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MultiPEM Toolbox: User Manual

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1 Introduction

This document explains use of the **Multi-Phenomenology Explosion Monitoring** (MultiPEM) 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 report¹ hereafter designated “WPA” for reference. Additional details on the application are found in a recent journal article². 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 imputation³. 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,

¹Williams, 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).

²Ford, 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.

³Plummer, 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 previously, 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<sup>4</sup>.

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.

---

<sup>4</sup>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 `pctype` 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 (`pctype` 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

$$\begin{aligned} \mathbf{E}_{S,11r} &= \begin{pmatrix} \mathbf{Z}_{11r,1} \\ \mathbf{Z}_{11r,2} \end{pmatrix} b_{1r,1}^{(S)} & \mathbf{E}_{P,11r} &= \begin{pmatrix} \mathbf{E}_{P,111r} \\ \mathbf{E}_{P,112r} \end{pmatrix} = \begin{bmatrix} \mathbf{Z}_{111r} & \mathbf{0}_2 \\ \mathbf{0}_5 & \mathbf{Z}_{112r} \end{bmatrix} \begin{pmatrix} b_{1r,11}^{(P)} \\ b_{1r,12}^{(P)} \end{pmatrix} \\ \mathbf{E}_{S,12r} &= \begin{pmatrix} \mathbf{Z}_{12r,1} \\ \mathbf{Z}_{12r,2} \\ \mathbf{Z}_{12r,3} \end{pmatrix} b_{1r,2}^{(S)} & \mathbf{E}_{P,12r} &= \begin{pmatrix} \mathbf{E}_{P,121r} \\ \mathbf{E}_{P,122r} \\ \mathbf{E}_{P,123r} \end{pmatrix} = \begin{bmatrix} \mathbf{Z}_{121r} & \mathbf{0}_4 & \mathbf{0}_4 \\ \mathbf{0}_3 & \mathbf{Z}_{122r} & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \mathbf{Z}_{123r} \end{bmatrix} \begin{pmatrix} b_{1r,21}^{(P)} \\ b_{1r,22}^{(P)} \\ b_{1r,23}^{(P)} \end{pmatrix}, \end{aligned}$$

where the default coefficient matrices are given by

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

for  $\mathbf{1}_q$  and  $\mathbf{0}_q$  the  $q$ -vectors of ones and zeros, respectively. The source and path random effects  $\{b_{1r,1}^{(S)}, b_{1r,2}^{(S)}\}$  and  $\{b_{1r,11}^{(P)}, b_{1r,12}^{(P)}, b_{1r,21}^{(P)}, b_{1r,22}^{(P)}, b_{1r,23}^{(P)}\}$  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 ( $\mathbf{E}_{P,11r}, \mathbf{E}_{P,12r}$ ) corresponding to the two sources above are replaced by the single path bias vector

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

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  $\{b_{1r,\{1,2\}1}^{(P)}, b_{1r,\{1,2\}2}^{(P)}, b_{1r,\{1,2\}3}^{(P)}\}$  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                                                                                                                             |
|---------------------|--------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <code>gdir</code>   | <code>none</code>  | directory location of global subroutines                                                                                                      |
| <code>adir</code>   | <code>none</code>  | directory location of application subroutines                                                                                                 |
| <code>rdir</code>   | <code>none</code>  | root directory location of data files                                                                                                         |
| <code>cdir</code>   | <code>none</code>  | directory locations (if relevant) and names of benchmark data files under <code>rdir</code>                                                   |
| <code>Rh</code>     | <code>none</code>  | vector with number of signatures for each phenomenology                                                                                       |
| <code>pbeta</code>  | <code>none</code>  | list containing empirical model common parameter counts by phenomenology                                                                      |
| <code>izmat</code>  | <code>FALSE</code> | user-provided code for computing variance component coefficient matrices                                                                      |
| <code>ieiv</code>   | <code>NULL</code>  | numerical identifier of phenomenologies utilizing errors-in-variables yields in analysis of benchmark data                                    |
| <code>seiv</code>   | <code>NULL</code>  | list containing identifiers of benchmark sources assigned errors-in-variables yields by phenomenology ( <code>ALL</code> – every source)      |
| <code>ewsd</code>   | <code>NULL</code>  | standard deviation of errors-in-variables Gaussian likelihood                                                                                 |
| <code>Th</code>     | <code>NULL</code>  | number of emplacement conditions for each phenomenology                                                                                       |
| <code>pbetat</code> | <code>NULL</code>  | list containing empirical model emplacement-dependent parameter counts by phenomenology                                                       |
| <code>ibetar</code> | <code>NULL</code>  | list containing locations of empirical model common parameters in full parameter vector by phenomenology                                      |
| <code>pvc_1</code>  | <code>NULL</code>  | list containing source variance component parameter counts by phenomenology                                                                   |
| <code>pvc_2</code>  | <code>NULL</code>  | list containing path variance component parameter counts by phenomenology                                                                     |
| <code>ptype</code>  | <code>NULL</code>  | list indicating treatment of path variance component parameter by phenomenology ( <code>Crossed</code> – common paths present across sources) |
| <code>cnames</code> | <code>NULL</code>  | 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  $\beta_{sr}$  is given as follows (WPA, §6.2, p. 11),

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

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  $\beta_{sr}$ , each element corresponding to each row of a matrix of covariates (having columns  $(w, h, \delta)$ ).

- 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  $\beta_{sr}$ , with rows corresponding to the rows of a matrix of covariates (having columns  $(w, h, \delta)$ ). If `eiv` is `TRUE` (Line 113 of Appendix A.1), the partial derivative of  $f_{sr}(\cdot)$  for log-yield  $w$  is also required,

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

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  $\beta_{sr}$ , 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                                                                                                                                                                      |
|-----------------------|-------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>p_cal</code>    | none        | environment storing all objects needed in log-likelihood calculations                                                                                                                  |
| <code>gdir</code>     | none        | directory location of global subroutines                                                                                                                                               |
| <code>adir</code>     | none        | directory location of application subroutines                                                                                                                                          |
| <code>f</code>        | none        | names of forward model functions for each signature by phenomenology                                                                                                                   |
| <code>nst</code>      | 10          | number of starting values for log-likelihood maximization                                                                                                                              |
| <code>ncor</code>     | 1           | number of cores for log-likelihood maximization                                                                                                                                        |
| <code>ci_lev</code>   | 0.95        | confidence interval levels for global forward model parameter inference                                                                                                                |
| <code>igrad</code>    | TRUE        | forward model Jacobian provided                                                                                                                                                        |
| <code>bfgs</code>     | TRUE        | log-likelihood maximization uses BFGS methods                                                                                                                                          |
| <code>igrck</code>    | TRUE        | conduct log-likelihood function gradient verification                                                                                                                                  |
| <code>g</code>        | NULL        | names of forward model Jacobian functions for each signature by phenomenology                                                                                                          |
| <code>iresp</code>    | NULL        | flags for modified calculation by signature in a common forward model for each relevant phenomenology                                                                                  |
| <code>fp_fm</code>    | NULL        | fixed inputs required by forward models                                                                                                                                                |
| <code>fopt_in</code>  | 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) |
| <code>Xst</code>      | NULL        | matrix of starting values for log-likelihood maximization if not generated by this function                                                                                            |
| <code>cst</code>      | NULL        | vector of starting values for global forward model parameters in log-likelihood maximization                                                                                           |
| <code>fopt_out</code> | NULL        | location to write output R data file with results of log-likelihood maximization                                                                                                       |
| <code>phen</code>     | NULL        | phenomenology number and type (if needed for postprocessing)                                                                                                                           |
| <code>pl</code>       | "multicore" | strategy for running parallel jobs using the <code>future</code> 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 gra-

dient function(s) for each signature. In this example, the *seismic* phenomenology utilizes a log-prior gradient function `lp_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,

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- 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  $\eta$  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<sup>5</sup> implemented in the R package `adaptMCMC`. `FME`

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<sup>5</sup>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<sup>6</sup> implemented in the R package FME. NUTS is the No-U-Turn Sampler of Hoffman and Gelman<sup>7</sup>. 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<sup>8</sup> (DIC) and the Predictive Information Criterion<sup>9</sup> (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.

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22:997-1008.

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

<sup>7</sup>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.

<sup>8</sup>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.

<sup>9</sup>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                                                                                                            |
|-----------------------|--------------------------|------------------------------------------------------------------------------------------------------------------------------|
| <code>p_cal</code>    | <code>none</code>        | environment storing all objects needed in log-posterior calculations                                                         |
| <code>gdir</code>     | <code>none</code>        | directory location of global subroutines                                                                                     |
| <code>adir</code>     | <code>none</code>        | directory location of application subroutines                                                                                |
| <code>nst</code>      | <code>10</code>          | number of starting values for log-posterior maximization                                                                     |
| <code>nburn</code>    | <code>10000</code>       | number of per core MCMC burn-in samples                                                                                      |
| <code>nmcmc</code>    | <code>20000</code>       | number of MCMC production samples                                                                                            |
| <code>nthin</code>    | <code>20</code>          | posterior sample thinning rate                                                                                               |
| <code>ncor_map</code> | <code>1</code>           | number of cores for log-posterior maximization                                                                               |
| <code>ncor_mc</code>  | <code>1</code>           | number of cores for generating parallel MCMC chains                                                                          |
| <code>igrad</code>    | <code>TRUE</code>        | forward model Jacobian provided                                                                                              |
| <code>igrck_pr</code> | <code>TRUE</code>        | conduct log-prior function gradient verification                                                                             |
| <code>igrck_po</code> | <code>TRUE</code>        | conduct log-posterior function gradient verification                                                                         |
| <code>bfgs</code>     | <code>TRUE</code>        | log-posterior maximization uses BFGS methods                                                                                 |
| <code>ibpr</code>     | <code>FALSE</code>       | prior density function(s) provided for signature within phenomenology forward model coefficients                             |
| <code>icpr</code>     | <code>FALSE</code>       | prior density function(s) provided for global forward model coefficients                                                     |
| <code>fpr.b</code>    | <code>NULL</code>        | location of functions computing log-prior density for signature within phenomenology forward model coefficients              |
| <code>fgpr.b</code>   | <code>NULL</code>        | location of functions computing gradients of log-prior density for signature within phenomenology forward model coefficients |
| <code>fpr.c</code>    | <code>NULL</code>        | location of functions computing log-prior density for global forward model coefficients                                      |
| <code>fgpr.c</code>   | <code>NULL</code>        | location of functions computing gradients of log-prior density for global forward model coefficients                         |
| <code>Xnom</code>     | <code>NULL</code>        | matrix of starting values for hyperparameters in log-posterior maximization if not generated by this function                |
| <code>imcmc</code>    | <code>"FME"</code>       | MCMC algorithm (current options: <code>"RAM"</code> , <code>"FME"</code> , <code>"NUTS"</code> )                             |
| <code>pl</code>       | <code>"multicore"</code> | strategy for running parallel jobs using the <code>future</code> 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,

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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<sup>10</sup> (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<sup>11</sup> (BIC) value based on benchmark data. Used for selecting among competing forward or error model specifications (WPA,

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<sup>10</sup>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.

<sup>11</sup>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;  $\mathbf{Alpha} = \mu$ ,  $\mathbf{Omega} = v$  (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;  $\text{Alpha} = \mu$ ,  $\text{Omega} = v$  (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  $\tau(\cdot)$  applied to transformed variables  $\tilde{\boldsymbol{\theta}}_0$  with the new event device parameters  $\boldsymbol{\theta}_0$  as its image,

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

- `j_tau`: Jacobian matrix of  $\tau(\cdot)$ ,

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

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`,

$$\log \text{abs}(\det(\mathbf{J}_\tau(\tilde{\boldsymbol{\theta}}_0)))$$

- `dlog_absdet_j_tau`: Gradient of the log absolute Jacobian determinant with respect to  $\tilde{\boldsymbol{\theta}}_0$
- `inv_tau`: Inverse function of  $\tau(\cdot)$

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  $\tilde{\boldsymbol{\theta}}_0 = (\tilde{w}, \tilde{h})$  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,

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- 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  $\theta_0$  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  $\theta_0$ . For relevant phenomenologies, parameter subsets are specified as integer vectors identifying the extracted elements of  $\theta_0$ . The forward models of all other phenomenologies depend on the full  $\theta_0$ . 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                                                                                    |
|---------------------|---------|------------------------------------------------------------------------------------------------------|
| <code>p_cal</code>  | none    | environment storing all objects needed in log-likelihood and log-posterior calculations              |
| <code>gdir</code>   | none    | directory location of global subroutines                                                             |
| <code>adir</code>   | none    | directory location of application subroutines                                                        |
| <code>rdir</code>   | none    | root directory location of data files                                                                |
| <code>ndir</code>   | none    | directory locations (if relevant) and names of new event data files under <code>rdir</code>          |
| <code>tnames</code> | none    | names of new event parameters                                                                        |
| <code>nimp</code>   | 1       | number of first stage imputation samples used in second stage new event parameter posterior sampling |
| <code>bopt</code>   | FALSE   | new event parameter bounds supplied to log-likelihood maximization                                   |
| <code>itr</code>    | FALSE   | bijective transform of new event parameters provided                                                 |
| <code>fp_tr</code>  | NULL    | fixed inputs to new event parameter transform                                                        |
| <code>tlb</code>    | NULL    | lower bounds for new event parameters                                                                |
| <code>tub</code>    | NULL    | upper bounds for new event parameters                                                                |
| <code>tsub</code>   | 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  $\theta_0$  previously) as their main argument. Forward model parameter values are passed in as fixed quantities. In this example, the *seismic* forward model  $f_{sr}^0(\cdot)$  as a function of the new event device parameters  $\theta_0 = (w, h)$  – for fixed parameters  $\beta_{sr}$  – is given by Equation (1). The function `f0_s` returns a vector of forward model calculations evaluated for the supplied value of  $\theta_0$  (fixed  $\beta_{sr}$  passed in as `params$beta`), each element corresponding to each row of a matrix of covariates (in this case, a column vector of ranges  $\delta$ ).

- 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  $\theta_0$  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  $\theta_0$ , for fixed parameters  $\beta_{sr}$ . 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  $\theta_0$  (fixed  $\beta_{sr}$  passed in as `params$beta`), with rows corresponding to the rows of a matrix of covariates (in this case, a column vector of ranges  $\delta$ ).

- 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                                                                                 |
|-----------------------|-------------|---------------------------------------------------------------------------------------------------|
| <code>p_cal</code>    | none        | environment storing all objects needed in log-likelihood calculations                             |
| <code>gdir</code>     | none        | directory location of global subroutines                                                          |
| <code>adir</code>     | none        | directory location of application subroutines                                                     |
| <code>f0</code>       | none        | names of forward model functions for each signature by phenomenology                              |
| <code>nst</code>      | 10          | number of starting values for log-likelihood maximization                                         |
| <code>ncor</code>     | 1           | number of cores for log-likelihood maximization                                                   |
| <code>ci_lev</code>   | 0.95        | confidence interval levels for new event parameter inference                                      |
| <code>igrad</code>    | TRUE        | forward model Jacobian provided                                                                   |
| <code>bfgs</code>     | TRUE        | log-likelihood maximization uses BFGS methods                                                     |
| <code>igrck</code>    | TRUE        | conduct log-likelihood function gradient verification                                             |
| <code>t_cal</code>    | NULL        | object required if bounds supplied to log-likelihood maximization                                 |
| <code>g0</code>       | NULL        | names of forward model Jacobian functions for each signature by phenomenology                     |
| <code>fopt_in</code>  | NULL        | location of input R data file providing an initial starting value for log-likelihood maximization |
| <code>Xst</code>      | NULL        | matrix of starting values for log-likelihood maximization if not generated by this function       |
| <code>tst</code>      | NULL        | vector of starting values for new event parameters in log-likelihood maximization                 |
| <code>fopt_out</code> | NULL        | location to write output R data file with results of log-likelihood maximization                  |
| <code>pl</code>       | "multicore" | strategy for running parallel jobs using the <b>future</b> 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<sup>12</sup> implemented in the R package `adaptMCMC`. `FME`

---

<sup>12</sup>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<sup>13</sup> implemented in the R package **FME**. **NUTS** is the No-U-Turn Sampler of Hoffman and Gelman<sup>14</sup>. 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<sup>15</sup>.

- 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 **nmc** (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.

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

<sup>14</sup>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.

<sup>15</sup>Golchi, S. and Loepky, 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                                                                                    |
|-----------------------|-------------|------------------------------------------------------------------------------------------------------|
| <code>p_cal</code>    | none        | environment storing all objects needed in log-posterior calculations                                 |
| <code>gdir</code>     | none        | directory location of global subroutines                                                             |
| <code>adir</code>     | none        | directory location of application subroutines                                                        |
| <code>nst</code>      | 10          | number of starting values for log-posterior maximization                                             |
| <code>nburn</code>    | 10000       | number of per core MCMC burn-in samples                                                              |
| <code>nmcmc</code>    | 20000       | number of MCMC production samples                                                                    |
| <code>nthin</code>    | 1           | posterior sample thinning rate per imputation, for multiple imputation                               |
| <code>ncor_map</code> | 1           | number of cores for log-posterior maximization                                                       |
| <code>ncor_mc</code>  | 1           | number of cores for multiple imputation, or for generating parallel MCMC chains if single imputation |
| <code>igrad</code>    | TRUE        | forward model Jacobian provided                                                                      |
| <code>igrck_pr</code> | TRUE        | conduct log-prior function gradient verification                                                     |
| <code>igrck_po</code> | TRUE        | conduct log-posterior function gradient verification                                                 |
| <code>bfgs</code>     | TRUE        | log-posterior maximization uses BFGS methods                                                         |
| <code>itpr</code>     | FALSE       | prior density function provided for new event parameters                                             |
| <code>fpr_t</code>    | NULL        | location of function computing log-prior density for new event parameters                            |
| <code>fgpr_t</code>   | NULL        | location of function computing gradients of log-prior density for new event parameters               |
| <code>imcmc</code>    | "FME"       | MCMC algorithm (current options: "RAM", "FME", "NUTS", "SMC")                                        |
| <code>pl</code>       | "multicore" | strategy for running parallel jobs using the <code>future</code> package                             |
| <code>ncor_smc</code> | NULL        | number of cores for inner parallelization of SMC code                                                |
| <code>lb_smc</code>   | NULL        | lower bounds of new event parameters for SMC sampling                                                |
| <code>ub_smc</code>   | NULL        | upper bounds of new event parameters for SMC sampling                                                |
| <code>t_cal</code>    | 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  $(\mathcal{I}_{\theta_0, \theta_0}^0)^{-1}$ ).
  - 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  $(\mathcal{I}_{\theta_0, \theta_0}^0)^{-1}$ ).
  - 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  $(\mathcal{I}_{\theta_0, \theta_0}^0)^{-1}$ ).
- 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$tmmap_0`: If `iBayes` is TRUE (Line 6 of Appendix A.7), maximum *a posteriori* estimate of transformed new event device parameters (i.e., on correct scale)
- `p_cal$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$tmmpi_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 `pctype` 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 (`pctype` 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

$$\begin{aligned}
\mathbf{E}_{S,11r} &= \begin{pmatrix} \mathbf{Z}_{11r,1} \\ \mathbf{Z}_{11r,2} \end{pmatrix} b_{1r,1}^{(S)} & \mathbf{E}_{P,11r} &= \begin{pmatrix} \mathbf{E}_{P,111r} \\ \mathbf{E}_{P,112r} \end{pmatrix} = \begin{bmatrix} \mathbf{Z}_{111r} & \mathbf{0}_2 \\ \mathbf{0}_5 & \mathbf{Z}_{112r} \end{bmatrix} \begin{pmatrix} b_{1r,11}^{(P)} \\ b_{1r,12}^{(P)} \end{pmatrix} \\
\mathbf{E}_{S,12r} &= \begin{pmatrix} \mathbf{Z}_{12r,1} \\ \mathbf{Z}_{12r,2} \\ \mathbf{Z}_{12r,3} \end{pmatrix} b_{1r,2}^{(S)} & \mathbf{E}_{P,12r} &= \begin{pmatrix} \mathbf{E}_{P,121r} \\ \mathbf{E}_{P,122r} \\ \mathbf{E}_{P,123r} \end{pmatrix} = \begin{bmatrix} \mathbf{Z}_{121r} & \mathbf{0}_4 & \mathbf{0}_4 \\ \mathbf{0}_3 & \mathbf{Z}_{122r} & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \mathbf{Z}_{123r} \end{bmatrix} \begin{pmatrix} b_{1r,21}^{(P)} \\ b_{1r,22}^{(P)} \\ b_{1r,23}^{(P)} \end{pmatrix},
\end{aligned}$$

where the default coefficient matrices are given by

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

for  $\mathbf{1}_q$  and  $\mathbf{0}_q$  the  $q$ -vectors of ones and zeros, respectively. The source and path random effects  $\{b_{1r,1}^{(S)}, b_{1r,2}^{(S)}\}$  and  $\{b_{1r,11}^{(P)}, b_{1r,12}^{(P)}, b_{1r,21}^{(P)}, b_{1r,22}^{(P)}, b_{1r,23}^{(P)}\}$  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 ( $\mathbf{E}_{P,11r}, \mathbf{E}_{P,12r}$ ) corresponding to the two sources above are replaced by the single path bias vector

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

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  $\{b_{1r,\{1,2\}1}^{(P)}, b_{1r,\{1,2\}2}^{(P)}, b_{1r,\{1,2\}3}^{(P)}\}$  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  $\tau(\cdot)$  applied to transformed variables  $\tilde{\theta}_0$  with the new event device parameters  $\theta_0$  as its image,

$$\theta_0 = \tau(\tilde{\theta}_0)$$

- \* `j_tau`: Jacobian matrix of  $\tau(\cdot)$ ,

$$\mathbf{J}_\tau(\tilde{\theta}_0) = \begin{bmatrix} \frac{\partial \tau_1(\tilde{\theta}_0)}{\partial \tilde{\theta}_{0,1}} & \dots & \frac{\partial \tau_1(\tilde{\theta}_0)}{\partial \tilde{\theta}_{0,q}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \tau_q(\tilde{\theta}_0)}{\partial \tilde{\theta}_{0,1}} & \dots & \frac{\partial \tau_q(\tilde{\theta}_0)}{\partial \tilde{\theta}_{0,q}} \end{bmatrix}$$

where  $q$  is the dimension of  $\theta_0$ .

