Manual for

BLUPF90 family of programs

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Introduction

BLUPF90 is a family of programs for mixed-model computations focusing on animal breeding applications. The programs can do data conditioning, estimate variances using several methods, calculate BLUP for very large data sets, calculate approximate reliabilities, and use SNP information for improved accuracy of breeding values and genome-wide association studies (GWAS).

The programs have been designed with 3 goals in mind:

1. Flexibility to support a large set of models found in animal breeding applications.
2. Simplicity of software to minimize errors and facilitate modifications.
3. Efficiency at the algorithmic level.

Aside from being used in hundreds of studies, the programs are utilized for commercial genetic evaluation in dairy, beef, pigs, chicken, fish, plants, and beyond by major companies/institutions/associations in the US and worldwide.

The programs are written in Fortran 90/95 and originated as exercises for a class taught by Ignacy Misztal at the University of Georgia. Over time, they have been upgraded and enhanced by many contributors. Details on programming and computing algorithms are available in an Interbull **paper** (Misztal, 1999) and as course notes. Old versions of source codes for nearly all programs are available **here**.

Additional information about the programs is available at **http://nce.ads.uga.edu/wiki/doku.php** as wiki pages. There is a BLUPF90 discussion group at **groups.io**.

List of programs from Wiki page

The latest binaries are available **here**.

All binaries for Linux, Mac OSX, and Windows are updated frequently. Always check for the most updated versions.

The **programs** support mixed models with multiple-correlated effects, multiple animal models and dominance.

BLUPF90+	– a combined program of blupf90, remlf90, and airemlf90
GIBBSF90+	– a combined program of gibbs2f90, gibbs3f90, thrgibbs1f90, and thrgibbs3f90
BLUPF90	– BLUP in memory
REMLF90	– accelerated EM REML
AIREMLF90	– Average Information REML with several options including EM-REML and heterogeneous residual variances (S. Tsuruta)
CBLUP90	– solutions for bivariate linear-threshold models
CBLUP90THR	– as above but with thresholds computed and many linear traits (B. Auvray)
CBLUP90REML	– as above but with quasi REML (B. Auvray)
GIBBSF90	– simple block implementation of Gibbs sampling
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
POSTGIBBSF90	– statistics and graphics for post-Gibbs analysis (S. Tsuruta)
THRGIBBSF90	– Gibbs sampling for any combination of categorical and linear traits (D. Lee)
THRGIBBS1F90	– as above but simplified with several options (S. Tsuruta)
THRGIBBS3F90	– as above with heterogeneous residual variances for linear traits
RENUMF90	– a renumbering program that also can check pedigrees and assign unknown parent groups; supports large datasets
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)
PREDICTF90	– a program to calculate adjusted y, $\hat{y}$, and residuals (I. Aguilar)
PREDF90	– a program to predict direct genomic values (DGV) and their reliabilities for animals based on genotypes and SNP solution
QCF90	– a quality-control tool on genotypes and pedigree information (Y. Masuda)
QXPAK	– joint analysis of QTL and polygenic effects (M. Perez-Enciso)

Available by request

MRF90	– Method R program suitable for very large data sets; contact T. Druet.
COXF90	– Bayesian Cox model – contact J. P. Sanchez (JuanPablo.Sanchez@irta.cat)
BLUPF90HYP	– BLUPF90 with hypothesis testing (F and Chi2 tests) – contact J. P. Sanchez as above

Available only under research agreement

BLUP90IOD2	– BLUP by iteration on data with support for very large models (S. Tsuruta)
BLUP90IOD3	– a combined program of BLUP90IOD2, BLUP90IOD2RR, BLUP90IOD2HR, and BLUP90MBE2 with new features
CBLUP90IOD	– BLUP by iteration on data for threshold-linear models
ACCF90	– approximation of accuracies for breeding values
ACCF90GS	– approximation of accuracies for genomic breeding values based on diagonals of **G**

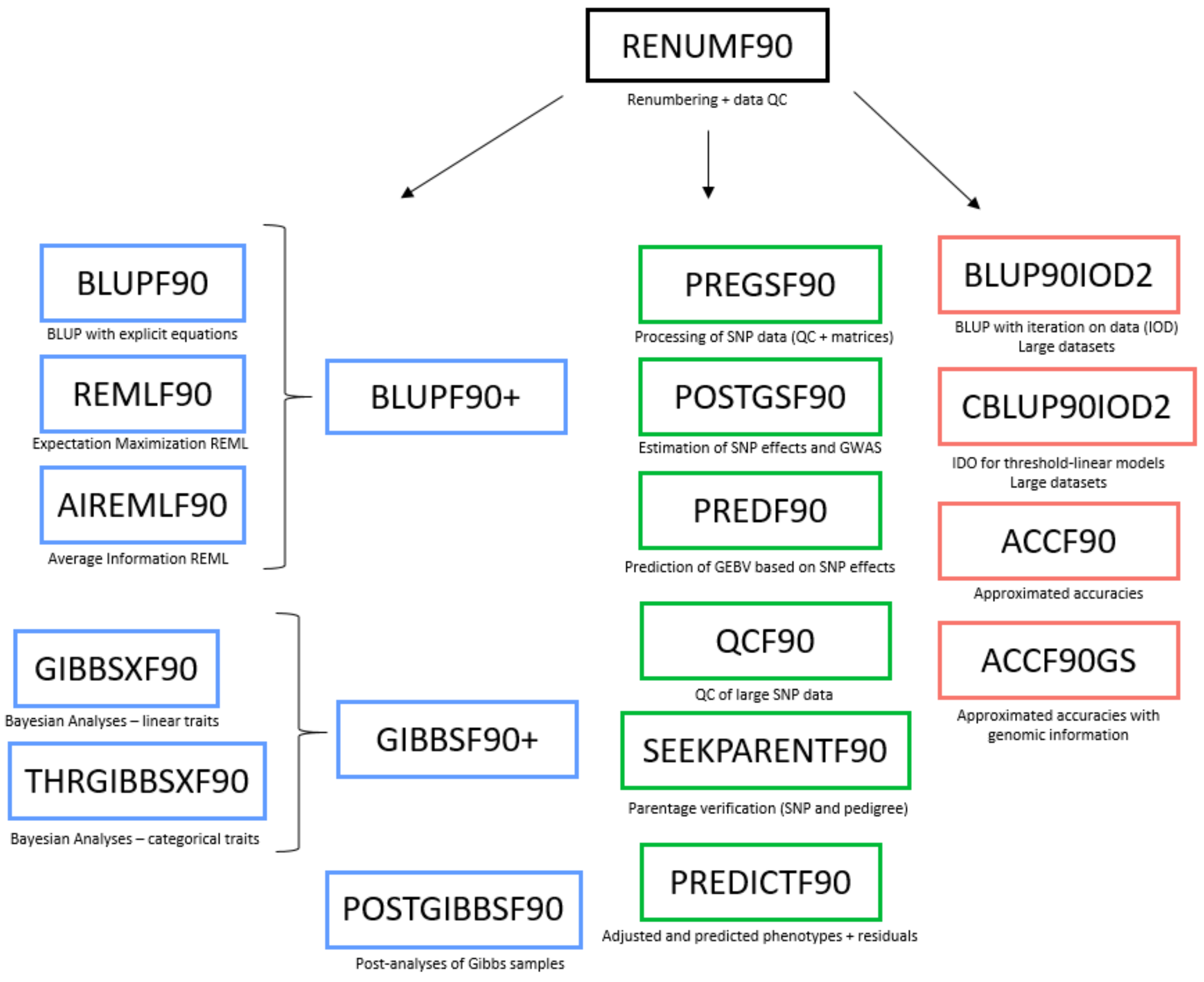
▪ **ACCF90GS2**	– new approximation of accuracies for genomic breeding values based on block sparse inversion
▪ BLUP90MBE	– BLUP by iteration on data with support for very large models for multi-breed evaluations
▪ **BLUP90ADJ**	– BLUP with a data preadjustment tool

Included in application programs

▪ **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)

Other programming contributions were made by Miguel Perez-Enciso `(user_file)` and François Guillaume (Jenkins hashing functions).

Main programs in a chart


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)
POSTGSF90
Estimation of SNP effects and GWAS
PREDF90
Prediction of GEBV based on SNP effects
QCF90
QC of large SNP data
SEEKPARENTF90
Parentage verification (SNP and pedigree)
PREDICTF90
Adjusted and predicted phenotypes + residuals
BLUP90IOD2
BLUP with iteration on data (IOD)
Large datasets
CBLUP90IOD2
IDO for threshold-linear models
Large datasets
ACCF90
Approximated accuracies
ACCF90GS
Approximated accuracies with
genomic information

Application programs (BLUP*, *REMLF90, THRGIBBS*, GIBBS*, POSTGIBBSF90, PREGSF90, POSTGSF90, and PREDICTF90) are driven by parameter files and require data files with effects renumbered from 1 consecutively. Some programs (PREDF90, QCF90, and SEEKPARENTF90) use command line instead of a parameter file.

Renumbering and quality control can be done by RENUMF90, which is also driven by a parameter file (different from the previous programs). Separation of renumbering and application programs allows supporting complicated models.

Some models are not directly supported by RENUMF90 and require tweaking the parameter file in the application programs.

Parameter file for application programs

The parameter file has keywords that are fixed (i.e., cannot be changed and should be typed exactly as shown here) followed by values, with the following structure. The example below comes from a 2-trait maternal model:

Keywords*	Description
DATAFILE	Name of file with phenotypes; free Fortran format (space-delimited file)
file.dat	
NUMBER OF TRAITS	Number of traits
2	
NUMBER OF EFFECTS	Number of effects in a model except for residual
6	
OBSERVATIONS(S)	Position(s) of observations in data file
1 2	
WEIGHTS	Position of weight on observations if used; otherwise blank
2	means that the weight is in column 2, and residual variance (R) is set to R/**weight**.
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]	
4 4 10 cross	**4 4** = crossclassified effect positions in data file for 2 traits; **10** = levels
5 0 100 cross	**5 0** = crossclassified effect, positions for 2 traits; **100** = levels
6 6 1 cov	**6 6** = covariable positions in data file
7 7 10 cov 4 4	**7 7** = covariable nested in effect position **4**; **10** = levels
8 8 1000 cross	**8 8** = crossclassified effect positions for 2 traits; **1000** = levels
0 9 1000 cross	**0 9** = crossclassified effect positions for 2 traits; **1000** = levels
RANDOM_RESIDUAL_VALUES	Residual variance or residual covariance matrix
10 1	For 2 trait model
1 10	
RANDOM_GROUP	List of effect numbers that form a group
5 6	For correlated random effects **5 6**
RANDOM_TYPE	Type of random effect
add_animal	**diagonal**, **add_sire**, **add_an_upg**, **add_an_upginb**, **par_domin**, or **user_file**
FILE	Pedigree file or other file associated with random effect; blank if none
file.ped	
(CO)VARIANCES	(Co)variance matrix for each random effect
10 1 0 1	For 2 trait, maternal model
1 10 0 1	
0 0 0 0	
1 1 0 10	

***Keywords need to be typed exactly (up to 20 characters).**
Hint: When preparing a new parameter file, consider modifying an existing file.

Note that this parameter file is for the application programs (BLUPF90, AIREMLF90, GIBBSF90, etc.) and not for RENUMF90. This program needs a different type of parameter file. See page 16 for details.

Description of effects

The effects are specified after the keyword:

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]

Each line contains the following:

- Position(s) of each effect in the data file; t positions for t traits
- Number of levels (assumed consecutive from 1)
- Type of effect: “cross” for cross-classified, and “cov” for covariable
  - Cross-classified uses integer numbers starting at 1
  - Covariable uses integer or real numbers
- For nested covariables, the following number (or t numbers for t traits) indicates the position of nesting in the data file
- Text after # can be used as a comment

Data and pedigree file should not have header; columns should be separated by at least one space (no TAB); hash (#) is interpreted as a comment initiator and should not be present inside the data and pedigree files. See page 15 for further details.

Consider the following dataset (copied to file.dat without the header):

i	j	k	y1	y2	x1
2	2	3	4.30	5.67	22.40
1	2	2	2.76	3.20	18.00
…	…	…	…	…	…
3	1	1	2.20	5.30	7.25

Let i go from 1 to 50, j from 1 to 80, and k from 1 to 200. The model:

$y1_{ij} = a_j + b_i + cx1 + e_{ij}$

will be specified in the parameter file as:

DATAFILE
file.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
3
OBSERVATIONS(S)
4
WEIGHTS

```
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
2 80 cross   # position 2, 80 levels
1 50 cross   # position 1, 50 levels
6 1 cov      # covariable on position 6, one level
……
```

By definition, a regular covariable has one level (i.e., a slope as regression).

For a similar model but with a nested covariable:

$$y1_{ij} = a_j + b_i + c_i x1 + e_{ij}$$

The description will change to:

```
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
2  80 cross   # position 2, 80 levels
1  50 cross   # position 1, 50 levels
6  50 cov 1   # covariable on position 6 nested in position 1; 50 levels
```

Assume a two-trait model:

$$y1_{ij} = a1_j + \qquad c1_i x1 + e1_{ij}$$
$$y2_{ij} = \qquad b2_i + c2_i x1 + e2_{ij}$$

This corresponds to:

```
……
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
3
……
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
2  0  80 cross     # position 2 for trait 1 only, 80 levels
0  1  50 cross     # position 1 for trait 2 only, 50 levels
6  6  50 cov 1 1   # covariable on position 6 for two traits nested in position 1
```

“0” in effect definitions means missing effect per trait.

The first two effects in the two-trait model above can be merged:

```
NUMBER_OF_EFFECTS
2
……
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
2  1  80 cross     # positions 2 and 1 for traits 1 and 2, 80 is max(50,80) levels
6  6  50 cov 1 1   # covariable in position 6 for two traits nested in position 1
```

Definition of random effects

RANDOM_GROUP defines one group of random effects. A group is one effect or multiple (correlated) effects that share the same covariance structure, e.g., direct-maternal effect or random regressions.

The structure of **RANDOM GROUP** is:

RANDOM_GROUP **5**	Corresponding to the effect number specified above; "**5**" means that the 5th effect is random. Or "**5 6**" means that 5th and 6th are correlated random effects.
or	
RANDOM_GROUP **5 6**	Corresponding to the effect number specified above; "**5 6**" means that 5th and 6th are correlated random effects.

RANDOM_TYPE defines a covariance structure: diagonal var() = s ⊗ **I** or **G** where s is a variance and **G** is a covariance matrix. For other types, see "Random effects and Pedigree files" on page 13.

Assume a model:

y = farm + animal_additive + permanent_environment + error

with var(animal_additive) = **A**⊗2.5, var(permanent_environment) = **I**⊗5.1, var(error) = **I**⊗13.7

With these effects:

```
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
3   100 cross   # effect 1: farm
2  1000 cross   # effect 2: additive genetic
2  1000 cross   # effect 3: permanent environment
RANDOM_RESIDUAL_VALUES
13.7
RANDOM_GROUP
2                   # this is for effect 2 on the effect list
RANDOM_TYPE
add_animal          # additive genetic
FILE
file.ped   # name of pedigree file
(CO)VARIANCES
2.5
RANDOM_GROUP
3                   # effect 3 on the effect list above
RANDOM_TYPE
diagonal  # permanent environment
FILE
                    # no file associated with diagonal structures
(CO)VARIANCES
5.1
```

Correlated effects

Assume a model:

y = farm + season + direct + maternal + error

var(direct,maternal)= $\mathbf{A}\otimes\begin{bmatrix}5 & 1\\1 & 6\end{bmatrix}$

with the effects as specified:

```
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
3    100 cross      # effect 1: farm
4      4 cross      # effect 2: season
2  1000 cross       # effect 3: direct
2  1000 cross       # effect 3: maternal
```

The distribution of the random effects is specified below:

```
…
RANDOM_GROUP
3  4                # direct and maternal effects
RANDOM_TYPE
add_animal          # additive genetic
FILE
file.ped            # name of pedigree file
(CO)VARIANCES
5  1
1  6
…
```

Random regression models may have many correlated random effects. Assume a data file with the following positions:

1 to 4: polynomials
5: animal number (1000 levels)
6: herd year season (50 levels)

```
…
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
6 50 cross          # herd year season
1 1000 cov 5        # first polynomial nested within the animal effect position 5
2 1000 cov 5        # second polynomial nested within the animal effect position 5
3 1000 cov 5        # third polynomial nested within the animal effect position 5
4 1000 cov 5        # fourth polynomial nested within the animal effect position 5
….
RANDOM_GROUP
2 3 4 5             # all covariables are correlated (effects 2, 3, 4, and 5 on the list above)
RANDOM_TYPE
add_animal          # additive genetic
FILE
file.ped            # name of pedigree file
(CO)VARIANCES
  (4 x 4 matrix)
```

Random effects and Pedigree files

There are a few types of additive genetic effects, each with a different pedigree format.

a) additive sire (**add_sire**)

The pedigree file has the following format:
sire number, sire's sire number, sire's maternal grandsire (MGS) number
where unknown sire's sire and/or sire's MGS numbers are replaced by 0.

b) additive animal (**add_animal**)

The pedigree file has the following format:
animal number, sire number, dam number
where unknown sire and/or dam numbers are replaced by 0.

c) additive animal with unknown parent groups (**add_an_upg**)

The pedigree file has the following format:
animal number, sire number, dam number, parent code
where sire and/or dam numbers can be replaced by unknown parent group numbers
parent code = 3 - number of known parents:

1 (both parents known)
2 (one parent known)
3 (both parents unknown)

d) additive animal with unknown parent groups and inbreeding (**add_an_upginb**)

The pedigree file has the following format:
animal number, sire number, dam number, inb/upg code
where sire and/or dam numbers can be replaced by unknown parent group numbers
inb/upg code = 4000 / [(1+ms)(1-Fs) + (1+md)(1-Fd)]

where ms (md) is 0 whenever sire (dam) is known, and 1 otherwise, and Fs(Fd) is the coefficient of inbreeding of the sire (dam). For example, the inb/upg code for the animal with both parents known is 2000. The code should be an integer value.

e) user provided matrix (**user_file**)

A file specified in FILE contains the inverse of a matrix in the following format:

row col value

as lower- or upper-triangular elements (but not full stored). The matrix is used directly by application programs. For example, to use a genomic relationship matrix **G**, the file needs to contain $\mathbf{G}^{-1}$.

f) user provided matrix with inversion (**user_file_inv**)

As above but the matrix in FILE is inverted by the application programs before being used. For example, to use a genomic relationship matrix **G**, the file needs to contain **G**. The inversion is by sparse matrix techniques, so it is efficient for sparse matrices but slow for dense matrices.

f) additive animal with selfing (**add_an_self**)

The pedigree file has the following format:
animal number, sire number, dam number, number of selfing generations
where unknown sire and/or dam numbers are replaced by 0.
This option fits some breeding structures in plants.

e) parental dominance (**par_domin**)

The pedigree class file has the following format:
s-d s-sd s-dd ss-d ds-d ss-sd ss-dd ds-sd ds-dd code
where x-y is a combination number of animals x and y, s is sire, d is dam, sd is sire of dam, etc. Code is a number of 0 to 255 and refers to the combination of missing subclasses. If one line is:

p s0 s1 s2 s3 s4 s5 s6 s7 code

then code = $\sum_{i=0}^{7}(a_i \times 2^i)$ where $a_i = 0$ if $s_i > 0$, or $a_i = 1$ otherwise.
For example, the code for a line with all nonzero parental subclasses is 255. For a line with only zero parental subclasses, if classes are ordered so that lines with zero parental subclasses, code=0. If lines are ordered so that p for parental classes with code = 0 are ordered last, they may be omitted and will be added automatically. The parental dominance file can be created by program **RENDOMN**.

Data and Pedigree files

All files are free format, with fields separated by spaces. By default, 0 is a missing value for all effects, including covariables.

Transferring a file from Windows (DOS) to Linux environment

Use “dos2unix” to convert the DOS (Windows) format to the UNIX (Linux) format if the programs show an error message while reading a file (“flip –u” can be also used instead of “dos2unix”).

Data file

a. Space(s) is a delimiter. At least one space between columns is required.
b. Dot (.) is just one character but not a missing value (default missing value = 0).
c. Check the data again, especially when converting from another format or software such as EXCEL, SAS, ...
d. For Gibbs sampling programs with “OPTION cont”, copy the previous output files somewhere else just in case making mistakes and replacing those files.

Pedigree file

a. An original pedigree file for RENUMF90 can include alpha-numeric characters with free format.
b. Remove duplicates.
c. Use 0 for unknown parent(s).

Error messages in the parameter file

a. Wrong data file name:
   Check outputs for the data file name and the number of records on the screen. The program will not stop if the wrong file name already exists.
b. Wrong pedigree file name:
   Check output for the pedigree file name and the number of animals on the screen. The program will not stop if the wrong file name exists.
c. Wrong positions or formats for observations and effects:
   Program may not stop and may get wrong results. Check outputs for the number of levels for each effect on the screen.
d. Missing or skipping one or more fixed lines in the parameter file:
   Program may stop. Check the missing line.
e. Misspelling:
   Program may stop. Correct the wrong spelling.
f. Missing an empty last line:
   Program may not stop. Parameter, data, and pedigree files may need one more extra line at the end of the file.
g. (Co)variance matrix is not symmetric, not positive definite, not right sized, ... :
   Program may not stop.
h. A good result does not mean that your parameter file is correct. Always double-check it!

RENUMF90 parameter file

Basic rules for RENUMF90 parameter file

RENUMF90 is a renumbering program to create input (data, pedigree, and parameter) files for BLUPF90 programs and provide basic statistics. Note that RENUMF90 uses a different type of parameter file as used in BLUPF90 or other programs. RENUMF90-specific parameter file should be prepared as follows:

- The file consists of pairs of **keyword** and the corresponding **value(s)**. The keyword is always capital.
- First 7 keywords are mandatory and must appear in the following order: **DATAFILE**, **TRAITS**, **FIELDS_PASSED TO OUTPUT**, **WEIGHT(S)**, **RESIDUAL_VARIANCE** and **EFFECT**. If you don't actually need **FIELDS_PASSED TO OUTPUT** and **WEIGHT(S)**, simply leave an empty line.
- The remaining keywords are optional but appear in the specific order shown below. For example, the **FILE** keyword must be followed by **FILE_POS** (or by **SNP_FILE** if **FILE_POS** is omitted; or by **PED_DEPTH** if both **FILE_POS** and **SNP_FILE** are omitted, and so on).
- Several **OPTION** lines can be included. RENUMF90 interpret a few options. Other options are simply passed through the template parameter file for BLUPF90 (*renf90.par*).

Parameter file

DATAFILE

f_1 # data file name – input files cannot contain character # because it is used as a comment.

TRAITS

t_1 t_2 t_3 ... # positions of traits in data file

FIELDS_PASSED TO OUTPUT

p_1 p_2 .. p_m # positions that are not renumbered; put empty line if not needed.

WEIGHT(S)

w # position of weight - fraction to the residual variance; put empty line if not needed.

RESIDUAL_VARIANCE

R # matrix of residual (co)variances

EFFECT

e_1 e_2 e_3 ... type form # e_1 e_2 e_3 ... = position of this effect for each trait
# type = 'cross' for crossclassified or 'cov' for covariables
# form = 'alpha' for alphanumeric or 'numer' for numeric (form is only for cross)

EFFECT

d_1 d_2 d_3 ... cov # d_1 d_2 d_3 ... = positions of covariables nested in the following cross-classified effects

NESTED

e_1 e_2 e_3 ... form # e_1 e_2 e_3 ... = positions of cross-classified effects nested
# form = 'alpha' for alphanumeric or 'numer' for numeric

RANDOM

random_type # 'diagonal', 'sire' or 'animal' for random effect

OPTIONAL

o_1 o_2 o_3 ... # 'pe' for permanent environment, 'mat' for maternal, and 'mpe' for maternal permanent environment

FILE

fped # pedigree file name

FILE_POS

animal sire dam alt_dam yob # positions of animal, sire, dam, alternate dam (recipient dam), and year of birth in pedigree file (default 1 2 3 0 0).

SNP_FILE

fsnp # specify a SNP file with ID and SNP information; the relationship matrix will include the genomic information; a fsnp file should start with ID with the same format as fped, and SNP info needs to start from a fixed column and include digits 0, 1, 2 and 5 (0, 1, and 2 for SNP count and 5 for missing SNP);
ID and SNP info need to be separated by at least one space; see more information in **http://nce.ads.uga.edu/wiki/doku.php?id=readme.pregsf90**.

PED_DEPTH

p # depth of pedigree search (default 3); all pedigrees are loaded if p = 0.

GEN_INT

min avg max # minimum, average, and maximum generation interval; applicable only if year of birth present in pedigree file; minimum and maximum used for pedigree checks; average used to predict year of birth of parent with missing pedigree.

REC_SEX

sex # if only one sex has records, specifies which parent it is; used for pedigree checks.

UPG_TYPE

t # 'yob': based on year of birth.
# 'in_pedigrees': the value of a missing parent should be -x, where x is UPG number that this missing parent should be allocated to; in this option, all known parents should have pedigree lines, i.e., each parent field should contain either the ID of a real parent, or a negative UPG number.
# ‘group’: it assigns different groups for sires and dams using a user-defined group label in the pedigree file. The field of the label should be specified as the 6th item in the FILE_POS entry.
# ‘group_unisex’: as above except assigning the same groups to sires and dams.
# 'internal', allocation is by a user-written function custom_upg (year_of_birth,sex,ID, parent_code).

INBREEDING

s # use of inbreeding coefficients to compute inb/upg code in the 4th column of the output pedigree file. Inbreeding calculation is default in RENUMF90 ≥ v1.157, even if this keyword is not used.

# 'pedigree': the program computes inbreeding coefficients with Meuwissen and Luo (1992) using the pedigree to be saved in renaddxx.ped; calculated inbreeding coefficients will be saved in a file "renf90.inb" with the original ID.
# 'file': the program reads inbreeding coefficients from an external file. You should put the filename after 'file' e.g. 'file inbreeding.txt'. The file has at least 2 columns: original_ID and inbreeding value (from 0.0 to 1.0). The program skips unnecessary IDs.
# 'self x': Calculates inbreeding with selfing
x is the column in the pedigree file with the number of selfing generations
# 'no-inbreeding': turn inbreeding calculation off in RENUMF90 ≥ v1.157.

(CO)VARIANCES
G # (co)variances for animal effects or animal + maternal effects
(CO)VARIANCES_PE
GPE # (co)variances for the PE effect
(CO)VARIANCES_MPE
GMPE # (co)variances for the MPE effect

Combining fields

How can we specify interactions? - Combining fields or interactions. Several fields in the data file can be combined into one using a **COMBINE** keyword.

COMBINE a b c .... # keywords COMBINE need to be on top of the parameter file (the first keyword). It can be placed after comments.

For example:
COMBINE 7 2 3 4
combines content of fields 2 3 4 into field 7; the data file is not changed, only the program treats field 7 as fields 2 3 4 put together (without spaces). The combined fields can be treated as "numeric" with the total length is < 9 or "alpha". The keyword is optional but must be placed in the top of the parameter file.

Hints: type `renumf90 --show-template` to have a template parameter file.
type `renumf90 --version` to see the version number.

Options

RENUMF90 parameter file can accept a few options. If the program detects non-RENUMF90 options, such option lines are simply transferred to *renf90.par*.

