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MultiPEM Toolbox: User Manual

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1 Introduction

This document explains use of the **Multi-P**henomenology **E**xplosion **M**onitoring (Multi-PEM) Toolbox, a collection of `R` scripts for estimating the unknown device parameters of a new event with uncertainty quantification. The methodology and application used for illustration in this user manual are fully documented in a Los Alamos National Laboratory technical report[1] hereafter designated "WPA" for reference. Additional details on the application are found in a recent journal article[2]. Two assessment types are available: *rapid* and *complete*.

Rapid assessments are conducted in two stages, as described in Section 2. In the first stage, benchmark data are used to estimate forward and error model parameters (WPA, §5.1) and (if relevant) errors-in-variables yield values for benchmark sources (WPA, §3, Equation (3)). Forward model parameters can be of two types: specific to signature within phenomenology and even emplacement condition, or global across more than one signature within phenomenology or across phenomenologies. In the second stage, new event data are used to estimate the unknown new event device parameters (WPA, §5.2) with uncertainty quantification.

Two options for treating the inferred first stage parameters in second stage Bayesian analysis are available: fixing them at their maximum likelihood estimate (default), or multiple imputation[3]. Multiple imputation involves utilizing several posterior samples (imputations) of the first stage parameters as fixed values in the second stage posterior sampling of the new event device parameters. Second stage sampling is conducted across imputations in parallel to improve computational efficiency. This method produces improved uncertainty quantification of the new event device parameters compared with the default treatment of the first stage parameters, at the expense of additional computation.

Complete assessments are conducted in a single stage, as described in Section 3. Benchmark and (if relevant) new event data are used simultaneously to estimate all forward model,

[1] Williams, B.J., Picard, R.R., & Anderson, D.N. (2023). Multi-phenomenology Yield Characterization. Los Alamos National Laboratory Technical Report LA-UR-23-21950 (rev.1).

[2] Ford, S.R., Bulaevskaya, V., Ramirez, A., Johannesson, G., & Rodgers, A.J. (2021). Joint Bayesian inference for near-surface explosion yield and height-of-burst, *J Geophys Res Solid Earth* 126:e2020JB020968.

[3] Plummer, M. (2015). Cuts in Bayesian graphical models, *Stat Comput* 25:37-43.

error model, and (if relevant) errors-in-variables yields and new event device parameters with uncertainty quantification on the latter.

As the name suggests, rapid assessments generally run substantially faster than complete assessments (even with multiple imputation), because the results of first stage analysis can be stored and incorporated into estimating a relatively low-dimensional space of new event device parameters whenever relevant new event data becomes available. On the other hand, complete assessments must be run on the full set of model and device parameters with benchmark and new event data every time the latter becomes available.

1.1 Running An Application in MultiPEM Toolbox

MultiPEM Toolbox applications can be run directly in `R`, or through Docker. The latter is useful if a common run environment is desired for multiple users. Details are provided here for the former, followed by brief remarks on the latter in the next subsection.

Begin with the following initial steps:

- Install the latest version of `R`
- Install the following auxillary `R` packages
  - `Matrix`
  - `numDeriv`
  - `doFuture`
  - `adaptMCMC`
  - `FME`
  - `abind` (optional for Sequential Monte Carlo (SMC) sampling)
  - `ramcmc` (optional for SMC sampling)

  For example, to install the `Matrix` package, run the command

  ```
  > install.packages("Matrix")
  ```

  inside an `R` session. The `FME` package requires `R` version 4.0 or higher (through its dependency on the `MASS` package) and its function `modMCMC` is used as the default posterior sampler in the run files associated with the rapid (`runMPEM_0.r`) and complete (`runMPEM.r`) assessments. If an older version of `R` is used, the `iMCMC` command in these run files should be changed from `"FME"` to `"RAM"`.
- Unpack the MultiPEM Toolbox package into the directory

  ```
  % ~/MultiPEM_Toolbox_Package
  ```

There are two MultiPEM analyses contained in the illustrative application (WPA, §6), named `3-Phen` and `4-Phen` below. The former estimates new event device parameters based on fusion of data from the *seismic*, *acoustic*, and *optical* phenomenologies, while the latter performs this same task but with addition of the *surface effects* (*crater*) phenomenology.

1.1.1 Rapid Assessments

The following steps may be invoked in sequential order to run the MultiPEM Toolbox on the illustrative application for rapid assessments. A similar workflow will pertain to any application. This application uses a single core for likelihood/posterior maximization and posterior sampling. Computation time can be significantly reduced by utilizing the multi-core options for these tasks as described in Section 2.

1. Create a symbolic link to the global code directory

```
% cd ./MultiPEM_Toolbox_Package/Runfiles
% # link to global code (used by all applications)
% ln -s ../Code/ Code
```

2. Create symbolic links to the application ("IYDT") data and code directories

```
% cd IYDT
% # link to application (IYDT) data files
% ln -s ../../Applications/Data/IYDT/ Data
% # link to application code (used by IYDT application)
% ln -s ../../Applications/Code/IYDT/ Code
```

3. Run the first stage analysis for each single phenomenology

   - Seismic (phenomenology 1)

```
% cd Seismic
% # link to phenomenology code (used by seismic
% # phenomenology to specify prior distribution
% # of the forward model coefficients (and its gradient))
% ln -s ../../../Applications/Code/IYDT/Phenomenology/ Code
% cd I-SUGAR-hob-0
% R CMD BATCH runMPEM.r runMPEM.out &
% # check status
% tail runMPEM.out
% # upon completion of run (~2 hours), copy
% # .RData file for use in all relevant future
% # seismic second stage rapid assessments
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% cp .RData .RData-s
```

   - Acoustic (2)

```
% cd ../../Acoustic/I-SUGAR-hob-0
% R CMD BATCH runMPEM.r runMPEM.out &
% # check status
```

```
% tail runMPEM.out
% # upon completion of run (~35 minutes), copy
% # .RData file for use in all relevant future
% # acoustic second stage rapid assessments
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% cp .RData .RData-a
```

- Optical (3)

```
% cd ../../Optical/I-EIV-SUGAR-hob-0
% R CMD BATCH runMPEM.r runMPEM.out &
% # check status
% tail runMPEM.out
% # upon completion of run (~1 hour), copy
% # .RData file for use in all relevant future
% # optical second stage rapid assessments
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% cp .RData .RData-o
```

- Surface Effects/Crater (4)

```
% cd ../../Crater
% # link to phenomenology code (used by crater
% # phenomenology to specify prior distribution
% # of log-yield (and its gradient))
% ln -s ../../../Applications/Code/IYDT/Phenomenology/ Code
% cd I-EIV-SUGAR-0
% R CMD BATCH runMPEM.r runMPEM.out &
% # check status
% tail runMPEM.out
% # upon completion of run (~5 minutes), copy
% # .RData file for use in all relevant future
% # crater second stage rapid assessments
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% cp .RData .RData-c
```

The `runMPEM.r` and `runMPEM.out` files are described in Section 2.1. The status of running code is checked by issuing the following command in the run directory,

```
% tail runMPEM.out
```

Successfully completed runs show the results of the `proc.time()` command at the end of the `runMPEM.out` file. Symbolic links are created to a phenomenology-specific code directory for `Seismic` and `Crater` prior to conducting the runs (see comments in above code). The `.RData` files resulting from each completed analysis should be copied and stored for use in relevant future second stage analyses (see comments in above code). Upon completion of these runs, copy each resulting `opt.RData` file to the `Opt` directory in each MultiPEM analysis, to be used as starting values for MultiPEM log-likelihood maximization.

```
% cd ../../3-Phen/Opt
% cp ../../Seismic/I-SUGAR-hob-0/opt.RData opt_1_0.RData
% cp ../../Acoustic/I-SUGAR-hob-0/opt.RData opt_2_0.RData
% cp ../../Optical/I-EIV-SUGAR-hob-0/opt.RData opt_3_eiv_0.RData
% cd ../../4-Phen/Opt
% cp ../../Seismic/I-SUGAR-hob-0/opt.RData opt_1_0.RData
% cp ../../Acoustic/I-SUGAR-hob-0/opt.RData opt_2_0.RData
% cp ../../Optical/I-EIV-SUGAR-hob-0/opt.RData opt_3_eiv_0.RData
% cp ../../Crater/I-EIV-SUGAR-0/opt.RData opt_4_eiv_0.RData
```

4. Run the second stage analysis for each single phenomenology, copying the `.RData` file from the first stage analysis into the run directories if necessary. For example, the two directories

   `./MultiPEM_Toolbox_Package/Runfiles/IYDT/Seismic/I-SUGAR-hob-0`

   `./MultiPEM_Toolbox_Package/Runfiles/IYDT/Seismic/I-SUGAR-hob-pi-0`

   contain two MultiPEM analyses for the new event device parameters. The first assumes a “flat” prior on these parameters, while the second assumes an informative prior (WPA, §6.6, pp. 18-19). However, both analyses use the same first stage results. To perform the second stage run for the informative prior, the first stage `.RData` file is copied into the run directory,

```
% cd ./MultiPEM_Toolbox_Package/Runfiles/IYDT/Seismic/I-SUGAR-hob-pi-0
% cp ../I-SUGAR-hob-0/.RData-s .RData
```

   and the analysis is run in the `I-EIV-SUGAR-hob-pi-0` directory as shown below.

   - Seismic (phenomenology 1)

```
% # noninformative prior distribution on new event
% # device parameters
% cd ../../Seismic/I-SUGAR-hob-0
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
% # informative prior distribution on new event
% # device parameters
% cd ../I-SUGAR-hob-pi-0
% cp ../I-SUGAR-hob-0/.RData-s .RData
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
```

```
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
```

- Acoustic (2)

```
% # noninformative prior distribution on new event
% # device parameters
% cd ../../Acoustic/I-SUGAR-hob-0
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
% # informative prior distribution on new event
% # device parameters
% cd ../I-SUGAR-hob-pi-0
% cp ../I-SUGAR-hob-0/.RData-a .RData
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
```

- Optical (3)

```
% # noninformative prior distribution on new event
% # device parameters
% cd ../../Optical/I-EIV-SUGAR-hob-0
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
% # informative prior distribution on new event
% # device parameters
% cd ../I-EIV-SUGAR-hob-pi-0
% cp ../I-EIV-SUGAR-hob-0/.RData-o .RData
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
```

- Surface Effects/Crater (4)

```
% # noninformative prior distribution on new event
% # device parameters
% cd ../../Crater/I-EIV-SUGAR-0
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
```

```
% # informative prior distribution on new event
% # device parameters
% cd ../I-EIV-SUGAR-pi-0
% cp ../I-EIV-SUGAR-0/.RData-c .RData
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
```

The `runMPEM_0.r` and `runMPEM_0.out` files are described in Section 2.2.

5. Run the first stage MultiPEM analysis (illustrated here for `4-Phen`)

```
% cd ../../4-Phen
% # link to phenomenology code (used by seismic
% # phenomenology to specify prior distribution
% # of the forward model coefficients (and its gradient))
% ln -s ../../../Applications/Code/IYDT/Phenomenology/ Code
% cd I-EIV-SUGAR-hob-0
% R CMD BATCH runMPEM.r runMPEM.out &
% # upon completion of run (~7 hours), copy
% # .RData file for use in all relevant future
% # multiPEM second stage rapid assessments
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% cp .RData .RData-4
```

The `runMPEM.r` and `runMPEM.out` files are described in Section 2.1. A symbolic link is created to a phenomenology-specific code directory prior to conducting the run (see comments in above code). The `.RData` file resulting from the completed analysis should be copied and stored for use in future second stage analyses (see comments in above code).

6. Run the second stage MultiPEM analyses, copying the `.RData` file from the first stage analysis into the run directories if necessary.

```
% # noninformative prior distribution on new event
% # device parameters
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
% # informative prior distribution on new event
% # device parameters
% cd ../I-EIV-SUGAR-hob-pi-0
% cp ../I-EIV-SUGAR-hob-0/.RData-4 .RData
% # if necessary, change iMCMC to "RAM" in runMPEM_0.r
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
```

```
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM_0.out file
```

The `runMPEM_0.r` and `runMPEM_0.out` files are described in Section 2.2.

1.1.2 Complete Assessments

The following steps may be invoked in sequential order to run the MultiPEM Toolbox on the illustrative application for complete assessments. A similar workflow will pertain to any application. This application uses a single core for likelihood/posterior maximization and posterior sampling. Computation time can be significantly reduced by utilizing the multi-core options for these tasks as described in Section 3.

1. Create a symbolic link to the global code directory

   ```
   % cd ./MultiPEM_Toolbox_Package/Runfiles
   % # link to global code (used by all applications)
   % # NOT REQUIRED IF LINK CREATED PREVIOUSLY
   % ln -s ../Code/ Code
   ```

2. Create symbolic links to the application ("IYDT") data and code directories

   ```
   % cd IYDT
   % # link to application (IYDT) data files
   % # NOT REQUIRED IF LINK CREATED PREVIOUSLY
   % ln -s ../../Applications/Data/IYDT/ Data
   % # link to application code (used by IYDT application)
   % # NOT REQUIRED IF LINK CREATED PREVIOUSLY
   % ln -s ../../Applications/Code/IYDT/ Code
   ```

3. Run the benchmark analysis for each single phenomenology

   - Seismic (phenomenology 1)

     ```
     % cd Seismic
     % # link to phenomenology code (used by seismic
     % # phenomenology to specify prior distribution
     % # of the forward model coefficients (and its gradient))
     % # NOT REQUIRED IF LINK CREATED PREVIOUSLY
     % ln -s ../../../Applications/Code/IYDT/Phenomenology/ Code
     % cd I
     % # if necessary, change iMCMC to "RAM" in runMPEM.r
     % R CMD BATCH runMPEM.r runMPEM.out &
     % # check status
     % tail runMPEM.out
     % # a completed run will show the results of proc.time()
     % # at the end of the runMPEM.out file
     ```

   - Acoustic (2)

```
% cd ../../Acoustic/I
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # check status
% tail runMPEM.out
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
```

- Optical (3)

```
% cd ../../Optical/I-EIV
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # check status
% tail runMPEM.out
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
```

- Surface Effects/Crater (4)

```
% cd ../../Crater
% # link to phenomenology code (used by crater
% # phenomenology to specify prior distribution
% # of log-yield (and its gradient))
% # NOT REQUIRED IF LINK CREATED PREVIOUSLY
% ln -s ../../../Applications/Code/IYDT/Phenomenology/ Code
% cd I-EIV
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # check status
% tail runMPEM.out
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
```

The `runMPEM.r` and `runMPEM.out` files are described in Section 3. The status of running code is checked by issuing the following command in the run directory,

```
% tail runMPEM.out
```

Successfully completed runs show the results of the `proc.time()` command at the end of the `runMPEM.out` file. Symbolic links are created to a phenomenology-specific code directory for `Seismic` and `Crater` prior to conducting the runs (see comments in above code; not required to recreate links if they were created previsously, e.g. for rapid assessments). Upon completion of the maximum likelihood estimation component of these runs (typically much earlier than the entire run), copy each resulting `opt.RData` file to the `Opt` directory in each MultiPEM analysis, to be used as starting values for MultiPEM log-likelihood maximization.

```
% cd ../../3-Phen/Opt
```

```
% cp ../../Seismic/I/opt.RData opt_1.RData
% cp ../../Acoustic/I/opt.RData opt_2.RData
% cp ../../Optical/I-EIV/opt.RData opt_3_eiv.RData
% cd ../../4-Phen/Opt
% cp ../../Seismic/I/opt.RData opt_1.RData
% cp ../../Acoustic/I/opt.RData opt_2.RData
% cp ../../Optical/I-EIV/opt.RData opt_3_eiv.RData
% cp ../../Crater/I-EIV/opt.RData opt_4_eiv.RData
```

4. Run the complete analysis for each single phenomenology

   - Seismic (phenomenology 1)

     ```
     % # noninformative prior distribution on new event
     % # device parameters
     % cd ../../Seismic/I-SUGAR-hob
     % # if necessary, change iMCMC to "RAM" in runMPEM.r
     % R CMD BATCH runMPEM.r runMPEM.out &
     % # a completed run will show the results of proc.time()
     % # at the end of the runMPEM.out file
     % # informative prior distribution on new event
     % # device parameters
     % cd ../I-SUGAR-hob-pi
     % # if necessary, change iMCMC to "RAM" in runMPEM.r
     % R CMD BATCH runMPEM.r runMPEM.out &
     % # a completed run will show the results of proc.time()
     % # at the end of the runMPEM.out file
     ```

   - Acoustic (2)

     ```
     % # noninformative prior distribution on new event
     % # device parameters
     % cd ../../Acoustic/I-SUGAR-hob
     % # if necessary, change iMCMC to "RAM" in runMPEM.r
     % R CMD BATCH runMPEM.r runMPEM.out &
     % # a completed run will show the results of proc.time()
     % # at the end of the runMPEM.out file
     % # informative prior distribution on new event
     % # device parameters
     % cd ../I-SUGAR-hob-pi
     % # if necessary, change iMCMC to "RAM" in runMPEM.r
     % R CMD BATCH runMPEM.r runMPEM.out &
     % # a completed run will show the results of proc.time()
     % # at the end of the runMPEM.out file
     ```

   - Optical (3)

     ```
     % # noninformative prior distribution on new event
     ```

```
% # device parameters
% cd ../../Optical/I-EIV-SUGAR-hob
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% # informative prior distribution on new event
% # device parameters
% cd ../I-EIV-SUGAR-hob-pi
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
```

- Surface Effects/Crater (4)

```
% # noninformative prior distribution on new event
% # device parameters
% cd ../../Crater/I-EIV-SUGAR
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% # informative prior distribution on new event
% # device parameters
% cd ../I-EIV-SUGAR-pi
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
```

5. Run the complete MultiPEM analysis (illustrated here for `4-Phen`)

```
% cd ../../4-Phen
% # link to phenomenology code (used by seismic
% # phenomenology to specify prior distribution
% # of the forward model coefficients (and its gradient))
% # NOT REQUIRED IF LINK CREATED PREVIOUSLY
% ln -s ../../../Applications/Code/IYDT/Phenomenology/ Code
% # noninformative prior distribution on new event
% # device parameters
% cd I-EIV-SUGAR-hob
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
% # informative prior distribution on new event
```

```
% # device parameters
% cd ../I-EIV-SUGAR-hob-pi
% # if necessary, change iMCMC to "RAM" in runMPEM.r
% R CMD BATCH runMPEM.r runMPEM.out &
% # a completed run will show the results of proc.time()
% # at the end of the runMPEM.out file
```

The `runMPEM.r` and `runMPEM.out` files are described in Section 3. A symbolic link is created to a phenomenology-specific code directory prior to conducting the run (see comments in above code; not required to recreate links if they were created previously, e.g. for rapid assessments).

1.2 Running MultiPEM Toolbox Through Docker

Applications can be run in the MultiPEM Toolbox through Docker, assuming Docker has been installed on the user's system. The basic steps are stated in the following `README` file,

```
% less ./Runfiles-Docker/README
```

First, a global Docker image is built. This installs the desired version of `R` with the required supporting packages, and incorporates the global subroutines. Second, an application-specific Docker image is built on top of the global image. This incorporates all application relevant subroutines and data. Third, single phenomenology or MultiPEM analysis-specific Docker images are built on top of the application image. These incorporate all run files and (if relevant) `R` data objects containing a starting value for optimization. Finally – for each single phenomenology or MultiPEM analysis – a Docker image is built on top of the analysis image and a Docker container is started to conduct the run, for each use case. Details are provided in the following `README` files for both rapid and complete assessments,

```
% less ./Runfiles-Docker/IYDT/Seismic/README
% less ./Runfiles-Docker/IYDT/Acoustic/README
% less ./Runfiles-Docker/IYDT/Optical/README
% less ./Runfiles-Docker/IYDT/Crater/README
% less ./Runfiles-Docker/IYDT/3-Phen/README
% less ./Runfiles-Docker/IYDT/4-Phen/README
```

As with the analyses of Section 1.1, all single phenomenology runs are conducted first, and (if needed) all optimization results are copied to the MultiPEM `Opt` directories prior to conducting the subsequent MultiPEM runs.

2 Rapid Assessment

Rapid assessments will be illustrated by examining the run files associated with a multi-phenomenology analysis in which signals from four phenomenologies are combined to infer the log-yield and height-of-burst (HOB)/depth-of-burial (DOB) of a near-surface nuclear explosion (WPA, §6).

```
% cd ./Runfiles/IYDT/4-Phen/I-EIV-SUGAR-hob-0
```

Rapid assessments consist of two stages. In the first stage, benchmark data are employed to estimate forward model parameters (e.g. regression coefficients) and error model parameters (e.g. source bias, path bias, observational error covariance), and (if relevant) errors-in-variables yield values of benchmark sources. This stage may be run for one or multiple scenarios of interest upon identification of relevant historical data for each scenario, and the resulting `.RData` file(s) stored for later use in processing new event data.

In the second stage, new event data are processed to infer unknown device parameters (e.g. yield, HOB/DOB, geolocation, event time) with uncertainty quantification. In Bayesian analysis, forward and error model parameters, and (if relevant) benchmark source errors-in-variables yields, may be treated in two ways:

- Fixed at values obtained from the first stage, or
- Imputed using posterior samples from the first stage[4].

Either approach results in rapid assessments being executed with far less compute time than complete assessments. The first approach has the potential consequence of underestimating uncertainty in the unknown device parameters of interest for the new event, which is avoided by selecting the second approach with the expense of additional compute time.

2.1 First Stage

The first stage analysis is defined in the `runMPEM.r` file, provided in the first three sections of Appendix A with line numbers referred to in the ensuing discussion. Appendix A.1 provides the preprocessing component of the first stage, Appendix A.2 provides the code employed to maximize the likelihood function of the benchmark data with respect to the parameters of the forward and error models, while Appendix A.3 provides the code employed to optionally sample the posterior distribution of these parameters.

The first stage analysis is run in batch mode as follows,

```
% R CMD BATCH runMPEM.r runMPEM.out &
```

The main features of the output file `runMPEM.out` are provided in Appendix A.4.

[4]Plummer, M. (2015). Cuts in Bayesian graphical models, *Stat Comput* 25:37-43.

2.1.1 Preprocessing

The preprocessing component of the first stage analysis in Appendix A.1 is primarily responsible for describing features of the benchmark data, and the parameters of the forward and error models.

- Line 12+: Load all R packages utilized by multiple supporting subroutines, most notably log-likelihood and log-prior calculations and their associated gradients.
- Line 23: Specify directory location (relative to run directory) of all global (application independent) subroutines.
- Line 26: Read in code performing first stage preprocessing of benchmark data.
- Line 29: Specify directory location (relative to run directory) of all application-specific subroutines.
- Line 32: Specify root directory (relative to run directory) containing all application-specific benchmark data files.
- Lines 35-38: A scalar or vector specifying the names of benchmark data files for each phenomenology, utilizing an ordering of the phenomenologies (for MultiPEM analysis) that is maintained throughout the input deck (as indicated here in Lines 41-44). Data files are text files (CSV formatted) containing all measured signatures (in the first column(s)) and input covariates (in succeeding column(s)) including all those required in forward and error model calculations. Directories specifying the exact locations of these files relative to the root data directory (Line 32) may also be included in the filenames.
- Line 47: Indicate if forward model parameters global to multiple signatures within phenomenology or across phenomenologies will be modeled. If `TRUE`, nominal values for these parameters may optionally be placed in the benchmark data file(s). If a subset of sources are to be assigned default values for some or all of these parameters, the value `NA` should be assigned to these parameters in the benchmark data file(s) for these sources, and the default values provided in the relevant forward model(s).
- Lines 49-52: If `calp` is `TRUE` (Line 47), provide a string vector of names for each of the global forward model parameters (Line 51).
- Line 55: A scalar or vector specifying the number of observed signatures for each phenomenology; in this example, 2 for each phenomenology.
- Lines 59-66: Specify the number of *common* forward model parameters within each phenomenology (WPA, §5.1, first paragraph). For a given forward model, common parameters maintain the same constant value within signature for every log-likelihood calculation. The `pbeta` object is initialized as a null list with elements for each phenomenology in the proper order (Line 59), initialized to zero vectors of length equal to the number of observed signatures (Line 60). Subsequent lines specify the number of common forward model parameters for each signature within each phenomenology. For example, the *acoustic* forward model for each signature contains 2 common forward

model parameters (Line 62).

- Lines 69-72: Specify if the forward model(s) for any phenomenology depend on event emplacement conditions (Line 69), followed by (if relevant) a vector indicating the number of distinct emplacement conditions considered for each phenomenology in the proper order (Line 71). This specification allows distinct forward model parameters to be associated with different emplacement conditions (as specified subsequently). If `Th` is `TRUE` (Line 69), a factor named `Type` must be present in the benchmark (and new event) data file for each relevant phenomenology, indicating the emplacement condition pertaining to each entry. In this example, the *seismic* and *acoustic* forward model parameters may vary for 3 distinct emplacements ("soft", "hard", and "wet" rock types), while the *optical* and *surface effects* forward models are independent of emplacement condition.

- Lines 76-91: Specify the number of *emplacement* dependent forward model parameters within each phenomenology if relevant (WPA, §5.1, first paragraph). For a given forward model, emplacement parameters remain constant within signature for log-likelihood calculations with a given emplacement condition, but may be modified within signature for each distinct emplacement. The `pbetat` object is initialized as a null list with elements for each phenomenology in the proper order (Line 77), initialized as null lists with elements for each emplacement condition (Line 79) if multiple emplacements are present. Subsequent lines specify the number of forward model parameters for each signature within each emplacement condition for each phenomenology. For example, the *seismic* forward model for each signature within each emplacement contains 5 forward model parameters (Line 84) allowed to vary across emplacements. `pbetat` must be specified if multiple emplacements are present for any phenomenology (at least one element of `Th` is greater than 1).

- Lines 95-110: Specify the location of *common* forward model parameters within the full parameter vector, for phenomenologies possessing both common and emplacement dependent parameters. The `ibetar` object is initialized as a null list with elements for each phenomenology in the proper order (Line 96), initialized as null lists with elements for each signature within each emplacement condition (Line 101) if multiple emplacements are present. Subsequent lines specify the position of common parameters in the full forward model parameter vector, for phenomenologies possessing both common and emplacement dependent forward model parameters. For example, the *acoustic* forward model parameter vector takes common parameter values in its first two positions for each signature within each emplacement condition (Line 107).

- Line 113: Indicate if errors-in-variables yield values for benchmark events will be modeled (WPA, §3, Equation (3); §A.4). If `TRUE`, this allows uncertain yields for benchmark events (often assumed known with certainty) to vary within user-specified guidelines.

- Lines 116-132: If relevant, specify details of errors-in-variables yield models for benchmark events.
  - Line 119: Specify phenomenologies for application of errors-in-variables yield models to benchmark events

- Lines 123-124: Provide the sources subject to errors-in-variables yield models for each phenomenology. The `seiv` object is initialized as a null list with elements for each phenomenology in the proper order (Line 123), with vectors indicating the relevant sources for each relevant phenomenology (Line 124). The `"ALL"` designation indicates that every source in the benchmark data set for the indicated phenomenology will be modeled with an errors-in-variables yield. `seiv` must be specified if `ieiv` is provided.
- Line 127: The standard deviation of the errors-in-variables Gaussian distribution for each benchmark event log-yield. For each event, the mean of this distribution is taken to be its provided (design or measured) log-yield. In this example, a "total" error (3 standard deviations) of 10% in each provided yield is allowed. Note that this error is relative because yields are treated on a logarithmic scale. `eiv_w_sd` must be specified if `ieiv` is provided.

- Lines 136-145: Specify if *source* random effects (WPA, §3, Equation (2); §4; §A.5) should be included in the error model (Line 136). If so, the `pvc_1` object is initialized as a null list with elements for each phenomenology in the proper order (Line 139), initialized to zero vectors of length equal to the number of observed signatures (Line 140). Subsequent lines specify the number of source random effects for each signature within each phenomenology. For example, the *seismic* error model for each signature contains a single source bias term (Line 142). If `pvc_1` is `TRUE` (Line 136), a factor named `Source` may be provided in the benchmark (and new event) data file for each relevant phenomenology, identifying the source pertaining to each entry. This factor must be present if there is more than one data entry for any source. In order to include source random effects in the error model for an observed signature, the benchmark data must contain more than one source, with at least one source containing more than one observation. A warning message will be printed to the log file if one of these conditions is violated.

- Lines 148-162: Specify if *path* random effects (WPA, §3, Equation (2); §4; §A.5), also referred to as *station* random effects, should be included in the error model (Line 148). If so, the `pvc_2` object is initialized as a null list with elements for each phenomenology in the proper order (Line 151), initialized to zero vectors of length equal to the number of observed signatures (Line 152). Subsequent lines specify the number of path random effects for each signature within each phenomenology. For example, the *seismic* error model for each signature contains a single path bias term (Line 154). The type of path random effect desired is specified by the `ptype` object, initialized as a null list with elements for each phenomenology in the proper order (Line 159). If `pvc_2` is `TRUE` (Line 148), a factor named `Path` must be provided in the benchmark (and new event) data file for each relevant phenomenology, identifying the source-to-sensor path pertaining to each entry. In order to include path random effects in the error model for an observed signature, the benchmark data must contain more than one path, with at least one path containing more than one observation. Additionally, specification of crossed path effects (`ptype` is `"Crossed"`) requires the signature to be observed from at least one common path for two or more sources, while specification of level 2 (within source) path effects requires more than one path for at least one source, with more than one observation for at least one of those paths. A warning message will be printed to the log file if one of these conditions is violated.

- Line 166: Indicate if the user is providing code to compute coefficient matrices for *source* or *path* random effects (WPA, §5.1). If `FALSE`, the functions `calc_zmat.r` and `calc_zmat_0.r` located in the global code directory,

  `MultiPEM_Toolbox_Package/Code`

  compute default coefficient matrices for the benchmark and new event data, respectively. If `TRUE`, then two user-provided functions of the same names must be placed in the application code directory; in this example,

  `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  Table 8 shows data for the first two *seismic* benchmark sources in this example.

Table 1: Data for seismic benchmark sources `HRI-1` and `HRI-2`.

`Y1`	`Y2`	`Source`	`Path`	`Type`	`lRange`	`W`	`HOB`
−15.091	−9.252	HRI-1	Path_1	1	6.932	6.291	5
−15.089	−9.180	HRI-1	Path_1	1	6.932	6.291	5
−15.836	−10.218	HRI-1	Path_2	1	7.570	6.291	5
−15.892	−10.180	HRI-1	Path_2	1	7.570	6.291	5
−16.176	−10.557	HRI-1	Path_2	1	7.800	6.291	5
−16.907	−11.366	HRI-1	Path_2	1	8.371	6.291	5
−16.931	−11.338	HRI-1	Path_2	1	8.371	6.291	5
−14.835	−9.199	HRI-2	Path_1	1	6.930	6.291	3
−14.860	−9.184	HRI-2	Path_1	1	6.930	6.291	3
−15.674	−10.089	HRI-2	Path_1	1	7.568	6.291	3
−15.754	−10.197	HRI-2	Path_1	1	7.568	6.291	3
−16.002	−10.530	HRI-2	Path_2	1	7.802	6.291	3
−16.060	−10.605	HRI-2	Path_2	1	7.802	6.291	3
−16.534	−11.115	HRI-2	Path_2	1	8.239	6.291	3
−16.741	−11.230	HRI-2	Path_3	1	8.373	6.291	3
−16.737	−11.288	HRI-2	Path_3	1	8.373	6.291	3
−17.208	−11.656	HRI-2	Path_3	1	8.738	6.291	3

If source and level 2 (within source) path random effects are included in the error model, the source and path bias vectors (WPA, §5.1, p. 7) associated with these sources (with

HRI-1 and HRI-2 designated as 1 and 2) are given by

$$\boldsymbol{E}_{S,11r} = \begin{pmatrix} \boldsymbol{Z}_{11r,1} \\ \boldsymbol{Z}_{11r,2} \end{pmatrix} b^{(S)}_{1r,1} \quad \boldsymbol{E}_{P,11r} = \begin{pmatrix} \boldsymbol{E}_{P,111r} \\ \boldsymbol{E}_{P,112r} \end{pmatrix} = \begin{bmatrix} \boldsymbol{Z}_{111r} & \mathbf{0}_2 \\ \mathbf{0}_5 & \boldsymbol{Z}_{112r} \end{bmatrix} \begin{pmatrix} b^{(P)}_{1r,11} \\ b^{(P)}_{1r,12} \end{pmatrix}$$

$$\boldsymbol{E}_{S,12r} = \begin{pmatrix} \boldsymbol{Z}_{12r,1} \\ \boldsymbol{Z}_{12r,2} \\ \boldsymbol{Z}_{12r,3} \end{pmatrix} b^{(S)}_{1r,2} \quad \boldsymbol{E}_{P,12r} = \begin{pmatrix} \boldsymbol{E}_{P,121r} \\ \boldsymbol{E}_{P,122r} \\ \boldsymbol{E}_{P,123r} \end{pmatrix} = \begin{bmatrix} \boldsymbol{Z}_{121r} & \mathbf{0}_4 & \mathbf{0}_4 \\ \mathbf{0}_3 & \boldsymbol{Z}_{122r} & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \boldsymbol{Z}_{123r} \end{bmatrix} \begin{pmatrix} b^{(P)}_{1r,21} \\ b^{(P)}_{1r,22} \\ b^{(P)}_{1r,23} \end{pmatrix},$$

where the default coefficient matrices are given by

$$\begin{aligned} \boldsymbol{Z}_{11r,1} &= \mathbf{1}_2 & \qquad \boldsymbol{Z}_{111r} &= \mathbf{1}_2 \\ \boldsymbol{Z}_{11r,2} &= \mathbf{1}_5 & \boldsymbol{Z}_{112r} &= \mathbf{1}_5 \\ \boldsymbol{Z}_{12r,1} &= \mathbf{1}_4 & \boldsymbol{Z}_{121r} &= \mathbf{1}_4 \\ \boldsymbol{Z}_{12r,2} &= \mathbf{1}_3 & \boldsymbol{Z}_{122r} &= \mathbf{1}_3 \\ \boldsymbol{Z}_{12r,3} &= \mathbf{1}_3 & \boldsymbol{Z}_{123r} &= \mathbf{1}_3 \end{aligned}$$

for $\mathbf{1}_q$ and $\mathbf{0}_q$ the q-vectors of ones and zeros, respectively. The source and path random effects $\{b^{(S)}_{1r,1}, b^{(S)}_{1r,2}\}$ and $\{b^{(P)}_{1r,11}, b^{(P)}_{1r,12}, b^{(P)}_{1r,21}, b^{(P)}_{1r,22}, b^{(P)}_{1r,23}\}$ are mutually independent realizations of their respective random effects distributions (WPA, §5.1, Equation (5), p. 7). For each signature, this structure indicates that there is a single source bias effect applied to every observation within each source, while observations from each path are adjusted by distinct (and independently distributed) path bias effects (signatures are collected from two and three paths respectively for HRI-1 and HRI-2).

If instead a signature is observed from one or more common source-to-sensor paths across two or more sources, referred to as "crossed paths" (ptype is "Crossed" (Line 159)) – assuming the source-to-sensor paths observed for the sources HRI-1 and HRI-2 are not present for any other source – the path bias vectors ($\boldsymbol{E}_{P,11r}, \boldsymbol{E}_{P,12r}$) corresponding to the two sources above are replaced by the single path bias vector

$$\boldsymbol{E}_{P,1\{1,2\}r} = \begin{bmatrix} \boldsymbol{Z}_{111r} & \mathbf{0}_2 & \mathbf{0}_2 \\ \mathbf{0}_5 & \boldsymbol{Z}_{112r} & \mathbf{0}_5 \\ \boldsymbol{Z}_{121r} & \mathbf{0}_4 & \mathbf{0}_4 \\ \mathbf{0}_3 & \boldsymbol{Z}_{122r} & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \boldsymbol{Z}_{123r} \end{bmatrix} \begin{pmatrix} b^{(P)}_{1r,\{1,2\}1} \\ b^{(P)}_{1r,\{1,2\}2} \\ b^{(P)}_{1r,\{1,2\}3} \end{pmatrix}.$$

The entry $\{1, 2\}$ for the source index indicates that sources 1 (HRI-1) and 2 (HRI-2) must be considered jointly as a group, due to covariance between their observed signatures induced by the common source-to-sensor propagation paths Path_1 and Path_2. The path random effects $\{b^{(P)}_{1r,\{1,2\}1}, b^{(P)}_{1r,\{1,2\}2}, b^{(P)}_{1r,\{1,2\}3}\}$ are mutually independent realizations of the path random effect distribution (WPA, §5.1, Equation (5), p. 7).