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

$$\log \text{abs}(\det(\mathbf{J}_\tau(\tilde{\theta}_0)))$$

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

- \* `inv_tau`: Inverse function of  $\tau(\cdot)$

In this example, the new event device parameters of inferential interest are log-yield  $w$  and height-of-burst  $h$ , that is  $\theta_0 = (w, h)$ . 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  $\tilde{\theta}_0 = (\tilde{w}, \tilde{h})$  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  $\theta_0$  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  $\theta_0$ . For relevant phenomenologies, parameter subsets are specified as integer vectors identifying the extracted elements of  $\theta_0$ . The forward models of all other phenomenologies depend on the full  $\theta_0$ . 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                                                                                                                       |
|---------------|---------|-----------------------------------------------------------------------------------------------------------------------------------------|
| <b>gdir</b>   | none    | directory location of global subroutines                                                                                                |
| <b>adir</b>   | none    | directory location of application subroutines                                                                                           |
| <b>rdir</b>   | none    | root directory location of data files                                                                                                   |
| <b>cdir</b>   | none    | directory locations (if relevant) and names of benchmark data files under <b>rdir</b>                                                   |
| <b>Rh</b>     | none    | vector with number of signatures for each phenomenology                                                                                 |
| <b>pbeta</b>  | none    | list containing empirical model common parameter counts by phenomenology                                                                |
| <b>bopt</b>   | FALSE   | parameter bounds supplied to log-likelihood maximization (currently implemented only for new event parameters)                          |
| <b>nev</b>    | FALSE   | analysis of new event                                                                                                                   |
| <b>itr</b>    | FALSE   | bijective transform of new event parameters provided                                                                                    |
| <b>izmat</b>  | FALSE   | user-provided code for computing variance component coefficient matrices                                                                |
| <b>ieiv</b>   | NULL    | numerical identifier of phenomenologies utilizing errors-in-variables yields in analysis of benchmark data                              |
| <b>seiv</b>   | NULL    | list containing identifiers of benchmark sources assigned errors-in-variables yields by phenomenology ( <b>ALL</b> – every source)      |
| <b>ewsd</b>   | NULL    | standard deviation of errors-in-variables Gaussian likelihood                                                                           |
| <b>Th</b>     | NULL    | number of emplacement conditions for each phenomenology                                                                                 |
| <b>pbetat</b> | NULL    | list containing empirical model emplacement-dependent parameter counts by phenomenology                                                 |
| <b>ibetar</b> | NULL    | list containing locations of empirical model common parameters in full parameter vector by phenomenology                                |
| <b>pvc_1</b>  | NULL    | list containing source variance component parameter counts by phenomenology                                                             |
| <b>pvc_2</b>  | NULL    | list containing path variance component parameter counts by phenomenology                                                               |
| <b>pptype</b> | NULL    | list indicating treatment of path variance component parameter by phenomenology ( <b>Crossed</b> – common paths present across sources) |
| <b>tnames</b> | NULL    | names of new event parameters                                                                                                           |
| <b>cnames</b> | NULL    | names of global forward model parameters                                                                                                |
| <b>fp_tr</b>  | NULL    | fixed inputs to new event parameter transform                                                                                           |
| <b>tlb</b>    | NULL    | lower bounds for new event parameters                                                                                                   |
| <b>tub</b>    | NULL    | upper bounds for new event parameters                                                                                                   |
| <b>ndir</b>   | NULL    | directory locations (if relevant) and names of new event data files under <b>rdir</b>                                                   |
| <b>tsub</b>   | 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  $\beta_{sr}$  and device parameters log-yield ( $w$ ) and HOB/DOB ( $h$ ) is given as follows (WPA, §6.2, p. 11),

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

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  $\delta$ . The function `f_s` returns a vector of forward model calculations evaluated for the supplied value of  $(\beta_{sr}, (w, h))$ , each element corresponding to each row of a matrix of covariates (in this case, a column vector of ranges  $\delta$ ).

- 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,



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,

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

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  $(\beta_{sr}, (w, h))$ , with rows corresponding to the rows of a matrix of covariates (in this case, a column vector of ranges  $\delta$ ). 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  $(\beta_{sr}, (w, h))$ , 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                                                                                                                                                                      |
|-----------------------|-------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>p_cal</code>    | none        | environment storing all objects needed in log-likelihood calculations                                                                                                                  |
| <code>gdir</code>     | none        | directory location of global subroutines                                                                                                                                               |
| <code>adir</code>     | none        | directory location of application subroutines                                                                                                                                          |
| <code>f</code>        | none        | names of forward model functions for each signature by phenomenology                                                                                                                   |
| <code>nst</code>      | 10          | number of starting values for log-likelihood maximization                                                                                                                              |
| <code>ncor</code>     | 1           | number of cores for log-likelihood maximization                                                                                                                                        |
| <code>ci_lev</code>   | 0.95        | confidence interval levels for global forward model and new event parameter inference                                                                                                  |
| <code>igrad</code>    | TRUE        | forward model Jacobian provided                                                                                                                                                        |
| <code>bfgs</code>     | TRUE        | log-likelihood maximization uses BFGS methods                                                                                                                                          |
| <code>igrck</code>    | TRUE        | conduct log-likelihood function gradient verification                                                                                                                                  |
| <code>t_cal</code>    | NULL        | object required if bounds supplied to log-likelihood maximization                                                                                                                      |
| <code>g</code>        | NULL        | names of forward model Jacobian functions for each signature by phenomenology                                                                                                          |
| <code>iresp</code>    | NULL        | flags for modified calculation by signature in a common forward model for each relevant phenomenology                                                                                  |
| <code>fp_fm</code>    | NULL        | fixed inputs required by forward models                                                                                                                                                |
| <code>fopt_in</code>  | 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) |
| <code>Xst</code>      | NULL        | matrix of starting values for log-likelihood maximization if not generated by this function                                                                                            |
| <code>tst</code>      | NULL        | vector of starting values for new event parameters in log-likelihood maximization                                                                                                      |
| <code>cst</code>      | NULL        | vector of starting values for global forward model parameters in log-likelihood maximization                                                                                           |
| <code>fopt_out</code> | NULL        | location to write output R data file with results of log-likelihood maximization                                                                                                       |
| <code>phen</code>     | NULL        | phenomenology number and type (if needed for postprocessing)                                                                                                                           |
| <code>pl</code>       | "multicore" | strategy for running parallel jobs using the <code>future</code> 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  $\eta$  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<sup>16</sup> implemented in the R package `adaptMCMC`. `FME` is the delayed rejection adaptive Metropolis algorithm of Haario, Laine, and Mira<sup>17</sup> implemented in the R package `FME`. `NUTS` is the No-U-Turn Sampler of Hoffman and Gelman<sup>18</sup>. 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<sup>19</sup> (DIC) and the Predictive Information Criterion<sup>20</sup> (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

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

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

<sup>18</sup>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.

<sup>19</sup>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.

<sup>20</sup>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                                                                                             |
|-----------------------|-------------|---------------------------------------------------------------------------------------------------------------|
| <code>p_cal</code>    | none        | environment storing all objects needed in log-posterior calculations                                          |
| <code>gdir</code>     | none        | directory location of global subroutines                                                                      |
| <code>adir</code>     | none        | directory location of application subroutines                                                                 |
| <code>nst</code>      | 10          | number of starting values for log-posterior maximization                                                      |
| <code>nburn</code>    | 10000       | number of per core MCMC burn-in samples                                                                       |
| <code>nmcmc</code>    | 20000       | number of MCMC production samples                                                                             |
| <code>nthin</code>    | 20          | posterior sample thinning rate                                                                                |
| <code>ncor_map</code> | 1           | number of cores for log-posterior maximization                                                                |
| <code>ncor_mc</code>  | 1           | number of cores for generating parallel MCMC chains                                                           |
| <code>igrad</code>    | TRUE        | forward model Jacobian provided                                                                               |
| <code>igrck_pr</code> | TRUE        | conduct log-prior function gradient verification                                                              |
| <code>igrck_po</code> | TRUE        | conduct log-posterior function gradient verification                                                          |
| <code>bfgs</code>     | TRUE        | log-posterior maximization uses BFGS methods                                                                  |
| <code>ibpr</code>     | FALSE       | prior density function(s) provided for forward model coefficients                                             |
| <code>icpr</code>     | FALSE       | prior density function(s) provided for global forward model coefficients                                      |
| <code>itpr</code>     | FALSE       | prior density function provided for new event parameters                                                      |
| <code>fpr_b</code>    | NULL        | location of functions computing log-prior density for forward model coefficients                              |
| <code>fgpr_b</code>   | NULL        | location of functions computing gradients of log-prior density for forward model coefficients                 |
| <code>fpr_c</code>    | NULL        | location of functions computing log-prior density for global forward model coefficients                       |
| <code>fgpr_c</code>   | NULL        | location of functions computing gradients of log-prior density for global forward model coefficients          |
| <code>fpr_t</code>    | NULL        | location of function computing log-prior density for new event parameters                                     |
| <code>fgpr_t</code>   | NULL        | location of function computing gradients of log-prior density for new event parameters                        |
| <code>Xnom</code>     | NULL        | matrix of starting values for hyperparameters in log-posterior maximization if not generated by this function |
| <code>imcmc</code>    | "FME"       | MCMC algorithm (current options: "RAM", "FME", "NUTS")                                                        |
| <code>pl</code>       | "multicore" | strategy for running parallel jobs using the <code>future</code> package                                      |
| <code>t_cal</code>    | 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<sup>21</sup> (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<sup>22</sup> (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.

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<sup>21</sup>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.

<sup>22</sup>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` =  $v$  (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;  $\text{Alpha} = \mu$ ,  $\text{Omega} = v$  (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$tmmap_0`: If `iBayes` is `TRUE` (Line 6 of Appendix B.3), maximum *a posteriori* estimate of transformed new event device parameters (i.e., on correct scale)
- `p_cal$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$tmmpi_0`: If `iBayes` is `TRUE` (Line 6 of Appendix B.3), posterior samples of transformed new event device parameters (i.e., on correct scale)
- `p_cal$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

```
1 #####
2 #
3 # This file is the input deck for MultiPEM Toolbox estimation of
4 # forward and error model parameters based on calibration data.
5 #
6 #####
7
8 #
9 # REQUIRED R PACKAGES
10 #
11
12 require(Matrix)
13
14 #
15 # END REQUIRED R PACKAGES
16 #
17
18 #
19 # PREPROCESSING
20 #
21
22 # Specify directory for general subroutines
23 gen_dir = "../..../Code"
24
25 # Source supporting R function
26 source(paste(gen_dir,"/prepro_cal.r",sep=""))
27
28 # Specify directory for application subroutines
29 app_dir = "../..../Code"
30
31 # Specify root data directory
32 dat_dir = "../..../Data"
33
34 # Specify calibration data directories
35 dat_cal = c("seismic_cal.csv",
36 "acoustic_cal.csv",
37 "optical_cal.csv",
38 "crater_cal.csv")
39
```

```

40 # Phenomenologies for this analysis
41 # 1 - seismic
42 # 2 - acoustic
43 # 3 - optical
44 # 4 - crater (surface effects)
45
46 # Indicate presence of calibration inference parameters
47 calp = FALSE
48
49 if(calp){
50 # Names of calibration inference parameters
51 #cal_par_names =
52 } else { cal_par_names = NULL }
53
54 # Specify number of responses for each phenomenology
55 Rh = c(2,2,2,2)
56
57 # Empirical model parameter count: common
58 # list with elements corresponding to phenomenologies
59 pbeta = vector("list",length(Rh))
60 for(hh in 1:length(Rh)){ pbeta[[hh]] = numeric(Rh[hh]) }
61 # phenomenology 2
62 pbeta[[2]] = c(2,2)
63 # phenomenology 3
64 pbeta[[3]] = c(2,2)
65 # phenomenology 4
66 pbeta[[4]] = c(2,2)
67
68 # Specify number of emplacement conditions for each phenomenology
69 Th = TRUE
70
71 if(Th){ Th = c(3,3,0,0)
72 } else { Th = NULL }
73
74 # Empirical model parameter count: emplacement condition
75 # list with elements corresponding to phenomenologies
76 if(!is.null(Th)){
77 pbetat = vector("list",length(Rh))
78 for(hh in 1:length(Rh)){
79 if(Th[hh] > 1){ pbetat[[hh]] = vector("list",Th[hh]) }
80 }
81 # phenomenology 1
82 for(tt in 1:Th[1]){
83 pbetat[[1]][[tt]] = numeric(Rh[1])
84 pbetat[[1]][[tt]] = c(5,5)

```

```

85 }
86 # phenomenology 2
87 for(tt in 1:Th[2]){
88 pbetat[[2]][[tt]] = numeric(Rh[2])
89 pbetat[[2]][[tt]] = c(1,1)
90 }
91 } else { pbetat = NULL }
92
93 # Locations of common parameters in full parameter vector
94 # list with elements corresponding to phenomenologies
95 if(!is.null(Th)){
96 ibetar = vector("list",length(Rh))
97 for(hh in 1:length(Rh)){
98 if(Th[hh] > 1){
99 # lists with elements for each response within
100 # emplacement condition
101 ibetar[[hh]] = vector("list",Th[hh]*Rh[hh])
102 }
103 }
104 # phenomenology 2
105 for(tt in 1:Th[2]){
106 for(rr in 1:Rh[2]){
107 ibetar[[2]][[(tt-1)*Rh[2]+rr]] = 1:2
108 }
109 }
110 } else { ibetar = NULL }
111
112 # Indicate analysis with errors-in-variables (eiv)
113 eiv = TRUE
114
115 # Specifications for errors-in-variables
116 if(eiv){
117 # Specify phenomenologies utilizing
118 # errors-in-variables yields
119 ieiv = 3:4
120
121 # Errors-in-variables source lists by
122 # phenomenology
123 seiv = vector("list",length(Rh))
124 for(hh in ieiv){ seiv[[hh]] = "ALL" }
125
126 # Set standard deviation of eiv Gaussian likelihood
127 eiv_w_sd = 0.1/3
128 } else {
129 ieiv = NULL

```



```

130 seiv = NULL
131 eiv_w_sd = NULL
132 }
133
134 # Specify Error Model
135 # Level 1 variance component parameter count
136 pvc_1 = TRUE
137
138 if(pvc_1){
139 pvc_1 = vector("list",length(Rh))
140 for(hh in 1:length(Rh)){ pvc_1[[hh]] = numeric(Rh[hh]) }
141 # phenomenology 1
142 pvc_1[[1]] = c(1,1)
143 # phenomenology 2
144 pvc_1[[2]] = c(1,1)
145 } else { pvc_1 = NULL }
146
147 # Level 2 variance component parameter count
148 pvc_2 = TRUE
149
150 if(pvc_2){
151 pvc_2 = vector("list",length(Rh))
152 for(hh in 1:length(Rh)){ pvc_2[[hh]] = numeric(Rh[hh]) }
153 # phenomenology 1
154 pvc_2[[1]] = c(1,1)
155 # phenomenology 2
156 #pvc_2[[2]] =
157
158 # path error models by phenomenology
159 ptype = vector("list",length(Rh))
160 # phenomenology 1
161 #ptype[[1]] =
162 } else { pvc_2 = NULL; ptype = NULL; }
163
164 # Set flag for user-provided code to calculate variance
165 # component coefficient matrices
166 calc_Z = FALSE
167
168 # Preprocessing for statistical analysis routines
169 p_cal = prepro_cal(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,
170 izmat=calc_Z,ieiv=ieiv,seiv=seiv,ewsd=eiv_w_sd,
171 Th=Th,pbetat=pbetat,ibetar=ibetar,pvc_1=pvc_1,
172 pvc_2=pvc_2,ptype=ptype,cnames=cal_par_names)
173 save.image()
174

```

```
175 #
176 # END PREPROCESSING
177 #
```

## A.2 Benchmark Data: Maximum Likelihood Estimation

```
1 #
2 # MAXIMUM LIKELIHOOD CALCULATION
3 #
4
5 # Source supporting R function
6 source(paste(gen_dir,"/calc_mle_cal.r",sep=""))
7
8 # Set seed for repeatability of analysis
9 set.seed(621)
10
11 # Names of forward models for each response
12 # by phenomenology
13 fm = vector("list",length(Rh))
14 fm[[1]] = c("f_s","f_s")
15 fm[[2]] = c("f_a","f_a")
16 fm[[3]] = c("f_o","f_o")
17 fm[[4]] = c("f_c","f_c")
18
19 # Indicate if forward model gradients provided
20 igrad = TRUE
21
22 if(igrad){
23 # Names of forward model gradients for each response
24 # by phenomenology
25 gfm = vector("list",length(Rh))
26 gfm[[1]] = c("g_s","g_s")
27 gfm[[2]] = c("g_a","g_a")
28 gfm[[3]] = c("g_o","g_o")
29 gfm[[4]] = c("g_c","g_c")
30 } else { gfm = NULL }
31
32 # Specifications for forward model calculations
33 # a) flags for modified forward model calculation by
34 # response for each relevant phenomenology
35 iResponse = TRUE
36
37 if(iResponse){
38 iResponse = vector("list",length(Rh))
39 iResponse[[1]] = c(TRUE,FALSE)
40 iResponse[[2]] = c(TRUE,FALSE)
41 } else { iResponse = NULL }
42
43 # b) fixed quantities required by forward models
```

```

44 fPars = TRUE
45
46 if(fPars){
47 fPars = vector("list",length(Rh))
48 fPars[[1]]$yield_scaling = 1/3
49 fPars[[2]]$yield_scaling = 1/3
50 fPars[[2]]$pressure_scaling = 1/3
51 fPars[[2]]$temp_scaling = 1/2
52 fPars[[3]]$yield_scaling = 1/3
53 fPars[[3]]$pressure_scaling = 1/3
54 fPars[[3]]$temp_scaling = 1/2
55 } else { fPars = NULL }
56
57 # Specify number of starting values for optimization
58 nstart = 10
59
60 # number of cores to use for optimization
61 ncores_mle = 1
62
63 # Indicate use of BFGS optimization methods
64 bfgs = TRUE
65
66 # Location of R data files with starting values
67 # for input to MLE optimization
68 opt_files_in = c("../Opt/opt_1_0.RData",
69 "../Opt/opt_2_0.RData",
70 "../Opt/opt_3_eiv_0.RData",
71 "../Opt/opt_4_eiv_0.RData")
72
73 # Location of R data file to write the results of
74 # MLE optimization
75 opt_files_out = "../opt.RData"
76
77 if(calp){
78 # Initial start value for calibration inference parameters
79 cst = FALSE
80
81 if(cst){
82 cst = numeric(p_cal$ncalp)
83 #cst[1] =
84 } else { cst = NULL }
85
86 # Confidence interval levels for calibration parameter inference
87 ci_lev = 0.95
88 } else {

```

```

89 cst = NULL
90 ci_lev = NULL
91 }
92
93 # Indicate phenomenology number and type (if needed
94 # for postprocessing)
95 Phen = TRUE
96
97 if(Phen){
98 Phen = matrix(c(1,"Seismic"),nrow=1)
99 } else { Phen = NULL }
100
101 # Indicator of MLE gradient check
102 mle_grad_ck = TRUE
103
104 # Strategy for running parallel jobs (future package)
105 parallel_plan = "multicore"
106
107 # MLE calculations
108 p_cal = calc_mle_cal(p_cal,gen_dir,app_dir,fm,nst=nstart,
109 ncor=ncores_mle,ci_lev=ci_lev,igrad=igrad,
110 bfgs=bfgs,igrck=mle_grad_ck,g=gfm,iresp=iResponse,
111 fp_fm=fPars,fopt_in=opt_files_in,Xst=NULL,
112 cst=cst,fopt_out=opt_files_out,phen=Phen,
113 pl=parallel_plan)
114 save.image()
115
116 #
117 # END MAXIMUM LIKELIHOOD CALCULATION
118 #

```

### A.3 Benchmark Data: Bayesian Analysis

```
1 #
2 # BAYESIAN ANALYSIS
3 #
4
5 # Specify if Bayesian analysis is to be conducted
6 iBayes = FALSE
7
8 if(iBayes){
9 # Source supporting R function
10 source(paste(gen_dir,"/calc_bayes_cal.r",sep=""))
11
12 # Indicator of prior distribution for forward model
13 # coefficients
14 iBetaPrior = TRUE
15
16 if(iBetaPrior){
17 # location of code for computing log-prior densities and gradients
18 prior_files_beta = "../Code/lp_beta_s.r"
19 if(igrad){
20 gr_prior_files_beta = "../Code/glp_beta_s.r"
21 } else { gr_prior_files_beta = NULL }
22
23 # prior distribution for phenomenology 1
24 # forward model coefficients
25 p_cal$h[[1]]$lp_betat = vector("list",Th[1])
26 for(tt in 1:Th[1]){
27 p_cal$h[[1]]$lp_betat[[tt]]$f = c("lp_s","lp_s")
28 if(igrad){
29 p_cal$h[[1]]$lp_betat[[tt]]$g = c("lq_s","lq_s")
30 }
31 }
32 } else {
33 prior_files_beta = NULL
34 gr_prior_files_beta = NULL
35 }
36
37 # Indicator of prior distribution for calibration parameters
38 iCalPrior = FALSE
39
40 if(calp && iCalPrior){
41 # location of code for computing log-prior densities and gradients
42 prior_files_calp = NULL
43 if(igrad){
```

```

44 gr_prior_files_calp = NULL
45 } else { gr_prior_files_calp = NULL }
46
47 # prior distribution for calibration parameters (calp)
48 p_callp_calpf = "lp_c"
49 if(igrad){ p_callp_calpg = "lq_c" }
50
51 # parameters for calibration parameter prior distribution
52 #p_cal$pi_c_mu =
53 #p_cal$pi_c_sd =
54 } else {
55 prior_files_calp = NULL
56 gr_prior_files_calp = NULL
57 }
58
59 # fixed scale parameters for variance component prior
60 # comment out if these parameters should vary
61 p_cal$A = 20
62
63 # eta parameter in Lewandowski-Kurowicka-Joe (LKJ) prior
64 # distribution for correlation parameters
65 p_callp_correta = 1
66
67 # FGSN parameters for errors-in-variables yields prior
68 # number of components
69 p_cal$K = 0
70 # total number of FGSN parameters
71 p_cal$p_fgsn = 0
72 if(eiv){
73 p_cal$K = 2
74 p_cal$p_fgsn = p_cal$K + 2
75 }
76
77 # specify Markov chain Monte Carlo (MCMC) algorithm
78 # options: "RAM", "FME", or "NUTS"
79 iMCMC = "FME"
80
81 # burn-in
82 nburn = 10000
83
84 # production
85 nmcmc = 20000
86
87 # posterior sample thinning rate
88 nthin = 20