OPTION alpha_size nn # new size
Changes the maximum size of character fields (default 20 characters).

OPTION max_string_readline nn

Changes the maximum length of characters in a line (default 800 characters).

OPTION max_field_readline nn
Changes the maximum number of fields capable in a line (default 100 fields).

OPTION missing x
It allows the indication that x represents a missing value (default is 0), for example if 0 is a valid record. This is only to represent the missing value in the data. If there are covariables in the data, 0 is treated as a value, not missing information. Missing pedigree is always 0 and cannot be changed to another value.

OPTION missing_in_weights
This indicates that, for a given trait, if a weight is 0, then the record value for that trait is converted to a "missing" in the output file *renf90.dat*. For instance, 0 when OPTION missing x is not used, or x otherwise.

OPTION no_basic_statistics
This causes the program to not compute descriptive statistics of the data (mean, minimum, correlations, …), which can take time for very large datasets.

OPTION inbreeding_method m
This allows the user to choose which method is used to compute inbreeding coefficients. Those inbreeding coefficients will be used later (in the other programs) to set up A-inverse. Acceptable values for m are:

1. Meuwissen and Luo (1992).
2. Modified Meuwissen & Luo by Sargolzaei and Iwaisaki (2004).
3. Modified Colleau by Salgolzaei et al. (2005).
4. Recursive tabular method.
5. Method of Tier (1990).
6. Parallel (OMP) version of Meuwissen and Luo (1992)
7. Recursive tabular with self-breeding generations.

The default is method 1. Method 6 can largely speed-up the computation, but it requires using many threads (e.g., OMP_NUM_THREADS=4).

The end of the parameter file for RENUMF90 can contain many lines with OPTION, those lines are passed to the parameter file *renf90.par* to be used by the other programs.

Output files

RENUMF90 generates several files.

- *renf90.par*: parameter template file for BLUPF90 and other application programs
- *renf90.dat*: data file for BLUPF90

- *renaddxx.ped*: pedigree file for BLUPF90; *xx* is an integer number that indicates the position of animal effect among all model effects in renf90.par. This file will be created only if **RANDOM animal** is specified
- *SNPfile_XrefID*: cross-reference file for genomic analysis, which contains renumbered ID and original ID; *SNPfile* is the original SNP marker file. This file will be created only if **SNP_FILE** is specified
- *renf90.inb*: inbreeding coefficients. Inbreeding calculation is default in RENUMF90 ≥ v1.157, even if the INBREEDING keyword is not used.
- *renf90.tables*: table relating the original code and the renumbered code
- *renf90.fields*: has detailed description of the effects in each field of renf90.dat.

Output pedigree file

The additive pedigree file built by RENUMF90 is renadd*xx*.ped. The pedigree file has the following structure:

1) animal number (from 1)
2) parent 1 number or unknown parent group number for parent 1
3) parent 2 number or unknown parent group number for parent 2
4) 3 minus number of known parents (this column is replaced by inbreeding code if **INBREEDING** is specified or by default in RENUMF90 ≥ v1.157)
5) known or estimated year of birth (0 if not provided)
6) number of known parents (for genotyped animals, if any: 10 + number of known parents)
7) number of records
8) number of progenies as parent 1
9) number of progenies as parent 2
10) original animal id

Example

Input file - data

```
aa 1 10
aa 2 12
bb 1 11
cc 1 12
cc 2 14
dd 2 13
ee 2 14
```

Pedigree file - ped

```
aa  ff  ee 2004
bb  hh  gg 2004
cc  hh  ii 2004
dd  ff  0  2004
ee  ff  0  2002
ff  0   0  2002
gg  ff  0  2002
```

```
hh  0   0  2002
ii  0   0  2002
kk  0   0  2000
```

Parameter file - testpar1

```
# Parameter file for program renumf90; it is translated to parameter file for BLUPF90 family of programs.
DATAFILE
data
TRAITS
3
FIELDS_PASSED TO OUTPUT
1  #passing original ID to the renumbered data file
WEIGHT(S)

RESIDUAL_VARIANCE
1
EFFECT
2 cross num
EFFECT
1 cross alpha
RANDOM
animal
FILE
ped
FILE_POS
1 2 3 0 4
PED_DEPTH
3
GEN_INT
1 2 10
UPG_TYPE
yob
2002 2003
(CO)VARIANCES
1
```

Output log

```
RENUMF90 version 1.157 with zlib
 testpar1
 datafile:data
 traits:           3
 fields passed:           1
 R
   1.000

 Processing effect  1 of type cross
 item_kind=num

 Processing effect  2 of type cross
 item_kind=alpha
 pedigree file name  "ped"
 positions of animal, sire, dam, alternate dam, yob, and group     1     2     3     0     4
0     0
```

```
 pedigree traced to generation            3
 Minimum, average and maximum generation intervals:     1    2   10
 Unknown parent groups separated by years:
        2002        2003
 Reading (CO)VARIANCES:           1 x           1

 Maximum size of character fields: 20

 Maximum size of record (max_string_readline): 8000

 Maximum number of fields for input file (max_field_readline): 100

 Pedigree search method (ped_search): convention

 Order of pedigree animals (animal_order): default

 Order of UPG (upg_order): default

 Missing observation code (missing): 0


 Using prime hash function
 hash tables for effects set up
 first 3 lines of the data file (up to 70 characters)
    aa 1 10
    aa 2 12
    bb 1 11
 read            7  records
 table with            2  elements sorted
 added count
 Effect group            1  of column            1  with            2  levels
 table expanded from        10000  to        10000  records
 added count
 Effect group            2  of column            1  with            5  levels
 wrote statistics in file "renf90.tables"

 Basic statistics for input data  (missing value code is '0')
 Pos  Min         Max         Mean        SD                 N
   2    1.0000      2.0000      1.5714     0.53452           7
   3    10.000      14.000      12.286      1.4960           7

 Correlation matrix
        2     3
  2   1.00  0.80
  3   0.80  1.00

 Counts of nonzero values (order as above)
          7         7
          7         7

 random effect   2
 type:animal
 opened output pedigree file "renadd02.ped"
 first 3 lines of the file (up to 70 characters)
    aa  ff  ee 2004
    bb  hh  gg 2004
    cc  hh  ii 2004
 read           10  pedigree records
 loaded            4  parent(s) in round            1

 Pedigree checks
ee: younger than parent 1 by      0 years
```

```
gg: younger than parent 1 by      0 years

 Unknown parent group allocation
 Equation   Group       #Animals   Years
       10       1       0             0-   2001
       11       2       8          2002-   2002
       12       3       1          2003-
 Max group = 3; Max UPG ID = 12

 Computations for inbreeding coefficients
 Tiny negative value will be replaced with 0 considered as numerical error.
 Wrote inbreeding file "renf90.inb" with original id

 Inbreeding statistics:
 the maximum inbreeding coefficient    =  0.2500
 average inbreeding for inbred animals =  0.2500   n = 1
                      for all animals =  0.0278   n = 9
 max upg           3

 Number of animals with records                  =           5
 Number of parents without records               =           4
 Total number of animals                         =           9

 Wrote parameter file "renf90.par"
 Wrote renumbered data "renf90.dat" 7 records
 Wrote field information "renf90.fields" for 4 fields in data
```

Output data file - renf90.dat

```
#observation, effect 1, animal number, original animal ID
 10 1 4 aa
 12 2 4 aa
 11 1 2 bb
 12 1 5 cc
 14 2 5 cc
 13 2 3 dd
 14 2 1 ee
```

Output pedigree file - renadd02.ped

```
Animal, sire, dam, inbreeding code (3-#unknown parents if no-inbreeding), birth year, #known
parents, #records, #progeny of sire, # progeny of dam, original animal ID
1 6 11 1333 2002 1 1 0 1 ee
2 8 7 2000 2004 2 1 0 0 bb
7 6 11 1333 2002 1 0 0 1 gg
3 6 12 1333 2004 1 1 0 0 dd
9 11 11 1000 2002 0 0 0 1 ii
4 6 1 2000 2004 2 2 0 0 aa
6 11 11 1000 2002 0 0 4 0 ff
5 8 9 2000 2004 2 2 0 0 cc
8 11 11 1000 2002 0 0 2 0 hh
```

Output 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      12 cross
RANDOM_RESIDUAL VALUES
   1.0000
 RANDOM_GROUP
    2
 RANDOM_TYPE
 add_an_upginb
 FILE
renadd02.ped
(CO)VARIANCES
   1.0000
```

Output tables after renumbering - renf90.tables

```
Effect group 1 of column 1 with 2 levels, effect # 1
 Value    #    consecutive number
1 3 1
2 4 2
```

Output tables after renumbering - renf90.fields

```
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
   4      passed          1        0          0           *       cov       *
```

Output tables after renumbering - renf90.inb

```
ee   0.000000       1
bb   0.000000       2
gg   0.000000       7
dd   0.000000       3
ii   0.000000       9
aa   0.250000       4
ff   0.000000       6
cc   0.000000       5
hh   0.000000       8
```

When to use which program and computing limits

BLUP

BLUPF90 sets up equations in memory. It can support a few million equations with a simple model but fewer equations with complicated models (multiple traits, maternal effects, random regression, etc). BLUPF90 uses three solvers, chosen with options. Preconditioned conjugate gradient (PCG) is the default solver and is usually the fastest one. Successive over-relaxation (SOR) requires less memory but usually converges slower. Sparse Cholesky (FSPAK) is usually the most accurate method but uses the most memory. The following options are available:

OPTION conv_crit 1e-12
Sets convergence criteria (default 1e-12).

OPTION maxrounds 10000
Sets maximum number of rounds (default 5000).

OPTION solv_method FSPAK
Selection of solving method: FSPAK, SOR, or PCG (default PCG).

OPTION r_factor 1.6
Sets relaxation factor for SOR (default 1.4). This factor helps speeding up convergence if the value is optimal; non-optimal values lead to poor convergence. It should be within [0,2].

OPTION sol se
Stores solutions and standard errors. If this option is used, the solving method will turn to FSPAK.

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

OPTION missing -999
Specify missing observations in the data file. Must be an integer value (default is 0).

OPTION blksize 3
Sets block size for preconditioner (default 1) to accelerate convergence (usually 2 to 5 times faster). For a multi-trait model, use the number of traits. This option is extremely important to ensure convergence in multi-trait models.

OPTION prior_solutions

The previous solution file will be used to start the iteration. Additional software is required to set up files correctly before using this option.

OPTION stdresidual
It stores y-hat and student residuals in "*yhat_student_residual*".

OPTION check_levels 0
Check levels (default 1 = true).

OPTION use_yams
Runs the program with YAMS (modified FSPAK). The computing time can be dramatically improved compared to using **solv_method** FSPAK

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 as used in GIBBS3F90.

OPTION hetres_var file
Combined with **hetres_int**, heterogeneous residual variances are read from **file**. The file has to contain residual (co)variances for each interval class.

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

OPTION snp_p_value
Computes the elements of the inverse of the Mixed Model Equations that are needed for exact GWAS with p-values using postGSf90. This requires quite a lot of memory and time.

OPTION omit_ainv
This causes the program to avoid computation of $\mathbf{A}^{-1}$. It is especially useful for GBLUP. For example, the following options can be used:

OPTION omit_ainv
OPTION TauOmega 1.0 0.0
OPTION AlphaBeta 0.95 0.05

With that, the program does not compute $\mathbf{A}^{-1}$ but calculates $\tau\mathbf{G}^{-1} - \omega\mathbf{A}_{22}^{-1}$; since $\omega = 0$, only $\mathbf{G}^{-1}$ will be included in the mixed model equations. **OPTION AlphaBeta 0.95 0.05** blends **G** with $\mathbf{A}_{22}$ as $0.95\mathbf{G} + 0.05\mathbf{A}_{22}^{-1}$ before inversion.

BLUP90IOD2

BLUP90IOD2 uses an iteration on data algorithm. It can handle hundreds of millions of equations with complicated models in a reasonable time. However, it is only available based on a research agreement with UGA. The following options are available:

OPTION conv_crit 1e-12
Sets convergence criteria (default 1e-12).

OPTION maxrounds 10000
Sets maximum number of rounds (default 5000).

OPTION blksize 3
Sets block size for preconditioner (default 1). The **blksize** number has to be the same as the number of traits for optimal performance.

OPTION init_eq 10
Sets the number of effects to be solved directly (default 0).

OPTION solv_method FSPAK
Solving method for initial equations (default DIRECT).

OPTION tol 1d-12
Tolerance to get a positive definite matrix (default 1d-12).

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

OPTION avgeps 50
Using the last 50 average eps for convergence.

OPTION cont 1
Restarts the program from the previous solutions.

OPTION missing -1
Sets the missing value (default 0).

OPTION restart 100
Sets the number of iteration to recompute residuals (default 100).

OPTION prior_solutions

Using the previous solution file to start the iteration. Additional software is required to use this option.

OPTION random_upg 1 2

Sets the UPG random. “1” is the computational algorithm used; only algorithm 1 is implemented. “2” is the weight (γ) for the group effects, the weight will be inverted (e.g., 1/2=0.5).

OPTION SNP_file snp

Specifies the SNP file name snp to use genotype data.

OPTION origID

Stores solutions with the original ID. The output is *trait effect level original_id solution*, and is stored in solutions.original. Be aware that this option may not in some programs.

Variance components estimation

There is not a single best choice for variance component estimation. The programs below offer choices for simple and complicated models. For advice on what works best under your circumstances, check this paper "**Reliable computing in estimation of variance components**".

REMLF90 uses expectation maximization (EM) REML. It is the most reliable algorithm for most problems but can take hundreds of rounds of iterations. REMLF90 was found to have problems converging with random regression models. In this case, using starting variances that are too large than too small usually helps. Also, EM does not calculate standard errors for the estimates. The following options are available:

OPTION conv_crit 1d-12
Convergence criterion (default 1d-12).

OPTION maxrounds 10000
Maximum rounds (default 5000).

OPTION sol se
Stores solutions and standard errors (se).

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

OPTION missing -999
Specifies missing observations (default 0).
This is only for data, not pedigree (always 0 for missing pedigrees). There is no missing covariable, so 0 is treated as a level.

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 is fixed.

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

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

AIREMLF90 uses Average Information (AI) REML. It usually converges much faster but sometimes does not converge. Very slow convergence usually indicates that the model is over parameterized, and there is insufficient information to estimate some variances. AI REML calculates standard errors for the estimates. The following options are available:

OPTION conv_crit 1d-12
Convergence criterion (default 1d-12).

OPTION maxrounds 500
Maximum rounds (default 5000). When it is zero, the program calculates BLUP without running REML.

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

OPTION tol 1d-18
Tolerance (or precision) for positive definite matrix and G-inverse subroutines (default 1d-14).

OPTION sol se
Stores solutions and standard errors (se).

OPTION missing -1
Sets the missing observation (default 0).

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 is fixed.

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

OPTION fact_once memory
Saves the Cholesky factor of LHS in memory. It greatly improves the computing time instead of memory consumption.

OPTION fact_once file
Saves Cholesky factor of LHS in a temporary file. It improves the computing time without extra memory.

OPTION approx_loglike
Skips the exact computation of log-likelihood. It would improve the computing time.

OPTION store_pev_pec 6
Stores standard errors and its covariances for correlated random effects such as direct-maternal and random regression effects in "*pev_pec_bf90*".

OPTION residual

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

Heterogeneous residual variances for a single trait

OPTION hetres_pos 10 11

Specifies the positions of covariables.

OPTION hetres_pol 4.0 0.1 0.1

Initial values of coefficients for heterogeneous residual variances. Use *ln*(a0, a1, a2, ...) to make these values. When the number of positions = the number of polynomials, the regressions do not include the intercept (e.g., linear spline).

Heterogeneous residual variances for multiple traits (the convergence will be very slow)

OPTION hetres_pos 10 10 11 11

Specifies positions of covariables (trait first).

OPTION hetres_pol 4.0 4.0 0.1 0.1 0.01 0.01

Initial values of coefficients for heterogeneous residual variances using ln(a0, a1, a2, …) to make these values (trait first). “4.0 4.0” are the intercept for first and second traits. “0.1 0.1” could be linear and “0.01 0.01” could be quadratic. To transform back to the original scale, use exp(a0+a1*X1+a2*X2).

OPTION SNP_file snp

Specifies the SNP file name **snp** to use genotype data.

Standard deviations for (co)variance functions including heritability

OPTION se_covar_function label function

Calculates SD for (co)variance functions by repeated sampling of parameter estimates from their asymptotic multivariate normal distribution, following idea presented by Meyer and Houle 2013. For details, see documentation at **http://nce.ads.uga.edu/wiki/doku.php?id=readme.aireml**.

OPTION samples_se_covar_function x

This allows the user to set the number of samples to calculate the standard error for functions of (co)variance components (default value is 10000).

GIBBSxF90 programs implement Bayesian methods. These methods potentially have better statistical properties. Also, they are more stable and use less memory for complicated models. After running any of the Gibbs sampling programs, samples can be analyzed (posterior means, SD, and convergence parameters) with the POSTGIBBSF90 program.

In practical cases, results from Gibbs samplers and REML are similar. Choose one or the other based on computing feasibility. If there are large differences beyond sampling errors, this indicates problems usually with the Gibbs sampler. Try longer chains or different priors.

Gibbs samplers may be slow to achieve convergence if initial values are far away from those at convergence, e.g., 100 times too low or too high. Before using more complicated models, Karin Meyer advocates using a series of simpler models.

GIBBS1F90 can run models with over 20 traits. However, if models are different per trait, the lines due to effects need to be modified. Also, with too many differences in models among traits, the program becomes increasingly slower.

GIBBS2F90 adds joint sampling of correlated effects. This results in faster mixing with random regression and maternal models. Memory requirements and CPU time per round are somewhat higher than in gibbs1f90.

Interactive inputs:

number of samples and length of burn-in?
In the first run, if you have no idea about the number of samples and burn-in, just type your guess (10000 or whatever) for samples and (0) for burn-in. You may need 2 or 3 runs to figure out the convergence.

Give n to store every n-th sample?
Gibbs samples are highly correlated, so you do not have to keep all samples (every 10th, 20th, 50th, ...).

The following options are available for **GIBBSxF90**:

OPTION fixed_var all 1 2 3
Stores all solutions and posterior means and SD for effects 1, 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 effects 1, 2, and 3 in "final_solutions" using fixed (known) variances.

OPTION solution all 1 2 3
Stores all solutions and posterior means and SD for effects 1, 2, and 3 in "all_solutions" and in "final_solutions" every round. Without numbers, all solutions for all effects are stored.
Caution: this option will create a huge output solution file when you run many rounds and/or use a large model.

OPTION solution mean 1 2 3
Posterior means and SD for effects 1, 2, and 3 are stored in "final_solutions".

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

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; where eff*x* corresponds to the effect number and db*x* 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
Specifies the SNP file name **snp** to use genotype data.

GIBBS3F90 adds estimation of heterogeneous residual covariances in classes. The computing costs usually increase with the number of classes.

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.

Other options are the same as for **GIBBS1F90** and **GIBBS2F90**. For **fixed_var all** or **fixed_var mean**, heterogeneous residual variances are read from a file '**hetres**'. This file name cannot be changed.

THRGIBBS1F90 is a Gibbs sampling program to analyze categorical and continuous traits simultaneously; categorical traits can be censored. The following options are available:

OPTION cat 0 0 2 5
"0" indicates 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 thresholds 0.0 1.0 2.0
Set the fixed thresholds. No need to set 0 for binary traits.

OPTION residual 1
Set the residual variance = 1.

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.

OPTION censored 1 0

Negative values of the last category in the data set indicate censored records. "1 0" determines that the first categorical trait is censored, and the second categorical trait is uncensored.

OPTION pos_def x.x

This specifies the tolerance x.x (default = 1d-08) for checking post-def for fixed effects.

Using the following options for ordered categorical data with right censored records:

OPTION cat 0 0 2 5
OPTION censored 1 0

The data file may look like

traits:	1	2	3	4
	1.71	11.1	1	1
	2.22	15.2	0	5
	3.29	16.4	2	1
	1.95	14.7	1	3
	2.25	20.8	-2	4
	3.64	19.2	1	5
	1.99	13.3	-1	2

Columns 1 and 2 are observations for linear traits and columns 3 and 4 are traits for 2 categories (binary) with censored records (negative values) and 5 categories.

Other options are the same as for **GIBBS1F90** and **GIBBS2F90**.

THRGIBBS3F90 works as THRGIBBS1f90 but with the estimation of heterogeneous residual covariances in classes as described for GIBBS3F90.

POSTGIBBSF90 is a program to calculate posterior means and SD and diagnose the convergence of the Gibbs chain. The program reads "**gibbs_samples**" and "**fort.99**" files from Gibbs sampling programs.

```
Read 1000 samples from round 10 to 10000

Burn-in?
1000            # in the first run, type 0 for burn-in to include all samples.
```

Give n to read every n-th sample? (1 means read all samples)

10 # Type the same number used with a Gibbs sampling program.
# You should not type 1 unless you have typed 1 in the Gibbs sampling program.

# samples after burn-in = 9000

Input files:

gibbs_samples, fort.99, and other files used in a parameter file from **(THR)GIBBSxF90**

Output files:

postgibbs_samples, postout, postmean, postsd

postgibbs_samples

A text file containing all Gibbs samples from **gibbs_samples** for other software (EXCEL, SAS, R, …) to calculate posterior means and SD, and to create graphs.

postmean

Posterior means

postsd

Posterior standard deviations

postout

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

                       ********  Posterior  Standard  Deviation  ********

Pos. eff1 eff2 trt1 trt2     PSD      Mean         PSD          Geweke      Autocorrelations     Independent
                                               Interval (95%)  diagnostic  lag: 1     10      50   # 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
```

where

"Pos."

position of each parameter in the parameter file.

"eff1" and "eff2"

effect number in the parameter file.

"trt1" and "trt2"

trait number in the parameter file (0 for residual).

"MCE"

Monte Carlo Error.

"Mean"

posterior means.

"HPD interval (95%)"

95% Highest Probability Density.

"Effective sample size"

at least > 10 is recommended; > 30 may be better.

"Median"

median of Gibbs samples.

"Mode"

when the distribution of the samples is not normal, "Mean" and “Mode” could be different.

"Independent chain size"

number of independent cycles of Gibbs samples.

"PSD"

Posterior Standard Deviation.

"PSD interval (95%)"

95% Posterior Standard Deviation interval.

"Geweke diagnostic"

the ratio between the first and second halves of the samples should be < 1.0, but it may not be helpful because it is < 1.0 most of the time.

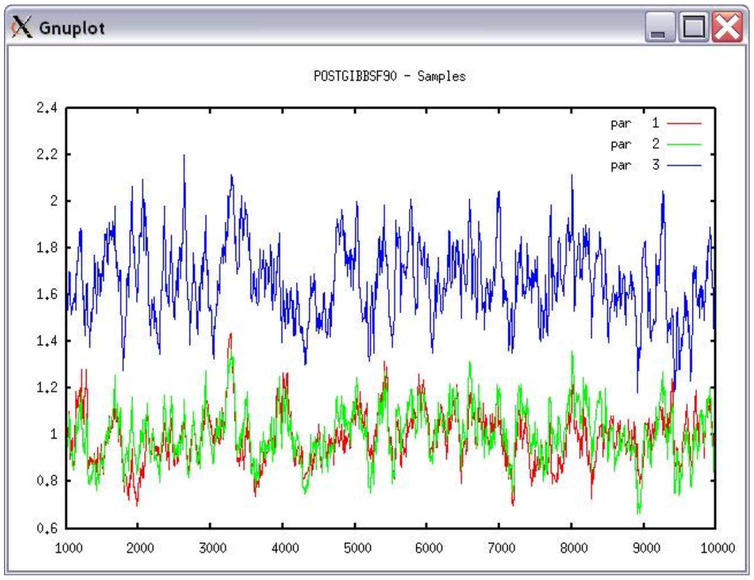
"Autocorrelations"

autocorrelations between two lags. High correlation implies samples are not independent.

"Independent # batches"

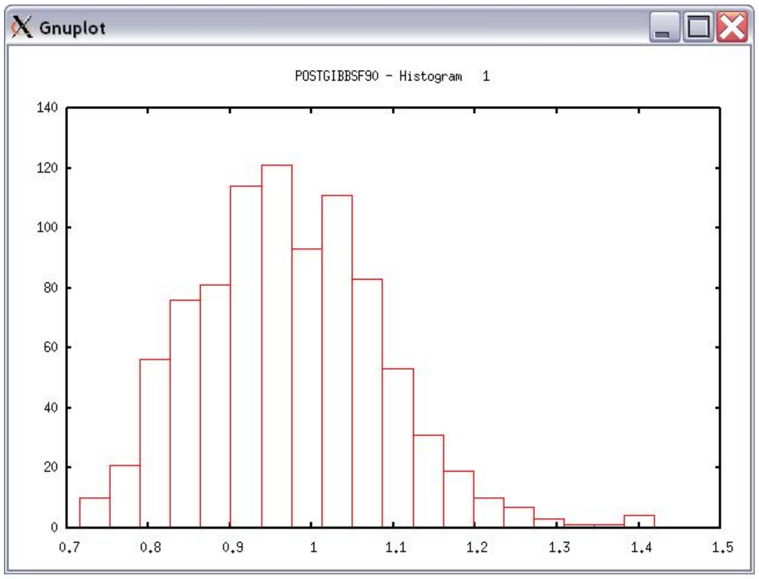
Hint 1: when eff1, eff2, trt1, trt2 are all -1, the values presented are for thresholds (if THRGIBBSXF90 is used).

```
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
Choose a graph for samples (= 1) or histogram (= 2); or exit (= 0)
2
Type position and # bins
1 20
```



The distribution should be usually normal (Mean = Mode = Median).