- Lines 169-172: Calls the preprocessing function prepro_cal for the benchmark data. Table 2 describes all inputs to this function with default values. Only inputs with no default values must be provided.

Table 2: Inputs to `prepro_cal` function.

Input	Default	Brief Description
`gdir`	none	directory location of global subroutines
`adir`	none	directory location of application subroutines
`rdir`	none	root directory location of data files
`cdir`	none	directory locations (if relevant) and names of benchmark data files under `rdir`
`Rh`	none	vector with number of signatures for each phenomenology
`pbeta`	none	list containing empirical model common parameter counts by phenomenology
`izmat`	`FALSE`	user-provided code for computing variance component coefficient matrices
`ieiv`	`NULL`	numerical identifier of phenomenologies utilizing errors-in-variables yields in analysis of benchmark data
`seiv`	`NULL`	list containing identifiers of benchmark sources assigned errors-in-variables yields by phenomenology (`ALL` – every source)
`ewsd`	`NULL`	standard deviation of errors-in-variables Gaussian likelihood
`Th`	`NULL`	number of emplacement conditions for each phenomenology
`pbetat`	`NULL`	list containing empirical model emplacement-dependent parameter counts by phenomenology
`ibetar`	`NULL`	list containing locations of empirical model common parameters in full parameter vector by phenomenology
`pvc_1`	`NULL`	list containing source variance component parameter counts by phenomenology
`pvc_2`	`NULL`	list containing path variance component parameter counts by phenomenology
`ptype`	`NULL`	list indicating treatment of path variance component parameter by phenomenology (`Crossed` – common paths present across sources)
`cnames`	`NULL`	names of global forward model parameters

2.1.2 Maximum Likelihood Estimation

The maximum likelihood estimation component of the first stage analysis in Appendix A.2 is responsible for utilizing benchmark data to estimate the parameters of the forward and error models, and possibly the yield of each benchmark source for phenomenologies adopting the errors-in-variables yield model (WPA, §A.4). The resulting estimates are supplied to all relevant second stage analyses.

- Line 6: Read in code performing first stage maximum likelihood estimation of forward and error model parameters, and (if relevant) benchmark source errors-in-variables yields, based on benchmark data.
- Line 9: User specified seed to ensure repeatability of maximum likelihood estimation.
- Lines 13-17: Provide names of forward models for each signature by phenomenology

(WPA, §6.1-6.4). The `fm` object is initialized as a null list with elements for each phenomenology in the proper order (Line 13). Subsequent lines specify the function names as vectors of strings having length equal to the number of signatures for each phenomenology (Lines 14-17). The code for all forward models from each phenomenology is concatenated into a single file named `forward.r` and placed in the application code directory; in this example,

`MultiPEM_Toolbox_Package/Applications/Code/IYDT`

Note that these forward models accept the parameters to be calibrated as their main argument. In this example, the *seismic* forward model $f_{sr}(\cdot)$ as a function of the parameters $\boldsymbol{\beta}_{sr}$ is given as follows (WPA, §6.2, p. 11),

$$\begin{aligned} \log(\tilde{d}_{sr}(\boldsymbol{\beta}_{sr})) &= \beta_{sr,1} + \beta_{sr,2}\log(\tilde{\delta}_s) + \beta_{sr,3}\,\text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \\ f_{sr}(\boldsymbol{\beta}_{sr}) &= \log(d_{sr}(\boldsymbol{\beta}_{sr})) \end{aligned} \tag{1}$$

for

$$\text{logistic}(x) = \frac{1}{1+\exp(-x)}\,.$$

The scaled signatures and covariates of this forward model are given by

$$\begin{aligned} \tilde{d}_{s1} &= d_{s1}\exp(-w/3) & \tilde{d}_{s2} &= d_{s2} \\ \tilde{\delta}_s &= \delta\exp(-w/3) & \tilde{h}_s &= h\exp(-w/3)\,, \end{aligned}$$

where d_{s1} and d_{s2} are P-wave displacement and maximum velocity, and the covariates $v = (w, h, \delta)$ are log-yield, HOB/DOB, and range. The function `f_s` returns a vector of forward model calculations evaluated for the supplied value of $\boldsymbol{\beta}_{sr}$, each element corresponding to each row of a matrix of covariates (having columns (w, h, δ)).

- Line 20: Indicate if forward model Jacobian matrices are provided for efficient log-likelihood maximization.

- Lines 22-30: If `igrad` is `TRUE`, names of forward model Jacobian functions must be provided for each signature by phenomenology. The `gfm` object is initialized as a null list with elements for each phenomenology in the proper order (Line 25). Subsequent lines specify the Jacobian function names as vectors of strings having length equal to the number of signatures for each phenomenology (Lines 26-29). The code for all forward model Jacobian functions from each phenomenology is concatenated into a single file named `jacobian.r` and placed in the application code directory; in this example,

  `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  Note that these Jacobian functions accept the parameters to be calibrated as their main argument. In this example, the gradient vector of the *seismic* forward model of Equation (1) is computed from the partial derivatives of $f_{sr}(\cdot)$ for each parameter as follows,

$$
\begin{aligned}
\frac{\partial f_{sr}}{\partial \beta_{sr,1}} &= 1 \\
\frac{\partial f_{sr}}{\partial \beta_{sr,2}} &= \log(\tilde{\delta}_s) \\
\frac{\partial f_{sr}}{\partial \beta_{sr,3}} &= \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \\
\frac{\partial f_{sr}}{\partial \beta_{sr,4}} &= \beta_{sr,3}\tilde{h}_s \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5}) \\
\frac{\partial f_{sr}}{\partial \beta_{sr,5}} &= \beta_{sr,3} \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5})
\end{aligned}
$$

The function `g_s` returns a Jacobian matrix (`jbeta_s`) of forward model gradients for the parameters, evaluated at the supplied value of $\boldsymbol{\beta}_{sr}$, with rows corresponding to the rows of a matrix of covariates (having columns (w, h, δ)). If `eiv` is `TRUE` (Line 113 of Appendix A.1), the partial derivative of $f_{sr}(\cdot)$ for log-yield w is also required,

$$
\begin{aligned}
\frac{\partial f_{sr}}{\partial w} = &-\frac{1}{3}\left(\beta_{sr,2} + \beta_{sr,3}\beta_{sr,4}\tilde{h}_s \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5})\right) \\
&+\frac{1}{3}\,\delta_1(r) \qquad (2)
\end{aligned}
$$

for $\delta_A(x)$ the indicator function of set A. The function `g_s` will also return a Jacobian vector (`jtheta_s`) of forward model partial derivatives for log-yield, evaluated at the supplied value of $\boldsymbol{\beta}_{sr}$, each element corresponding to each row of the same covariate matrix used in the calculation of `jbeta_s`.

- Line 35: Indicate if the same forward model function is used to compute multiple signatures, and signature-specific code within this function is required.
- Lines 37-41: If `iResponse` is `TRUE` (Line 35), initialize `iResponse` to a null list with elements for each phenomenology in the proper order (Line 38). For each relevant phenomenology, subsequent lines provide vectors of length equal to the number of signatures, each element of which is a tag identifying code specific to the corresponding signature. This mechanism is utilized for the *seismic* (Line 39) and *acoustic* (Line 40) phenomenologies.
- Line 44: Indicate if fixed inputs are to be provided to the forward models for at least one phenomenology.
- Lines 46-55: If `fPars` is `TRUE` (Line 44), initialize `fPars` to a null list with elements for each phenomenology in the proper order (Line 47). For each relevant phenomenology, subsequent lines provide the value(s) of all fixed inputs. For example, the *optical* forward model requires fixed values for `yield_scaling` (Line 52), `pressure_scaling` (Line 53), and `temp_scaling` (Line 54).

- Line 58: Specify the number of starting parameter vectors for the log-likelihood maximization routine.
- Line 61: Specify the number of cores to use for parallel optimization (across distinct starting values) of the benchmark data log-likelihood function.
- Line 64: Specify if the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is to be used for maximization of the log-likelihood function. If `TRUE`, functions to compute forward model Jacobian matrices analytically must be provided, or numerical gradients will be utilized (generally increasing compute time). If `FALSE`, the gradient-free Nelder-Mead simplex algorithm will be utilized for optimization, which is generally much slower computationally than BFGS with analytical gradients.
- Lines 68-71: If relevant, specifies the location (relative to the run directory) of parameter values or estimates to be used as the first starting value for log-likelihood maximization. These values are stored in a `.RData` object as a list, with elements corresponding to within signature forward model (e.g. common parameters `beta`, emplacement-dependent parameters `tbeta`) and error model (e.g. source variance components `vc_1`, path variance components `vc_2`, observation error parameters `eps`) quantities of interest. If relevant, global forward model parameter estimates (`calp`) and benchmark source errors-in-variables yield estimates (`w_eiv`) are also provided. For multi-phenomenology analyses, values or estimates from individual phenomenologies may be input in the proper order, and they will be concatenated appropriately.
- Line 75: If desired, name of output `.RData` file to store optimization results from this run. The elements of the list to be written are described in the previous item.
- Lines 77-91: If `calp` is `TRUE` (Line 47 of Appendix A.1), provides specifications for maximum likelihood estimation of global forward model parameters.
  - Line 79: If `cst` is `TRUE`, specifies an initial starting value for the global forward model parameters (Lines 82-83) for log-likelihood maximization. This value supersedes the value read in from the first file provided in the string vector `opt_files_in` (Line 68), if the `calp` list element is provided.
  - Line 87: Specifies the level of confidence intervals for the true values of each global forward model parameter from the maximum likelihood estimate and the estimated Fisher information matrix.
- Line 95: Indicate if phenomenology specific code is required in the postprocessing function.
- Lines 97-99: If `Phen` is `TRUE` (Line 95), specifies a matrix in which the first column provides the numerical phenomenology indicator (see Lines 41-44 of the preprocessing code in Appendix A.1), and the second column provides the phenomenology name in string format. In this example, specific code is required to process results for the *seismic* phenomenology (Line 98).
- Line 102: Indicate if gradient verification is to be conducted on the log-likelihood function. If `TRUE` and `igrad` is `TRUE` (Line 20), analytical and numerical gradients

at the optimal parameter value, and other randomly sampled parameter values, are compared for consistency.

- Line 105: Specify the strategy for running parallel jobs using the `future` package in `R`. The available options are given by starting an `R` session and issuing the following commands,

```
% R
> require(future)
> help(plan)
```

- Lines 108-113: Calls the log-likelihood maximization function `calc_mle_cal` for the benchmark data. Table 3 describes all inputs to this function with default values. Only inputs with no default values must be provided.

2.1.3 Bayesian Analysis

The optional Bayesian inference component of the analysis in Appendix A.3 is responsible for sampling forward and error model parameters, and benchmark source errors-in-variables yields (if relevant) from their joint posterior distribution using benchmark data. This Bayesian component must be run if multiple imputation of forward and error model parameters is desired in second stage Bayesian inference for new event device parameters.

- Line 6: Indicate if first stage Bayesian analysis is to be conducted. If second stage multiple imputation is desired, `iBayes` must be `TRUE`.
- Line 10: Read in code performing Bayesian analysis on forward and error model parameters, and benchmark source errors-in-variables yields (if relevant), using benchmark data.
- Line 14: Indicate if a log-prior density for the signature within phenomenology forward model parameters is supplied by the user (WPA, §6.5, p. 15). If `iBetaPrior` is `FALSE`, a "flat prior" (uniform on the domain) on these parameters is assumed.
- Lines 16-35: If relevant, specify details of user-provided log-prior distributions for signature within phenomenology forward model parameters. For each relevant phenomenology, the list object `lp_beta` is used for common coefficients, while the list object `lp_betat` is used for emplacement-dependent coefficients (as demonstrated below in this application).
  - Line 18: Specify location(s) of log-prior function(s). Must be provided if `iBetaPrior` is `TRUE` (Line 14). In this example, a single log-prior function is provided, located at

    ```
    ../Code/lp_beta_s.r
    ```

  - Line 20: If `igrad` is `TRUE` (Line 20 of Appendix A.2), specify location(s) of the log-prior gradient function(s). In this example, a single log-prior gradient function is provided, located at

    ```
    ../Code/glp_beta_s.r
    ```

Table 3: Inputs to `calc_mle_cal` function.

Input	Default	Brief Description
`p_cal`	none	environment storing all objects needed in log-likelihood calculations
`gdir`	none	directory location of global subroutines
`adir`	none	directory location of application subroutines
`f`	none	names of forward model functions for each signature by phenomenology
`nst`	10	number of starting values for log-likelihood maximization
`ncor`	1	number of cores for log-likelihood maximization
`ci_lev`	0.95	confidence interval levels for global forward model parameter inference
`igrad`	`TRUE`	forward model Jacobian provided
`bfgs`	`TRUE`	log-likelihood maximization uses BFGS methods
`igrck`	`TRUE`	conduct log-likelihood function gradient verification
`g`	`NULL`	names of forward model Jacobian functions for each signature by phenomenology
`iresp`	`NULL`	flags for modified calculation by signature in a common forward model for each relevant phenomenology
`fp_fm`	`NULL`	fixed inputs required by forward models
`fopt_in`	`NULL`	location of input `R` data file(s) providing an initial starting value for log-likelihood maximization (if multiple files, starting value created by concatenating over phenomenologies)
`Xst`	`NULL`	matrix of starting values for log-likelihood maximization if not generated by this function
`cst`	`NULL`	vector of starting values for global forward model parameters in log-likelihood maximization
`fopt_out`	`NULL`	location to write output `R` data file with results of log-likelihood maximization
`phen`	`NULL`	phenomenology number and type (if needed for postprocessing)
`pl`	`"multicore"`	strategy for running parallel jobs using the `future` package

- Line 25: For each relevant phenomenology, initialize a null list `lp_betat` of length equal to the number of emplacement conditions containing distinct forward model parameters.

- Line 27: For each relevant phenomenology and emplacement condition, provide the name(s) of the log-prior function(s) for each signature. In this example, the *seismic* phenomenology utilizes a log-prior function `lp_s` for each signature within each emplacement condition.

- Line 29: If `igrad` is `TRUE` (Line 20 of Appendix A.2), then for each relevant phenomenology and emplacement condition, provide the name(s) of the log-prior gradient function(s) for each signature. In this example, the *seismic* phenomenology utilizes a log-prior gradient function `lq_s` for each signature within each emplacement condition.

- Line 38: If `calp` is `TRUE` (Line 47 of Appendix A.1), indicate if a log-prior density for the global forward model parameters is supplied by the user. If `iCalPrior` is `FALSE`, a "flat prior" (uniform on the domain) on these parameters is assumed.
- Lines 40-57: If relevant, specify details of user-provided log-prior distributions for global forward model parameters.
  - Line 42: Specify location of log-prior function. If `NULL`, utilize the default log-prior function contained in the file `lp_c.r` placed in the application code directory; in this example,

    `MultiPEM_Toolbox_Package/Applications/Code/IYDT`
  - Line 44: If `igrad` is `TRUE` (Line 20 of Appendix A.2), specify location of the log-prior gradient function. If `NULL`, utilize the default log-prior gradient function contained in the file `glp_c.r` placed in the application code directory; in this example,

    `MultiPEM_Toolbox_Package/Applications/Code/IYDT`
  - Line 48: Provide the name of the log-prior function.
  - Line 49: If `igrad` is `TRUE` (Line 20 of Appendix A.2), provide the name of the log-prior gradient function.
  - Lines 52-53: Specify all fixed quantities required for calculation of the log-prior density.
- Line 61: Specify a *fixed* value for the scale parameter `A` of half-Cauchy prior distribution(s) for the *source* and *path* variance component parameters if relevant (WPA, §6.5, p. 15; §6.6, p. 17). Prior distributions for a non-empty collection of variance component parameters are taken to be mutually independent. Comment out if this parameter is to be sampled from its posterior distribution.
- Line 65: Specify a *fixed* value for the shape parameter η of the Lewandowski-Kurowicka-Joe (LKJ) prior distribution for the observational error model correlation parameters (WPA, §6.5, p. 15; §6.6, p. 17).
- Line 73: If `eiv` is `TRUE` (Line 113 of Appendix A.1), specify a *fixed* value for the parameter that controls the number of modes in the *flexible generalized skew-normal* (FGSN) prior distribution for the errors-in-variables yields of the benchmark events (WPA, §6.5, p. 15; §6.6, p. 23).
- Line 79: Select the Markov chain Monte Carlo (MCMC) algorithm to use for posterior sampling, from one of three options: `RAM`, `FME`, and `NUTS`. `RAM` is the robust adaptive Metropolis algorithm of Vihola[5] implemented in the `R` package `adaptMCMC`. `FME`

[5] Vihola, M. (2012). Robust adaptive Metropolis algorithm with coerced acceptance rate. *Stat Comput*

is the delayed rejection adaptive Metropolis algorithm of Haario, Laine, and Mira[6] implemented in the `R` package `FME`. `NUTS` is the No-U-Turn Sampler of Hoffman and Gelman[7]. The `NUTS` option requires the analytical gradient of the log-posterior density, which in turn requires `igrad` to be `TRUE` (Line 20 of Appendix A.2).

- Line 82: Specify the per core sample size of the burn-in period for MCMC sampling (pre-equilibrium stage of Markov chain). These samples are discarded prior to any inference using the posterior samples.
- Line 85: Specify the sample size of the MCMC production run. These samples are kept for posterior inference.
- Line 88: Specify the rate at which MCMC production samples are thinned for estimation of the Deviance Information Criterion[8] (DIC) and the Predictive Information Criterion[9] (PIC). In this example, the `nthin` value of `20` indicates that every 20-th production sample is kept for DIC and PIC estimation.
- Line 91: Specify the number of cores to use for parallel optimization (across distinct starting values) of the benchmark data log-posterior function. By default, this optimization uses the same number of distinct starting values as optimization of the benchmark data log-likelihood function (Line 58 of Appendix A.2).
- Line 94: Specify the number of cores used to run parallel MCMC chains. The burn-in period for each chain is determined by `nburn` (Line 82), while the `nmcmc` (Line 85) production runs are split between the `ncores_mc` processors and combined at the conclusion of the runs.
- Line 97: Indicate if gradient verification is to be conducted on the log-prior function. If `TRUE` and `igrad` is `TRUE` (Line 20 of Appendix A.2), analytical and numerical gradients at the maximum *a posteriori* parameter value, and other randomly sampled parameter values, are compared for consistency.
- Line 100: Indicate if gradient verification is to be conducted on the log-posterior function. If `TRUE` and `igrad` is `TRUE` (Line 20 of Appendix A.2), analytical and numerical gradients at the maximum *a posteriori* parameter value, and other randomly sampled parameter values, are compared for consistency.
- Lines 103-112: Calls the Bayesian analysis function `calc_bayes_cal` for the benchmark data. Table 4 describes all inputs to this function with default values. Only inputs with no default values must be provided.

22:997-1008.

[6]Haario, H., Laine, M., and Mira, A. (2006). DRAM: Efficient adaptive MCMC. *Stat Comput* 16:339-354.

[7]Hoffman, M. D. and Gelman, A. (2014). The No-U-Turn Sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. *J Mach Learn Res* 15:1593-1623.

[8]Spiegelhalter, D.J., Best, N.G., Carlin, B.P., & van der Linde, A. (2002). Bayesian measures of model complexity and fit (with discussion), *J R Stat Soc Ser B* 64:583-639.

[9]Ando, T. (2011). Predictive Bayesian model selection, *Am J Math Manag Sci* 31:13-38.

Table 4: Inputs to calc_bayes_cal function.

Input	Default	Brief Description
p_cal	none	environment storing all objects needed in log-posterior calculations
gdir	none	directory location of global subroutines
adir	none	directory location of application subroutines
nst	10	number of starting values for log-posterior maximization
nburn	10000	number of per core MCMC burn-in samples
nmcmc	20000	number of MCMC production samples
nthin	20	posterior sample thinning rate
ncor_map	1	number of cores for log-posterior maximization
ncor_mc	1	number of cores for generating parallel MCMC chains
igrad	TRUE	forward model Jacobian provided
igrck_pr	TRUE	conduct log-prior function gradient verification
igrck_po	TRUE	conduct log-posterior function gradient verification
bfgs	TRUE	log-posterior maximization uses BFGS methods
ibpr	FALSE	prior density function(s) provided for signature within phenomenology forward model coefficients
icpr	FALSE	prior density function(s) provided for global forward model coefficients
fpr_b	NULL	location of functions computing log-prior density for signature within phenomenology forward model coefficients
fgpr_b	NULL	location of functions computing gradients of log-prior density for signature within phenomenology forward model coefficients
fpr_c	NULL	location of functions computing log-prior density for global forward model coefficients
fgpr_c	NULL	location of functions computing gradients of log-prior density for global forward model coefficients
Xnom	NULL	matrix of starting values for hyperparameters in log-posterior maximization if not generated by this function
imcmc	"FME"	MCMC algorithm (current options: "RAM", "FME", "NUTS")
pl	"multicore"	strategy for running parallel jobs using the future package

2.1.4 Output

The output file runMPEM.out from the first stage analysis contains a summary of (if relevant) global forward model parameters, (if relevant) errors-in-variables yield estimates for the relevant benchmark sources, signature within phenomenology forward and error model parameter estimates, and (if relevant) posterior samples derived from the benchmark data. The desired output is supplied by the user function print_sumstats.r, placed in the application code directory; in this example,

```
MultiPEM_Toolbox_Package/Applications/Code/IYDT
```

The output presented in Appendix A.4 contains the most pertinent information extracted from the full file.

- Lines 6-17: Output from the preprocessing function `prepro_cal`. These warning messages explain which variance component models are allowed (if any) for each signature of each phenomenology based on the structure of the benchmark data. In this example, only *source* random effects are allowed for each *acoustic* signature (Lines 6-9), while no random effects are allowed for *optical* or *surface effects* phenomenologies (Lines 10-17). There are no warning messages for *seismic* signatures, indicating source and *path* random effects are allowed.
- Lines 26-241: Output from the maximum likelihood estimation function `calc_mle_cal`:
  - Line 28: Convergence code from the `R` optimization function `optim`. In this example, '0' indicates successful completion.
  - Line 29: Number of optimization restarts in which the relative absolute maximum log-likelihood difference is $\leq 10^{-8}$. The algorithm exits after 2 such restarts, which is attained in this example.
  - Lines 34-37: Maximum likelihood estimates of errors-in-variables yields for the relevant benchmark sources. Source names (Lines 34 and 36) are given above yield estimates (Lines 35 and 37). Errors-in-variables yields are only estimated if `eiv` is `TRUE` (Line 113 of Appendix A.1).
  - Lines 41-63: Maximum likelihood estimates of *common* forward model parameters for each signature of each phenomenology (where present).
  - Lines 67-113: Maximum likelihood estimates of *emplacement-dependent* forward model parameters for each signature of each phenomenology (where present).
  - Lines 117-131: Maximum likelihood estimates of *source* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
  - Lines 135-141: Maximum likelihood estimates of *path* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
  - Lines 145-191: Maximum likelihood estimates of observational error variances for each signature, and correlations between signatures, for each phenomenology (WPA, §A.5).
  - Line 193: Akaike Information Criterion[10] (AIC) value based on benchmark data. Used for selecting among competing forward or error model specifications (WPA, §6.5, p. 15; §6.6, Tables 4 and 5, p. 18).
  - Line 195: Bayesian Information Criterion[11] (BIC) value based on benchmark data. Used for selecting among competing forward or error model specifications (WPA,

[10] Akaike, H. (1973). Information Theory and an Extension of the Maximum Likelihood Principle. In: Petrov, B.N. & Csaki, F., Eds., International Symposium on Information Theory, 267-281.

[11] Schwarz, G. (1978). Estimating the dimension of a model, *Ann Stat* 6:461-464.

§6.5, p. 15; §6.6, Tables 4 and 5, p. 18).

  - Lines 200-241: Example of log-likelihood gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
    * Lines 201-219: Analytic gradient calculation
    * Lines 221-239: Numerical gradient calculation using the `R` package `numDeriv`
    * Line 241: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients

- Lines 256-1286: Output from the Bayesian analysis function `calc_bayes_cal`:
  - Line 258: Convergence code from the `R` optimization function `optim`. In this example, '0' indicates successful completion.
  - Line 259: Number of optimization restarts in which the relative absolute maximum log-posterior difference is $\leq 10^{-8}$. The algorithm exits after 2 such restarts, which is attained in this example.
  - Lines 264-267: Maximum *a posteriori* estimates of errors-in-variables yields for the relevant benchmark sources. Source names (Lines 264 and 266) are given above yield estimates (Lines 265 and 267). Errors-in-variables yields are only estimated if `eiv` is `TRUE` (Line 113 of Appendix A.1).
  - Lines 271-293: Maximum *a posteriori* estimates of *common* forward model parameters for each signature of each phenomenology (where present).
  - Lines 297-343: Maximum *a posteriori* estimates of *emplacement-dependent* forward model parameters for each signature of each phenomenology (where present).
  - Lines 347-361: Maximum *a posteriori* estimates of *source* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
  - Lines 365-371: Maximum *a posteriori* estimates of *path* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
  - Lines 375-421: Maximum *a posteriori* estimates of observational error variances for each signature, and correlations between signatures, for each phenomenology (WPA, §A.5).
  - Lines 425-427: Maximum *a posteriori* estimates of FGSN prior distribution parameters (WPA, §6.6, p. 23; `Alpha` $= \mu$, `Omega` $= \upsilon$ (two coefficients)).
  - Lines 431-474: Example of log-prior gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
    * Lines 432-451: Analytic gradient calculation
    * Lines 453-472: Numerical gradient calculation using the `R` package `numDeriv`

  * Line 474: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients

- Lines 478-521: Example of log-posterior gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
  * Lines 479-498: Analytic gradient calculation
  * Lines 500-519: Numerical gradient calculation using the `R` package `numDeriv`
  * Line 521: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients
- Line 525: Acceptance rate of the Delayed Rejection Adaptive Metropolis (DRAM) posterior sampling method implemented in `R` package `FME`. Note that one delayed rejection step is allowed in the default implementation.
- Lines 531-583: Means and user specified quantiles of samples from the marginal posterior distributions of errors-in-variables yields for the relevant benchmark sources. The ordering of benchmark sources is provided with the maximum *a posteriori* estimates (Lines 264 and 266). Errors-in-variables yields are only estimated if `eiv` is `TRUE` (Line 113 of Appendix A.1).
- Lines 587-669: Means and user specified quantiles of samples from the marginal posterior distributions of *common* forward model parameters for each signature of each phenomenology (where present).
- Lines 673-875: Means and user specified quantiles of samples from the marginal posterior distributions of *emplacement-dependent* forward model parameters for each signature of each phenomenology (where present).
- Lines 879-933: Means and user specified quantiles of samples from the marginal posterior distributions of *source* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 937-963: Means and user specified quantiles of samples from the marginal posterior distributions of *path* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 967-1241: Means and user specified quantiles of samples from the marginal posterior distributions of observational error variances for each signature, and correlations between signatures, for each phenomenology (WPA, §A.5).
- Lines 1245-1282: Means and user specified quantiles of samples from the marginal posterior distributions of FGSN prior distribution parameters (WPA, §6.6, p. 23; `Alpha` $= \mu$, `Omega` $= \upsilon$ (two coefficients)).
- Line 1284: DIC value based on benchmark data. Used for selecting among competing forward or error model specifications (WPA, §6.5, pp. 15-16; §6.6, Tables 4 and 5, p. 18).

– Line 1286: PIC value based on benchmark data. Used for selecting among competing forward or error model specifications (WPA, §6.5, pp. 15-16; §6.6, Tables 4 and 5, p. 18).

The `p_cal` environment resulting from this run contains several elements of potential interest for additional post-processing:

- `p_cal$mle_cal`: Maximum likelihood estimate of (if relevant) unbounded global forward model parameters (i.e., on scale used by the optimizer), benchmark source errors-in-variables yields (if relevant), and signature within phenomenology forward and error model parameters based on benchmark data
- `p_cal$mle_calp`: If `calp` is `TRUE` (Line 47 of Appendix A.1), maximum likelihood estimate of unbounded global forward model parameters based on benchmark data
- `p_cal$Sigma_mle_cal$II_calp`: If `calp` is `TRUE` (Line 47 of Appendix A.1), estimated asymptotic covariance matrix of `p_cal$mle_calp`, adjusted for estimation of signature within phenomenology forward model parameters, and (if relevant) benchmark source errors-in-variables yields
- `p_cal$map_cal`: If `iBayes` is `TRUE` (Line 6 of Appendix A.3), maximum *a posteriori* estimate of (if relevant) unbounded global forward model parameters (i.e., on scale used by the optimizer), benchmark source errors-in-variables yields (if relevant), and signature within phenomenology forward and error model parameters based on benchmark data
- `p_cal$map_calp`: If `iBayes` is `TRUE` (Line 6 of Appendix A.3), and `calp` is `TRUE` (Line 47 of Appendix A.1), maximum *a posteriori* estimate of unbounded global forward model parameters based on benchmark data
- `p_cal$mpi`: If `iBayes` is `TRUE` (Line 6 of Appendix A.3), posterior samples of unbounded global forward model parameters (if relevant), benchmark source errors-in-variables yields (if relevant), and signature within phenomenology forward and error model parameters based on benchmark data
- `p_cal$mpi_calp`: If `iBayes` is `TRUE` (Line 6 of Appendix A.3), and `calp` is `TRUE` (Line 47 of Appendix A.1), posterior samples of unbounded global forward model parameters based on benchmark data

2.2 Second Stage

The second stage analysis is defined in the `runMPEM_0.r` file, provided in Appendix A with line numbers referred to in the ensuing discussion. Appendix A.5 provides the preprocessing component of the second stage, Appendix A.6 provides the code employed to maximize the likelihood function of the new event data with respect to the new event device parameters, while Appendix A.7 provides the code employed to optionally sample the posterior distribution of these parameters.

The second stage analysis is run in batch mode as follows,

```
% R CMD BATCH runMPEM_0.r runMPEM_0.out &
```

This job requires the .RData file from the completion of the first stage run to be copied into the second stage run directory. The main features of the output file runMPEM_0.out are provided in Appendix A.8.

2.2.1 Preprocessing

The preprocessing component of the second stage analysis in Appendix A.5 is primarily responsible for describing features of the new event data and device parameters of inferential interest.

- Line 13+: Load all R packages utilized by multiple supporting subroutines, most notably log-likelihood and log-prior calculations and their associated gradients.
- Line 24: Specify directory location (relative to run directory) of all global (application independent) subroutines.
- Line 27: Read in code performing second stage preprocessing of new event data.
- Line 30: Specify directory location (relative to run directory) of all application-specific subroutines.
- Line 33: Specify root directory (relative to run directory) containing all application-specific new event data files.
- Lines 36-39: A scalar or vector specifying the names of new event data files for each phenomenology, utilizing an ordering of the phenomenologies (for MultiPEM analysis) that is consistent with first stage preprocessing and maintained throughout the input deck (as indicated here in Lines 42-45). Data files are text files (CSV formatted) containing all measured signatures (in the first column(s)) and input covariates (in succeeding column(s)) including all those required in forward and error model calculations, but excepting the new event device parameters that are unknown and subject to second stage inference. Directories specifying the exact locations of these files relative to the root data directory (Line 33) may also be included in the filenames.
- Line 48: Specify the names of the new event device parameters of inferential interest as a vector of strings. This information is utilized in postprocessing.
- Line 52: Number of first stage within signature forward and error model parameter posterior samples utilized in the multiple imputation algorithm for generating second stage new event device parameter posterior samples. If nimpute is set to 1 (default), the first stage maximum likelihood estimate of the within signature forward and error model parameters is used in place of the imputation samples.
- Line 55: Specify if bounded optimization of new event device parameters is to be conducted. The default is to optimize all new event device parameters on an unbounded input space, transforming them to their input domain (specified subsequently in this preprocessing file) as necessary for forward model calculations. If opt_B is TRUE, the new event device parameters are optimized directly on their input domain.

- Line 58: Indicate if the new event device parameters are subjected to a user-provided bijective transformation supplied to assist likelihood maximization or posterior sampling. If `itransform` is `TRUE`, the code implementing this transformation is concatenated into a single file named `transform.r` and placed in the application code directory; in this example,

  `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  The functions that must be provided in `transform.r` include the following:

  - `tau`: Function $\boldsymbol{\tau}(\cdot)$ applied to transformed variables $\widetilde{\boldsymbol{\theta}}_0$ with the new event device parameters $\boldsymbol{\theta}_0$ as its image,
  $$\boldsymbol{\theta}_0 = \boldsymbol{\tau}(\widetilde{\boldsymbol{\theta}}_0)$$
  - `j_tau`: Jacobian matrix of $\boldsymbol{\tau}(\cdot)$,
  $$\boldsymbol{J}_{\boldsymbol{\tau}}(\widetilde{\boldsymbol{\theta}}_0) = \begin{bmatrix} \dfrac{\partial \tau_1(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,1}} & \cdots & \dfrac{\partial \tau_1(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,q}} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial \tau_q(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,1}} & \cdots & \dfrac{\partial \tau_q(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,q}} \end{bmatrix}$$
  where q is the dimension of $\boldsymbol{\theta}_0$.
  - `log_absdet_j_tau`: Logarithm of the absolute value of the determinant of the Jacobian matrix computed from `j_tau`,
  $$\log \mathrm{abs}(\det(\boldsymbol{J}_{\boldsymbol{\tau}}(\widetilde{\boldsymbol{\theta}}_0)))$$
  - `dlog_absdet_j_tau`: Gradient of the log absolute Jacobian determinant with respect to $\widetilde{\boldsymbol{\theta}}_0$
  - `inv_tau`: Inverse function of $\boldsymbol{\tau}(\cdot)$

  In this example, the new event device parameters of inferential interest are log-yield w and height-of-burst h, that is $\boldsymbol{\theta}_0 = (w, h)$. The relevant forward models are functions of a scaled height-of-burst, $\tilde{h} = h \exp(-w/3)$, suggesting the possible utility of likelihood maximization or posterior sampling in terms of $\widetilde{\boldsymbol{\theta}}_0 = (\tilde{w}, \tilde{h})$ for $\tilde{w} = w$.

- Lines 61-68: If `itransform` is `TRUE` (Line 58), and if `tPars` is `TRUE` (Line 62), initialize `tPars` to a null list (Line 65). Subsequent lines provide the value(s) for all fixed inputs required to compute the function `tau` (see previous item). In this example, a `yield_scaling` value is required (Line 66).

- Lines 72-75: Specify lower and upper bounds for the new event device parameters if needed. By default, lower bounds are set to $-\infty$ (Line 72) and upper bounds to $+\infty$ (Line 74). In this example, the second parameter (height-of-burst) is restricted to the range $(-10, 160)$ (Lines 73 and 75). Note that likelihood maximization and posterior sampling are conducted on an unbounded parameter space. If lower or upper bounds are specified for any parameter, they are applied just prior to objective function calculations using the `transform` function of the `transform.r` file located in the global code directory,

```
MultiPEM_Toolbox_Package/Code
```

- Lines 78-83: If `tsub` is `TRUE` (Line 78), the forward model for at least one phenomenology depends only on a subset of the full vector $\boldsymbol{\theta}_0$ of new event device parameters. The `tsub` object is initialized to a null list with elements for each phenomenology in the proper order (Line 81). The `theta_names` vector (Line 48) describes the order of elements in $\boldsymbol{\theta}_0$. For relevant phenomenologies, parameter subsets are specified as integer vectors identifying the extracted elements of $\boldsymbol{\theta}_0$. The forward models of all other phenomenologies depend on the full $\boldsymbol{\theta}_0$. In this example, the *surface effects* (*crater*) phenomenology only depends on log-yield (Line 82), while the other phenomenologies depend on both log-yield and height-of-burst.
- Lines 86-88: Calls the preprocessing function `prepro_0` for the new event data. Table 5 describes all inputs to this function with default values. Only inputs with no default values must be provided.

Table 5: Inputs to `prepro_0` function.

