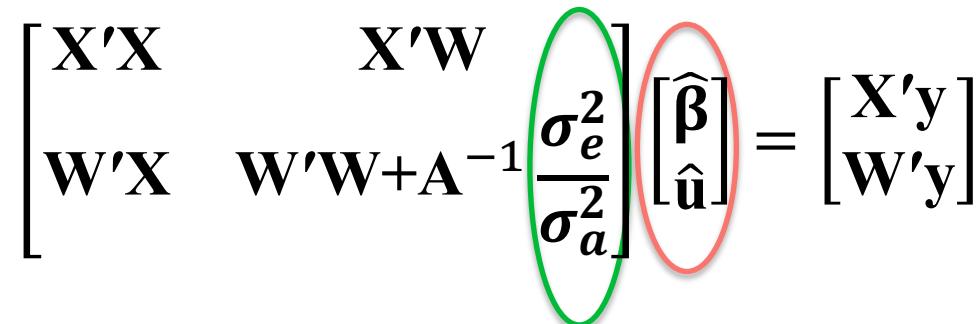
```
$awk '{ if ($1==1 && $2==2) print $3,$4}' solutions | sort +0 -1 > sol.temp  
$awk '{print $1,$10}' renadd02.ped | sort +0 -1 > ids.temp  
$join -1 +1 -2 +1 ids.temp sol.temp > renumbered_original_EBV
```

# remIf90

and

# airemIf90

Variance components estimation

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


# remlf90 and airemlf90

- REML = restricted/residual maximum likelihood
  - Patterson and Thompson (1971)
- Most used method to estimate variance components in breeding and genetics
- BLUPF90 family has 2 REML programs
  - remlf90: expectation-maximization (EM) algorithm
  - airemlf90: average information (AI) algorithm
- remlf90 and airemlf90 use the same parameter file as blupf90

# remlf90

$$y = \mathbf{X}\beta + \mathbf{Z}u + e$$

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

Inverse of LHS for  
animal effect

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

# animals  
(rank of A)

- This method requires iterations:
  - 1) set initial variance components
  - 2) compute  $\hat{\beta}$  and  $\hat{\mathbf{u}}$  via mixed model equations
  - 3) update variance components with above equations
  - 4) go to 1 or stop if the parameters do not change anymore

# remlf90

- 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  $\mathbf{C}^{\mathbf{u}\mathbf{u}}$

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

# airemlf90

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

Vector of variance components  
Hessian Matrix  
Gradient (score vector)

Average-information algorithm uses this matrix as Hessian,

$$\mathbf{H}(\theta) = \mathcal{I}_A(\theta) = \begin{bmatrix} -\frac{1}{2}\mathbf{y}'\mathbf{P}\mathbf{Z}\mathbf{A}\mathbf{Z}'\mathbf{P}\mathbf{Z}\mathbf{A}\mathbf{Z}'\mathbf{P}\mathbf{y} & -\frac{1}{2}\mathbf{y}'\mathbf{P}\mathbf{Z}\mathbf{A}\mathbf{Z}'\mathbf{P}\mathbf{P}\mathbf{y} \\ -\frac{1}{2}\mathbf{y}'\mathbf{P}\mathbf{P}\mathbf{Z}\mathbf{A}\mathbf{Z}'\mathbf{P}\mathbf{y} & -\frac{1}{2}\mathbf{y}'\mathbf{P}\mathbf{P}\mathbf{P}\mathbf{y} \end{bmatrix}$$

Gradient

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

expensive

# airemlf90

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

# Options for remlf90 and airemlf90

```
OPTION conv_crit 1d-12
```

Convergence criterion (default 1d-10).

```
OPTION maxrounds 10000
```

Maximum rounds (default 5000).

```
OPTION sol se
```

Store solutions and se.

```
OPTION residual
```

y-hat and residuals will be included in "yhat\_residual".

```
OPTION missing -999
```

Specify missing observations (default 0) in integer.

```
OPTION use_yams
```

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

```
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.

# Options for airemlf90

```
OPTION EM-REML 10
```

Run EM-REML (REMLF90) for first 10 rounds to get initial variances within the parameter space (default 0).

```
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 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".

## Heterogeneous residual variances for a single trait

```
OPTION hetres_pos 10 11
```

Specify the column positions of (two) covariables in the data file.

```
OPTION hetres_pol 4.0 0.1 0.1
```

Initial values of coefficients for heterogeneous residual variances using  $\ln(a_0, a_1, a_2, \dots)$  to make these values.