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

*** Log Marginal Density for Bayes Factor ***
after 900 burn-in
log(p) = -179448.742766031
```

This value could be used when calculating Bayes Factor and/or DIC.

Combined programs

BLUPF90+

This software combines BLUPF90, REMLF90, and AIREMLF90. Therefore, it can take options used in each of these programs.

It has some new features such as the computation of reliabilities of (G)EBV based on PEV, and the ability to save solutions with original ID.

The default of this software is to run BLUP, unless variance components estimation options are used.
Hint: type `blupf90+ --help` to see all the BLUPF90+ options
or `blupf90+ --help-genomic` to see genomic options BLUPF90+ can take.

Specific options

OPTION method VCE
Runs AIREMLF90 for variance component estimation.

OPTION EM-REML x
Runs EM-REML (REMLF90) for first x rounds to get initial variances within the parameter space. After 100 rounds, it will switch to AI-REML (AIREMLF90) and continue until convergence. If the program converges within 100 rounds, it will show only the results from AI-REML
Examples:
OPTION EM-REML n
….Runs AI rounds until convergence or x after n EM rounds, showing AI output
OPTION EM-REML or OPTION EM-REML pure
….Runs EM until convergence or x, showing EM output, which is equivalent to REMLF90
OPTION EM-REML AI or ai
….Runs EM until convergence and then switches to AI rounds until AI convergence or x, showing AI output

OPTION store_accuracy eff
Stores reliabilities based on PEV, where eff is the number of the animal effect. By default, it uses inbreeding (F) in the denominator of the reliability formula: reliability = 1-PEV/(σ_u^2 (1+F)). It uses inbreeding based on the relationship matrix that is being used in the mixed model equations.

OPTION acctype 1.0
Select 1.0 for dairy cattle (Reliability) or 0.5 for beef cattle (BIF accuracy) (default 1.0).

OPTION correct_accuracy_by_inbreeding filename
filename is the name of the inbreeding file if other than renf90.inb

OPTION correct_accuracy_by_inbreeding_direct 0
This option turns off the inbreeding correction in the reliability formula.

OPTION origID
Stores solutions with the original ID. The output is *trait effect level original_id solution*, and is stored in solutions.original.

OPTION store_accuracy eff orig
Stores reliabilities based on PEV, where **eff** is the number of the animal effect, and **orig** should be used to output reliabilities with original ID. Combine with OPTION origID if solutions should also be output with original ID. The resulting file, acc_bf90, contains: trait, effect, level, original_ID, solutions, reliabilities.

OPTION set_eig 1d-12
It allows to set a tolerance (or precision) for positive definite matrix and g-inverse subroutines (default is 1d-18).

Click **here** for more details on BLUPF90+

GIBBSF90+
This software combines GIBBS1F90, GIBBS2F90, GIBBS3F90, THRGIBBS1F90, and THRGIBBS3F90.
It takes any options from the above Gibbs programs.
Click **here** for more details on GIBBSF90+

Genomic programs

PREGSF90

PreGSF90 is an interface program to the genomic module to process the genomic information for the BLUPF90 family of programs. This software performs quality control of genomic data and constructs and inverts the genomic relationship matrix (**G**) and the pedigree relationship matrix for genotyped animals ($\mathbf{A}_{22}$). When the inverse of the relationship matrix based on the pedigree information (**A**) in the mixed model equations is replaced by the inverse of the realized relationship matrix (**H**), which combines pedigree and genomic information, BLUP becomes single-step GBLUP (**ssGBLUP**). The main difference between $\mathbf{A}^{-1}$ and $\mathbf{H}^{-1}$ is the structure of $\mathbf{G}^{-1} - \mathbf{A}_{22}^{-1}$ added for the genotyped animals. Some of the options for **PREGSF90** can be also used with **BLUPF90**, (**AI**)**REMLF90**, **GIBBS1F90**, **GIBBS2F90**, **GIBBS3F90**, **THRGIBBS1F90**, **BLUPF90+**, **GIBBSF90+**, **BLUP90IOD2**, and **BLUP90IOD3**.

Input files
OPTION SNP_file <file>
This option invokes the genomic routine in the application programs. The SNP file should contain
Field 1 - animal ID with the same format as in pedigree file

Field 2 - genotypes with 0, 1, 2, and 5 (missing) or real values for gene content (or genotype probability) 0.120.890.54 (i.e., 0.12 0.89 0.54 without spaces). Be aware that some quality control steps are turned off when using genotype probabilities.

Two Fields (animal ID and SNP) need to be separated by at least one space, and Field 2 should have fixed format (i.e., all rows of genotypes should start at the same column number or position).

```
 80    2110101100201201101101011011111211111210100
 8014 21110101511101120221110111511112101112210100
 516  21100101202252021120210121102111202212111101
 181  21110111112201120550200020101022212211111100
```

The renumbered ID file for genotypes named after the genotype file, e.g., **file_XrefID**, is created by RENUMF90 (using the SNP file), containing the renumbered ID and the original ID, which follows the same order as in the SNP file:

```
1732 80
8474 8014
406 516
9441 181
```

The pedigree file from RENUMF90 looks like:

```
1732 11010 10584 1 3 12  1 0 0 80
8474  8691  9908 1 3 12  1 0 0 8014
 406  8691  9825 1 3 12  1 0 2 516
9441  8691  8829 1 3 12  1 0 0 181
```

Map file for SNP can be used as optional:

OPTION map_file <file>: reads SNP map information from the file.
The file should have a header with the following column names:

SNP_ID #identification of the SNP (alphanumeric)
CHR #chromosome number (numeric), starting from 1
POS #position bp (numeric)

Extra columns are possible (optional).
The first SNP in the Map file corresponds to the first SNP in the genotype file, and so on.
Example:

```
SNP_ID CHR POS
    1    1   1201
    2    1   8004
    3    1  12006
    4    1  16008
```

The map file is useful to check for Mendelian conflicts and HWE (with also **OPTION sex_chr**) and for **POSTGSF90** (**ssGWAS**).

With other options, the program can read **G** or its inverse, $\mathbf{A}_{22}$ or its inverse, etc.

Output files

By default, **PREGSf90** runs quality control and creates GimA22i in binary format for use by other application programs, specifying **OPTION readGimA22i**. With **OPTION saveAscii**, this file can be stored as ASCII format: i, j, $\mathbf{G}^{-1} - \mathbf{A}_{22}^{-1}$.

“freqdata.count” contains allele frequencies in the original genotype file with the format: SNP number (related to the genotype file) and allele frequency as mentioned above.

“freqdata.count.after.clean” contains allele frequencies as used in calculations with the format: SNP number (related to the genotype file), allele frequency, and exclusion code.
Exclusion codes:

1: Call Rate
2: MAF
3: Monomorphic
4: Excluded by request
5: Mendelian error
6: HWE
7: High Correlation with other(s) SNP

“Gen_call_rate” contains a list of animals excluded with call rate below the threshold.

“Gen_conflicts” contains a report of animals with Mendelian conflicts with their parents.

The program can store files such as **G** or its inverse, **A**$_{22}$ or its inverse, or other reports from QC as specified by their respective OPTIONs.

Options for creating the genomic relationship Matrix (G)

The genomic relationship matrix, **G**, can be created in different ways.

OPTION whichG x
Specifies how **G** is created.
The variable x can be
1: $\mathbf{G} = \frac{\mathbf{ZZ'}}{k}$; VanRaden, 2008 (default)
2: $\mathbf{G} = \frac{\mathbf{ZDZ'}}{n}$; Amin et al., 2007; Leuttenger et al., 2003; where $\mathbf{D} = \frac{1}{2p(1-p)}$
3: As 2 with modification UAR from Yang et al., 2010

OPTION whichfreq x
Specifies which frequency is used for centering **Z** to create **G**.
The variable x can be
0: read from file “freqdata” or from the other file using **OPTION FreqFile**

1: 0.5
2: current calculated from genotypes (default)

OPTION whichfreqScale x
Specifies which frequency is used to scale **G**. This can be applied to use different allele frequencies to center and scale **G**. The variable x can be:
0: read from file as specified using **OPTION FreqFile**
1: 0.5
2: current calculated from genotypes (default)

OPTION FreqFile <file>
Reads allele frequencies from a file. For example, based on allele frequencies calculated by estfreq.f90 (VanRaden, 2009) with format:
Field 1 – SNP number (sequential marker number)
Field 2 – allele frequency as a real value from 0 to 1
Example:

```
1   0.525333
2   0.293667
3   0.448333
4   0.510667
```

where SNP corresponds to the index of SNP based on the same order as in the genotype file.
If **whichfreq** is set to 0, the default file name is "freqdata".

OPTION whichScale x
Specifies how **G** is scaled.
The variable x can be
1: $2\sum\{p(1-p)\}$; VanRaden, 2008 (default)
2: $\frac{tr(\mathbf{ZZ'})}{n}$; Legarra, 2009, Hayes, 2009
3: correction; Gianola et al., 2009

OPTION weightedG <file>
Reads weights from a file to create weighted genomic relationships.
With weights, Z* = Z sqrt(D) ⇒ **G** = Z*Z*' = ZDZ'. Format:
Field 1 – weight
Example:

```
0.7837836E-01
0.4900770E-01
0.7538282
1.0
```

Each weight corresponds to each SNP marker defined in the map file.
Weights can be extracted from the output of **POSTGSF90**.

OPTION maxsnp x

Sets the maximum length of string to read marker data from a file. It is only necessary if greater than default (400,000).

*Quality Control (QC) for **G***

By default the following QC can be run:

MAF
Call rate (SNPs and animals)
Monomorphic
Parent-progeny conflicts (SNPs and animals)

Parameters can be modified with the following options:

OPTION minfreq x

Ignores all SNP with MAF < x (default value = 0.05).

OPTION callrate x

Ignores SNP with call rates < x (number of calls / number of individuals with genotypes). The default value is 0.90.

OPTION callrateAnim x

Ignores genotypes with call rates < x (number of calls / number of SNPs). Default value is 0.90.

OPTION monomorphic x

Ignores monomorphic SNPs. Optional parameter x can be used to enable (1) or disable (0) the check. The default value is 1.

OPTION hwe x

Checks departure of heterozygous from Hardy-Weinberg equilibrium. By default, this QC is not run. The optional parameter x can be the maximum difference between observed and expected frequency (default value = 0.15) as used in Wiggans et al. (2009) in JDS.

OPTION high_correlation x y

Checks for highly correlated SNP. By default, this QC is not run. The optional parameter x can be the maximum difference in allele frequency to check a pair of loci. If no value is set, 0.025 is used. Decrease this value to speed up the calculation. A pair of loci is considered highly correlated if all genotypes are the same (0-0, 1-1, 2-2) or the opposite (0-2, 1-1, 2-0) (Wiggans et al., 2009. JDS). The optional parameter y can be used to set a threshold to check the number of identical samples out of the number of genotypes (default values: x=0.025, y=0.995).

OPTION verify_parentage x

Verifies parent-progeny Mendelian conflicts and writes a report into the "Gen_conflicts" file. The optional parameter x can be
0: no action
1: only detects
2: detects and searches for an alternate parent; no change to any file. This option is implemented in the **SeekParentF90** program.
3: detects and eliminates progenies with conflicts (default).

OPTION exclusion_threshold x
Sets the number of parent-progeny exclusions as percentage. All SNP are used to determine wrong relationships (default value = 2).

OPTION exclusion_threshold_snp x
Sets the number of parent-progeny exclusions for each locus as percentage. A pair of genotyped animals is evaluated to exclude SNP from the analysis (default value = 10).

OPTION number_parent_progeny_evaluations x
Sets the number of minimum pair of parent-progeny evaluations to exclude SNP due to parent-progeny exclusion (default value = 100).

OPTION outparent_progeny x
Creates a full log file "Gen_conflicts_all" with all pairs of parent-progeny tested for Mendelian conflicts.

OPTION excludeCHR n1 n2 n3 …
Excludes all SNP from chromosomes n1, n2, n3, … A map file must be provided (see **OPTION map_file**).

OPTION includeCHR n1 n2 n3 …
Include all SNP from chromosomes n1, n2, n3, … A map file must be provided (see **OPTION map_file**).

OPTION excludeSample n1 n2 n3 …
Exclude genotype samples n1, n2, n3, … Where n1, n2, n3, … are row number of individuals in the genotype file.

OPTION sex_chr n
Chromosomes with a number greater or equal to n are not considered as autosomes. If this option is used, sex chromosomes will not be used for checking parent-progeny, Mendelian conflicts, and HWE. A map file must be provided (see **OPTION map_file**).

OPTION threshold_duplicate_samples x
Sets the threshold to issue warning for possible duplicate samples if G(i,j) / sqrt(G(i,i) * G(j,j)) > x (default value = 0.9).

OPTION high_threshold_diagonal_g x

Checks for extremely large diagonals in the genomic relationship matrix. If optional x is present, the threshold will be set (default value = 1.6).

OPTION low_threshold_diagonal_g x

Checks for extremely low diagonals in the genomic relationship matrix. If optional x is present, the threshold will be set (default value = 0.7).

OPTION plotpca print/noprint

Plots the first two principal components to look for stratification in the population. With noprint the program will save the first two principal components of **G** without showing the PCA plot on the screen; otherwise, (print) it will print on the screen.

OPTION extra_info_pca <file> col

Reads the column col to plot with different colors for different classes from the file. The file should contain at least one variable with different classes for each genotyped individual, and the order should match the order of the genotype file. Variables could be alphanumeric and separated by one or more spaces.

OPTION calculate_LD

Calculates LD as the squared correlation of allele counts for two SNP.
Results are stored in “ld_results”, columns: snp_i, chr_i, pos_i, freq_i, snp_j, chr_j, pos_j,freq_j, dist_ij, Rsq_ij

OPTION LD_by_chr

Calculates LD within chromosome.

OPTION LD_by_pos x

Calculates LD within chromosome and windows of SNP based on position. Optional parameter x defines with windows size in Bp, default value 200000

OPTION filter_by_LD x

Filters SNP with Rsq > threshold. Optional parameter x define the threshold. default value 0.8

OPTION thr_output_LD x

Threshold to print out Rsq between pair of SNP Optional parameter x define the threshold. default value 0.1

OPTION saveCleanSNPs *

Saves clean genotype data with excluded SNP and animals based on the OPTIONS specified.
*_clean files are created:

- gt_clean
- gt_clean_XrefID

*_removed files are created:

- gt_SNPs_removed
- gt_Animals_removed

where “gt” is the genotype file.

OPTION no_quality_control

Turns off all quality control. It speeds up computations when the QC was previously performed.

OPTION outcallrate

Prints all call rate information for SNP and individuals. The files “callrate” for SNP and “callrate_a” for individuals are created.

OPTION h2_gene_content

This allows to check if the heritability of gene content is equal to 1.00 as described in Forneris et al. (2015). Markers whose estimated heritability is < 0.98 and significant p-value for the LRT ($p < 0.01$) will be removed, and a file “h2_gc_test” will be created with heritability and status of each marker. The test is useful for homogenous populations (breeds) but theory does not hold for crossbred animals. This test uses explicitly inv($\mathbf{A}_{22}$) so it is not suitable for very large populations.

Quality Control for Off-diagonal of A_{22} and $\mathbf{G}$

OPTION thrWarnCorAG x

Sets the threshold to issue warning if correlation between $\mathbf{A}_{22}$ and $\mathbf{G}$ < x (default value = 0.5).

OPTION thrStopCorAG x

Sets the threshold to stop the analysis if correlation between $\mathbf{A}_{22}$ and $\mathbf{G}$ < x (default value = 0.3).

OPTION thrCorAG x

Sets the threshold to calculate correlation between $\mathbf{A}_{22}$ and $\mathbf{G}$ for only $\mathbf{A}_{22} \geq$ x (default value = 0.02).

*Options for **H***

The options includes different weights to create $\mathbf{G}^{-1} - \mathbf{A}_{22}^{-1}$ as

$$\tau(\alpha\mathbf{G} + \beta\mathbf{A}_{22} + \gamma\mathbf{I} + \delta\mathbf{1}\mathbf{1}')^{-1} - \omega\mathbf{A}_{22}^{-1}$$

where the parameters are to scale the genomic information to be compatible with the pedigree information, to make matrices invertible in the presence of clones, and to control bias. The default values are: tau (τ) = 1, alpha (α) = 0.95, beta (β) = 0.05, gamma (γ) = 0, delta (δ) = 0, and omega (ω) = 1. Options to change these defaults are specified with:

OPTION TauOmega tau omega

OPTION AlphaBeta alpha beta
OPTION GammaDelta gamma delta

Hint: OPTION TauOmega was needed when inbreeding was not considered for $\mathbf{A}^{-1}$. Because inbreeding is now considered for $\mathbf{A}^{-1}$, we recommend not using this option anymore.

OPTION tunedG x
Scales **G** based on $\mathbf{A}_{22}$. The variable x can be:
0: no scaling
1: mean(diag(**G**))=1 and mean(offdiag(**G**))=0
2: mean(diag(**G**))=mean(diag($\mathbf{A}_{22}$)) and mean(offdiag(**G**))=mean(offdiag($\mathbf{A}_{22}$)) (default)
3: mean(**G**)=mean($\mathbf{A}_{22}$)
4: rescale **G** using the first adjustment as in Powell et al. (2010) or Vitezica et al. (2011).

Options to extract the diagonal of H

The diagonal of **H** contains an improved estimator of inbreeding: $\mathrm{F_H} = diag(\mathbf{H}) - 1$. For genotyped animals, $\mathrm{F_H} = \mathrm{F_G}$ (because $diag(\mathbf{H}) = diag(\mathbf{G})$). For non-genotyped animals $diag(\mathbf{H})$ also includes pedigree-based estimates of genomic inbreeding. To extract $diag(\mathbf{H})$ the following options can be used:

OPTION saveDiagH
It outputs the diagonal of **H** with renumbered id's.

OPTION saveDiagHOrig
It outputs the diagonal of **H** with original and renumbered id's.

The user can choose one of two equivalent methods:

OPTION methodDiagH 1
OPTION methodDiagH 2

OPTION methodDiagH 1 does a sparse inversion of $\mathbf{H}^{-1}$ (default) which is very fast for medium size pedigrees. **OPTION methodDiagH 2** uses the third method described in Legarra et al. (2019) to compute $\mathbf{M} = \mathbf{A}_{22}^{-1}(\mathbf{G} - \mathbf{A}_{22})\mathbf{A}_{22}^{-1}$. This method is **recommended** for large pedigrees. The output depends on the used method. Method 1 shows only individual id and $diag(\mathbf{H})$ and method 2 outputs individual id and the values of $diag(\mathbf{H})$ and $diag(\mathbf{A})$, and the difference $diag(\mathbf{H}) - diag(\mathbf{A})$.

General control of PREGSF90

OPTION num_threads_pregs n
Specifies number of threads to be used with MKL-OpenMP for creation and inversion of matrices.

OPTION num_theads_iod n
Specifies number of threads to be used with MKL-OpenMP in BLUP90IOD for matrix-vector multiplications in the PCG algorithm.

OPTION graphics s
Allows to generate plots with GNUPLOT. If optional parameter s is present, set the time in seconds to show the plot. Avoid using in batch programs!!!

OPTION msg x
Sets the level of verbose; 0 minimal; 1 prints lots of diagnostics on the screen.

Save and Read options:

OPTION saveAscii
Saves intermediate matrices (GimA22i, G, Gi, etc.) into files as ASCII (default = binary).

OPTION saveHinv
Saves $\mathbf{H}^{-1}$ in "Hinv.txt" (format: i, j, val; where i, j, are the index level for the additive genetic effect).

OPTION saveAinv
Saves $\mathbf{A}^{-1}$ in "Ainv.txt" (format: i, j, val; where i, j, are the index level for the additive genetic effect).

The following options use the information of the original ID (alphanumeric) stored in the 10th column of the "renaddxx.ped" file created by **RENUMF90**.

OPTION saveHinvOrig
Saves $\mathbf{H}^{-1}$ with original IDs

OPTION saveAinvOrig
Saves $\mathbf{A}^{-1}$ with original IDs

OPTION saveDiagGOrig
Saves diagonal of **G** in "DiagGOrig.txt" (format: id, val; where id is the original ID).

OPTION saveGOrig
Saves **G** in "G_Orig.txt" (format: id_i, id_j, val; where id_i and id_j are the original IDs).

OPTION saveA22Orig
Saves $\mathbf{A}_{22}$ in "A22_Orig.txt" (format: id_i, id_j, val; where id_i and id_j are the original IDs).

OPTION readOrigId
Reads information from "renaddxx.ped" file, original ID, and possibly year of birth for its use in parent-

progeny conflict. Only needed if none of the previous “save*Orig” is present.

OPTION saveGimA22iRen

Saves GimA22i matrix in GimA22i_Ren.txt (format: id_i, id_j, val; where id_i and id_j are the IDs as stored in the first column of renaddXX.ped).

OPTION saveGimA22iOrig

Saves GimA22i matrix in GimA22i_Orig.txt (format: id_i, id_j, val; where id_i and id_j are the IDs as stored in the original pedigree file and in column 10 of renaddXX.ped).

OPTION savePLINK

Saves genotypes in PLINK format files: toPLINK.ped and toPLINK.map.

OPTION no_full_binary

Saves the elements of half-matrix instead of the full matrix. It is useful to keep the compatibility with the older versions of preGSf90. The newer versions save the matrix in a more efficient way, where reading the information from the binary file is not trivial (i.e., not as *i, j, val* anymore).

The following options are used to save and read intermediate files:

OPTION readGimA22i <file>

Reads $\mathbf{G}^{-1} - \mathbf{A}_{22}^{-1}$ from a file. This option can be used in the application programs (BLUPF90, REMLF90, etc.) to use the information already stored in the GimA22i file (default filename). In general, methods used to create and invert matrices in such programs do not use an optimized version. For a large number of genotyped animals, run first PREGSf90 and read stored matrices in the application programs.

The optional file can be used to specify a different file name (other than GimA22i) or a path. For example,

OPTION readGimA22i ../../pregsrun/GimA22i

Other intermediate matrices files can be stored for inspection or for use in BLUPF90 programs as **user_file** type of random effect. See **tricks** and **REMLF90** for details.

Individual output options:

OPTION saveA22

Saves $\mathbf{A}_{22}$ in “A22”.

OPTION saveA22Inverse

Saves $\mathbf{A}_{22}^{-1}$ in “A22i”.

OPTION saveA22InverseOrig

Saves $\mathbf{A}_{22}^{-1}$ with original id’s (format id_i, id_j, and value).

OPTION saveG all

If optional all is present, all intermediate matrices for **G** will be saved in separate files. If omitting all, only the final **G** will be saved in "G".

OPTION saveGInverse

Saves $\mathbf{G}^{-1}$ in "Gi".

OPTION saveGInverseOrig

Saves $\mathbf{G}^{-1}$ with original id's (format id_i,id_j, and value).

OPTION saveGmA22

Saves $\mathbf{G} - \mathbf{A}_{22}$ in "GmA22". This option is obsolete.

OPTION readG <file>

Reads $\mathbf{G}$ from "G" by default, or from a user-supplied **file**.

OPTION readGInverse <file>

Reads $\mathbf{G}^{-1}$ from "Gi" by default, or from a user-supplied **file**. See the caution below.

OPTION readA22 <file>

Reads $\mathbf{A}_{22}$ from "A22" by default, or from a user-supplied **file**.

OPTION readA22Inverse <file>

Reads $\mathbf{A}_{22}^{-1}$ from "A22i" by default, or from a user-supplied **file**. See the caution below.

OPTION readGmA22 <file>

Reads $\mathbf{G} - \mathbf{A}_{22}$ from "GmA22" by default, or from user-supplied **file**. This option is obsolete.

Caution:

With the options **readGInverse** and **readA22Inverse** combined **OPTION TauOmega tau omega**, the program applies τ to the loaded $\mathbf{G}^{-1}$ and ω to the loaded $\mathbf{A}_{22}^{-1}$ regardless of whether the matrices have been already scaled with τ or ω. In other words, the loaded matrix could be scaled twice if the user used τ or ω both in saving and reading the matrix. Be careful to use the scaling factors combined with the input/output options.

Hint: OPTION TauOmega was needed when inbreeding was not considered for $\mathbf{A}^{-1}$. Because inbreeding is now considered for $\mathbf{A}^{-1}$, we recommend not using this option anymore.

POSTGSF90

Basic options

The program calculates SNP effects using the ssGBLUP framework (**Wang et al., 2012**). The program needs **OPTION map_file** to assign SNP to their location for Manhattan plots, so chromosomes are visualized in different colors. The following options for **POSTGSF90** (ssGWAS) are available:

OPTION Manhattan_plot
Plots the Manhattan plot (SNP effects) for each trait and correlated effects using **GNUPLOT**.

OPTION Manhattan_plot_R
Plots the Manhattan plot (SNP effects) for each trait and correlated effects using R. TIF images are created: manplot_Sft1e2.tif (note: t1e2 corresponds to trait 1, effect 2).

OPTION Manhattan_plot_R_format format
Controls the format type to create images in R. The format values accepted are: pdf (default), png, or tif.

OPTION plotsnp n
Controls the values of SNP effects to use in Manhattan plots
1: plots regular SNP effects: abs(val)
2: plots standardized SNP effects: abs(val/sd) (default)

OPTION SNP_moving_average n
Solutions for SNP effects will be by moving average of n adjacent SNPs.

OPTION windows_variance n
Calculates the variance explained by n adjacent SNPs.

Hint: When this option is used, the sum of variance explained by n adjacent SNPs (column 8 of snp_sol or column 3 of chrsnpvar) is not 100%. This is because moving variance is used. If windows size is 20, the proportion of variance assigned to SNP 1 is calculated from SNP 1 to 20, for SNP 2 it goes from 2 to 21, for SNP 3 it goes from 3 to 22, and so forth. A file called windows_variance has variance that sums to 100% in column 9.

OPTION windows_variance_mbp n
Calculates the variance explained by n Mb window of adjacent SNPs.

OPTION windows_variance_type n
Sets windows type for variances calculations
1: moving windows
2: exclusive windows

OPTION which_weight x

Generates a weight variable to construct a weighted genomic relationship matrix $\mathbf{G} = \mathbf{ZDZ}'$

1: w = y^2 * (2(p(1-p)))

2: w = y^2

3: experimental with the degree of brief

4: w = C**(abs(y_i)/sqrt(var(**y**))-2) from VanRaden et al. (2009)

nonlinearA: same as 4

where y is the SNP solution, with scaled weight = w * nSnp/sum(w); and C is 1.125 by default (enable to change it using the second argument of the option line (**OPTION which_weight nonlinearA value**), e.g., OPTION which_weight nonlinearA 1.2

OPTION solutions_postGS x

Sets the file name for the solutions file (default = solutions).

OPTION postgs_trt_eff x1 x2

Computes postGS solutions (SNP solutions, variance explained, etc.) for only trait: x1 and effect: x2

OPTION snp_p_value

Computes p-values for GWAS from elements of the inverse of the Mixed Model Equations previously obtained from blupf90. This requires quite a lot of memory and time. See **Aguilar et al. (2019)** for more details.

OPTION snp_var

Creates a file with prediction error covariance (PEC) for SNP to be used in **PREDF90** to compute reliability for indirect predictions. This option works when **OPTION snp_p_value** is used in BLUPF90+.

*Output files for **POSTGSF90**:*

"snp_sol" contains solutions of SNP and weights

1: trait

2: effect

3: SNP

4: Chromosome

5: Position

6: SNP solution

7: weight (can be used as the weight to calculate the weighted **G** matrix)

8: variance explained by n adjacent SNP (if **OPTION windows_variance** is used)

9: variance of the SNP solution (used to compute the p-value if **OPTION snp_p_value** is used)

"chrsnp" contains data to create the plot by GNUPLOT

1: trait

2: effect
3: values of SNP effects to use in Manhattan plots, i.e., (abs(SNP_i)/var(SNP))
4: SNP
5: Chromosome
6: Position

“chrsnp_pval” contains data to create the plot by GNUPLOT
1: trait
2: effect
3: -log10(p-value)
4: SNP
5: Chromosome
6: Position

“chrsnpvar” contains data to create plot by GNUPLOT
1: trait
2: effect
3: variance explained by n adjacent SNP
4: SNP
5: Chromosome
6: Position

“windows_segment” contains information of windows segments used to get variance explained
1: label
2: window size (number of SNP)
3: Start SNP number for the window
4: End SNP number for the window
5: identification of window: (ChrNumber)'_'(startPositionMBP)
6: Start (ChrNumber)'_'(Position) for the window
7: End (ChrNumber)'_'(Position) for the window

“windows_variance” contains variance explained for the biggest non-overlapping windows segments
1: trait
2: effect
3: Start SNP number or SNP name for the window
4: End SNP number or SNP name for the window
5: window size (number of SNP)
6: Start (ChrNumber)'_'(Position) for the window
7: End (ChrNumber)'_'(Position) for the window
8: identification of window: (ChrNumber)'_'(startPositionMBP)
9: variance explained by n adjacents SNP

“snp_pred” contains allele frequencies + SNP effects

Graphic control files:

Several files are created to generate graphics using either GNUPLOT or R.

File names rules
“Sft1e2.R”. The first letter indicates “S” for solutions of SNP, “V” for variance explained, and “P” for p-values.
“t1e2” indicates that the file is for the trait 1 and the effect 2.

Filename extension

- xxx.gnuplot => GNUPLOT
- xxx.R => R programs
- xxx.pdf => image
- xxx.png => image
- xxx.tif => image

Misc. options:

OPTION num_threads_pregs n
Specify the number of threads n to be used with MKL-OpenMP for creating and inverting matrices

OPTION num_threads_iod n
Specify the number of threads n to be used with MKL-OpenMP in ''BLUP90IOD'' program
for matrix-vector multiplications in the PCG algorithm

OPTION graphics s
Allows to generate plots with ''GNUPLOT'' program.
If present optional parameter s, set the time in seconds to show the plot.
Avoid using in batch programs!

OPTION msg x
x set level of verbose; 0 minimal; 1 gives more diagnostic information

PREDF90

Predicts direct genomic value (DGV) for young animals based on only genotypes i.e. $\hat{\mathbf{u}} = \mathbf{Z}\hat{\mathbf{a}}$, where $\hat{\mathbf{u}}$ is DGV and $\hat{\mathbf{a}}$ is the SNP effects. The prediction is based on SNP effects obtained from **POSTGSF90**. For young animals that were not included in the previous analysis, DGV can be calculated using the “snp_pred” file from **POSTGSF90**. PREDF90 requires some output files from POSTGSF90 and a genotype file for the animals to be predicted. It does not accept a parameter file but takes command-line options.

PREDF90 does not accept a parameter file but takes command-line options.

--snpfile name
Provides the SNP file for animals to be indirectly predicted. PREDF90 will ask for the SNP file name if this command is not present. The SNP file has the same format as for PREGSF90.

--acc
Computes reliability for indirect predictions. It requires OPTION snp_p_value in BLUPF90+ and OPTION snp_var in POSTGSf90. It reads “snp_var”, a file with SNP PEC created by POSTGSF90.

--acc_type
Select 1.0 for dairy cattle (Reliability) or 0.5 for beef cattle (BIF accuracy) (default 1.0).

--use_diagG_acc
Uses inbreeding (F) from **G** in the denominator of the reliability formula: reliability = 1-PEV/(σ_u^2(1+F)).

--use_mu_hat
Adds the base ($\hat{\mu}$) for DGV so the values are comparable to GEBV. See **Legarra et al. (2021)** and **Lourenco et al. (2018)** for more details.

--use_var_mu_hat
Considers the variance of $\hat{\mu}$ when calculating the reliability of DGV and is automatically turned on if --use_mu_hat and --acc are present.

--help
Shows the main options.

Usage:

predf90 --snpfile new_genotypes.txt --use_mu_hat --acc --use_diagG_acc

With these commands, predf90 will compute indirect predictions for the animals in new_genotypes.txt, including $\hat{\mu}$ (i.e., DGV = $\hat{\mu} + \mathbf{Z\hat{a}}$), computing reliabilities adjusted for inbreeding in **G**.

Input files:

This program automatically detects and read the following files:

“snp_pred”

- information about the random effect (number of traits + correlated effects)
- gene frequencies
- solutions of SNP effects

SNP_file_for_animals_to_predict
SNP file for animals to have DGV predicted. This file has the same format as used in PREGSF90 and POSTGSF90.

Output file:

"SNP_predictions"
- ID, call rate, DGV, reliability (if --acc is present)

Constant parameters that cannot be changed by the users**:**

1. alpha - fraction of **G** used (default=0.95); affects scale of prediction
2. callrate - to be used later for discarding genotypes with poor quality (default=0.7)

PREDICTF90

This program computes adjusted phenotypes. It reads the blupf90 parameter file, the solutions file, and the data file. It needs **OPTION include_effects x1 x2 x3** followed by the effects (**x1 x2 x3**) that should NOT be used to adjust phenotypes (y). It computes:

y_star = y adjusted by the effects not mentioned in **OPTION include_effects x1 x2 x3** (i.e., the included effects)
y_hat = sum of estimates of the included effects
residual = y - included effects (not a true residual)

Example: y = herd + age + animal + e
If the parameter file has OPTION include_effects 3.

y_star = y - herd_hat - age_hat *(y – effects to be adjusted for)*
y_hat = animal_hat *(effect to keep)*

Which makes cor(y_hat,y_star) = cor(ebv, adjusted y), in this example, which is a measure of accuracy. However, this is done based on one dataset. Real validations are done between a benchmark computed with a complete dataset (e.g., adjusted phenotypes here) and a prediction using a reduced dataset (e.g., the ebv here).

It outputs the correlation between y_hat and y_star, for instance cor(ystar,yhat)=cor(u+e, uhat) and outputs these columns into a file, together with animal id (if there is animal in the model) or record number (if not).

In addition, if animal effect is in the model, it produces a file with ebvs from the solutions file.

Output file:

"yhat_residual"
The main file is yhat_residual, which has corrected phenotypes and predicted residuals. The number of columns in this file depend on the number of traits (N).

Column 1: Animal ID (renumbered i.e., same as the 1st column in renaddxx.ped)
Column 2 to N+1: "y_star" explained above
Column N+2 to 2N+1: "y_hat" explained above
Column 2N+2 to 3N+1: "residual" explained above

Demonstration for genomic analysis

Data were simulated by D. Lourenco and the files are available here:
https://github.com/danielall/Data_ssGBLUP

Preparation with RENUMF90

"renum.par" for **RENUMF90**