Input	Default	Brief Description
`p_cal`	none	environment storing all objects needed in log-likelihood and log-posterior calculations
`gdir`	none	directory location of global subroutines
`adir`	none	directory location of application subroutines
`rdir`	none	root directory location of data files
`ndir`	none	directory locations (if relevant) and names of new event data files under `rdir`
`tnames`	none	names of new event parameters
`nimp`	1	number of first stage imputation samples used in second stage new event parameter posterior sampling
`bopt`	`FALSE`	new event parameter bounds supplied to log-likelihood maximization
`itr`	`FALSE`	bijective transform of new event parameters provided
`fp_tr`	`NULL`	fixed inputs to new event parameter transform
`tlb`	`NULL`	lower bounds for new event parameters
`tub`	`NULL`	upper bounds for new event parameters
`tsub`	`NULL`	list containing index sets identifying new event parameter subsets by phenomenology if relevant

- Lines 89-95: If `opt_B` is `TRUE` (Line 55), the preprocessor function `prepro_0` returns a list (designated here as `tmp`) with objects `p_cal` and `t_cal`, which are then assigned as follows

```
% p_cal = tmp$p_cal
% t_cal = tmp$t_cal
```

and both are utilized for maximum likelihood estimation and Bayesian analysis. Otherwise, p_cal is the only object returned,

```
% p_cal = tmp$p_cal
```

and utilized in subsequent analyses.

2.2.2 Maximum Likelihood Estimation

The maximum likelihood estimation component of the second stage analysis in Appendix A.6 is responsible for integrating calibrated within signature forward and error model parameter values from the first stage with new event data to estimate new event device parameters of interest with uncertainty quantification (WPA, §A.2).

- Line 6: Read in code performing second stage maximum likelihood estimation and uncertainty quantification of new event device parameters, using calibrated within signature forward and error model parameters from the first stage.
- Line 9: User specified seed to ensure repeatability of maximum likelihood estimation.
- Lines 13-17: Provide names of forward models for each signature by phenomenology (WPA, §6.1-6.4). The `fm0` object is initialized as a null list with elements for each phenomenology in the proper order (Line 13). Subsequent lines specify the function names as vectors of strings having length equal to the number of signatures for each phenomenology (Lines 14-17). The code for all forward models from each phenomenology is concatenated into a single file named `forward_0.r` and placed in the application code directory; in this example,

  ```
  MultiPEM_Toolbox_Package/Applications/Code/IYDT
  ```

  Note that these forward models compute the same signatures as those used in the first stage. However, they accept only the new event device parameters of inferential interest (designated $\boldsymbol{\theta}_0$ previously) as their main argument. Forward model parameter values are passed in as fixed quantities. In this example, the *seismic* forward model $f^0_{sr}(\cdot)$ as a function of the new event device parameters $\boldsymbol{\theta}_0 = (w, h)$ – for fixed parameters $\boldsymbol{\beta}_{sr}$ – is given by Equation (1). The function `f0_s` returns a vector of forward model calculations evaluated for the supplied value of $\boldsymbol{\theta}_0$ (fixed $\boldsymbol{\beta}_{sr}$ passed in as `params$beta`), each element corresponding to each row of a matrix of covariates (in this case, a column vector of ranges δ).
- Line 20: Indicate if forward model Jacobian matrices are provided for efficient log-likelihood maximization.
- Lines 22-30: If `igrad` is `TRUE` (Line 20), names of forward model Jacobian functions must be provided for each signature by phenomenology. The `gfm0` object is initialized as a null list with elements for each phenomenology in the proper order (Line 25). Subsequent lines specify the Jacobian function names as vectors of strings having length equal to the number of signatures for each phenomenology (Lines 26-29). The code for all forward model Jacobian functions from each phenomenology is concatenated into

a single file named `jacobian_0.r` and placed in the application code directory; in this example,

`MultiPEM_Toolbox_Package/Applications/Code/IYDT`

Note that these Jacobian functions accept only the new event device parameters of inferential interest (designated $\boldsymbol{\theta}_0$ previously) as their main argument. Forward model parameter values are passed in as fixed quantities. In this example, the gradient vector of the *seismic* forward model (see description above) is computed from the partial derivatives of $f_{sr}^0(\cdot)$ for each new event device parameter in $\boldsymbol{\theta}_0$, for fixed parameters $\boldsymbol{\beta}_{sr}$. The partial derivative for log-yield w is given in Equation (2). For HOB/DOB h,

$$\frac{\partial f_{sr}^0}{\partial h} = \beta_{sr,3}\beta_{sr,4}\exp(-w/3) \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5})$$

The function `g0_s` returns a Jacobian matrix (`jtheta_s`) of forward model gradients for the new event device parameters, evaluated at the supplied value of $\boldsymbol{\theta}_0$ (fixed $\boldsymbol{\beta}_{sr}$ passed in as `params$beta`), with rows corresponding to the rows of a matrix of covariates (in this case, a column vector of ranges δ).

- Line 33: Specify the number of starting new event device parameter vectors for the log-likelihood maximization routine.
- Line 36: Specify the number of cores to use for parallel optimization (across distinct starting values) of the new event data log-likelihood function.
- Line 39: Specify if the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is to be used for maximization of the log-likelihood function. If `TRUE`, functions to compute forward model Jacobian matrices analytically must be provided, or numerical gradients will be utilized (generally increasing compute time). If `FALSE`, the gradient-free Nelder-Mead simplex algorithm will be utilized for optimization, which is generally much slower computationally than BFGS with analytical gradients.
- Line 43: If relevant, specifies the location (relative to the run directory) of parameter values or estimates to be used as the first starting value for log-likelihood maximization. These values are stored in a `.RData` object as a list, with an element corresponding to new event device parameters (`theta0`).
- Line 47: If desired, name of output `.RData` file to store optimization results from this run. The element of the list to be written are described in the previous item.
- Lines 50-55: If `tst` is `TRUE` (Line 50), specifies an initial starting value for the new event device parameters (Lines 53-54) for log-likelihood maximization. This value supersedes the value read in from `opt_files_in` (Line 43), if provided.
- Line 58: Specify the level of confidence intervals computed for the true values of each new event device parameter from the maximum likelihood estimate and the estimated Fisher information matrix (WPA, §A.2, Equation (19); §A.4, Equation (21)).
- Line 61: Indicate if gradient verification is to be conducted on the log-likelihood function. If `TRUE` and `igrad` is `TRUE` (Line 20), analytical and numerical gradients at the

optimal parameter value, and other randomly sampled parameter values, are compared for consistency.

- Line 64: Specify the strategy for running parallel jobs using the `future` package in `R`. The available options are given by starting an `R` session and issuing the following commands,

```
% R
> require(future)
> help(plan)
```

- Lines 67-71: Calls the log-likelihood maximization function `calc_mle_0` for the new event data. Table 6 describes all inputs to this function with default values. Only inputs with no default values must be provided.

Table 6: Inputs to `calc_mle_0` function.

Input	Default	Brief Description
`p_cal`	none	environment storing all objects needed in log-likelihood calculations
`gdir`	none	directory location of global subroutines
`adir`	none	directory location of application subroutines
`f0`	none	names of forward model functions for each signature by phenomenology
`nst`	10	number of starting values for log-likelihood maximization
`ncor`	1	number of cores for log-likelihood maximization
`ci_lev`	0.95	confidence interval levels for new event parameter inference
`igrad`	`TRUE`	forward model Jacobian provided
`bfgs`	`TRUE`	log-likelihood maximization uses BFGS methods
`igrck`	`TRUE`	conduct log-likelihood function gradient verification
`t_cal`	`NULL`	object required if bounds supplied to log-likelihood maximization
`g0`	`NULL`	names of forward model Jacobian functions for each signature by phenomenology
`fopt_in`	`NULL`	location of input `R` data file providing an initial starting value for log-likelihood maximization
`Xst`	`NULL`	matrix of starting values for log-likelihood maximization if not generated by this function
`tst`	`NULL`	vector of starting values for new event parameters in log-likelihood maximization
`fopt_out`	`NULL`	location to write output `R` data file with results of log-likelihood maximization
`pl`	`"multicore"`	strategy for running parallel jobs using the `future` package

2.2.3 Bayesian Analysis

The optional Bayesian inference component of the second stage analysis in Appendix A.7 is responsible for integrating calibrated within signature forward and error model parameter values from the first stage with new event data to sample new event device parameters of interest from their posterior distribution. Imputation of first stage parameters results in more complete uncertainty quantification, but is computationally more intensive than employing the maximum likelihood estimate (default). Estimates of the new event device parameters with uncertainty quantification are computed from the posterior samples.

- Line 6: Indicate if Bayesian analysis is to be conducted.
- Line 10: Read in code performing second stage Bayesian analysis on new event device parameters, using calibrated within signature forward and error model parameters from the first stage.
- Line 13: Indicate if a log-prior density for the new event device parameters is supplied by the user (WPA, §6.5, p. 15; §6.6, pp. 18-19). If `iTheta0Prior` is `FALSE`, a "flat prior" (uniform on the domain) on these parameters is assumed.
- Lines 15-35: If relevant, specify details of user-provided log-prior distributions for new event device parameters.
  - Line 17: Specify location of log-prior function. If `NULL`, utilize the default log-prior function contained in the file `lp_0.r` placed in the application code directory; in this example,

    `MultiPEM_Toolbox_Package/Applications/Code/IYDT`
  - Line 19: If `igrad` is `TRUE` (Line 20 of Appendix A.6), specify location of the log-prior gradient function. If `NULL`, utilize the default log-prior gradient function contained in the file `glp_0.r` placed in the application code directory; in this example,

    `MultiPEM_Toolbox_Package/Applications/Code/IYDT`
  - Line 23: Provide the name of the log-prior function.
  - Line 24: If `igrad` is `TRUE` (Line 20 of Appendix A.6), provide the name of the log-prior gradient function.
  - Lines 26-31: Specify all fixed quantities required for calculation of the log-prior density. In this example, the mean (Line 27) and standard deviation (Line 28) of the Gaussian prior distribution for log-yield, and the mean (Line 30) and standard deviation (Line 31) of the Gaussian prior distribution for height-of-burst, are specified.
- Line 39: Select the Markov chain Monte Carlo (MCMC) algorithm to use for posterior sampling, from one of four options: `RAM`, `FME`, `NUTS`, and `SMC`. `RAM` is the robust adaptive Metropolis algorithm of Vihola[12] implemented in the `R` package `adaptMCMC`. `FME`

[12] Vihola, M. (2012). Robust adaptive Metropolis algorithm with coerced acceptance rate. *Stat Comput*

is the delayed rejection adaptive Metropolis algorithm of Haario, Laine, and Mira[13] implemented in the `R` package `FME`. `NUTS` is the No-U-Turn Sampler of Hoffman and Gelman[14]. The `NUTS` option requires the analytical gradient of the log-posterior density, which in turn requires `igrad` to be `TRUE` (Line 20 of Appendix A.6). `SMC` is a Sequential Monte Carlo (SMC) method adapted for sampling challenging posterior distributions (e.g. multi-modal) of low-dimensional parameter spaces[15].

- Line 42: Specify the per core sample size of the burn-in period for MCMC sampling (pre-equilibrium stage of Markov chain). These samples are discarded prior to any inference using the posterior samples.
- Line 45: Specify the sample size of the MCMC production run. These samples are kept for posterior inference.
- Line 48: Specify the rate at which MCMC production samples are thinned when multiple imputation of first stage parameters is invoked for improved uncertainty quantification of second stage parameters.
- Line 51: Specify the number of cores to use for parallel optimization (across distinct starting values) of the new event data log-posterior function. By default, this optimization uses the same number of distinct starting values as optimization of the new event data log-likelihood function (Line 33 of Appendix A.6).
- Line 54: Specify the number of cores used to run multiple imputations simultaneously or parallel MCMC chains for a single imputation. The burn-in period for each chain is determined by `nburn` (Line 42), while `nmcmc` (Line 45) production runs are generated for each imputed first stage parameter value, or split between the `ncores_mc` processors and combined at the conclusion of the runs for a single imputation.
- Line 57: Indicate if gradient verification is to be conducted on the log-prior function. If `TRUE` and `igrad` is `TRUE` (Line 20 of Appendix A.6), analytical and numerical gradients at the maximum *a posteriori* parameter value, and other randomly sampled parameter values, are compared for consistency.
- Line 60: Indicate if gradient verification is to be conducted on the log-posterior function. If `TRUE` and `igrad` is `TRUE` (Line 20 of Appendix A.6), analytical and numerical gradients at the maximum *a posteriori* parameter value, and other randomly sampled parameter values, are compared for consistency.
- Line 65: If `iMCMC` is `"SMC"` (Line 39), specify the number of cores to be used in the inner parallelization of the Sequential Monte Carlo (SMC) code for posterior sampling of the new event device parameters. SMC is advantageous if the posterior distribution of these parameters is multi-modal.

22:997-1008.

[13] Haario, H., Laine, M., and Mira, A. (2006). DRAM: Efficient adaptive MCMC. *Stat Comput* 16:339-354.

[14] Hoffman, M. D. and Gelman, A. (2014). The No-U-Turn Sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. *J Mach Learn Res* 15:1593-1623.

[15] Golchi, S. and Loeppky, J.L. (2016). Monte Carlo based Designs for Constrained Domains. arXiv:1512.07328v2 [stat.ME], 8 Aug. 2016.

- Line 67: Lower bounds of new event device parameters (on infinite domain) for SMC sampling. For infinite values, lower bounds are determined from the maximum likelihood estimate (MLE) of these parameters and its uncertainty.
- Line 68: Upper bounds of new event device parameters (on infinite domain) for SMC sampling. For infinite values, upper bounds are determined from the MLE of these parameters and its uncertainty.
- Lines 71-79: Calls the Bayesian analysis function `calc_bayes_0` for the new event data. Table 7 describes all inputs to this function with default values. Only inputs with no default values must be provided.

Table 7: Inputs to `calc_bayes_0` function.

Input	Default	Brief Description
`p_cal`	none	environment storing all objects needed in log-posterior calculations
`gdir`	none	directory location of global subroutines
`adir`	none	directory location of application subroutines
`nst`	10	number of starting values for log-posterior maximization
`nburn`	10000	number of per core MCMC burn-in samples
`nmcmc`	20000	number of MCMC production samples
`nthin`	1	posterior sample thinning rate per imputation, for multiple imputation
`ncor_map`	1	number of cores for log-posterior maximization
`ncor_mc`	1	number of cores for multiple imputation, or for generating parallel MCMC chains if single imputation
`igrad`	`TRUE`	forward model Jacobian provided
`igrck_pr`	`TRUE`	conduct log-prior function gradient verification
`igrck_po`	`TRUE`	conduct log-posterior function gradient verification
`bfgs`	`TRUE`	log-posterior maximization uses BFGS methods
`itpr`	`FALSE`	prior density function provided for new event parameters
`fpr_t`	`NULL`	location of function computing log-prior density for new event parameters
`fgpr_t`	`NULL`	location of function computing gradients of log-prior density for new event parameters
`imcmc`	`"FME"`	MCMC algorithm (current options: `"RAM"`, `"FME"`, `"NUTS"`, `"SMC"`)
`pl`	`"multicore"`	strategy for running parallel jobs using the `future` package
`ncor_smc`	`NULL`	number of cores for inner parallelization of SMC code
`lb_smc`	`NULL`	lower bounds of new event parameters for SMC sampling
`ub_smc`	`NULL`	upper bounds of new event parameters for SMC sampling
`t_cal`	`NULL`	object required if bounds supplied to log-posterior maximization

2.2.4 Output

The output file `runMPEM_0.out` from the second stage analysis contains a summary of new event device parameter estimates and (if relevant) posterior samples derived from the new event data, based on fixed (or multiply imputed) within signature forward and error model parameter values from the first stage analysis derived from the benchmark data. The desired output is supplied by the user function `print_sumstats_0.r`, placed in the application code directory; in this example,

`MultiPEM_Toolbox_Package/Applications/Code/IYDT`

The output presented in Appendix A.8 contains the most pertinent information extracted from the full file.

- Lines 7-62: Output from the maximum likelihood estimation function `calc_mle_0`:
  - Line 9: Convergence code from the `R` optimization function `optim`. In this example, '0' indicates successful completion.
  - Line 10: Number of optimization restarts in which the relative absolute maximum log-likelihood difference is $\leq 10^{-8}$. The algorithm exits after 2 such restarts, which is attained in this example.
  - Line 18: Maximum likelihood estimates of the new event device parameters; in this example, log-yield (`W`) and height-of-burst (`HOB`).
  - Line 23: Standard errors of the maximum likelihood estimates of the new event device parameters, adjusted for estimation of the forward model parameters and (if relevant) benchmark source errors-in-variables yields in the first stage (WPA, §A.2, Equation (19); §A.4, Equation (21)).
  - Line 28: Standard errors of the maximum likelihood estimates of the new event device parameters, assuming the forward model parameters and (if relevant) benchmark source errors-in-variables yields are known with certainty (set to their first stage values) (WPA, §A.2, p. 36, calculated from $(\mathcal{I}^0_{\boldsymbol{\theta}_0,\boldsymbol{\theta}_0})^{-1}$).
  - Lines 32-34: Correlation matrix of the maximum likelihood estimates of the new event device parameters, adjusted for estimation of the forward model parameters and (if relevant) benchmark source errors-in-variables yields in the first stage (WPA, §A.2, Equation (19); §A.4, Equation (21)).
  - Lines 38-40: Correlation matrix of the maximum likelihood estimates of the new event device parameters, assuming the forward model parameters and (if relevant) benchmark source errors-in-variables yields are known with certainty (set to their first stage values) (WPA, §A.2, p. 36, calculated from $(\mathcal{I}^0_{\boldsymbol{\theta}_0,\boldsymbol{\theta}_0})^{-1}$).
  - Lines 45-46: 95% confidence intervals for the unknown true values of the new event device parameters, based on standard errors adjusted for estimation of the forward model parameters and (if relevant) benchmark source errors-in-variables yields in the first stage (WPA, §A.2, Equation (19); §A.4, Equation (21)).

  - Lines 51-52: 95% confidence intervals for the unknown true values of the new event device parameters, based on standard errors assuming the forward model parameters and (if relevant) benchmark source errors-in-variables yields are known with certainty (set to their first stage values) (WPA, §A.2, p. 36, calculated from $(\mathcal{I}^0_{\boldsymbol{\theta}_0,\boldsymbol{\theta}_0})^{-1}$).
  - Lines 57-62: Example of log-likelihood gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
    * Line 58: Analytic gradient calculation
    * Line 60: Numerical gradient calculation using the `R` package `numDeriv`
    * Line 62: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients
- Lines 75-132: Output from the Bayesian analysis function `calc_bayes_0`:
  - Line 77: Convergence code from the `R` optimization function `optim`. In this example, '0' indicates successful completion.
  - Line 78: Number of optimization restarts in which the relative absolute maximum log-posterior difference is $\leq 10^{-8}$. The algorithm exits after 2 such restarts, which is attained in this example.
  - Line 86: Maximum *a posteriori* estimates of the new event device parameters.
  - Lines 90-95: Example of log-prior gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
    * Line 91: Analytic gradient calculation
    * Line 93: Numerical gradient calculation using the `R` package `numDeriv`
    * Line 95: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients
  - Lines 99-104: Example of log-posterior gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
    * Line 100: Analytic gradient calculation
    * Line 102: Numerical gradient calculation using the `R` package `numDeriv`
    * Line 104: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients
  - Line 108: Acceptance rate of the Delayed Rejection Adaptive Metropolis (DRAM) posterior sampling method implemented in `R` package `FME`. Note that one delayed rejection step is allowed in the default implementation.
  - Line 114: Means of samples from the new event device parameter marginal posterior distributions.

- Line 116: Standard deviations of samples from the new event device parameter marginal posterior distributions.
- Lines 118-126: User specified quantiles of samples from the new event device parameter marginal posterior distributions.
- Lines 130-132: Correlation matrix of samples from the new event device parameter joint posterior distribution.

The `p_cal` environment resulting from this run contains several elements of potential interest for additional post-processing:

- `p_cal$mle`: Maximum likelihood estimate of unbounded new event device parameters (i.e., on scale used by the optimizer)
- `p_cal$Sigma_mle_0$II_nev_it`: Estimated asymptotic covariance matrix of `p_cal$mle`, adjusted for first stage estimation of quantities stated below
- `p_cal$Sigma_mle_0$II_nev_0_it`: Estimated asymptotic covariance matrix of `p_cal$mle`, assuming first stage estimates of quantities stated below are known with certainty
- `p_cal$tmle_0`: Maximum likelihood estimate of transformed new event device parameters (i.e., on correct scale)
- `p_cal$Sigma_mle_0$II_nev`: Estimated asymptotic covariance matrix of `p_cal$tmle_0`, adjusted for first stage estimation of quantities stated below
- `p_cal$Sigma_mle_0$II_nev_0`: Estimated asymptotic covariance matrix of `p_cal$tmle_0`, assuming first stage estimates of quantities stated below are known with certainty
- `p_cal$Sigma_mle_0$II_calp`: If `calp` is `TRUE` (Line 47 of Appendix A.1), estimated asymptotic covariance matrix of `p_cal$mle_calp`, adjusted for estimation of new event device parameters and first stage estimation of quantities stated below
- `p_cal$map`: If `iBayes` is `TRUE` (Line 6 of Appendix A.7), maximum *a posteriori* estimate of unbounded new event device parameters (i.e., on scale used by the optimizer)
- `p_cal$tmap_0`: If `iBayes` is `TRUE` (Line 6 of Appendix A.7), maximum *a posteriori* estimate of transformed new event device parameters (i.e., on correct scale)
- `p_cal$mpi`: For multiple imputation (`nimpute` > 1; Line 52 of Appendix A.5)), first stage posterior samples of (if relevant) unbounded global forward model parameters, (if relevant) benchmark source errors-in-variables yields, and signature within phenomenology forward and error model parameters based on benchmark data, used as second stage imputation values of these parameters if `iBayes` is `TRUE` (Line 6 of Appendix A.7)
- `p_cal$tmpi_0`: If `iBayes` is `TRUE` (Line 6 of Appendix A.7), posterior samples of transformed new event device parameters (i.e., on correct scale)

The maximum likelihood-based quantities use maximum likelihood estimates for the forward and error model parameters and (if relevant) the benchmark source errors-in-variables yields from the first stage analysis.

3 Complete Assessment

Complete assessments will be illustrated by examining the run files associated with a multi-phenomenology analysis in which signals from four phenomenologies are combined to infer the log-yield and height-of-burst (HOB)/depth-of-burial (DOB) of a near-surface nuclear explosion (WPA, §6).

```
% cd ./Runfiles/IYDT/4-Phen/I-EIV-SUGAR-hob
```

Complete assessments involve combining benchmark and (if relevant) new event data to simultaneously estimate global (if relevant) and signature within phenomenology forward model parameters (e.g. regression coefficients), error model parameters (e.g. source bias, path bias, observational error covariance), errors-in-variables yield values of benchmark sources (if relevant), and (if relevant) new event device parameters (e.g. yield, HOB/DOB, geolocation, event time) with uncertainty quantification. Complete assessments are more computationally intensive than rapid assessments, as they require that all parameters are inferred simultaneously for each new event of interest.

The analysis is defined in the `runMPEM.r` file, provided in Appendix B with line numbers referred to in the ensuing discussion. Appendix B.1 provides the preprocessing component, Appendix B.2 provides the code employed to maximize the likelihood function of the data with respect to all of the forward model, error model, (if relevant) errors-in-variables yield, and (if relevant) new event device parameters, while Appendix B.3 provides the code employed to optionally sample the posterior distribution of these parameters.

The complete analysis is run in batch mode as follows,

```
% R CMD BATCH runMPEM.r runMPEM.out &
```

The main features of the output file `runMPEM.out` are provided in Appendix B.4.

3.0.1 Preprocessing

The preprocessing component of the analysis in Appendix B.1 is primarily responsible for describing features of the benchmark and (if relevant) new event data and all parameters of inferential interest.

- Line 12+: Load all `R` packages utilized by multiple supporting subroutines, most notably log-likelihood and log-prior calculations and their associated gradients.
- Line 23: Specify directory location (relative to run directory) of all global (application independent) subroutines.
- Line 26: Read in code performing preprocessing of benchmark and (if relevant) new event data.
- Line 29: Specify directory location (relative to run directory) of all application-specific subroutines.
- Line 32: Specify root directory (relative to run directory) containing all application-specific benchmark and (if relevant) new event data files.

- Lines 35-38: A scalar or vector specifying the names of benchmark data files for each phenomenology, utilizing an ordering of the phenomenologies (for MultiPEM analysis) that is maintained throughout the input deck (as indicated here in Lines 41-44). Data files are text files (CSV formatted) containing all measured signatures (in the first column(s)) and input covariates (in succeeding column(s)) including all those required in forward and error model calculations. Directories specifying the exact locations of these files relative to the root data directory (Line 32) may also be included in the filenames.

- Line 47: Indicate if forward model parameters global to multiple signatures within phenomenology or across phenomenologies will be modeled. If `TRUE`, nominal values for these parameters may optionally be placed in the benchmark data file(s). If a subset of sources are to be assigned default values for some or all of these parameters, the value `NA` should be assigned to these parameters in the benchmark data file(s) for these sources, and the default values provided in the relevant forward model(s).

- Lines 49-52: If `calp` is `TRUE` (Line 47), provide a string vector of names for each of the global forward model parameters (Line 51).

- Line 55: A scalar or vector specifying the number of observed signatures for each phenomenology; in this example, 2 for each phenomenology.

- Lines 59-66: Specify the number of *common* forward model parameters within each phenomenology (WPA, §5.1, first paragraph). For a given forward model, common parameters maintain the same constant value within signature for every log-likelihood calculation. The `pbeta` object is initialized as a null list with elements for each phenomenology in the proper order (Line 59), initialized to zero vectors of length equal to the number of observed signatures (Line 60). Subsequent lines specify the number of common forward model parameters for each signature within each phenomenology. For example, the *acoustic* forward model for each signature contains 2 common forward model parameters (Line 62).

- Lines 69-72: Specify if the forward model(s) for any phenomenology depend on event emplacement conditions (Line 69), followed by (if relevant) a vector indicating the number of distinct emplacement conditions considered for each phenomenology in the proper order (Line 71). This specification allows distinct forward model parameters to be associated with different emplacement conditions (as specified subsequently). If `Th` is `TRUE` (Line 69), a factor named `Type` must be present in the benchmark and (if relevant) new event data files for each relevant phenomenology, indicating the emplacement condition pertaining to each entry. In this example, the *seismic* and *acoustic* forward model parameters may vary for 3 distinct emplacements ("soft", "hard", and "wet" rock types), while the *optical* and *surface effects* forward models are independent of emplacement condition.

- Lines 76-91: Specify the number of *emplacement* dependent forward model parameters within each phenomenology if relevant (WPA, §5.1, first paragraph). For a given forward model, emplacement parameters remain constant within signature for log-likelihood calculations with a given emplacement condition, but may be modified within signature for each distinct emplacement. The `pbetat` object is initialized as a null list with elements for each phenomenology in the proper order (Line 77), initialized as null lists with elements for each emplacement condition (Line 79) if multiple emplacements are present. Subsequent lines specify the number of forward model parameters for each signature within each emplacement condition for each phenomenology. For example, the *seismic* forward model for each signature within each emplacement contains 5 forward model parameters (Line 84) allowed to vary across emplacements. `pbetat` must be specified if multiple emplacements are present for any phenomenology (at least one element of `Th` is greater than 1).

- Lines 95-110: Specify the location of *common* forward model parameters within the full parameter vector, for phenomenologies possessing both common and emplacement dependent parameters. The `ibetar` object is initialized as a null list with elements for each phenomenology in the proper order (Line 96), initialized as null lists with elements for each signature within each emplacement condition (Line 101) if multiple emplacements are present. Subsequent lines specify the position of common parameters in the full forward model parameter vector, for phenomenologies possessing both common and emplacement dependent forward model parameters. For example, the *acoustic* forward model parameter vector takes common parameter values in its first two positions for each signature within each emplacement condition (Line 107).
- Line 113: Indicate if errors-in-variables yield values for benchmark events will be modeled (WPA, §3, Equation (3); §A.4). If `TRUE`, this allows uncertain yields for benchmark events (often assumed known with certainty) to vary within user-specified guidelines.
- Lines 116-132: If relevant, specify details of errors-in-variables yield models for benchmark events.
  - Line 119: Specify phenomenologies for application of errors-in-variables yield models to benchmark events
  - Lines 123-124: Provide the sources subject to errors-in-variables yield models for each phenomenology. The `seiv` object is initialized as a null list with elements for each phenomenology in the proper order (Line 123), with vectors indicating the relevant sources for each relevant phenomenology (Line 124). The `"ALL"` designation indicates that every source in the benchmark data set for the indicated phenomenology will be modeled with an errors-in-variables yield. `seiv` must be specified if `ieiv` is provided.
  - Line 127: The standard deviation of the errors-in-variables Gaussian distribution for each benchmark event log-yield. For each event, the mean of this distribution is taken to be its provided (design or measured) log-yield. In this example, a "total" error (3 standard deviations) of 10% in each provided yield is allowed. Note that this error is relative because yields are treated on a logarithmic scale. `eiv_w_sd` must be specified if `ieiv` is provided.
- Lines 136-145: Specify if *source* random effects (WPA, §3, Equation (2); §4; §A.5) should be included in the error model (Line 136). If so, the `pvc_1` object is initialized

as a null list with elements for each phenomenology in the proper order (Line 139), initialized to zero vectors of length equal to the number of observed signatures (Line 140). Subsequent lines specify the number of source random effects for each signature within each phenomenology. For example, the *seismic* error model for each signature contains a single source bias term (Line 142). If `pvc_1` is `TRUE` (Line 136), a factor named `Source` may be provided in the benchmark and (if relevant) new event data files for each relevant phenomenology, identifying the source pertaining to each entry. This factor must be present if there is more than one data entry for any source. In order to include source random effects in the error model for an observed signature, the benchmark data must contain more than one source, with at least one source containing more than one observation. A warning message will be printed to the log file if one of these conditions is violated.

- Lines 148-162: Specify if *path* random effects (WPA, §3, Equation (2); §4; §A.5), also referred to as *station* random effects, should be included in the error model (Line 148). If so, the `pvc_2` object is initialized as a null list with elements for each phenomenology in the proper order (Line 151), initialized to zero vectors of length equal to the number of observed signatures (Line 152). Subsequent lines specify the number of path random effects for each signature within each phenomenology. For example, the *seismic* error model for each signature contains a single path bias term (Line 154). The type of path random effect desired is specified by the `ptype` object, initialized as a null list with elements for each phenomenology in the proper order (Line 159). If `pvc_2` is `TRUE` (Line 148), a factor named `Path` must be provided in the benchmark (and new event) data file for each relevant phenomenology, identifying the source-to-sensor path pertaining to each entry. In order to include path random effects in the error model for an observed signature, the benchmark data must contain more than one path, with at least one path containing more than one observation. Additionally, specification of crossed path effects (`ptype` is `"Crossed"`) requires the signature to be observed from at least one common path for two or more sources, while specification of level 2 (within source) path effects requires more than one path for at least one source, with more than one observation for at least one of those paths. A warning message will be printed to the log file if one of these conditions is violated.

- Line 166: Indicate if the user is providing code to compute coefficient matrices for *source* or *path* random effects (WPA, §5.1). If `FALSE`, the function `calc_zmat.r` located in the global code directory,

  `MultiPEM_Toolbox_Package/Code`

  computes default coefficient matrices for the benchmark and (if relevant) new event data. If `TRUE`, then a user-provided function of the same name must be placed in the application code directory; in this example,

  `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  Table 8 shows data for the first two *seismic* benchmark sources in this example.

  If source and level 2 (within source) path random effects are included in the error model,

Table 8: Data for seismic benchmark sources `HRI-1` and `HRI-2`.

Y1	Y2	Source	Path	Type	lRange	W	HOB
−15.091	−9.252	HRI-1	Path_1	1	6.932	6.291	5
−15.089	−9.180	HRI-1	Path_1	1	6.932	6.291	5
−15.836	−10.218	HRI-1	Path_2	1	7.570	6.291	5
−15.892	−10.180	HRI-1	Path_2	1	7.570	6.291	5
−16.176	−10.557	HRI-1	Path_2	1	7.800	6.291	5
−16.907	−11.366	HRI-1	Path_2	1	8.371	6.291	5
−16.931	−11.338	HRI-1	Path_2	1	8.371	6.291	5
−14.835	−9.199	HRI-2	Path_1	1	6.930	6.291	3
−14.860	−9.184	HRI-2	Path_1	1	6.930	6.291	3
−15.674	−10.089	HRI-2	Path_1	1	7.568	6.291	3
−15.754	−10.197	HRI-2	Path_1	1	7.568	6.291	3
−16.002	−10.530	HRI-2	Path_2	1	7.802	6.291	3
−16.060	−10.605	HRI-2	Path_2	1	7.802	6.291	3
−16.534	−11.115	HRI-2	Path_2	1	8.239	6.291	3
−16.741	−11.230	HRI-2	Path_3	1	8.373	6.291	3
−16.737	−11.288	HRI-2	Path_3	1	8.373	6.291	3
−17.208	−11.656	HRI-2	Path_3	1	8.738	6.291	3

the source and path bias vectors (WPA, §5.1, p. 7) associated with these sources (with `HRI-1` and `HRI-2` designated as 1 and 2) are given by

$$\boldsymbol{E}_{S,11r} = \begin{pmatrix} \boldsymbol{Z}_{11r,1} \\ \boldsymbol{Z}_{11r,2} \end{pmatrix} b^{(S)}_{1r,1} \qquad \boldsymbol{E}_{P,11r} = \begin{pmatrix} \boldsymbol{E}_{P,111r} \\ \boldsymbol{E}_{P,112r} \end{pmatrix} = \begin{bmatrix} \boldsymbol{Z}_{111r} & \mathbf{0}_2 \\ \mathbf{0}_5 & \boldsymbol{Z}_{112r} \end{bmatrix} \begin{pmatrix} b^{(P)}_{1r,11} \\ b^{(P)}_{1r,12} \end{pmatrix}$$

$$\boldsymbol{E}_{S,12r} = \begin{pmatrix} \boldsymbol{Z}_{12r,1} \\ \boldsymbol{Z}_{12r,2} \\ \boldsymbol{Z}_{12r,3} \end{pmatrix} b^{(S)}_{1r,2} \quad \boldsymbol{E}_{P,12r} = \begin{pmatrix} \boldsymbol{E}_{P,121r} \\ \boldsymbol{E}_{P,122r} \\ \boldsymbol{E}_{P,123r} \end{pmatrix} = \begin{bmatrix} \boldsymbol{Z}_{121r} & \mathbf{0}_4 & \mathbf{0}_4 \\ \mathbf{0}_3 & \boldsymbol{Z}_{122r} & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \boldsymbol{Z}_{123r} \end{bmatrix} \begin{pmatrix} b^{(P)}_{1r,21} \\ b^{(P)}_{1r,22} \\ b^{(P)}_{1r,23} \end{pmatrix},$$

where the default coefficient matrices are given by

$$\begin{aligned} \boldsymbol{Z}_{11r,1} &= \mathbf{1}_2 & \qquad \boldsymbol{Z}_{111r} &= \mathbf{1}_2 \\ \boldsymbol{Z}_{11r,2} &= \mathbf{1}_5 & \boldsymbol{Z}_{112r} &= \mathbf{1}_5 \\ \boldsymbol{Z}_{12r,1} &= \mathbf{1}_4 & \boldsymbol{Z}_{121r} &= \mathbf{1}_4 \\ \boldsymbol{Z}_{12r,2} &= \mathbf{1}_3 & \boldsymbol{Z}_{122r} &= \mathbf{1}_3 \\ \boldsymbol{Z}_{12r,3} &= \mathbf{1}_3 & \boldsymbol{Z}_{123r} &= \mathbf{1}_3 \end{aligned}$$

for $\mathbf{1}_q$ and $\mathbf{0}_q$ the q-vectors of ones and zeros, respectively. The source and path random effects $\{b^{(S)}_{1r,1}, b^{(S)}_{1r,2}\}$ and $\{b^{(P)}_{1r,11}, b^{(P)}_{1r,12}, b^{(P)}_{1r,21}, b^{(P)}_{1r,22}, b^{(P)}_{1r,23}\}$ are mutually independent realizations of their respective random effects distributions (WPA, §5.1, Equation (5), p. 7). For each signature, this structure indicates that there is a single source bias effect applied to every observation within each source, while observations from each path are adjusted by distinct (and independently distributed) path bias effects (signatures are collected from two and three paths respectively for `HRI-1` and `HRI-2`).