To transform back to the original scale, use  $\exp(a_0 + a_1 * X_1 + a_2 * X_2)$

log-residual function (Foulley and Quaas, 1995)

# Options for airemlf90

```
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
```

# Does REML 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 AIREMLF90 does not converge but REMLF90 converges with the same data set and the same model:
  - run REMLF90 again but with a smaller starting value to check the estimate because it could be an artifact
  - use OPTION EM-REML inside airemlf90:  
OPTION EM-REML xx  
where xx is the number of rounds of EM

# gibbsf90

## Bayes Theorem

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

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

prior probability of unknown  $\theta$

posterior probability of unknown  $\theta$  with known  $y$

- Basic idea of Gibbs sampling:
- Gibbs sampling is a 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
}
```

# gibbsXf90

- gibbs1f90: faster for multiple trait models
- gibbs2f90: better for correlated random effects
- gibbs3f90: for heterogeneous residual variance
- 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**

```
gibbs1f90 gibbs1.par --rounds 10000 --burnin 0 --thin 10
```

# gibbsXf90

- Procedure
  - Run gibbsXf90 to estimate variance components
  - Run postgibbsf90 to process the samples and verify convergence
  - Run gibbsXf90 with new variance components to estimate breeding values (2k to 10k rounds)

# gibbsXf90

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

All solutions and posterior means and SD for effects for effects1, 2, and 3 are stored in "all\_solutions" and in "final\_solutions" every round using fixed variances. Without numbers, all solutions for all effects are stored.

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

Posterior means and SD for effects1, 2, and 3 in "final\_solutions".

```
OPTION solution all 1 2 3
```

Caution: this option will create a huge output solution file when you run many rounds and/or use a large model. All solutions and posterior means and SD for effects1, 2, and 3 are stored in "all\_solutions" and in "final\_solutions" every round. Without numbers, all solutions for all effects are stored.

```
OPTION solution mean 1 2 3
```

Caution: this option will create a huge output solution file when you run many rounds and/or use a large model. Posterior means and SD for effects1, 2, and 3 in "final\_solutions".

```
OPTION cont 10000
```

10000 is the number of samples run previously when restarting the program from the last run.

# gibbsXf90

```
OPTION prior 5 2 -1 5
```

The (co)variance priors are specified in the parameter file.

Degree of belief for all random effects should be specified using the following structure:

```
OPTION prior eff1 db1 eff2 db2 ... effn dbn -1 dbres
```

effx correspond to the effect number and dbx to the degree of belief for this random effect, -1 corresponds to the degree of belief of the residual variance.

In this example 2 is the degree of belief for the 5th effect, and 5 is the degree of belief for the residual.

```
OPTION seed 123 321
```

Two seeds for a random number generator can be specified.

```
OPTION SNP_file.snp
```

Specify the SNP file name to use genotype data.

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

# gibbs3f90

```
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.

# gibbs3f90

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
```

# thrgibbsXf90

- thrgibbs1f90: Gibbs sampler for mixed threshold-linear models  
Thresholds and variances can be estimated or assumed
- thrgibbs3f90: for heterogeneous residual variance
- 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**

```
thrgibbs1f90 gibbs1.par --rounds 10000 --burnin 0 --thin 10
```

# thrgibbsXf90

## Options

```
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 save_halfway_samples 5000
```

The program saves every "5000" samples to restart or recover the job right after the last saved samples. It is useful when the program accidentally stopped.

To restart, add `OPTION cont 1` to your parameter file and run `thrgibbs1f90` again

```
OPTION thresholds 0.0 1.0 2.0
```

Set the fixed thresholds. No need to set 0 for binary traits.