```
# Parameter file for renumf90
# Data file = phenotypes.txt
#  1     2     3     4   5
#  animal, sex ,phenotype, TBV,  generation
# Pedigree file = pedigree.txt
#   1      2     3
#  animal   sire   dam
# SNP file = genotypes.txt
# SNP 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  #animal
RANDOM
animal
FILE
pedigree.txt
SNP_FILE
genotypes.txt
(CO)VARIANCES
0.40
OPTION map_file gen_map.txt
```

Run RENUMF90

```
RENUMF90 version 1.157 with zlib
 renum.par
...    ...    ...
 Inbreeding statistics:
 the maximum inbreeding coefficient    =  0.3125
 average inbreeding for inbred animals =  0.0621   n = 1292
                      for all animals =  0.0067   n = 12010

 Number of animals with records                  =        10000
 Number of animals with genotypes                =         2024
 Number of animals with records or genotypes     =        10000
 Number of animals with genotypes and no records =            0
 Number of parents without records or genotypes  =         2010
 Total number of animals                         =        12010

 Wrote cross reference IDs for SNP file "genotypes.txt_XrefID"

 Wrote parameter file "renf90.par"
 Wrote renumbered data "renf90.dat" 10000 records
 Wrote field information "renf90.fields" for 3 fields in data
```

“renf90.par” from RENUMF90

```
# 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
```

Analysis with BLUPF90

Run BLUPF90

```
     BLUPF90 ver. 1.71

 Parameter file:             renf90.par
 Data file:                  renf90.dat
 Number of Traits             1
 Number of Effects            2
 Position of Observations      1
 Position of Weights           0
 Value of Missing Trait/Observation           0
 name of parameter file?renf90.par
  ... ... ...
 *---------------------------------------------------------------*
 *                 Genomic Library: Version 1.308                *
 *                                                               *
 *            Optimized OpenMP Version -  4 threads              *
 *                                                               *
 *  Modified relationship matrix (H) created for effect:   2     *
 *---------------------------------------------------------------*

 Read 12010 animals from pedigree file: "renadd02.ped"
 Number of Genotyped Animals: 2024
  ... ... ...
 round =    55  convergence =  0.1126E-11
 round =    56  convergence =  0.5045E-12
   56 iterations,   convergence criterion= 0.5045E-12
 solutions stored in file: "solutions"
```

Analysis with POSTGSF90

Run POSTGSF90

```
 name of parameter file?renf90.par

     postGSf90 ver. 1.77
... ... ...
 Solutions read from file: "solutions"
 Solutions for SNPs in file: "snp_sol"
 Files for pedictions by SNP effects in file: "snp_pred"
```

Indirect Predictions with PREDF90

Run PREDF90

```
predf90 1.13
Predicts EBVs from genotypes based on results from single-step evaluation
... ... ...
Number of SNP:     4500
Number of traits:   1
number of correlated traits:   1
... ... ...
MU_hat to adjust Za
   Trait: 1
   Correlated effect: 1
   mu_hat:     0.1443
... ... ...
        3000  SNP
The genotype file contains   45000 SNP starting from position  14

 Firts 10 genotypes: Id, EBV
 UGA42014       0.4649608
 UGA42019       0.6343889
 UGA42029      -0.1096066
 UGA42039       0.9360114
 UGA42047       0.6454658
 UGA42051       0.5041275
 UGA42052       1.7737031E-02
 UGA42056       0.9935431
 UGA42057       0.2609830

 Processed  2024 genotypes
 Average calling rate: 1.00


$head -5 SNP_predictions
UGA42014       1.00       0.46496075
UGA42019       1.00       0.63438886
UGA42029       1.00      -0.10960658
UGA42039       1.00       0.93601137
UGA42047       1.00       0.64546579
```

Computing adjusted phenotypes with PREDICTF90

Run PREDICTF90

This program is used to calculate adjusted y, ŷ, and residuals using the same parameter file and "solutions" as BLUPF90

Output files:
"yhat_residual"
Format: record #, adjusted y, ŷ, residual
"bvs.dat"
The same format as "solutions" including (G)EBV.

```
# BLUPF90 parameter file created by RENF90 and extended to work with PREDICTF90
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
OPTION include_effects 2   #phenotypes will be adjusted for all effects but effect number 2 (animal)
```

Run PREDICTF90

name of parameter file?
pred.par

```
 *** include effects to predict Yhat n, effects           1         2

    PREDICTF90 ver. 1.6
. . .   . . .   . . .
Animal Effect:           2
  y(s), yhat(s), residual(s) in written in "yhat_residual" file
      10000 records read
 Trait:           1       10000
   mean Y        8.662515402103672E-002  var Y         0.934465837702133
   mean Yhat      8.662514367382973E-002  var Yhat      0.181142370417667
   cov (Y,Yhat)   0.344475853966058       corr (Y,Yhat)  0.837272925060839
 wrote bvs for animals in data in file "bvs.dat"
```

Hints:

1) The effect that goes into OPTION include_effects (e.g., OPTION include_effects 2) is included in the Yhat. In this small example with 1 trait, the format of yhat_residual is: Animal_id, Y, Yhat, residual
Where: Y = Phenotype – μ

Yhat = EBV (or animal effect)
Residual = Phenotype - EBV

2) When 2 traits are used in the model, the format of yhat_residual is:
Animal_id, Y1, Y2, Yhat1, Yhat2, residual1, residual2

3) corr (Y,Yhat) should not be used as a measure of predictivity because it uses adjusted phenotypes and EBVs from the same dataset. Usually, predictivity requires phenotypes adjusted for fixed effects in the complete data (benchmark) and (G)EBVs calculated from the reduced data (without records for validation animals). The regular predictivity measure is: corr[Y_from_PREDICTf90, (G)EBV_reduced]

For this small example with 1 trait, a general Linux bash code is:

```
$awk '{print $1,$2}' ebv_complete/yhat_residual | sort +0 -1 > Y
$awk '{if ($2==2) print $3,$4}' ebv_reduced/solutions | sort +0 -1 > ebv.temp
$awk '{if ($2==2) print $3,$4}' gebv_reduced/solutions | sort +0 -1 > gebv.temp
$join -1 +1 -2 +1 Y validation_animals > file1.temp
$join -1 +1 -2 +1 file1.temp ebv.temp > file2.temp
$join -1 +1 -2 +1 file2.temp gebv.temp > Y_ebv_gebv
```

#obs: `validation_animals` is a file that contains sorted ids for validation animals

An R code to calculate correlations is:

```
pred <- read.table("Y_ebv_gebv",header=F)
ebv_predictivity <- cor(pred[,2],pred[,3]); ebv_predictivity
gebv_predictivity <- cor(pred[,2],pred[,4]); gebv_predictivity
```

Examples of parameter files

Sire model without A matrix

DATAFILE
test.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 cross
2 3 cross
RANDOM_RESIDUAL VALUES

```
10
RANDOM_GROUP
2
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1
```

Sire model with A matrix

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 cross
2 3 cross
RANDOM_RESIDUAL VALUES
10
RANDOM_GROUP
2
RANDOM_TYPE
add_sire
FILE
sire.ped
(CO)VARIANCES
1
```

Two-trait sire model

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
3 4
WEIGHT(S)
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 2 cross
2 2 3 cross
RANDOM_RESIDUAL VALUES
```

10 1
1 5
RANDOM_GROUP
2
RANDOM_TYPE
add_sire
FILE
sire.ped
(CO)VARIANCES
1 0.1
0.1 1

Animal model

DATAFILE
test.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 cross
5 10 cross
RANDOM_RESIDUAL VALUES
10
RANDOM_GROUP
2
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1

Multiple trait animal model
# Example 1: two-trait animal model

DATAFILE
test.dat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
3 4
WEIGHT(S)

```
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 2 cross
5 5 10 cross
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
2
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1
0.1 1
```

# Example 2: different model for each trait

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
3
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 2 cross
5 5 10 cross
6 7 30 cross
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
2
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1
0.1 1
RANDOM_GROUP
3
RANDOM_TYPE
diagonal
FILE
```

```
(CO)VARIANCES
1 0
0 1
```

Animal model with UPG

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 2 cross
5 5 13 cross
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
2
RANDOM_TYPE
add_an_upg
FILE
animal.ped
(CO)VARIANCES
1 0.1
0.1 1
```

Animal model with inbreeding

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 2 cross
5 5 13 cross
RANDOM_RESIDUAL VALUES
10 1
```

```
1 5
RANDOM_GROUP
2
RANDOM_TYPE
add_an_upginb
FILE
animal.ped
(CO)VARIANCES
1 0.1
0.1 1
```

Repeatability model – single trait

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
3
OBSERVATION(S)
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 cross
5 5 cross
5 5 cross
RANDOM_RESIDUAL VALUES
10
RANDOM_GROUP
2
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1
RANDOM_GROUP
3
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1
```

Repeatability model – two traits

```
DATAFILE
test.dat
```

```
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
3
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 2 cross
5 5 5 cross
5 5 5 cross
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
2
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1
0.1 1
RANDOM_GROUP
3
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0.1
0.1 1
```

Maternal effect model

```
DATAFILE
maternal.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
4
OBSERVATION(S)
4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
3 946 cross
1 22473 cross
2 22473 cross
```

```
2 22473 cross
RANDOM_RESIDUAL VALUES
1050
RANDOM_GROUP
2 3
RANDOM_TYPE
add_animal
FILE
maternal.ped
(CO)VARIANCES
450 -100
-100 340
RANDOM_GROUP
4
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
370
```

# For (THR)GIBBSxF90
# Example 1 – declaring the random, diagonal effect separately for effects 4 and 5.

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
5
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 0 2 cross
0 2 2 cross
5 5 10 cross
6 0 30 cross
0 7 20 cross
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
3
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
```

```
1 0.1
0.1 1
RANDOM_GROUP
4
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0
0 0
RANDOM_GROUP
5
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
0 0
0 1
```

# Example 2 – joint declaration for the random, diagonal effects 4 and 5.

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
5
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 0 2 cross
0 2 2 cross
5 5 10 cross
6 0 30 cross
0 7 30 cross
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
3
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1
```

```
0.1 1
RANDOM_GROUP
4 5
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 1
```

# Dominance model

```
DATAFILE
dom.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
4
OBSERVATION(S)
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 cross
4 1 cov
2 30001 cross
5 10412 cross
RANDOM_RESIDUAL VALUES
100
RANDOM_GROUP
3
RANDOM_TYPE
add_an_upginb
FILE
add.ped
(CO)VARIANCES
10
RANDOM_GROUP
4
RANDOM_TYPE
par_dom
FILE
dom.ped
(CO)VARIANCES
2
```

Random regression model

# Single trait

```
DATAFILE
data_score
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
10
OBSERVATION(S)
9
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
 1    788 cross
 2     32 cross
 5      1 cov
 6      1 cov
 3  15097 cross
 5  15097 cov  3
 6  15097 cov  3
 3  81883 cross
 5  81883 cov  3
 6  81883 cov  3
RANDOM_RESIDUAL VALUES
 100
RANDOM_GROUP
5 6 7
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
 100  1    1
 1    10   1
 1    1    10
RANDOM_GROUP
8 9 10
RANDOM_TYPE
add_an_upg
FILE
ped_score
(CO)VARIANCES
 100  1    1
 1    10   1
 1    1    10
```

# Two traits

```
DATAFILE
test.dat1
NUMBER_OF_TRAITS
```

```
2
NUMBER_OF_EFFECTS
9
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 2 cross
6 6 1 cov
7 7 1 cov
2 2 5 cross
6 6 5 cov 2 2
7 7 5 cov 2 2
2 2 10 cross
6 6 10 cov 2 2
7 7 10 cov 2 2
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
4 5 6
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0.1 0.1 0.1 0.1 0.1
0.1 1 0.1 0.1 0.1 0.1
0.1 0.1 1 0.1 0.1 0.1
0.1 0.1 0.1 1 0.1 0.1
0.1 0.1 0.1 0.1 1 0.1
0.1 0.1 0.1 0.1 0.1 1
RANDOM_GROUP
7 8 9
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1 0.1 0.1 0.1 0.1
0.1 1 0.1 0.1 0.1 0.1
0.1 0.1 1 0.1 0.1 0.1
0.1 0.1 0.1 1 0.1 0.1
0.1 0.1 0.1 0.1 1 0.1
0.1 0.1 0.1 0.1 0.1 1
```

# Example 3

```
DATAFILE
```

```
test.dat2
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
10
OBSERVATION(S)
3 4
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 1 2 cross
6 6 1 cov
7 7 1 cov
8 8 1 cov
6 6 5 cov 2 2
7 7 5 cov 2 2
8 8 5 cov 2 2
6 6 10 cov 2 2
7 7 10 cov 2 2
8 8 10 cov 2 2
RANDOM_RESIDUAL VALUES
10 1
1 5
RANDOM_GROUP
5 6 7
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0.1 0.1 0.1 0.1 0.1
0.1 1 0.1 0.1 0.1 0.1
0.1 0.1 1 0.1 0.1 0.1
0.1 0.1 0.1 1 0.1 0.1
0.1 0.1 0.1 0.1 1 0.1
0.1 0.1 0.1 0.1 0.1 1
RANDOM_GROUP
8 9 10
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1 0.1 0.1 0.1 0.1
0.1 1 0.1 0.1 0.1 0.1
0.1 0.1 1 0.1 0.1 0.1
0.1 0.1 0.1 1 0.1 0.1
0.1 0.1 0.1 0.1 1 0.1
0.1 0.1 0.1 0.1 0.1 1
```

Random regression model with heterogeneous residual variances

### using airemlf90

# Example 1: with intercept

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
9
OBSERVATION(S)
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 cross
6 1 cov
7 1 cov
5 5 cross
6 5 cov 5
7 5 cov 5
5 10 cross
6 10 cov 5
7 10 cov 5
RANDOM_RESIDUAL VALUES
10
RANDOM_GROUP
4 5 6
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0.1 0.1
0.1 1 0.1
0.1 0.1 1
RANDOM_GROUP
7 8 9
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1 0.1
0.1 1 0.1
0.1 0.1 1
OPTION hetres_pos 6 7
OPTION hetres_pol 4.0 1.0 0.1
```

# Example 2: with no intercept

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
7
OBSERVATION(S)
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 cross
6 1 cov
7 1 cov
6 5 cov 5
7 5 cov 5
6 10 cov 5
7 10 cov 5
RANDOM_RESIDUAL VALUES
10
RANDOM_GROUP
4 5
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0.1
0.1 1
RANDOM_GROUP
6 7
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1
0.1 1
OPTION hetres_pos 6 7
OPTION hetres_pol 1.0 0.1
```

### using GIBBS3F90

```
DATAFILE
test.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
9
OBSERVATION(S)
```

```
3
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT NESTED]
1 2 cross
6 1 cov
7 1 cov
5 5 cross
6 5 cov 5
7 5 cov 5
5 10 cross
6 10 cov 5
7 10 cov 5
RANDOM_RESIDUAL VALUES
10
RANDOM_GROUP
4 5 6
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
1 0.1 0.1
0.1 1 0.1
0.1 0.1 1
RANDOM_GROUP
7 8 9
RANDOM_TYPE
add_animal
FILE
animal.ped
(CO)VARIANCES
1 0.1 0.1
0.1 1 0.1
0.1 0.1 1
OPTION hetres_int 8 5
```

Competitive model (i.e., social interaction effects)

```
DATAFILE
competition.dat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
19
OBSERVATION(S)
24
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT[EFFECT NESTED]
```

```
2 88 cross
3 362 cross
21 2409 cross
4 8004 cross
22 0 cov 5
22 0 cov 6
22 0 cov 7
22 0 cov 8
22 0 cov 9
22 0 cov 10
22 0 cov 11
22 0 cov 12
22 0 cov 13
22 0 cov 14
22 0 cov 15
22 0 cov 16
22 0 cov 17
22 0 cov 18
22 8004 cov 19
RANDOM_RESIDUAL VALUES
1225.8
RANDOM_GROUP
4 5
RANDOM_TYPE
add_animal
FILE
renadd04.ped
(CO)VARIANCES
267.03 25.313
25.313 104.44
RANDOM_GROUP
2
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
89.187
RANDOM_GROUP
3
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
167.34
```

Appendix A (single trait animal model)

Single trait "USDA-type" animal model. The files used in this example are available **here**.

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

where

y_{ijkl}	- production yield
hys_i	- fixed herd year season
hs_{ij}	- random herd x sire interaction
p_k	- random permanent environment
a_k	- random animal

and

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

Data file (ic)

Format: animal/hys/p/hs/y

```
 1  1  1  1  10
 2  1  2  1  11
 3  2  3  2  15
 4  2  4  3  13
 5  3  5  4  14
 6  3  6  3  12
```

Pedigree file (is)

Format: animal/dam/sire/code

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

Parameter file

```
# Example of single-trait animal model with one fixed effect
DATAFILE
ic
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
4
OBSERVATION(S)
5
WEIGHT(S)
```

```
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT  [EFFECT NESTED]
2 3 cross
3 6 cross
4 4 cross
1 14 cross
RANDOM_RESIDUAL VALUES
1
RANDOM_GROUP
2
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
.1
RANDOM_GROUP
3
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
.05
RANDOM_GROUP
4
RANDOM_TYPE
add_an_upg
FILE
is
(CO)VARIANCES
.5
```

Execution

```
name of parameter file?exiap

     BLUPF90 1.00

 Parameter file:             exiap
 Data file:                  ic
 Number of Traits             1
 Number of Effects            4
 Position of Observations      5
 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      1                    14
 Residual (co)variance Matrix
     1.000
 Random Effect      2
 Type of Random Effect:      diagonal
 trait   effect    (CO)VARIANCES
  1       2       0.100

 Random Effect      3
 Type of Random Effect:      diagonal
 trait   effect    (CO)VARIANCES
  1       3       0.050

 Random Effect      4
 Type of Random Effect:      additive animal
 Pedigree File:              is
 trait   effect    (CO)VARIANCES
  1       4       0.500

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

 Data record length = 5
 original G
   0.10
 inverted G
  10.00
 original G
   0.05
 inverted G
  20.00
 original G
   0.50
 inverted G
   2.00
 solutions stored in file: "solutions"

trait/effect level  solution
  1  1       1     11.8589
  1  1       2     13.7539
  1  1       3     14.7086
  1  2       1     -0.0088
  1  2       2      0.0088
  1  2       3     -0.0159
  1  2       4      0.0159
  1  2       5      0.0321
  1  2       6     -0.0321
  1  3       1      0.0000
  1  3       2     -0.0079
  1  3       3     -0.0081
  1  3       4      0.0161
  1  4       1     -1.7627
  1  4       2     -0.9553
  1  4       3      1.4288
  1  4       4     -0.9206
  1  4       5     -1.0781
  1  4       6     -2.3474
  1  4       7      0.8511
  1  4       8     -0.1521
  1  4       9      3.8926
  1  4      10     -2.7717
```

```
1  4      11      0.8528
1  4      12     -3.1911
1  4      13      7.9976
1  4      14     -6.3340
```

Appendix B (multiple trait sire model)

Example of multiple trait sire model (from L.R. Schaeffer notes of 1985).

Models

Trait 1: $y_{1i}=h_i+s_{1j}+e_{1ijk}$

Trait 2: $y_{2i}=\mu+s_{2j}+e_{2jk}$

where

h - fixed herd

s - random sire

and

var(s)=A[8 6; 6 17], var(e)=I[10 10; 10 20]

Data file (lrsdat)

Format: h/μ/s/y_1/y_2

```
1 0 1 3.4 0
2 0 2 1.3 0
1 1 3 .8 50.3
2 1 4 4.5 52.6
0 1 5  0 55.0
```

Pedigree file (lrsrel)

Format: bull/sire/MGS

```
1 3 0
2 0 5
3 0 0
4 0 0
5 0 0
```

Parameter file (lrsex)

```
# Example of two trait sire model with unequal models
DATAFILE
lrsdat
NUMBER_OF_TRAITS
2
NUMBER_OF_EFFECTS
2
OBSERVATION(S)
4 5
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT  [EFFECT NESTED]
1 2 2 cross
3 3 5 cross
```

RANDOM_RESIDUAL VALUES
10 10
10 20
RANDOM_GROUP
2
RANDOM_TYPE
add_sire
FILE
lrsrel
(CO)VARIANCES
8 6
6 17

Execution

```
name of parameter file?lrsex

     BLUPF90 1.00

 Parameter file:             lrsex
 Data file:                  lrsdat
 Number of Traits             2
 Number of Effects            2
 Position of Observations      4  5
 Position of Weight (1)        0
 Value of Missing Trait/Observation           0

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


 Residual (co)variance Matrix
   10.000    10.000
   10.000    20.000

 Random Effect      1
 Type of Random Effect:      additive sire
 Pedigree File:              lrsrel
 trait   effect    (CO)VARIANCES
  1       2       8.000     6.000
  2       2       6.000    17.000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

 Data record length = 5
 original G
   8.00   6.00
   6.00  17.00
 inverted G
   0.17  -0.06
  -0.06   0.08

solutions stored in file: "solutions"
```

```
trait/effect level  solution
  1  1       1      2.3877
  2  1       1     52.4449
  1  1       2      3.2180
  2  1       2      0.0000
  1  2       1      0.2243
  2  2       1     -0.0210
  1  2       2     -0.8217
  2  2       2     -0.3866
  1  2       3     -0.4969
  2  2       3     -0.7512
  1  2       4      0.6178
  2  2       4     -0.0769
  1  2       5      0.2217
  2  2       5      1.0851
```

Appendix C (test-day model)

This test-day model example comes from the paper of Schaeffer and Dekkers (WCGALP94 18:443). The files used in this example are available **here**.

Model

$y_{ijkl} = h_i + \beta_1 X_{1j} + \beta_2 X_{2j} + a_k + \gamma_{1k} X_{1j} + \gamma_{2k} X_{2j} + e_{ijkl}$

where

y_{ijkl}	- yield of test day
h_i	- test day effect
X_{1j}	- days in milk
X_{2j}	- log(days in milk)
β_1, β_2	- fixed regressions
a_k	- random animal
γ_{1k}, γ_{2k}	- random regressions for each animal

and

$var(e_{ijkl}) = 1; var(a_k, \gamma_{1k}, \gamma_{2k}) = [\ 2.25\ 4\ -.7;\ 4\ 1375\ 12;\ -.7\ 12\ 94]^{-1}$

<u>Data file (lrsrrdat)</u>

Format: h/a/X_1/X_2/y