If instead a signature is observed from one or more common source-to-sensor paths across two or more sources, referred to as "crossed paths" (`ptype` is `"Crossed"` (Line 159)) – assuming the source-to-sensor paths observed for the sources `HRI-1` and `HRI-2` are not present for any other source – the path bias vectors ($\boldsymbol{E}_{P,11r}, \boldsymbol{E}_{P,12r}$) corresponding to the two sources above are replaced by the single path bias vector

$$\boldsymbol{E}_{P,1\{1,2\}r} = \begin{bmatrix} \boldsymbol{Z}_{111r} & \boldsymbol{0}_2 & \boldsymbol{0}_2 \\ \boldsymbol{0}_5 & \boldsymbol{Z}_{112r} & \boldsymbol{0}_5 \\ \boldsymbol{Z}_{121r} & \boldsymbol{0}_4 & \boldsymbol{0}_4 \\ \boldsymbol{0}_3 & \boldsymbol{Z}_{122r} & \boldsymbol{0}_3 \\ \boldsymbol{0}_3 & \boldsymbol{0}_3 & \boldsymbol{Z}_{123r} \end{bmatrix} \begin{pmatrix} b^{(P)}_{1r,\{1,2\}1} \\ b^{(P)}_{1r,\{1,2\}2} \\ b^{(P)}_{1r,\{1,2\}3} \end{pmatrix}.$$

The entry $\{1, 2\}$ for the source index indicates that sources 1 (`HRI-1`) and 2 (`HRI-2`) must be considered jointly as a group, due to covariance between their observed signatures induced by the common source-to-sensor propagation paths `Path_1` and `Path_2`. The path random effects $\{b^{(P)}_{1r,\{1,2\}1}, b^{(P)}_{1r,\{1,2\}2}, b^{(P)}_{1r,\{1,2\}3}\}$ are mutually independent realizations of the path random effect distribution (WPA, §5.1, Equation (5), p. 7).

- Line 170: Specify if bounded optimization of any unknown parameters is to be conducted. This option is currently only supported for new event device parameters. The default is to optimize all new event device parameters on an unbounded input space, transforming them to their input domain (specified subsequently in this preprocessing file) as necessary for forward model calculations. If `opt_B` is `TRUE`, the new event device parameters are optimized directly on their input domain.

- Line 173: Indicate if new event device parameters are to be estimated with uncertainty quantification simultaneously from the benchmark and new event data. If `nev` is `FALSE`, only forward and error model parameters, and benchmark source errors-in-variables yields (if relevant), are inferred from the benchmark data.

- Lines 176-221: If relevant, specify details of new event device parameters and location(s) of new event data.

  – Lines 178-181: A scalar or vector specifying the names of new event data files for each phenomenology, utilizing an ordering of the phenomenologies (for MultiPEM analysis) that is consistent with the benchmark data files and maintained throughout the input deck (as indicated here in Lines 41-44). Data files are text files (CSV formatted) containing all measured signatures (in the first column(s)) and input covariates (in succeeding column(s)) including all those required in forward and error model calculations, but excepting the new event device parameters that are unknown and subject to inference. Directories specifying the exact locations of these files relative to the root data directory (Line 32) may also be included in the filenames. Must be provided if `nev` is `TRUE` (Line 173).

  – Line 184: Specify the names of the new event device parameters of inferential interest as a vector of strings. This information is utilized in postprocessing, and must be provided if `nev` is `TRUE` (Line 173).

- Line 187: Indicate if the new event device parameters are subjected to a user-provided bijective transformation supplied to assist likelihood maximization or posterior sampling. If `itransform` is `TRUE`, the code implementing this transformation is concatenated into a single file named `transform.r` and placed in the application code directory; in this example,

  `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  The functions that must be provided in `transform.r` include the following:

  * `tau`: Function $\boldsymbol{\tau}(\cdot)$ applied to transformed variables $\widetilde{\boldsymbol{\theta}}_0$ with the new event device parameters $\boldsymbol{\theta}_0$ as its image,

  $$\boldsymbol{\theta}_0 = \boldsymbol{\tau}(\widetilde{\boldsymbol{\theta}}_0)$$

  * `j_tau`: Jacobian matrix of $\boldsymbol{\tau}(\cdot)$,

  $$\boldsymbol{J}_{\boldsymbol{\tau}}(\widetilde{\boldsymbol{\theta}}_0) = \begin{bmatrix} \dfrac{\partial \tau_1(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,1}} & \cdots & \dfrac{\partial \tau_1(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,q}} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial \tau_q(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,1}} & \cdots & \dfrac{\partial \tau_q(\widetilde{\boldsymbol{\theta}}_0)}{\partial \tilde{\theta}_{0,q}} \end{bmatrix}$$

    where q is the dimension of $\boldsymbol{\theta}_0$.

  * `log_absdet_j_tau`: Logarithm of the absolute value of the determinant of the Jacobian matrix computed from `j_tau`,

  $$\log \operatorname{abs}(\det(\boldsymbol{J}_{\boldsymbol{\tau}}(\widetilde{\boldsymbol{\theta}}_0)))$$

  * `dlog_absdet_j_tau`: Gradient of the log absolute Jacobian determinant with respect to $\widetilde{\boldsymbol{\theta}}_0$

  * `inv_tau`: Inverse function of $\boldsymbol{\tau}(\cdot)$

  In this example, the new event device parameters of inferential interest are log-yield w and height-of-burst h, that is $\boldsymbol{\theta}_0 = (w, h)$. The relevant forward models are functions of a scaled height-of-burst, $\tilde{h} = h \exp(-w/3)$, suggesting the possible utility of likelihood maximization or posterior sampling in terms of $\widetilde{\boldsymbol{\theta}}_0 = (\tilde{w}, \tilde{h})$ for $\tilde{w} = w$.

- Lines 190-197: If `itransform` is `TRUE` (Line 187), and if `tPars` is `TRUE` (Line 191), initialize `tPars` to a null list (Line 194). Subsequent lines provide the value(s) for all fixed inputs required to compute the function `tau` (see previous item). In this example, a `yield_scaling` value is required (Line 195).

- Lines 201-204: Specify lower and upper bounds for the new event device parameters if needed. By default, lower bounds are set to $-\infty$ (Line 201) and upper bounds to $+\infty$ (Line 203). In this example, the second parameter (height-of-burst) is restricted to the range $(-10, 160)$ (Lines 202 and 204). Note that likelihood maximization and posterior sampling are conducted on an unbounded parameter space. If lower or upper bounds are specified for any parameter, they are applied just prior to objective function calculations using the `transform` function of the `transform.r` file located in the global code directory,

  `MultiPEM_Toolbox_Package/Code`

- Lines 207-212: If `tsub` is `TRUE` (Line 207), the forward model for at least one phenomenology depends only on a subset of the full vector $\boldsymbol{\theta}_0$ of new event device parameters. The `tsub` object is initialized to a null list with elements for each phenomenology in the proper order (Line 210). The `theta_names` vector (Line 184) describes the order of elements in $\boldsymbol{\theta}_0$. For relevant phenomenologies, parameter subsets are specified as integer vectors identifying the extracted elements of $\boldsymbol{\theta}_0$. The forward models of all other phenomenologies depend on the full $\boldsymbol{\theta}_0$. In this example, the *surface effects* (*crater*) phenomenology only depends on log-yield (Line 211), while the other phenomenologies depend on both log-yield and height-of-burst.

- Lines 224-229: Calls the preprocessing function `prepro` for the benchmark and (if relevant) new event data. Table 9 describes all inputs to this function with default values. Only inputs with no default values must be provided.

- Lines 230-236: If `opt_B` is `TRUE` (Line 170), the preprocessor function `prepro` returns a list (designated here as `tmp`) with objects `p_cal` and `t_cal`, which are then assigned as follows

  ```
  % p_cal = tmp$p_cal
  % t_cal = tmp$t_cal
  ```

  and both are utilized for maximum likelihood estimation and Bayesian analysis. Otherwise, `p_cal` is the only object returned,

  ```
  % p_cal = tmp$p_cal
  ```

  and utilized in subsequent analyses.

3.0.2 Maximum Likelihood Estimation

The maximum likelihood estimation component of the complete analysis in Appendix B.2 is responsible for utilizing benchmark and (if relevant) new event data to simultaneously estimate the parameters of the forward and error models, possibly the yield of each benchmark source for phenomenologies adopting the errors-in-variables yield model, and (if relevant) the new event device parameters (WPA, §A.1-A.2). If `nev` is `TRUE` (Line 168 of Appendix B.1), quantification of uncertainty in the new event device parameter estimates is provided, adjusting for asymptotically dependent quantities.

Table 9: Inputs to prepro function.

Input	Default	Brief Description
gdir	none	directory location of global subroutines
adir	none	directory location of application subroutines
rdir	none	root directory location of data files
cdir	none	directory locations (if relevant) and names of benchmark data files under rdir
Rh	none	vector with number of signatures for each phenomenology
pbeta	none	list containing empirical model common parameter counts by phenomenology
bopt	FALSE	parameter bounds supplied to log-likelihood maximization (currently implemented only for new event parameters)
nev	FALSE	analysis of new event
itr	FALSE	bijective transform of new event parameters provided
izmat	FALSE	user-provided code for computing variance component coefficient matrices
ieiv	NULL	numerical identifier of phenomenologies utilizing errors-in-variables yields in analysis of benchmark data
seiv	NULL	list containing identifiers of benchmark sources assigned errors-in-variables yields by phenomenology (ALL – every source)
ewsd	NULL	standard deviation of errors-in-variables Gaussian likelihood
Th	NULL	number of emplacement conditions for each phenomenology
pbetat	NULL	list containing empirical model emplacement-dependent parameter counts by phenomenology
ibetar	NULL	list containing locations of empirical model common parameters in full parameter vector by phenomenology
pvc_1	NULL	list containing source variance component parameter counts by phenomenology
pvc_2	NULL	list containing path variance component parameter counts by phenomenology
ptype	NULL	list indicating treatment of path variance component parameter by phenomenology (Crossed – common paths present across sources)
tnames	NULL	names of new event parameters
cnames	NULL	names of global forward model parameters
fp_tr	NULL	fixed inputs to new event parameter transform
tlb	NULL	lower bounds for new event parameters
tub	NULL	upper bounds for new event parameters
ndir	NULL	directory locations (if relevant) and names of new event data files under rdir
tsub	NULL	list containing index sets identifying new event parameter subsets by phenomenology if relevant

- Line 6: Read in code performing simultaneous maximum likelihood estimation of forward and error model parameters, benchmark source errors-in-variables yields (if relevant), and new event device parameters (if relevant), based on benchmark and (if relevant) new event data.
- Line 9: User specified seed to ensure repeatability of maximum likelihood estimation.
- Lines 13-17: Provide names of forward models for each signature by phenomenology (WPA, §6.1-6.4). The `fm` object is initialized as a null list with elements for each phenomenology in the proper order (Line 13). Subsequent lines specify the function names as vectors of strings having length equal to the number of signatures for each phenomenology (Lines 14-17). The code for all forward models from each phenomenology is concatenated into a single file named `forward.r` and placed in the application code directory; in this example,

  `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  Note that these forward models accept a vector of calibration and device parameters as their main argument. In this example, the *seismic* forward model $f_{sr}(\cdot)$ as a function of the parameters $\boldsymbol{\beta}_{sr}$ and device parameters log-yield (w) and HOB/DOB (h) is given as follows (WPA, §6.2, p. 11),

  $$\begin{aligned} \log(\tilde{d}_{sr}(\boldsymbol{\beta}_{sr},(w,h))) &= \beta_{sr,1}+\beta_{sr,2}\log(\tilde{\delta}_s)+\beta_{sr,3}\,\text{logistic}(\beta_{sr,4}\tilde{h}_s+\beta_{sr,5}) \\ f_{sr}(\boldsymbol{\beta}_{sr},(w,h)) &= \log(d_{sr}(\boldsymbol{\beta}_{sr},(w,h))) \end{aligned} \tag{3}$$

  for

  $$\text{logistic}(x)=\frac{1}{1+\exp(-x)}\,.$$

  The scaled signatures and covariates of this forward model are given by

  $$\begin{aligned} \tilde{d}_{s1} &= d_{s1}\exp(-w/3) & \tilde{d}_{s2} &= d_{s2} \\ \tilde{\delta}_s &= \delta\exp(-w/3) & \tilde{h}_s &= h\exp(-w/3)\,, \end{aligned}$$

  where d_{s1} and d_{s2} are P-wave displacement and maximum velocity, and the covariate is range δ. The function `f_s` returns a vector of forward model calculations evaluated for the supplied value of $(\boldsymbol{\beta}_{sr},(w,h))$, each element corresponding to each row of a matrix of covariates (in this case, a column vector of ranges δ).
- Line 20: Indicate if forward model Jacobian matrices are provided for efficient log-likelihood maximization.
- Lines 22-30: If `igrad` is `TRUE` (Line 20), names of forward model Jacobian functions must be provided for each signature by phenomenology. The `gfm` object is initialized as a null list with elements for each phenomenology in the proper order (Line 25). Subsequent lines specify the Jacobian function names as vectors of strings having length equal to the number of signatures for each phenomenology (Lines 26-29). The code for all forward model Jacobian functions from each phenomenology is concatenated into a single file named `jacobian.r` and placed in the application code directory; in this example,

`MultiPEM_Toolbox_Package/Applications/Code/IYDT`

Note that these Jacobian functions accept a vector of calibration and device parameters as their main argument. In this example, the gradient vector of the *seismic* forward model of Equation (3) is computed from the partial derivatives of $f_{sr}(\cdot)$ for each parameter as follows,

$$\begin{aligned}
\frac{\partial f_{sr}}{\partial \beta_{sr,1}} &= 1 \\
\frac{\partial f_{sr}}{\partial \beta_{sr,2}} &= \log(\tilde{\delta}_s) \\
\frac{\partial f_{sr}}{\partial \beta_{sr,3}} &= \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \\
\frac{\partial f_{sr}}{\partial \beta_{sr,4}} &= \beta_{sr,3}\tilde{h}_s \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5}) \\
\frac{\partial f_{sr}}{\partial \beta_{sr,5}} &= \beta_{sr,3} \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5}) \,,
\end{aligned}$$

and each device parameter as follows,

$$\begin{aligned}
\frac{\partial f_{sr}}{\partial w} =& -\frac{1}{3}\left(\beta_{sr,2} + \beta_{sr,3}\beta_{sr,4}\tilde{h}_s \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5})\right) \\
&+ \frac{1}{3}\,\delta_1(r) \\
\frac{\partial f_{sr}}{\partial h} =& \ \beta_{sr,3}\beta_{sr,4}\exp(-w/3) \times \text{logistic}(\beta_{sr,4}\tilde{h}_s + \beta_{sr,5}) \times \text{logistic}(-\beta_{sr,4}\tilde{h}_s - \beta_{sr,5})
\end{aligned}$$

for $\delta_A(x)$ the indicator function of set A. The function `g_s` returns a Jacobian matrix (`jbeta_s`) of forward model gradients for the parameters, evaluated at the supplied value of $(\boldsymbol{\beta}_{sr}, (w, h))$, with rows corresponding to the rows of a matrix of covariates (in this case, a column vector of ranges δ). If relevant, `g_s` will also return a Jacobian matrix (`jtheta_s`) of forward model gradients for the device parameters, evaluated at the supplied value of $(\boldsymbol{\beta}_{sr}, (w, h))$, each element corresponding to each row of the same covariate matrix used in the calculation of `jbeta_s`.

- Line 35: Indicate if the same forward model function is used to compute multiple signatures, and signature-specific code within this function is required.
- Lines 37-41: If `iResponse` is `TRUE` (Line 35), initialize `iResponse` to a null list with elements for each phenomenology in the proper order (Line 38). For each relevant phenomenology, subsequent lines provide vectors of length equal to the number of signatures, each element of which is a tag identifying code specific to the corresponding signature. This mechanism is utilized for the *seismic* (Line 39) and *acoustic* (Line 40) phenomenologies.
- Line 44: Indicate if fixed inputs are to be provided to the forward models for at least one phenomenology.

- Lines 46-55: If `fPars` is `TRUE` (Line 44), initialize `fPars` to a null list with elements for each phenomenology in the proper order (Line 47). For each relevant phenomenology, subsequent lines provide the value(s) of all fixed inputs. For example, the *optical* forward model requires fixed values for `yield_scaling` (Line 52), `pressure_scaling` (Line 53), and `temp_scaling` (Line 54).

- Line 58: Specify the number of starting parameter vectors for the log-likelihood maximization routine.

- Line 61: Specify the number of cores to use for parallel optimization (across distinct starting values) of the benchmark and (if relevant) new event data log-likelihood function.

- Line 64: Specify if the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is to be used for maximization of the log-likelihood function. If `TRUE`, functions to compute forward model Jacobian matrices analytically must be provided, or numerical gradients will be utilized (generally increasing compute time). If `FALSE`, the gradient-free Nelder-Mead simplex algorithm will be utilized for optimization, which is generally much slower computationally than BFGS with analytical gradients.

- Lines 68-71: If relevant, specifies the location (relative to the run directory) of parameter values or estimates to be used as the first starting value for log-likelihood maximization. These values are stored in a `.RData` object as a list, with elements corresponding to forward model (e.g. global parameters `calp`, within signature common parameters `beta`, within signature emplacement-dependent parameters `tbeta`) and error model (e.g. source variance components `vc_1`, path variance components `vc_2`, observation error parameters `eps`) quantities of interest. If relevant, benchmark source errors-in-variables yield estimates (`w_eiv`) are also provided. For multi-phenomenology analyses, values or estimates from individual phenomenologies may be input in the proper order, and they will be concatenated appropriately.

- Line 75: If desired, name of output `.RData` file to store optimization results from this run. The elements of the list to be written are described in the previous item.

- Lines 77-85: If `calp` is `TRUE` (Line 47 of Appendix B.1), and if `cst` is `TRUE` (Line 79), specifies an initial starting value for the global forward model parameters (Lines 82-83) for log-likelihood maximization. This value supersedes the value read in from the first file provided in the string vector `opt_files_in` (Line 68), if the `calp` list element is provided.

- Lines 87-95: If `nev` is `TRUE` (Line 168 of Appendix B.1), and if `tst` is `TRUE` (Line 89), specifies an initial starting value for the new event device parameters (Lines 92-93) for log-likelihood maximization. This value supersedes the value read in from the first file provided in the string vector `opt_files_in` (Line 68), if the `theta0` list element is provided.

- Line 97-100: Specify the level of confidence intervals for (a) the true values of each global forward model parameter from the maximum likelihood estimate and the estimated Fisher information matrix, and/or (b) the true values of each new event device parameter from the maximum likelihood estimate and the estimated Fisher information matrix (WPA, §A.2, Equation (19); §A.4, Equation (21)).

- Line 104: Indicate if phenomenology specific code is required in the postprocessing function.
- Lines 106-108: If `Phen` is `TRUE` (Line 104), specifies a matrix in which the first column provides the numerical phenomenology indicator (see Lines 41-44 of the preprocessing code in Appendix B.1), and the second column provides the phenomenology name in string format. In this example, specific code is required to process results for the *seismic* phenomenology (Line 107).
- Line 111: Indicate if gradient verification is to be conducted on the log-likelihood function. If `TRUE` and `igrad` is `TRUE` (Line 20), analytical and numerical gradients at the optimal parameter value, and other randomly sampled parameter values, are compared for consistency.
- Line 114: Specify the strategy for running parallel jobs using the `future` package in `R`. The available options are given by starting an `R` session and issuing the following commands,

```
% R
> require(future)
> help(plan)
```

- Lines 117-121: Calls the log-likelihood maximization function `calc_mle` for the benchmark and (if relevant) new event data. Table 10 describes all inputs to this function with default values. Only inputs with no default values must be provided.

3.0.3 Bayesian Analysis

The optional Bayesian inference component of the analysis in Appendix B.3 is responsible for sampling forward and error model parameters, benchmark source errors-in-variables yields (if relevant), and new event device parameters (if relevant) from their joint posterior distribution, using benchmark and (if relevant) new event data simultaneously. If `nev` is `TRUE` (Line 168 of Appendix B.1), estimates of new event device parameters with uncertainty quantification are computed from these samples.

- Line 6: Indicate if Bayesian analysis is to be conducted.
- Line 10: Read in code performing Bayesian analysis on forward and error model parameters, benchmark source errors-in-variables yields (if relevant), and new event device parameters (if relevant), using benchmark and (if relevant) new event data.
- Line 14: Indicate if a log-prior density for the signature within phenomenology forward model parameters is supplied by the user (WPA, §6.5, p. 15). If `iBetaPrior` is `FALSE`, a "flat prior" (uniform on the domain) on these parameters is assumed.
- Lines 16-35: If relevant, specify details of user-provided log-prior distributions for signature within phenomenology forward model parameters. For each relevant phe-

Table 10: Inputs to calc_mle function.

Input	Default	Brief Description
p_cal	none	environment storing all objects needed in log-likelihood calculations
gdir	none	directory location of global subroutines
adir	none	directory location of application subroutines
f	none	names of forward model functions for each signature by phenomenology
nst	10	number of starting values for log-likelihood maximization
ncor	1	number of cores for log-likelihood maximization
ci_lev	0.95	confidence interval levels for global forward model and new event parameter inference
igrad	TRUE	forward model Jacobian provided
bfgs	TRUE	log-likelihood maximization uses BFGS methods
igrck	TRUE	conduct log-likelihood function gradient verification
t_cal	NULL	object required if bounds supplied to log-likelihood maximization
g	NULL	names of forward model Jacobian functions for each signature by phenomenology
iresp	NULL	flags for modified calculation by signature in a common forward model for each relevant phenomenology
fp_fm	NULL	fixed inputs required by forward models
fopt_in	NULL	location of input R data file(s) providing an initial starting value for log-likelihood maximization (if multiple files, starting value created by concatenating over phenomenologies)
Xst	NULL	matrix of starting values for log-likelihood maximization if not generated by this function
tst	NULL	vector of starting values for new event parameters in log-likelihood maximization
cst	NULL	vector of starting values for global forward model parameters in log-likelihood maximization
fopt_out	NULL	location to write output R data file with results of log-likelihood maximization
phen	NULL	phenomenology number and type (if needed for postprocessing)
pl	"multicore"	strategy for running parallel jobs using the future package

nomenology, the list object lp_beta is used for common coefficients, while the list object lp_betat is used for emplacement-dependent coefficients (as demonstrated below in this application).

- Line 18: Specify location(s) of log-prior function(s). Must be provided if iBetaPrior is TRUE (Line 14). In this example, a single log-prior function is provided, located at

```
../Code/lp_beta_s.r
```

   - Line 20: If `igrad` is `TRUE` (Line 20 of Appendix B.2), specify location(s) of the log-prior gradient function(s). In this example, a single log-prior gradient function is provided, located at

```
../Code/glp_beta_s.r
```

   - Line 25: For each relevant phenomenology, initialize a null list `lp_betat` of length equal to the number of emplacement conditions containing distinct forward model parameters.
   - Line 27: For each relevant phenomenology and emplacement condition, provide the name(s) of the log-prior function(s) for each signature. In this example, the *seismic* phenomenology utilizes a log-prior function `lp_s` for each signature within each emplacement condition.
   - Line 29: If `igrad` is `TRUE` (Line 20 of Appendix B.2), then for each relevant phenomenology and emplacement condition, provide the name(s) of the log-prior gradient function(s) for each signature. In this example, the *seismic* phenomenology utilizes a log-prior gradient function `lq_s` for each signature within each emplacement condition.

- Line 38: If `calp` is `TRUE` (Line 47 of Appendix B.1), indicate if a log-prior density for the global forward model parameters is supplied by the user. If `iCalPrior` is `FALSE`, a "flat prior" (uniform on the domain) on these parameters is assumed.
- Lines 40-57: If relevant, specify details of user-provided log-prior distributions for global forward model parameters.
   - Line 42: Specify location of log-prior function. If `NULL`, utilize the default log-prior function contained in the file `lp_c.r` placed in the application code directory; in this example,

```
MultiPEM_Toolbox_Package/Applications/Code/IYDT
```

   - Line 44: If `igrad` is `TRUE` (Line 20 of Appendix B.2), specify location of the log-prior gradient function. If `NULL`, utilize the default log-prior gradient function contained in the file `glp_c.r` placed in the application code directory; in this example,

```
MultiPEM_Toolbox_Package/Applications/Code/IYDT
```

   - Line 48: Provide the name of the log-prior function.
   - Line 49: If `igrad` is `TRUE` (Line 20 of Appendix B.2), provide the name of the log-prior gradient function.
   - Lines 52-53: Specify all fixed quantities required for calculation of the log-prior density.

- Line 60: If `nev` is `TRUE` (Line 168 of Appendix B.1), indicate if a log-prior density for the new event device parameters is supplied by the user (WPA, §6.5, p. 15; §6.6, pp. 18-19). If `iTheta0Prior` is `FALSE`, a "flat prior" (uniform on the domain) on these parameters is assumed.

- Lines 62-82: If relevant, specify details of user-provided log-prior distributions for new event device parameters.

  - Line 64: Specify location of log-prior function. If `NULL`, utilize the default log-prior function contained in the file `lp_0.r` placed in the application code directory; in this example,

    `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  - Line 66: If `igrad` is `TRUE` (Line 20 of Appendix B.2), specify location of the log-prior gradient function. If `NULL`, utilize the default log-prior gradient function contained in the file `glp_0.r` placed in the application code directory; in this example,

    `MultiPEM_Toolbox_Package/Applications/Code/IYDT`

  - Line 70: Provide the name of the log-prior function.

  - Line 71: If `igrad` is `TRUE` (Line 20 of Appendix B.2), provide the name of the log-prior gradient function.

  - Lines 73-78: Specify all fixed quantities required for calculation of the log-prior density. In this example, the mean (Line 74) and standard deviation (Line 75) of the Gaussian prior distribution for log-yield, and the mean (Line 77) and standard deviation (Line 78) of the Gaussian prior distribution for height-of-burst, are specified.

- Line 86: Specify a *fixed* value for the scale parameter `A` of half-Cauchy prior distribution(s) for the *source* and *path* variance component parameters if relevant (WPA, §6.5, p. 15; §6.6, p. 17). Prior distributions for a non-empty collection of variance component parameters are taken to be mutually independent. Comment out if this parameter is to be sampled from its posterior distribution.

- Line 90: Specify a *fixed* value for the shape parameter η of the Lewandowski-Kurowicka-Joe (LKJ) prior distribution for the observational error model correlation parameters (WPA, §6.5, p. 15; §6.6, p. 17).

- Line 98: If `eiv` is `TRUE` (Line 113 of Appendix B.1), specify a *fixed* value for the parameter that controls the number of modes in the *flexible generalized skew-normal* (FGSN) prior distribution for the errors-in-variables yields of the benchmark events (WPA, §6.5, p. 15; §6.6, p. 23).

- Line 104: Select the Markov chain Monte Carlo (MCMC) algorithm to use for posterior sampling, from one of three options: `RAM`, `FME`, and `NUTS`. `RAM` is the robust adaptive Metropolis algorithm of Vihola[16] implemented in the `R` package `adaptMCMC`. `FME` is the delayed rejection adaptive Metropolis algorithm of Haario, Laine, and Mira[17] implemented in the `R` package `FME`. `NUTS` is the No-U-Turn Sampler of Hoffman and Gelman[18]. The `NUTS` option requires the analytical gradient of the log-posterior density, which in turn requires `igrad` to be `TRUE` (Line 20 of Appendix B.2).

- Line 107: Specify the per core sample size of the burn-in period for MCMC sampling (pre-equilibrium stage of Markov chain). These samples are discarded prior to any inference using the posterior samples.

- Line 110: Specify the sample size of the MCMC production run. These samples are kept for posterior inference.

- Line 113: Specify the rate at which MCMC production samples are thinned for estimation of the Deviance Information Criterion[19] (DIC) and the Predictive Information Criterion[20] (PIC). In this example, the `nthin` value of `20` indicates that every 20-th production sample is kept for DIC and PIC estimation.

- Line 116: Specify the number of cores to use for parallel optimization (across distinct starting values) of the benchmark and (if relevant) new event data log-posterior function. By default, this optimization uses the same number of distinct starting values as optimization of the benchmark and (if relevant) new event data log-likelihood function (Line 58 of Appendix B.2).

- Line 119: Specify the number of cores used to run parallel MCMC chains. The burn-in period for each chain is determined by `nburn` (Line 107), while the `nmcmc` (Line 110) production runs are split between the `ncores_mc` processors and combined at the conclusion of the runs.

- Line 122: Indicate if gradient verification is to be conducted on the log-prior function. If `TRUE` and `igrad` is `TRUE` (Line 20 of Appendix B.2), analytical and numerical gradients at the maximum *a posteriori* parameter value, and other randomly sampled parameter values, are compared for consistency.

- Line 125: Indicate if gradient verification is to be conducted on the log-posterior function. If `TRUE` and `igrad` is `TRUE` (Line 20 of Appendix B.2), analytical and numerical gradients at the maximum *a posteriori* parameter value, and other randomly sampled parameter values, are compared for consistency.

- Lines 128-138: Calls the Bayesian analysis function `calc_bayes` for the new event data. Table 11 describes all inputs to this function with default values. Only inputs with no

[16] Vihola, M. (2012). Robust adaptive Metropolis algorithm with coerced acceptance rate. *Stat Comput* 22:997-1008.

[17] Haario, H., Laine, M., and Mira, A. (2006). DRAM: Efficient adaptive MCMC. *Stat Comput* 16:339-354.

[18] Hoffman, M. D. and Gelman, A. (2014). The No-U-Turn Sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. *J Mach Learn Res* 15:1593-1623.

[19] Spiegelhalter, D.J., Best, N.G., Carlin, B.P., & van der Linde, A. (2002). Bayesian measures of model complexity and fit (with discussion), *J R Stat Soc Ser B* 64:583-639.

[20] Ando, T. (2011). Predictive Bayesian model selection, *Am J Math Manag Sci* 31:13-38.

default values must be provided.

Table 11: Inputs to `calc_bayes` function.

Input	Default	Brief Description
`p_cal`	none	environment storing all objects needed in log-posterior calculations
`gdir`	none	directory location of global subroutines
`adir`	none	directory location of application subroutines
`nst`	10	number of starting values for log-posterior maximization
`nburn`	10000	number of per core MCMC burn-in samples
`nmcmc`	20000	number of MCMC production samples
`nthin`	20	posterior sample thinning rate
`ncor_map`	1	number of cores for log-posterior maximization
`ncor_mc`	1	number of cores for generating parallel MCMC chains
`igrad`	`TRUE`	forward model Jacobian provided
`igrck_pr`	`TRUE`	conduct log-prior function gradient verification
`igrck_po`	`TRUE`	conduct log-posterior function gradient verification
`bfgs`	`TRUE`	log-posterior maximization uses BFGS methods
`ibpr`	`FALSE`	prior density function(s) provided for forward model coefficients
`icpr`	`FALSE`	prior density function(s) provided for global forward model coefficients
`itpr`	`FALSE`	prior density function provided for new event parameters
`fpr_b`	`NULL`	location of functions computing log-prior density for forward model coefficients
`fgpr_b`	`NULL`	location of functions computing gradients of log-prior density for forward model coefficients
`fpr_c`	`NULL`	location of functions computing log-prior density for global forward model coefficients
`fgpr_c`	`NULL`	location of functions computing gradients of log-prior density for global forward model coefficients
`fpr_t`	`NULL`	location of function computing log-prior density for new event parameters
`fgpr_t`	`NULL`	location of function computing gradients of log-prior density for new event parameters
`Xnom`	`NULL`	matrix of starting values for hyperparameters in log-posterior maximization if not generated by this function
`imcmc`	`"FME"`	MCMC algorithm (current options: `"RAM"`, `"FME"`, `"NUTS"`)
`pl`	`"multicore"`	strategy for running parallel jobs using the `future` package
`t_cal`	`NULL`	object required if bounds supplied to log-posterior maximization

3.0.4 Output

The output file runMPEM.out from the complete analysis contains a summary of (if relevant) global forward model parameters, (if relevant) errors-in-variables yield estimates for the relevant benchmark sources, signature within phenomenology forward and error model parameter estimates, as well as (if relevant) new event device parameter estimates derived from the benchmark and (if relevant) new event data simultaneously. The desired output is supplied by the user function print_sumstats.r, placed in the application code directory; in this example,

MultiPEM_Toolbox_Package/Applications/Code/IYDT

The output presented in Appendix B.4 contains the most pertinent information extracted from the full file.

- Lines 8-19: Output from the preprocessing function prepro. These warning messages explain which variance component models are allowed (if any) for each signature of each phenomenology based on the structure of the benchmark data. In this example, only *source* random effects are allowed for each *acoustic* signature (Lines 8-11), while no random effects are allowed for *optical* or *surface effects* phenomenologies (Lines 12-19). There are no warning messages for *seismic* signatures, indicating source and *path* random effects are allowed.
- Lines 27-267: Output from the maximum likelihood estimation function calc_mle:
  - Line 29: Convergence code from the R optimization function optim. In this example, '0' indicates successful completion.
  - Line 30: Number of optimization restarts in which the relative absolute maximum log-likelihood difference is $\leq 10^{-8}$. The algorithm exits after 2 such restarts, which is attained in this example.
  - Line 38: Maximum likelihood estimates of the new event device parameters; in this example, log-yield (W) and height-of-burst (HOB).
  - Line 43: Standard errors of the maximum likelihood estimates of the new event device parameters, adjusted for estimation of the forward model parameters and (if relevant) benchmark source errors-in-variables yields (WPA, §A.2, Equation (19); §A.4, Equation (21)).
  - Lines 47-49: Correlation matrix of the maximum likelihood estimates of the new event device parameters, adjusted for estimation of the forward model parameters and (if relevant) benchmark source errors-in-variables yields (WPA, §A.2, Equation (19); §A.4, Equation (21)).
  - Lines 53-55: 95% confidence intervals for the unknown true values of the new event device parameters, based on standard errors adjusted for estimation of the forward model parameters and (if relevant) benchmark source errors-in-variables yields (WPA, §A.2, Equation (19); §A.4, Equation (21)).

- Lines 60-63: Maximum likelihood estimates of errors-in-variables yields for the relevant benchmark sources. Source names (Lines 60 and 62) are given above yield estimates (Lines 61 and 63). Errors-in-variables yields are only estimated if `eiv` is `TRUE` (Line 113 of Appendix B.1).
- Lines 67-89: Maximum likelihood estimates of *common* forward model parameters for each signature of each phenomenology (where present).
- Lines 93-139: Maximum likelihood estimates of *emplacement-dependent* forward model parameters for each signature of each phenomenology (where present).
- Lines 143-157: Maximum likelihood estimates of *source* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 161-167: Maximum likelihood estimates of *path* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 171-217: Maximum likelihood estimates of observational error variances for each signature, and correlations between signatures, for each phenomenology (WPA, §A.5).
- Line 219: Akaike Information Criterion[21] (AIC) value based on benchmark and (if relevant) new event data. Used for selecting among competing forward or error model specifications (WPA, §6.5, p. 15; §6.6, Tables 4 and 5, p. 18).
- Line 221: Bayesian Information Criterion[22] (BIC) value based on benchmark and (if relevant) new event data. Used for selecting among competing forward or error model specifications (WPA, §6.5, p. 15; §6.6, Tables 4 and 5, p. 18).
- Lines 226-267: Example of log-likelihood gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
  * Lines 227-245: Analytic gradient calculation
  * Lines 247-265: Numerical gradient calculation using the `R` package `numDeriv`
  * Line 267: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients

• Lines 283-1344: Output from the Bayesian analysis function `calc_bayes`:

- Line 285: Convergence code from the `R` optimization function `optim`. In this example, '0' indicates successful completion.
- Line 286: Number of optimization restarts in which the relative absolute maximum log-posterior difference is $\leq 10^{-8}$. The algorithm exits after 2 such restarts, which is attained in this example.

[21] Akaike, H. (1973). Information Theory and an Extension of the Maximum Likelihood Principle. In: Petrov, B.N. & Csaki, F., Eds., International Symposium on Information Theory, 267-281.