```

```

89
90 # number of cores to use for optimization
91 ncores_map = 1
92
93 # number of cores to use for generating parallel MCMC chains
94 ncores_mc = 1
95
96 # Indicator of prior gradient check
97 prior_grad_ck = TRUE
98
99 # Indicator of posterior gradient check
100 post_grad_ck = TRUE
101
102 # Bayesian calculations
103 p_cal = calc_bayes_cal(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
104 nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
105 ncor_mc=ncores_mc,igrad=igrad,
106 igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
107 bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
108 fpr_b=prior_files_beta,
109 fgpr_b=gr_prior_files_beta,
110 fpr_c=prior_files_calp,
111 fgpr_c=gr_prior_files_calp,
112 Xnom=NULL,imcmc=iMCMC,pl=parallel_plan)
113 save.image()
114 }
115
116 #
117 # END BAYESIAN ANALYSIS
118 #

```



## A.4 Benchmark Data: Output File

```

1 > # Preprocessing for statistical analysis routines
2 > p_cal = prepro_cal(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,
3 + izmat=calc_Z,ieiv=ieiv,seiv=seiv,ewsd=eiv_w_sd,
4 + Th=Th,pbetat=pbetat,ibetar=ibetar,pvc_1=pvc_1,
5 + pvc_2=pvc_2,ptype=ptype,cnames=cal_par_names)
6 [1] "Warning: Insufficient Paths for Level 2 Variance Component models with
7 Phenomenology 2 and Response 1."
8 [1] "Warning: Insufficient Paths for Level 2 Variance Component models with
9 Phenomenology 2 and Response 2."
10 [1] "Warning: Insufficient number of observations per Source for Variance
11 Component models with Phenomenology 3 and Response 1."
12 [1] "Warning: Insufficient number of observations per Source for Variance
13 Component models with Phenomenology 3 and Response 2."
14 [1] "Warning: Insufficient number of observations per Source for Variance
15 Component models with Phenomenology 4 and Response 1."
16 [1] "Warning: Insufficient number of observations per Source for Variance
17 Component models with Phenomenology 4 and Response 2."
18
19 > # MLE calculations
20 > p_cal = calc_mle_cal(p_cal,gen_dir,app_dir,fm,nst=nstart,
21 + ncor=ncores_mle,ci_lev=ci_lev,igrad=igrad,
22 + bfgs=bfgs,igrck=mle_grad_ck,g=gfm,iresp=iResponse,
23 + fp_fm=fPars,fopt_in=opt_files_in,Xst=NULL,
24 + cst=cst,fopt_out=opt_files_out,phen=Phen,
25 + pl=parallel_plan)
26 [1] "MLE CONVERGENCE STATUS"
27
28 [1] 0
29 [1] 2
30 [1] "MAXIMUM LIKELIHOOD SUMMARY"
31
32 [1] "ERRORS-IN-VARIABLES YIELDS"
33
34 7 8 9 10 11 13 14 16 17 20 21 22 23
35 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
36 24 25 28 29 30 31 33 34 35 36 37 38 39
37 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
38
39 [1] "COMMON COEFFICIENTS"
40
41 [1] "Phenomenology: 2; Response: 1"
42
43 [1] 6.67 -1.14

```

```

44
45 [1] "Phenomenology: 2; Response: 2"
46
47 [1] -5.08 0.23
48
49 [1] "Phenomenology: 3; Response: 1"
50
51 [1] -11.07 1.89
52
53 [1] "Phenomenology: 3; Response: 2"
54
55 [1] -8.64 1.72
56
57 [1] "Phenomenology: 4; Response: 1"
58
59 [1] -3.34 0.43
60
61 [1] "Phenomenology: 4; Response: 2"
62
63 [1] -2.64 0.29
64
65 [1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"
66
67 [1] "Phenomenology: 1; Emplacement: 1; Response: 1"
68
69 [1] -10.07 -1.31 -1.43 3.52 0.39
70
71 [1] "Phenomenology: 1; Emplacement: 1; Response: 2"
72
73 [1] -1.52 -1.44 -1.23 2.31 0.65
74
75 [1] "Phenomenology: 1; Emplacement: 2; Response: 1"
76
77 [1] -11.48 -1.09 -3.59 4.32 0.16
78
79 [1] "Phenomenology: 1; Emplacement: 2; Response: 2"
80
81 [1] -2.33 -1.22 -7.78 1.32 -1.36
82
83 [1] "Phenomenology: 1; Emplacement: 3; Response: 1"
84
85 [1] -9.53 -1.16 -4.47 4.95 0.34
86
87 [1] "Phenomenology: 1; Emplacement: 3; Response: 2"
88

```

```

89 [1] -2.85 -0.71 -2.11 2.68 0.13
90
91 [1] "Phenomenology: 2; Emplacement: 1; Response: 1"
92
93 [1] 3.87
94
95 [1] "Phenomenology: 2; Emplacement: 1; Response: 2"
96
97 [1] -0.17
98
99 [1] "Phenomenology: 2; Emplacement: 2; Response: 1"
100
101 [1] 3.11
102
103 [1] "Phenomenology: 2; Emplacement: 2; Response: 2"
104
105 [1] -0.9
106
107 [1] "Phenomenology: 2; Emplacement: 3; Response: 1"
108
109 [1] 2.16
110
111 [1] "Phenomenology: 2; Emplacement: 3; Response: 2"
112
113 [1] -0.94
114
115 [1] "LEVEL 1 VARIANCE COMPONENTS"
116
117 [1] "Phenomenology: 1; Response: 1"
118
119 [1] 0.0011
120
121 [1] "Phenomenology: 1; Response: 2"
122
123 [1] 0.0017
124
125 [1] "Phenomenology: 2; Response: 1"
126
127 [1] 0.0038
128
129 [1] "Phenomenology: 2; Response: 2"
130
131 [1] 0.0016
132
133 [1] "LEVEL 2 VARIANCE COMPONENTS"

```

```

134
135 [1] "Phenomenology: 1; Response: 1"
136
137 [1] 0.001
138
139 [1] "Phenomenology: 1; Response: 2"
140
141 [1] 9e-04
142
143 [1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"
144
145 [1] "Phenomenology 1"
146
147 [1] "Variances"
148
149 [1] 0.0021 0.0034
150
151 [1] "Correlations"
152
153 [,1] [,2]
154 [1,] 1 0.28
155 [2,] 0 1.00
156
157 [1] "Phenomenology 2"
158
159 [1] "Variances"
160
161 [1] 1e-03 3e-04
162
163 [1] "Correlations"
164
165 [,1] [,2]
166 [1,] 1 -0.25
167 [2,] 0 1.00
168
169 [1] "Phenomenology 3"
170
171 [1] "Variances"
172
173 [1] 0.0011 0.0011
174
175 [1] "Correlations"
176
177 [,1] [,2]
178 [1,] 1 0.93

```

```

179 [2,] 0 1.00
180
181 [1] "Phenomenology 4"
182
183 [1] "Variances"
184
185 [1] 0.0260 0.0077
186
187 [1] "Correlations"
188
189 [,1] [,2]
190 [1,] 1 0.73
191 [2,] 0 1.00
192
193 [1] "AIC = -5840.98"
194
195 [1] "BIC = -5511.71"
196
197 Loading required package: numDeriv
198 [1] "CHECK LOG-LIKELIHOOD GRADIENTS"
199
200 [1] "Analytic gradient"
201 [1] -8.431868e-04 -7.038053e-07 -5.595059e-05 -2.702571e-04 4.145765e-04
202 [6] -6.877652e-04 -5.414314e-05 1.630249e-04 -7.642356e-04 -2.549322e-03
203 [11] -9.760283e-04 3.702140e-04 -1.655408e-05 -2.803807e-03 -1.524976e-03
204 [16] -1.081318e-03 -2.981360e-03 4.701484e-04 7.538052e-04 2.782379e-04
205 [21] 6.314769e-04 -4.285824e-04 8.941258e-04 6.184055e-04 3.258050e-04
206 [26] -4.870028e-04 -1.503716e-03 -7.324998e-02 -2.978359e-02 -5.224518e-01
207 [31] 1.255690e-01 5.041580e-02 -1.384946e-01 -4.589536e-02 -2.084526e-03
208 [36] -3.723123e-02 4.302576e-03 8.161440e-02 -2.400975e-03 -8.966039e-03
209 [41] -2.170289e-03 -1.693288e-04 5.219861e-04 -6.309496e-04 2.186223e-03
210 [46] 2.912214e-04 2.204081e-05 3.314070e-04 -1.062880e-02 -7.688789e-02
211 [51] -6.298861e-03 -6.976100e-04 7.529508e-03 1.421339e-03 3.434872e-02
212 [56] 1.317798e-02 -3.648180e-04 -2.097170e-02 7.638015e-03 5.206311e-02
213 [61] 3.562170e-03 1.863806e-03 -1.890228e-03 1.781585e-03 1.291352e-02
214 [66] 2.920229e-03 6.897676e-04 1.963322e-04 7.009887e-04 -1.052502e-03
215 [71] -3.373052e-04 3.676417e-04 -5.854999e-04 6.978043e-04 -2.989961e-05
216 [76] -2.478198e-04 -6.438579e-05 1.975623e-04 3.884852e-04 -1.331501e-04
217 [81] 7.588398e-04 -1.283586e-03 4.477531e-03 5.487680e-04 -9.010081e-04
218 [86] 1.037655e-01 6.236496e-03 -1.749379e-04 -1.290433e-02 2.277553e-04
219 [91] 3.282681e-04 1.789334e-03
220 [1] "Numerical gradient"
221 [1] -8.431866e-04 -7.061032e-07 -5.596042e-05 -2.702460e-04 4.145769e-04
222 [6] -6.877675e-04 -5.413925e-05 1.630274e-04 -7.642502e-04 -2.549334e-03
223 [11] -9.760306e-04 3.702130e-04 -1.656036e-05 -2.803783e-03 -1.524965e-03

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224 [16] -1.081294e-03 -2.981438e-03 4.701524e-04 7.538070e-04 2.782443e-04
225 [21] 6.314669e-04 -4.285834e-04 8.941207e-04 6.183993e-04 3.257979e-04
226 [26] -4.869988e-04 -1.503741e-03 -7.325015e-02 -2.978351e-02 -5.224522e-01
227 [31] 1.255690e-01 5.041530e-02 -1.384947e-01 -4.589501e-02 -2.084511e-03
228 [36] -3.723102e-02 4.302586e-03 8.161507e-02 -2.400988e-03 -8.966151e-03
229 [41] -2.171152e-03 -1.693386e-04 5.216883e-04 -6.309502e-04 2.186201e-03
230 [46] 2.909891e-04 2.202312e-05 3.314891e-04 -1.062881e-02 -7.688785e-02
231 [51] -6.298773e-03 -6.975891e-04 7.529809e-03 1.421349e-03 3.434873e-02
232 [56] 1.317800e-02 -3.647383e-04 -2.097168e-02 7.638015e-03 5.206300e-02
233 [61] 3.562154e-03 1.863808e-03 -1.890134e-03 1.781589e-03 1.291348e-02
234 [66] 2.920191e-03 6.897655e-04 1.962526e-04 7.009899e-04 -1.052988e-03
235 [71] -3.372905e-04 3.676777e-04 -5.856120e-04 6.976661e-04 -2.991824e-05
236 [76] -2.478187e-04 -6.428826e-05 1.975601e-04 3.884810e-04 -1.331631e-04
237 [81] 7.588249e-04 -1.283589e-03 4.476626e-03 5.487913e-04 -9.010005e-04
238 [86] 1.037792e-01 6.235949e-03 -1.747034e-04 -1.290695e-02 2.279298e-04
239 [91] 3.282717e-04 1.789455e-03
240 [1] "Difference"
241 [1] -1.374109e-05 2.622069e-06
242
243 + # Bayesian calculations
244 + p_cal = calc_bayes_cal(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
245 + nmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
246 + ncor_mc=ncores_mc,igrad=igrad,
247 + igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
248 + bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
249 + fpr_b=prior_files_beta,
250 + fgpr_b=gr_prior_files_beta,
251 + fpr_c=prior_files_calp,
252 + fgpr_c=gr_prior_files_calp,
253 + Xnom=NULL,imcmc=iMCMC,pl=parallel_plan)
254 + save.image()
255 + }
256 [1] "MAP CONVERGENCE STATUS"
257
258 [1] 0
259 [1] 2
260 [1] "MAXIMUM A POSTERIORI SUMMARY"
261
262 [1] "ERRORS-IN-VARIABLES YIELDS"
263
264 7 8 9 10 11 13 14 16 17 20 21 22 23
265 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
266 24 25 28 29 30 31 33 34 35 36 37 38 39
267 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
268

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269 [1] "COMMON COEFFICIENTS"
270
271 [1] "Phenomenology: 2; Response: 1"
272
273 [1] 6.67 -1.14
274
275 [1] "Phenomenology: 2; Response: 2"
276
277 [1] -5.08 0.23
278
279 [1] "Phenomenology: 3; Response: 1"
280
281 [1] -11.07 1.89
282
283 [1] "Phenomenology: 3; Response: 2"
284
285 [1] -8.64 1.72
286
287 [1] "Phenomenology: 4; Response: 1"
288
289 [1] -3.35 0.43
290
291 [1] "Phenomenology: 4; Response: 2"
292
293 [1] -2.64 0.29
294
295 [1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"
296
297 [1] "Phenomenology: 1; Emplacement: 1; Response: 1"
298
299 [1] -10.07 -1.31 -1.43 3.51 0.39
300
301 [1] "Phenomenology: 1; Emplacement: 1; Response: 2"
302
303 [1] -1.51 -1.44 -1.24 2.26 0.63
304
305 [1] "Phenomenology: 1; Emplacement: 2; Response: 1"
306
307 [1] -11.48 -1.09 -3.62 4.18 0.15
308
309 [1] "Phenomenology: 1; Emplacement: 2; Response: 2"
310
311 [1] -2.16 -1.22 -56.31 0.93 -3.42
312
313 [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

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314
315 [1] -9.53 -1.16 -4.47 4.95 0.34
316
317 [1] "Phenomenology: 1; Emplacement: 3; Response: 2"
318
319 [1] -2.85 -0.71 -2.17 2.60 0.08
320
321 [1] "Phenomenology: 2; Emplacement: 1; Response: 1"
322
323 [1] 3.87
324
325 [1] "Phenomenology: 2; Emplacement: 1; Response: 2"
326
327 [1] -0.17
328
329 [1] "Phenomenology: 2; Emplacement: 2; Response: 1"
330
331 [1] 3.11
332
333 [1] "Phenomenology: 2; Emplacement: 2; Response: 2"
334
335 [1] -0.9
336
337 [1] "Phenomenology: 2; Emplacement: 3; Response: 1"
338
339 [1] 2.16
340
341 [1] "Phenomenology: 2; Emplacement: 3; Response: 2"
342
343 [1] -0.94
344
345 [1] "LEVEL 1 VARIANCE COMPONENTS"
346
347 [1] "Phenomenology: 1; Response: 1"
348
349 [1] 0.0012
350
351 [1] "Phenomenology: 1; Response: 2"
352
353 [1] 0.0017
354
355 [1] "Phenomenology: 2; Response: 1"
356
357 [1] 0.0039
358

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359 [1] "Phenomenology: 2; Response: 2"
360
361 [1] 0.0016
362
363 [1] "LEVEL 2 VARIANCE COMPONENTS"
364
365 [1] "Phenomenology: 1; Response: 1"
366
367 [1] 0.001
368
369 [1] "Phenomenology: 1; Response: 2"
370
371 [1] 0.001
372
373 [1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"
374
375 [1] "Phenomenology 1"
376
377 [1] "Variances"
378
379 [1] 0.0021 0.0034
380
381 [1] "Correlations"
382
383 [,1] [,2]
384 [1,] 1 0.27
385 [2,] 0 1.00
386
387 [1] "Phenomenology 2"
388
389 [1] "Variances"
390
391 [1] 1e-03 3e-04
392
393 [1] "Correlations"
394
395 [,1] [,2]
396 [1,] 1 -0.25
397 [2,] 0 1.00
398
399 [1] "Phenomenology 3"
400
401 [1] "Variances"
402
403 [1] 1e-03 9e-04

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404
405 [1] "Correlations"
406
407 [,1] [,2]
408 [1,] 1 0.92
409 [2,] 0 1.00
410
411 [1] "Phenomenology 4"
412
413 [1] "Variances"
414
415 [1] 0.0218 0.0059
416
417 [1] "Correlations"
418
419 [,1] [,2]
420 [1,] 1 0.59
421 [2,] 0 1.00
422
423 [1] "FGSN PRIOR PARAMETERS"
424
425 [1] "Alpha = 17.33"
426 [1] "Lambda squared = 8"
427 [1] "Omega = -1.66" "Omega = 0.56"
428
429 [1] "CHECK LOG-PRIOR GRADIENTS"
430
431 [1] "Analytic gradient"
432 [1] -1.055466e-01 -8.327724e-02 -1.787279e-01 -2.140887e-01 -3.507367e-01
433 [6] 1.997990e+00 -5.483409e-01 -4.466296e-01 -1.832292e-01 3.561637e-01
434 [11] 5.548120e-02 -5.553768e-01 1.865502e-01 1.979674e-02 -1.646971e-01
435 [16] 3.490028e-01 2.182226e+00 -5.901511e-01 -3.792248e-01 -6.430252e-01
436 [21] -5.276501e-01 3.937098e-01 2.550063e-01 -2.494903e-01 1.570684e-01
437 [26] -7.524566e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
438 [31] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
439 [36] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
440 [41] 1.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
441 [46] 1.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
442 [51] 7.751886e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
443 [56] 1.572709e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
444 [61] 6.610821e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
445 [66] 1.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
446 [71] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 4.999971e-01
447 [76] 4.999956e-01 4.999902e-01 4.999959e-01 4.999974e-01 4.999975e-01
448 [81] 0.000000e+00 -7.753342e-01 -1.413558e+01 -4.440892e-16 -8.113389e-01

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449 [86] 4.223002e+01 2.220446e-16 1.518082e+00 -9.080578e+01 0.000000e+00
450 [91] 5.581077e-02 -2.313183e+01 1.965379e-02 -3.608055e-03 2.519400e-03
451 [96] 1.691543e-02
452 [1] "Numerical gradient"
453 [1] -1.055466e-01 -8.327723e-02 -1.787279e-01 -2.140887e-01 -3.507367e-01
454 [6] 1.997990e+00 -5.483409e-01 -4.466296e-01 -1.832292e-01 3.561637e-01
455 [11] 5.548120e-02 -5.553768e-01 1.865502e-01 1.979674e-02 -1.646971e-01
456 [16] 3.490028e-01 2.182226e+00 -5.901511e-01 -3.792248e-01 -6.430252e-01
457 [21] -5.276501e-01 3.937098e-01 2.550063e-01 -2.494903e-01 1.570684e-01
458 [26] -7.524566e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
459 [31] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
460 [36] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
461 [41] 1.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
462 [46] 1.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
463 [51] 7.751886e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
464 [56] 1.572709e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
465 [61] 6.610821e-01 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
466 [66] 1.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
467 [71] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 4.999971e-01
468 [76] 4.999956e-01 4.999902e-01 4.999959e-01 4.999974e-01 4.999975e-01
469 [81] 0.000000e+00 -7.753342e-01 -1.413558e+01 0.000000e+00 -8.113389e-01
470 [86] 4.223002e+01 -2.776737e-20 1.518082e+00 -9.080578e+01 0.000000e+00
471 [91] 5.581077e-02 -2.313183e+01 1.965379e-02 -3.608056e-03 2.519400e-03
472 [96] 1.691543e-02
473 [1] "Difference"
474 [1] -3.718726e-08 4.307974e-07
475
476 [1] "CHECK LOG-POSTERIOR GRADIENTS"
477
478 [1] "Analytic gradient"
479 [1] -0.143725992 -0.060385357 -0.128368006 0.021998510 -0.025658369
480 [6] -0.036306696 -0.050177600 -0.085249094 0.015305390 0.103565181
481 [11] -0.201184644 0.035028210 0.057834796 0.119313668 -0.047274099
482 [16] -0.138810545 0.143130873 0.012883495 0.027928439 0.031038567
483 [21] 0.009257306 0.048872686 0.042925809 0.021272475 0.044293980
484 [26] -0.012342070 0.055484797 0.464397999 0.145253071 3.136130832
485 [31] -0.085779845 0.227551255 -0.021211292 0.153970860 -0.008353076
486 [36] -0.072768259 -0.001231599 -0.129250679 -0.066407399 0.009340489
487 [41] 0.057159667 0.001311732 -0.005017758 -0.025711262 -0.061502299
488 [46] 0.006932307 0.033351768 -0.022771865 0.151675870 -0.235282410
489 [51] -1.248225356 -0.037197888 -0.473227835 0.096449963 -0.414093631
490 [56] -0.154049649 -0.678058084 -0.964376932 -0.004970885 0.022785614
491 [61] 0.058071746 -0.001887512 0.008393102 0.006164484 0.041256854
492 [66] 0.017139968 0.011643573 -0.012383597 -0.015343286 0.063412903
493 [71] -0.035682482 -0.037305676 -0.076071754 0.021156892 0.012114242

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494 [76] 0.007195484 -0.007422780 0.002099905 -0.003198358 -0.002760457
495 [81] 0.032427579 0.010586708 0.047392728 -0.038438158 -0.030227541
496 [86] -0.839483224 -0.016865095 -0.038679600 -0.002776678 0.016996863
497 [91] 0.028550901 -0.031829322 0.019653787 -0.003608055 0.002519400
498 [96] 0.016915435
499 [1] "Numerical gradient"
500 [1] -0.143726008 -0.060385354 -0.128368009 0.021998512 -0.025658378
501 [6] -0.036306692 -0.050177604 -0.085249091 0.015305380 0.103565176
502 [11] -0.201184641 0.035028212 0.057834794 0.119313685 -0.047274109
503 [16] -0.138810540 0.143130810 0.012883498 0.027928440 0.031038559
504 [21] 0.009257302 0.048872688 0.042925807 0.021272464 0.044293981
505 [26] -0.012342073 0.055484827 0.464398287 0.145253137 3.136132448
506 [31] -0.085779761 0.227551232 -0.021211309 0.153970961 -0.008353068
507 [36] -0.072768079 -0.001231649 -0.129250734 -0.066407414 0.009340623
508 [41] 0.057159404 0.001311717 -0.005018124 -0.025711252 -0.061502296
509 [46] 0.006931771 0.033351792 -0.022771965 0.151675863 -0.235282339
510 [51] -1.248225359 -0.037197899 -0.473227186 0.096449898 -0.414093621
511 [56] -0.154049648 -0.678058194 -0.964376936 -0.004970892 0.022785708
512 [61] 0.058071708 -0.001887510 0.008392921 0.006164449 0.041256794
513 [66] 0.017139825 0.011643578 -0.012383603 -0.015343273 0.063411939
514 [71] -0.035682449 -0.037305829 -0.076071821 0.021156943 0.012114223
515 [76] 0.007195512 -0.007422785 0.002099886 -0.003198378 -0.002760494
516 [81] 0.032427562 0.010586659 0.047382834 -0.038438287 -0.030227440
517 [86] -0.839521589 -0.016865429 -0.038679788 -0.002761438 0.016996873
518 [91] 0.028550994 -0.031826601 0.019653788 -0.003608078 0.002519406
519 [96] 0.016915378
520 [1] "Difference"
521 [1] -1.524005e-05 3.836539e-05
522
523 [1] "ACCEPTANCE RATES:"
524
525 [1] "Core 1: 0.8553666666666667"
526
527 [1] "POSTERIOR SUMMARY"
528
529 [1] "ERRORS-IN-VARIABLES YIELDS"
530
531 [1] "POSTERIOR MEAN: 16.28" "POSTERIOR MEAN: 16.21" "POSTERIOR MEAN: 16.51"
532 [4] "POSTERIOR MEAN: 16.61" "POSTERIOR MEAN: 17" "POSTERIOR MEAN: 12.21"
533 [7] "POSTERIOR MEAN: 17.57" "POSTERIOR MEAN: 17.27" "POSTERIOR MEAN: 16.52"
534 [10] "POSTERIOR MEAN: 14.5" "POSTERIOR MEAN: 15.75" "POSTERIOR MEAN: 17.6"
535 [13] "POSTERIOR MEAN: 15.23" "POSTERIOR MEAN: 15.87" "POSTERIOR MEAN: 16.46"
536 [16] "POSTERIOR MEAN: 14.53" "POSTERIOR MEAN: 12.13" "POSTERIOR MEAN: 17.71"
537 [19] "POSTERIOR MEAN: 23.08" "POSTERIOR MEAN: 23.41" "POSTERIOR MEAN: 17.51"
538 [22] "POSTERIOR MEAN: 21.96" "POSTERIOR MEAN: 22.34" "POSTERIOR MEAN: 16.71"

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539 [25] "POSTERIOR MEAN: 21.02" "POSTERIOR MEAN: 18.52"

540

541 [1] "LEVEL 2.5%: 16.27" "LEVEL 2.5%: 16.21" "LEVEL 2.5%: 16.49"

542 [4] "LEVEL 2.5%: 16.6" "LEVEL 2.5%: 16.99" "LEVEL 2.5%: 12.21"

543 [7] "LEVEL 2.5%: 17.55" "LEVEL 2.5%: 17.26" "LEVEL 2.5%: 16.51"

544 [10] "LEVEL 2.5%: 14.48" "LEVEL 2.5%: 15.74" "LEVEL 2.5%: 17.58"

545 [13] "LEVEL 2.5%: 15.22" "LEVEL 2.5%: 15.86" "LEVEL 2.5%: 16.46"

546 [16] "LEVEL 2.5%: 14.51" "LEVEL 2.5%: 12.12" "LEVEL 2.5%: 17.7"

547 [19] "LEVEL 2.5%: 23.05" "LEVEL 2.5%: 23.4" "LEVEL 2.5%: 17.49"

548 [22] "LEVEL 2.5%: 21.94" "LEVEL 2.5%: 22.33" "LEVEL 2.5%: 16.7"

549 [25] "LEVEL 2.5%: 21.01" "LEVEL 2.5%: 18.51"

550

551 [1] "LEVEL 5%: 16.28" "LEVEL 5%: 16.21" "LEVEL 5%: 16.49" "LEVEL 5%: 16.6"

552 [5] "LEVEL 5%: 16.99" "LEVEL 5%: 12.21" "LEVEL 5%: 17.56" "LEVEL 5%: 17.26"

553 [9] "LEVEL 5%: 16.51" "LEVEL 5%: 14.48" "LEVEL 5%: 15.74" "LEVEL 5%: 17.59"

554 [13] "LEVEL 5%: 15.23" "LEVEL 5%: 15.86" "LEVEL 5%: 16.46" "LEVEL 5%: 14.51"

555 [17] "LEVEL 5%: 12.12" "LEVEL 5%: 17.7" "LEVEL 5%: 23.06" "LEVEL 5%: 23.4"

556 [21] "LEVEL 5%: 17.49" "LEVEL 5%: 21.94" "LEVEL 5%: 22.33" "LEVEL 5%: 16.7"

557 [25] "LEVEL 5%: 21.01" "LEVEL 5%: 18.51"

558

559 [1] "LEVEL 50%: 16.28" "LEVEL 50%: 16.21" "LEVEL 50%: 16.51" "LEVEL 50%: 16.61"

560 [5] "LEVEL 50%: 17" "LEVEL 50%: 12.21" "LEVEL 50%: 17.57" "LEVEL 50%: 17.27"

561 [9] "LEVEL 50%: 16.52" "LEVEL 50%: 14.5" "LEVEL 50%: 15.75" "LEVEL 50%: 17.59"

562 [13] "LEVEL 50%: 15.24" "LEVEL 50%: 15.87" "LEVEL 50%: 16.46" "LEVEL 50%: 14.53"

563 [17] "LEVEL 50%: 12.13" "LEVEL 50%: 17.71" "LEVEL 50%: 23.08" "LEVEL 50%: 23.41"

564 [21] "LEVEL 50%: 17.51" "LEVEL 50%: 21.96" "LEVEL 50%: 22.34" "LEVEL 50%: 16.71"

565 [25] "LEVEL 50%: 21.02" "LEVEL 50%: 18.52"

566

567 [1] "LEVEL 95%: 16.29" "LEVEL 95%: 16.22" "LEVEL 95%: 16.52" "LEVEL 95%: 16.62"

568 [5] "LEVEL 95%: 17.01" "LEVEL 95%: 12.22" "LEVEL 95%: 17.59" "LEVEL 95%: 17.28"

569 [9] "LEVEL 95%: 16.53" "LEVEL 95%: 14.51" "LEVEL 95%: 15.75" "LEVEL 95%: 17.6"

570 [13] "LEVEL 95%: 15.24" "LEVEL 95%: 15.89" "LEVEL 95%: 16.47" "LEVEL 95%: 14.54"

571 [17] "LEVEL 95%: 12.14" "LEVEL 95%: 17.72" "LEVEL 95%: 23.09" "LEVEL 95%: 23.43"

572 [21] "LEVEL 95%: 17.52" "LEVEL 95%: 21.97" "LEVEL 95%: 22.35" "LEVEL 95%: 16.72"

573 [25] "LEVEL 95%: 21.03" "LEVEL 95%: 18.52"

574

575 [1] "LEVEL 97.5%: 16.3" "LEVEL 97.5%: 16.22" "LEVEL 97.5%: 16.52"

576 [4] "LEVEL 97.5%: 16.62" "LEVEL 97.5%: 17.01" "LEVEL 97.5%: 12.22"

577 [7] "LEVEL 97.5%: 17.59" "LEVEL 97.5%: 17.28" "LEVEL 97.5%: 16.53"

578 [10] "LEVEL 97.5%: 14.52" "LEVEL 97.5%: 15.76" "LEVEL 97.5%: 17.61"

579 [13] "LEVEL 97.5%: 15.24" "LEVEL 97.5%: 15.89" "LEVEL 97.5%: 16.47"

580 [16] "LEVEL 97.5%: 14.54" "LEVEL 97.5%: 12.15" "LEVEL 97.5%: 17.72"

581 [19] "LEVEL 97.5%: 23.1" "LEVEL 97.5%: 23.43" "LEVEL 97.5%: 17.53"

582 [22] "LEVEL 97.5%: 21.98" "LEVEL 97.5%: 22.35" "LEVEL 97.5%: 16.72"

583 [25] "LEVEL 97.5%: 21.03" "LEVEL 97.5%: 18.52"