```
1 1 73 1.42985 26
1 2 34 2.19395 29
1 3 8 3.64087 37
2 1 123 0.908127 23
2 2 84 1.28949 18
2 3 58 1.65987 25
2 4 5 4.11087 44
3 1 178 0.538528 21
3 2 139 0.785838 8
3 3 113 0.992924 19
3 4 60 1.62597 29
4 2 184 0.505376 1
4 3 158 0.657717 15
4 4 105 1.06635 22
4 5 14 3.08125 35
5 3 218 0.335817 11
5 4 165 0.614366 14
5 5 74 1.41625 23
5 6 31 2.28632 28
6 3 268 0.129325 7
6 4 215 0.349674 8
6 5 124 0.90003 17
6 6 81 1.32586 22
```

<u>Pedigree file (lrsrrel)</u>

Format: animal/sire/dam

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

```
5 11 7
6 11 1
7 0 0
8 0 0
9 0 0
10 0 0
11 0 0
```

Parameter file (exlrsrr)

```
# Example of single-trait random-regression model
DATAFILE
lrsrrdat
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
6
OBSERVATION(S)
5
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT  [EFFECT NESTED]
1 6 cross
3 1 cov
4 1 cov
2 11 cross
3 11 cov 2
4 11 cov 2
RANDOM_RESIDUAL VALUES
1
RANDOM_GROUP
4 5 6
RANDOM_TYPE
add_animal
FILE
lrsrrrel
(CO)VARIANCES
 .447906   -0.001334    0.003506
 -0.001334    0.000732   -0.000103
  0.003506   -0.000103    .010678
```

Execution

```
name of parameter file?exlrsrr

     BLUPF90 1.00

 Parameter file:             exlrsrr
 Data file:                  lrsrrdat
 Number of Traits             1
 Number of Effects            6
 Position of Observations      5
 Position of Weight (1)        0
 Value of Missing Trait/Observation           0

EFFECTS
```

```
 #  type                position (2)        levels   [positions for nested]
 1  cross-classified      1                    6
 2  covariable            3                    1
 3  covariable            4                    1
 4  cross-classified      2                   11
 5  covariable            3                   11     2
 6  covariable            4                   11     2

 Residual (co)variance Matrix
     1.000

 correlated random effects     4  5  6
 Type of Random Effect:      additive animal
 Pedigree File:              lrsrrrel
 trait   effect    (CO)VARIANCES
  1       4       0.448    -0.001     0.004
  1       5      -0.001     0.001     0.000
  1       6       0.004     0.000     0.011

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

 Data record length = 5
 original G
   0.45   0.00   0.00
   0.00   0.00   0.00
   0.00   0.00   0.01
 inverted G
   2.25   4.00  -0.70
   4.001375.09  11.95
  -0.70  11.95  94.00
 solutions stored in file: "solutions"

trait/effect level  solution
  1  1       1     19.9496
  1  1       2     20.3729
  1  1       3     20.6095
  1  1       4     19.7278
  1  1       5     18.6035
  1  1       6     17.8500
  1  2       1     -0.0498
  1  3       1      5.2912
  1  4       1     -0.4430
  1  4       2      0.2704
  1  4       3     -0.7288
  1  4       4      1.1019
  1  4       5     -0.1626
  1  4       6     -0.4828
  1  4       7     -0.0988
  1  4       8      0.4574
  1  4       9     -0.6288
  1  4      10      0.4574
  1  4      11     -0.1872
  1  5       1      0.0369
  1  5       2     -0.0661
  1  5       3      0.0068
  1  5       4     -0.0054
  1  5       5      0.0069
  1  5       6      0.0167
  1  5       7      0.0133
```

```
1  5       8     -0.0238
1  5       9      0.0350
1  5      10     -0.0238
1  5      11     -0.0008
1  6       1     -0.0370
1  6       2      0.0325
1  6       3     -0.0479
1  6       4      0.0767
1  6       5     -0.0149
1  6       6     -0.0377
1  6       7     -0.0103
1  6       8      0.0364
1  6       9     -0.0480
1  6      10      0.0364
1  6      11     -0.0145
```

Appendix D (multibreed maternal effect model)

This model was used for studies on multibreed evaluation in beef cattle. It is provided as an example of a model with maternal effect and different models per trait.

Model (in concise form, with most indices omitted)

$$
\begin{aligned}
y_1 &= cg_1 + bt + mbt + a + M \quad\quad\; + e\\
y_2 &= cg_2 + bt + mbt + a + M + pe + e\\
y_3 &= cg_3 + bt + mbt + a + \quad\quad\quad\quad\; e
\end{aligned}
$$

where

$y_{1\text{-}3}$	- birth weight, weaning weight, and gain
$cg_{1\text{-}3}$	- contemporary groups separate for each trait
br	- breed type
mbt	- maternal breed type
a	- additive effect
m	- maternal effect
pe	- permanent environmental effect of the dam

<u>Data file (data.out)</u>

Format:

1. contemporary group for trait 1
2. contemporary group for trait 2
3. contemporary group for trait 3
4. animal breed type
5. maternal breed type
6. animal id
7. dam id
8. birth weight
9. weaning weight
10. gain

<u>Pedigree file (pedi.outok)</u>

Format:

animal
sire or unknown parent group
dam or unknown parent group
“1 + number of missing parents”

Parameter file (param.out)

```
DATAFILE
data.out
NUMBER_OF_TRAITS
3
NUMBER_OF_EFFECTS
6
OBSERVATION(S)
8 9 10
WEIGHT(S)


EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT [EFFECT
NESTED]
 1 2 3   133085 cross
 4 4 4     181 cross
 5 5 0     165 cross
 6 6 6  1724112 cross
 7 7 0  1724112 cross
 0 7 0  1724112 cross
RANDOM_RESIDUAL VALUES
26.3    40.7    20.3
40.7    1312.9  141.9
20.3    141.9   1246.3
RANDOM_GROUP
4 5
RANDOM_TYPE
add_an_upg
FILE
pedi.outok
(CO)VARIANCES
22.9    36.3    18.6    -4.6    0.0     0.0
36.6    500.2   110.8   0.0     -91.6   0.0
18.6    110.8   313.0   0.0     0.0     0.0
-4.6    0.0     0.0     10.1    0.0     0.0
0.0     -91.6   0.0     0.0     419.1   0.0
0.0     0.0     0.0     0.0     0.0     0.0
RANDOM_GROUP
2
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
0.263   0.0     0.0
0.0     13.129  0.0
0.0     0.0     12.463
RANDOM_GROUP
3
RANDOM_TYPE
diagonal
```

```
FILE

(CO)VARIANCES
0.263   0.0     0.0
0.0     13.129  0.0
0.0     0.0     0.0
RANDOM_GROUP
6
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
0.0     0.0     0.0
0.0     45.5    0.0
0.0     0.0     0.0
```

Appendix E (random regression model)

A single-trait random regression model for test-day milk is using cubic Legendre polynomials.

Model

$$y_{ijkl}=hym_{ij}+\sum_{m=1}^{4}\alpha_m(l)h_{im}+\sum_{m=1}^{4}\alpha_m(l)u_{km}+\sum_{m=1}^{4}\alpha_m(l)pe_{im}+e_{ijkl}$$

where

y_{ijkl}	- test day milk
hym_{ij}	- hear-year-test for herd i and year-test j
h_i	- effects of herd i
$\alpha_m(l)$	- value of m-th Legendre polynomial at point corresponding to DIM=l
u	- additive effects
pe	- permanent environmental effects

Data file (datarr)

Format:

1.herd

2. hear-year-test

3-6. values of Legendre polynomials

7. weight for residuals: 100/var(e_{ijkl})

8. test day

9. animal

Relationship file (pedirr)

Format:

animal

sire

dam

Parameter file (exrr3)

```
DATAFILE
datarr
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
13
OBSERVATION(S)
8
WEIGHT(S)
7
EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT
```

```
2   3726 cross          #herd-year-test
3 84 cov 1                          #herd
4 84 cov 1
5 84 cov 1
6 84 cov 1
3 21874 cov 9                       #additive
4 21874 cov 9
5 21874 cov 9
6 21874 cov 9
3 21874 cov 9                       #pe
4 21874 cov 9
5 21874 cov 9
6 21874 cov 9
RANDOM_RESIDUAL VALUES
100
RANDOM_GROUP
6 7 8 9
RANDOM_TYPE
add_animal
FILE
pedirr
(CO)VARIANCES
(4 x 4 matrix)
RANDOM_GROUP
10 11 12 13
RANDOM_TYPE
diagonal
FILE

(CO)VARIANCES
(4 x 4 matrix)
```

Appendix F (terminal cross model)

A terminal cross model by Fernando et al. and Lo et al.

breed A:	ya	=	cga	+	ua			+	ea
breed B:	yb	=	cgb	+			ub	+	eb
cross:	yab	=	cgab	+	uaab	+	ubab	+	eab

Data file (data_cross)

1. cg A (85 levels)
2. cg B (110 levels)
3. cg crossbred (87 levels)
4. animal - breed A (2400 animals) or parent from breed A
5. animal - breed B (3000 animals) or parent from breed B
6. ya
7. yb
8. yc

Pedigree files: pedig_A for breed A and pedig_B for breed B

Parameter file

```
# Example of a terminal-cross model
DATAFILE
data-cross
NUMBER_OF_TRAITS
3
NUMBER_OF_EFFECTS
3
OBSERVATION(S)
6 7 8
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT  [EFFECT NESTED]
1 2 3 110 cross
4 0 4 2400 cross
0 5 5 3000 cross
RANDOM_RESIDUAL VALUES
100 0 0
0 100 0
0 0 100
RANDOM_GROUP
2
RANDOM_TYPE
add_animal
FILE
pedig_A
(CO)VARIANCES
 (3 x 3 matrix)
```

```
RANDOM_GROUP
3
RANDOM_TYPE
add_animal
FILE
pedig_B
(CO)VARIANCES
 (3 x 3 matrix)
```

Appendix G (competitive model)

Example of a competitive model (a la Muir and Schinkel)

y=cg + a +c1 + c2 +..+c5 + e

ci is the effect of the i-th competitor; assumed pen size of up to 6.

<u>Datafile (data_comp)</u>

1. y
2. cg (max 120)
3. animal (max 3000)
4. competitor 1
5. c 2

...

8. c 5

If pen size is less than 6, unused fields set to 0.

<u>Parameter file</u>

```
# Example of a competitive model
DATAFILE
data_comp
NUMBER_OF_TRAITS
1
NUMBER_OF_EFFECTS
7
OBSERVATION(S)
1
WEIGHT(S)

EFFECTS: POSITIONS_IN_DATAFILE NUMBER_OF_LEVELS TYPE_OF_EFFECT  [EFFECT NESTED]
2 120 cross
3 3000 cross
4 0 cross
5 0 cross
6 0 cross
7 0 cross
8 3000 cross
RANDOM_RESIDUAL VALUES
50
RANDOM_GROUP
2 3
RANDOM_TYPE
add_animal
FILE
```

The 2nd effect (position 3 in the data) is additive direct effect and 3rd to 7th effects (positions 4 to 8 in the data) are competitive effects (animal ID for competitors).

```
pedig
(CO)VARIANCES
40 -10
-10 10
```

The covariance matrix contains variance for the second effect, variance for effects 3 to 7 (accumulated to 7), and covariance between direct and competitive effects.

Appendix H (genomic model)

Example of evaluation /variance component estimation using phenotypic, pedigree and genomic information in single-step evaluation

Files simulated by Huiyu Wang using program QMSim by Mehdi Sargolzaei & Flavio Schenkel.

Parameter file for renumbering program RENUMF90

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

WEIGHT(S)

RESIDUAL_VARIANCE
 0.9038
EFFECT
1 cross alpha  #fixed effect
EFFECT
2 cross alpha  #animal
RANDOM
animal
FILE
pedigree
SNP_FILE
marker.geno.clean
 (CO)VARIANCES
   0.9951E-01
```

Phenotypes.txt – phenotype file
Single trait in position 3
Fixed effect in position 1 read as alphanumeric
Random animal effect in position 3
Pedigree file pedigrees
SNP file marker.geno.clean

Phenotype file

```
phenotypes.txt

1 1 4.16 0
1 2 3.47 0
1 3 4.5 0
1 4 4.97 0
1 5 5.98 0
1 6 6.63 0
1 7 3.32 0
1 8 5.85 0
1 9 4.77 0
1 10 4.22 0
```

Pedigree file

```
pedigree

1 0 0 0
2 0 0 0
3 0 0 0
4 0 0 0
5 0 0 0
```

```
6 0 0 0
7 0 0 0
8 0 0 0
9 0 0 0
10 0 0 0
```

SNP file for the first 50 SNP

```
$cut -c1-50 marker.geno.clean|head -10
```

```
 8002 21101011002012011011010110111111211111210100
 8014 21110101111101120221110111111112101112210100
 8016 21100101202202021120210121102111202212111101
 8018 21110111112201120210200020101022212211111100
 8024 21110102201201111220210111102122201221111111
 8038 11110000102100120201211121201022112111121111
 8041 22210001201201121110210121202111102102121001
 8063 20110101202202020212221110110112022201212002 1
 8065 21110101111112111221110101010220212001110012
 8083 10111011110010111111110112100111121011010121
```

Run RENUMF90

```
RENUMF90 version 1.86
name of parameter file?renum.par
renum.par
datafile:phenotypes.txt
traits:           3
fields passed:           4
R
 0.9038

Processing effect  1 of type cross
item_kind=alpha

Processing effect  2 of type cross
item_kind=alpha
pedigree file name  "pedigree"
positions of animal, sire, dam, alternate dam and yob           1           2
          3           0           0
SNP file name  "marker.geno.clean"
all pedigrees to be included
Reading (CO)VARIANCES:           1 x           1

Maximum size of character fields: 20

Maximum size of record (max_string_readline): 800

Maximum number of fields innput file (max_field_readline): 100

hash tables for effects set up
table expanded from        10000  to        20000  records
table expanded from        20000  to        40000  records
read        15800  records
table with            1  elements sorted
added count
Effect group            1  of column           1  with            1  levels
table expanded from        10000  to        10000  records
added count
Effect group            2  of column           1  with        15800  levels
wrote statistics in file "renf90.tables"

Basic statistics for input data  (missing value code is 0)
Pos  Min         Max         Mean        SD                 N
  3   0.73000      8.8300      4.9793      1.0069       15800
```

```
random effect with SNPs  2
type: animal
file: marker.geno.clean
read SNPs        1500  records
Effect group            2  of column            1  with        15800  levels

random effect   2
type:animal
opened output pedigree file "renadd02.ped"
read        15800  pedigree records

Pedigree checks

Number of animals with records:       15800
Number of animals with genotypes:        1500
Number of animals with records or genotypes:       15800
Number of animals with genotypes and no records           0
Number of parents without records or genotypes:           0
Total number of animals:       15800

Wrote cross reference IDs for SNP file "marker.geno.clean_XrefID"

Wrote parameter file "renf90.par"
Wrote renumbered data "renf90.dat"
```

Parameter file for application programs with renumbered fields

renf90.par

renf90.dat – phenotype file
Single trait in position 1
Two effects in model
Fixed effect in position 1 cross-classified with 1 level (μ)
Animal effect in position 3
Second effect (Random Group 2) is additive-animal with
renadd02.ped – pedigree file
SNP file marker.geno.clean

```
# BLUPF90 parameter file created by RENF90
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       1 cross
 3    15800 cross
RANDOM_RESIDUAL VALUES
 0.9038
 RANDOM_GROUP
       2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.9951E-01
OPTION SNP_file marker.geno.clean
```

Renumbered pedigree file

```
renadd02.ped
```

```
1 5742 14705 1 0 2 1 0 0 14670
2 2302 1384 1 0 2 1 0 0 12367
3 4248 15309 1 0 12 1 0 2 9123
4 4241 3492 1 0 2 1 0 0 7455
5 14459 14202 1 0 2 1 0 0 5736
6 1029 1292 1 0 2 1 0 3 5877
7 10876 7596 1 0 2 1 0 0 9638
8 13589 12642 1 0 2 1 0 0 14136
9 7070 11562 1 0 2 1 0 0 6010
10 6449 2448 1 0 2 1 0 0 15498
```

Renumbered phenotype file

renf90.dat

```
4.16 1 5903 0
3.47 1 3628 0
4.5 1 1329 0
4.97 1 14808 0
5.98 1 12481 0
6.63 1 10205 0
3.32 1 7935 0
5.85 1 5639 0
4.77 1 3348 0
4.22 1 1951 0
```

Run BLUPF90

```
name of parameter file?renf90.par

* SNP file: marker.geno.clean
* SNP Xref file: marker.geno.clean_XrefID
* Frequency to Center Z=M-p to create G=ZZ'/k (default whichfreq = 2):
          2
    BLUPF90 1.42

Parameter file:             renf90.par
Data file:                  renf90.dat
Number of Traits             1
Number of Effects            2
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                                                 1
 2  cross-classified     3                                             15800

Residual (co)variance Matrix
0.90380

Random Effect(s)    2
Type of Random Effect:      additive animal
Pedigree File:              renadd02.ped
trait   effect    (CO)VARIANCES
 1       2    0.9951E-01

REMARKS
 (1) Weight position 0 means no weights utilized
 (2) Effect positions of 0 for some effects and traits means that such
     effects are missing for specified traits

Data record length =            3
# equations =        15801
G
0.99510E-01
```

```
read        15800  records in   3.5994001E-02  s,         31601  nonzeroes
 read        15800  additive pedigrees

*--------------------------------------------------------------*
*                 Setup Genomic: Version 1.76                  *
*                                                              *
*  Modified relationship matrix (H) created for effect:   2    *
*--------------------------------------------------------------*

Read 15800 animals from pedigree file
Pedigree was in not chronological order (parent first format), reodering will be performed!!!

Current OPTIONS

Genomic Matrix
  Make/Read   Which  Save Test File       StorageType
     Make        1     F     F   G  densem

Rel. Matrix A22
  Make/Read   Which  Save Test File       StorageType
     Make        4     F     F   A22  densem

Inv. Genomic Matrix
  Make/Read   Which  Save Test File       StorageType
     Make        9     F     F   Gi  densem

Inv. Rel. Matrix A22
  Make/Read   Which  Save Test File       StorageType
     Make        9     F     F   A22i  densem

Genomic - A22 Matrix
  Make/Read   Which  Save Test File       StorageType
     None        9     F     F   GmA22  densem

Inv. Genomic- A22 Matrix
  Make/Read   Which  Save Test File       StorageType
     Make        0     F     F   GimA22i  densem

Other options
   Allele Frequency file:    freqdata
   Center Allele Frequency:  2
   Scale  Allele Frequency:  2
   Scale  Method:            1
   Regression G on A:              F
   Tuned G Method:          2

   Creation of GimA22i
      tau inv(alpha G + beta A22 + gamma I + delta) - omega inv(A22)
            alpha,beta         0.950   0.050
            gamma,delta        0.000   0.000
            tau,omega          1.000   1.000

Number of Genotyped Animals        1500

Creating A22
   Extracting subset of: 3432 pedigrees from: 15800 elapsed time:     0.0000
   Calculating Inbreeding by M&L function.. elapsed time  1.0000020E-03
   Calculating A22 Matrix by Colleau ...elapsed time  0.3299500
```

Statistics for A22

```
Statistic of Rel. Matrix A22
                           N       Mean       Min       Max       Var
    Diagonal            1500      1.001     1.000     1.250     0.000
    Off-diagonal     2248500      0.003     0.000     0.750     0.001
```

Statistics for SNP file

```
Reading SNP file
```

```
   Column position in file for the first marker:            7
   Format to read SNP file: (6x,400000i1)
   Number of SNPs :        3000
   Number of Genotyped animals:         1500
   Reading SNP file elapsed time  0.4639290

Statistics of alleles frequencies in the current population
   N:           3000
   Mean:       0.501
   Min:        0.132
   Max:        0.890
   Var:        0.014
```

Several quality checks performed; no error messages as all files for this example have been simulated

```
Quality Control - Check call rate for animals


Quality Control - Check Parent-Progeny Mendelian conflicts
   Total animals: 15800 - Genotyped animals: 1500
   Number of Individual - Sire pairs: 470
   Number of Individual - Dams pairs: 256
   Number of Individual - Sire - Dam trios: 152

Checking SNPs for Mendelian conflicts
Total number of parent-progeny evaluations:          726
Number of SNPs with Mendelian conflicts: 0

Checking Animals for Mendelian conflicts

Statistics of alleles frequencies in the current population after
    Quality Control (MAF, monomorphic, call rate)
   N:           3000
   Mean:       0.501
   Min:        0.132
   Max:        0.890
   Var:        0.014

    Locus      Freq      0-2p      1-2p      2-2p
        1  0.751333 -1.502667 -0.502667  0.497333
        2  0.382333 -0.764667  0.235333  1.235333
        3  0.568667 -1.137333 -0.137333  0.862667
        4  0.680000 -1.360000 -0.360000  0.640000
        5  0.184333 -0.368667  0.631333  1.631333
        6  0.298333 -0.596667  0.403333  1.403333
        7  0.392000 -0.784000  0.216000  1.216000
        8  0.379667 -0.759333  0.240667  1.240667
        9  0.596667 -1.193333 -0.193333  0.806667
       10  0.352333 -0.704667  0.295333  1.295333
Genotypes missings (%):  0.0000000E+00

Average denom. (scale):   1415.90178466665
Center Matrix elapsed:   8.3986998E-02

Creating G Matrix

Calculating G Matrix
   Wall time: 08-05-2011  16h 57m 34s 213
MMP - OPTML
Elapsed time   18.47419
   Wall time: 08-05-2011  16h 58m 09s 371
```

Statistics of G calculated assuming current allele frequencies

```
Statistic of Genomic Matrix
                          N       Mean       Min       Max       Var
    Diagonal           1500      0.999     0.889     1.463     0.002
    Off-diagonal    2248500     -0.001    -0.147     0.830     0.002


Correlation of Genomic Inbreeding and Pedigree Inbreeding
```

```
    Correlation:     0.3220

All elements - Diagonal / Off-Diagonal
   Estimating Regression Coefficients G = b0 11' + b1 A + e
   Regression coefficients b0 b1 =     -0.004     0.997

   Correlation all elements G & A     0.644


Off-Diagonal
   Using 70386 elements from A22 >= 0.02000

   Estimating Regression Coefficients G = b0 11' + b1 A + e
   Regression coefficients b0 b1 =     -0.006     1.000

   Correlation Off-Diagonal elements G & A     0.660


Blend G as alpha*G + beta*A22: (alpha,beta)     0.950     0.050

Statistic of Genomic Matrix
                            N      Mean       Min       Max       Var
    Diagonal             1500     0.999     0.894     1.446     0.002
    Off-diagonal      2248500     0.000    -0.139     0.820     0.002

Frequency - Diagonal of G
   N:         1500
   Mean:         0.999
   Min:          0.894
   Max:          1.446
   Range:        0.028
   Class:      20

 #Class       Class   Count
       1   0.8942         9
       2   0.9218        86
       3   0.9494       343
       4   0.9770       480
       5    1.005       361
       6    1.032       139
       7    1.060        51
       8    1.087        16
       9    1.115         6
      10    1.142         2
      11    1.170         1
      12    1.198         1
      13    1.225         1
      14    1.253         1
      15    1.280         0
      16    1.308         0
      17    1.336         0
      18    1.363         2
      19    1.391         0
      20    1.418         1
      21    1.446         0


Scale G matrix according to A22 -  Method: 2
   Diagonal A:     1.001    Offdiagonal A:     0.003    All A:     0.004    Difference:    0.998
   Diagonal G:     0.999    Offdiagonal G:     0.000    All G:     0.000    Difference:    0.999
   Diff G Diag - G OffDiag:     0.999    (da-oa)/(dg-og):     0.998
   Diff A OffDiag - G OffDiag:     0.004
   Diff A all - G all:     0.004
   New Alpha:    0.948    New Beta:    0.050    :New Delta    0.004

------------------------------
 Final Pedrigree-Based Matrix
------------------------------

Statistic of Rel. Matrix A22
```

Correlations of off-diagonal elements of G and A22 is 0.660;
low numbers indicated genotyped mistakes or poor pedigrees

Diagonal elements of G should be 1± 0.2. Too large or too small elements indicate:
Genotyping mistakes
Mixed lines
See Simeone et al. (2011)

```
                          N       Mean        Min        Max        Var
    Diagonal           1500      1.001      1.000      1.250      0.000
    Off-diagonal    2248500      0.003      0.000      0.750      0.001
```

Statistics of G after scaling as in Chen et al (2011) or Vitezica et al. (2011)
Statistics should be same as for A22.

```
----------------------
 Final Genomic Matrix
----------------------

Statistic of Genomic Matrix
                          N       Mean        Min        Max        Var
    Diagonal           1500      1.001      0.896      1.447      0.002
    Off-diagonal    2248500      0.003     -0.134      0.822      0.002


Correlation of Genomic Inbreeding and Pedigree Inbreeding
    Correlation:      0.3363

All elements - Diagonal / Off-Diagonal
   Estimating Regression Coefficients G = b0 11' + b1 A + e
   Regression coefficients b0 b1 =      0.000      0.995

   Correlation all elements G & A     0.663

Off-Diagonal
   Using 70386 elements from A22 >= 0.02000

   Estimating Regression Coefficients G = b0 11' + b1 A + e
   Regression coefficients b0 b1 =     -0.001      0.998

   Correlation Off-Diagonal elements G & A     0.679

Creating A22-inverse
   Wall time: 08-05-2011  16h 58m 10s 866
Inverse using ginv2
elapsed time   3.54446100000000
   Wall time: 08-05-2011  16h 58m 17s 691
```

Statistics of A_{22}^{-1}

```
Statistic of Inv. Rel. Matrix A22
                          N       Mean        Min        Max        Var
    Diagonal           1500      1.607      1.056      9.221      0.575
    Off-diagonal    2248500     -0.001     -1.067      0.533      0.001


Creating G-inverse
   Wall time: 08-05-2011  16h 58m 17s 987
Inverse using ginv2
elapsed time   4.24635400000000
   Wall time: 08-05-2011  16h 58m 26s 044
```