[22] Schwarz, G. (1978). Estimating the dimension of a model, *Ann Stat* 6:461-464.

- Line 294: Maximum *a posteriori* estimates of the new event device parameters.
- Lines 299-302: Maximum *a posteriori* estimates of errors-in-variables yields for the relevant benchmark sources. Source names (Lines 299 and 301) are given above yield estimates (Lines 300 and 302). Errors-in-variables yields are only estimated if `eiv` is `TRUE` (Line 113 of Appendix B.1).
- Lines 306-328: Maximum *a posteriori* estimates of *common* forward model parameters for each signature of each phenomenology (where present).
- Lines 332-378: Maximum *a posteriori* estimates of *emplacement-dependent* forward model parameters for each signature of each phenomenology (where present).
- Lines 382-396: Maximum *a posteriori* estimates of *source* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 400-406: Maximum *a posteriori* estimates of *path* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 410-456: Maximum *a posteriori* estimates of observational error variances for each signature, and correlations between signatures, for each phenomenology (WPA, §A.5).
- Lines 460-462: Maximum *a posteriori* estimates of FGSN prior distribution parameters (WPA, §6.6, p. 23; `Alpha` $= \mu$, `Omega` $= \upsilon$ (two coefficients)).
- Lines 466-509: Example of log-prior gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
  * Lines 467-486: Analytic gradient calculation
  * Lines 488-507: Numerical gradient calculation using the `R` package `numDeriv`
  * Line 509: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients
- Lines 514-556: Example of log-posterior gradient verification at a single sampled parameter vector. Additional checks were deleted for brevity.
  * Lines 514-533: Analytic gradient calculation
  * Lines 535-554: Numerical gradient calculation using the `R` package `numDeriv`
  * Line 556: Largest negative (first entry) and positive (second entry) differences between the analytic and numerical gradients
- Line 560: Acceptance rate of the Delayed Rejection Adaptive Metropolis (DRAM) posterior sampling method implemented in `R` package `FME`. Note that one delayed rejection step is allowed in the default implementation.

- Line 566: Means of samples from the new event device parameter marginal posterior distributions.
- Line 568: Standard deviations of samples from the new event device parameter marginal posterior distributions.
- Lines 570-578: User specified quantiles of samples from the new event device parameter marginal posterior distributions.
- Lines 582-584: Correlation matrix of samples from the new event device parameter joint posterior distribution.
- Lines 588-640: Means and user specified quantiles of samples from the marginal posterior distributions of errors-in-variables yields for the relevant benchmark sources. The ordering of benchmark sources is provided with the maximum *a posteriori* estimates (Lines 299 and 301). Errors-in-variables yields are only estimated if `eiv` is `TRUE` (Line 113 of Appendix B.1).
- Lines 644-726: Means and user specified quantiles of samples from the marginal posterior distributions of *common* forward model parameters for each signature of each phenomenology (where present).
- Lines 730-933: Means and user specified quantiles of samples from the marginal posterior distributions of *emplacement-dependent* forward model parameters for each signature of each phenomenology (where present).
- Lines 937-991: Means and user specified quantiles of samples from the marginal posterior distributions of *source* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 995-1021: Means and user specified quantiles of samples from the marginal posterior distributions of *path* random effect (error model) variance component parameters for each signature of each phenomenology (where present).
- Lines 1025-1299: Means and user specified quantiles of samples from the marginal posterior distributions of observational error variances for each signature, and correlations between signatures, for each phenomenology (WPA, §A.5).
- Lines 1303-1340: Means and user specified quantiles of samples from the marginal posterior distributions of FGSN prior distribution parameters (WPA, §6.6, p. 23; `Alpha` $= \mu$, `Omega` $= \upsilon$ (two coefficients)).
- Line 1342: DIC value based on benchmark and (if relevant) new event data. Used for selecting among competing forward or error model specifications (WPA, §6.5, pp. 15-16; §6.6, Tables 4 and 5, p. 18).
- Line 1344: PIC value based on benchmark and (if relevant) new event data. Used for selecting among competing forward or error model specifications (WPA, §6.5, pp. 15-16; §6.6, Tables 4 and 5, p. 18).

The p_cal environment resulting from this run contains several elements of potential interest for additional post-processing:

- p_cal$mle: Maximum likelihood estimate of (if relevant) unbounded new event device parameters (i.e., on scale used by the optimizer), unbounded global forward model parameters (if relevant), benchmark source errors-in-variables yields (if relevant), and signature within phenomenology forward and error model parameters
- p_cal$Sigma_mle_0$II_nev_it: If relevant, estimated asymptotic covariance matrix of new event device parameter elements of p_cal$mle
- p_cal$tmle_0: If relevant, maximum likelihood estimate of transformed new event device parameters (i.e., on correct scale)
- p_cal$Sigma_mle_0$II_nev: If relevant, estimated asymptotic covariance matrix of p_cal$tmle_0
- p_cal$mle_calp: If calp is TRUE (Line 47 of Appendix B.1), maximum likelihood estimate of unbounded global forward model parameters
- p_cal$Sigma_mle_cal$II_calp: If nev is FALSE (Line 168 of Appendix B.1) and calp is TRUE (Line 47 of Appendix B.1), estimated asymptotic covariance matrix of p_cal$mle_calp, adjusted for estimation of signature within phenomenology forward model parameters, and (if relevant) benchmark source errors-in-variables yields
- p_cal$Sigma_mle_0$II_calp: If nev is TRUE (Line 168 of Appendix B.1) and calp is TRUE (Line 47 of Appendix B.1), estimated asymptotic covariance matrix of p_cal$mle_calp, adjusted for estimation of new event device parameters, signature within phenomenology forward model parameters, and (if relevant) benchmark source errors-in-variables yields
- p_cal$map: If iBayes is TRUE (Line 6 of Appendix B.3), maximum *a posteriori* estimate of (if relevant) unbounded new event device parameters (i.e., on scale used by the optimizer), unbounded global forward model parameters (if relevant), benchmark source errors-in-variables yields (if relevant), and signature within phenomenology forward and error model parameters
- p_cal$tmap_0: If iBayes is TRUE (Line 6 of Appendix B.3), maximum *a posteriori* estimate of transformed new event device parameters (i.e., on correct scale)
- p_cal$map_calp: If iBayes is TRUE (Line 6 of Appendix B.3) and calp is TRUE (Line 47 of Appendix B.1), maximum *a posteriori* estimate of unbounded global forward model parameters
- p_cal$tmpi_0: If iBayes is TRUE (Line 6 of Appendix B.3), posterior samples of transformed new event device parameters (i.e., on correct scale)
- p_cal$mpi_calp: If iBayes is TRUE (Line 6 of Appendix B.3) and calp is TRUE (Line 47 of Appendix B.1), posterior samples of unbounded global forward model parameters

A Rapid Assessment Run Files

This appendix provides example run files and output files for rapid assessments.

A.1 Benchmark Data: Preprocessing

```
###########################################################################
#                                                                         #
# This file is the input deck for MultiPEM Toolbox estimation of          #
# forward and error model parameters based on calibration data.           #
#                                                                         #
###########################################################################

#
# REQUIRED R PACKAGES
#

require(Matrix)

#
# END REQUIRED R PACKAGES
#

#
# PREPROCESSING
#

# Specify directory for general subroutines
gen_dir = "../../../Code"

# Source supporting R function
source(paste(gen_dir,"/prepro_cal.r",sep=""))

# Specify directory for application subroutines
app_dir = "../../Code"

# Specify root data directory
dat_dir = "../../Data"

# Specify calibration data directories
dat_cal = c("seismic_cal.csv",
            "acoustic_cal.csv",
            "optical_cal.csv",
            "crater_cal.csv")

```

```
# Phenomenologies for this analysis
# 1 - seismic
# 2 - acoustic
# 3 - optical
# 4 - crater (surface effects)

# Indicate presence of calibration inference parameters
calp = FALSE

if( calp ){
  # Names of calibration inference parameters
  #cal_par_names =
} else { cal_par_names = NULL }

# Specify number of responses for each phenomenology
Rh = c(2,2,2,2)

# Empirical model parameter count: common
# list with elements corresponding to phenomenologies
pbeta = vector("list",length(Rh))
for( hh in 1:length(Rh) ){ pbeta[[hh]] = numeric(Rh[hh]) }
# phenomenology 2
pbeta[[2]] = c(2,2)
# phenomenology 3
pbeta[[3]] = c(2,2)
# phenomenology 4
pbeta[[4]] = c(2,2)

# Specify number of emplacement conditions for each phenomenology
Th = TRUE

if( Th ){ Th = c(3,3,0,0)
} else { Th = NULL }

# Empirical model parameter count: emplacement condition
# list with elements corresponding to phenomenologies
if( !is.null(Th) ){
  pbetat = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){
    if( Th[hh] > 1 ){ pbetat[[hh]] = vector("list",Th[hh]) }
  }
  # phenomenology 1
  for( tt in 1:Th[1] ){
    pbetat[[1]][[tt]] = numeric(Rh[1])
    pbetat[[1]][[tt]] = c(5,5)
```

```
  }
  # phenomenology 2
  for( tt in 1:Th[2] ){
    pbetat[[2]][[tt]] = numeric(Rh[2])
    pbetat[[2]][[tt]] = c(1,1)
  }
} else { pbetat = NULL }

# Locations of common parameters in full parameter vector
# list with elements corresponding to phenomenologies
if( !is.null(Th) ){
  ibetar = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){
    if( Th[hh] > 1 ){
      # lists with elements for each response within
      # emplacement condition
      ibetar[[hh]] = vector("list",Th[hh]*Rh[hh])
    }
  }
  # phenomenology 2
  for( tt in 1:Th[2] ){
    for( rr in 1:Rh[2] ){
      ibetar[[2]][[(tt-1)*Rh[2]+rr]] = 1:2
    }
  }
} else { ibetar = NULL }

# Indicate analysis with errors-in-variables (eiv)
eiv = TRUE

# Specifications for errors-in-variables
if( eiv ){
  # Specify phenomenologies utilizing
  # errors-in-variables yields
  ieiv = 3:4

  # Errors-in-variables source lists by
  # phenomenology
  seiv = vector("list",length(Rh))
  for( hh in ieiv ){ seiv[[hh]] = "ALL" }

  # Set standard deviation of eiv Gaussian likelihood
  eiv_w_sd = 0.1/3
} else {
  ieiv = NULL
```

```
  seiv = NULL
  eiv_w_sd = NULL
}

# Specify Error Model
# Level 1 variance component parameter count
pvc_1 = TRUE

if( pvc_1 ){
  pvc_1 = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){ pvc_1[[hh]] = numeric(Rh[hh]) }
  # phenomenology 1
  pvc_1[[1]] = c(1,1)
  # phenomenology 2
  pvc_1[[2]] = c(1,1)
} else { pvc_1 = NULL }

# Level 2 variance component parameter count
pvc_2 = TRUE

if( pvc_2 ){
  pvc_2 = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){ pvc_2[[hh]] = numeric(Rh[hh]) }
  # phenomenology 1
  pvc_2[[1]] = c(1,1)
  # phenomenology 2
  #pvc_2[[2]] =

  # path error models by phenomenology
  ptype = vector("list",length(Rh))
  # phenomenology 1
  #ptype[[1]] =
} else { pvc_2 = NULL; ptype = NULL; }

# Set flag for user-provided code to calculate variance
# component coefficient matrices
calc_Z = FALSE

# Preprocessing for statistical analysis routines
p_cal = prepro_cal(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,
                   izmat=calc_Z,ieiv=ieiv,seiv=seiv,ewsd=eiv_w_sd,
                   Th=Th,pbetat=pbetat,ibetar=ibetar,pvc_1=pvc_1,
                   pvc_2=pvc_2,ptype=ptype,cnames=cal_par_names)
save.image()

```

```
#
# END PREPROCESSING
#
```

A.2 Benchmark Data: Maximum Likelihood Estimation

```
#
# MAXIMUM LIKELIHOOD CALCULATION
#

# Source supporting R function
source(paste(gen_dir,"/calc_mle_cal.r",sep=""))

# Set seed for repeatability of analysis
set.seed(621)

# Names of forward models for each response
# by phenomenology
fm = vector("list",length(Rh))
fm[[1]] = c("f_s","f_s")
fm[[2]] = c("f_a","f_a")
fm[[3]] = c("f_o","f_o")
fm[[4]] = c("f_c","f_c")

# Indicate if forward model gradients provided
igrad = TRUE

if( igrad ){
  # Names of forward model gradients for each response
  # by phenomenology
  gfm = vector("list",length(Rh))
  gfm[[1]] = c("g_s","g_s")
  gfm[[2]] = c("g_a","g_a")
  gfm[[3]] = c("g_o","g_o")
  gfm[[4]] = c("g_c","g_c")
} else { gfm = NULL }

# Specifications for forward model calculations
# a) flags for modified forward model calculation by
#    response for each relevant phenomenology
iResponse = TRUE

if( iResponse ){
  iResponse = vector("list",length(Rh))
  iResponse[[1]] = c(TRUE,FALSE)
  iResponse[[2]] = c(TRUE,FALSE)
} else { iResponse = NULL }

# b) fixed quantities required by forward models
```

```
fPars = TRUE

if( fPars ){
  fPars = vector("list",length(Rh))
  fPars[[1]]$yield_scaling = 1/3
  fPars[[2]]$yield_scaling = 1/3
  fPars[[2]]$pressure_scaling = 1/3
  fPars[[2]]$temp_scaling = 1/2
  fPars[[3]]$yield_scaling = 1/3
  fPars[[3]]$pressure_scaling = 1/3
  fPars[[3]]$temp_scaling = 1/2
} else { fPars = NULL }

# Specify number of starting values for optimization
nstart = 10

# number of cores to use for optimization
ncores_mle = 1

# Indicate use of BFGS optimization methods
bfgs = TRUE

# Location of R data files with starting values
# for input to MLE optimization
opt_files_in = c("../Opt/opt_1_0.RData",
                 "../Opt/opt_2_0.RData",
                 "../Opt/opt_3_eiv_0.RData",
                 "../Opt/opt_4_eiv_0.RData")

# Location of R data file to write the results of
# MLE optimization
opt_files_out = "./opt.RData"

if( calp ){
  # Initial start value for calibration inference parameters
  cst = FALSE

  if( cst ){
    cst = numeric(p_cal$ncalp)
    #cst[1] =
  } else { cst = NULL }

  # Confidence interval levels for calibration parameter inference
  ci_lev = 0.95
} else {
```

```
  cst = NULL
  ci_lev = NULL
}

# Indicate phenomenology number and type (if needed
# for postprocessing)
Phen = TRUE

if( Phen ){
  Phen = matrix(c(1,"Seismic"),nrow=1)
} else { Phen = NULL }

# Indicator of MLE gradient check
mle_grad_ck = TRUE

# Strategy for running parallel jobs (future package)
parallel_plan = "multicore"

# MLE calculations
p_cal = calc_mle_cal(p_cal,gen_dir,app_dir,fm,nst=nstart,
                     ncor=ncores_mle,ci_lev=ci_lev,igrad=igrad,
                     bfgs=bfgs,igrck=mle_grad_ck,g=gfm,iresp=iResponse,
                     fp_fm=fPars,fopt_in=opt_files_in,Xst=NULL,
                     cst=cst,fopt_out=opt_files_out,phen=Phen,
                     pl=parallel_plan)
save.image()

#
# END MAXIMUM LIKELIHOOD CALCULATION
#
```

A.3 Benchmark Data: Bayesian Analysis

```
#
# BAYESIAN ANALYSIS
#

# Specify if Bayesian analysis is to be conducted
iBayes = FALSE

if( iBayes ){
  # Source supporting R function
  source(paste(gen_dir,"/calc_bayes_cal.r",sep=""))

  # Indicator of prior distribution for forward model
  # coefficients
  iBetaPrior = TRUE

  if( iBetaPrior ){
    # location of code for computing log-prior densities and gradients
    prior_files_beta = "../Code/lp_beta_s.r"
    if( igrad ){
      gr_prior_files_beta = "../Code/glp_beta_s.r"
    } else { gr_prior_files_beta = NULL }

    # prior distribution for phenomenology 1
    # forward model coefficients
    p_cal$h[[1]]$lp_betat = vector("list",Th[1])
    for( tt in 1:Th[1] ){
      p_cal$h[[1]]$lp_betat[[tt]]$f = c("lp_s","lp_s")
      if( igrad ){
        p_cal$h[[1]]$lp_betat[[tt]]$g = c("lq_s","lq_s")
      }
    }
  } else {
    prior_files_beta = NULL
    gr_prior_files_beta = NULL
  }

  # Indicator of prior distribution for calibration parameters
  iCalPrior = FALSE

  if( calp && iCalPrior ){
    # location of code for computing log-prior densities and gradients
    prior_files_calp = NULL
    if( igrad ){
```

```
      gr_prior_files_calp = NULL
    } else { gr_prior_files_calp = NULL }

    # prior distribution for calibration parameters (calp)
    p_cal$lp_calp$f = "lp_c"
    if( igrad ){ p_cal$lp_calp$g = "lq_c" }

    # parameters for calibration parameter prior distribution
    #p_cal$pi_c_mu =
    #p_cal$pi_c_sd =
  } else {
    prior_files_calp = NULL
    gr_prior_files_calp = NULL
  }

  # fixed scale parameters for variance component prior
  # comment out if these parameters should vary
  p_cal$A = 20

  # eta parameter in Lewandowski-Kurowicka-Joe (LKJ) prior
  # distribution for correlation parameters
  p_cal$lp_corr$eta = 1

  # FGSN parameters for errors-in-variables yields prior
  # number of components
  p_cal$K = 0
  # total number of FGSN parameters
  p_cal$p_fgsn = 0
  if( eiv ){
    p_cal$K = 2
    p_cal$p_fgsn = p_cal$K + 2
  }

  # specify Markov chain Monte Carlo (MCMC) algorithm
  # options: "RAM", "FME", or "NUTS"
  iMCMC = "FME"

  # burn-in
  nburn = 10000

  # production
  nmcmc = 20000

  # posterior sample thinning rate
  nthin = 20
```

```
  # number of cores to use for optimization
  ncores_map = 1

  # number of cores to use for generating parallel MCMC chains
  ncores_mc = 1

  # Indicator of prior gradient check
  prior_grad_ck = TRUE

  # Indicator of posterior gradient check
  post_grad_ck = TRUE

  # Bayesian calculations
  p_cal = calc_bayes_cal(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
                         nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
                         ncor_mc=ncores_mc,igrad=igrad,
                         igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
                         bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
                         fpr_b=prior_files_beta,
                         fgpr_b=gr_prior_files_beta,
                         fpr_c=prior_files_calp,
                         fgpr_c=gr_prior_files_calp,
                         Xnom=NULL,imcmc=iMCMC,pl=parallel_plan)
  save.image()
}

#
# END BAYESIAN ANALYSIS
#
```

A.4 Benchmark Data: Output File

```
> # Preprocessing for statistical analysis routines
> p_cal = prepro_cal(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,
+                    izmat=calc_Z,ieiv=ieiv,seiv=seiv,ewsd=eiv_w_sd,
+                    Th=Th,pbetat=pbetat,ibetar=ibetar,pvc_1=pvc_1,
+                    pvc_2=pvc_2,ptype=ptype,cnames=cal_par_names)
[1] "Warning: Insufficient Paths for Level 2 Variance Component models with
     Phenomenology 2 and Response 1."
[1] "Warning: Insufficient Paths for Level 2 Variance Component models with
     Phenomenology 2 and Response 2."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 3 and Response 1."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 3 and Response 2."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 4 and Response 1."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 4 and Response 2."

> # MLE calculations
> p_cal = calc_mle_cal(p_cal,gen_dir,app_dir,fm,nst=nstart,
+                      ncor=ncores_mle,ci_lev=ci_lev,igrad=igrad,
+                      bfgs=bfgs,igrck=mle_grad_ck,g=gfm,iresp=iResponse,
+                      fp_fm=fPars,fopt_in=opt_files_in,Xst=NULL,
+                      cst=cst,fopt_out=opt_files_out,phen=Phen,
+                      pl=parallel_plan)
[1] "MLE CONVERGENCE STATUS"

[1] 0
[1] 2
[1] "MAXIMUM LIKELIHOOD SUMMARY"

[1] "ERRORS-IN-VARIABLES YIELDS"

    7     8     9    10    11    13    14    16    17    20    21    22    23
16.29 16.21 16.51 16.61 17.00 12.21 17.57 17.27 16.52 14.50 15.75 17.59 15.23
   24    25    28    29    30    31    33    34    35    36    37    38    39
15.88 16.46 14.52 12.13 17.70 23.07 23.42 17.51 21.96 22.34 16.71 21.02 18.52

[1] "COMMON COEFFICIENTS"

        [1] "Phenomenology: 2; Response: 1"

        [1]  6.67 -1.14
```

```
        [1] "Phenomenology: 2; Response: 2"

        [1] -5.08  0.23

        [1] "Phenomenology: 3; Response: 1"

        [1] -11.07   1.89

        [1] "Phenomenology: 3; Response: 2"

        [1] -8.64  1.72

        [1] "Phenomenology: 4; Response: 1"

        [1] -3.34  0.43

        [1] "Phenomenology: 4; Response: 2"

        [1] -2.64  0.29

[1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

        [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

        [1] -10.07  -1.31  -1.43   3.52   0.39

        [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

        [1] -1.52 -1.44 -1.23  2.31  0.65

        [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

        [1] -11.48  -1.09  -3.59   4.32   0.16

        [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

        [1] -2.33 -1.22 -7.78  1.32 -1.36

        [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

        [1] -9.53 -1.16 -4.47  4.95  0.34

        [1] "Phenomenology: 1; Emplacement: 3; Response: 2"
```

```
        [1] -2.85 -0.71 -2.11  2.68  0.13

        [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

        [1] 3.87

        [1] "Phenomenology: 2; Emplacement: 1; Response: 2"

        [1] -0.17

        [1] "Phenomenology: 2; Emplacement: 2; Response: 1"

        [1] 3.11

        [1] "Phenomenology: 2; Emplacement: 2; Response: 2"

        [1] -0.9

        [1] "Phenomenology: 2; Emplacement: 3; Response: 1"

        [1] 2.16

        [1] "Phenomenology: 2; Emplacement: 3; Response: 2"

        [1] -0.94

[1] "LEVEL 1 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] 0.0011

        [1] "Phenomenology: 1; Response: 2"

        [1] 0.0017

        [1] "Phenomenology: 2; Response: 1"

        [1] 0.0038

        [1] "Phenomenology: 2; Response: 2"

        [1] 0.0016

[1] "LEVEL 2 VARIANCE COMPONENTS"
```

```
        [1] "Phenomenology: 1; Response: 1"

        [1] 0.001

        [1] "Phenomenology: 1; Response: 2"

        [1] 9e-04

[1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"

[1] "Phenomenology 1"

[1] "Variances"

[1] 0.0021 0.0034

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.28
[2,]    0 1.00

[1] "Phenomenology 2"

[1] "Variances"

[1] 1e-03 3e-04

[1] "Correlations"

     [,1]  [,2]
[1,]    1 -0.25
[2,]    0  1.00

[1] "Phenomenology 3"

[1] "Variances"

[1] 0.0011 0.0011

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.93
```

```
[2,]    0 1.00

[1] "Phenomenology 4"

[1] "Variances"

[1] 0.0260 0.0077

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.73
[2,]    0 1.00

[1] "AIC = -5840.98"

[1] "BIC = -5511.71"

Loading required package: numDeriv
[1] "CHECK LOG-LIKELIHOOD GRADIENTS"

[1] "Analytic gradient"
 [1] -8.431868e-04 -7.038053e-07 -5.595059e-05 -2.702571e-04  4.145765e-04
 [6] -6.877652e-04 -5.414314e-05  1.630249e-04 -7.642356e-04 -2.549322e-03
[11] -9.760283e-04  3.702140e-04 -1.655408e-05 -2.803807e-03 -1.524976e-03
[16] -1.081318e-03 -2.981360e-03  4.701484e-04  7.538052e-04  2.782379e-04
[21]  6.314769e-04 -4.285824e-04  8.941258e-04  6.184055e-04  3.258050e-04
[26] -4.870028e-04 -1.503716e-03 -7.324998e-02 -2.978359e-02 -5.224518e-01
[31]  1.255690e-01  5.041580e-02 -1.384946e-01 -4.589536e-02 -2.084526e-03
[36] -3.723123e-02  4.302576e-03  8.161440e-02 -2.400975e-03 -8.966039e-03
[41] -2.170289e-03 -1.693288e-04  5.219861e-04 -6.309496e-04  2.186223e-03
[46]  2.912214e-04  2.204081e-05  3.314070e-04 -1.062880e-02 -7.688789e-02
[51] -6.298861e-03 -6.976100e-04  7.529508e-03  1.421339e-03  3.434872e-02
[56]  1.317798e-02 -3.648180e-04 -2.097170e-02  7.638015e-03  5.206311e-02
[61]  3.562170e-03  1.863806e-03 -1.890228e-03  1.781585e-03  1.291352e-02
[66]  2.920229e-03  6.897676e-04  1.963322e-04  7.009887e-04 -1.052502e-03
[71] -3.373052e-04  3.676417e-04 -5.854999e-04  6.978043e-04 -2.989961e-05
[76] -2.478198e-04 -6.438579e-05  1.975623e-04  3.884852e-04 -1.331501e-04
[81]  7.588398e-04 -1.283586e-03  4.477531e-03  5.487680e-04 -9.010081e-04
[86]  1.037655e-01  6.236496e-03 -1.749379e-04 -1.290433e-02  2.277553e-04
[91]  3.282681e-04  1.789334e-03
[1] "Numerical gradient"
 [1] -8.431866e-04 -7.061032e-07 -5.596042e-05 -2.702460e-04  4.145769e-04
 [6] -6.877675e-04 -5.413925e-05  1.630274e-04 -7.642502e-04 -2.549334e-03
[11] -9.760306e-04  3.702130e-04 -1.656036e-05 -2.803783e-03 -1.524965e-03
```

```
[16] -1.081294e-03 -2.981438e-03  4.701524e-04  7.538070e-04  2.782443e-04
[21]  6.314669e-04 -4.285834e-04  8.941207e-04  6.183993e-04  3.257979e-04
[26] -4.869988e-04 -1.503741e-03 -7.325015e-02 -2.978351e-02 -5.224522e-01
[31]  1.255690e-01  5.041530e-02 -1.384947e-01 -4.589501e-02 -2.084511e-03
[36] -3.723102e-02  4.302586e-03  8.161507e-02 -2.400988e-03 -8.966151e-03
[41] -2.171152e-03 -1.693386e-04  5.216883e-04 -6.309502e-04  2.186201e-03
[46]  2.909891e-04  2.202312e-05  3.314891e-04 -1.062881e-02 -7.688785e-02
[51] -6.298773e-03 -6.975891e-04  7.529809e-03  1.421349e-03  3.434873e-02
[56]  1.317800e-02 -3.647383e-04 -2.097168e-02  7.638015e-03  5.206300e-02
[61]  3.562154e-03  1.863808e-03 -1.890134e-03  1.781589e-03  1.291348e-02
[66]  2.920191e-03  6.897655e-04  1.962526e-04  7.009899e-04 -1.052988e-03
[71] -3.372905e-04  3.676777e-04 -5.856120e-04  6.976661e-04 -2.991824e-05
[76] -2.478187e-04 -6.428826e-05  1.975601e-04  3.884810e-04 -1.331631e-04
[81]  7.588249e-04 -1.283589e-03  4.476626e-03  5.487913e-04 -9.010005e-04
[86]  1.037792e-01  6.235949e-03 -1.747034e-04 -1.290695e-02  2.279298e-04
[91]  3.282717e-04  1.789455e-03
[1] "Difference"
[1] -1.374109e-05  2.622069e-06

+   # Bayesian calculations
+   p_cal = calc_bayes_cal(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
+                          nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
+                          ncor_mc=ncores_mc,igrad=igrad,
+                          igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
+                          bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
+                          fpr_b=prior_files_beta,
+                          fgpr_b=gr_prior_files_beta,
+                          fpr_c=prior_files_calp,
+                          fgpr_c=gr_prior_files_calp,
+                          Xnom=NULL,imcmc=iMCMC,pl=parallel_plan)
+   save.image()
+ }
[1] "MAP CONVERGENCE STATUS"

[1] 0
[1] 2
[1] "MAXIMUM A POSTERIORI SUMMARY"

[1] "ERRORS-IN-VARIABLES YIELDS"

    7     8     9    10    11    13    14    16    17    20    21    22    23
16.28 16.21 16.51 16.61 17.00 12.21 17.57 17.27 16.52 14.50 15.75 17.59 15.23
   24    25    28    29    30    31    33    34    35    36    37    38    39
15.87 16.46 14.53 12.13 17.71 23.08 23.41 17.51 21.96 22.34 16.71 21.02 18.52

```

```
[1] "COMMON COEFFICIENTS"

        [1] "Phenomenology: 2; Response: 1"

        [1]  6.67 -1.14

        [1] "Phenomenology: 2; Response: 2"

        [1] -5.08  0.23

        [1] "Phenomenology: 3; Response: 1"

        [1] -11.07   1.89

        [1] "Phenomenology: 3; Response: 2"

        [1] -8.64  1.72

        [1] "Phenomenology: 4; Response: 1"

        [1] -3.35  0.43

        [1] "Phenomenology: 4; Response: 2"

        [1] -2.64  0.29

[1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

        [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

        [1] -10.07  -1.31  -1.43   3.51   0.39

        [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

        [1] -1.51 -1.44 -1.24  2.26  0.63

        [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

        [1] -11.48  -1.09  -3.62   4.18   0.15

        [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

        [1]  -2.16  -1.22 -56.31   0.93  -3.42

        [1] "Phenomenology: 1; Emplacement: 3; Response: 1"
```

```
        [1] -9.53 -1.16 -4.47  4.95  0.34

        [1] "Phenomenology: 1; Emplacement: 3; Response: 2"

        [1] -2.85 -0.71 -2.17  2.60  0.08

        [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

        [1] 3.87

        [1] "Phenomenology: 2; Emplacement: 1; Response: 2"

        [1] -0.17

        [1] "Phenomenology: 2; Emplacement: 2; Response: 1"

        [1] 3.11

        [1] "Phenomenology: 2; Emplacement: 2; Response: 2"

        [1] -0.9

        [1] "Phenomenology: 2; Emplacement: 3; Response: 1"

        [1] 2.16

        [1] "Phenomenology: 2; Emplacement: 3; Response: 2"

        [1] -0.94

[1] "LEVEL 1 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] 0.0012

        [1] "Phenomenology: 1; Response: 2"

        [1] 0.0017

        [1] "Phenomenology: 2; Response: 1"

        [1] 0.0039
```

```
         [1] "Phenomenology: 2; Response: 2"

         [1] 0.0016

[1] "LEVEL 2 VARIANCE COMPONENTS"

         [1] "Phenomenology: 1; Response: 1"

         [1] 0.001

         [1] "Phenomenology: 1; Response: 2"

         [1] 0.001

[1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"

[1] "Phenomenology 1"

[1] "Variances"

[1] 0.0021 0.0034

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.27
[2,]    0 1.00

[1] "Phenomenology 2"

[1] "Variances"

[1] 1e-03 3e-04

[1] "Correlations"

     [,1]  [,2]
[1,]    1 -0.25
[2,]    0  1.00

[1] "Phenomenology 3"

[1] "Variances"

[1] 1e-03 9e-04
```

```
[1] "Correlations"

     [,1] [,2]
[1,]    1 0.92
[2,]    0 1.00

[1] "Phenomenology 4"

[1] "Variances"

[1] 0.0218 0.0059

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.59
[2,]    0 1.00

[1] "FGSN PRIOR PARAMETERS"

[1] "Alpha = 17.33"
[1] "Lambda squared = 8"
[1] "Omega = -1.66" "Omega = 0.56"

[1] "CHECK LOG-PRIOR GRADIENTS"

[1] "Analytic gradient"
 [1] -1.055466e-01 -8.327724e-02 -1.787279e-01 -2.140887e-01 -3.507367e-01
 [6]  1.997990e+00 -5.483409e-01 -4.466296e-01 -1.832292e-01  3.561637e-01
[11]  5.548120e-02 -5.553768e-01  1.865502e-01  1.979674e-02 -1.646971e-01
[16]  3.490028e-01  2.182226e+00 -5.901511e-01 -3.792248e-01 -6.430252e-01
[21] -5.276501e-01  3.937098e-01  2.550063e-01 -2.494903e-01  1.570684e-01
[26] -7.524566e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[31]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[36]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[41]  1.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[46]  1.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[51]  7.751886e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[56]  1.572709e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[61]  6.610821e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[66]  1.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[71]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  4.999971e-01
[76]  4.999956e-01  4.999902e-01  4.999959e-01  4.999974e-01  4.999975e-01
[81]  0.000000e+00 -7.753342e-01 -1.413558e+01 -4.440892e-16 -8.113389e-01
```

```
[86]  4.223002e+01  2.220446e-16  1.518082e+00 -9.080578e+01  0.000000e+00
[91]  5.581077e-02 -2.313183e+01  1.965379e-02 -3.608055e-03  2.519400e-03
[96]  1.691543e-02
[1] "Numerical gradient"
 [1] -1.055466e-01 -8.327723e-02 -1.787279e-01 -2.140887e-01 -3.507367e-01
 [6]  1.997990e+00 -5.483409e-01 -4.466296e-01 -1.832292e-01  3.561637e-01
[11]  5.548120e-02 -5.553768e-01  1.865502e-01  1.979674e-02 -1.646971e-01
[16]  3.490028e-01  2.182226e+00 -5.901511e-01 -3.792248e-01 -6.430252e-01
[21] -5.276501e-01  3.937098e-01  2.550063e-01 -2.494903e-01  1.570684e-01
[26] -7.524566e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[31]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[36]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[41]  1.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[46]  1.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[51]  7.751886e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[56]  1.572709e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[61]  6.610821e-01  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[66]  1.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[71]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  4.999971e-01
[76]  4.999956e-01  4.999902e-01  4.999959e-01  4.999974e-01  4.999975e-01
[81]  0.000000e+00 -7.753342e-01 -1.413558e+01  0.000000e+00 -8.113389e-01
[86]  4.223002e+01 -2.776737e-20  1.518082e+00 -9.080578e+01  0.000000e+00
[91]  5.581077e-02 -2.313183e+01  1.965379e-02 -3.608056e-03  2.519400e-03
[96]  1.691543e-02
[1] "Difference"
[1] -3.718726e-08  4.307974e-07

[1] "CHECK LOG-POSTERIOR GRADIENTS"

[1] "Analytic gradient"
 [1] -0.143725992 -0.060385357 -0.128368006  0.021998510 -0.025658369
 [6] -0.036306696 -0.050177600 -0.085249094  0.015305390  0.103565181
[11] -0.201184644  0.035028210  0.057834796  0.119313668 -0.047274099
[16] -0.138810545  0.143130873  0.012883495  0.027928439  0.031038567
[21]  0.009257306  0.048872686  0.042925809  0.021272475  0.044293980
[26] -0.012342070  0.055484797  0.464397999  0.145253071  3.136130832
[31] -0.085779845  0.227551255 -0.021211292  0.153970860 -0.008353076
[36] -0.072768259 -0.001231599 -0.129250679 -0.066407399  0.009340489
[41]  0.057159667  0.001311732 -0.005017758 -0.025711262 -0.061502299
[46]  0.006932307  0.033351768 -0.022771865  0.151675870 -0.235282410
[51] -1.248225356 -0.037197888 -0.473227835  0.096449963 -0.414093631
[56] -0.154049649 -0.678058084 -0.964376932 -0.004970885  0.022785614
[61]  0.058071746 -0.001887512  0.008393102  0.006164484  0.041256854
[66]  0.017139968  0.011643573 -0.012383597 -0.015343286  0.063412903
[71] -0.035682482 -0.037305676 -0.076071754  0.021156892  0.012114242
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[76]  0.007195484 -0.007422780  0.002099905 -0.003198358 -0.002760457
[81]  0.032427579  0.010586708  0.047392728 -0.038438158 -0.030227541
[86] -0.839483224 -0.016865095 -0.038679600 -0.002776678  0.016996863
[91]  0.028550901 -0.031829322  0.019653787 -0.003608055  0.002519400
[96]  0.016915435
[1] "Numerical gradient"
 [1] -0.143726008 -0.060385354 -0.128368009  0.021998512 -0.025658378
 [6] -0.036306692 -0.050177604 -0.085249091  0.015305380  0.103565176
[11] -0.201184641  0.035028212  0.057834794  0.119313685 -0.047274109
[16] -0.138810540  0.143130810  0.012883498  0.027928440  0.031038559
[21]  0.009257302  0.048872688  0.042925807  0.021272464  0.044293981
[26] -0.012342073  0.055484827  0.464398287  0.145253137  3.136132448
[31] -0.085779761  0.227551232 -0.021211309  0.153970961 -0.008353068
[36] -0.072768079 -0.001231649 -0.129250734 -0.066407414  0.009340623
[41]  0.057159404  0.001311717 -0.005018124 -0.025711252 -0.061502296
[46]  0.006931771  0.033351792 -0.022771965  0.151675863 -0.235282339
[51] -1.248225359 -0.037197899 -0.473227186  0.096449898 -0.414093621
[56] -0.154049648 -0.678058194 -0.964376936 -0.004970892  0.022785708
[61]  0.058071708 -0.001887510  0.008392921  0.006164449  0.041256794
[66]  0.017139825  0.011643578 -0.012383603 -0.015343273  0.063411939
[71] -0.035682449 -0.037305829 -0.076071821  0.021156943  0.012114223
[76]  0.007195512 -0.007422785  0.002099886 -0.003198378 -0.002760494
[81]  0.032427562  0.010586659  0.047382834 -0.038438287 -0.030227440
[86] -0.839521589 -0.016865429 -0.038679788 -0.002761438  0.016996873
[91]  0.028550994 -0.031826601  0.019653788 -0.003608078  0.002519406
[96]  0.016915378
[1] "Difference"
[1] -1.524005e-05  3.836539e-05

[1] "ACCEPTANCE RATES:"

[1] "Core 1: 0.855366666666667"

[1] "POSTERIOR SUMMARY"

[1] "ERRORS-IN-VARIABLES YIELDS"

 [1] "POSTERIOR MEAN: 16.28" "POSTERIOR MEAN: 16.21" "POSTERIOR MEAN: 16.51"
 [4] "POSTERIOR MEAN: 16.61" "POSTERIOR MEAN: 17"    "POSTERIOR MEAN: 12.21"
 [7] "POSTERIOR MEAN: 17.57" "POSTERIOR MEAN: 17.27" "POSTERIOR MEAN: 16.52"
[10] "POSTERIOR MEAN: 14.5"  "POSTERIOR MEAN: 15.75" "POSTERIOR MEAN: 17.6"
[13] "POSTERIOR MEAN: 15.23" "POSTERIOR MEAN: 15.87" "POSTERIOR MEAN: 16.46"
[16] "POSTERIOR MEAN: 14.53" "POSTERIOR MEAN: 12.13" "POSTERIOR MEAN: 17.71"
[19] "POSTERIOR MEAN: 23.08" "POSTERIOR MEAN: 23.41" "POSTERIOR MEAN: 17.51"
[22] "POSTERIOR MEAN: 21.96" "POSTERIOR MEAN: 22.34" "POSTERIOR MEAN: 16.71"
```