```

584
585 [1] "COMMON COEFFICIENTS"
586
587 [1] "Phenomenology: 2; Response: 1"
588
589 [1] "POSTERIOR MEAN: 6.67" "POSTERIOR MEAN: -1.14"
590
591 [1] "LEVEL 2.5%: 6.67" "LEVEL 2.5%: -1.14"
592
593 [1] "LEVEL 5%: 6.67" "LEVEL 5%: -1.14"
594
595 [1] "LEVEL 50%: 6.67" "LEVEL 50%: -1.14"
596
597 [1] "LEVEL 95%: 6.68" "LEVEL 95%: -1.14"
598
599 [1] "LEVEL 97.5%: 6.68" "LEVEL 97.5%: -1.14"
600
601 [1] "Phenomenology: 2; Response: 2"
602
603 [1] "POSTERIOR MEAN: -5.08" "POSTERIOR MEAN: 0.23"
604
605 [1] "LEVEL 2.5%: -5.08" "LEVEL 2.5%: 0.23"
606
607 [1] "LEVEL 5%: -5.08" "LEVEL 5%: 0.23"
608
609 [1] "LEVEL 50%: -5.08" "LEVEL 50%: 0.23"
610
611 [1] "LEVEL 95%: -5.08" "LEVEL 95%: 0.23"
612
613 [1] "LEVEL 97.5%: -5.08" "LEVEL 97.5%: 0.23"
614
615 [1] "Phenomenology: 3; Response: 1"
616
617 [1] "POSTERIOR MEAN: -11.07" "POSTERIOR MEAN: 1.89"
618
619 [1] "LEVEL 2.5%: -11.09" "LEVEL 2.5%: 1.88"
620
621 [1] "LEVEL 5%: -11.08" "LEVEL 5%: 1.88"
622
623 [1] "LEVEL 50%: -11.07" "LEVEL 50%: 1.89"
624
625 [1] "LEVEL 95%: -11.06" "LEVEL 95%: 1.91"
626
627 [1] "LEVEL 97.5%: -11.06" "LEVEL 97.5%: 1.91"
628

```

629 [1] "Phenomenology: 3; Response: 2"

630

631 [1] "POSTERIOR MEAN: -8.64" "POSTERIOR MEAN: 1.72"

632

633 [1] "LEVEL 2.5%: -8.65" "LEVEL 2.5%: 1.7"

634

635 [1] "LEVEL 5%: -8.65" "LEVEL 5%: 1.7"

636

637 [1] "LEVEL 50%: -8.64" "LEVEL 50%: 1.72"

638

639 [1] "LEVEL 95%: -8.63" "LEVEL 95%: 1.73"

640

641 [1] "LEVEL 97.5%: -8.63" "LEVEL 97.5%: 1.73"

642

643 [1] "Phenomenology: 4; Response: 1"

644

645 [1] "POSTERIOR MEAN: -3.34" "POSTERIOR MEAN: 0.43"

646

647 [1] "LEVEL 2.5%: -3.53" "LEVEL 2.5%: 0.42"

648

649 [1] "LEVEL 5%: -3.5" "LEVEL 5%: 0.42"

650

651 [1] "LEVEL 50%: -3.35" "LEVEL 50%: 0.43"

652

653 [1] "LEVEL 95%: -3.16" "LEVEL 95%: 0.44"

654

655 [1] "LEVEL 97.5%: -3.12" "LEVEL 97.5%: 0.44"

656

657 [1] "Phenomenology: 4; Response: 2"

658

659 [1] "POSTERIOR MEAN: -2.63" "POSTERIOR MEAN: 0.29"

660

661 [1] "LEVEL 2.5%: -2.77" "LEVEL 2.5%: 0.28"

662

663 [1] "LEVEL 5%: -2.74" "LEVEL 5%: 0.28"

664

665 [1] "LEVEL 50%: -2.63" "LEVEL 50%: 0.29"

666

667 [1] "LEVEL 95%: -2.52" "LEVEL 95%: 0.3"

668

669 [1] "LEVEL 97.5%: -2.5" "LEVEL 97.5%: 0.3"

670

671 [1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

672

673 [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

674 [1] "POSTERIOR MEAN: -10.07" "POSTERIOR MEAN: -1.31" "POSTERIOR MEAN: -1.43"

675 [4] "POSTERIOR MEAN: 3.51" "POSTERIOR MEAN: 0.38"

676

677 [1] "LEVEL 2.5%: -10.1" "LEVEL 2.5%: -1.31" "LEVEL 2.5%: -1.46"

678 [4] "LEVEL 2.5%: 3.39" "LEVEL 2.5%: 0.35"

679

680 [1] "LEVEL 5%: -10.09" "LEVEL 5%: -1.31" "LEVEL 5%: -1.46" "LEVEL 5%: 3.42"

681 [5] "LEVEL 5%: 0.36"

682

683 [1] "LEVEL 50%: -10.07" "LEVEL 50%: -1.31" "LEVEL 50%: -1.43"

684 [4] "LEVEL 50%: 3.51" "LEVEL 50%: 0.38"

685

686 [1] "LEVEL 95%: -10.05" "LEVEL 95%: -1.31" "LEVEL 95%: -1.41"

687 [4] "LEVEL 95%: 3.6" "LEVEL 95%: 0.41"

688

689 [1] "LEVEL 97.5%: -10.04" "LEVEL 97.5%: -1.31" "LEVEL 97.5%: -1.41"

690 [4] "LEVEL 97.5%: 3.62" "LEVEL 97.5%: 0.42"

691

692 [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

693

694 [1] "POSTERIOR MEAN: -1.52" "POSTERIOR MEAN: -1.44" "POSTERIOR MEAN: -1.24"

695 [4] "POSTERIOR MEAN: 2.26" "POSTERIOR MEAN: 0.63"

696

697 [1] "LEVEL 2.5%: -1.56" "LEVEL 2.5%: -1.45" "LEVEL 2.5%: -1.28"

698 [4] "LEVEL 2.5%: 2.13" "LEVEL 2.5%: 0.59"

699

700 [1] "LEVEL 5%: -1.55" "LEVEL 5%: -1.45" "LEVEL 5%: -1.27" "LEVEL 5%: 2.15"

701 [5] "LEVEL 5%: 0.6"

702

703 [1] "LEVEL 50%: -1.51" "LEVEL 50%: -1.44" "LEVEL 50%: -1.24" "LEVEL 50%: 2.25"

704 [5] "LEVEL 50%: 0.63"

705

706 [1] "LEVEL 95%: -1.48" "LEVEL 95%: -1.44" "LEVEL 95%: -1.21" "LEVEL 95%: 2.38"

707 [5] "LEVEL 95%: 0.67"

708

709 [1] "LEVEL 97.5%: -1.48" "LEVEL 97.5%: -1.44" "LEVEL 97.5%: -1.2"

710 [4] "LEVEL 97.5%: 2.4" "LEVEL 97.5%: 0.68"

711

712 [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

713

714 [1] "POSTERIOR MEAN: -11.48" "POSTERIOR MEAN: -1.09" "POSTERIOR MEAN: -3.62"

715 [4] "POSTERIOR MEAN: 4.18" "POSTERIOR MEAN: 0.15"

716

717 [1] "LEVEL 2.5%: -11.5" "LEVEL 2.5%: -1.1" "LEVEL 2.5%: -3.8"

718



719 [4] "LEVEL 2.5%: 3.5" "LEVEL 2.5%: 0.06"

720

721 [1] "LEVEL 5%: -11.5" "LEVEL 5%: -1.1" "LEVEL 5%: -3.77" "LEVEL 5%: 3.59"

722 [5] "LEVEL 5%: 0.08"

723

724 [1] "LEVEL 50%: -11.48" "LEVEL 50%: -1.09" "LEVEL 50%: -3.62"

725 [4] "LEVEL 50%: 4.17" "LEVEL 50%: 0.15"

726

727 [1] "LEVEL 95%: -11.46" "LEVEL 95%: -1.09" "LEVEL 95%: -3.48"

728 [4] "LEVEL 95%: 4.79" "LEVEL 95%: 0.22"

729

730 [1] "LEVEL 97.5%: -11.45" "LEVEL 97.5%: -1.09" "LEVEL 97.5%: -3.45"

731 [4] "LEVEL 97.5%: 4.89" "LEVEL 97.5%: 0.23"

732

733 [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

734

735 [1] "POSTERIOR MEAN: -2.16" "POSTERIOR MEAN: -1.22" "POSTERIOR MEAN: -55.75"

736 [4] "POSTERIOR MEAN: 0.93" "POSTERIOR MEAN: -3.41"

737

738 [1] "LEVEL 2.5%: -2.28" "LEVEL 2.5%: -1.23" "LEVEL 2.5%: -67.22"

739 [4] "LEVEL 2.5%: 0.87" "LEVEL 2.5%: -3.66"

740

741 [1] "LEVEL 5%: -2.26" "LEVEL 5%: -1.23" "LEVEL 5%: -65.77" "LEVEL 5%: 0.88"

742 [5] "LEVEL 5%: -3.62"

743

744 [1] "LEVEL 50%: -2.16" "LEVEL 50%: -1.22" "LEVEL 50%: -55.44"

745 [4] "LEVEL 50%: 0.93" "LEVEL 50%: -3.41"

746

747 [1] "LEVEL 95%: -2.07" "LEVEL 95%: -1.21" "LEVEL 95%: -47.11"

748 [4] "LEVEL 95%: 0.99" "LEVEL 95%: -3.22"

749

750 [1] "LEVEL 97.5%: -2.05" "LEVEL 97.5%: -1.21" "LEVEL 97.5%: -46.03"

751 [4] "LEVEL 97.5%: 1" "LEVEL 97.5%: -3.2"

752

753 [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

754

755 [1] "POSTERIOR MEAN: -9.53" "POSTERIOR MEAN: -1.16" "POSTERIOR MEAN: -4.47"

756 [4] "POSTERIOR MEAN: 4.96" "POSTERIOR MEAN: 0.34"

757

758 [1] "LEVEL 2.5%: -9.56" "LEVEL 2.5%: -1.16" "LEVEL 2.5%: -4.49"

759 [4] "LEVEL 2.5%: 4.89" "LEVEL 2.5%: 0.33"

760

761 [1] "LEVEL 5%: -9.55" "LEVEL 5%: -1.16" "LEVEL 5%: -4.49" "LEVEL 5%: 4.9"

762 [5] "LEVEL 5%: 0.33"

763

764 [1] "LEVEL 50%: -9.53" "LEVEL 50%: -1.16" "LEVEL 50%: -4.47" "LEVEL 50%: 4.96"  
765 [5] "LEVEL 50%: 0.34"  
766  
767 [1] "LEVEL 95%: -9.5" "LEVEL 95%: -1.15" "LEVEL 95%: -4.45" "LEVEL 95%: 5.01"  
768 [5] "LEVEL 95%: 0.35"  
769  
770 [1] "LEVEL 97.5%: -9.5" "LEVEL 97.5%: -1.15" "LEVEL 97.5%: -4.44"  
771 [4] "LEVEL 97.5%: 5.02" "LEVEL 97.5%: 0.35"  
772  
773 [1] "Phenomenology: 1; Emplacement: 3; Response: 2"  
774  
775 [1] "POSTERIOR MEAN: -2.85" "POSTERIOR MEAN: -0.71" "POSTERIOR MEAN: -2.16"  
776 [4] "POSTERIOR MEAN: 2.61" "POSTERIOR MEAN: 0.09"  
777  
778 [1] "LEVEL 2.5%: -2.89" "LEVEL 2.5%: -0.71" "LEVEL 2.5%: -2.36"  
779 [4] "LEVEL 2.5%: 2.34" "LEVEL 2.5%: -0.05"  
780  
781 [1] "LEVEL 5%: -2.88" "LEVEL 5%: -0.71" "LEVEL 5%: -2.33" "LEVEL 5%: 2.38"  
782 [5] "LEVEL 5%: -0.03"  
783  
784 [1] "LEVEL 50%: -2.85" "LEVEL 50%: -0.71" "LEVEL 50%: -2.16" "LEVEL 50%: 2.61"  
785 [5] "LEVEL 50%: 0.09"  
786  
787 [1] "LEVEL 95%: -2.81" "LEVEL 95%: -0.7" "LEVEL 95%: -2.01" "LEVEL 95%: 2.84"  
788 [5] "LEVEL 95%: 0.2"  
789  
790 [1] "LEVEL 97.5%: -2.8" "LEVEL 97.5%: -0.7" "LEVEL 97.5%: -1.99"  
791 [4] "LEVEL 97.5%: 2.88" "LEVEL 97.5%: 0.21"  
792  
793 [1] "Phenomenology: 2; Emplacement: 1; Response: 1"  
794  
795 [1] "POSTERIOR MEAN: 3.87"  
796  
797 [1] "LEVEL 2.5%: 3.86"  
798  
799 [1] "LEVEL 5%: 3.86"  
800  
801 [1] "LEVEL 50%: 3.87"  
802  
803 [1] "LEVEL 95%: 3.88"  
804  
805 [1] "LEVEL 97.5%: 3.88"  
806  
807 [1] "Phenomenology: 2; Emplacement: 1; Response: 2"  
808

809 [1] "POSTERIOR MEAN: -0.17"  
810  
811 [1] "LEVEL 2.5%: -0.19"  
812  
813 [1] "LEVEL 5%: -0.19"  
814  
815 [1] "LEVEL 50%: -0.17"  
816  
817 [1] "LEVEL 95%: -0.15"  
818  
819 [1] "LEVEL 97.5%: -0.15"  
820  
821 [1] "Phenomenology: 2; Emplacement: 2; Response: 1"  
822  
823 [1] "POSTERIOR MEAN: 3.11"  
824  
825 [1] "LEVEL 2.5%: 3.09"  
826  
827 [1] "LEVEL 5%: 3.09"  
828  
829 [1] "LEVEL 50%: 3.11"  
830  
831 [1] "LEVEL 95%: 3.14"  
832  
833 [1] "LEVEL 97.5%: 3.14"  
834  
835 [1] "Phenomenology: 2; Emplacement: 2; Response: 2"  
836  
837 [1] "POSTERIOR MEAN: -0.9"  
838  
839 [1] "LEVEL 2.5%: -0.96"  
840  
841 [1] "LEVEL 5%: -0.95"  
842  
843 [1] "LEVEL 50%: -0.9"  
844  
845 [1] "LEVEL 95%: -0.86"  
846  
847 [1] "LEVEL 97.5%: -0.85"  
848  
849 [1] "Phenomenology: 2; Emplacement: 3; Response: 1"  
850  
851 [1] "POSTERIOR MEAN: 2.16"  
852  
853 [1] "LEVEL 2.5%: 2.14"

854  
855 [1] "LEVEL 5%: 2.14"  
856  
857 [1] "LEVEL 50%: 2.16"  
858  
859 [1] "LEVEL 95%: 2.17"  
860  
861 [1] "LEVEL 97.5%: 2.18"  
862  
863 [1] "Phenomenology: 2; Emplacement: 3; Response: 2"  
864  
865 [1] "POSTERIOR MEAN: -0.94"  
866  
867 [1] "LEVEL 2.5%: -0.99"  
868  
869 [1] "LEVEL 5%: -0.98"  
870  
871 [1] "LEVEL 50%: -0.94"  
872  
873 [1] "LEVEL 95%: -0.9"  
874  
875 [1] "LEVEL 97.5%: -0.9"  
876  
877 [1] "LEVEL 1 VARIANCE COMPONENTS"  
878  
879 [1] "Phenomenology: 1; Response: 1"  
880  
881 [1] "POSTERIOR MEAN: 0.0012"  
882  
883 [1] "LEVEL 2.5%: 9e-04"  
884  
885 [1] "LEVEL 5%: 9e-04"  
886  
887 [1] "LEVEL 50%: 0.0012"  
888  
889 [1] "LEVEL 95%: 0.0015"  
890  
891 [1] "LEVEL 97.5%: 0.0015"  
892  
893 [1] "Phenomenology: 1; Response: 2"  
894  
895 [1] "POSTERIOR MEAN: 0.0017"  
896  
897 [1] "LEVEL 2.5%: 0.0016"  
898

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899 [1] "LEVEL 5%: 0.0017"
900
901 [1] "LEVEL 50%: 0.0017"
902
903 [1] "LEVEL 95%: 0.0019"
904
905 [1] "LEVEL 97.5%: 0.0019"
906
907 [1] "Phenomenology: 2; Response: 1"
908
909 [1] "POSTERIOR MEAN: 0.0039"
910
911 [1] "LEVEL 2.5%: 0.0035"
912
913 [1] "LEVEL 5%: 0.0036"
914
915 [1] "LEVEL 50%: 0.0039"
916
917 [1] "LEVEL 95%: 0.0043"
918
919 [1] "LEVEL 97.5%: 0.0044"
920
921 [1] "Phenomenology: 2; Response: 2"
922
923 [1] "POSTERIOR MEAN: 0.0016"
924
925 [1] "LEVEL 2.5%: 0.0015"
926
927 [1] "LEVEL 5%: 0.0015"
928
929 [1] "LEVEL 50%: 0.0016"
930
931 [1] "LEVEL 95%: 0.0018"
932
933 [1] "LEVEL 97.5%: 0.0018"
934
935 [1] "LEVEL 2 VARIANCE COMPONENTS"
936
937 [1] "Phenomenology: 1; Response: 1"
938
939 [1] "POSTERIOR MEAN: 0.001"
940
941 [1] "LEVEL 2.5%: 9e-04"
942
943 [1] "LEVEL 5%: 9e-04"

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944
945 [1] "LEVEL 50%: 0.001"
946
947 [1] "LEVEL 95%: 0.0012"
948
949 [1] "LEVEL 97.5%: 0.0013"
950
951 [1] "Phenomenology: 1; Response: 2"
952
953 [1] "POSTERIOR MEAN: 0.001"
954
955 [1] "LEVEL 2.5%: 8e-04"
956
957 [1] "LEVEL 5%: 8e-04"
958
959 [1] "LEVEL 50%: 0.001"
960
961 [1] "LEVEL 95%: 0.0012"
962
963 [1] "LEVEL 97.5%: 0.0012"
964
965 [1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"
966
967 [1] "Phenomenology 1"
968
969 [1] "POSTERIOR MEAN:"
970
971 [1] "Variances"
972
973 [1] 0.0021 0.0034
974
975 [1] "Correlations"
976
977 [,1] [,2]
978 [1,] 1 0.27
979 [2,] 0 1.00
980
981 [1] "Variances"
982
983 [1] "LEVEL 2.5%: 0.002" "LEVEL 2.5%: 0.0032"
984
985 [1] "Correlations"
986
987 [1] "LEVEL 2.5%:"
988 [,1] [,2]

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989 [1,] 1 0.26
990 [2,] 0 1.00
991
992 [1] "Variances"
993
994 [1] "LEVEL 5%: 0.002" "LEVEL 5%: 0.0032"
995
996 [1] "Correlations"
997
998 [1] "LEVEL 5%:"
999 [,1] [,2]
1000 [1,] 1 0.26
1001 [2,] 0 1.00
1002
1003 [1] "Variances"
1004
1005 [1] "LEVEL 50%: 0.0021" "LEVEL 50%: 0.0034"
1006
1007 [1] "Correlations"
1008
1009 [1] "LEVEL 50%:"
1010 [,1] [,2]
1011 [1,] 1 0.27
1012 [2,] 0 1.00
1013
1014 [1] "Variances"
1015
1016 [1] "LEVEL 95%: 0.0022" "LEVEL 95%: 0.0035"
1017
1018 [1] "Correlations"
1019
1020 [1] "LEVEL 95%:"
1021 [,1] [,2]
1022 [1,] 1 0.28
1023 [2,] 0 1.00
1024
1025 [1] "Variances"
1026
1027 [1] "LEVEL 97.5%: 0.0022" "LEVEL 97.5%: 0.0036"
1028
1029 [1] "Correlations"
1030
1031 [1] "LEVEL 97.5%:"
1032 [,1] [,2]
1033 [1,] 1 0.28