Statistics of G^{-1}
2 x diag(G^{-1} - A_{22}^{-1}) is approx. measure of extra genomic info in terms of effective daughters

```
Statistic of Inv. Genomic Matrix
                          N       Mean        Min        Max        Var
    Diagonal           1500      8.007      3.597     64.893     21.055
    Off-diagonal    2248500     -0.005    -12.697      6.632      0.056


Creating GimA22i in file: "GimA22i"
Calculating GmA22/GimA22i Matrix Densem storage
Calculating GmA22/GimA22i Matrix...elapsed time  0.1269817
```

```
 Setup Genomic Done.
 wGimA22i   1.00000000000000
hash matrix increased from 100000 to 150000 % filled:     0.9000
hash matrix increased from 150000 to 225000 % filled:     0.9000
hash matrix increased from 225000 to 337500 % filled:     0.9000
hash matrix increased from 337500 to 506250 % filled:     0.9000
hash matrix increased from 506250 to 759375 % filled:     0.9000
hash matrix increased from 759375 to 1139062 % filled:     0.9000
hash matrix increased from 1139062 to 1708593 % filled:     0.9000
 finished peds in    30.68333      s,       1193064  nonzeroes
 round            1    convergence=  3.234776127905992E-004
 round            2    convergence=  1.615955145159698E-005
 round            3    convergence=  9.675137058360991E-006
 round            4    convergence=  6.533482675941447E-006
 round            5    convergence=  2.711751165983321E-006
………..
………..
 round           64    convergence=  2.721030958617683E-012
 round           65    convergence=  1.931029578758311E-012
 round           66    convergence=  1.610472992188148E-012
 round           67    convergence=  1.259204136643006E-012
 round           68    convergence=  9.025592862452768E-013
          68  iterations,   convergence criterion=  9.025592862452768E-013
 solutions stored in file: "solutions"
```

Solution file

```
solutions

trait/effect level  solution
   1   1         1      4.97591211
   1   2         1      0.10194865
   1   2         2      0.33749439
   1   2         3      0.04475742
   1   2         4     -0.31055520
   1   2         5      0.22368631
   1   2         6     -0.09454804
   1   2         7     -0.03186435
   1   2         8      0.18033163
```

Variance component estimation by AIREMLF90

```
 name of parameter file?renf90.par

 * SNP file: marker.geno.clean
 * SNP Xref file: marker.geno.clean_XrefID
 * Frequency to Center Z=M-p to create G=ZZ'/k (default whichfreq = 2):
           2
     AI-REMLF90 ver. 1.96

 Parameter file:             renf90.par
 Data file:                  renf90.dat
 Number of Traits             1
 Number of Effects            2
 Position of Observations      1
 Position of Weight (1)        0
 Value of Missing Trait/Observation           0

………..
………..

Statistic of Inv. Genomic Matrix
                           N       Mean        Min        Max        Var
    Diagonal            1500      8.007      3.597     64.893     21.055
    Off-diagonal     2248500     -0.005    -12.697      6.632      0.056


 Creating GimA22i in file: "GimA22i"
 Calculating GmA22/GimA22i Matrix Densem storage
 Calculating GmA22/GimA22i Matrix...elapsed time  0.1089821
 Setup Genomic Done.
 wGimA22i   1.00000000000000
hash matrix increased from 85428 to 128142 % filled:     0.9000
hash matrix increased from 128142 to 192213 % filled:     0.9000
hash matrix increased from 192213 to 288319 % filled:     0.9000
hash matrix increased from 288319 to 432478 % filled:     0.9000
hash matrix increased from 432478 to 648717 % filled:     0.9000
hash matrix increased from 648717 to 973075 % filled:     0.9000
hash matrix increased from 973075 to 1459612 % filled:     0.9000
hash matrix increased from 85428 to 128142 % filled:     0.9000
hash matrix increased from 128142 to 192213 % filled:     0.9000
hash matrix increased from 192213 to 288319 % filled:     0.9000
hash matrix increased from 288319 to 432478 % filled:     0.9000
hash matrix increased from 432478 to 648717 % filled:     0.9000
hash matrix increased from 648717 to 973075 % filled:     0.9000
hash matrix increased from 973075 to 1459612 % filled:     0.9000
 finished peds in    32.01313      s,       1193064  nonzeroes
 rank=       15801
              **************
              **** FSPAK ***
              **************
              MPE / IM / MAE
                  Jun 1994

             SPARSE STATISTICS
     DIMENSION OF MATRIX     =                    15801
     RANK                    =                    15801
     STORAGE AVAILABLE       =                  7061497
     MAXIMUM NEEDED          =                  7061497
     NZE IN UPPER TRIANGULAR =                  1208865
     NZE IN FACTOR           =                  1521840
     NO. OF CALLS NUM FACT   =                        1
     NO. OF CALLS SOLVE      =                        1
     NO. OF CALLS SPARS SOLV =                        0
     NO. OF CALLS DET / LDET =                        1
     NO. OF CALLS SPARS INV  =                        1
     TOTAL CPU TIME IN FSPAK =                 9.465561
     TIME FOR FINDING ORDER  =                 2.568611
     TIME FOR SYMBOLIC FAC   =                 0.676899
     TIME FOR NUMERICAL FAC  =                 2.017693
     TIME FOR SOLVE          =                 0.008995
     TIME FOR SPARSE SOLVE   =                 0.000000
     TIME FOR SPARSE INVERSE =                 4.147369
 -2logL =    43515.7413644011       : AIC =    43519.7413644011
  In round            1  convergence=  0.423851780381002
  delta convergence=  0.252173522062583
 new R
  0.58510
 new G
  0.28516
 -2logL =    53013.2734486053       : AIC =    53017.2734486053
  In round            2  convergence=  0.141351613622645
  delta convergence=  0.117430758820623
 new R
  0.52205
 new G
  0.45696
 -2logL =    52800.6601605267       : AIC =    52804.6601605267
  In round            3  convergence=  1.725330565925358E-002
  delta convergence=  4.769938966058494E-002
 new R
  0.49575
 new G
  0.52606
 -2logL =    52785.2479463395       : AIC =    52789.2479463395
  In round            4  convergence=  1.101891763451498E-004
  delta convergence=  3.662497104484009E-003
 new R
  0.49400
 new G
  0.53164
 -2logL =    52785.1635385807       : AIC =    52789.1635385807
  In round            5  convergence=  2.804695847240073E-009
  delta convergence=  1.777604045032979E-005
 new R
  0.49400
 new G
  0.53167
```

Estimates of variance components

```
Final Estimates
 Genetic variance(s) for effect  2
  0.53167
 Residual variance(s)
  0.49400
 inverse of AI matrix (Sampling Variance)
  0.40448E-03 -0.17367E-03
 -0.17367E-03  0.14702E-03
 Correlations from inverse of AI matrix
   1.0000     -0.71219
 -0.71219       1.0000
 SE for R
  0.12125E-01
 SE for G
  0.20112E-01
 solutions stored in file: "solutions"
```

Appendix I (complete genomic analysis)

Data files are available at **http://nce.ads.uga.edu/wiki/doku.php?id=course_materials_-_from_uga_2014**.

Using **RENUMF90, PREGSF90, BLUPF90** (**BLUP**), **BLUPF90** (**ssGBLUP**), **PREDICTF90, POSTGSF90** (**ssGWAS**)

Simulated data

Single trait with heritability of 0.30 and phenotypic variance = 1.0

Five generations

Total of 994 parents from generations 1 to 4 were genotyped

Three hundred progeny from 5th generation had genotypes and pedigree, but phenotypes were removed for traditional and genomic evaluations

Data Structure:

#Animal Generation Sex Mu QTL Residual Phenotype (Phenotype = Mu + QTL + Residual)

```
1 0 1 1 -0.826104  1.586661 1.76056
2 0 1 1 -1.093034 -0.451821 -0.544855
3 0 1 1 -0.135824  0.984936 1.84911
4 0 1 1  0.044242 -0.802145 0.242097
5 0 1 1  0.342068  0.028434 1.3705
               .
               .
6095 5 1 1  1.801324 -0.494822 2.3065
6096 5 2 1  0.772964  0.791936 2.5649
6097 5 2 1  0.748241  0.285815 2.03406
6098 5 1 1  1.042522 -1.606656 0.435866
6099 5 1 1  0.891319  0.179843 2.07116
6100 5 1 1  0.745873  0.034715 1.78059
```

Pedigree: 6100 animals

#Animal Sire Dam

```
1 0 0
2 0 0
3 0 0
4 0 0
5 0 0
   .
   .
6095 4576 4403
6096 4576 4065
6097 4576 2263
6098 4576 4150
6099 4576 3690
6100 4576 4311
```

Genotypes: 1294 animals genotyped for 1000 SNP across 5 chromosomes

# Animal $SNP_1SNP_2SNP_3SNP_4SNP_5…SNP_{1000}$

```
6100   22212…1
```

Map:

#SNP order chromosome position

```
1 1 10010
2 1 16722
3 1 33444
4 1 50166
5 1 66888
        .
        .
1000 5 299878
```

Parameter file for RENUMF90

```
DATAFILE
newdata.txt
TRAITS
 7
FIELDS_PASSED TO OUTPUT
2
WEIGHT(S)

RESIDUAL_VARIANCE
0.70
EFFECT
4 cross alpha    #mu
EFFECT
1  cross alpha    #animal
RANDOM
animal
FILE
ped.txt
FILE_POS
1 2 3 0 0
SNP_FILE
snp.txt
PED_DEPTH
0
(CO)VARIANCES
0.30
OPTION map_file map.txt
```

Log file for RENUMF90

```
RENUMF90 version 1.104
 name of parameter file? renum.par
 datafile:newdata.txt
 traits:           7
 fields passed:           2
 R
  0.7000

 Processing effect  1 of type cross
 item_kind=alpha

 Processing effect  2 of type cross
```

```
item_kind=alpha
pedigree file name  "ped.txt"
positions of animal, sire, dam, alternate dam and yob    1    2    3    0    0
SNP file name  "snp.txt"
all pedigrees to be included
Reading (CO)VARIANCES:           1 x           1

Maximum size of character fields: 20

Maximum size of record (max_string_readline): 800

Maximum number of fields for input file (max_field_readline): 100

hash tables for effects set up
read         6100  records
table with             1  elements sorted
added count
Effect group             1  of column           1  with            1  levels
table expanded from         10000  to         10000  records
added count
Effect group             2  of column           1  with         6100  levels
wrote statistics in file "renf90.tables"

Basic statistics for input data  (missing value code is 0)
Pos  Min         Max         Mean        SD                 N
  7   -2.8883      5.0863      1.0042     0.99034        6100

random effect with SNPs  2
type: animal
file: snp.txt
read SNPs        1294  records
Effect group             2  of column           1  with         6100  levels

random effect   2
type:animal
opened output pedigree file "renadd02.ped"
read         6100  pedigree records

Pedigree checks

Number of animals with records:        6100
Number of animals with genotypes:        1294
Number of animals with records or genotypes:        6100
Number of animals with genotypes and no records           0
Number of parents without records or genotypes:           0
Total number of animals:        6100

Wrote cross reference IDs for SNP file "snp.txt_XrefID"

Wrote parameter file "renf90.par"
Wrote renumbered data "renf90.dat"
```

Parameter file for PREGSF90 without quality control

```
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       1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
   2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.30000
OPTION SNP_file snp.txt
OPTION map_file map.txt
OPTION no_quality_control
```

Log file for PREGSF90 without quality control

```
name of parameter file?
renf90.par

     preGS 1.10

 Parameter file:             renf90.par
 Data file:                  renf90.dat
 Number of Traits             1
 Number of Effects            2
 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                                                 1
 2  cross-classified     3                                              6100

 Residual (co)variance Matrix
 0.70000

 Random Effect(s)    2
 Type of Random Effect:      additive animal
 Pedigree File:              renadd02.ped
 trait   effect    (CO)VARIANCES
  1       2    0.3000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

Options read from parameter file:

 * SNP file: snp.txt
 * SNP Xref file: snp.txt_XrefID
 * Map file: map.txt
 * No Quality Control Checks !!!!! (default .false.):  T

 *---------------------------------------------------------------*
 *                Genomic Library: Version 1.164                 *
 *                                                               *
 *                  Optimized OpenMP Version                     *
 *                                                               *
 *  Modified relationship matrix (H) created for effect:   2     *
 *---------------------------------------------------------------*

 Read 6100 animals from pedigree file: "renadd02.ped"
 Number of Genotyped Animals: 1294

Creating A22
    Extracting subset of: 2312 pedigrees from: 6100 elapsed time:     0.0150
    Calculating A22 Matrix by Colleau OpenMP...elapsed time: .0190
    Numbers of threads=8 16

 Reading SNP file
    Column position in file for the first marker: 8
    Format to read SNP file: (7x,400000i1)
    Number of SNPs: 1000
    Number of Genotyped animals: 1294
    Reading SNP file elapsed time: .06

 Statistics of alleles frequencies in the current population
    N:           1000
    Mean:       0.504
    Min:        0.043
    Max:        0.929
    Var:        0.032

 Reading MAP file: "map.txt" - 1000 SNPs out of 1000

    Min and max # of chromosome: 1 5

    Min and max # of SNP: 1 1000

 Genotypes missings (%):  0.000

 Calculating G Matrix
    Dgemm MKL #threads=     8   16 Elapsed omp_get_time:     0.7359

 Scale by Sum(2pq). Average:   435.221580281360

 Blend G as alpha*G + beta*A22: (alpha,beta)     0.950     0.050

 Frequency - Diagonal of G
    N:        1294
    Mean:        0.999
    Min:         0.895
    Max:         1.468
    Range:       0.029
    Class:     20

#Class       Class   Count
       1  0.8949         27
       2  0.9236        109
       3  0.9523        300
       4  0.9810        380
       5   1.010         287
       6   1.038         137
       7   1.067          33
       8   1.096          14
       9   1.124           3
      10   1.153           1
      11   1.182           0
      12   1.210           2
      13   1.239           0
      14   1.268           0
      15   1.296           0
      16   1.325           0
      17   1.354           0
      18   1.382           0
      19   1.411           0
      20   1.440           1
      21   1.468           0


 Check for diagonal of genomic relationship matrix

 Check for diagonal of genomic relationship matrix, genotypes not removed: 0

 ------------------------------
  Final Pedrigree-Based Matrix
 ------------------------------

 Statistic of Rel. Matrix A22
                           N      Mean       Min       Max       Var
     Diagonal           1294     1.001     1.000     1.250     0.000
     Off-diagonal    1673142     0.005     0.000     0.750     0.001

 ----------------------
  Final Genomic Matrix
 ----------------------

 Statistic of Genomic Matrix
                           N      Mean       Min       Max       Var
     Diagonal           1294     1.001     0.898     1.469     0.002
     Off-diagonal    1673142     0.005    -0.158     0.791     0.002

 Correlation of Genomic Inbreeding and Pedigree Inbreeding
     Correlation:     0.2177

All elements - Diagonal / Off-Diagonal
    Estimating Regression Coefficients G = b0 11' + b1 A + e
    Regression coefficients b0 b1 =      0.000     0.991

    Correlation all elements G & A     0.717

 Off-Diagonal
    Using 83426 elements from A22 >= .02000

    Estimating Regression Coefficients G = b0 11' + b1 A + e
    Regression coefficients b0 b1 =     -0.003     0.999

    Correlation Off-Diagonal elements G & A     0.777

 Creating A22-inverse
    Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1071

 ----------------------
```

```
  Final A22 Inv Matrix
 ----------------------

 Statistic of Inv. Rel. Matrix A22
                           N      Mean        Min        Max        Var
     Diagonal           1294     1.851      1.067      5.812      0.431
     Off-diagonal    1673142    -0.001     -1.200      0.600      0.001


 Creating G-inverse
    Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1050

 --------------------------
  Final Genomic Inv Matrix
 --------------------------

 Statistic of Inv. Genomic Matrix
                           N      Mean        Min        Max        Var
     Diagonal           1294    13.457      5.827     45.588     27.985
     Off-diagonal    1673142    -0.010    -13.500      6.896      0.226

 Check for diagonal of Inverse Genomic - Inverse of pedigree relationship matrix

 Saving GimA22i in file: "GimA22i"

------------------------------
  Final G Inv - A22 Inv Matrix
 ------------------------------

 Statistic of Inv. Genomic- A22 Matrix
                           N      Mean        Min        Max        Var
     Diagonal           1294    11.606      4.746     40.310     21.707
     Off-diagonal    1673142    -0.009    -12.500      6.396      0.211

*-------------------------*
* Setup Genomic Done !!! *
*-------------------------*
```

Parameter file for PREGSF90 with quality control

```
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       1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
   2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
  0.30000
OPTION SNP_file snp.txt
OPTION map_file map.txt
```

Log file for PREGSF90 with quality control

```
name of parameter file?
renf90.par

     preGS 1.10

 Parameter file:             renf90.par
 Data file:                  renf90.dat
 Number of Traits             1
 Number of Effects            2
 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                                                   1
 2  cross-classified     3                                                6100

 Residual (co)variance Matrix
 0.70000

 Random Effect(s)    2
 Type of Random Effect:      additive animal
 Pedigree File:              renadd02.ped
 trait   effect    (CO)VARIANCES
  1        2    0.3000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

Options read from parameter file:

 * SNP file: snp.txt
 * SNP Xref file: snp.txt_XrefID
 * Map file: map.txt

 *---------------------------------------------------------------*
 *                 Genomic Library: Version 1.164                *
 *                                                               *
 *                   Optimized OpenMP Version                    *
 *                                                               *
 *  Modified relationship matrix (H) created for effect:   2     *
 *---------------------------------------------------------------*

 Read 6100 animals from pedigree file: "renadd02.ped"
 Number of Genotyped Animals: 1294

 Creating A22
```

```
   Extracting subset of: 2312 pedigrees from: 6100 elapsed time:     0.0160
   Calculating A22 Matrix by Colleau OpenMP...elapsed time: .0189
   Numbers of threads=8 16

Reading SNP file
   Column position in file for the first marker: 8
   Format to read SNP file: (7x,400000i1)
   Number of SNPs: 1000
   Number of Genotyped animals: 1294
   Reading SNP file elapsed time: .06

Statistics of alleles frequencies in the current population
   N:           1000
   Mean:       0.504
   Min:        0.043
   Max:        0.929
   Var:        0.032

Reading MAP file: "map.txt" - 1000 SNPs out of 1000

   Min and max # of chromosome: 1 5

   Min and max # of SNP: 1 1000

Quality Control - SNPs with Call Rate < callrate ( 0.90) will removed: 0

Quality Control - SNPs with MAF < minfreq ( 0.05) will removed: 1

Quality Control - Monomorphic SNPs will be removed: 0

Quality Control - Removed Animals with Call rate < callrate ( 0.90): 0

Quality Control - Check Parent-Progeny Mendelian conflicts

   Total animals: 6100 - Genotyped animals: 1294 - Effective: 1294

   Number of pairs Individual - Sire: 450
   Number of pairs Individual - Dam: 440
   Number of trios Individual - Sire - Dam: 206

   No sex Chromosome information is available
   Parent-progeny conflicts or HWE could eliminate SNPs in sex Chr
   Provide map information and sex Chr to checks using autosomes

Checking SNPs for Mendelian conflicts

   Total number of effective SNP: 999
   Total number of parent-progeny evaluations: 890
   Number of SNPs with Mendelian conflicts: 0

Checking Animals for Mendelian conflicts

   Total number of effective SNP for checks on Animals: 999

   Number of Parent-Progeny Mendelian Conflicts: 0

Number of effective SNPs (after QC): 999

Number of effective Indiviuals (after QC): 1294

Statistics of alleles frequencies in the current population after
Quality Control (MAF, monomorphic, call rate, HWE, Mendelian conflicts)
```

```
   N:            999
   Mean:       0.504
   Min:        0.051
   Max:        0.929
   Var:        0.032

Genotypes missings (%):  0.100

Genotypes missings after cleannig (%):  0.000

Calculating G Matrix
   Dgemm MKL #threads=     8   16 Elapsed omp_get_time:     0.9840

Scale by Sum(2pq). Average:   435.140185710293

Blend G as alpha*G + beta*A22: (alpha,beta)     0.950     0.050

Frequency - Diagonal of G
   N:        1294
   Mean:        0.999
   Min:         0.895
   Max:         1.469
   Range:       0.029
   Class:     20

 #Class       Class   Count
      1  0.8951        27
      2  0.9238       109
      3  0.9524       304
      4  0.9811       379
      5   1.010       285
      6   1.038       137
      7   1.067        32
      8   1.096        14
      9   1.125         3
     10   1.153         1
     11   1.182         0
     12   1.211         2
     13   1.239         0
     14   1.268         0
     15   1.297         0
     16   1.325         0
     17   1.354         0
     18   1.383         0
     19   1.411         0
     20   1.440         1
     21   1.469         0

Check for diagonal of genomic relationship matrix

Check for diagonal of genomic relationship matrix, genotypes not removed: 0

------------------------------
 Final Pedrigree-Based Matrix
------------------------------

Statistic of Rel. Matrix A22
                          N      Mean       Min       Max       Var
    Diagonal           1294     1.001     1.000     1.250     0.000
    Off-diagonal    1673142     0.005     0.000     0.750     0.001

----------------------
```

```
 Final Genomic Matrix
---------------------

Statistic of Genomic Matrix
                          N      Mean       Min       Max       Var
    Diagonal           1294     1.001     0.898     1.470     0.002
    Off-diagonal    1673142     0.005    -0.158     0.791     0.002

Correlation of Genomic Inbreeding and Pedigree Inbreeding
    Correlation:     0.2180

All elements - Diagonal / Off-Diagonal
   Estimating Regression Coefficients G = b0 11' + b1 A + e
   Regression coefficients b0 b1 =      0.000     0.991

   Correlation all elements G & A     0.717

Off-Diagonal
   Using 83426 elements from A22 >= .02000

   Estimating Regression Coefficients G = b0 11' + b1 A + e
   Regression coefficients b0 b1 =     -0.003     0.999

   Correlation Off-Diagonal elements G & A     0.777

Creating A22-inverse
   Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1068
----------------------
 Final A22 Inv Matrix
---------------------

Statistic of Inv. Rel. Matrix A22
                          N      Mean       Min       Max       Var
    Diagonal           1294     1.851     1.067     5.812     0.431
    Off-diagonal    1673142    -0.001    -1.200     0.600     0.001

Creating G-inverse
   Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1047

-------------------------
 Final Genomic Inv Matrix
-------------------------

Statistic of Inv. Genomic Matrix
                          N      Mean       Min       Max       Var
    Diagonal           1294    13.466     5.863    45.587    28.023
    Off-diagonal    1673142    -0.010   -13.521     6.897     0.227

Check for diagonal of Inverse Genomic - Inverse of pedigree relationship matrix

Saving GimA22i in file: "GimA22i"

------------------------------
 Final G Inv - A22 Inv Matrix
------------------------------

Statistic of Inv. Genomic- A22 Matrix
                          N      Mean       Min       Max       Var
    Diagonal           1294    11.615     4.782    40.309    21.740
    Off-diagonal    1673142    -0.009   -12.521     6.397     0.211

*------------------------*
```

```
* Setup Genomic Done !!! *
*------------------------*
```

Parameter file for PREGSF90 with quality control, removing SNP from chromosome 5 and saving the clean SNP file

```
 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        1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
    2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.30000
OPTION SNP_file snp.txt
OPTION map_file map.txt
OPTION excludeCHR 5
OPTION saveCleanSNPs
```

Log file for PREGSF90 with quality control, removing SNP from chromosome 5 and saving the clean SNP file

```
name of parameter file?
renf90.par

     preGS 1.10

 Parameter file:             renf90.par
 Data file:                  renf90.dat
 Number of Traits             1
 Number of Effects            2
 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                                                    1
 2  cross-classified     3                                                 6100
 Residual (co)variance Matrix
 0.70000

 Random Effect(s)    2
 Type of Random Effect:      additive animal
 Pedigree File:              renadd02.ped
 trait   effect    (CO)VARIANCES
  1       2    0.3000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

Options read from parameter file:

 * SNP file: snp.txt
 * SNP Xref file: snp.txt_XrefID
 * Map file: map.txt
 * Save Clean SNP data to (SNP_file)_clean file (default .false.)
 * Exclude Chromosomes (default .false.): 5

 *-------------------------------------------------------------*
 *                 Genomic Library: Version 1.164              *
 *                                                             *
 *                   Optimized OpenMP Version                  *
 *                                                             *
 *  Modified relationship matrix (H) created for effect:   2    *
 *-------------------------------------------------------------*

 Read 6100 animals from pedigree file: "renadd02.ped"
 Number of Genotyped Animals: 1294

 Creating A22
    Extracting subset of: 2312 pedigrees from: 6100 elapsed time:     0.0150
    Calculating A22 Matrix by Colleau OpenMP...elapsed time: .0190
    Numbers of threads=8 16

 Reading SNP file
    Column position in file for the first marker: 8
    Format to read SNP file: (7x,400000i1)
    Number of SNPs: 1000
    Number of Genotyped animals: 1294
    Reading SNP file elapsed time: .06

 Statistics of alleles frequencies in the current population
    N:           1000
    Mean:       0.504
    Min:        0.043
    Max:        0.929
    Var:        0.032

 Reading MAP file: "map.txt" - 1000 SNPs out of 1000

    Min and max # of chromosome: 1 5

    Min and max # of SNP: 1 1000

 Excluded 199 SNPs from 1 chromosomes: 5

 Quality Control - SNPs with Call Rate < callrate ( 0.90) will removed: 199
 Quality Control - SNPs with MAF < minfreq ( 0.05) will removed: 1

 Quality Control - Monomorphic SNPs will be removed: 0

 Quality Control - Removed Animals with Call rate < callrate ( 0.90): 0

 Quality Control - Check Parent-Progeny Mendelian conflicts

    Total animals: 6100 - Genotyped animals: 1294 - Effective: 1294

    Number of pairs Individual - Sire: 450
    Number of pairs Individual - Dam: 440
    Number of trios Individual - Sire - Dam: 206

    No sex Chromosome information is available
    Parent-progeny conflicts or HWE could eliminate SNPs in sex Chr
    Provide map information and sex Chr to checks using autosomes

 Checking SNPs for Mendelian conflicts

    Total number of effective SNP: 801
    Total number of parent-progeny evaluations: 890
    Number of SNPs with Mendelian conflicts: 0

 Checking Animals for Mendelian conflicts

    Total number of effective SNP for checks on Animals: 801

    Number of Parent-Progeny Mendelian Conflicts: 0

 Number of effective SNPs (after QC): 801
```

Number of effective SNP was reduced to 801 after removing chromosome 5

```
Number of effective Indiviuals (after QC): 1294

Statistics of alleles frequencies in the current population after
Quality Control (MAF, monomorphic, call rate, HWE, Mendelian conflicts)
   N:             801
   Mean:        0.503
   Min:         0.051
   Max:         0.928
   Var:         0.032

List of SNPs removed in: "snp.txt_SNPs_removed"

Clean genotype file was created: "snp.txt_clean"
```