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[25] "POSTERIOR MEAN: 21.02" "POSTERIOR MEAN: 18.52"

 [1] "LEVEL 2.5%: 16.27" "LEVEL 2.5%: 16.21" "LEVEL 2.5%: 16.49"
 [4] "LEVEL 2.5%: 16.6"  "LEVEL 2.5%: 16.99" "LEVEL 2.5%: 12.21"
 [7] "LEVEL 2.5%: 17.55" "LEVEL 2.5%: 17.26" "LEVEL 2.5%: 16.51"
[10] "LEVEL 2.5%: 14.48" "LEVEL 2.5%: 15.74" "LEVEL 2.5%: 17.58"
[13] "LEVEL 2.5%: 15.22" "LEVEL 2.5%: 15.86" "LEVEL 2.5%: 16.46"
[16] "LEVEL 2.5%: 14.51" "LEVEL 2.5%: 12.12" "LEVEL 2.5%: 17.7"
[19] "LEVEL 2.5%: 23.05" "LEVEL 2.5%: 23.4"  "LEVEL 2.5%: 17.49"
[22] "LEVEL 2.5%: 21.94" "LEVEL 2.5%: 22.33" "LEVEL 2.5%: 16.7"
[25] "LEVEL 2.5%: 21.01" "LEVEL 2.5%: 18.51"

 [1] "LEVEL 5%: 16.28" "LEVEL 5%: 16.21" "LEVEL 5%: 16.49" "LEVEL 5%: 16.6"
 [5] "LEVEL 5%: 16.99" "LEVEL 5%: 12.21" "LEVEL 5%: 17.56" "LEVEL 5%: 17.26"
 [9] "LEVEL 5%: 16.51" "LEVEL 5%: 14.48" "LEVEL 5%: 15.74" "LEVEL 5%: 17.59"
[13] "LEVEL 5%: 15.23" "LEVEL 5%: 15.86" "LEVEL 5%: 16.46" "LEVEL 5%: 14.51"
[17] "LEVEL 5%: 12.12" "LEVEL 5%: 17.7"  "LEVEL 5%: 23.06" "LEVEL 5%: 23.4"
[21] "LEVEL 5%: 17.49" "LEVEL 5%: 21.94" "LEVEL 5%: 22.33" "LEVEL 5%: 16.7"
[25] "LEVEL 5%: 21.01" "LEVEL 5%: 18.51"

 [1] "LEVEL 50%: 16.28" "LEVEL 50%: 16.21" "LEVEL 50%: 16.51" "LEVEL 50%: 16.61"
 [5] "LEVEL 50%: 17"    "LEVEL 50%: 12.21" "LEVEL 50%: 17.57" "LEVEL 50%: 17.27"
 [9] "LEVEL 50%: 16.52" "LEVEL 50%: 14.5"  "LEVEL 50%: 15.75" "LEVEL 50%: 17.59"
[13] "LEVEL 50%: 15.24" "LEVEL 50%: 15.87" "LEVEL 50%: 16.46" "LEVEL 50%: 14.53"
[17] "LEVEL 50%: 12.13" "LEVEL 50%: 17.71" "LEVEL 50%: 23.08" "LEVEL 50%: 23.41"
[21] "LEVEL 50%: 17.51" "LEVEL 50%: 21.96" "LEVEL 50%: 22.34" "LEVEL 50%: 16.71"
[25] "LEVEL 50%: 21.02" "LEVEL 50%: 18.52"

 [1] "LEVEL 95%: 16.29" "LEVEL 95%: 16.22" "LEVEL 95%: 16.52" "LEVEL 95%: 16.62"
 [5] "LEVEL 95%: 17.01" "LEVEL 95%: 12.22" "LEVEL 95%: 17.59" "LEVEL 95%: 17.28"
 [9] "LEVEL 95%: 16.53" "LEVEL 95%: 14.51" "LEVEL 95%: 15.75" "LEVEL 95%: 17.6"
[13] "LEVEL 95%: 15.24" "LEVEL 95%: 15.89" "LEVEL 95%: 16.47" "LEVEL 95%: 14.54"
[17] "LEVEL 95%: 12.14" "LEVEL 95%: 17.72" "LEVEL 95%: 23.09" "LEVEL 95%: 23.43"
[21] "LEVEL 95%: 17.52" "LEVEL 95%: 21.97" "LEVEL 95%: 22.35" "LEVEL 95%: 16.72"
[25] "LEVEL 95%: 21.03" "LEVEL 95%: 18.52"

 [1] "LEVEL 97.5%: 16.3"  "LEVEL 97.5%: 16.22" "LEVEL 97.5%: 16.52"
 [4] "LEVEL 97.5%: 16.62" "LEVEL 97.5%: 17.01" "LEVEL 97.5%: 12.22"
 [7] "LEVEL 97.5%: 17.59" "LEVEL 97.5%: 17.28" "LEVEL 97.5%: 16.53"
[10] "LEVEL 97.5%: 14.52" "LEVEL 97.5%: 15.76" "LEVEL 97.5%: 17.61"
[13] "LEVEL 97.5%: 15.24" "LEVEL 97.5%: 15.89" "LEVEL 97.5%: 16.47"
[16] "LEVEL 97.5%: 14.54" "LEVEL 97.5%: 12.15" "LEVEL 97.5%: 17.72"
[19] "LEVEL 97.5%: 23.1"  "LEVEL 97.5%: 23.43" "LEVEL 97.5%: 17.53"
[22] "LEVEL 97.5%: 21.98" "LEVEL 97.5%: 22.35" "LEVEL 97.5%: 16.72"
[25] "LEVEL 97.5%: 21.03" "LEVEL 97.5%: 18.52"
```

```
[1] "COMMON COEFFICIENTS"

        [1] "Phenomenology: 2; Response: 1"

        [1] "POSTERIOR MEAN: 6.67"  "POSTERIOR MEAN: -1.14"

        [1] "LEVEL 2.5%: 6.67"  "LEVEL 2.5%: -1.14"

        [1] "LEVEL 5%: 6.67"  "LEVEL 5%: -1.14"

        [1] "LEVEL 50%: 6.67"  "LEVEL 50%: -1.14"

        [1] "LEVEL 95%: 6.68"  "LEVEL 95%: -1.14"

        [1] "LEVEL 97.5%: 6.68"  "LEVEL 97.5%: -1.14"

        [1] "Phenomenology: 2; Response: 2"

        [1] "POSTERIOR MEAN: -5.08" "POSTERIOR MEAN: 0.23"

        [1] "LEVEL 2.5%: -5.08" "LEVEL 2.5%: 0.23"

        [1] "LEVEL 5%: -5.08" "LEVEL 5%: 0.23"

        [1] "LEVEL 50%: -5.08" "LEVEL 50%: 0.23"

        [1] "LEVEL 95%: -5.08" "LEVEL 95%: 0.23"

        [1] "LEVEL 97.5%: -5.08" "LEVEL 97.5%: 0.23"

        [1] "Phenomenology: 3; Response: 1"

        [1] "POSTERIOR MEAN: -11.07" "POSTERIOR MEAN: 1.89"

        [1] "LEVEL 2.5%: -11.09" "LEVEL 2.5%: 1.88"

        [1] "LEVEL 5%: -11.08" "LEVEL 5%: 1.88"

        [1] "LEVEL 50%: -11.07" "LEVEL 50%: 1.89"

        [1] "LEVEL 95%: -11.06" "LEVEL 95%: 1.91"

        [1] "LEVEL 97.5%: -11.06" "LEVEL 97.5%: 1.91"
```

```
        [1] "Phenomenology: 3; Response: 2"

        [1] "POSTERIOR MEAN: -8.64" "POSTERIOR MEAN: 1.72"

        [1] "LEVEL 2.5%: -8.65" "LEVEL 2.5%: 1.7"

        [1] "LEVEL 5%: -8.65" "LEVEL 5%: 1.7"

        [1] "LEVEL 50%: -8.64" "LEVEL 50%: 1.72"

        [1] "LEVEL 95%: -8.63" "LEVEL 95%: 1.73"

        [1] "LEVEL 97.5%: -8.63" "LEVEL 97.5%: 1.73"

        [1] "Phenomenology: 4; Response: 1"

        [1] "POSTERIOR MEAN: -3.34" "POSTERIOR MEAN: 0.43"

        [1] "LEVEL 2.5%: -3.53" "LEVEL 2.5%: 0.42"

        [1] "LEVEL 5%: -3.5" "LEVEL 5%: 0.42"

        [1] "LEVEL 50%: -3.35" "LEVEL 50%: 0.43"

        [1] "LEVEL 95%: -3.16" "LEVEL 95%: 0.44"

        [1] "LEVEL 97.5%: -3.12" "LEVEL 97.5%: 0.44"

        [1] "Phenomenology: 4; Response: 2"

        [1] "POSTERIOR MEAN: -2.63" "POSTERIOR MEAN: 0.29"

        [1] "LEVEL 2.5%: -2.77" "LEVEL 2.5%: 0.28"

        [1] "LEVEL 5%: -2.74" "LEVEL 5%: 0.28"

        [1] "LEVEL 50%: -2.63" "LEVEL 50%: 0.29"

        [1] "LEVEL 95%: -2.52" "LEVEL 95%: 0.3"

        [1] "LEVEL 97.5%: -2.5" "LEVEL 97.5%: 0.3"

[1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

        [1] "Phenomenology: 1; Emplacement: 1; Response: 1"
```

```
      [1] "POSTERIOR MEAN: -10.07" "POSTERIOR MEAN: -1.31"  "POSTERIOR MEAN: -1.43"
[4] "POSTERIOR MEAN: 3.51"   "POSTERIOR MEAN: 0.38"

      [1] "LEVEL 2.5%: -10.1" "LEVEL 2.5%: -1.31" "LEVEL 2.5%: -1.46"
[4] "LEVEL 2.5%: 3.39"  "LEVEL 2.5%: 0.35"

      [1] "LEVEL 5%: -10.09" "LEVEL 5%: -1.31"  "LEVEL 5%: -1.46"  "LEVEL 5%: 3.42"
[5] "LEVEL 5%: 0.36"

      [1] "LEVEL 50%: -10.07" "LEVEL 50%: -1.31"  "LEVEL 50%: -1.43"
[4] "LEVEL 50%: 3.51"   "LEVEL 50%: 0.38"

      [1] "LEVEL 95%: -10.05" "LEVEL 95%: -1.31"  "LEVEL 95%: -1.41"
[4] "LEVEL 95%: 3.6"    "LEVEL 95%: 0.41"

      [1] "LEVEL 97.5%: -10.04" "LEVEL 97.5%: -1.31"  "LEVEL 97.5%: -1.41"
[4] "LEVEL 97.5%: 3.62"   "LEVEL 97.5%: 0.42"

      [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

      [1] "POSTERIOR MEAN: -1.52" "POSTERIOR MEAN: -1.44" "POSTERIOR MEAN: -1.24"
[4] "POSTERIOR MEAN: 2.26"  "POSTERIOR MEAN: 0.63"

      [1] "LEVEL 2.5%: -1.56" "LEVEL 2.5%: -1.45" "LEVEL 2.5%: -1.28"
[4] "LEVEL 2.5%: 2.13"  "LEVEL 2.5%: 0.59"

      [1] "LEVEL 5%: -1.55" "LEVEL 5%: -1.45" "LEVEL 5%: -1.27" "LEVEL 5%: 2.15"
[5] "LEVEL 5%: 0.6"

      [1] "LEVEL 50%: -1.51" "LEVEL 50%: -1.44" "LEVEL 50%: -1.24" "LEVEL 50%: 2.25"
[5] "LEVEL 50%: 0.63"

      [1] "LEVEL 95%: -1.48" "LEVEL 95%: -1.44" "LEVEL 95%: -1.21" "LEVEL 95%: 2.38"
[5] "LEVEL 95%: 0.67"

      [1] "LEVEL 97.5%: -1.48" "LEVEL 97.5%: -1.44" "LEVEL 97.5%: -1.2"
[4] "LEVEL 97.5%: 2.4"   "LEVEL 97.5%: 0.68"

      [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

      [1] "POSTERIOR MEAN: -11.48" "POSTERIOR MEAN: -1.09"  "POSTERIOR MEAN: -3.62"
[4] "POSTERIOR MEAN: 4.18"   "POSTERIOR MEAN: 0.15"

      [1] "LEVEL 2.5%: -11.5" "LEVEL 2.5%: -1.1"  "LEVEL 2.5%: -3.8"
```

```
[4] "LEVEL 2.5%: 3.5"   "LEVEL 2.5%: 0.06"

        [1] "LEVEL 5%: -11.5" "LEVEL 5%: -1.1"  "LEVEL 5%: -3.77" "LEVEL 5%: 3.59"
[5] "LEVEL 5%: 0.08"

        [1] "LEVEL 50%: -11.48" "LEVEL 50%: -1.09"  "LEVEL 50%: -3.62"
[4] "LEVEL 50%: 4.17"   "LEVEL 50%: 0.15"

        [1] "LEVEL 95%: -11.46" "LEVEL 95%: -1.09"  "LEVEL 95%: -3.48"
[4] "LEVEL 95%: 4.79"   "LEVEL 95%: 0.22"

        [1] "LEVEL 97.5%: -11.45" "LEVEL 97.5%: -1.09"  "LEVEL 97.5%: -3.45"
[4] "LEVEL 97.5%: 4.89"   "LEVEL 97.5%: 0.23"

        [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

        [1] "POSTERIOR MEAN: -2.16"  "POSTERIOR MEAN: -1.22"  "POSTERIOR MEAN: -55.75"
[4] "POSTERIOR MEAN: 0.93"   "POSTERIOR MEAN: -3.41"

        [1] "LEVEL 2.5%: -2.28"  "LEVEL 2.5%: -1.23"  "LEVEL 2.5%: -67.22"
[4] "LEVEL 2.5%: 0.87"   "LEVEL 2.5%: -3.66"

        [1] "LEVEL 5%: -2.26"  "LEVEL 5%: -1.23"  "LEVEL 5%: -65.77" "LEVEL 5%: 0.88"
[5] "LEVEL 5%: -3.62"

        [1] "LEVEL 50%: -2.16"  "LEVEL 50%: -1.22"  "LEVEL 50%: -55.44"
[4] "LEVEL 50%: 0.93"   "LEVEL 50%: -3.41"

        [1] "LEVEL 95%: -2.07"  "LEVEL 95%: -1.21"  "LEVEL 95%: -47.11"
[4] "LEVEL 95%: 0.99"   "LEVEL 95%: -3.22"

        [1] "LEVEL 97.5%: -2.05"  "LEVEL 97.5%: -1.21"  "LEVEL 97.5%: -46.03"
[4] "LEVEL 97.5%: 1"      "LEVEL 97.5%: -3.2"

        [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

        [1] "POSTERIOR MEAN: -9.53" "POSTERIOR MEAN: -1.16" "POSTERIOR MEAN: -4.47"
[4] "POSTERIOR MEAN: 4.96"  "POSTERIOR MEAN: 0.34"

        [1] "LEVEL 2.5%: -9.56" "LEVEL 2.5%: -1.16" "LEVEL 2.5%: -4.49"
[4] "LEVEL 2.5%: 4.89"  "LEVEL 2.5%: 0.33"

        [1] "LEVEL 5%: -9.55" "LEVEL 5%: -1.16" "LEVEL 5%: -4.49" "LEVEL 5%: 4.9"
[5] "LEVEL 5%: 0.33"
```

```
      [1] "LEVEL 50%: -9.53" "LEVEL 50%: -1.16" "LEVEL 50%: -4.47" "LEVEL 50%: 4.96"
[5] "LEVEL 50%: 0.34"

      [1] "LEVEL 95%: -9.5"  "LEVEL 95%: -1.15" "LEVEL 95%: -4.45" "LEVEL 95%: 5.01"
[5] "LEVEL 95%: 0.35"

      [1] "LEVEL 97.5%: -9.5"  "LEVEL 97.5%: -1.15" "LEVEL 97.5%: -4.44"
[4] "LEVEL 97.5%: 5.02"  "LEVEL 97.5%: 0.35"

      [1] "Phenomenology: 1; Emplacement: 3; Response: 2"

      [1] "POSTERIOR MEAN: -2.85" "POSTERIOR MEAN: -0.71" "POSTERIOR MEAN: -2.16"
[4] "POSTERIOR MEAN: 2.61"  "POSTERIOR MEAN: 0.09"

      [1] "LEVEL 2.5%: -2.89" "LEVEL 2.5%: -0.71" "LEVEL 2.5%: -2.36"
[4] "LEVEL 2.5%: 2.34"  "LEVEL 2.5%: -0.05"

      [1] "LEVEL 5%: -2.88" "LEVEL 5%: -0.71" "LEVEL 5%: -2.33" "LEVEL 5%: 2.38"
[5] "LEVEL 5%: -0.03"

      [1] "LEVEL 50%: -2.85" "LEVEL 50%: -0.71" "LEVEL 50%: -2.16" "LEVEL 50%: 2.61"
[5] "LEVEL 50%: 0.09"

      [1] "LEVEL 95%: -2.81" "LEVEL 95%: -0.7"  "LEVEL 95%: -2.01" "LEVEL 95%: 2.84"
[5] "LEVEL 95%: 0.2"

      [1] "LEVEL 97.5%: -2.8"  "LEVEL 97.5%: -0.7"  "LEVEL 97.5%: -1.99"
[4] "LEVEL 97.5%: 2.88"  "LEVEL 97.5%: 0.21"

      [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

      [1] "POSTERIOR MEAN: 3.87"

      [1] "LEVEL 2.5%: 3.86"

      [1] "LEVEL 5%: 3.86"

      [1] "LEVEL 50%: 3.87"

      [1] "LEVEL 95%: 3.88"

      [1] "LEVEL 97.5%: 3.88"

      [1] "Phenomenology: 2; Emplacement: 1; Response: 2"
```

```
[1] "POSTERIOR MEAN: -0.17"

[1] "LEVEL 2.5%: -0.19"

[1] "LEVEL 5%: -0.19"

[1] "LEVEL 50%: -0.17"

[1] "LEVEL 95%: -0.15"

[1] "LEVEL 97.5%: -0.15"

[1] "Phenomenology: 2; Emplacement: 2; Response: 1"

[1] "POSTERIOR MEAN: 3.11"

[1] "LEVEL 2.5%: 3.09"

[1] "LEVEL 5%: 3.09"

[1] "LEVEL 50%: 3.11"

[1] "LEVEL 95%: 3.14"

[1] "LEVEL 97.5%: 3.14"

[1] "Phenomenology: 2; Emplacement: 2; Response: 2"

[1] "POSTERIOR MEAN: -0.9"

[1] "LEVEL 2.5%: -0.96"

[1] "LEVEL 5%: -0.95"

[1] "LEVEL 50%: -0.9"

[1] "LEVEL 95%: -0.86"

[1] "LEVEL 97.5%: -0.85"

[1] "Phenomenology: 2; Emplacement: 3; Response: 1"

[1] "POSTERIOR MEAN: 2.16"

[1] "LEVEL 2.5%: 2.14"
```

```
        [1] "LEVEL 5%: 2.14"

        [1] "LEVEL 50%: 2.16"

        [1] "LEVEL 95%: 2.17"

        [1] "LEVEL 97.5%: 2.18"

        [1] "Phenomenology: 2; Emplacement: 3; Response: 2"

        [1] "POSTERIOR MEAN: -0.94"

        [1] "LEVEL 2.5%: -0.99"

        [1] "LEVEL 5%: -0.98"

        [1] "LEVEL 50%: -0.94"

        [1] "LEVEL 95%: -0.9"

        [1] "LEVEL 97.5%: -0.9"

[1] "LEVEL 1 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] "POSTERIOR MEAN: 0.0012"

        [1] "LEVEL 2.5%: 9e-04"

        [1] "LEVEL 5%: 9e-04"

        [1] "LEVEL 50%: 0.0012"

        [1] "LEVEL 95%: 0.0015"

        [1] "LEVEL 97.5%: 0.0015"

        [1] "Phenomenology: 1; Response: 2"

        [1] "POSTERIOR MEAN: 0.0017"

        [1] "LEVEL 2.5%: 0.0016"
```

```
        [1] "LEVEL 5%: 0.0017"

        [1] "LEVEL 50%: 0.0017"

        [1] "LEVEL 95%: 0.0019"

        [1] "LEVEL 97.5%: 0.0019"

        [1] "Phenomenology: 2; Response: 1"

        [1] "POSTERIOR MEAN: 0.0039"

        [1] "LEVEL 2.5%: 0.0035"

        [1] "LEVEL 5%: 0.0036"

        [1] "LEVEL 50%: 0.0039"

        [1] "LEVEL 95%: 0.0043"

        [1] "LEVEL 97.5%: 0.0044"

        [1] "Phenomenology: 2; Response: 2"

        [1] "POSTERIOR MEAN: 0.0016"

        [1] "LEVEL 2.5%: 0.0015"

        [1] "LEVEL 5%: 0.0015"

        [1] "LEVEL 50%: 0.0016"

        [1] "LEVEL 95%: 0.0018"

        [1] "LEVEL 97.5%: 0.0018"

[1] "LEVEL 2 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] "POSTERIOR MEAN: 0.001"

        [1] "LEVEL 2.5%: 9e-04"

        [1] "LEVEL 5%: 9e-04"
```

```
        [1] "LEVEL 50%: 0.001"

        [1] "LEVEL 95%: 0.0012"

        [1] "LEVEL 97.5%: 0.0013"

        [1] "Phenomenology: 1; Response: 2"

        [1] "POSTERIOR MEAN: 0.001"

        [1] "LEVEL 2.5%: 8e-04"

        [1] "LEVEL 5%: 8e-04"

        [1] "LEVEL 50%: 0.001"

        [1] "LEVEL 95%: 0.0012"

        [1] "LEVEL 97.5%: 0.0012"

[1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"

[1] "Phenomenology 1"

[1] "POSTERIOR MEAN:"

[1] "Variances"

[1] 0.0021 0.0034

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.27
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 2.5%: 0.002"  "LEVEL 2.5%: 0.0032"

[1] "Correlations"

        [1] "LEVEL 2.5%:"
             [,1] [,2]
```

```
[1,]    1 0.26
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 5%: 0.002"  "LEVEL 5%: 0.0032"

[1] "Correlations"

        [1] "LEVEL 5%:"
             [,1] [,2]
[1,]    1 0.26
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 50%: 0.0021" "LEVEL 50%: 0.0034"

[1] "Correlations"

        [1] "LEVEL 50%:"
             [,1] [,2]
[1,]    1 0.27
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 95%: 0.0022" "LEVEL 95%: 0.0035"

[1] "Correlations"

        [1] "LEVEL 95%:"
             [,1] [,2]
[1,]    1 0.28
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 97.5%: 0.0022" "LEVEL 97.5%: 0.0036"

[1] "Correlations"

        [1] "LEVEL 97.5%:"
             [,1] [,2]
[1,]    1 0.28
```

```
[2,]    0 1.00

[1] "Phenomenology 2"

[1] "POSTERIOR MEAN:"

[1] "Variances"

[1] 1e-03 3e-04

[1] "Correlations"

     [,1]  [,2]
[1,]    1 -0.25
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 2.5%: 0.001" "LEVEL 2.5%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 2.5%:"
             [,1] [,2]
[1,]    1 -0.3
[2,]    0  1.0

[1] "Variances"

        [1] "LEVEL 5%: 0.001" "LEVEL 5%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 5%:"
             [,1]  [,2]
[1,]    1 -0.29
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 50%: 0.001" "LEVEL 50%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 50%:"
```

```
             [,1]  [,2]
[1,]    1 -0.25
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 95%:"
             [,1]  [,2]
[1,]    1 -0.21
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 97.5%: 0.0011" "LEVEL 97.5%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 97.5%:"
             [,1]  [,2]
[1,]    1 -0.21
[2,]    0  1.00

[1] "Phenomenology 3"

[1] "POSTERIOR MEAN:"

[1] "Variances"

[1] 1e-03 9e-04

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.92
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 2.5%: 8e-04" "LEVEL 2.5%: 8e-04"

[1] "Correlations"
```

```
        [1] "LEVEL 2.5%:"
             [,1] [,2]
[1,]    1  0.9
[2,]    0  1.0

[1] "Variances"

        [1] "LEVEL 5%: 9e-04" "LEVEL 5%: 8e-04"

[1] "Correlations"

        [1] "LEVEL 5%:"
             [,1] [,2]
[1,]    1  0.9
[2,]    0  1.0

[1] "Variances"

        [1] "LEVEL 50%: 0.001" "LEVEL 50%: 9e-04"

[1] "Correlations"

        [1] "LEVEL 50%:"
             [,1] [,2]
[1,]    1 0.92
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 0.0011"

[1] "Correlations"

        [1] "LEVEL 95%:"
             [,1] [,2]
[1,]    1 0.93
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 97.5%: 0.0012" "LEVEL 97.5%: 0.0011"

[1] "Correlations"
```

```
        [1] "LEVEL 97.5%:"
             [,1] [,2]
[1,]    1 0.93
[2,]    0 1.00

[1] "Phenomenology 4"

[1] "POSTERIOR MEAN:"

[1] "Variances"

[1] 0.0223 0.0061

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.59
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 2.5%: 0.0163" "LEVEL 2.5%: 0.0045"

[1] "Correlations"

        [1] "LEVEL 2.5%:"
             [,1] [,2]
[1,]    1 0.45
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 5%: 0.0169" "LEVEL 5%: 0.0046"

[1] "Correlations"

        [1] "LEVEL 5%:"
             [,1] [,2]
[1,]    1 0.47
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 50%: 0.022" "LEVEL 50%: 0.006"
```

```
[1] "Correlations"

        [1] "LEVEL 50%:"
             [,1] [,2]
[1,]    1  0.6
[2,]    0  1.0

[1] "Variances"

        [1] "LEVEL 95%: 0.029"  "LEVEL 95%: 0.0077"

[1] "Correlations"

        [1] "LEVEL 95%:"
             [,1] [,2]
[1,]    1  0.7
[2,]    0  1.0

[1] "Variances"

        [1] "LEVEL 97.5%: 0.0307" "LEVEL 97.5%: 0.008"

[1] "Correlations"

        [1] "LEVEL 97.5%:"
             [,1] [,2]
[1,]    1 0.71
[2,]    0 1.00

[1] "FGSN PRIOR PARAMETERS"

[1] "POSTERIOR MEAN:"

[1] "Alpha = 17.33"
[1] "Lambda squared = 8"
[1] "Omega = -1.67" "Omega = 0.56"

[1] "Alpha:"
[1] "LEVEL 2.5%: 17.13"

[1] "LEVEL 5%: 17.16"

[1] "LEVEL 50%: 17.33"

[1] "LEVEL 95%: 17.48"
```

```
[1] "LEVEL 97.5%: 17.51"

[1] "Lambda squared:"
[1] "LEVEL 2.5%: 7.83"

[1] "LEVEL 5%: 7.85"

[1] "LEVEL 50%: 8"

[1] "LEVEL 95%: 8.13"

[1] "LEVEL 97.5%: 8.15"

[1] "Omega:"
[1] "LEVEL 2.5%: -1.94" "LEVEL 2.5%: 0.49"

[1] "LEVEL 5%: -1.9" "LEVEL 5%: 0.5"

[1] "LEVEL 50%: -1.67" "LEVEL 50%: 0.56"

[1] "LEVEL 95%: -1.42" "LEVEL 95%: 0.62"

[1] "LEVEL 97.5%: -1.37" "LEVEL 97.5%: 0.63"

[1] "DIC = -6011.41"

[1] "PIC = -6005.05"
```

A.5 New Event Data: Preprocessing

```
###########################################################################
#                                                                         #
# This file is the input deck for MultiPEM Toolbox rapid post-           #
# detonation analysis, based on using fixed values of the forward and    #
# error model parameters obtained from calibration data.                 #
#                                                                         #
###########################################################################

#
# REQUIRED R PACKAGES
#

require(Matrix)

#
# END REQUIRED R PACKAGES
#

#
# PREPROCESSING
#

# Specify directory for general subroutines
gen_dir = "../../../Code"

# Source supporting R function
source(paste(gen_dir,"/prepro_0.r",sep=""))

# Specify directory for application subroutines
app_dir = "../../Code"

# Specify root data directory
dat_dir = "../../Data"

# Specify new event data directories
dat_new = c("seismic_new.csv",
            "acoustic_new.csv",
            "optical_new.csv",
            "crater_new.csv")

# Phenomenologies for this analysis
# 1 - seismic
# 2 - acoustic
```

```
# 3 - optical
# 4 - crater (surface effects)

# Names of new event inference parameters
theta_names = c("W","HOB")

# Number of calibration parameter imputations utilized in
# Markov chain Monte Carlo (MCMC) for new event parameters
nimpute = 1

# Set flag for bounded optimization
opt_B = FALSE

# Indicate nev parameter transform
itransform = FALSE

# Specify fixed parameters for nev parameter transform
if( itransform ){
  tPars = TRUE

  if( tPars ){
    tPars = vector("list",0)
    tPars$yield_scaling = 1/3
  } else { tPars = NULL }
} else { tPars = NULL }

# Set up parameter constraints
# lower and upper bounds (use -Inf and Inf if unbounded)
lb_theta0 = rep(-Inf,length(theta_names))
lb_theta0[2] = -10
ub_theta0 = rep(Inf,length(theta_names))
ub_theta0[2] = 160

# Set up parameter subsets by phenomenology
tsub = TRUE

if( tsub ) {
  tsub = vector("list",length(Rh))
  tsub[[4]] = 1 # only log-yield for crater
} else { tsub = NULL }

# Preprocessing for statistical analysis routines
tmp = prepro_0(p_cal,gen_dir,app_dir,dat_dir,dat_new,theta_names,
               nimp=nimpute,bopt=opt_B,itr=itransform,fp_tr=tPars,
               tlb=lb_theta0,tub=ub_theta0,tsub=tsub)
```

```
if( opt_B ){
  p_cal = tmp$p_cal
  t_cal = tmp$t_cal
} else {
  p_cal = tmp
  t_cal = NULL
}
rm(tmp)
save.image()

#
# END PREPROCESSING
#
```

A.6 New Event Data: Maximum Likelihood Estimation

```
#
# MAXIMUM LIKELIHOOD CALCULATION
#

# Source supporting R function
source(paste(gen_dir,"/calc_mle_0.r",sep=""))

# Set seed for repeatability of analysis
set.seed(631)

# Names of forward models for each response
# by phenomenology
fm0 = vector("list",length(Rh))
fm0[[1]] = c("f0_s","f0_s")
fm0[[2]] = c("f0_a","f0_a")
fm0[[3]] = c("f0_o","f0_o")
fm0[[4]] = c("f0_c","f0_c")

# Indicate if forward model gradients provided
igrad = TRUE

if( igrad ){
  # Names of forward model gradients for each response
  # by phenomenology
  gfm0 = vector("list",length(Rh))
  gfm0[[1]] = c("g0_s","g0_s")
  gfm0[[2]] = c("g0_a","g0_a")
  gfm0[[3]] = c("g0_o","g0_o")
  gfm0[[4]] = c("g0_c","g0_c")
} else { gfm0 = NULL }

# Specify number of starting values for optimization
nstart = 10

# number of cores to use for optimization
ncores_mle = 1

# Indicate use of BFGS optimization methods
bfgs = TRUE

# Location of R data files with starting values
# for input to MLE optimization
opt_files_in = NULL
```

```
# Location of R data file to write the results of
# MLE optimization
opt_files_out = "./opt_nev.RData"

# Initial start value for theta0
tst = TRUE

if( tst ){
  tst = numeric(p_cal$ntheta0)
  tst[2] = runif(1,-1.e-6,1.e-6)
} else { tst = NULL }

# Confidence interval levels for new event parameter inference
ci_lev = 0.95

# Indicator of MLE gradient check
mle_grad_ck = TRUE

# Strategy for running parallel jobs (future package)
parallel_plan = "multicore"

# MLE calculations
p_cal = calc_mle_0(p_cal,gen_dir,app_dir,fm0,nst=nstart,ncor=ncores_mle,
                   ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,
                   igrck=mle_grad_ck,t_cal=t_cal,g0=gfm0,
                   fopt_in=opt_files_in,Xst=NULL,tst=tst,
                   fopt_out=opt_files_out,pl=parallel_plan)
save.image()

#
# END MAXIMUM LIKELIHOOD CALCULATION
#
```

A.7 New Event Data: Bayesian Analysis

```
#
# BAYESIAN ANALYSIS
#

# Specify if Bayesian analysis is to be conducted
iBayes = TRUE

if( iBayes ){
  # Source supporting R function
  source(paste(gen_dir,"/calc_bayes_0.r",sep=""))

  # Indicator of prior distribution for theta0
  iTheta0Prior = FALSE

  if( iTheta0Prior ){
    # location of code for computing log-prior densities and gradients
    prior_files_theta0 = NULL
    if( igrad ){
      gr_prior_files_theta0 = NULL
    } else { gr_prior_files_theta0 = NULL }

    # prior distribution for new event parameters (theta0)
    p_cal$lp_theta0$f = "lp_0"
    if( igrad ){ p_cal$lp_theta0$g = "lq_0" }