```

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1034 [2,] 0 1.00
1035
1036 [1] "Phenomenology 2"
1037
1038 [1] "POSTERIOR MEAN:"
1039
1040 [1] "Variances"
1041
1042 [1] 1e-03 3e-04
1043
1044 [1] "Correlations"
1045
1046 [,1] [,2]
1047 [1,] 1 -0.25
1048 [2,] 0 1.00
1049
1050 [1] "Variances"
1051
1052 [1] "LEVEL 2.5%: 0.001" "LEVEL 2.5%: 3e-04"
1053
1054 [1] "Correlations"
1055
1056 [1] "LEVEL 2.5%:"
1057 [,1] [,2]
1058 [1,] 1 -0.3
1059 [2,] 0 1.0
1060
1061 [1] "Variances"
1062
1063 [1] "LEVEL 5%: 0.001" "LEVEL 5%: 3e-04"
1064
1065 [1] "Correlations"
1066
1067 [1] "LEVEL 5%:"
1068 [,1] [,2]
1069 [1,] 1 -0.29
1070 [2,] 0 1.00
1071
1072 [1] "Variances"
1073
1074 [1] "LEVEL 50%: 0.001" "LEVEL 50%: 3e-04"
1075
1076 [1] "Correlations"
1077
1078 [1] "LEVEL 50%:"

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1079 [,1] [,2]
1080 [1,] 1 -0.25
1081 [2,] 0 1.00
1082
1083 [1] "Variances"
1084
1085 [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 3e-04"
1086
1087 [1] "Correlations"
1088
1089 [1] "LEVEL 95%:"
1090 [,1] [,2]
1091 [1,] 1 -0.21
1092 [2,] 0 1.00
1093
1094 [1] "Variances"
1095
1096 [1] "LEVEL 97.5%: 0.0011" "LEVEL 97.5%: 3e-04"
1097
1098 [1] "Correlations"
1099
1100 [1] "LEVEL 97.5%:"
1101 [,1] [,2]
1102 [1,] 1 -0.21
1103 [2,] 0 1.00
1104
1105 [1] "Phenomenology 3"
1106
1107 [1] "POSTERIOR MEAN:"
1108
1109 [1] "Variances"
1110
1111 [1] 1e-03 9e-04
1112
1113 [1] "Correlations"
1114
1115 [,1] [,2]
1116 [1,] 1 0.92
1117 [2,] 0 1.00
1118
1119 [1] "Variances"
1120
1121 [1] "LEVEL 2.5%: 8e-04" "LEVEL 2.5%: 8e-04"
1122
1123 [1] "Correlations"

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1124
1125 [1] "LEVEL 2.5%:"
1126 [,1] [,2]
1127 [1,] 1 0.9
1128 [2,] 0 1.0
1129
1130 [1] "Variances"
1131
1132 [1] "LEVEL 5%: 9e-04" "LEVEL 5%: 8e-04"
1133
1134 [1] "Correlations"
1135
1136 [1] "LEVEL 5%:"
1137 [,1] [,2]
1138 [1,] 1 0.9
1139 [2,] 0 1.0
1140
1141 [1] "Variances"
1142
1143 [1] "LEVEL 50%: 0.001" "LEVEL 50%: 9e-04"
1144
1145 [1] "Correlations"
1146
1147 [1] "LEVEL 50%:"
1148 [,1] [,2]
1149 [1,] 1 0.92
1150 [2,] 0 1.00
1151
1152 [1] "Variances"
1153
1154 [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 0.0011"
1155
1156 [1] "Correlations"
1157
1158 [1] "LEVEL 95%:"
1159 [,1] [,2]
1160 [1,] 1 0.93
1161 [2,] 0 1.00
1162
1163 [1] "Variances"
1164
1165 [1] "LEVEL 97.5%: 0.0012" "LEVEL 97.5%: 0.0011"
1166
1167 [1] "Correlations"
1168

```

```

1169 [1] "LEVEL 97.5%:"
1170 [,1] [,2]
1171 [1,] 1 0.93
1172 [2,] 0 1.00
1173
1174 [1] "Phenomenology 4"
1175
1176 [1] "POSTERIOR MEAN:"
1177
1178 [1] "Variances"
1179
1180 [1] 0.0223 0.0061
1181
1182 [1] "Correlations"
1183
1184 [,1] [,2]
1185 [1,] 1 0.59
1186 [2,] 0 1.00
1187
1188 [1] "Variances"
1189
1190 [1] "LEVEL 2.5%: 0.0163" "LEVEL 2.5%: 0.0045"
1191
1192 [1] "Correlations"
1193
1194 [1] "LEVEL 2.5%:"
1195 [,1] [,2]
1196 [1,] 1 0.45
1197 [2,] 0 1.00
1198
1199 [1] "Variances"
1200
1201 [1] "LEVEL 5%: 0.0169" "LEVEL 5%: 0.0046"
1202
1203 [1] "Correlations"
1204
1205 [1] "LEVEL 5%:"
1206 [,1] [,2]
1207 [1,] 1 0.47
1208 [2,] 0 1.00
1209
1210 [1] "Variances"
1211
1212 [1] "LEVEL 50%: 0.022" "LEVEL 50%: 0.006"
1213

```

```

1214 [1] "Correlations"
1215
1216 [1] "LEVEL 50%:"
1217 [,1] [,2]
1218 [1,] 1 0.6
1219 [2,] 0 1.0
1220
1221 [1] "Variances"
1222
1223 [1] "LEVEL 95%: 0.029" "LEVEL 95%: 0.0077"
1224
1225 [1] "Correlations"
1226
1227 [1] "LEVEL 95%:"
1228 [,1] [,2]
1229 [1,] 1 0.7
1230 [2,] 0 1.0
1231
1232 [1] "Variances"
1233
1234 [1] "LEVEL 97.5%: 0.0307" "LEVEL 97.5%: 0.008"
1235
1236 [1] "Correlations"
1237
1238 [1] "LEVEL 97.5%:"
1239 [,1] [,2]
1240 [1,] 1 0.71
1241 [2,] 0 1.00
1242
1243 [1] "FGSN PRIOR PARAMETERS"
1244
1245 [1] "POSTERIOR MEAN:"
1246
1247 [1] "Alpha = 17.33"
1248 [1] "Lambda squared = 8"
1249 [1] "Omega = -1.67" "Omega = 0.56"
1250
1251 [1] "Alpha:"
1252 [1] "LEVEL 2.5%: 17.13"
1253
1254 [1] "LEVEL 5%: 17.16"
1255
1256 [1] "LEVEL 50%: 17.33"
1257
1258 [1] "LEVEL 95%: 17.48"

```

```

1259
1260 [1] "LEVEL 97.5%: 17.51"
1261
1262 [1] "Lambda squared:"
1263 [1] "LEVEL 2.5%: 7.83"
1264
1265 [1] "LEVEL 5%: 7.85"
1266
1267 [1] "LEVEL 50%: 8"
1268
1269 [1] "LEVEL 95%: 8.13"
1270
1271 [1] "LEVEL 97.5%: 8.15"
1272
1273 [1] "Omega:"
1274 [1] "LEVEL 2.5%: -1.94" "LEVEL 2.5%: 0.49"
1275
1276 [1] "LEVEL 5%: -1.9" "LEVEL 5%: 0.5"
1277
1278 [1] "LEVEL 50%: -1.67" "LEVEL 50%: 0.56"
1279
1280 [1] "LEVEL 95%: -1.42" "LEVEL 95%: 0.62"
1281
1282 [1] "LEVEL 97.5%: -1.37" "LEVEL 97.5%: 0.63"
1283
1284 [1] "DIC = -6011.41"
1285
1286 [1] "PIC = -6005.05"

```

## A.5 New Event Data: Preprocessing

```
1 #####
2 #
3 # This file is the input deck for MultiPEM Toolbox rapid post-
4 # detonation analysis, based on using fixed values of the forward and
5 # error model parameters obtained from calibration data.
6 #
7 #####
8
9 #
10 # REQUIRED R PACKAGES
11 #
12
13 require(Matrix)
14
15 #
16 # END REQUIRED R PACKAGES
17 #
18
19 #
20 # PREPROCESSING
21 #
22
23 # Specify directory for general subroutines
24 gen_dir = "../..../Code"
25
26 # Source supporting R function
27 source(paste(gen_dir,"/prepro_0.r",sep=""))
28
29 # Specify directory for application subroutines
30 app_dir = "../..../Code"
31
32 # Specify root data directory
33 dat_dir = "../..../Data"
34
35 # Specify new event data directories
36 dat_new = c("seismic_new.csv",
37 "acoustic_new.csv",
38 "optical_new.csv",
39 "crater_new.csv")
40
41 # Phenomenologies for this analysis
42 # 1 - seismic
43 # 2 - acoustic
```

```

44 # 3 - optical
45 # 4 - crater (surface effects)
46
47 # Names of new event inference parameters
48 theta_names = c("W","HOB")
49
50 # Number of calibration parameter imputations utilized in
51 # Markov chain Monte Carlo (MCMC) for new event parameters
52 nimpute = 1
53
54 # Set flag for bounded optimization
55 opt_B = FALSE
56
57 # Indicate nev parameter transform
58 itransform = FALSE
59
60 # Specify fixed parameters for nev parameter transform
61 if(itransform){
62 tPars = TRUE
63
64 if(tPars){
65 tPars = vector("list",0)
66 tPars$yield_scaling = 1/3
67 } else { tPars = NULL }
68 } else { tPars = NULL }
69
70 # Set up parameter constraints
71 # lower and upper bounds (use -Inf and Inf if unbounded)
72 lb_theta0 = rep(-Inf,length(theta_names))
73 lb_theta0[2] = -10
74 ub_theta0 = rep(Inf,length(theta_names))
75 ub_theta0[2] = 160
76
77 # Set up parameter subsets by phenomenology
78 tsub = TRUE
79
80 if(tsub) {
81 tsub = vector("list",length(Rh))
82 tsub[[4]] = 1 # only log-yield for crater
83 } else { tsub = NULL }
84
85 # Preprocessing for statistical analysis routines
86 tmp = prepro_0(p_cal,gen_dir,app_dir,dat_dir,dat_new,theta_names,
87 nimp=nimpute,bopt=opt_B,itr=itransform,fp_tr=tPars,
88 tlb=lb_theta0,tub=ub_theta0,tsub=tsub)

```

```
89 if(opt_B){
90 p_cal = tmp$p_cal
91 t_cal = tmp$t_cal
92 } else {
93 p_cal = tmp
94 t_cal = NULL
95 }
96 rm(tmp)
97 save.image()
98
99 #
100 # END PREPROCESSING
101 #
```



## A.6 New Event Data: Maximum Likelihood Estimation

```
1 #
2 # MAXIMUM LIKELIHOOD CALCULATION
3 #
4
5 # Source supporting R function
6 source(paste(gen_dir,"/calc_mle_0.r",sep=""))
7
8 # Set seed for repeatability of analysis
9 set.seed(631)
10
11 # Names of forward models for each response
12 # by phenomenology
13 fm0 = vector("list",length(Rh))
14 fm0[[1]] = c("f0_s","f0_s")
15 fm0[[2]] = c("f0_a","f0_a")
16 fm0[[3]] = c("f0_o","f0_o")
17 fm0[[4]] = c("f0_c","f0_c")
18
19 # Indicate if forward model gradients provided
20 igrad = TRUE
21
22 if(igrad){
23 # Names of forward model gradients for each response
24 # by phenomenology
25 gfm0 = vector("list",length(Rh))
26 gfm0[[1]] = c("g0_s","g0_s")
27 gfm0[[2]] = c("g0_a","g0_a")
28 gfm0[[3]] = c("g0_o","g0_o")
29 gfm0[[4]] = c("g0_c","g0_c")
30 } else { gfm0 = NULL }
31
32 # Specify number of starting values for optimization
33 nstart = 10
34
35 # number of cores to use for optimization
36 ncores_mle = 1
37
38 # Indicate use of BFGS optimization methods
39 bfgs = TRUE
40
41 # Location of R data files with starting values
42 # for input to MLE optimization
43 opt_files_in = NULL
```

```

44
45 # Location of R data file to write the results of
46 # MLE optimization
47 opt_files_out = "./opt_nev.RData"
48
49 # Initial start value for theta0
50 tst = TRUE
51
52 if(tst){
53 tst = numeric(p_cal$ntheta0)
54 tst[2] = runif(1,-1.e-6,1.e-6)
55 } else { tst = NULL }
56
57 # Confidence interval levels for new event parameter inference
58 ci_lev = 0.95
59
60 # Indicator of MLE gradient check
61 mle_grad_ck = TRUE
62
63 # Strategy for running parallel jobs (future package)
64 parallel_plan = "multicore"
65
66 # MLE calculations
67 p_cal = calc_mle_0(p_cal,gen_dir,app_dir,fm0,nst=nstart,ncor=ncores_mle,
68 ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,
69 igrck=mle_grad_ck,t_cal=t_cal,g0=gfm0,
70 fopt_in=opt_files_in,Xst=NULL,tst=tst,
71 fopt_out=opt_files_out,pl=parallel_plan)
72 save.image()
73
74 #
75 # END MAXIMUM LIKELIHOOD CALCULATION
76 #

```

## A.7 New Event Data: Bayesian Analysis

```
1 #
2 # BAYESIAN ANALYSIS
3 #
4
5 # Specify if Bayesian analysis is to be conducted
6 iBayes = TRUE
7
8 if(iBayes){
9 # Source supporting R function
10 source(paste(gen_dir,"/calc_bayes_0.r",sep=""))
11
12 # Indicator of prior distribution for theta0
13 iTheta0Prior = FALSE
14
15 if(iTheta0Prior){
16 # location of code for computing log-prior densities and gradients
17 prior_files_theta0 = NULL
18 if(igrad){
19 gr_prior_files_theta0 = NULL
20 } else { gr_prior_files_theta0 = NULL }
21
22 # prior distribution for new event parameters (theta0)
23 p_callp_theta0f = "lp_0"
24 if(igrad){ p_callp_theta0g = "lq_0" }
25
26 # parameters for log yield parameter prior (Gaussian)
27 p_cal$pi_w_mu = (log(10)+log(10000000))/2
28 p_cal$pi_w_sd = (log(10000000)-log(10))/6
29 # parameters for HOB/DOB parameter prior (Gaussian)
30 p_cal$pi_h_mu = 0
31 p_cal$pi_h_sd = 160/3
32 } else {
33 prior_files_theta0 = NULL
34 gr_prior_files_theta0 = NULL
35 }
36
37 # specify MCMC algorithm
38 # options: "RAM", "FME", "NUTS", or "SMC"
39 iMCMC = "FME"
40
41 # burn-in
42 nburn = 10000
43
```