```
OPTION residual 1
```

The residual variance can be set to 1 but not necessary for categorical traits more than 2 categories. For binary traits, the residual variance is automatically set to 1, so no need to use this option.

# postgibbsf90

- Basic idea of post Gibbs analysis:
- Summarize and visualize the samples drawn by gibbsXf90
- 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

number of independent cycles of Gibbs samples

Pos.	eff1	eff2	trt1	trt2	MCE	Monte	Carlo	Error by	Time Series	*****	Mode	Independent chain size
						Mean	HPD Interval (95%)		Effective sample size	Median		
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

Pos.	eff1	eff2	trt1	trt2	PSD	Mean	*****	P	Lower and upper bounds of Mean ± 1.96PSD	ratio	ratio between first half and second half of the samples ; should be < 1.0	Independent # batches	
							PSD	Diagnostic	Autocorrelations				
							Interval (95%)	lag: 1	10	50			
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
```

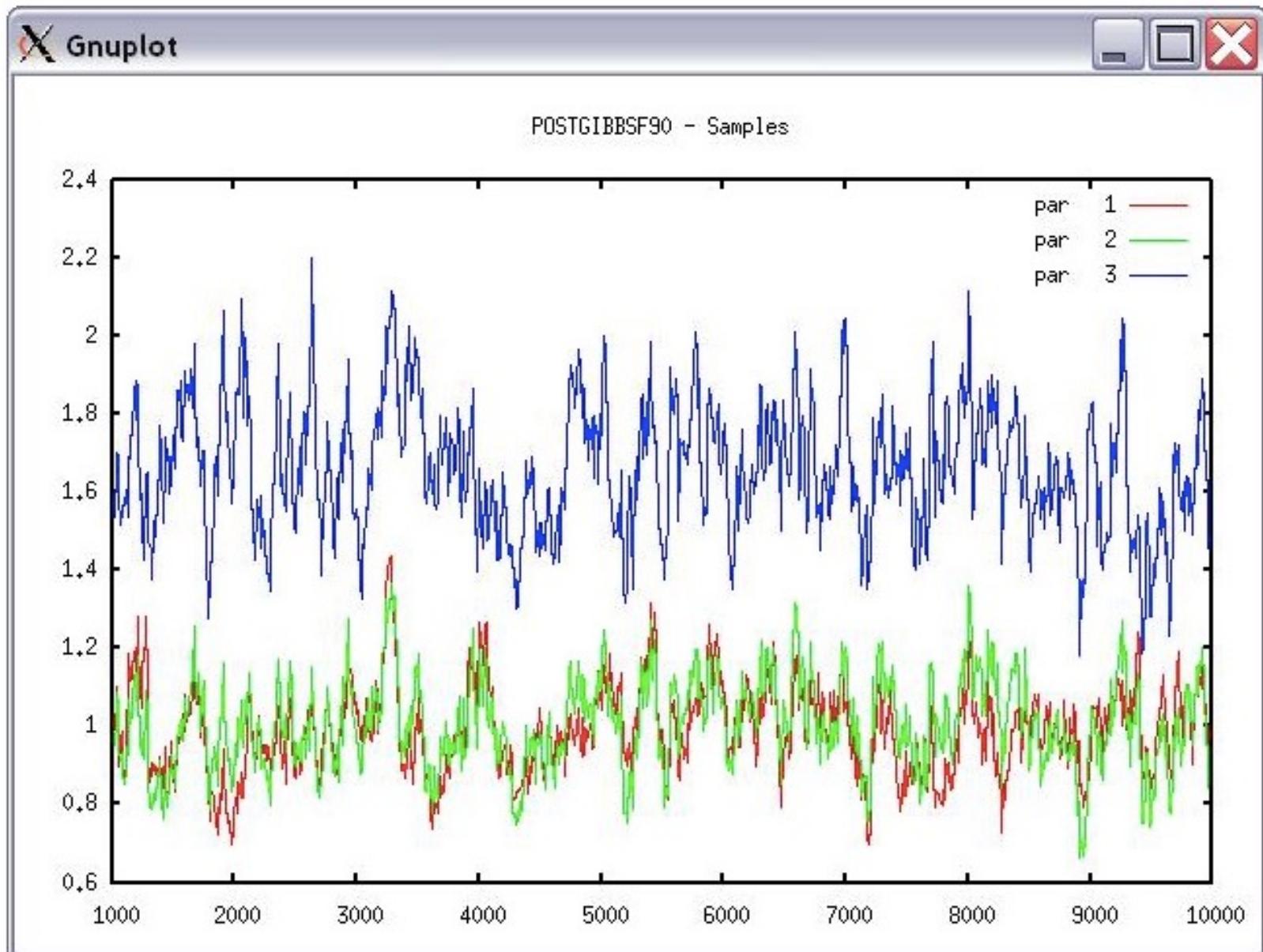
```
If the graph is stable (not increasing or decreasing), the convergence is met.
```

```
All samples before that point should be discarded as burn-in.
```