    # parameters for log yield parameter prior (Gaussian)
    p_cal$pi_w_mu = (log(10)+log(10000000))/2
    p_cal$pi_w_sd = (log(10000000)-log(10))/6
    # parameters for HOB/DOB parameter prior (Gaussian)
    p_cal$pi_h_mu = 0
    p_cal$pi_h_sd = 160/3
  } else {
    prior_files_theta0 = NULL
    gr_prior_files_theta0 = NULL
  }

  # specify MCMC algorithm
  # options: "RAM", "FME", "NUTS", or "SMC"
  iMCMC = "FME"

  # burn-in
  nburn = 10000

```

```
  # production
  nmcmc = 20000

  # posterior sample thinning rate (for multiple imputation)
  nthin = 1

  # number of cores to use for optimization
  ncores_map = 1

  # number of cores to use for generating parallel MCMC chains
  ncores_mc = 1

  # Indicator of prior gradient check
  prior_grad_ck = TRUE

  # Indicator of posterior gradient check
  post_grad_ck = TRUE

  # Options for Sequential Monte Carlo (SMC) sampling
  # (iMCMC = "SMC")
  # number of cores to use for parallelization within SMC algorithm
  ncores_smc = NULL
  # new event parameter ranges for initial SMC sample
  lb_smc = rep(-Inf,length(theta_names))
  ub_smc = rep(Inf,length(theta_names))

  # Bayesian calculations
  p_cal = calc_bayes_0(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
                       nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
                       ncor_mc=ncores_mc,igrad=igrad,
                       igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
                       bfgs=bfgs,itpr=iTheta0Prior,
                       fpr_t=prior_files_theta0,
                       fgpr_t=gr_prior_files_theta0,imcmc=iMCMC,
                       pl=parallel_plan,ncor_smc=ncores_smc,
                       lb_smc=lb_smc,ub_smc=ub_smc,t_cal=t_cal)
  save.image()
}

#
# END BAYESIAN ANALYSIS
#
```

A.8 New Event Data: Output File

```
> # MLE calculations
> p_cal = calc_mle_0(p_cal,gen_dir,app_dir,fm0,nst=nstart,ncor=ncores_mle,
+                     ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,
+                     igrck=mle_grad_ck,t_cal=t_cal,g0=gfm0,
+                     fopt_in=opt_files_in,Xst=NULL,tst=tst,
+                     fopt_out=opt_files_out,pl=parallel_plan)
[1] "MLE CONVERGENCE STATUS"

[1] 0
[1] 2
[1] "MAXIMUM LIKELIHOOD SUMMARY"

[1] "NEW EVENT INFERENCE PARAMETERS"

[1] "ESTIMATE: "

    W   HOB
14.02 -2.70

[1] "STANDARD DEVIATION: "

   W  HOB
0.05 1.97

[1] "STANDARD DEVIATION FIXED MODEL PARAMETERS: "

   W  HOB
0.05 1.79

[1] "CORRELATION MATRIX: "

        W   HOB
W    1.00 -0.43
HOB -0.43  1.00

[1] "CORRELATION MATRIX FIXED MODEL PARAMETERS: "

        W   HOB
W    1.00 -0.36
HOB -0.36  1.00

[1] "95%: CONFIDENCE INTERVAL:"

```

```
       W   HOB
lb 13.92 -5.46
ub 14.13  3.30

[1] "95%: CONFIDENCE INTERVAL FIXED MODEL PARAMETERS:"

         W   HOB
lb_0 13.93 -5.28
ub_0 14.11  2.52

Loading required package: numDeriv
[1] "CHECK LOG-LIKELIHOOD GRADIENTS"

[1] "Analytic gradient"
[1] 3.612240e-06 1.545468e-07
[1] "Numerical gradient"
[1] 3.611856e-06 1.526450e-07
[1] "Difference"
[1] 3.836284e-10 1.901811e-09

+   # Bayesian calculations
+   p_cal = calc_bayes_0(p_cal,gen_dir,app_dir,nburn=nburn,nmcmc=nmcmc,
+                        nthin=nthin,ncor=ncores_mc,igrad=igrad,
+                        igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
+                        bfgs=bfgs,itpr=iTheta0Prior,
+                        fpr_t=prior_files_theta0,
+                        fgpr_t=gr_prior_files_theta0,imcmc=iMCMC,
+                        pl=parallel_plan,ncor_smc=ncores_smc,
+                        lb_smc=lb_smc,ub_smc=ub_smc,t_cal=t_cal)
+   save.image()
+ }
[1] "MAP CONVERGENCE STATUS"

[1] 0
[1] 2
[1] "MAXIMUM A POSTERIORI SUMMARY"

[1] "NEW EVENT INFERENCE PARAMETERS"

[1] "ESTIMATE: "

    W   HOB
14.02 -2.11

[1] "CHECK LOG-PRIOR GRADIENTS"
```

```

[1] "Analytic gradient"
[1] 0.000000 0.682004
[1] "Numerical gradient"
[1] 0.000000 0.682004
[1] "Difference"
[1] 0.000000e+00 7.597145e-12

[1] "CHECK LOG-POSTERIOR GRADIENTS"

[1] "Analytic gradient"
[1] 4.523644e-06 3.942643e-06
[1] "Numerical gradient"
[1] 4.524224e-06 3.942255e-06
[1] "Difference"
[1] -5.799625e-10  3.878053e-10

[1] "ACCEPTANCE RATES:"

[1] "Core 1: 0.816366666666667"

[1] "POSTERIOR SUMMARY"

[1] "NEW EVENT INFERENCE PARAMETERS"

[1] "POSTERIOR MEAN: 14.03" "POSTERIOR MEAN: -0.77"

[1] "POSTERIOR SD: 0.05" "POSTERIOR SD: 3.04"

[1] "LEVEL 2.5%: 13.94" "LEVEL 2.5%: -5.54"

[1] "LEVEL 5%: 13.95" "LEVEL 5%: -5.03"

[1] "LEVEL 50%: 14.03" "LEVEL 50%: -1.42"

[1] "LEVEL 95%: 14.1" "LEVEL 95%: 4.48"

[1] "LEVEL 97.5%: 14.12" "LEVEL 97.5%: 5.25"

[1] "CORRELATION MATRIX:"

    W HOB
W   1   0
HOB 0   1
```

B Complete Assessment Run Files

This appendix provides an example run file and output file for complete assessments.

B.1 Preprocessing

```
##########################################################################
#                                                                        #
# This file is the input deck for MultiPEM Toolbox complete post-       #
# detonation analysis.                                                   #
#                                                                        #
##########################################################################

#
# REQUIRED R PACKAGES
#

require(Matrix)

#
# END REQUIRED R PACKAGES
#

#
# PREPROCESSING
#

# Specify directory for general subroutines
gen_dir = "../../../Code"

# Source supporting R function
source(paste(gen_dir,"/prepro.r",sep=""))

# Specify directory for application subroutines
app_dir = "../../Code"

# Specify root data directory
dat_dir = "../../Data"

# Specify calibration data directories
dat_cal = c("seismic_cal.csv",
            "acoustic_cal.csv",
            "optical_cal.csv",
            "crater_cal.csv")

```

```
# Phenomenologies for this analysis
# 1 - seismic
# 2 - acoustic
# 3 - optical
# 4 - crater (surface effects)

# Indicate presence of calibration inference parameters
calp = FALSE

if( calp ){
  # Names of calibration inference parameters
  #cal_par_names =
} else { cal_par_names = NULL }

# Specify number of responses for each phenomenology
Rh = c(2,2,2,2)

# Empirical model parameter count: common
# list with elements corresponding to phenomenologies
pbeta = vector("list",length(Rh))
for( hh in 1:length(Rh) ){ pbeta[[hh]] = numeric(Rh[hh]) }
# phenomenology 2
pbeta[[2]] = c(2,2)
# phenomenology 3
pbeta[[3]] = c(2,2)
# phenomenology 4
pbeta[[4]] = c(2,2)

# Specify number of emplacement conditions for each phenomenology
Th = TRUE

if( Th ){ Th = c(3,3,0,0)
} else { Th = NULL }

# Empirical model parameter count: emplacement condition
# list with elements corresponding to phenomenologies
if( !is.null(Th) ){
  pbetat = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){
    if( Th[hh] > 1 ){ pbetat[[hh]] = vector("list",Th[hh]) }
  }
  # phenomenology 1
  for( tt in 1:Th[1] ){
    pbetat[[1]][[tt]] = numeric(Rh[1])
    pbetat[[1]][[tt]] = c(5,5)
```

```
  }
  # phenomenology 2
  for( tt in 1:Th[2] ){
    pbetat[[2]][[tt]] = numeric(Rh[2])
    pbetat[[2]][[tt]] = c(1,1)
  }
} else { pbetat = NULL }

# Locations of common parameters in full parameter vector
# list with elements corresponding to phenomenologies
if( !is.null(Th) ){
  ibetar = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){
    if( Th[hh] > 1 ){
      # lists with elements for each response within
      # emplacement condition
      ibetar[[hh]] = vector("list",Th[hh]*Rh[hh])
    }
  }
  # phenomenology 2
  for( tt in 1:Th[2] ){
    for( rr in 1:Rh[2] ){
      ibetar[[2]][[(tt-1)*Rh[2]+rr]] = 1:2
    }
  }
} else { ibetar = NULL }

# Indicate analysis with errors-in-variables (eiv)
eiv = TRUE

# Specifications for errors-in-variables
if( eiv ){
  # Specify phenomenologies utilizing
  # errors-in-variables yields
  ieiv = 3:4

  # Errors-in-variables source lists by
  # phenomenology
  seiv = vector("list",length(Rh))
  for( hh in ieiv ){ seiv[[hh]] = "ALL" }

  # Set standard deviation of eiv Gaussian likelihood
  eiv_w_sd = 0.1/3
} else {
  ieiv = NULL
```

```
  seiv = NULL
  eiv_w_sd = NULL
}

# Specify Error Model
# Level 1 variance component parameter count
pvc_1 = TRUE

if( pvc_1 ){
  pvc_1 = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){ pvc_1[[hh]] = numeric(Rh[hh]) }
  # phenomenology 1
  pvc_1[[1]] = c(1,1)
  # phenomenology 2
  pvc_1[[2]] = c(1,1)
} else { pvc_1 = NULL }

# Level 2 variance component parameter count
pvc_2 = TRUE

if( pvc_2 ){
  pvc_2 = vector("list",length(Rh))
  for( hh in 1:length(Rh) ){ pvc_2[[hh]] = numeric(Rh[hh]) }
  # phenomenology 1
  pvc_2[[1]] = c(1,1)
  # phenomenology 2
  #pvc_2[[2]] =

  # path error models by phenomenology
  ptype = vector("list",length(Rh))
  # phenomenology 1
  #ptype[[1]] =
} else { pvc_2 = NULL; ptype = NULL; }

# Set flag for user-provided code to calculate variance
# component coefficient matrices
calc_Z = FALSE

# Set flag for bounded optimization
# currently only supported for new event parameters
opt_B = FALSE

# Indicate analysis of new event (nev)
nev = TRUE

```

```
# Specifications for new event
if( nev ){
  # Specify new event data directories
  dat_new = c("seismic_new.csv",
              "acoustic_new.csv",
              "optical_new.csv",
              "crater_new.csv")

  # Names of new event inference parameters
  theta_names = c("W","HOB")

  # Indicate nev parameter transform
  itransform = FALSE

  # Specify fixed parameters for nev parameter transform
  if( itransform ){
    tPars = TRUE

    if( tPars ){
      tPars = vector("list",0)
      tPars$yield_scaling = 1/3
    } else { tPars = NULL }
  } else { tPars = NULL }

  # Set up parameter constraints
  # lower and upper bounds (use -Inf and Inf if unbounded)
  lb_theta0 = rep(-Inf,length(theta_names))
  lb_theta0[2] = -10
  ub_theta0 = rep(Inf,length(theta_names))
  ub_theta0[2] = 160

  # Set up parameter subsets by phenomenology
  tsub = TRUE

  if( tsub ){
    tsub = vector("list",length(Rh))
    tsub[[4]] = 1 # only log-yield for crater
  } else { tsub = NULL }
} else {
  dat_new = NULL
  theta_names = NULL
  itransform = FALSE
  tPars = NULL
  lb_theta0 = NULL
  ub_theta0 = NULL
```

```
  tsub = NULL
}

# Preprocessing for statistical analysis routines
tmp = prepro(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,bopt=opt_B,
             nev=nev,itr=itransform,izmat=calc_Z,ieiv=ieiv,seiv=seiv,
             ewsd=eiv_w_sd,Th=Th,pbetat=pbetat,ibetar=ibetar,
             pvc_1=pvc_1,pvc_2=pvc_2,ptype=ptype,tnames=theta_names,
             cnames=cal_par_names,fp_tr=tPars,tlb=lb_theta0,
             tub=ub_theta0,ndir=dat_new,tsub=tsub)
if( opt_B ){
  p_cal = tmp$p_cal
  t_cal = tmp$t_cal
} else {
  p_cal = tmp
  t_cal = NULL
}
rm(tmp)
save.image()

#
# END PREPROCESSING
#
```

B.2 Maximum Likelihood Estimation

```
#
# MAXIMUM LIKELIHOOD CALCULATION
#

# Source supporting R function
source(paste(gen_dir,"/calc_mle.r",sep=""))

# Set seed for repeatability of analysis
set.seed(611)

# Names of forward models for each response
# by phenomenology
fm = vector("list",length(Rh))
fm[[1]] = c("f_s","f_s")
fm[[2]] = c("f_a","f_a")
fm[[3]] = c("f_o","f_o")
fm[[4]] = c("f_c","f_c")

# Indicate if forward model gradients provided
igrad = TRUE

if( igrad ){
  # Names of forward model gradients for each response
  # by phenomenology
  gfm = vector("list",length(Rh))
  gfm[[1]] = c("g_s","g_s")
  gfm[[2]] = c("g_a","g_a")
  gfm[[3]] = c("g_o","g_o")
  gfm[[4]] = c("g_c","g_c")
} else { gfm = NULL }

# Specifications for forward model calculations
# a) flags for modified forward model calculation by
#    response for each relevant phenomenology
iResponse = TRUE

if( iResponse ){
  iResponse = vector("list",length(Rh))
  iResponse[[1]] = c(TRUE,FALSE)
  iResponse[[2]] = c(TRUE,FALSE)
} else { iResponse = NULL }

# b) fixed quantities required by forward models
```

```
fPars = TRUE

if( fPars ){
  fPars = vector("list",length(Rh))
  fPars[[1]]$yield_scaling = 1/3
  fPars[[2]]$yield_scaling = 1/3
  fPars[[2]]$pressure_scaling = 1/3
  fPars[[2]]$temp_scaling = 1/2
  fPars[[3]]$yield_scaling = 1/3
  fPars[[3]]$pressure_scaling = 1/3
  fPars[[3]]$temp_scaling = 1/2
} else { fPars = NULL }

# Specify number of starting values for optimization
nstart = 10

# number of cores to use for optimization
ncores_mle = 1

# Indicate use of BFGS optimization methods
bfgs = TRUE

# Location of R data files with starting values
# for input to MLE optimization
opt_files_in = c("../Opt/opt_1.RData",
                 "../Opt/opt_2.RData",
                 "../Opt/opt_3_eiv.RData",
                 "../Opt/opt_4_eiv.RData")

# Location of R data file to write the results of
# MLE optimization
opt_files_out = "./opt.RData"

if( calp ){
  # Initial start value for calibration inference parameters
  cst = FALSE

  if( cst ){
    cst = numeric(p_cal$ncalp)
    #cst[1] =
  } else { cst = NULL }
} else { cst = NULL }

if( nev ){
  # Initial start value for theta0
```

```
  tst = TRUE

  if( tst ){
    tst = numeric(p_cal$ntheta0)
    tst[2] = runif(1,-1.e-6,1.e-6)
  } else { tst = NULL }
} else { tst = NULL }

if( calp || nev ){
  # Confidence interval levels
  ci_lev = 0.95
} else { ci_lev = NULL }

# Indicate phenomenology number and type (if needed
# for postprocessing)
Phen = TRUE

if( Phen ){
  Phen = matrix(c(1,"Seismic"),nrow=1)
} else { Phen = NULL }

# Indicator of MLE gradient check
mle_grad_ck = TRUE

# Strategy for running parallel jobs (future package)
parallel_plan = "multicore"

# MLE calculations
p_cal = calc_mle(p_cal,gen_dir,app_dir,fm,nst=nstart,ncor=ncores_mle,
                 ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,igrck=mle_grad_ck,
                 t_cal=t_cal,g=gfm,iresp=iResponse,fp_fm=fPars,
                 fopt_in=opt_files_in,Xst=NULL,tst=tst,cst=cst,
                 fopt_out=opt_files_out,phen=Phen,pl=parallel_plan)
save.image()

#
# END MAXIMUM LIKELIHOOD CALCULATION
#
```

B.3 Bayesian Analysis

```
#
# BAYESIAN ANALYSIS
#

# Specify if Bayesian analysis is to be conducted
iBayes = TRUE

if( iBayes ){
  # Source supporting R function
  source(paste(gen_dir,"/calc_bayes.r",sep=""))

  # Indicator of prior distribution for forward model
  # coefficients
  iBetaPrior = TRUE

  if( iBetaPrior ){
    # location of code for computing log-prior densities and gradients
    prior_files_beta = "../Code/lp_beta_s.r"
    if( igrad ){
      gr_prior_files_beta = "../Code/glp_beta_s.r"
    } else { gr_prior_files_beta = NULL }

    # prior distribution for phenomenology 1
    # forward model coefficients
    p_cal$h[[1]]$lp_betat = vector("list",Th[1])
    for( tt in 1:Th[1] ){
      p_cal$h[[1]]$lp_betat[[tt]]$f = c("lp_s","lp_s")
      if( igrad ){
        p_cal$h[[1]]$lp_betat[[tt]]$g = c("lq_s","lq_s")
      }
    }
  } else {
    prior_files_beta = NULL
    gr_prior_files_beta = NULL
  }

  # Indicator of prior distribution for calibration parameters
  iCalPrior = TRUE

  if( calp && iCalPrior ){
    # location of code for computing log-prior densities and gradients
    prior_files_calp = NULL
    if( igrad ){
```

```
      gr_prior_files_calp = NULL
    } else { gr_prior_files_calp = NULL }

    # prior distribution for calibration parameters (calp)
    p_cal$lp_calp$f = "lp_c"
    if( igrad ){ p_cal$lp_calp$g = "lq_c" }

    # parameters for calibration parameter prior distribution
    #p_cal$pi_c_mu =
    #p_cal$pi_c_sd =
  } else {
    prior_files_calp = NULL
    gr_prior_files_calp = NULL
  }

  # Indicator of prior distribution for theta0
  iTheta0Prior = FALSE

  if( nev && iTheta0Prior ){
    # location of code for computing log-prior densities and gradients
    prior_files_theta0 = NULL
    if( igrad ){
      gr_prior_files_theta0 = NULL
    } else { gr_prior_files_theta0 = NULL }

    # prior distribution for new event parameters (theta0)
    p_cal$lp_theta0$f = "lp_0"
    if( igrad ){ p_cal$lp_theta0$g = "lq_0" }

    # parameters for log yield parameter prior (Gaussian)
    p_cal$pi_w_mu = (log(10)+log(10000000))/2
    p_cal$pi_w_sd = (log(10000000)-log(10))/6
    # parameters for HOB/DOB parameter prior (Gaussian)
    p_cal$pi_h_mu = 0
    p_cal$pi_h_sd = 160/3
  } else {
    prior_files_theta0 = NULL
    gr_prior_files_theta0 = NULL
  }

  # fixed scale parameters for variance component prior
  # comment out if these parameters should vary
  p_cal$A = 20

  # eta parameter in Lewandowski-Kurowicka-Joe (LKJ) prior
```

```
# distribution for correlation parameters
p_cal$lp_corr$eta = 1

# FGSN parameters for errors-in-variables yields prior
# number of components
p_cal$K = 0
# total number of FGSN parameters
p_cal$p_fgsn = 0
if( eiv ){
  p_cal$K = 2
  p_cal$p_fgsn = p_cal$K + 2
}

# specify Markov chain Monte Carlo (MCMC) algorithm
# options: "RAM", "FME", or "NUTS"
iMCMC = "FME"

# burn-in
nburn = 10000

# production
nmcmc = 20000

# posterior sample thinning rate
nthin = 20

# number of cores to use for optimization
ncores_map = 1

# number of cores to use for generating parallel MCMC chains
ncores_mc = 1

# Indicator of prior gradient check
prior_grad_ck = TRUE

# Indicator of posterior gradient check
post_grad_ck = TRUE

# Bayesian calculations
p_cal = calc_bayes(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
                   nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
                   ncor_mc=ncores_mc,igrad=igrad,
                   igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
                   bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
                   itpr=iTheta0Prior,fpr_b=prior_files_beta,
```

```
                     fgpr_b=gr_prior_files_beta,fpr_c=prior_files_calp,
                     fgpr_c=gr_prior_files_calp,
                     fpr_t=prior_files_theta0,
                     fgpr_t=gr_prior_files_theta0,Xnom=NULL,
                     imcmc=iMCMC,pl=parallel_plan,t_cal=t_cal)
  save.image()
}

#
# END BAYESIAN ANALYSIS
#
```

B.4 Output File

```
> # Preprocessing for statistical analysis routines
> tmp = prepro(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,bopt=opt_B,
+               nev=nev,itr=itransform,izmat=calc_Z,ieiv=ieiv,seiv=seiv,
+               ewsd=eiv_w_sd,Th=Th,pbetat=pbetat,ibetar=ibetar,
+               pvc_1=pvc_1,pvc_2=pvc_2,ptype=ptype,tnames=theta_names,
+               cnames=cal_par_names,fp_tr=tPars,tlb=lb_theta0,
+               tub=ub_theta0,ndir=dat_new,tsub=tsub)
[1] "Warning: Insufficient Paths for Level 2 Variance Component models with
     Phenomenology 2 and Response 1."
[1] "Warning: Insufficient Paths for Level 2 Variance Component models with
     Phenomenology 2 and Response 2."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 3 and Response 1."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 3 and Response 2."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 4 and Response 1."
[1] "Warning: Insufficient number of observations per Source for Variance
     Component models with Phenomenology 4 and Response 2."

> # MLE calculations
> p_cal = calc_mle(p_cal,gen_dir,app_dir,fm,nst=nstart,ncor=ncores_mle,
+                   ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,igrck=mle_grad_ck,
+                   t_cal=t_cal,g=gfm,iresp=iResponse,fp_fm=fPars,
+                   fopt_in=opt_files_in,Xst=NULL,tst=tst,cst=cst,
+                   fopt_out=opt_files_out,phen=Phen,pl=parallel_plan)
[1] "MLE CONVERGENCE STATUS"

[1] 0
[1] 2
[1] "MAXIMUM LIKELIHOOD SUMMARY"

[1] "NEW EVENT INFERENCE PARAMETERS"

[1] "ESTIMATE: "

    W   HOB
14.02 -2.62

[1] "STANDARD DEVIATION: "

   W  HOB
0.05 1.93
```

```

[1] "CORRELATION MATRIX: "

        W   HOB
W    1.00 -0.44
HOB -0.44  1.00

[1] "95%: CONFIDENCE INTERVAL:"

       W   HOB
lb 13.92 -5.35
ub 14.12  3.18


[1] "ERRORS-IN-VARIABLES YIELDS"

    7     8     9    10    11    13    14    16    17    20    21    22    23
16.29 16.21 16.51 16.61 17.00 12.21 17.57 17.27 16.52 14.50 15.75 17.59 15.23
   24    25    28    29    30    31    33    34    35    36    37    38    39
15.88 16.46 14.52 12.13 17.71 23.08 23.42 17.51 21.96 22.34 16.71 21.02 18.52

[1] "COMMON COEFFICIENTS"

        [1] "Phenomenology: 2; Response: 1"

        [1]  6.67 -1.14

        [1] "Phenomenology: 2; Response: 2"

        [1] -5.08  0.23

        [1] "Phenomenology: 3; Response: 1"

        [1] -11.07   1.89

        [1] "Phenomenology: 3; Response: 2"

        [1] -8.64  1.71

        [1] "Phenomenology: 4; Response: 1"

        [1] -3.31  0.43

        [1] "Phenomenology: 4; Response: 2"

```

```
        [1] -2.38  0.28

[1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

        [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

        [1] -10.07  -1.31  -1.43   3.53   0.40

        [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

        [1] -1.52 -1.44 -1.23  2.29  0.63

        [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

        [1] -11.48  -1.09  -3.59   4.32   0.16

        [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

        [1]  -2.19  -1.22 -26.48   0.99  -2.65

        [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

        [1] -9.53 -1.16 -4.47  4.95  0.34

        [1] "Phenomenology: 1; Emplacement: 3; Response: 2"

        [1] -2.85 -0.71 -2.10  2.68  0.13

        [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

        [1] 3.87

        [1] "Phenomenology: 2; Emplacement: 1; Response: 2"

        [1] -0.17

        [1] "Phenomenology: 2; Emplacement: 2; Response: 1"

        [1] 3.12

        [1] "Phenomenology: 2; Emplacement: 2; Response: 2"

        [1] -0.9

        [1] "Phenomenology: 2; Emplacement: 3; Response: 1"
```

```
        [1] 2.16

        [1] "Phenomenology: 2; Emplacement: 3; Response: 2"

        [1] -0.94

[1] "LEVEL 1 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] 0.0011

        [1] "Phenomenology: 1; Response: 2"

        [1] 0.0016

        [1] "Phenomenology: 2; Response: 1"

        [1] 0.0037

        [1] "Phenomenology: 2; Response: 2"

        [1] 0.0015

[1] "LEVEL 2 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] 0.001

        [1] "Phenomenology: 1; Response: 2"

        [1] 9e-04

[1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"

[1] "Phenomenology 1"

[1] "Variances"

[1] 0.0021 0.0034

[1] "Correlations"
```

```
     [,1] [,2]
[1,]    1 0.27
[2,]    0 1.00

[1] "Phenomenology 2"

[1] "Variances"

[1] 1e-03 3e-04

[1] "Correlations"

     [,1]  [,2]
[1,]    1 -0.25
[2,]    0  1.00

[1] "Phenomenology 3"

[1] "Variances"

[1] 0.0011 0.0010

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.93
[2,]    0 1.00

[1] "Phenomenology 4"

[1] "Variances"

[1] 0.0222 0.0087

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.65
[2,]    0 1.00

[1] "AIC = -5913.11"

[1] "BIC = -5573.35"

Loading required package: numDeriv
```

```
[1] "CHECK LOG-LIKELIHOOD GRADIENTS"

[1] "Analytic gradient"
 [1]  5.112159e-04 -2.542508e-05 -1.863792e-03  6.228479e-04 -1.625812e-03
 [6]  1.907117e-03  2.310639e-04  8.065429e-04 -8.404374e-05 -9.984542e-04
[11] -4.226071e-04 -1.989370e-03 -1.157463e-03  1.812303e-03  3.537858e-03
[16] -2.784636e-03  7.371172e-04  7.547859e-04 -1.494877e-03  4.223703e-03
[21]  1.534175e-03 -2.357543e-03  1.895850e-03 -3.989834e-04  1.732983e-03
[26]  9.354533e-04 -4.440143e-05  9.331977e-06 -2.694365e-03 -4.299476e-02
[31] -1.507931e-02 -2.445686e-01 -3.765500e-02 -7.708215e-04  2.986042e-02
[36]  6.118387e-03 -6.676220e-04 -1.555101e-02  1.448662e-03  2.788605e-02
[41]  9.125824e-04  2.695089e-04 -2.401801e-03 -1.526986e-04 -4.231445e-04
[46] -1.511128e-03  1.417248e-03  1.029923e-03 -1.364681e-04  3.342011e-04
[51] -1.656650e-02 -1.223063e-01  4.508649e-02  3.934503e-03 -7.615629e-03
[56]  1.978269e-03  1.821235e-03  4.439611e-03  1.006111e-02  4.886488e-03
[61] -3.438471e-04  2.571739e-03  1.720799e-03  2.864180e-04 -7.508282e-04
[66]  9.688080e-04  2.185358e-03 -1.105926e-03  1.041878e-04 -4.157820e-04
[71]  5.369795e-04 -4.609019e-04  2.385899e-04 -6.059969e-05  3.177182e-04
[76]  2.788174e-04  5.402526e-04  2.458910e-04 -3.436638e-05 -1.133472e-04
[81] -3.018574e-04 -1.905102e-04  1.069394e-04  5.970366e-04 -5.390348e-04
[86]  6.469861e-04  2.939823e-05  1.613974e-01  8.178509e-04  6.931910e-04
[91]  2.285890e-02 -1.018627e-04  4.539666e-05  2.014041e-04
[1] "Numerical gradient"
 [1]  5.112092e-04 -2.539405e-05 -1.863777e-03  6.228507e-04 -1.625809e-03
 [6]  1.907111e-03  2.310578e-04  8.065436e-04 -8.404145e-05 -9.984549e-04
[11] -4.225894e-04 -1.989392e-03 -1.157464e-03  1.812304e-03  3.537854e-03
[16] -2.784620e-03  7.370990e-04  7.547591e-04 -1.494772e-03  4.223713e-03
[21]  1.534173e-03 -2.357541e-03  1.895848e-03 -3.989830e-04  1.732981e-03
[26]  9.354541e-04 -4.440477e-05  9.337693e-06 -2.694363e-03 -4.299474e-02
[31] -1.507930e-02 -2.445664e-01 -3.765495e-02 -7.709241e-04  2.986035e-02
[36]  6.117932e-03 -6.675813e-04 -1.555099e-02  1.448742e-03  2.788585e-02
[41]  9.125534e-04  2.693702e-04 -2.401588e-03 -1.526865e-04 -4.228457e-04
[46] -1.511103e-03  1.417144e-03  1.029829e-03 -1.364287e-04  3.343325e-04
[51] -1.656650e-02 -1.223064e-01  4.508646e-02  3.934508e-03 -7.616756e-03
[56]  1.978321e-03  1.821328e-03  4.439639e-03  1.006101e-02  4.886500e-03
[61] -3.438479e-04  2.571653e-03  1.720924e-03  2.864399e-04 -7.508463e-04
[66]  9.688664e-04  2.185367e-03 -1.105973e-03  1.041493e-04 -4.163252e-04
[71]  5.369532e-04 -4.615999e-04  2.386148e-04 -6.041131e-05  3.177212e-04
[76]  2.789338e-04  5.402541e-04  2.458948e-04 -3.428431e-05 -1.133899e-04
[81] -3.018444e-04 -1.905103e-04  1.069402e-04  5.970440e-04 -5.336226e-04
[86]  6.470927e-04  2.945024e-05  1.614883e-01  8.171414e-04  6.932402e-04
[91]  2.286268e-02 -1.016709e-04  4.562640e-05  2.005773e-04
[1] "Difference"
[1] -9.084942e-05  1.126289e-06
```

```
+   # Bayesian calculations
+   p_cal = calc_bayes(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
+                      nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
+                      ncor_mc=ncores_mc,igrad=igrad,
+                      igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
+                      bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
+                      itpr=iTheta0Prior,fpr_b=prior_files_beta,
+                      fgpr_b=gr_prior_files_beta,fpr_c=prior_files_calp,
+                      fgpr_c=gr_prior_files_calp,
+                      fpr_t=prior_files_theta0,
+                      fgpr_t=gr_prior_files_theta0,Xnom=NULL,
+                      imcmc=iMCMC,pl=parallel_plan,t_cal=t_cal)
+   save.image()
+ }
[1] "MAP CONVERGENCE STATUS"

[1] 0
[1] 2
[1] "MAXIMUM A POSTERIORI SUMMARY"

[1] "NEW EVENT INFERENCE PARAMETERS"

[1] "ESTIMATE: "

    W   HOB
14.01  2.30


[1] "ERRORS-IN-VARIABLES YIELDS"

    7     8     9    10    11    13    14    16    17    20    21    22    23
16.28 16.21 16.50 16.61 17.00 12.21 17.57 17.27 16.52 14.50 15.75 17.60 15.24
   24    25    28    29    30    31    33    34    35    36    37    38    39
15.87 16.46 14.53 12.13 17.71 23.08 23.41 17.51 21.96 22.34 16.71 21.02 18.52

[1] "COMMON COEFFICIENTS"

        [1] "Phenomenology: 2; Response: 1"

        [1]  6.67 -1.14

        [1] "Phenomenology: 2; Response: 2"

        [1] -5.08  0.23

```

```
        [1] "Phenomenology: 3; Response: 1"

        [1] -11.07   1.89

        [1] "Phenomenology: 3; Response: 2"

        [1] -8.64  1.71

        [1] "Phenomenology: 4; Response: 1"

        [1] -3.31  0.43

        [1] "Phenomenology: 4; Response: 2"

        [1] -2.38  0.28

[1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

        [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

        [1] -10.06  -1.31  -1.44   3.49   0.38

        [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

        [1] -1.50 -1.44 -1.25  2.24  0.61

        [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

        [1] -11.48  -1.09  -3.60   4.25   0.16

        [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

        [1]   -2.13   -1.22 -159.29    0.90   -4.47

        [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

        [1] -9.53 -1.16 -4.47  4.95  0.34

        [1] "Phenomenology: 1; Emplacement: 3; Response: 2"

        [1] -2.85 -0.71 -2.15  2.61  0.10

        [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

        [1] 3.87
```

```
        [1] "Phenomenology: 2; Emplacement: 1; Response: 2"

        [1] -0.17

        [1] "Phenomenology: 2; Emplacement: 2; Response: 1"

        [1] 3.11

        [1] "Phenomenology: 2; Emplacement: 2; Response: 2"

        [1] -0.91

        [1] "Phenomenology: 2; Emplacement: 3; Response: 1"

        [1] 2.16

        [1] "Phenomenology: 2; Emplacement: 3; Response: 2"

        [1] -0.94

[1] "LEVEL 1 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] 0.0012

        [1] "Phenomenology: 1; Response: 2"

        [1] 0.0017

        [1] "Phenomenology: 2; Response: 1"

        [1] 0.0039

        [1] "Phenomenology: 2; Response: 2"

        [1] 0.0016

[1] "LEVEL 2 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] 0.001
```

```
        [1] "Phenomenology: 1; Response: 2"

        [1] 0.001

[1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"

[1] "Phenomenology 1"

[1] "Variances"

[1] 0.0021 0.0034

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.27
[2,]    0 1.00

[1] "Phenomenology 2"

[1] "Variances"

[1] 1e-03 3e-04

[1] "Correlations"

     [,1]  [,2]
[1,]    1 -0.25
[2,]    0  1.00

[1] "Phenomenology 3"

[1] "Variances"

[1] 9e-04 9e-04

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.92
[2,]    0 1.00

[1] "Phenomenology 4"

[1] "Variances"
```

```
[1] 0.0196 0.0071

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.52
[2,]    0 1.00

[1] "FGSN PRIOR PARAMETERS"

[1] "Alpha = 17.33"
[1] "Lambda squared = 8.05"
[1] "Omega = -1.65" "Omega = 0.56"

[1] "CHECK LOG-PRIOR GRADIENTS"

[1] "Analytic gradient"
 [1]  0.000000e+00  7.980369e-01 -1.043263e-01 -8.247890e-02 -1.766663e-01
 [6] -2.122515e-01 -3.470393e-01  1.996855e+00 -5.420832e-01 -4.415773e-01
[11] -1.814653e-01  3.548269e-01  5.536912e-02 -5.491970e-01  1.851314e-01
[16]  1.968395e-02 -1.633027e-01  3.474537e-01  2.182895e+00 -5.838604e-01
[21] -3.733141e-01 -6.350369e-01 -5.217498e-01  3.876847e-01  2.520478e-01
[26] -2.463583e-01  1.526028e-01 -7.433990e-01  0.000000e+00  0.000000e+00
[31]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[36]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[41]  0.000000e+00  0.000000e+00  1.000000e+00  0.000000e+00  0.000000e+00
[46]  0.000000e+00  0.000000e+00  1.000000e+00  0.000000e+00  0.000000e+00
[51]  0.000000e+00  0.000000e+00  7.782174e-01  0.000000e+00  0.000000e+00
[56]  0.000000e+00  0.000000e+00  9.276835e-02  0.000000e+00  0.000000e+00
[61]  0.000000e+00  0.000000e+00  6.610552e-01  0.000000e+00  0.000000e+00
[66]  0.000000e+00  0.000000e+00  1.000000e+00  0.000000e+00  0.000000e+00
[71]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[76]  0.000000e+00  4.999971e-01  4.999957e-01  4.999904e-01  4.999960e-01
[81]  4.999974e-01  4.999976e-01 -2.220446e-16 -7.766602e-01 -1.404975e+01
[86]  0.000000e+00 -8.150896e-01  4.186579e+01 -4.440892e-16  1.514024e+00
[91] -9.310054e+01 -4.440892e-16 -1.766204e-01 -1.871582e+01 -3.044490e-02
[96] -2.429394e-02 -7.026312e-02 -1.405367e-01
[1] "Numerical gradient"
 [1]  0.000000e+00  7.980369e-01 -1.043263e-01 -8.247890e-02 -1.766663e-01
 [6] -2.122515e-01 -3.470393e-01  1.996855e+00 -5.420832e-01 -4.415773e-01
[11] -1.814653e-01  3.548269e-01  5.536912e-02 -5.491970e-01  1.851314e-01
[16]  1.968395e-02 -1.633027e-01  3.474538e-01  2.182895e+00 -5.838604e-01
[21] -3.733141e-01 -6.350369e-01 -5.217498e-01  3.876847e-01  2.520478e-01
[26] -2.463583e-01  1.526028e-01 -7.433990e-01  0.000000e+00  0.000000e+00
```