```

44 # production
45 nmcmc = 20000
46
47 # posterior sample thinning rate (for multiple imputation)
48 nthin = 1
49
50 # number of cores to use for optimization
51 ncores_map = 1
52
53 # number of cores to use for generating parallel MCMC chains
54 ncores_mc = 1
55
56 # Indicator of prior gradient check
57 prior_grad_ck = TRUE
58
59 # Indicator of posterior gradient check
60 post_grad_ck = TRUE
61
62 # Options for Sequential Monte Carlo (SMC) sampling
63 # (iMCMC = "SMC")
64 # number of cores to use for parallelization within SMC algorithm
65 ncores_smc = NULL
66 # new event parameter ranges for initial SMC sample
67 lb_smc = rep(-Inf,length(theta_names))
68 ub_smc = rep(Inf,length(theta_names))
69
70 # Bayesian calculations
71 p_cal = calc_bayes_0(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
72 nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
73 ncor_mc=ncores_mc,igrad=igrad,
74 igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
75 bfgs=bfgs,itpr=iTheta0Prior,
76 fpr_t=prior_files_theta0,
77 fgpr_t=gr_prior_files_theta0,imcmc=iMCMC,
78 pl=parallel_plan,ncor_smc=ncores_smc,
79 lb_smc=lb_smc,ub_smc=ub_smc,t_cal=t_cal)
80 save.image()
81 }
82
83 #
84 # END BAYESIAN ANALYSIS
85 #

```

## A.8 New Event Data: Output File

```
1 > # MLE calculations
2 > p_cal = calc_mle_0(p_cal,gen_dir,app_dir,fm0,nst=nstart,ncor=ncores_mle,
3 + ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,
4 + igrck=mle_grad_ck,t_cal=t_cal,g0=gfm0,
5 + fopt_in=opt_files_in,Xst=NULL,tst=tst,
6 + fopt_out=opt_files_out,pl=parallel_plan)
7 [1] "MLE CONVERGENCE STATUS"
8
9 [1] 0
10 [1] 2
11 [1] "MAXIMUM LIKELIHOOD SUMMARY"
12
13 [1] "NEW EVENT INFERENCE PARAMETERS"
14
15 [1] "ESTIMATE: "
16
17 W HOB
18 14.02 -2.70
19
20 [1] "STANDARD DEVIATION: "
21
22 W HOB
23 0.05 1.97
24
25 [1] "STANDARD DEVIATION FIXED MODEL PARAMETERS: "
26
27 W HOB
28 0.05 1.79
29
30 [1] "CORRELATION MATRIX: "
31
32 W HOB
33 W 1.00 -0.43
34 HOB -0.43 1.00
35
36 [1] "CORRELATION MATRIX FIXED MODEL PARAMETERS: "
37
38 W HOB
39 W 1.00 -0.36
40 HOB -0.36 1.00
41
42 [1] "95%: CONFIDENCE INTERVAL:"
43
```

```

44 W HOB
45 lb 13.92 -5.46
46 ub 14.13 3.30
47
48 [1] "95%: CONFIDENCE INTERVAL FIXED MODEL PARAMETERS:"
49
50 W HOB
51 lb_0 13.93 -5.28
52 ub_0 14.11 2.52
53
54 Loading required package: numDeriv
55 [1] "CHECK LOG-LIKELIHOOD GRADIENTS"
56
57 [1] "Analytic gradient"
58 [1] 3.612240e-06 1.545468e-07
59 [1] "Numerical gradient"
60 [1] 3.611856e-06 1.526450e-07
61 [1] "Difference"
62 [1] 3.836284e-10 1.901811e-09
63
64 + # Bayesian calculations
65 + p_cal = calc_bayes_0(p_cal,gen_dir,app_dir,nburn=nburn,nmcmc=nmcmc,
66 + nthin=nthin,ncor=ncores_mc,igrad=igrad,
67 + igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
68 + bfgs=bfgs,itpr=iTheta0Prior,
69 + fpr_t=prior_files_theta0,
70 + fgpr_t=gr_prior_files_theta0,imcmc=iMCMC,
71 + pl=parallel_plan,ncor_smc=ncores_smc,
72 + lb_smc=lb_smc,ub_smc=ub_smc,t_cal=t_cal)
73 + save.image()
74 + }
75 [1] "MAP CONVERGENCE STATUS"
76
77 [1] 0
78 [1] 2
79 [1] "MAXIMUM A POSTERIORI SUMMARY"
80
81 [1] "NEW EVENT INFERENCE PARAMETERS"
82
83 [1] "ESTIMATE: "
84
85 W HOB
86 14.02 -2.11
87
88 [1] "CHECK LOG-PRIOR GRADIENTS"

```

```

89
90 [1] "Analytic gradient"
91 [1] 0.000000 0.682004
92 [1] "Numerical gradient"
93 [1] 0.000000 0.682004
94 [1] "Difference"
95 [1] 0.000000e+00 7.597145e-12
96
97 [1] "CHECK LOG-POSTERIOR GRADIENTS"
98
99 [1] "Analytic gradient"
100 [1] 4.523644e-06 3.942643e-06
101 [1] "Numerical gradient"
102 [1] 4.524224e-06 3.942255e-06
103 [1] "Difference"
104 [1] -5.799625e-10 3.878053e-10
105
106 [1] "ACCEPTANCE RATES:"
107
108 [1] "Core 1: 0.8163666666666667"
109
110 [1] "POSTERIOR SUMMARY"
111
112 [1] "NEW EVENT INFERENCE PARAMETERS"
113
114 [1] "POSTERIOR MEAN: 14.03" "POSTERIOR MEAN: -0.77"
115
116 [1] "POSTERIOR SD: 0.05" "POSTERIOR SD: 3.04"
117
118 [1] "LEVEL 2.5%: 13.94" "LEVEL 2.5%: -5.54"
119
120 [1] "LEVEL 5%: 13.95" "LEVEL 5%: -5.03"
121
122 [1] "LEVEL 50%: 14.03" "LEVEL 50%: -1.42"
123
124 [1] "LEVEL 95%: 14.1" "LEVEL 95%: 4.48"
125
126 [1] "LEVEL 97.5%: 14.12" "LEVEL 97.5%: 5.25"
127
128 [1] "CORRELATION MATRIX:"
129
130 W HOB
131 W 1 0
132 HOB 0 1

```

## B Complete Assessment Run Files

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

### B.1 Preprocessing

```
1 #####
2 #
3 # This file is the input deck for MultiPEM Toolbox complete post-
4 # detonation analysis.
5 #
6 #####
7
8 #
9 # REQUIRED R PACKAGES
10 #
11
12 require(Matrix)
13
14 #
15 # END REQUIRED R PACKAGES
16 #
17
18 #
19 # PREPROCESSING
20 #
21
22 # Specify directory for general subroutines
23 gen_dir = "../..../Code"
24
25 # Source supporting R function
26 source(paste(gen_dir,"/prepro.r",sep=""))
27
28 # Specify directory for application subroutines
29 app_dir = "../..../Code"
30
31 # Specify root data directory
32 dat_dir = "../..../Data"
33
34 # Specify calibration data directories
35 dat_cal = c("seismic_cal.csv",
36 "acoustic_cal.csv",
37 "optical_cal.csv",
38 "crater_cal.csv")
39
```



```

40 # Phenomenologies for this analysis
41 # 1 - seismic
42 # 2 - acoustic
43 # 3 - optical
44 # 4 - crater (surface effects)
45
46 # Indicate presence of calibration inference parameters
47 calp = FALSE
48
49 if(calp){
50 # Names of calibration inference parameters
51 #cal_par_names =
52 } else { cal_par_names = NULL }
53
54 # Specify number of responses for each phenomenology
55 Rh = c(2,2,2,2)
56
57 # Empirical model parameter count: common
58 # list with elements corresponding to phenomenologies
59 pbeta = vector("list",length(Rh))
60 for(hh in 1:length(Rh)){ pbeta[[hh]] = numeric(Rh[hh]) }
61 # phenomenology 2
62 pbeta[[2]] = c(2,2)
63 # phenomenology 3
64 pbeta[[3]] = c(2,2)
65 # phenomenology 4
66 pbeta[[4]] = c(2,2)
67
68 # Specify number of emplacement conditions for each phenomenology
69 Th = TRUE
70
71 if(Th){ Th = c(3,3,0,0)
72 } else { Th = NULL }
73
74 # Empirical model parameter count: emplacement condition
75 # list with elements corresponding to phenomenologies
76 if(!is.null(Th)){
77 pbetat = vector("list",length(Rh))
78 for(hh in 1:length(Rh)){
79 if(Th[hh] > 1){ pbetat[[hh]] = vector("list",Th[hh]) }
80 }
81 # phenomenology 1
82 for(tt in 1:Th[1]){
83 pbetat[[1]][[tt]] = numeric(Rh[1])
84 pbetat[[1]][[tt]] = c(5,5)

```

```

85 }
86 # phenomenology 2
87 for(tt in 1:Th[2]){
88 pbetat[[2]][[tt]] = numeric(Rh[2])
89 pbetat[[2]][[tt]] = c(1,1)
90 }
91 } else { pbetat = NULL }
92
93 # Locations of common parameters in full parameter vector
94 # list with elements corresponding to phenomenologies
95 if(!is.null(Th)){
96 ibetar = vector("list",length(Rh))
97 for(hh in 1:length(Rh)){
98 if(Th[hh] > 1){
99 # lists with elements for each response within
100 # emplacement condition
101 ibetar[[hh]] = vector("list",Th[hh]*Rh[hh])
102 }
103 }
104 # phenomenology 2
105 for(tt in 1:Th[2]){
106 for(rr in 1:Rh[2]){
107 ibetar[[2]][[(tt-1)*Rh[2]+rr]] = 1:2
108 }
109 }
110 } else { ibetar = NULL }
111
112 # Indicate analysis with errors-in-variables (eiv)
113 eiv = TRUE
114
115 # Specifications for errors-in-variables
116 if(eiv){
117 # Specify phenomenologies utilizing
118 # errors-in-variables yields
119 ieiv = 3:4
120
121 # Errors-in-variables source lists by
122 # phenomenology
123 seiv = vector("list",length(Rh))
124 for(hh in ieiv){ seiv[[hh]] = "ALL" }
125
126 # Set standard deviation of eiv Gaussian likelihood
127 eiv_w_sd = 0.1/3
128 } else {
129 ieiv = NULL

```

```

130 seiv = NULL
131 eiv_w_sd = NULL
132 }
133
134 # Specify Error Model
135 # Level 1 variance component parameter count
136 pvc_1 = TRUE
137
138 if(pvc_1){
139 pvc_1 = vector("list",length(Rh))
140 for(hh in 1:length(Rh)){ pvc_1[[hh]] = numeric(Rh[hh]) }
141 # phenomenology 1
142 pvc_1[[1]] = c(1,1)
143 # phenomenology 2
144 pvc_1[[2]] = c(1,1)
145 } else { pvc_1 = NULL }
146
147 # Level 2 variance component parameter count
148 pvc_2 = TRUE
149
150 if(pvc_2){
151 pvc_2 = vector("list",length(Rh))
152 for(hh in 1:length(Rh)){ pvc_2[[hh]] = numeric(Rh[hh]) }
153 # phenomenology 1
154 pvc_2[[1]] = c(1,1)
155 # phenomenology 2
156 #pvc_2[[2]] =
157
158 # path error models by phenomenology
159 ptype = vector("list",length(Rh))
160 # phenomenology 1
161 #ptype[[1]] =
162 } else { pvc_2 = NULL; ptype = NULL; }
163
164 # Set flag for user-provided code to calculate variance
165 # component coefficient matrices
166 calc_Z = FALSE
167
168 # Set flag for bounded optimization
169 # currently only supported for new event parameters
170 opt_B = FALSE
171
172 # Indicate analysis of new event (nev)
173 nev = TRUE
174

```

```

175 # Specifications for new event
176 if(nev){
177 # Specify new event data directories
178 dat_new = c("seismic_new.csv",
179 "acoustic_new.csv",
180 "optical_new.csv",
181 "crater_new.csv")
182
183 # Names of new event inference parameters
184 theta_names = c("W","HOB")
185
186 # Indicate nev parameter transform
187 itransform = FALSE
188
189 # Specify fixed parameters for nev parameter transform
190 if(itransform){
191 tPars = TRUE
192
193 if(tPars){
194 tPars = vector("list",0)
195 tPars$yield_scaling = 1/3
196 } else { tPars = NULL }
197 } else { tPars = NULL }
198
199 # Set up parameter constraints
200 # lower and upper bounds (use -Inf and Inf if unbounded)
201 lb_theta0 = rep(-Inf,length(theta_names))
202 lb_theta0[2] = -10
203 ub_theta0 = rep(Inf,length(theta_names))
204 ub_theta0[2] = 160
205
206 # Set up parameter subsets by phenomenology
207 tsub = TRUE
208
209 if(tsub){
210 tsub = vector("list",length(Rh))
211 tsub[[4]] = 1 # only log-yield for crater
212 } else { tsub = NULL }
213 } else {
214 dat_new = NULL
215 theta_names = NULL
216 itransform = FALSE
217 tPars = NULL
218 lb_theta0 = NULL
219 ub_theta0 = NULL

```

```

220 tsub = NULL
221 }
222
223 # Preprocessing for statistical analysis routines
224 tmp = prepro(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,bopt=opt_B,
225 nev=nev,itr=itransform,izmat=calc_Z,ieiv=ieiv,seiv=seiv,
226 ewsd=eiv_w_sd,Th=Th,pbetat=pbetat,ibetar=ibetar,
227 pvc_1=pvc_1,pvc_2=pvc_2,ptype=ptype,tnames=theta_names,
228 cnames=cal_par_names,fp_tr=tPars,tlb=lb_theta0,
229 tub=ub_theta0,ndir=dat_new,tsub=tsub)
230 if(opt_B){
231 p_cal = tmp$p_cal
232 t_cal = tmp$t_cal
233 } else {
234 p_cal = tmp
235 t_cal = NULL
236 }
237 rm(tmp)
238 save.image()
239
240 #
241 # END PREPROCESSING
242 #

```

## B.2 Maximum Likelihood Estimation

```
1 #
2 # MAXIMUM LIKELIHOOD CALCULATION
3 #
4
5 # Source supporting R function
6 source(paste(gen_dir,"/calc_mle.r",sep=""))
7
8 # Set seed for repeatability of analysis
9 set.seed(611)
10
11 # Names of forward models for each response
12 # by phenomenology
13 fm = vector("list",length(Rh))
14 fm[[1]] = c("f_s","f_s")
15 fm[[2]] = c("f_a","f_a")
16 fm[[3]] = c("f_o","f_o")
17 fm[[4]] = c("f_c","f_c")
18
19 # Indicate if forward model gradients provided
20 igrad = TRUE
21
22 if(igrad){
23 # Names of forward model gradients for each response
24 # by phenomenology
25 gfm = vector("list",length(Rh))
26 gfm[[1]] = c("g_s","g_s")
27 gfm[[2]] = c("g_a","g_a")
28 gfm[[3]] = c("g_o","g_o")
29 gfm[[4]] = c("g_c","g_c")
30 } else { gfm = NULL }
31
32 # Specifications for forward model calculations
33 # a) flags for modified forward model calculation by
34 # response for each relevant phenomenology
35 iResponse = TRUE
36
37 if(iResponse){
38 iResponse = vector("list",length(Rh))
39 iResponse[[1]] = c(TRUE,FALSE)
40 iResponse[[2]] = c(TRUE,FALSE)
41 } else { iResponse = NULL }
42
43 # b) fixed quantities required by forward models
```

```

44 fPars = TRUE
45
46 if(fPars){
47 fPars = vector("list",length(Rh))
48 fPars[[1]]$yield_scaling = 1/3
49 fPars[[2]]$yield_scaling = 1/3
50 fPars[[2]]$pressure_scaling = 1/3
51 fPars[[2]]$temp_scaling = 1/2
52 fPars[[3]]$yield_scaling = 1/3
53 fPars[[3]]$pressure_scaling = 1/3
54 fPars[[3]]$temp_scaling = 1/2
55 } else { fPars = NULL }
56
57 # Specify number of starting values for optimization
58 nstart = 10
59
60 # number of cores to use for optimization
61 ncores_mle = 1
62
63 # Indicate use of BFGS optimization methods
64 bfgs = TRUE
65
66 # Location of R data files with starting values
67 # for input to MLE optimization
68 opt_files_in = c("../Opt/opt_1.RData",
69 "../Opt/opt_2.RData",
70 "../Opt/opt_3_eiv.RData",
71 "../Opt/opt_4_eiv.RData")
72
73 # Location of R data file to write the results of
74 # MLE optimization
75 opt_files_out = "../opt.RData"
76
77 if(calp){
78 # Initial start value for calibration inference parameters
79 cst = FALSE
80
81 if(cst){
82 cst = numeric(p_cal$ncalp)
83 #cst[1] =
84 } else { cst = NULL }
85 } else { cst = NULL }
86
87 if(nev){
88 # Initial start value for theta0

```

```

89 tst = TRUE
90
91 if(tst){
92 tst = numeric(p_cal$ntheta0)
93 tst[2] = runif(1,-1.e-6,1.e-6)
94 } else { tst = NULL }
95 } else { tst = NULL }
96
97 if(calp || nev){
98 # Confidence interval levels
99 ci_lev = 0.95
100 } else { ci_lev = NULL }
101
102 # Indicate phenomenology number and type (if needed
103 # for postprocessing)
104 Phen = TRUE
105
106 if(Phen){
107 Phen = matrix(c(1,"Seismic"),nrow=1)
108 } else { Phen = NULL }
109
110 # Indicator of MLE gradient check
111 mle_grad_ck = TRUE
112
113 # Strategy for running parallel jobs (future package)
114 parallel_plan = "multicore"
115
116 # MLE calculations
117 p_cal = calc_mle(p_cal,gen_dir,app_dir,fm,nst=nstart,ncor=ncores_mle,
118 ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,igrck=mle_grad_ck,
119 t_cal=t_cal,g=gfm,iresp=iResponse,fp_fm=fPars,
120 fopt_in=opt_files_in,Xst=NULL,tst=tst,cst=cst,
121 fopt_out=opt_files_out,phen=Phen,pl=parallel_plan)
122 save.image()
123
124 #
125 # END MAXIMUM LIKELIHOOD CALCULATION
126 #

```



## B.3 Bayesian Analysis

```
1 #
2 # BAYESIAN ANALYSIS
3 #
4
5 # Specify if Bayesian analysis is to be conducted
6 iBayes = TRUE
7
8 if(iBayes){
9 # Source supporting R function
10 source(paste(gen_dir,"/calc_bayes.r",sep=""))
11
12 # Indicator of prior distribution for forward model
13 # coefficients
14 iBetaPrior = TRUE
15
16 if(iBetaPrior){
17 # location of code for computing log-prior densities and gradients
18 prior_files_beta = "../Code/lp_beta.s.r"
19 if(igrad){
20 gr_prior_files_beta = "../Code/glp_beta.s.r"
21 } else { gr_prior_files_beta = NULL }
22
23 # prior distribution for phenomenology 1
24 # forward model coefficients
25 p_cal$h[[1]]$lp_betat = vector("list",Th[1])
26 for(tt in 1:Th[1]){
27 p_cal$h[[1]]$lp_betat[[tt]]$f = c("lp_s","lp_s")
28 if(igrad){
29 p_cal$h[[1]]$lp_betat[[tt]]$g = c("lq_s","lq_s")
30 }
31 }
32 } else {
33 prior_files_beta = NULL
34 gr_prior_files_beta = NULL
35 }
36
37 # Indicator of prior distribution for calibration parameters
38 iCalPrior = TRUE
39
40 if(calp && iCalPrior){
41 # location of code for computing log-prior densities and gradients
42 prior_files_calp = NULL
43 if(igrad){
```

```

44 gr_prior_files_calp = NULL
45 } else { gr_prior_files_calp = NULL }
46
47 # prior distribution for calibration parameters (calp)
48 p_callp_calpf = "lp_c"
49 if(igrad){ p_callp_calpg = "lq_c" }
50
51 # parameters for calibration parameter prior distribution
52 #p_cal$pi_c_mu =
53 #p_cal$pi_c_sd =
54 } else {
55 prior_files_calp = NULL
56 gr_prior_files_calp = NULL
57 }
58
59 # Indicator of prior distribution for theta0
60 iTheta0Prior = FALSE
61
62 if(nev && iTheta0Prior){
63 # location of code for computing log-prior densities and gradients
64 prior_files_theta0 = NULL
65 if(igrad){
66 gr_prior_files_theta0 = NULL
67 } else { gr_prior_files_theta0 = NULL }
68
69 # prior distribution for new event parameters (theta0)
70 p_callp_theta0f = "lp_0"
71 if(igrad){ p_callp_theta0g = "lq_0" }
72
73 # parameters for log yield parameter prior (Gaussian)
74 p_cal$pi_w_mu = (log(10)+log(10000000))/2
75 p_cal$pi_w_sd = (log(10000000)-log(10))/6
76 # parameters for HOB/DOB parameter prior (Gaussian)
77 p_cal$pi_h_mu = 0
78 p_cal$pi_h_sd = 160/3
79 } else {
80 prior_files_theta0 = NULL
81 gr_prior_files_theta0 = NULL
82 }
83
84 # fixed scale parameters for variance component prior
85 # comment out if these parameters should vary
86 p_cal$A = 20
87
88 # eta parameter in Lewandowski-Kurowicka-Joe (LKJ) prior

```