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

```
2
```

# postgibbsf90



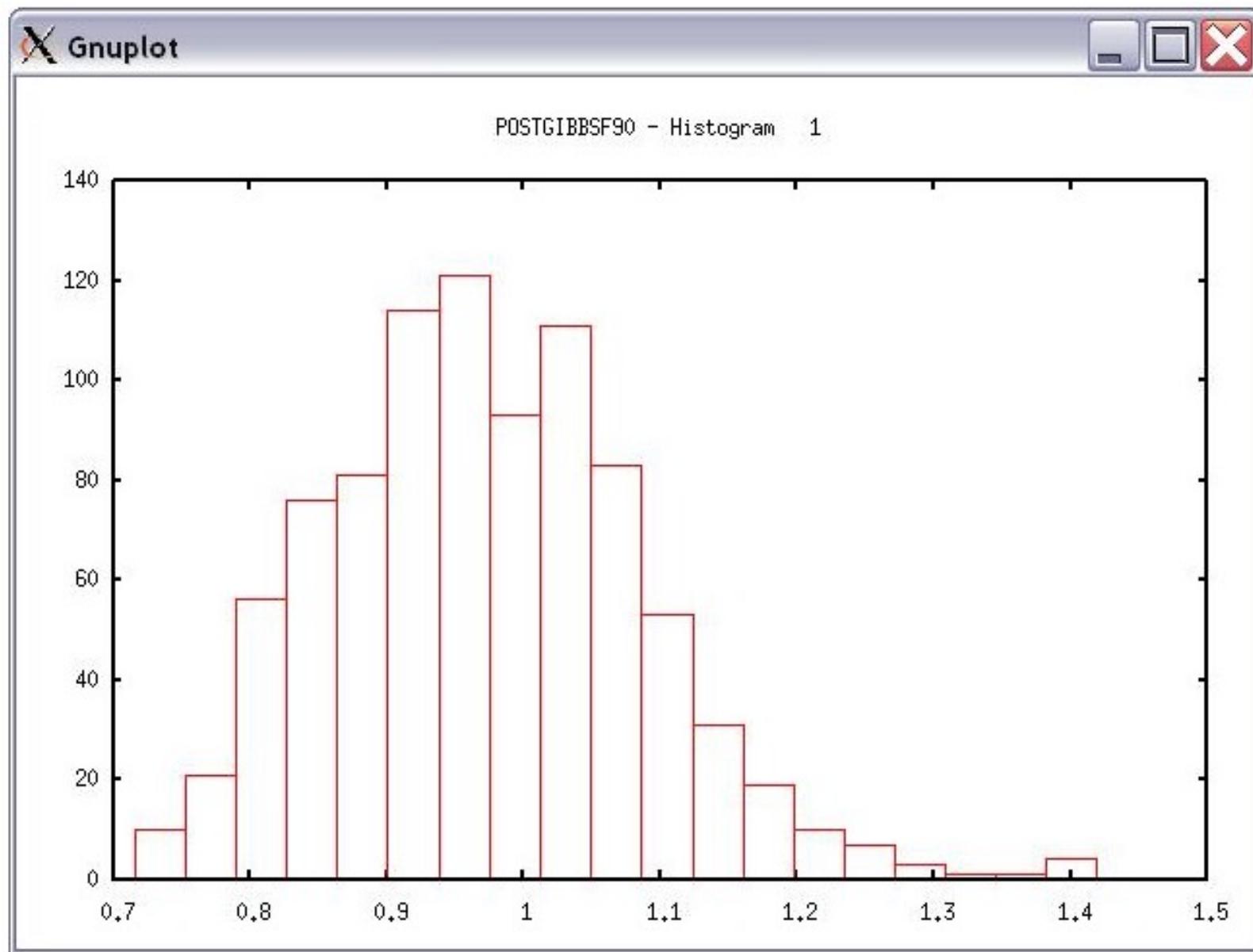
# postgibbsf90

```
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**

```
echo renf90.par | renumf90 | tee renf.log
```

## **blupf90**

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

## **airemlf90**

```
echo renf90.par | airemlf90 | tee aireml.log
```

# Run in background + Save output

```
$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
```

```
$vi gibbs.sh  
#type the following commands inside gibbs.sh  
    gibbs2f90 <<AA > gibbs.log  
    renf90.par  
    1000 0  
    10  
    AA  
#save and exit  
$bash gibbs.sh & #can replace bash by sh
```