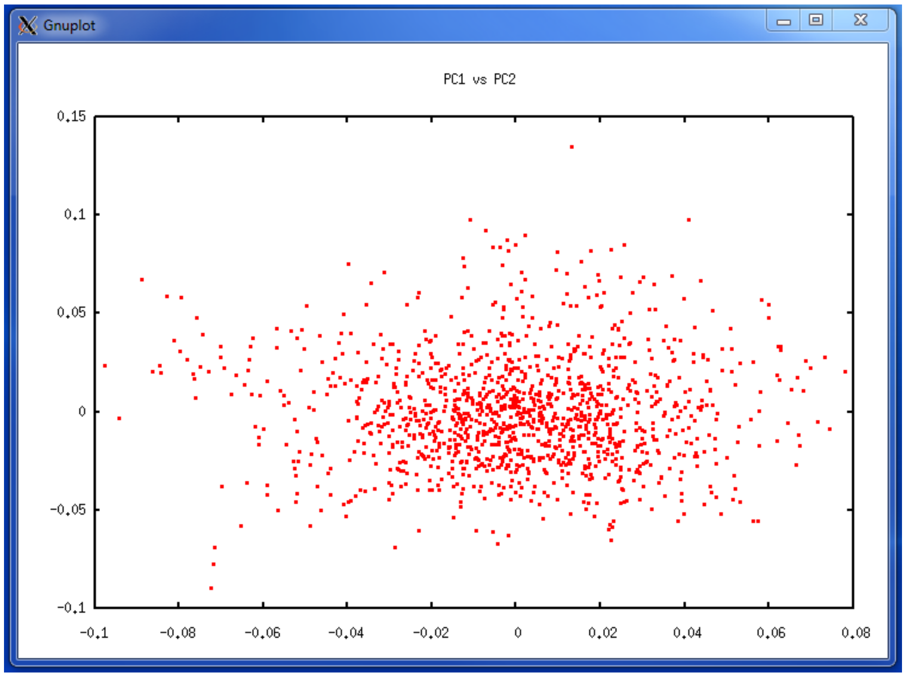
New files with clean genotypes

```
Cross reference ID file was created: "snp.txt_clean_XrefID"

Genotypes missings (%): 19.900

Genotypes missings after cleannig (%):  0.000

Calculating G Matrix
   Dgemm MKL #threads=     8   16 Elapsed omp_get_time:     0.8764

Scale by Sum(2pq). Average:   349.571560214902

Blend G as alpha*G + beta*A22: (alpha,beta)     0.950     0.050

Frequency - Diagonal of G
   N:         1294
   Mean:         1.000
   Min:         0.874
   Max:         1.593
   Range:       0.036
   Class:     20

 #Class       Class   Count
      1  0.8741         17
      2  0.9100        107
      3  0.9460        341
      4  0.9819        419
      5   1.018        281
      6   1.054         98
      7   1.090         20
      8   1.126          4
      9   1.162          4
     10   1.198          1
     11   1.234          0
     12   1.270          1
     13   1.306          0
     14   1.342          0
     15   1.377          0
     16   1.413          0
     17   1.449          0
     18   1.485          0
     19   1.521          0
     20   1.557          1
     21   1.593          0

Check for diagonal of genomic relationship matrix

Check for diagonal of genomic relationship matrix, genotypes not removed: 0

------------------------------
 Final Pedrigree-Based Matrix
------------------------------

Statistic of Rel. Matrix A22
                           N      Mean       Min       Max       Var
    Diagonal            1294     1.001     1.000     1.250     0.000
    Off-diagonal     1673142     0.005     0.000     0.750     0.001

----------------------
 Final Genomic Matrix
----------------------

Statistic of Genomic Matrix
                           N      Mean       Min       Max       Var
    Diagonal            1294     1.001     0.876     1.593     0.002
    Off-diagonal     1673142     0.005    -0.169     0.861     0.003

Correlation of Genomic Inbreeding and Pedigree Inbreeding
    Correlation:     0.2092

All elements - Diagonal / Off-Diagonal
   Estimating Regression Coefficients G = b0 11' + b1 A + e
   Regression coefficients b0 b1 =      0.000     0.991

   Correlation all elements G & A     0.677

Off-Diagonal
   Using 83426 elements from A22 >= .02000
```

```
    Estimating Regression Coefficients G = b0 11' + b1 A + e
    Regression coefficients b0 b1 =     -0.002     0.996

    Correlation Off-Diagonal elements G & A     0.742

 Creating A22-inverse
    Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1409

 ----------------------
  Final A22 Inv Matrix
 ----------------------

 Statistic of Inv. Rel. Matrix A22
                           N       Mean        Min        Max        Var
     Diagonal           1294      1.851      1.067      5.812      0.431
     Off-diagonal    1673142     -0.001     -1.200      0.600      0.001

 Creating G-inverse
    Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1370

 --------------------------
  Final Genomic Inv Matrix
 --------------------------

 Statistic of Inv. Genomic Matrix
                           N       Mean        Min        Max        Var
     Diagonal           1294     17.075      7.840     56.092     43.645
     Off-diagonal    1673142     -0.013    -16.499      8.893      0.309

 Check for diagonal of Inverse Genomic - Inverse of pedigree relationship matrix

 Saving GimA22i in file: "GimA22i"

 ------------------------------
  Final G Inv - A22 Inv Matrix
 ------------------------------

 Statistic of Inv. Genomic- A22 Matrix
                           N       Mean        Min        Max        Var
     Diagonal           1294     15.223      6.759     51.043     35.648
     Off-diagonal    1673142     -0.012    -15.499      8.393      0.289

*-------------------------*
* Setup Genomic Done !!! *
*-------------------------*
```

Parameter file for PREGSF90 with quality control and PCA analysis

Include extra option: **OPTION plotpca**



Parameter file for BLUPF90 without genomic information

```
DATAFILE
 renf90_5.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        1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
   2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.30000
OPTION conv_crit 1e-15
```

renf90_5.dat has phenotypes for all animals, but generation 5

Linux code to remove phenotypes for those animals:
$awk '{ if ($4==5) print 0,$2,$3,$4; else print $1,$2,$3,$4}' renf90.dat > renf90_5.dat

Default convergence criteria = 1e-12

Log file for BLUPF90 without genomic information

```
name of parameter file?
```

```
renf90.par
 * convergence criterion (default=1e-12):  1.0000000E-15

     BLUPF90 1.48

 Parameter file:             renf90.par
 Data file:                  renf90_5.dat
 Number of Traits             1
 Number of Effects            2
 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                                                    1
 2  cross-classified     3                                                 6100

 Residual (co)variance Matrix
 0.70000

 Random Effect(s)    2
 Type of Random Effect:      additive animal
 Pedigree File:              renadd02.ped
 trait   effect    (CO)VARIANCES
  1       2    0.3000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

 Data record length =            3
 # equations =         6101
 G
 0.30000
 read         6100  records in   1.4997000E-02  s,                    12201
  nonzeroes
  read          6100  additive pedigrees
 finished peds in   1.9996000E-02  s,                    27178  nonzeroes
round =     1  convergence =  0.1730E-03
round =     2  convergence =  0.7971E-03
round =     3  convergence =  0.5923E-04
round =     4  convergence =  0.6219E-04
round =     5  convergence =  0.2122E-04
        .
        .
        .
round =    40  convergence =  0.1230E-13
round =    41  convergence =  0.3164E-14
round =    42  convergence =  0.2804E-14
round =    43  convergence =  0.1081E-14
round =    44  convergence =  0.5761E-15
   44 iterations,   convergence criterion= 0.5761E-15
 solutions stored in file: "solutions"
```

Solutions for BLUPF90 without genomic information

```
trait/effect level  solution
   1   1         1      1.02176505
   1   2         1     -0.24665178
   1   2         2      0.16420973
   1   2         3      0.32371581
   1   2         4      0.00318130
   1   2         5     -0.13277100
```

The solution file (solutions) has 4 columns:

1) Trait [only 1 trait in this example]
2) Effect [we have 2 effects: overall mean (effect 1) and additive genetic direct (effect 2)]
3) Level [number of the level for each effect in the model]
4) Solution

EBV accuracy

If accuracy of EBV is desired, it can be calculated based on standard errors (se) for EBV. **BLUPF90** has an option for calculating se:

OPTION sol se

Solutions for BLUPF90 with option to calculate se

```
trait/effect level  solution          s.e.
   1   2         1      1.02176504      0.02496866
   1   2         1     -0.24665117      0.39158195
   1   2         2      0.16421026      0.40488662
   1   2         3      0.32371755      0.29405286
   1   2         4      0.00318218      0.38229658
   1   2         5     -0.13277154      0.46566701
```

The solution file now includes a 5th column with EBV standard errors

Parameter file for BLUPF90 with genomic information (ssGBLUP)

```
DATAFILE
 renf90_5.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       1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
    2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.30000
OPTION SNP_file snp.txt
OPTION map_file map.txt
OPTION conv_crit 1e-15
```

Log file for BLUPF90 with genomic information (ssGBLUP)

```
name of parameter file?
renf90.par
 * convergence criterion (default=1e-12):  1.0000000E-15


Options read from parameter file:

 * SNP file: snp.txt
 * SNP Xref file:snp.txt_XrefID
 * Map file: map.txt
     BLUPF90 1.48

 Parameter file:             renf90.par
 Data file:                  renf90_5.dat
 Number of Traits             1
 Number of Effects            2
 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                                                 1
 2  cross-classified     3                                              6100

 Residual (co)variance Matrix
 0.70000

 Random Effect(s)    2
 Type of Random Effect:      additive animal
 Pedigree File:              renadd02.ped
 trait   effect    (CO)VARIANCES
  1       2    0.3000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

 Data record length =            3
 # equations =         6101
 G
 0.30000
 read         6100  records in   0.1499770      s,                   12201
  nonzeroes
  read         6100  additive pedigrees

 *--------------------------------------------------------------*
 *                 Genomic Library: Version 1.164               *
 *                                                              *
 *                   Optimized OpenMP Version                   *
 *                                                              *
 *  Modified relationship matrix (H) created for effect:   2    *
 *--------------------------------------------------------------*

 Read 6100 animals from pedigree file: "renadd02.ped"
 Number of Genotyped Animals: 1294

 Creating A22
```

```
   Extracting subset of: 2312 pedigrees from: 6100 elapsed time:     0.0150
   Calculating A22 Matrix by Colleau OpenMP...elapsed time: .0346
   Numbers of threads=8 16

Reading SNP file
   Column position in file for the first marker: 8
   Format to read SNP file: (7x,400000i1)
   Number of SNPs: 1000
   Number of Genotyped animals: 1294
   Reading SNP file elapsed time: .06

Statistics of alleles frequencies in the current population
   N:           1000
   Mean:       0.504
   Min:        0.043
   Max:        0.929
   Var:        0.032

Reading MAP file: "map.txt" - 1000 SNPs out of 1000

   Min and max # of chromosome: 1 5

   Min and max # of SNP: 1 1000

Quality Control - SNPs with Call Rate < callrate ( 0.90) will removed: 0

Quality Control - SNPs with MAF < minfreq ( 0.05) will removed: 1

Quality Control - Monomorphic SNPs will be removed: 0

Quality Control - Removed Animals with Call rate < callrate ( 0.90): 0

Quality Control - Check Parent-Progeny Mendelian conflicts

   Total animals: 6100 - Genotyped animals: 1294 - Effective: 1294

   Number of pairs Individual - Sire: 450
   Number of pairs Individual - Dam: 440
   Number of trios Individual - Sire - Dam: 206

   No sex Chromosome information is available
   Parent-progeny conflicts or HWE could eliminate SNPs in sex Chr
   Provide map information and sex Chr to checks using autosomes

Checking SNPs for Mendelian conflicts

   Total number of effective SNP: 999
   Total number of parent-progeny evaluations: 890
   Number of SNPs with Mendelian conflicts: 0

Checking Animals for Mendelian conflicts

   Total number of effective SNP for checks on Animals: 999

   Number of Parent-Progeny Mendelian Conflicts: 0

Number of effective SNPs (after QC): 999

Number of effective Indiviuals (after QC): 1294

Statistics of alleles frequencies in the current population after
Quality Control (MAF, monomorphic, call rate, HWE, Mendelian conflicts)
```

```
   N:            999
   Mean:       0.504
   Min:        0.051
   Max:        0.929
   Var:        0.032

Genotypes missings (%):  0.100

Genotypes missings after cleannig (%):  0.000

Calculating G Matrix
   Dgemm MKL #threads=     8   16 Elapsed omp_get_time:     1.0240

Scale by Sum(2pq). Average:   435.140185710293

Blend G as alpha*G + beta*A22: (alpha,beta)     0.950     0.050

Frequency - Diagonal of G
   N:        1294
   Mean:        0.999
   Min:         0.895
   Max:         1.469
   Range:       0.029
   Class:     20

 #Class       Class   Count
      1  0.8951          27
      2  0.9238         109
      3  0.9524         304
      4  0.9811         379
      5   1.010         285
      6   1.038         137
      7   1.067          32
      8   1.096          14
      9   1.125           3
     10   1.153           1
     11   1.182           0
     12   1.211           2
     13   1.239           0
     14   1.268           0
     15   1.297           0
     16   1.325           0
     17   1.354           0
     18   1.383           0
     19   1.411           0
     20   1.440           1
     21   1.469           0


Check for diagonal of genomic relationship matrix


Check for diagonal of genomic relationship matrix, genotypes not removed: 0

------------------------------
 Final Pedrigree-Based Matrix
------------------------------

Statistic of Rel. Matrix A22
                          N      Mean       Min       Max       Var
    Diagonal           1294     1.001     1.000     1.250     0.000
    Off-diagonal    1673142     0.005     0.000     0.750     0.001
 ---------------------
  Final Genomic Matrix
 ---------------------

 Statistic of Genomic Matrix
                           N      Mean       Min       Max       Var
     Diagonal           1294     1.001     0.898     1.470     0.002
     Off-diagonal    1673142     0.005    -0.158     0.791     0.002


 Correlation of Genomic Inbreeding and Pedigree Inbreeding
     Correlation:     0.2180

All elements - Diagonal / Off-Diagonal
    Estimating Regression Coefficients G = b0 11' + b1 A + e
    Regression coefficients b0 b1 =      0.000     0.991

    Correlation all elements G & A     0.717

 Off-Diagonal
    Using 83426 elements from A22 >= .02000

    Estimating Regression Coefficients G = b0 11' + b1 A + e
    Regression coefficients b0 b1 =     -0.003     0.999

    Correlation Off-Diagonal elements G & A     0.777


 Creating A22-inverse
    Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1059

 ---------------------
  Final A22 Inv Matrix
 ---------------------

 Statistic of Inv. Rel. Matrix A22
                           N      Mean       Min       Max       Var
     Diagonal           1294     1.851     1.067     5.812     0.431
     Off-diagonal    1673142    -0.001    -1.200     0.600     0.001


 Creating G-inverse
    Inverse LAPACK MKL dpotrf/i  #threads=    8   16 Elapsed omp_get_time:     0.1093

 -------------------------
  Final Genomic Inv Matrix
 -------------------------

 Statistic of Inv. Genomic Matrix
                           N      Mean       Min       Max       Var
     Diagonal           1294    13.466     5.863    45.587    28.023
     Off-diagonal    1673142    -0.010   -13.521     6.897     0.227


 Check for diagonal of Inverse Genomic - Inverse of pedigree relationship matrix
-----------------------------
  Final G Inv - A22 Inv Matrix
 -----------------------------

 Statistic of Inv. Genomic- A22 Matrix
```

```
                           N        Mean         Min         Max         Var
     Diagonal           1294      11.615       4.782      40.309      21.740
     Off-diagonal    1673142      -0.009     -12.521       6.397       0.211


*------------------------*
* Setup Genomic Done !!! *
*------------------------*

hash matrix increased from          131072 to          262144 % filled:      0.8000
hash matrix increased from          262144 to          524288 % filled:      0.8000
hash matrix increased from          524288 to         1048576 % filled:      0.8000
hash matrix increased from         1048576 to         2097152 % filled:      0.8000
 finished peds in    25.61810      s,                  861721  nonzeroes
round =      1  convergence =  0.6397E-03
round =      2  convergence =  0.4280E-03
round =      3  convergence =  0.3112E-03
round =      4  convergence =  0.9994E-04
round =      5  convergence =  0.8129E-04
        .
        .
        .
round =     90  convergence =  0.3590E-14
round =     91  convergence =  0.2549E-14
round =     92  convergence =  0.2022E-14
round =     93  convergence =  0.1453E-14
round =     94  convergence =  0.9599E-15
   94 iterations,   convergence criterion= 0.9599E-15
 solutions stored in file: "solutions"
```

Solutions for BLUPF90 with genomic information (ssGBLUP)

The solution file has the same format as in blupf90 without genomic information. The option for calculating se for EBV can also be used here.

Parameter file for PREDICTF90

Predictivity can be measured as correlation between adjusted phenotypes and (G)EBV. In this example we show how to use PREDICTF90 to adjust phenotypes for genotyped animals in the validation population.

1) Adjusting phenotypes

As this program needs solution file, it can be run in the same folder as BLUP with complete data

Parameter file:

pred.dat is the data file only for genotyped animals in the 5th generation (validation animals). Lines can be extracted from renf90.dat

```
DATAFILE
 pred.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      1 cross
 3    6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
   2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.30000
OPTION include_effects 2
```

Log file for adjusting phenotypes for genotyped animals in 5th generation

```
name of parameter file?
pred.par

 *** include effets to predict Yhat n, effects            1           2
     PREDICTF90 1.3

 Parameter file:             gen.par
 Data file:                  pred.dat
 Number of Traits             1
 Number of Effects            2
 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                                                 1
 2  cross-classified     3                                              6100

 Residual (co)variance Matrix
 0.70000

 Random Effect(s)    2
 Type of Random Effect:      additive animal
 Pedigree File:              renadd02.ped
 trait   effect    (CO)VARIANCES
  1       2    0.3000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
      effects are missing for specified traits

 Data record length =            3
 # equations =          6101
 *** effets to include in Yhat (T/F):  F T
 solutions read from file: soltutions
 Animal Effect:            2
 y(s), yhat(s), residual(s) in written in "yhat_residual" file
         300 records read
 Trait:            1         300
    mean Y        -5.204056186291079E-002  var Y          0.979795877964320
    mean Yhat     -1.187536126623551E-002  var Yhat       7.349890384221654E-002
```

```
   cov (Y,Yhat)   8.232182257800019E-002  corr (Y,Yhat)  0.306765659847626
 wrote bvs for animals in data in file "bvs.dat"
```

Output files from PREDICTF90

yhat_residual

yhat_residual has 4 columns: animal | y | yhat | residual

```
 4644      -0.266520       0.415535       0.339710
 2176      -0.418925       0.094263       0.508577
```

Because OPTION include_effects 2 was used:
y is phenotype minus all effects other than animal
yhat receives the second effect, which is the animal effect
residual is phenotype minus animal effect

bvs.dat

bvs.dat has 4 columns: trait | effect | Animal | solution (EBV)

```
1  2    4644      0.415535
1  2    2176      0.094263
```

Hint: corr (Y,Yhat) from the output of PREDICTF90 (`corr (Y,Yhat)  0.306765659847626`) should not be used as a measure of predictivity because it uses adjusted phenotypes and EBVs from the same dataset. Usually, predictivity requires phenotypes adjusted for fixed effects in the complete data (benchmark) and (G)EBVs calculated from the reduced data (without records for validation animals). The regular predictivity measure is: corr[Y_from_PREDICTf90, (G)EBV_reduced]

For this small example with 1 trait, a general Linux code to merge files is:

```
$awk '{print $1,$2}' ebv_complete/yhat_residual | sort +0 -1 > Y
$awk '{if ($2==2) print $3,$4}' ebv_reduced/solutions | sort +0 -1 > ebv.temp
$awk '{if ($2==2) print $3,$4}' gebv_reduced/solutions | sort +0 -1 > gebv.temp
$join -1 +1 -2 +1 Y ebv.temp > file1.temp
$join -1 +1 -2 +1 file1.temp gebv.temp > Y_ebv_gebv
```

An R code to calculate correlations is:

```
pred <- read.table("Y_ebv_gebv",header=F)
ebv_predictivity <- cor(pred[,2],pred[,3]); ebv_predictivity
gebv_predictivity <- cor(pred[,2],pred[,4]); gebv_predictivity
```

Parameter files for GWAS using ssGBLUP (ssGWAS)

Run BLUPF90 with genomic information and salve G^{-1} and A_{22}^{-1}

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       1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
    2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.30000
OPTION SNP_file snp.txt
OPTION map_file map.txt
OPTION no_quality_control
OPTION saveGInverse
OPTION saveA22Inverse
OPTION weightedG wei
```

Weights for SNP can be updated by an iterative process, where the initial weights are all equal to 1.

Linux code to get initial weights for 1000 SNP:

```
$awk 'BEGIN { for (i==1;i<1000;i++) print 1}' > wei
```

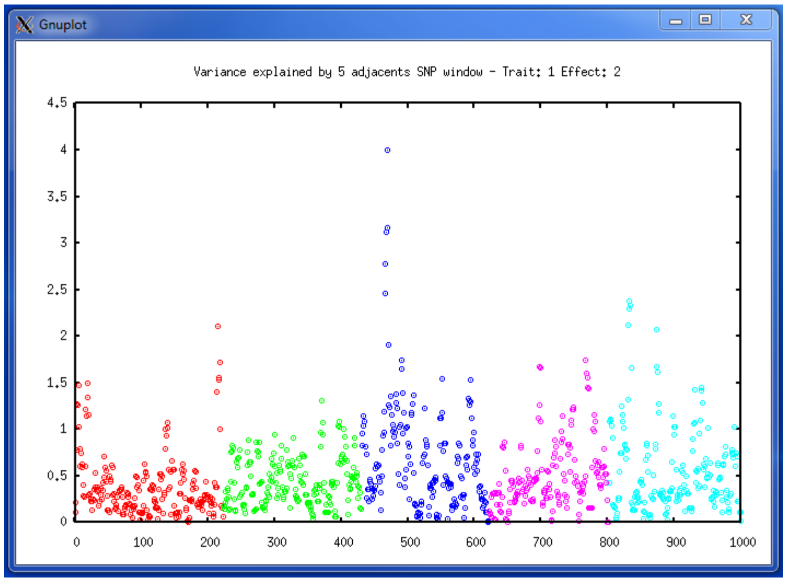
Run POSTGSF90 and read G^{-1} and A_{22}^{-1}

```
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       1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
    2
 RANDOM_TYPE
 add_animal
 FILE
renadd02.ped
(CO)VARIANCES
 0.30000
```

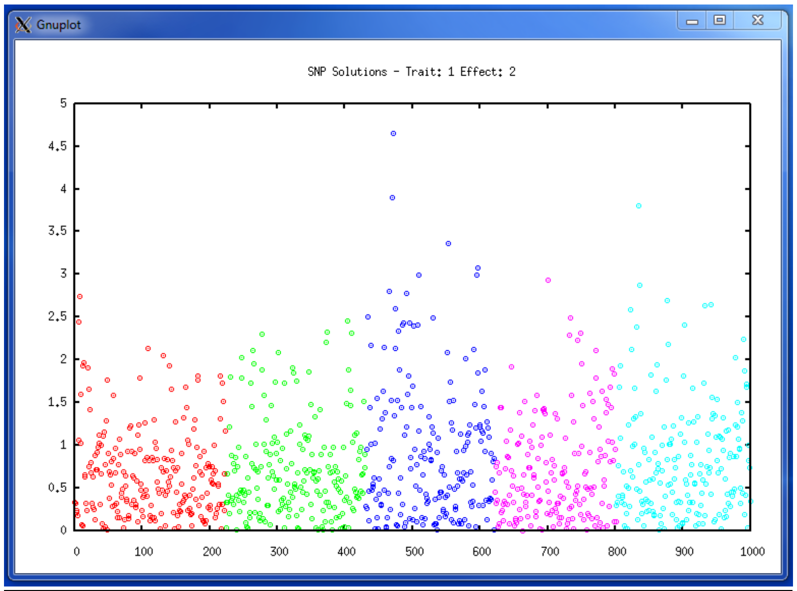
OPTION SNP_file snp.txt
OPTION map_file map.txt
OPTION no_quality_control
OPTION Manhattan_plot
OPTION readGInverse
OPTION readA22Inverse
OPTION weightedG wei
OPTION windows_variance 5

Moving average of SNP effects can be obtained by using the following option:
OPTION SNP_moving_average n
where n is the number of SNP

Manhattan plots for SNP windows variance



Manhattan plots for SNP effect using moving average of 2 SNP



Output files for ssGWAS

snp_sol

```
   1     2     1     1     0   0.7001368E-02   0.2209213      0.1119293     0.1126648E-03
   1     2     2     1     0  -0.1359349E-01   0.5065436      0.2104747     0.2118577E-03
   1     2     3     1     0   0.8714214E-02   0.3917027      0.7757968     0.7808942E-03
   1     2     4     1     0  -0.4223401E-02   0.6873333E-01  1.271113      0.1279465E-02
   1     2     5     1     0   0.5471629E-03   0.1539137E-02  1.261010      0.1269296E-02
```

snp_sol has 9 columns because “OPTION windows_variance” was used:
trait | effect | SNP | chromosome | position | SNP_solution | weight | % of variance explained by n adjacent SNP | variance explained by n adjacent SNP

chrsnpvar

```
  1     2     0.1119293459     1     1     0
  1     2     0.2104747339     2     1     0
  1     2     0.7757968029     3     1     0
  1     2     1.2711127978     4     1     0
  1     2     1.2610103595     5     1     0
```

chrsnpvar has 6 columns:
trait | effect | % of variance explained by n adjacent SNP | SNP | chromosome | position

This file is used by POSTGSF90 for Manhattan plots

Appendix J (custom relationship matrices)

When a relationship (or dispersion) matrix cannot be created within the application programs, it can be prepared separately and then included as a custom relationship matrix. Two options exist for inclusion of such a matrix. Option user_file incorporates this matrix directly. Option user_file_inv incorporates the inverse of this matrix.

The example below presents a model from the previous Appendix with matrix $\mathbf{H}^{-1}$ created externally and then read as a custom matrix. The custom matrix (Hinverse.txt) is stored as below, with each line containing: row, column and value.

```
 1     1   3.0000
 1   422  -1.0000
 1   870   0.5000
 1  4326  -1.0000
 1  4612  -1.0000
 .    .        .
 .    .        .
6096 6100 -0.0527
6097 6097  2.5000
6098 6098 11.0000
6099 6099  2.0000
6100 6100 12.0236
```

Parameter file for BLUPF90 with a custom relationship matrix

```
DATAFILE
 renf90_5.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       1 cross
 3     6100 cross
RANDOM_RESIDUAL VALUES
 0.70000
 RANDOM_GROUP
    2
 RANDOM_TYPE
user_file
 FILE
Hinverse.txt
(CO)VARIANCES
 0.30000
OPTION conv_crit 1e-15
```

Log file for BLUPF90 with a custom relationship matrix

```
name of parameter file?
user.par
 * convergence criterion (default=1e-12):  1.0000000E-15

    BLUPF90 1.48

 Parameter file:           user.par
 Data file:  renf90_5.dat
 Number of Traits           1
 Number of Effects          2
 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                                   1
 2  cross-classified     3                                6100

 Residual (co)variance Matrix
 0.70000

 Random Effect(s)    2
 Type of Random Effect:      user defined from file
 User File:                Hinverse.txt
 trait   effect    (CO)VARIANCES
  1       2    0.3000

 REMARKS
  (1) Weight position 0 means no weights utilized
  (2) Effect positions of 0 for some effects and traits means that such
     effects are missing for specified traits

 Data record length =          3
 # equations =        6101
 G
 0.30000
 read        6100  records in   4.7991998E-02  s,                 12201  nonzeroes
…
 g_usr_inv: read       855620  elements
 largest row, column, diagonal:       6100       6100       6100
…
 finished peds in    1.776729       s,                861721  nonzeroes
round =     1  convergence =  0.5737E-03
…
round =    80  convergence =  0.9128E-15
   80 iterations,   convergence criterion= 0.9128E-15
 solutions stored in file: "solutions"
```

The name of custom matrix used is shown here

Appendix K (selected programming details)

This section provides some programming insights into an early version of the blupf90 program. The model is completely described in the module MODEL.