```

89 # distribution for correlation parameters
90 p_callp_correta = 1
91
92 # FGSN parameters for errors-in-variables yields prior
93 # number of components
94 p_cal$K = 0
95 # total number of FGSN parameters
96 p_cal$p_fgsn = 0
97 if(eiv){
98 p_cal$K = 2
99 p_cal$p_fgsn = p_cal$K + 2
100 }
101
102 # specify Markov chain Monte Carlo (MCMC) algorithm
103 # options: "RAM", "FME", or "NUTS"
104 iMCMC = "FME"
105
106 # burn-in
107 nburn = 10000
108
109 # production
110 nmcmc = 20000
111
112 # posterior sample thinning rate
113 nthin = 20
114
115 # number of cores to use for optimization
116 ncores_map = 1
117
118 # number of cores to use for generating parallel MCMC chains
119 ncores_mc = 1
120
121 # Indicator of prior gradient check
122 prior_grad_ck = TRUE
123
124 # Indicator of posterior gradient check
125 post_grad_ck = TRUE
126
127 # Bayesian calculations
128 p_cal = calc_bayes(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
129 nmcmc=nmcmc,nthin=nthin,ncor_map=ncores_map,
130 ncor_mc=ncores_mc,igrad=igrad,
131 igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
132 bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
133 itpr=iTheta0Prior,fpr_b=prior_files_beta,

```

```

134 fgpr_b=gr_prior_files_beta,fpr_c=prior_files_calp,
135 fgpr_c=gr_prior_files_calp,
136 fpr_t=prior_files_theta0,
137 fgpr_t=gr_prior_files_theta0,Xnom=NULL,
138 imcmc=iMCMC,pl=parallel_plan,t_cal=t_cal)
139 save.image()
140 }
141
142 #
143 # END BAYESIAN ANALYSIS
144 #

```

## B.4 Output File

```
1 > # Preprocessing for statistical analysis routines
2 > tmp = prepro(gen_dir,app_dir,dat_dir,dat_cal,Rh,pbeta,bopt=opt_B,
3 + nev=nev,itr=itransform,izmat=calc_Z,ieiv=ieiv,seiv=seiv,
4 + ewsd=eiv_w_sd,Th=Th,pbetat=pbetat,ibetar=ibetar,
5 + pvc_1=pvc_1,pvc_2=pvc_2,ptype=ptype,tname=theta_names,
6 + cnames=cal_par_names,fp_tr=tPars,tlb=lb_theta0,
7 + tub=ub_theta0,ndir=dat_new,tsub=tsub)
8 [1] "Warning: Insufficient Paths for Level 2 Variance Component models with
9 Phenomenology 2 and Response 1."
10 [1] "Warning: Insufficient Paths for Level 2 Variance Component models with
11 Phenomenology 2 and Response 2."
12 [1] "Warning: Insufficient number of observations per Source for Variance
13 Component models with Phenomenology 3 and Response 1."
14 [1] "Warning: Insufficient number of observations per Source for Variance
15 Component models with Phenomenology 3 and Response 2."
16 [1] "Warning: Insufficient number of observations per Source for Variance
17 Component models with Phenomenology 4 and Response 1."
18 [1] "Warning: Insufficient number of observations per Source for Variance
19 Component models with Phenomenology 4 and Response 2."
20
21 > # MLE calculations
22 > p_cal = calc_mle(p_cal,gen_dir,app_dir,fm,nst=nstart,ncor=ncores_mle,
23 + ci_lev=ci_lev,igrad=igrad,bfgs=bfgs,igrck=mle_grad_ck,
24 + t_cal=t_cal,g=gfm,iresp=iResponse,fp_fm=fPars,
25 + fopt_in=opt_files_in,Xst=NULL,tst=tst,cst=cst,
26 + fopt_out=opt_files_out,phen=Phen,pl=parallel_plan)
27 [1] "MLE CONVERGENCE STATUS"
28
29 [1] 0
30 [1] 2
31 [1] "MAXIMUM LIKELIHOOD SUMMARY"
32
33 [1] "NEW EVENT INFERENCE PARAMETERS"
34
35 [1] "ESTIMATE: "
36
37 W HOB
38 14.02 -2.62
39
40 [1] "STANDARD DEVIATION: "
41
42 W HOB
43 0.05 1.93
```

```

44
45 [1] "CORRELATION MATRIX: "
46
47 W HOB
48 W 1.00 -0.44
49 HOB -0.44 1.00
50
51 [1] "95%: CONFIDENCE INTERVAL:"
52
53 W HOB
54 lb 13.92 -5.35
55 ub 14.12 3.18
56
57
58 [1] "ERRORS-IN-VARIABLES YIELDS"
59
60 7 8 9 10 11 13 14 16 17 20 21 22 23
61 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
62 24 25 28 29 30 31 33 34 35 36 37 38 39
63 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
64
65 [1] "COMMON COEFFICIENTS"
66
67 [1] "Phenomenology: 2; Response: 1"
68
69 [1] 6.67 -1.14
70
71 [1] "Phenomenology: 2; Response: 2"
72
73 [1] -5.08 0.23
74
75 [1] "Phenomenology: 3; Response: 1"
76
77 [1] -11.07 1.89
78
79 [1] "Phenomenology: 3; Response: 2"
80
81 [1] -8.64 1.71
82
83 [1] "Phenomenology: 4; Response: 1"
84
85 [1] -3.31 0.43
86
87 [1] "Phenomenology: 4; Response: 2"
88

```

89           [1] -2.38 0.28

90

91 [1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

92

93           [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

94

95           [1] -10.07 -1.31 -1.43 3.53 0.40

96

97           [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

98

99           [1] -1.52 -1.44 -1.23 2.29 0.63

100

101           [1] "Phenomenology: 1; Emplacement: 2; Response: 1"

102

103           [1] -11.48 -1.09 -3.59 4.32 0.16

104

105           [1] "Phenomenology: 1; Emplacement: 2; Response: 2"

106

107           [1] -2.19 -1.22 -26.48 0.99 -2.65

108

109           [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

110

111           [1] -9.53 -1.16 -4.47 4.95 0.34

112

113           [1] "Phenomenology: 1; Emplacement: 3; Response: 2"

114

115           [1] -2.85 -0.71 -2.10 2.68 0.13

116

117           [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

118

119           [1] 3.87

120

121           [1] "Phenomenology: 2; Emplacement: 1; Response: 2"

122

123           [1] -0.17

124

125           [1] "Phenomenology: 2; Emplacement: 2; Response: 1"

126

127           [1] 3.12

128

129           [1] "Phenomenology: 2; Emplacement: 2; Response: 2"

130

131           [1] -0.9

132

133           [1] "Phenomenology: 2; Emplacement: 3; Response: 1"

```

134
135 [1] 2.16
136
137 [1] "Phenomenology: 2; Emplacement: 3; Response: 2"
138
139 [1] -0.94
140
141 [1] "LEVEL 1 VARIANCE COMPONENTS"
142
143 [1] "Phenomenology: 1; Response: 1"
144
145 [1] 0.0011
146
147 [1] "Phenomenology: 1; Response: 2"
148
149 [1] 0.0016
150
151 [1] "Phenomenology: 2; Response: 1"
152
153 [1] 0.0037
154
155 [1] "Phenomenology: 2; Response: 2"
156
157 [1] 0.0015
158
159 [1] "LEVEL 2 VARIANCE COMPONENTS"
160
161 [1] "Phenomenology: 1; Response: 1"
162
163 [1] 0.001
164
165 [1] "Phenomenology: 1; Response: 2"
166
167 [1] 9e-04
168
169 [1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"
170
171 [1] "Phenomenology 1"
172
173 [1] "Variances"
174
175 [1] 0.0021 0.0034
176
177 [1] "Correlations"
178

```



```

179 [,1] [,2]
180 [1,] 1 0.27
181 [2,] 0 1.00
182
183 [1] "Phenomenology 2"
184
185 [1] "Variances"
186
187 [1] 1e-03 3e-04
188
189 [1] "Correlations"
190
191 [,1] [,2]
192 [1,] 1 -0.25
193 [2,] 0 1.00
194
195 [1] "Phenomenology 3"
196
197 [1] "Variances"
198
199 [1] 0.0011 0.0010
200
201 [1] "Correlations"
202
203 [,1] [,2]
204 [1,] 1 0.93
205 [2,] 0 1.00
206
207 [1] "Phenomenology 4"
208
209 [1] "Variances"
210
211 [1] 0.0222 0.0087
212
213 [1] "Correlations"
214
215 [,1] [,2]
216 [1,] 1 0.65
217 [2,] 0 1.00
218
219 [1] "AIC = -5913.11"
220
221 [1] "BIC = -5573.35"
222
223 Loading required package: numDeriv

```

```

224 [1] "CHECK LOG-LIKELIHOOD GRADIENTS"
225
226 [1] "Analytic gradient"
227 [1] 5.112159e-04 -2.542508e-05 -1.863792e-03 6.228479e-04 -1.625812e-03
228 [6] 1.907117e-03 2.310639e-04 8.065429e-04 -8.404374e-05 -9.984542e-04
229 [11] -4.226071e-04 -1.989370e-03 -1.157463e-03 1.812303e-03 3.537858e-03
230 [16] -2.784636e-03 7.371172e-04 7.547859e-04 -1.494877e-03 4.223703e-03
231 [21] 1.534175e-03 -2.357543e-03 1.895850e-03 -3.989834e-04 1.732983e-03
232 [26] 9.354533e-04 -4.440143e-05 9.331977e-06 -2.694365e-03 -4.299476e-02
233 [31] -1.507931e-02 -2.445686e-01 -3.765500e-02 -7.708215e-04 2.986042e-02
234 [36] 6.118387e-03 -6.676220e-04 -1.555101e-02 1.448662e-03 2.788605e-02
235 [41] 9.125824e-04 2.695089e-04 -2.401801e-03 -1.526986e-04 -4.231445e-04
236 [46] -1.511128e-03 1.417248e-03 1.029923e-03 -1.364681e-04 3.342011e-04
237 [51] -1.656650e-02 -1.223063e-01 4.508649e-02 3.934503e-03 -7.615629e-03
238 [56] 1.978269e-03 1.821235e-03 4.439611e-03 1.006111e-02 4.886488e-03
239 [61] -3.438471e-04 2.571739e-03 1.720799e-03 2.864180e-04 -7.508282e-04
240 [66] 9.688080e-04 2.185358e-03 -1.105926e-03 1.041878e-04 -4.157820e-04
241 [71] 5.369795e-04 -4.609019e-04 2.385899e-04 -6.059969e-05 3.177182e-04
242 [76] 2.788174e-04 5.402526e-04 2.458910e-04 -3.436638e-05 -1.133472e-04
243 [81] -3.018574e-04 -1.905102e-04 1.069394e-04 5.970366e-04 -5.390348e-04
244 [86] 6.469861e-04 2.939823e-05 1.613974e-01 8.178509e-04 6.931910e-04
245 [91] 2.285890e-02 -1.018627e-04 4.539666e-05 2.014041e-04
246 [1] "Numerical gradient"
247 [1] 5.112092e-04 -2.539405e-05 -1.863777e-03 6.228507e-04 -1.625809e-03
248 [6] 1.907111e-03 2.310578e-04 8.065436e-04 -8.404145e-05 -9.984549e-04
249 [11] -4.225894e-04 -1.989392e-03 -1.157464e-03 1.812304e-03 3.537854e-03
250 [16] -2.784620e-03 7.370990e-04 7.547591e-04 -1.494772e-03 4.223713e-03
251 [21] 1.534173e-03 -2.357541e-03 1.895848e-03 -3.989830e-04 1.732981e-03
252 [26] 9.354541e-04 -4.440477e-05 9.337693e-06 -2.694363e-03 -4.299474e-02
253 [31] -1.507930e-02 -2.445664e-01 -3.765495e-02 -7.709241e-04 2.986035e-02
254 [36] 6.117932e-03 -6.675813e-04 -1.555099e-02 1.448742e-03 2.788585e-02
255 [41] 9.125534e-04 2.693702e-04 -2.401588e-03 -1.526865e-04 -4.228457e-04
256 [46] -1.511103e-03 1.417144e-03 1.029829e-03 -1.364287e-04 3.343325e-04
257 [51] -1.656650e-02 -1.223064e-01 4.508646e-02 3.934508e-03 -7.616756e-03
258 [56] 1.978321e-03 1.821328e-03 4.439639e-03 1.006101e-02 4.886500e-03
259 [61] -3.438479e-04 2.571653e-03 1.720924e-03 2.864399e-04 -7.508463e-04
260 [66] 9.688664e-04 2.185367e-03 -1.105973e-03 1.041493e-04 -4.163252e-04
261 [71] 5.369532e-04 -4.615999e-04 2.386148e-04 -6.041131e-05 3.177212e-04
262 [76] 2.789338e-04 5.402541e-04 2.458948e-04 -3.428431e-05 -1.133899e-04
263 [81] -3.018444e-04 -1.905103e-04 1.069402e-04 5.970440e-04 -5.336226e-04
264 [86] 6.470927e-04 2.945024e-05 1.614883e-01 8.171414e-04 6.932402e-04
265 [91] 2.286268e-02 -1.016709e-04 4.562640e-05 2.005773e-04
266 [1] "Difference"
267 [1] -9.084942e-05 1.126289e-06
268

```

```

269 + # Bayesian calculations
270 + p_cal = calc_bayes(p_cal,gen_dir,app_dir,nst=nstart,nburn=nburn,
271 + nmcmmc=nmcmmc,nthin=nthin,ncor_map=ncores_map,
272 + ncor_mc=ncores_mc,igrad=igrad,
273 + igrck_pr=prior_grad_ck,igrck_po=post_grad_ck,
274 + bfgs=bfgs,ibpr=iBetaPrior,icpr=iCalPrior,
275 + itpr=iTheta0Prior,fpr_b=prior_files_beta,
276 + fgpr_b=gr_prior_files_beta,fpr_c=prior_files_calp,
277 + fgpr_c=gr_prior_files_calp,
278 + fpr_t=prior_files_theta0,
279 + fgpr_t=gr_prior_files_theta0,Xnom=NULL,
280 + imcmc=iMCMC,pl=parallel_plan,t_cal=t_cal)
281 + save.image()
282 + }
283 [1] "MAP CONVERGENCE STATUS"
284
285 [1] 0
286 [1] 2
287 [1] "MAXIMUM A POSTERIORI SUMMARY"
288
289 [1] "NEW EVENT INFERENCE PARAMETERS"
290
291 [1] "ESTIMATE: "
292
293 W HOB
294 14.01 2.30
295
296
297 [1] "ERRORS-IN-VARIABLES YIELDS"
298
299 7 8 9 10 11 13 14 16 17 20 21 22 23
300 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
301 24 25 28 29 30 31 33 34 35 36 37 38 39
302 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
303
304 [1] "COMMON COEFFICIENTS"
305
306 [1] "Phenomenology: 2; Response: 1"
307
308 [1] 6.67 -1.14
309
310 [1] "Phenomenology: 2; Response: 2"
311
312 [1] -5.08 0.23
313

```

314 [1] "Phenomenology: 3; Response: 1"  
 315  
 316 [1] -11.07 1.89  
 317  
 318 [1] "Phenomenology: 3; Response: 2"  
 319  
 320 [1] -8.64 1.71  
 321  
 322 [1] "Phenomenology: 4; Response: 1"  
 323  
 324 [1] -3.31 0.43  
 325  
 326 [1] "Phenomenology: 4; Response: 2"  
 327  
 328 [1] -2.38 0.28  
 329  
 330 [1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"  
 331  
 332 [1] "Phenomenology: 1; Emplacement: 1; Response: 1"  
 333  
 334 [1] -10.06 -1.31 -1.44 3.49 0.38  
 335  
 336 [1] "Phenomenology: 1; Emplacement: 1; Response: 2"  
 337  
 338 [1] -1.50 -1.44 -1.25 2.24 0.61  
 339  
 340 [1] "Phenomenology: 1; Emplacement: 2; Response: 1"  
 341  
 342 [1] -11.48 -1.09 -3.60 4.25 0.16  
 343  
 344 [1] "Phenomenology: 1; Emplacement: 2; Response: 2"  
 345  
 346 [1] -2.13 -1.22 -159.29 0.90 -4.47  
 347  
 348 [1] "Phenomenology: 1; Emplacement: 3; Response: 1"  
 349  
 350 [1] -9.53 -1.16 -4.47 4.95 0.34  
 351  
 352 [1] "Phenomenology: 1; Emplacement: 3; Response: 2"  
 353  
 354 [1] -2.85 -0.71 -2.15 2.61 0.10  
 355  
 356 [1] "Phenomenology: 2; Emplacement: 1; Response: 1"  
 357  
 358 [1] 3.87

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359
360 [1] "Phenomenology: 2; Emplacement: 1; Response: 2"
361
362 [1] -0.17
363
364 [1] "Phenomenology: 2; Emplacement: 2; Response: 1"
365
366 [1] 3.11
367
368 [1] "Phenomenology: 2; Emplacement: 2; Response: 2"
369
370 [1] -0.91
371
372 [1] "Phenomenology: 2; Emplacement: 3; Response: 1"
373
374 [1] 2.16
375
376 [1] "Phenomenology: 2; Emplacement: 3; Response: 2"
377
378 [1] -0.94
379
380 [1] "LEVEL 1 VARIANCE COMPONENTS"
381
382 [1] "Phenomenology: 1; Response: 1"
383
384 [1] 0.0012
385
386 [1] "Phenomenology: 1; Response: 2"
387
388 [1] 0.0017
389
390 [1] "Phenomenology: 2; Response: 1"
391
392 [1] 0.0039
393
394 [1] "Phenomenology: 2; Response: 2"
395
396 [1] 0.0016
397
398 [1] "LEVEL 2 VARIANCE COMPONENTS"
399
400 [1] "Phenomenology: 1; Response: 1"
401
402 [1] 0.001
403

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```

404 [1] "Phenomenology: 1; Response: 2"
405
406 [1] 0.001
407
408 [1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"
409
410 [1] "Phenomenology 1"
411
412 [1] "Variances"
413
414 [1] 0.0021 0.0034
415
416 [1] "Correlations"
417
418 [,1] [,2]
419 [1,] 1 0.27
420 [2,] 0 1.00
421
422 [1] "Phenomenology 2"
423
424 [1] "Variances"
425
426 [1] 1e-03 3e-04
427
428 [1] "Correlations"
429
430 [,1] [,2]
431 [1,] 1 -0.25
432 [2,] 0 1.00
433
434 [1] "Phenomenology 3"
435
436 [1] "Variances"
437
438 [1] 9e-04 9e-04
439
440 [1] "Correlations"
441
442 [,1] [,2]
443 [1,] 1 0.92
444 [2,] 0 1.00
445
446 [1] "Phenomenology 4"
447
448 [1] "Variances"

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449
450 [1] 0.0196 0.0071
451
452 [1] "Correlations"
453
454 [,1] [,2]
455 [1,] 1 0.52
456 [2,] 0 1.00
457
458 [1] "FGSN PRIOR PARAMETERS"
459
460 [1] "Alpha = 17.33"
461 [1] "Lambda squared = 8.05"
462 [1] "Omega = -1.65" "Omega = 0.56"
463
464 [1] "CHECK LOG-PRIOR GRADIENTS"
465
466 [1] "Analytic gradient"
467 [1] 0.000000e+00 7.980369e-01 -1.043263e-01 -8.247890e-02 -1.766663e-01
468 [6] -2.122515e-01 -3.470393e-01 1.996855e+00 -5.420832e-01 -4.415773e-01
469 [11] -1.814653e-01 3.548269e-01 5.536912e-02 -5.491970e-01 1.851314e-01
470 [16] 1.968395e-02 -1.633027e-01 3.474537e-01 2.182895e+00 -5.838604e-01
471 [21] -3.733141e-01 -6.350369e-01 -5.217498e-01 3.876847e-01 2.520478e-01
472 [26] -2.463583e-01 1.526028e-01 -7.433990e-01 0.000000e+00 0.000000e+00
473 [31] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
474 [36] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
475 [41] 0.000000e+00 0.000000e+00 1.000000e+00 0.000000e+00 0.000000e+00
476 [46] 0.000000e+00 0.000000e+00 1.000000e+00 0.000000e+00 0.000000e+00
477 [51] 0.000000e+00 0.000000e+00 7.782174e-01 0.000000e+00 0.000000e+00
478 [56] 0.000000e+00 0.000000e+00 9.276835e-02 0.000000e+00 0.000000e+00
479 [61] 0.000000e+00 0.000000e+00 6.610552e-01 0.000000e+00 0.000000e+00
480 [66] 0.000000e+00 0.000000e+00 1.000000e+00 0.000000e+00 0.000000e+00
481 [71] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
482 [76] 0.000000e+00 4.999971e-01 4.999957e-01 4.999904e-01 4.999960e-01
483 [81] 4.999974e-01 4.999976e-01 -2.220446e-16 -7.766602e-01 -1.404975e+01
484 [86] 0.000000e+00 -8.150896e-01 4.186579e+01 -4.440892e-16 1.514024e+00
485 [91] -9.310054e+01 -4.440892e-16 -1.766204e-01 -1.871582e+01 -3.044490e-02
486 [96] -2.429394e-02 -7.026312e-02 -1.405367e-01
487 [1] "Numerical gradient"
488 [1] 0.000000e+00 7.980369e-01 -1.043263e-01 -8.247890e-02 -1.766663e-01
489 [6] -2.122515e-01 -3.470393e-01 1.996855e+00 -5.420832e-01 -4.415773e-01
490 [11] -1.814653e-01 3.548269e-01 5.536912e-02 -5.491970e-01 1.851314e-01
491 [16] 1.968395e-02 -1.633027e-01 3.474538e-01 2.182895e+00 -5.838604e-01
492 [21] -3.733141e-01 -6.350369e-01 -5.217498e-01 3.876847e-01 2.520478e-01
493 [26] -2.463583e-01 1.526028e-01 -7.433990e-01 0.000000e+00 0.000000e+00