```
[31]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[36]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[41]  0.000000e+00  0.000000e+00  1.000000e+00  0.000000e+00  0.000000e+00
[46]  0.000000e+00  0.000000e+00  1.000000e+00  0.000000e+00  0.000000e+00
[51]  0.000000e+00  0.000000e+00  7.782174e-01  0.000000e+00  0.000000e+00
[56]  0.000000e+00  0.000000e+00  9.276835e-02  0.000000e+00  0.000000e+00
[61]  0.000000e+00  0.000000e+00  6.610552e-01  0.000000e+00  0.000000e+00
[66]  0.000000e+00  0.000000e+00  1.000000e+00  0.000000e+00  0.000000e+00
[71]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[76]  0.000000e+00  4.999971e-01  4.999957e-01  4.999904e-01  4.999960e-01
[81]  4.999974e-01  4.999976e-01  0.000000e+00 -7.766602e-01 -1.404975e+01
[86]  0.000000e+00 -8.150896e-01  4.186579e+01  2.753625e-20  1.514024e+00
[91] -9.310054e+01  1.333140e-16 -1.766204e-01 -1.871582e+01 -3.044490e-02
[96] -2.429394e-02 -7.026312e-02 -1.405367e-01
[1] "Difference"
[1] -5.909749e-08  7.107675e-07

[1] "CHECK LOG-POSTERIOR GRADIENTS"

[1] "Analytic gradient"
 [1]  0.0652554710  0.2809128777  0.2776747288  0.1913483992  0.1640543443
 [6]  0.4110787063  0.3053493374  0.2732904664  0.0689460969  0.0034688791
[11] -0.3275711254 -0.5398117514  0.1307987365  0.3776565007  0.1278625292
[16] -1.0163032877 -0.3003047036 -0.5183880602 -0.4898692700  0.3585217007
[21]  0.1201606000 -0.0253855445  0.3277713035 -0.0943793983  0.1286572477
[26]  0.0709557394 -0.2406661285 -0.1030212436  0.2253706895  0.0874951338
[31] -0.0918057138  0.7026903265 -0.1706238390  1.2547660142 -0.0055983437
[36]  0.8590244663 -0.0192460560  0.4013458092 -0.0654405703 -0.5828461460
[41]  0.1246405443 -0.0227052968 -0.0380441080  0.0041646414  0.0634785826
[46] -0.0197653236  0.0154455135  0.1004165465 -0.0645952411  0.0333200130
[51] -0.0217611223  0.1961083586  0.3975783892  0.0062887012 -0.0368259828
[56]  0.0234689167 -0.1709389850  0.0385639350 -0.0001195893 -0.2933159601
[61] -0.0091858079  0.0182733107  0.0555022779  0.0462591964 -0.0944073914
[66] -0.0296077888  0.1329141126  0.2394165121  0.0738754511 -0.0903148613
[71]  0.0482421120 -0.3823240575 -0.0177985898  0.0577506753 -0.1026839723
[76]  0.0120394755  0.0211923436  0.0150026326 -0.0237693383 -0.0250745269
[81]  0.0140009614  0.0128335916  0.0898737506  0.0054301676  0.0055953664
[86]  0.0285555250 -0.0256819332  0.6947476606  0.3170921643  0.3694779435
[91] -0.1589376117 -0.0032056661  0.0286115155  1.1214529943 -0.0304449029
[96] -0.0242939414 -0.0702631185 -0.1405366559
[1] "Numerical gradient"
 [1]  0.0652554649  0.2809128894  0.2776747326  0.1913483933  0.1640543491
 [6]  0.4110787091  0.3053493421  0.2732904738  0.0689461035  0.0034688910
[11] -0.3275711180 -0.5398117334  0.1307987382  0.3776564972  0.1278625377
[16] -1.0163032755 -0.3003047094 -0.5183880474 -0.4898692439  0.3585217045
```

```
[21]  0.1201605998 -0.0253855458  0.3277713020 -0.0943793913  0.1286572464
[26]  0.0709557483 -0.2406661286 -0.1030212465  0.2253706584  0.0874950308
[31] -0.0918056653  0.7026919885 -0.1706238980  1.2547656219 -0.0055983545
[36]  0.8590243042 -0.0192460637  0.4013454211 -0.0654405498 -0.5828455748
[41]  0.1246405538 -0.0227052931 -0.0380437658  0.0041647257  0.0634790314
[46] -0.0197652454  0.0154455414  0.1004166175 -0.0645952838  0.0333197483
[51] -0.0217611143  0.1961083798  0.3975782937  0.0062887030 -0.0368266050
[56]  0.0234689285 -0.1709390734  0.0385639399 -0.0001195863 -0.2933159334
[61] -0.0091857966  0.0182732944  0.0555020405  0.0462592100 -0.0944077022
[66] -0.0296077430  0.1329142502  0.2394164763  0.0738755689 -0.0903175582
[71]  0.0482421097 -0.3823248767 -0.0177985940  0.0577507259 -0.1026839206
[76]  0.0120396687  0.0211923580  0.0150026541 -0.0237692800 -0.0250745786
[81]  0.0140009232  0.0128335996  0.0898737813  0.0054301772  0.0055855654
[86]  0.0285555874 -0.0256819816  0.6947811056  0.3170917052  0.3694781757
[91] -0.1589561195 -0.0032054142  0.0286116001  1.1214522097 -0.0304449021
[96] -0.0242939549 -0.0702630914 -0.1405367301
[1] "Difference"
[1] -3.344501e-05  1.850774e-05

[1] "ACCEPTANCE RATES:"

[1] "Core 1: 0.852566666666667"

[1] "POSTERIOR SUMMARY"

[1] "NEW EVENT INFERENCE PARAMETERS"

[1] "POSTERIOR MEAN: 14.01" "POSTERIOR MEAN: 2.26"

[1] "POSTERIOR SD: 0.01" "POSTERIOR SD: 0.69"

[1] "LEVEL 2.5%: 13.98" "LEVEL 2.5%: 0.99"

[1] "LEVEL 5%: 13.99" "LEVEL 5%: 1.18"

[1] "LEVEL 50%: 14.01" "LEVEL 50%: 2.23"

[1] "LEVEL 95%: 14.03" "LEVEL 95%: 3.47"

[1] "LEVEL 97.5%: 14.04" "LEVEL 97.5%: 3.69"

[1] "CORRELATION MATRIX:"

       W  HOB
W   1.00 0.89
```

```
HOB 0.89 1.00

[1] "ERRORS-IN-VARIABLES YIELDS"

 [1] "POSTERIOR MEAN: 16.28" "POSTERIOR MEAN: 16.21" "POSTERIOR MEAN: 16.51"
 [4] "POSTERIOR MEAN: 16.61" "POSTERIOR MEAN: 17"    "POSTERIOR MEAN: 12.21"
 [7] "POSTERIOR MEAN: 17.57" "POSTERIOR MEAN: 17.27" "POSTERIOR MEAN: 16.52"
[10] "POSTERIOR MEAN: 14.5"  "POSTERIOR MEAN: 15.75" "POSTERIOR MEAN: 17.6"
[13] "POSTERIOR MEAN: 15.24" "POSTERIOR MEAN: 15.87" "POSTERIOR MEAN: 16.46"
[16] "POSTERIOR MEAN: 14.53" "POSTERIOR MEAN: 12.13" "POSTERIOR MEAN: 17.71"
[19] "POSTERIOR MEAN: 23.08" "POSTERIOR MEAN: 23.41" "POSTERIOR MEAN: 17.51"
[22] "POSTERIOR MEAN: 21.96" "POSTERIOR MEAN: 22.34" "POSTERIOR MEAN: 16.71"
[25] "POSTERIOR MEAN: 21.02" "POSTERIOR MEAN: 18.52"

 [1] "LEVEL 2.5%: 16.27" "LEVEL 2.5%: 16.2"  "LEVEL 2.5%: 16.49"
 [4] "LEVEL 2.5%: 16.59" "LEVEL 2.5%: 16.97" "LEVEL 2.5%: 12.2"
 [7] "LEVEL 2.5%: 17.56" "LEVEL 2.5%: 17.25" "LEVEL 2.5%: 16.5"
[10] "LEVEL 2.5%: 14.48" "LEVEL 2.5%: 15.74" "LEVEL 2.5%: 17.58"
[13] "LEVEL 2.5%: 15.22" "LEVEL 2.5%: 15.86" "LEVEL 2.5%: 16.45"
[16] "LEVEL 2.5%: 14.51" "LEVEL 2.5%: 12.12" "LEVEL 2.5%: 17.7"
[19] "LEVEL 2.5%: 23.06" "LEVEL 2.5%: 23.4"  "LEVEL 2.5%: 17.5"
[22] "LEVEL 2.5%: 21.94" "LEVEL 2.5%: 22.32" "LEVEL 2.5%: 16.69"
[25] "LEVEL 2.5%: 21"    "LEVEL 2.5%: 18.5"

 [1] "LEVEL 5%: 16.27" "LEVEL 5%: 16.2"  "LEVEL 5%: 16.49" "LEVEL 5%: 16.59"
 [5] "LEVEL 5%: 16.98" "LEVEL 5%: 12.2"  "LEVEL 5%: 17.56" "LEVEL 5%: 17.25"
 [9] "LEVEL 5%: 16.51" "LEVEL 5%: 14.49" "LEVEL 5%: 15.74" "LEVEL 5%: 17.59"
[13] "LEVEL 5%: 15.22" "LEVEL 5%: 15.86" "LEVEL 5%: 16.45" "LEVEL 5%: 14.52"
[17] "LEVEL 5%: 12.12" "LEVEL 5%: 17.7"  "LEVEL 5%: 23.07" "LEVEL 5%: 23.4"
[21] "LEVEL 5%: 17.5"  "LEVEL 5%: 21.95" "LEVEL 5%: 22.33" "LEVEL 5%: 16.69"
[25] "LEVEL 5%: 21.01" "LEVEL 5%: 18.5"

 [1] "LEVEL 50%: 16.28" "LEVEL 50%: 16.21" "LEVEL 50%: 16.51" "LEVEL 50%: 16.61"
 [5] "LEVEL 50%: 17"    "LEVEL 50%: 12.21" "LEVEL 50%: 17.57" "LEVEL 50%: 17.27"
 [9] "LEVEL 50%: 16.52" "LEVEL 50%: 14.5"  "LEVEL 50%: 15.74" "LEVEL 50%: 17.6"
[13] "LEVEL 50%: 15.24" "LEVEL 50%: 15.87" "LEVEL 50%: 16.46" "LEVEL 50%: 14.53"
[17] "LEVEL 50%: 12.13" "LEVEL 50%: 17.71" "LEVEL 50%: 23.08" "LEVEL 50%: 23.41"
[21] "LEVEL 50%: 17.51" "LEVEL 50%: 21.96" "LEVEL 50%: 22.34" "LEVEL 50%: 16.71"
[25] "LEVEL 50%: 21.02" "LEVEL 50%: 18.52"

 [1] "LEVEL 95%: 16.29" "LEVEL 95%: 16.22" "LEVEL 95%: 16.52" "LEVEL 95%: 16.62"
 [5] "LEVEL 95%: 17.01" "LEVEL 95%: 12.23" "LEVEL 95%: 17.58" "LEVEL 95%: 17.28"
 [9] "LEVEL 95%: 16.53" "LEVEL 95%: 14.51" "LEVEL 95%: 15.75" "LEVEL 95%: 17.61"
[13] "LEVEL 95%: 15.25" "LEVEL 95%: 15.88" "LEVEL 95%: 16.47" "LEVEL 95%: 14.54"
[17] "LEVEL 95%: 12.14" "LEVEL 95%: 17.72" "LEVEL 95%: 23.09" "LEVEL 95%: 23.43"
```

```
[21] "LEVEL 95%: 17.52" "LEVEL 95%: 21.97" "LEVEL 95%: 22.35" "LEVEL 95%: 16.72"
[25] "LEVEL 95%: 21.03" "LEVEL 95%: 18.53"

 [1] "LEVEL 97.5%: 16.3"  "LEVEL 97.5%: 16.22" "LEVEL 97.5%: 16.52"
 [4] "LEVEL 97.5%: 16.63" "LEVEL 97.5%: 17.02" "LEVEL 97.5%: 12.23"
 [7] "LEVEL 97.5%: 17.59" "LEVEL 97.5%: 17.29" "LEVEL 97.5%: 16.53"
[10] "LEVEL 97.5%: 14.51" "LEVEL 97.5%: 15.76" "LEVEL 97.5%: 17.61"
[13] "LEVEL 97.5%: 15.25" "LEVEL 97.5%: 15.89" "LEVEL 97.5%: 16.48"
[16] "LEVEL 97.5%: 14.54" "LEVEL 97.5%: 12.14" "LEVEL 97.5%: 17.72"
[19] "LEVEL 97.5%: 23.09" "LEVEL 97.5%: 23.43" "LEVEL 97.5%: 17.52"
[22] "LEVEL 97.5%: 21.98" "LEVEL 97.5%: 22.35" "LEVEL 97.5%: 16.73"
[25] "LEVEL 97.5%: 21.03" "LEVEL 97.5%: 18.53"

[1] "COMMON COEFFICIENTS"

        [1] "Phenomenology: 2; Response: 1"

        [1] "POSTERIOR MEAN: 6.67"  "POSTERIOR MEAN: -1.14"

        [1] "LEVEL 2.5%: 6.66"  "LEVEL 2.5%: -1.14"

        [1] "LEVEL 5%: 6.66"  "LEVEL 5%: -1.14"

        [1] "LEVEL 50%: 6.67"  "LEVEL 50%: -1.14"

        [1] "LEVEL 95%: 6.68"  "LEVEL 95%: -1.14"

        [1] "LEVEL 97.5%: 6.68"  "LEVEL 97.5%: -1.14"

        [1] "Phenomenology: 2; Response: 2"

        [1] "POSTERIOR MEAN: -5.08" "POSTERIOR MEAN: 0.23"

        [1] "LEVEL 2.5%: -5.08" "LEVEL 2.5%: 0.23"

        [1] "LEVEL 5%: -5.08" "LEVEL 5%: 0.23"

        [1] "LEVEL 50%: -5.08" "LEVEL 50%: 0.23"

        [1] "LEVEL 95%: -5.08" "LEVEL 95%: 0.23"

        [1] "LEVEL 97.5%: -5.08" "LEVEL 97.5%: 0.23"

        [1] "Phenomenology: 3; Response: 1"

```

```
[1] "POSTERIOR MEAN: -11.07" "POSTERIOR MEAN: 1.89"

[1] "LEVEL 2.5%: -11.08" "LEVEL 2.5%: 1.87"

[1] "LEVEL 5%: -11.08" "LEVEL 5%: 1.88"

[1] "LEVEL 50%: -11.07" "LEVEL 50%: 1.89"

[1] "LEVEL 95%: -11.06" "LEVEL 95%: 1.91"

[1] "LEVEL 97.5%: -11.06" "LEVEL 97.5%: 1.91"

[1] "Phenomenology: 3; Response: 2"

[1] "POSTERIOR MEAN: -8.64" "POSTERIOR MEAN: 1.71"

[1] "LEVEL 2.5%: -8.64" "LEVEL 2.5%: 1.7"

[1] "LEVEL 5%: -8.64" "LEVEL 5%: 1.7"

[1] "LEVEL 50%: -8.64" "LEVEL 50%: 1.71"

[1] "LEVEL 95%: -8.63" "LEVEL 95%: 1.72"

[1] "LEVEL 97.5%: -8.63" "LEVEL 97.5%: 1.72"

[1] "Phenomenology: 4; Response: 1"

[1] "POSTERIOR MEAN: -3.31" "POSTERIOR MEAN: 0.43"

[1] "LEVEL 2.5%: -3.39" "LEVEL 2.5%: 0.43"

[1] "LEVEL 5%: -3.38" "LEVEL 5%: 0.43"

[1] "LEVEL 50%: -3.31" "LEVEL 50%: 0.43"

[1] "LEVEL 95%: -3.24" "LEVEL 95%: 0.43"

[1] "LEVEL 97.5%: -3.23" "LEVEL 97.5%: 0.43"

[1] "Phenomenology: 4; Response: 2"

[1] "POSTERIOR MEAN: -2.37" "POSTERIOR MEAN: 0.28"

[1] "LEVEL 2.5%: -2.45" "LEVEL 2.5%: 0.27"
```

```
        [1] "LEVEL 5%: -2.43" "LEVEL 5%: 0.27"

        [1] "LEVEL 50%: -2.37" "LEVEL 50%: 0.28"

        [1] "LEVEL 95%: -2.31" "LEVEL 95%: 0.28"

        [1] "LEVEL 97.5%: -2.3" "LEVEL 97.5%: 0.28"

[1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

        [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

        [1] "POSTERIOR MEAN: -10.06" "POSTERIOR MEAN: -1.31"  "POSTERIOR MEAN: -1.44"
[4] "POSTERIOR MEAN: 3.5"    "POSTERIOR MEAN: 0.38"

        [1] "LEVEL 2.5%: -10.07" "LEVEL 2.5%: -1.31"  "LEVEL 2.5%: -1.47"
[4] "LEVEL 2.5%: 3.29"   "LEVEL 2.5%: 0.32"

        [1] "LEVEL 5%: -10.07" "LEVEL 5%: -1.31"  "LEVEL 5%: -1.46"  "LEVEL 5%: 3.32"
[5] "LEVEL 5%: 0.33"

        [1] "LEVEL 50%: -10.06" "LEVEL 50%: -1.31"  "LEVEL 50%: -1.44"
[4] "LEVEL 50%: 3.5"    "LEVEL 50%: 0.38"

        [1] "LEVEL 95%: -10.05" "LEVEL 95%: -1.31"  "LEVEL 95%: -1.41"
[4] "LEVEL 95%: 3.68"   "LEVEL 95%: 0.43"

        [1] "LEVEL 97.5%: -10.05" "LEVEL 97.5%: -1.31"  "LEVEL 97.5%: -1.4"
[4] "LEVEL 97.5%: 3.72"   "LEVEL 97.5%: 0.44"

        [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

        [1] "POSTERIOR MEAN: -1.5"  "POSTERIOR MEAN: -1.44" "POSTERIOR MEAN: -1.25"
[4] "POSTERIOR MEAN: 2.24"  "POSTERIOR MEAN: 0.6"

        [1] "LEVEL 2.5%: -1.52" "LEVEL 2.5%: -1.45" "LEVEL 2.5%: -1.28"
[4] "LEVEL 2.5%: 2.18"  "LEVEL 2.5%: 0.53"

        [1] "LEVEL 5%: -1.52" "LEVEL 5%: -1.45" "LEVEL 5%: -1.27" "LEVEL 5%: 2.19"
[5] "LEVEL 5%: 0.55"

        [1] "LEVEL 50%: -1.5"  "LEVEL 50%: -1.44" "LEVEL 50%: -1.25" "LEVEL 50%: 2.24"
[5] "LEVEL 50%: 0.6"
```

```
        [1] "LEVEL 95%: -1.49" "LEVEL 95%: -1.44" "LEVEL 95%: -1.23" "LEVEL 95%: 2.28"
[5] "LEVEL 95%: 0.67"

        [1] "LEVEL 97.5%: -1.49" "LEVEL 97.5%: -1.44" "LEVEL 97.5%: -1.22"
[4] "LEVEL 97.5%: 2.29"  "LEVEL 97.5%: 0.68"

        [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

        [1] "POSTERIOR MEAN: -11.48" "POSTERIOR MEAN: -1.09"  "POSTERIOR MEAN: -3.61"
[4] "POSTERIOR MEAN: 4.23"   "POSTERIOR MEAN: 0.15"

        [1] "LEVEL 2.5%: -11.51" "LEVEL 2.5%: -1.1"   "LEVEL 2.5%: -3.76"
[4] "LEVEL 2.5%: 3.65"   "LEVEL 2.5%: 0.09"

        [1] "LEVEL 5%: -11.5" "LEVEL 5%: -1.1"  "LEVEL 5%: -3.74" "LEVEL 5%: 3.73"
[5] "LEVEL 5%: 0.1"

        [1] "LEVEL 50%: -11.48" "LEVEL 50%: -1.09"  "LEVEL 50%: -3.6"
[4] "LEVEL 50%: 4.23"   "LEVEL 50%: 0.15"

        [1] "LEVEL 95%: -11.45" "LEVEL 95%: -1.09"  "LEVEL 95%: -3.49"
[4] "LEVEL 95%: 4.7"    "LEVEL 95%: 0.21"

        [1] "LEVEL 97.5%: -11.45" "LEVEL 97.5%: -1.09"  "LEVEL 97.5%: -3.46"
[4] "LEVEL 97.5%: 4.79"   "LEVEL 97.5%: 0.22"

        [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

        [1] "POSTERIOR MEAN: -2.13"   "POSTERIOR MEAN: -1.22"
[3] "POSTERIOR MEAN: -165.12" "POSTERIOR MEAN: 0.9"
[5] "POSTERIOR MEAN: -4.5"

        [1] "LEVEL 2.5%: -2.18"  "LEVEL 2.5%: -1.23"  "LEVEL 2.5%: -205.6"
[4] "LEVEL 2.5%: 0.85"   "LEVEL 2.5%: -4.74"

        [1] "LEVEL 5%: -2.17"   "LEVEL 5%: -1.22"   "LEVEL 5%: -200.61"
[4] "LEVEL 5%: 0.85"    "LEVEL 5%: -4.71"

        [1] "LEVEL 50%: -2.13"   "LEVEL 50%: -1.22"   "LEVEL 50%: -164.39"
[4] "LEVEL 50%: 0.9"     "LEVEL 50%: -4.5"

        [1] "LEVEL 95%: -2.1"    "LEVEL 95%: -1.22"   "LEVEL 95%: -131.19"
[4] "LEVEL 95%: 0.94"    "LEVEL 95%: -4.29"

        [1] "LEVEL 97.5%: -2.09"   "LEVEL 97.5%: -1.21"   "LEVEL 97.5%: -127.28"
```

```
[4] "LEVEL 97.5%: 0.94"    "LEVEL 97.5%: -4.27"

        [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

        [1] "POSTERIOR MEAN: -9.53" "POSTERIOR MEAN: -1.16" "POSTERIOR MEAN: -4.47"
[4] "POSTERIOR MEAN: 4.95"  "POSTERIOR MEAN: 0.34"

        [1] "LEVEL 2.5%: -9.54" "LEVEL 2.5%: -1.16" "LEVEL 2.5%: -4.51"
[4] "LEVEL 2.5%: 4.9"   "LEVEL 2.5%: 0.31"

        [1] "LEVEL 5%: -9.54" "LEVEL 5%: -1.16" "LEVEL 5%: -4.5"  "LEVEL 5%: 4.91"
[5] "LEVEL 5%: 0.32"

        [1] "LEVEL 50%: -9.53" "LEVEL 50%: -1.16" "LEVEL 50%: -4.47" "LEVEL 50%: 4.95"
[5] "LEVEL 50%: 0.34"

        [1] "LEVEL 95%: -9.51" "LEVEL 95%: -1.16" "LEVEL 95%: -4.43" "LEVEL 95%: 5"
[5] "LEVEL 95%: 0.36"

        [1] "LEVEL 97.5%: -9.51" "LEVEL 97.5%: -1.15" "LEVEL 97.5%: -4.42"
[4] "LEVEL 97.5%: 5.01"  "LEVEL 97.5%: 0.36"

        [1] "Phenomenology: 1; Emplacement: 3; Response: 2"

        [1] "POSTERIOR MEAN: -2.85" "POSTERIOR MEAN: -0.71" "POSTERIOR MEAN: -2.17"
[4] "POSTERIOR MEAN: 2.6"   "POSTERIOR MEAN: 0.09"

        [1] "LEVEL 2.5%: -2.88" "LEVEL 2.5%: -0.71" "LEVEL 2.5%: -2.38"
[4] "LEVEL 2.5%: 2.43"  "LEVEL 2.5%: -0.11"

        [1] "LEVEL 5%: -2.87" "LEVEL 5%: -0.71" "LEVEL 5%: -2.34" "LEVEL 5%: 2.45"
[5] "LEVEL 5%: -0.07"

        [1] "LEVEL 50%: -2.84" "LEVEL 50%: -0.71" "LEVEL 50%: -2.16" "LEVEL 50%: 2.61"
[5] "LEVEL 50%: 0.09"

        [1] "LEVEL 95%: -2.82" "LEVEL 95%: -0.7"  "LEVEL 95%: -2"    "LEVEL 95%: 2.75"
[5] "LEVEL 95%: 0.25"

        [1] "LEVEL 97.5%: -2.81" "LEVEL 97.5%: -0.7"  "LEVEL 97.5%: -1.97"
[4] "LEVEL 97.5%: 2.78"  "LEVEL 97.5%: 0.27"

        [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

        [1] "POSTERIOR MEAN: 3.87"
```

```
[1] "LEVEL 2.5%: 3.85"

[1] "LEVEL 5%: 3.85"

[1] "LEVEL 50%: 3.87"

[1] "LEVEL 95%: 3.89"

[1] "LEVEL 97.5%: 3.89"

[1] "Phenomenology: 2; Emplacement: 1; Response: 2"

[1] "POSTERIOR MEAN: -0.17"

[1] "LEVEL 2.5%: -0.19"

[1] "LEVEL 5%: -0.18"

[1] "LEVEL 50%: -0.17"

[1] "LEVEL 95%: -0.15"

[1] "LEVEL 97.5%: -0.14"

[1] "Phenomenology: 2; Emplacement: 2; Response: 1"

[1] "POSTERIOR MEAN: 3.11"

[1] "LEVEL 2.5%: 3.11"

[1] "LEVEL 5%: 3.11"

[1] "LEVEL 50%: 3.11"

[1] "LEVEL 95%: 3.12"

[1] "LEVEL 97.5%: 3.12"

[1] "Phenomenology: 2; Emplacement: 2; Response: 2"

[1] "POSTERIOR MEAN: -0.9"

[1] "LEVEL 2.5%: -0.95"
```

```
        [1] "LEVEL 5%: -0.94"

        [1] "LEVEL 50%: -0.9"

        [1] "LEVEL 95%: -0.86"

        [1] "LEVEL 97.5%: -0.85"

        [1] "Phenomenology: 2; Emplacement: 3; Response: 1"

        [1] "POSTERIOR MEAN: 2.16"

        [1] "LEVEL 2.5%: 2.14"

        [1] "LEVEL 5%: 2.14"

        [1] "LEVEL 50%: 2.16"

        [1] "LEVEL 95%: 2.17"

        [1] "LEVEL 97.5%: 2.17"

        [1] "Phenomenology: 2; Emplacement: 3; Response: 2"

        [1] "POSTERIOR MEAN: -0.94"

        [1] "LEVEL 2.5%: -0.99"

        [1] "LEVEL 5%: -0.98"

        [1] "LEVEL 50%: -0.94"

        [1] "LEVEL 95%: -0.91"

        [1] "LEVEL 97.5%: -0.9"

[1] "LEVEL 1 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] "POSTERIOR MEAN: 0.0012"

        [1] "LEVEL 2.5%: 0.001"

        [1] "LEVEL 5%: 0.001"
```

```
[1] "LEVEL 50%: 0.0012"
[1] "LEVEL 95%: 0.0014"
[1] "LEVEL 97.5%: 0.0014"
[1] "Phenomenology: 1; Response: 2"
[1] "POSTERIOR MEAN: 0.0017"
[1] "LEVEL 2.5%: 0.0014"
[1] "LEVEL 5%: 0.0014"
[1] "LEVEL 50%: 0.0017"
[1] "LEVEL 95%: 0.002"
[1] "LEVEL 97.5%: 0.0021"
[1] "Phenomenology: 2; Response: 1"
[1] "POSTERIOR MEAN: 0.0038"
[1] "LEVEL 2.5%: 0.0034"
[1] "LEVEL 5%: 0.0034"
[1] "LEVEL 50%: 0.0038"
[1] "LEVEL 95%: 0.0043"
[1] "LEVEL 97.5%: 0.0044"
[1] "Phenomenology: 2; Response: 2"
[1] "POSTERIOR MEAN: 0.0016"
[1] "LEVEL 2.5%: 0.0014"
[1] "LEVEL 5%: 0.0014"
[1] "LEVEL 50%: 0.0016"
```

```
        [1] "LEVEL 95%: 0.0018"

        [1] "LEVEL 97.5%: 0.0019"

[1] "LEVEL 2 VARIANCE COMPONENTS"

        [1] "Phenomenology: 1; Response: 1"

        [1] "POSTERIOR MEAN: 0.001"

        [1] "LEVEL 2.5%: 9e-04"

        [1] "LEVEL 5%: 9e-04"

        [1] "LEVEL 50%: 0.001"

        [1] "LEVEL 95%: 0.0011"

        [1] "LEVEL 97.5%: 0.0012"

        [1] "Phenomenology: 1; Response: 2"

        [1] "POSTERIOR MEAN: 0.001"

        [1] "LEVEL 2.5%: 9e-04"

        [1] "LEVEL 5%: 9e-04"

        [1] "LEVEL 50%: 0.001"

        [1] "LEVEL 95%: 0.001"

        [1] "LEVEL 97.5%: 0.001"

[1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"

[1] "Phenomenology 1"

[1] "POSTERIOR MEAN:"

[1] "Variances"

[1] 0.0021 0.0034

[1] "Correlations"
```

```
     [,1] [,2]
[1,]    1 0.27
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 2.5%: 0.002"  "LEVEL 2.5%: 0.0033"

[1] "Correlations"

        [1] "LEVEL 2.5%:"
             [,1] [,2]
[1,]    1 0.26
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 5%: 0.002"  "LEVEL 5%: 0.0033"

[1] "Correlations"

        [1] "LEVEL 5%:"
             [,1] [,2]
[1,]    1 0.26
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 50%: 0.0021" "LEVEL 50%: 0.0034"

[1] "Correlations"

        [1] "LEVEL 50%:"
             [,1] [,2]
[1,]    1 0.27
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 95%: 0.0021" "LEVEL 95%: 0.0035"

[1] "Correlations"

        [1] "LEVEL 95%:"
```

```
                [,1] [,2]
[1,]    1 0.29
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 97.5%: 0.0021" "LEVEL 97.5%: 0.0035"

[1] "Correlations"

        [1] "LEVEL 97.5%:"
             [,1] [,2]
[1,]    1 0.29
[2,]    0 1.00

[1] "Phenomenology 2"

[1] "POSTERIOR MEAN:"

[1] "Variances"

[1] 1e-03 3e-04

[1] "Correlations"

     [,1]  [,2]
[1,]    1 -0.25
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 2.5%: 0.001" "LEVEL 2.5%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 2.5%:"
             [,1]  [,2]
[1,]    1 -0.29
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 5%: 0.001" "LEVEL 5%: 3e-04"

[1] "Correlations"
```

```
        [1] "LEVEL 5%:"
             [,1]  [,2]
[1,]    1 -0.28
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 50%: 0.001" "LEVEL 50%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 50%:"
             [,1]  [,2]
[1,]    1 -0.26
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 95%:"
             [,1]  [,2]
[1,]    1 -0.22
[2,]    0  1.00

[1] "Variances"

        [1] "LEVEL 97.5%: 0.0011" "LEVEL 97.5%: 3e-04"

[1] "Correlations"

        [1] "LEVEL 97.5%:"
             [,1]  [,2]
[1,]    1 -0.22
[2,]    0  1.00

[1] "Phenomenology 3"

[1] "POSTERIOR MEAN:"

[1] "Variances"
```

```
[1] 9e-04 9e-04

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.91
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 2.5%: 8e-04" "LEVEL 2.5%: 7e-04"

[1] "Correlations"

        [1] "LEVEL 2.5%:"
             [,1] [,2]
[1,]    1 0.89
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 5%: 8e-04" "LEVEL 5%: 8e-04"

[1] "Correlations"

        [1] "LEVEL 5%:"
             [,1] [,2]
[1,]    1 0.89
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 50%: 9e-04" "LEVEL 50%: 9e-04"

[1] "Correlations"

        [1] "LEVEL 50%:"
             [,1] [,2]
[1,]    1 0.92
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 0.001"
```

```
[1] "Correlations"

         [1] "LEVEL 95%:"
              [,1] [,2]
[1,]    1 0.93
[2,]    0 1.00

[1] "Variances"

         [1] "LEVEL 97.5%: 0.0011" "LEVEL 97.5%: 0.001"

[1] "Correlations"

         [1] "LEVEL 97.5%:"
              [,1] [,2]
[1,]    1 0.93
[2,]    0 1.00

[1] "Phenomenology 4"

[1] "POSTERIOR MEAN:"

[1] "Variances"

[1] 0.0201 0.0071

[1] "Correlations"

     [,1] [,2]
[1,]    1 0.53
[2,]    0 1.00

[1] "Variances"

         [1] "LEVEL 2.5%: 0.0156" "LEVEL 2.5%: 0.0056"

[1] "Correlations"

         [1] "LEVEL 2.5%:"
              [,1] [,2]
[1,]    1  0.4
[2,]    0  1.0

[1] "Variances"
```

```
        [1] "LEVEL 5%: 0.0162" "LEVEL 5%: 0.0058"

[1] "Correlations"

        [1] "LEVEL 5%:"
             [,1] [,2]
[1,]    1 0.42
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 50%: 0.02"   "LEVEL 50%: 0.0071"

[1] "Correlations"

        [1] "LEVEL 50%:"
             [,1] [,2]
[1,]    1 0.53
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 95%: 0.0244" "LEVEL 95%: 0.0086"

[1] "Correlations"

        [1] "LEVEL 95%:"
             [,1] [,2]
[1,]    1 0.63
[2,]    0 1.00

[1] "Variances"

        [1] "LEVEL 97.5%: 0.0253" "LEVEL 97.5%: 0.0088"

[1] "Correlations"

        [1] "LEVEL 97.5%:"
             [,1] [,2]
[1,]    1 0.65
[2,]    0 1.00

[1] "FGSN PRIOR PARAMETERS"

[1] "POSTERIOR MEAN:"
```

```
[1] "Alpha = 17.32"
[1] "Lambda squared = 8.03"
[1] "Omega = -1.68" "Omega = 0.57"

[1] "Alpha:"
[1] "LEVEL 2.5%: 17.25"

[1] "LEVEL 5%: 17.26"

[1] "LEVEL 50%: 17.32"

[1] "LEVEL 95%: 17.38"

[1] "LEVEL 97.5%: 17.39"

[1] "Lambda squared:"
[1] "LEVEL 2.5%: 7.4"

[1] "LEVEL 5%: 7.51"

[1] "LEVEL 50%: 8.01"

[1] "LEVEL 95%: 8.57"

[1] "LEVEL 97.5%: 8.68"

[1] "Omega:"
[1] "LEVEL 2.5%: -1.93" "LEVEL 2.5%: 0.48"

[1] "LEVEL 5%: -1.9" "LEVEL 5%: 0.49"

[1] "LEVEL 50%: -1.68" "LEVEL 50%: 0.57"

[1] "LEVEL 95%: -1.46" "LEVEL 95%: 0.65"

[1] "LEVEL 97.5%: -1.41" "LEVEL 97.5%: 0.66"

[1] "DIC = -6086.65"

[1] "PIC = -6080.32"
```