```
module model
implicit none

!        Types of effects
integer,parameter::effcross=0,& !effects can be cross-classified
                   effcov=1     !or covariables

!        Types of random effects
integer,  parameter ::  g_fixed=1,&       ! fixed effect
                        g_diag=2, &       ! diagonal
                        g_A=3, &          ! additive animal
                        g_A_UPG=4, &      ! additive animal with unknown
                                          !       parent groups
                      & g_A_UPG_INB=5, &  ! additive animal with unknown
                                          !       parent groups and inbreeding
                      & g_As=6,&          ! additive sire
                        g_PD =7, &         ! parental dominance
                        g_last=8          ! last type

character (40)     ::   parfile, &     !name of parameter file
                        datafile       !name of data set

integer :: ntrait,&                  !number of traits
           neff,&                    !number of effects
           miss=0                      !value of missing trait/effect


integer,allocatable :: pos_y(:)        !positions of observations
integer ::             pos_weight      ! position of weight of records; zero if none


integer,allocatable :: pos_eff(:,:),&  !positions of effects for each trait
                       nlev(:),&       !number of levels
                       effecttype(:),& !type of effects
                       nestedcov(:,:),&!position of nesting effect for each trait
                                       ! if the effect is nested covariable
                     & randomtype(:),& ! status of each effect, as above
                       randomnumb(:)   ! number of consecutive correlated effects

character (40),allocatable::  randomfile(:)   ! name of file associated with given
                                                   ! effect

real, allocatable  ::  r(:,:),&        !residual (co)variance matrix
                       rinv(:,:),&     ! and its inverse
                       g(:,:,:)      ! The random (co)variance matrix for each trait
end module model
```

The core of the program is presented below.

```
program BLUPF90
use model;use sparsem; use sparseop
implicit none
real,allocatable :: y(:),&                          ! observation value
                    indata(:)                       ! one line of input data

real ::             weight_y                        ! weight for records

type (sparse_hashm)::xx               ! X'X in sparse hash form
type (sparse_ija):: xx_ija           ! X'X in IJA form, for use with FSPAK only
real, allocatable:: xy(:),sol(:)        !X'Y and solutions

real,allocatable :: weight_cov(:,:)
integer,allocatable:: address(:,:)      ! start and address of each effect
integer :: neq,io,&                     ! number of equations and io-status
           data_len,&                   ! length of data record to read
           i,j,k,l                      ! extra variables
real::  val, dat_eff

!
call read_parameters
call print_parameters
neq=ntrait*sum(nlev)
data_len=max(pos_weight,maxval(pos_y),maxval(pos_eff))
print*,'Data record length = ',data_len
allocate (xy(neq), sol(neq),address(neff,ntrait),&
          weight_cov(neff,ntrait),y(ntrait),indata(data_len))
call zerom(xx,neq); xy=0
!
call setup_g                    ! invert R matrices

open(50,file=datafile)         !data file

! Contributions from records
do
   read(50,*,iostat=io)indata
   if (io.ne.0) exit
   call decode_record
   call find_addresses
   call find_rinv
   do i=1,neff
       do j=1,neff
          do k=1,ntrait
             do l=1,ntrait
                 val=weight_cov(i,k)*weight_cov(j,l)*weight_y*rinv(k,l)
                 call addm(val,address(i,k),address(j,l),xx)
             enddo
          enddo
       enddo
       do k=1,ntrait
          do l=1,ntrait
              xy(address(i,k))=xy(address(i,k))+rinv(k,l)*y(l)*weight_cov(i,k) &
                                                          *weight_y
          enddo
       enddo
   enddo
enddo
!
!     Random effects' contributions
do i=1,neff
   select case (randomtype(i))
     case (g_fixed)
        continue                ! fixed effect, do nothing
     case (g_diag)
        call add_g_diag(i)
     case (g_A, g_As, g_A_UPG,g_A_UPG_INB)
        call add_g_add(randomtype(i),i)
     case (g_PD)
        call add_g_domin(i)
     case default
       print*,'unimplemented random type',randomtype(i)
   endselect
enddo

if (neq < 15) then
   print*,'left hand side'
   call printm(xx)
   print  '( '' right hand side:'' ,100f8.1)',xy
endif
```

```
 call solve_iterm(xx,xy,sol)

! Comment the line above and uncomments the lines below only if
! solutions by FSPAK are desired
!xx_ija=xx;
!call fspak90(‘solve’,xx_ija,xy,sol)


if (neq <15) print  '( '' solution:'' ,100f7.3)',sol

call store_solutions
```

Modules and Libraries

Module DENSEOP

Subroutines and functions for dense matrix manipulation in Fortran 90.
Uses F90 LAPACK implementation by Alan Miller for some low level routines.

Written by: Tomasz Strabel & Ignacy Misztal, University of Georgia e-mail: strabel@au.poznan.pl, ignacy@uga.edu, Oct/5/98-June 8, 2006

The module implements matrix operations on dense general and symmetric matrices. Each subroutine/function is overloaded to work with several types of arguments. The module is primarily designed for matrix operations where timing and memory requirements are not critical.

Symmetric matrices

Each of the functions/subroutines works with full-stored and packed (half-stored) matrices. Each matrix or vector can be single or double precision. However, in one function/subroutine, all arguments should be of the same precision, and all matrices should be stored the same way.

Subroutines

`call chol(a,rank)`	- Cholesky decomposition
`call inverse_s(A,rank)`	- Generalized inverse: AI = A-
`call eigen(A,d,V)`	- Eigenvalues and eigenvectors: A =V diag(d)*V'
`call solve_s(A,b,x)`	- Generalized solutions: x: Ax=b

The optional variable rank returns the rank of the matrix.

Functions

`fchol(A)`	- Cholesky decomposition
`finverse_s(A)`	- Generalized inverse
`fsolve_s(A,b)`	- Generalized solve
`fdet_s(A)`	- Determinant of A

Procedures for symmetric matrices work with generalized matrices. Redundant rows/columns equations are determined by operational zero, which is kept in global variable denseop_tol with default value is 10-

10. To change the limit, change the value of the variable in the application program, e.g., denseop_tol=1d-12

Conversions

Let A be a square matrix and AP be a packed matrix

`call packit(A,AP)` - Conversion from square to packed form; only lower-diagonal elements are used.
`call unpackit(AP,A)` - Conversion from packed to square form; the matrix is assumed symmetric.

General matrices

Each matrix or vector can be single or double precision. However, in one function/subroutine, all arguments should be of the same precision. All matrices are assumed full-rank.

Subroutines

`call inverse(A)` - Inverse: AI = A-1 call solve(A,b,x) - Solutions: x: Ax=b

Functions

`AI=finverse(A)` - Returns inverse: AI = Ax=fsolve(A,b) - Computes solutions: x: Ax=b

Printing

`call printmat(matrix, text, fmt, un)` print any type of matrix using the specified format fmt and preceded by text. Both text and fmt are optional. If optional un is present, the output is send to file with unit un.
Warning: The printmat function prints the symmetric packed matrices in full. If a half-stored matrix is in packed form, it will be printed as full-stored matrix.

Additional subroutines and functions

The subroutine(s) and functions below work only with double precision arguments (r8) and fullstored matrices.
`call pos_def(x,text,min_eig,stat)` Corrects X if it is not “sufficiently” positive-definite; ignores rows/columns with 0 elements only.

X - real (r8) symmetric square matrix

text - optional character variable that is printed if X is corrected min_eig - optional real (r8) variable that sets the minimum relative eigenvalue in X; if min_eig is missing, 1e-5 is used.

stat - optional logical variable that is set to .true. if X was corrected and .false. if not.

`A = diag(b)` - creates square diagonal real (r8) matrix with values of real (r8) vector b on diagonal

`b = diag(A)` - creates real (r8) vector b containing diagonals of real (r8) matrix A

`A=kron(B,C)` - A = B “Kronecker product” C; works with real(r4) and real (r8) matrices

Technical details

The basic operations are done in full storage and double precision. Operations with other formats and precision are obtained by conversions. Computing of eigenvalues/eignevectors and general matrix operations use parts of LAPACK subroutines as converted by Alan Miller. These subroutines may contain many more functionality than necessary and may be trimmed to reduce size of the object code.

The modules consist of two files:
lapack90r.f90 - Part of LAPACK denseop.f90 - Interfaces, subroutines, functions and conversion codes.
For compilation, module kind in file kind.f90 that contains definitions of single and double precision is also needed.

In the BLUPF90 distribution, these files are included in directory libs and are compiled as denseop.a. One way to use the denseop module is via a Makefile from an application program in the blupf90 package.

Example (exdense.f90)

Program Example:

```
use kinds; use denseop
real (r4):: xpacked4(3)=(/1,3,10/)     ! Symmetric packed single
precision
real (r4)::x4(2,2)    ! Full single precision
real (r8)::x8(2,2)    ! Full double precision
call printmat(xpacked4,’ X ‘)
call printmat(fchol(xpacked4),’ Cholesky(X) ‘,’(10(f10.2))')
x4=xpacked4
x8=x4
print*,’ Determinant(xpacked4)=’,fdet_s(xpacked4)
print*,’ Determinant(x8)=’,fdet_s(x8)
print*,’ Determinant(x4)=’,fdet_s(x4)
end
```

Compilation

To compile standalone:

```
      f90 kind.f90 lapack90r.f90 denseop.f90 exdense.f90
```

This assumes that all files are in the same directory.
To compile in subdirectory of the blupf90 distribution under Linux/Absoft,

```
      f90 -p  ../libs exdense.f90  ../libs/denseop.a
```

where option -p specifies library directory. This option (-p) is different under different platforms. See documentation on blupf90 distribution for details.

Module SPARSEM

Collection of sparse matrix modules for Fortran 90 useful in animal breeding problems

Written by: Ignacy Misztal, University of Georgia e-mail: ignacy@uga.edu,
9/4/1997 - 5/25/2007

Introduction

Traditionally, programming in animal breeding is done in 2 stages: in a matrix language and in a regular programming language. Programs in a matrix language such as IML SAS, Matlab, Mathematica or APL are reasonably simple and useful for creating examples but inefficient for large problems. Programs in a regular programming language such as Fortran or C/C++ are much more efficient but could take much longer to write and require substantial training.

Matrix languages are easy to deal with matrices partly because usually only one format is usually supported: dense rectangular. Operations on such matrices are easy to specify and program, but large matrices require large memory and long running time. Also, memory and computations are equal whether matrices are sparse (contain very few nonzero elements) or not. In animal breeding, many matrices are sparse. If that sparsity is taken into account, the memory requirements and computations can decrease dramatically. Unfortunately, there is more than one format for storing sparse matrices, and some computations are fast with one format and but not with another one. Also, the storage formats and operations are considerably more complicated than dense rectangular matrices. A library to handle multiple matrix formats and multiple operations would contain many subroutines, each with a long list of arguments. Such a library would involve considerable learning, and many details associated with the library would create many opportunities for making a mistake.

One matrix package, Matlab, has some forms of sparse-matrix storage and operations included.

Modern programming languages with "object-oriented" features, such as C++ or Fortran 90, have abilities to create classes/modules, where many implementation details on specific data structures can be hidden. A technique called overloading allows single function/subroutine to work with different formats of its arguments. Therefore, the number of details to remember can be drastically reduced. Subsequently, programming can be done much easier and quicker.

SPARSEM is a module for Fortran 90 that enables programming common sparse matrix operations almost as easily as with dense matrices. It supports two dense matrix formats, useful for testing, and two sparse matrix formats. Changing a program from dense to sparse-matrix format using DENSEM can be as simple as changing one declaration line. SPARSEM incorporates an interface to FSPAK, which enables efficient sparse matrix factorization, solving, sparse inversion and calculation of determinant on matrices much larger than possible with dense matrix structures.

Matrix formats

Four matrix formats are available.
DENSEM - dense square matrix.
DENSE_SYMM -dense symmetric upper-stored.
    It has approximately only half memory requirements of the dense square matrix.
SPARSE_HASHM - sparse triple accessed by hash algorithm.
    This is a very efficient format for set-up and for iterative-solving of sparse matrices.
SPARSE_IJA - Sparse IJA.
    This is a memory-efficient format for sparse matrices used by sparse matrix packages. Format IJA cannot easily be set up directly but can be derived by conversion from the hash format.

For more information on all these formats see Duff et al, George and Liu, or my class notes.

A popular format that is not included here is linked list. That format is reasonably efficient for creating and computing with sparse matrices if the number of nonzero elements per row is not too high and the matrix is not too large. However, the combination of hash plus ija is generally more efficient.

Matrix operations

The following subroutines/functions are supported. All real scalars and vectors are single precision unless indicated otherwise.

Operation	**Description**	**Comments**
call init(x)	Initialize x	Required by standard but usually not necessary because on most systems pointers are initialized automatically
call zerom(x,n)	Allocate storage for x as an n*n matrix and zero it	If x was set before, it is reallocated[1]

call reset(x)	Deallocates storage	
call addm(a,i,j,x)	Add to matrix: x(i,j)=x(i,j)+a	Does not work on SPARSE_IJA
call setm(a,i,j,x)	sets element of matrix: x(i,j)=a	Does not work on SPARSE_IJA
y=getm(i,j,x)	find element of matrix: y=x(I,j)	real(4) function; returns lower-diagonal elements of upper-stored matrix
x=y	Conversion between formats	Conversion from sparse to dense formats may require too much storage
call printm(x)	Prints x as square matrix	print(x,'internal') prints sparse matrices in internal format
call solve_iterm(x,rs,sol)	Solves: x sol=rs iteratively by SOR	
call default_iter (conv,maxround,relax, zerosol)	Changes default iteration parameters	All parameters are optional; default values are: conv(ergence criterion)=1e-10, max round(s)=1000, relax(ation factor)=1.0, zerosol(utions ar beginning of iteration) = .true.
x=block(y,i1,i2,j1,j2)	Selects block from y: x=y(i1:i1,j1:j2)	does not work on dense_symm format; may not work with unsymmetric blocks from symmetric matrices
q=quadrf(u,x,v)	q=u'Xv	real(8) function; does not work on dense_symm format
tr=trace(x,y)	Self explanatory	real(8) function; x and y must be in same formats; works on densem and sparse_ija formats only
tr=traceblock(x,y,i1,i2,j1, j2)	tr=trace(xy(i1:i2,j1:j2))	Works as a block-trace combination; produces correct results when blocks of y are nonsymmetric

[1]The hash matrix is allocated for a default number of elements. If the default is too small, the hash matrix is enlarged automatically. To change the default p elements, use call zerom(x,n,p). One matrix element in hash format takes 12 bytes, and for efficient operation there should be at least 10% more nonzero elements available than used.

All operations assume that the densem type is general while all the other types are upperstored.

Operations tr, quadf work with both upper- and full-stored matrices but the block operation works literally, i.e., selecting a lower block would return an empty matrix and selecting an upper block would return only an upper-stored matrix. This could be a source of incompatibility between densem and other formats that use the block operation without taking its limitations into consideration. Potential problems can be noticed in examples by printing matrices of interest.

Storage type

Matrices in the hash or ija format are half-stored by default. To change the storage type to full, add the option 'f' to the addm subroutine: `call addm(a,i,j,x,'f')`

The subsequent conversion to the ija format will also be full-stored. For conversion from half-stored hash matrix to full-stored ija, please see a documentation for the GIBBS module.

The printing and other functions/subroutines have been designed for half-stored hash and ija matrices. Results may not be correct with full-stored matrices.

Numerical accuracy

Module KINDS defines precision r4 to be equivalent to real*4, and r8 to be equivalent to r8. Precision rh can be set up to r4 or r8 dependent on whether memory or precision is more important.

Formats DENSEM, DENSE_SYMM, and SPARSE_IJA use precision r8. Format
SPARSE_HASHM uses precision rh. Whenever the precision of numbers in SPARSEM functions/subroutines is not specified, it is of type rh. Setting rh to r4 is useful when memory usage needs to be reduced, e.g., for large BLUP programs. Setting rh to r8 is necessary when numerical accuracy is important, e.g., in variance component programs, and is usually a safer choice.

Diagnostics

Printing of some diagnostic messages depends on the value of an integer variable sparsem_msg. The value of 3 means maximum diagnostic messages while the value of 0 means no diagnostic messages. The default is 2. This variable can be set in any part of the application program using the module SPARSEM.

FSPAK90

FSPAK is a sparse matrix package written in F77 that performs operations on sparse matrices in format SPARSE_IJA. Operations include solving a system of linear equations by factorization, calculating a (log)determinant or finding a sparse inverse of a matrix. A sparse inverse is such a matrix that contains inverse values only for those elements that were nonzero in the original matrix. For sparse matrices, FSPAK is very efficient computationally.

FSPAK90 is a F90 interface written to simplify the use of FSPAK.

A complete call to FSPAK90 is:

```
      call fspak90(operation,ija,rs,sol,det,msglev,maxmem,rank)
```

where

operation=	"factorize"	- calculate sparse factorization
	"invert"	- calculate sparse inverse
	"solve"	- solve a system of equation
	"reset"	- reset the storage
	"det"	- calculate determinant
	"stat"	- print statistics
	"fact_mult"	- multiplication by Cholesky factor of the reordered matrix (if LL=IJA; sol=L*rs)
	"inv_fact_mult"	- solve the system formed by the Cholesky factor of the reordered matrix (sol: L*sol=rs)

ija = matrix in SPARSE_IJA form
rs = real (r4) or (r8) vector of right hand side,
sol = real (r4) or (r8), identical to precision of rs, vector of solutions
det = real (r8) determinant or log-determinant
msglev= message level from 0 (minimum) to 3 (maximum); default=0 maxmem=maximum memory available in the system; default=infinite
rank=rank of matrix

All the arguments of fspak90 except "operation" and "ija" are optional except when they are needed in a specific "operation". Thus, rs and sol are needed for solving and det for "det" or "ldet".

Examples:

To solve:

```
      call fspak90('solve',ija,rs,sol)
```

for both rs and sol either in single or double precision; all. Preceding steps are done automatically.

To solve using double precision right hand side and solutions:
```
       call fspak90('solve',ija,rs8=rs,sol8=sol)
```
To sparse invert:
```
       call fspak90('invert',ija)
```
To obtain the determinant d:
```
       call fspak90('det',ija,det=d)
```
To obtain the log determinant ld:
```
       call fspak90('ldet',ija,det=ld)
```
To obtain rank r with any operation:
```
       call fspak90(.....,rank=r)
```
To force new factorization, when the input matrix has changed: `call`
```
       fspak90('factor',ija)
```
To deallocate the internal memory:
```
       call fspak90('reset')
```
To limit memory to a maximum od maxmem, e.g., 20,000k, with any operation `call`
```
       fspak90(..............,maxmem=20000)
```

Note that only relevant arguments for each step need to be included in calling FSPAK90. Reordering is performed the first time when FSPAK90 is called. Subsequent factorization except after the option "reset" will reuse the ordering. Subsequent solves will reuse the factorization.
Additionally:

To sample y from N(0,A) where x~N(0,1)
```
       call fspak90('fact_mult',A,rs8=x,sol8=y)
```
To sample y from N(0,A^{-1}) where x~N(0,1)
```
       call fspak90('inv_fact_mult',A,rs8=x,sol8=y)
```
For details of the last operations, see Appendix S2

Additional subroutines and functions:

Function

y=mult(A,x)

y=mult(x,A)

Implements the matrix by vector multiplication for all matrix formats except dense_symm, and for double precision x and y.

Subroutine

call multmatscal(A,x)

Implements A=A*x for all matrix formats except dense_symm, and for double precision x.

<u>Hints on using SPARSEM</u>

Initially all the matrices can be implemented in DENSEM format. After the program works well with an example, convert all data structures for potentially large matrices to sparse formats and verify that same results are obtained.

Compiling

Matrix types and functions subroutine are defined in module sparsem. Subroutine fspak90 is in module sparseop. Program xx.f90 can be compiled as

```
      f90 -Maa xx.f90 aa/sparsem.a
```

where aa is the directory containing the modules and the library, and M is the option to include module directory.

Beginning in May, 1999, SPARSEM is part of a programming package that includes BLUPF90, REMLF90, GIBSF90 etc. Compilation for several Unix environments is automated by makefiles. To find details, read Readme and Installation files in the package distributions. To create application with SPARSEM and possibly other modules, create a subdirectory in the main directory of the package, and adapt a makefile from the existing directory, e.g., blup.

Sample Programs

Dense matrix solution program

```
program test_sparse_structures use
sparsem; use kinds type (densem)::x
integer,parameter ::n=5
integer :: i,j
real (rh):: rs(n),sol(n),val

call init(x)
call zerom(x,n)

! set up a sample matrix do
i=1,n
  rs(i)=n+1-i
  val=10.0*i/i
  call addm(val,i,i,x)
  do j=i+1,n
    val=10.0*i/j
    call addm(val,i,j,x); call addm(val,j,i,x)
  enddo
enddo
```

```
print*,'rs: ',rs print*,'matrix' ; call printm(y) call
solve_iterm(y,rs,sol) !solve iteratively
print*,'sol: ',sol
end
```

Triangular dense matrix iterative-solution program

```
......
type (dense_symm)::x
.......
```

(The rest of the program remains identical)

Sparse hash matrix iterative-solution program

```
......
type (sparse_hashm)::x
.......
```

Sparse IJA matrix iterative-solution program

Matrix in ija form cannot be set up directly but can be converted from hash form.

```
......
type (sparse_hashm)::x type
(sparse_ija)::y
...
y=x         !conversion
call reset(x) ! Optional statement to release storage
print*,'rs: ',rs print*,'matrix' ; call printm(y) call
solve_iterm(y,rs,sol)

end
```

Sparse IJA matrix finite-solution and inversion program with FSPACK90

```
...
use sparsem use sparseop !fspak90 is in module sparseop .....
call fspak90('solve',y,rs,sol) ....
!now invert call
fspak90('invert',y)
call printm(y)
end
```

References

George, A. and Liu, J.W.H. (1981) Computer solution of large sparse positive definite systems. Prentice-Hall, Englewood Cliffs, N.J.

Appendix S1

Definitions of structure (type)

```
type densem     !traditional dense square matrix
      integer :: n
      real(8) ,pointer::x(:,:)
end type densem

type dense_symm       !upper stored symmetric dense matrix
      integer ::n
      real(8) ,pointer::x(:)
end type dense_symm

type sparse_hashm
    integer:: n,&         ! for compatibility mainly
              nel,&       ! number of elements             filled,&
              ! number of filled elements            status      !
              1 if ready to hash, 2 if in sorted
                          ! order
real (rh) , pointer :: x(:,:)
end type sparse_hashm

type sparse_ija
     integer :: n,&      ! number of equations
                nel      ! number of nonzeroes
      integer, pointer::ia(:),ja(:)    !will be ia(n+1), ja(m)
      real (8), pointer::a(:)          !will be a(m)
end type
```

Accessing structures

Structures can be accessed within the application program using the "%" symbol. This is useful, e.g., when using Fortran 77 programs. The example below shows how to use a determinant program written in F77.

```
type (densem):: z
integer::i,j
real (rh)::value

call init(z)
call zerom(x,2)
```

```
! initialize z
do i=1,2
   do j=1,2
     value=i**j/10.
     call addm(value, i,j,z)
   enddo
enddo

print*, det(z%n,z%x)
end

function det(n,x)
!calculate determinant for a 2x2 matrix
integer n
real (r8):: x(n,n),det !
det= x(1,1)*x(2,2)/x(1,2)/x(2,1)
end
```

Library

The following files are compiled into the library:

kind.f90	- definitions of precisions
sparse.f90	- type definitions + main subroutines,
sparse2.f	- supporting subroutines (in f77),
fspak.f90	- f90 interface to fspak
fspak.f	- main fspak subroutine (in f77),
fspaksub.f	- supporting fspak subroutines (in f77),
sparssub.f	- low-level subroutines from the book of George and Liu (in f77),
second.f	- timing subroutine specific to each computer (in f77).

Subroutines second() specific to other computers can be found in the FSPAK manual.

Appendix S2

Multiplication and solving using factors

Let A be a matrix. Factorization produced by FSPAK is L:

A=P'LL'P

where P is a reordering matrix chosen to minimize the size of L:

PP'=P'P=I

Operation "fact_mult" multiplies the factor by a vector:

y=P' L P x

Operation " inv_fact_mult" solves the system of equation:

P'L' Py=x

This is equivalent to:

y= P' (L'^{-1}) Px

Both operations were programmed by Juan Pablo Sanchez. The operations are useful for generation of large random samples from a multivariate normal distribution. They may be useful in Gibbs sampler algorithms when setting up and factorization of the system of equations in each round are feasible.

Module Prob

Probability routines for use in threshold models and Gibbs sampling

Written by: Ignacy Misztal and Deukhwan Lee, University of Georgia e-mail: ignacy@uga.edu, 04/29/99-04/19/2001

Module Prob is a collection of random number generators / probabilities / truncated distributions useful for Gibbs sampling and for threshold models. The module uses features of Fortran 90 to simplify programnming and high-level optimization to reduce running time, with simplicity being as important as efficiency. To understand the module fully, please read the documentation on SPARSEM and on BLUPF90.

Module prob uses high-quality generators from public domain package RANLIB for random number generators. Some low level code is from Luis Varona.

Subroutines/functions

call set_seed(n)
Sets seed for random number generator to integer n. If this subroutine is not called, the seed will be selected by the system.

```
x=gen_uniform(a,b)
```
a,b - both real (r*) or both integers or both missing.
If a,b are missing, generates samples from uniform(0,1) distribution
If a,b are real (r8), generates samples from uniform(a,b) distribution
If a,b are integers, generates random integer between a and b

```
x=gen_normal(mean,var)
```
mean - (r8) scalar or vector
var - (r8) scalar or square matrix
x - (r8) scalar or square matrix
Generates x=N(mean,Var) when mean and var are scalars, or x=MVN(mean,Var) when mean is a vector and Var is a matrix. Arguments mean and var are optional. If they are missing, sampling is from N(0,1)

```
x=gen_invwishart(inv_q_form,df)
```
inv_q_form - (r8) scalar or square matrix containing inverse of quadratic form
df - an integer containing degrees of freedom
Generates samples from inverted chi square or inverted Wishart distributions.

```
y=normal(x)
```
x - real(r8) scalar
y - real (r8) contains density(X) for N(0,1)

```
y=normal_cdf(x)
```
x - real (r8) scalar
y - real (r8) cumulative distribution function for N(0,1)

```
y=normal_invcdf(x)
```
x - real (r8) scalar in the range of <0,1>
y - real (r8) as in: x=normal_cdf(y)

```
y=generate_trunc_normal(a,b,mean,var)
```
y - real (r8) scalar or vector
a,b - real (r8) lower and upper bound of random samples
mean - real(r8) scalar or vectors of mean, optional if scalar
var - real(r8) variance or covariance matrix, optional if scalar

If mean and var are missing, generates random samples from N(0,1) distribution truncated to interval <a,b>.

If mean and var are scalars, generates random samples from N(mean,var) distribution truncated to interval <a,b>.

If mean is a vector and var is a matrix, generates random samples from MVN(mean,var) distribution with first dimension truncated to interval <a,b>.

Other functions/subroutines

New functions/subroutines are added to Module prob periodically. Please see program prob.f90 for details.

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