```

```

494 [31] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
495 [36] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
496 [41] 0.000000e+00 0.000000e+00 1.000000e+00 0.000000e+00 0.000000e+00
497 [46] 0.000000e+00 0.000000e+00 1.000000e+00 0.000000e+00 0.000000e+00
498 [51] 0.000000e+00 0.000000e+00 7.782174e-01 0.000000e+00 0.000000e+00
499 [56] 0.000000e+00 0.000000e+00 9.276835e-02 0.000000e+00 0.000000e+00
500 [61] 0.000000e+00 0.000000e+00 6.610552e-01 0.000000e+00 0.000000e+00
501 [66] 0.000000e+00 0.000000e+00 1.000000e+00 0.000000e+00 0.000000e+00
502 [71] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
503 [76] 0.000000e+00 4.999971e-01 4.999957e-01 4.999904e-01 4.999960e-01
504 [81] 4.999974e-01 4.999976e-01 0.000000e+00 -7.766602e-01 -1.404975e+01
505 [86] 0.000000e+00 -8.150896e-01 4.186579e+01 2.753625e-20 1.514024e+00
506 [91] -9.310054e+01 1.333140e-16 -1.766204e-01 -1.871582e+01 -3.044490e-02
507 [96] -2.429394e-02 -7.026312e-02 -1.405367e-01
508 [1] "Difference"
509 [1] -5.909749e-08 7.107675e-07
510
511 [1] "CHECK LOG-POSTERIOR GRADIENTS"
512
513 [1] "Analytic gradient"
514 [1] 0.0652554710 0.2809128777 0.2776747288 0.1913483992 0.1640543443
515 [6] 0.4110787063 0.3053493374 0.2732904664 0.0689460969 0.0034688791
516 [11] -0.3275711254 -0.5398117514 0.1307987365 0.3776565007 0.1278625292
517 [16] -1.0163032877 -0.3003047036 -0.5183880602 -0.4898692700 0.3585217007
518 [21] 0.1201606000 -0.0253855445 0.3277713035 -0.0943793983 0.1286572477
519 [26] 0.0709557394 -0.2406661285 -0.1030212436 0.2253706895 0.0874951338
520 [31] -0.0918057138 0.7026903265 -0.1706238390 1.2547660142 -0.0055983437
521 [36] 0.8590244663 -0.0192460560 0.4013458092 -0.0654405703 -0.5828461460
522 [41] 0.1246405443 -0.0227052968 -0.0380441080 0.0041646414 0.0634785826
523 [46] -0.0197653236 0.0154455135 0.1004165465 -0.0645952411 0.0333200130
524 [51] -0.0217611223 0.1961083586 0.3975783892 0.0062887012 -0.0368259828
525 [56] 0.0234689167 -0.1709389850 0.0385639350 -0.0001195893 -0.2933159601
526 [61] -0.0091858079 0.0182733107 0.0555022779 0.0462591964 -0.0944073914
527 [66] -0.0296077888 0.1329141126 0.2394165121 0.0738754511 -0.0903148613
528 [71] 0.0482421120 -0.3823240575 -0.0177985898 0.0577506753 -0.1026839723
529 [76] 0.0120394755 0.0211923436 0.0150026326 -0.0237693383 -0.0250745269
530 [81] 0.0140009614 0.0128335916 0.0898737506 0.0054301676 0.0055953664
531 [86] 0.0285555250 -0.0256819332 0.6947476606 0.3170921643 0.3694779435
532 [91] -0.1589376117 -0.0032056661 0.0286115155 1.1214529943 -0.0304449029
533 [96] -0.0242939414 -0.0702631185 -0.1405366559
534 [1] "Numerical gradient"
535 [1] 0.0652554649 0.2809128894 0.2776747326 0.1913483933 0.1640543491
536 [6] 0.4110787091 0.3053493421 0.2732904738 0.0689461035 0.0034688910
537 [11] -0.3275711180 -0.5398117334 0.1307987382 0.3776564972 0.1278625377
538 [16] -1.0163032755 -0.3003047094 -0.5183880474 -0.4898692439 0.3585217045

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539 [21] 0.1201605998 -0.0253855458 0.3277713020 -0.0943793913 0.1286572464
540 [26] 0.0709557483 -0.2406661286 -0.1030212465 0.2253706584 0.0874950308
541 [31] -0.0918056653 0.7026919885 -0.1706238980 1.2547656219 -0.0055983545
542 [36] 0.8590243042 -0.0192460637 0.4013454211 -0.0654405498 -0.5828455748
543 [41] 0.1246405538 -0.0227052931 -0.0380437658 0.0041647257 0.0634790314
544 [46] -0.0197652454 0.0154455414 0.1004166175 -0.0645952838 0.0333197483
545 [51] -0.0217611143 0.1961083798 0.3975782937 0.0062887030 -0.0368266050
546 [56] 0.0234689285 -0.1709390734 0.0385639399 -0.0001195863 -0.2933159334
547 [61] -0.0091857966 0.0182732944 0.0555020405 0.0462592100 -0.0944077022
548 [66] -0.0296077430 0.1329142502 0.2394164763 0.0738755689 -0.0903175582
549 [71] 0.0482421097 -0.3823248767 -0.0177985940 0.0577507259 -0.1026839206
550 [76] 0.0120396687 0.0211923580 0.0150026541 -0.0237692800 -0.0250745786
551 [81] 0.0140009232 0.0128335996 0.0898737813 0.0054301772 0.0055855654
552 [86] 0.0285555874 -0.0256819816 0.6947811056 0.3170917052 0.3694781757
553 [91] -0.1589561195 -0.0032054142 0.0286116001 1.1214522097 -0.0304449021
554 [96] -0.0242939549 -0.0702630914 -0.1405367301
555 [1] "Difference"
556 [1] -3.344501e-05 1.850774e-05
557
558 [1] "ACCEPTANCE RATES:"
559
560 [1] "Core 1: 0.8525666666666667"
561
562 [1] "POSTERIOR SUMMARY"
563
564 [1] "NEW EVENT INFERENCE PARAMETERS"
565
566 [1] "POSTERIOR MEAN: 14.01" "POSTERIOR MEAN: 2.26"
567
568 [1] "POSTERIOR SD: 0.01" "POSTERIOR SD: 0.69"
569
570 [1] "LEVEL 2.5%: 13.98" "LEVEL 2.5%: 0.99"
571
572 [1] "LEVEL 5%: 13.99" "LEVEL 5%: 1.18"
573
574 [1] "LEVEL 50%: 14.01" "LEVEL 50%: 2.23"
575
576 [1] "LEVEL 95%: 14.03" "LEVEL 95%: 3.47"
577
578 [1] "LEVEL 97.5%: 14.04" "LEVEL 97.5%: 3.69"
579
580 [1] "CORRELATION MATRIX:"
581
582 W HOB
583 W 1.00 0.89

```

584 HOB 0.89 1.00

585

586 [1] "ERRORS-IN-VARIABLES YIELDS"

587

588 [1] "POSTERIOR MEAN: 16.28" "POSTERIOR MEAN: 16.21" "POSTERIOR MEAN: 16.51"

589 [4] "POSTERIOR MEAN: 16.61" "POSTERIOR MEAN: 17" "POSTERIOR MEAN: 12.21"

590 [7] "POSTERIOR MEAN: 17.57" "POSTERIOR MEAN: 17.27" "POSTERIOR MEAN: 16.52"

591 [10] "POSTERIOR MEAN: 14.5" "POSTERIOR MEAN: 15.75" "POSTERIOR MEAN: 17.6"

592 [13] "POSTERIOR MEAN: 15.24" "POSTERIOR MEAN: 15.87" "POSTERIOR MEAN: 16.46"

593 [16] "POSTERIOR MEAN: 14.53" "POSTERIOR MEAN: 12.13" "POSTERIOR MEAN: 17.71"

594 [19] "POSTERIOR MEAN: 23.08" "POSTERIOR MEAN: 23.41" "POSTERIOR MEAN: 17.51"

595 [22] "POSTERIOR MEAN: 21.96" "POSTERIOR MEAN: 22.34" "POSTERIOR MEAN: 16.71"

596 [25] "POSTERIOR MEAN: 21.02" "POSTERIOR MEAN: 18.52"

597

598 [1] "LEVEL 2.5%: 16.27" "LEVEL 2.5%: 16.2" "LEVEL 2.5%: 16.49"

599 [4] "LEVEL 2.5%: 16.59" "LEVEL 2.5%: 16.97" "LEVEL 2.5%: 12.2"

600 [7] "LEVEL 2.5%: 17.56" "LEVEL 2.5%: 17.25" "LEVEL 2.5%: 16.5"

601 [10] "LEVEL 2.5%: 14.48" "LEVEL 2.5%: 15.74" "LEVEL 2.5%: 17.58"

602 [13] "LEVEL 2.5%: 15.22" "LEVEL 2.5%: 15.86" "LEVEL 2.5%: 16.45"

603 [16] "LEVEL 2.5%: 14.51" "LEVEL 2.5%: 12.12" "LEVEL 2.5%: 17.7"

604 [19] "LEVEL 2.5%: 23.06" "LEVEL 2.5%: 23.4" "LEVEL 2.5%: 17.5"

605 [22] "LEVEL 2.5%: 21.94" "LEVEL 2.5%: 22.32" "LEVEL 2.5%: 16.69"

606 [25] "LEVEL 2.5%: 21" "LEVEL 2.5%: 18.5"

607

608 [1] "LEVEL 5%: 16.27" "LEVEL 5%: 16.2" "LEVEL 5%: 16.49" "LEVEL 5%: 16.59"

609 [5] "LEVEL 5%: 16.98" "LEVEL 5%: 12.2" "LEVEL 5%: 17.56" "LEVEL 5%: 17.25"

610 [9] "LEVEL 5%: 16.51" "LEVEL 5%: 14.49" "LEVEL 5%: 15.74" "LEVEL 5%: 17.59"

611 [13] "LEVEL 5%: 15.22" "LEVEL 5%: 15.86" "LEVEL 5%: 16.45" "LEVEL 5%: 14.52"

612 [17] "LEVEL 5%: 12.12" "LEVEL 5%: 17.7" "LEVEL 5%: 23.07" "LEVEL 5%: 23.4"

613 [21] "LEVEL 5%: 17.5" "LEVEL 5%: 21.95" "LEVEL 5%: 22.33" "LEVEL 5%: 16.69"

614 [25] "LEVEL 5%: 21.01" "LEVEL 5%: 18.5"

615

616 [1] "LEVEL 50%: 16.28" "LEVEL 50%: 16.21" "LEVEL 50%: 16.51" "LEVEL 50%: 16.61"

617 [5] "LEVEL 50%: 17" "LEVEL 50%: 12.21" "LEVEL 50%: 17.57" "LEVEL 50%: 17.27"

618 [9] "LEVEL 50%: 16.52" "LEVEL 50%: 14.5" "LEVEL 50%: 15.74" "LEVEL 50%: 17.6"

619 [13] "LEVEL 50%: 15.24" "LEVEL 50%: 15.87" "LEVEL 50%: 16.46" "LEVEL 50%: 14.53"

620 [17] "LEVEL 50%: 12.13" "LEVEL 50%: 17.71" "LEVEL 50%: 23.08" "LEVEL 50%: 23.41"

621 [21] "LEVEL 50%: 17.51" "LEVEL 50%: 21.96" "LEVEL 50%: 22.34" "LEVEL 50%: 16.71"

622 [25] "LEVEL 50%: 21.02" "LEVEL 50%: 18.52"

623

624 [1] "LEVEL 95%: 16.29" "LEVEL 95%: 16.22" "LEVEL 95%: 16.52" "LEVEL 95%: 16.62"

625 [5] "LEVEL 95%: 17.01" "LEVEL 95%: 12.23" "LEVEL 95%: 17.58" "LEVEL 95%: 17.28"

626 [9] "LEVEL 95%: 16.53" "LEVEL 95%: 14.51" "LEVEL 95%: 15.75" "LEVEL 95%: 17.61"

627 [13] "LEVEL 95%: 15.25" "LEVEL 95%: 15.88" "LEVEL 95%: 16.47" "LEVEL 95%: 14.54"

628 [17] "LEVEL 95%: 12.14" "LEVEL 95%: 17.72" "LEVEL 95%: 23.09" "LEVEL 95%: 23.43"

629 [21] "LEVEL 95%: 17.52" "LEVEL 95%: 21.97" "LEVEL 95%: 22.35" "LEVEL 95%: 16.72"  
630 [25] "LEVEL 95%: 21.03" "LEVEL 95%: 18.53"  
631  
632 [1] "LEVEL 97.5%: 16.3" "LEVEL 97.5%: 16.22" "LEVEL 97.5%: 16.52"  
633 [4] "LEVEL 97.5%: 16.63" "LEVEL 97.5%: 17.02" "LEVEL 97.5%: 12.23"  
634 [7] "LEVEL 97.5%: 17.59" "LEVEL 97.5%: 17.29" "LEVEL 97.5%: 16.53"  
635 [10] "LEVEL 97.5%: 14.51" "LEVEL 97.5%: 15.76" "LEVEL 97.5%: 17.61"  
636 [13] "LEVEL 97.5%: 15.25" "LEVEL 97.5%: 15.89" "LEVEL 97.5%: 16.48"  
637 [16] "LEVEL 97.5%: 14.54" "LEVEL 97.5%: 12.14" "LEVEL 97.5%: 17.72"  
638 [19] "LEVEL 97.5%: 23.09" "LEVEL 97.5%: 23.43" "LEVEL 97.5%: 17.52"  
639 [22] "LEVEL 97.5%: 21.98" "LEVEL 97.5%: 22.35" "LEVEL 97.5%: 16.73"  
640 [25] "LEVEL 97.5%: 21.03" "LEVEL 97.5%: 18.53"  
641  
642 [1] "COMMON COEFFICIENTS"  
643  
644 [1] "Phenomenology: 2; Response: 1"  
645  
646 [1] "POSTERIOR MEAN: 6.67" "POSTERIOR MEAN: -1.14"  
647  
648 [1] "LEVEL 2.5%: 6.66" "LEVEL 2.5%: -1.14"  
649  
650 [1] "LEVEL 5%: 6.66" "LEVEL 5%: -1.14"  
651  
652 [1] "LEVEL 50%: 6.67" "LEVEL 50%: -1.14"  
653  
654 [1] "LEVEL 95%: 6.68" "LEVEL 95%: -1.14"  
655  
656 [1] "LEVEL 97.5%: 6.68" "LEVEL 97.5%: -1.14"  
657  
658 [1] "Phenomenology: 2; Response: 2"  
659  
660 [1] "POSTERIOR MEAN: -5.08" "POSTERIOR MEAN: 0.23"  
661  
662 [1] "LEVEL 2.5%: -5.08" "LEVEL 2.5%: 0.23"  
663  
664 [1] "LEVEL 5%: -5.08" "LEVEL 5%: 0.23"  
665  
666 [1] "LEVEL 50%: -5.08" "LEVEL 50%: 0.23"  
667  
668 [1] "LEVEL 95%: -5.08" "LEVEL 95%: 0.23"  
669  
670 [1] "LEVEL 97.5%: -5.08" "LEVEL 97.5%: 0.23"  
671  
672 [1] "Phenomenology: 3; Response: 1"  
673

674 [1] "POSTERIOR MEAN: -11.07" "POSTERIOR MEAN: 1.89"

675

676 [1] "LEVEL 2.5%: -11.08" "LEVEL 2.5%: 1.87"

677

678 [1] "LEVEL 5%: -11.08" "LEVEL 5%: 1.88"

679

680 [1] "LEVEL 50%: -11.07" "LEVEL 50%: 1.89"

681

682 [1] "LEVEL 95%: -11.06" "LEVEL 95%: 1.91"

683

684 [1] "LEVEL 97.5%: -11.06" "LEVEL 97.5%: 1.91"

685

686 [1] "Phenomenology: 3; Response: 2"

687

688 [1] "POSTERIOR MEAN: -8.64" "POSTERIOR MEAN: 1.71"

689

690 [1] "LEVEL 2.5%: -8.64" "LEVEL 2.5%: 1.7"

691

692 [1] "LEVEL 5%: -8.64" "LEVEL 5%: 1.7"

693

694 [1] "LEVEL 50%: -8.64" "LEVEL 50%: 1.71"

695

696 [1] "LEVEL 95%: -8.63" "LEVEL 95%: 1.72"

697

698 [1] "LEVEL 97.5%: -8.63" "LEVEL 97.5%: 1.72"

699

700 [1] "Phenomenology: 4; Response: 1"

701

702 [1] "POSTERIOR MEAN: -3.31" "POSTERIOR MEAN: 0.43"

703

704 [1] "LEVEL 2.5%: -3.39" "LEVEL 2.5%: 0.43"

705

706 [1] "LEVEL 5%: -3.38" "LEVEL 5%: 0.43"

707

708 [1] "LEVEL 50%: -3.31" "LEVEL 50%: 0.43"

709

710 [1] "LEVEL 95%: -3.24" "LEVEL 95%: 0.43"

711

712 [1] "LEVEL 97.5%: -3.23" "LEVEL 97.5%: 0.43"

713

714 [1] "Phenomenology: 4; Response: 2"

715

716 [1] "POSTERIOR MEAN: -2.37" "POSTERIOR MEAN: 0.28"

717

718 [1] "LEVEL 2.5%: -2.45" "LEVEL 2.5%: 0.27"

719 [1] "LEVEL 5%: -2.43" "LEVEL 5%: 0.27"

720

721 [1] "LEVEL 50%: -2.37" "LEVEL 50%: 0.28"

722

723 [1] "LEVEL 95%: -2.31" "LEVEL 95%: 0.28"

724

725 [1] "LEVEL 97.5%: -2.3" "LEVEL 97.5%: 0.28"

726

727 [1] "EMPLACEMENT CONDITION DEPENDENT COEFFICIENTS"

728

729 [1] "Phenomenology: 1; Emplacement: 1; Response: 1"

730

731 [1] "POSTERIOR MEAN: -10.06" "POSTERIOR MEAN: -1.31" "POSTERIOR MEAN: -1.44"

732 [4] "POSTERIOR MEAN: 3.5" "POSTERIOR MEAN: 0.38"

733

734 [1] "LEVEL 2.5%: -10.07" "LEVEL 2.5%: -1.31" "LEVEL 2.5%: -1.47"

735 [4] "LEVEL 2.5%: 3.29" "LEVEL 2.5%: 0.32"

736

737 [1] "LEVEL 5%: -10.07" "LEVEL 5%: -1.31" "LEVEL 5%: -1.46" "LEVEL 5%: 3.32"

738 [5] "LEVEL 5%: 0.33"

739

740 [1] "LEVEL 50%: -10.06" "LEVEL 50%: -1.31" "LEVEL 50%: -1.44"

741 [4] "LEVEL 50%: 3.5" "LEVEL 50%: 0.38"

742

743 [1] "LEVEL 95%: -10.05" "LEVEL 95%: -1.31" "LEVEL 95%: -1.41"

744 [4] "LEVEL 95%: 3.68" "LEVEL 95%: 0.43"

745

746 [1] "LEVEL 97.5%: -10.05" "LEVEL 97.5%: -1.31" "LEVEL 97.5%: -1.4"

747 [4] "LEVEL 97.5%: 3.72" "LEVEL 97.5%: 0.44"

748

749 [1] "Phenomenology: 1; Emplacement: 1; Response: 2"

750

751 [1] "POSTERIOR MEAN: -1.5" "POSTERIOR MEAN: -1.44" "POSTERIOR MEAN: -1.25"

752 [4] "POSTERIOR MEAN: 2.24" "POSTERIOR MEAN: 0.6"

753

754 [1] "LEVEL 2.5%: -1.52" "LEVEL 2.5%: -1.45" "LEVEL 2.5%: -1.28"

755 [4] "LEVEL 2.5%: 2.18" "LEVEL 2.5%: 0.53"

756

757 [1] "LEVEL 5%: -1.52" "LEVEL 5%: -1.45" "LEVEL 5%: -1.27" "LEVEL 5%: 2.19"

758 [5] "LEVEL 5%: 0.55"

759

760 [1] "LEVEL 50%: -1.5" "LEVEL 50%: -1.44" "LEVEL 50%: -1.25" "LEVEL 50%: 2.24"

761 [5] "LEVEL 50%: 0.6"

762

763

764 [1] "LEVEL 95%: -1.49" "LEVEL 95%: -1.44" "LEVEL 95%: -1.23" "LEVEL 95%: 2.28"  
765 [5] "LEVEL 95%: 0.67"  
766  
767 [1] "LEVEL 97.5%: -1.49" "LEVEL 97.5%: -1.44" "LEVEL 97.5%: -1.22"  
768 [4] "LEVEL 97.5%: 2.29" "LEVEL 97.5%: 0.68"  
769  
770 [1] "Phenomenology: 1; Emplacement: 2; Response: 1"  
771  
772 [1] "POSTERIOR MEAN: -11.48" "POSTERIOR MEAN: -1.09" "POSTERIOR MEAN: -3.61"  
773 [4] "POSTERIOR MEAN: 4.23" "POSTERIOR MEAN: 0.15"  
774  
775 [1] "LEVEL 2.5%: -11.51" "LEVEL 2.5%: -1.1" "LEVEL 2.5%: -3.76"  
776 [4] "LEVEL 2.5%: 3.65" "LEVEL 2.5%: 0.09"  
777  
778 [1] "LEVEL 5%: -11.5" "LEVEL 5%: -1.1" "LEVEL 5%: -3.74" "LEVEL 5%: 3.73"  
779 [5] "LEVEL 5%: 0.1"  
780  
781 [1] "LEVEL 50%: -11.48" "LEVEL 50%: -1.09" "LEVEL 50%: -3.6"  
782 [4] "LEVEL 50%: 4.23" "LEVEL 50%: 0.15"  
783  
784 [1] "LEVEL 95%: -11.45" "LEVEL 95%: -1.09" "LEVEL 95%: -3.49"  
785 [4] "LEVEL 95%: 4.7" "LEVEL 95%: 0.21"  
786  
787 [1] "LEVEL 97.5%: -11.45" "LEVEL 97.5%: -1.09" "LEVEL 97.5%: -3.46"  
788 [4] "LEVEL 97.5%: 4.79" "LEVEL 97.5%: 0.22"  
789  
790 [1] "Phenomenology: 1; Emplacement: 2; Response: 2"  
791  
792 [1] "POSTERIOR MEAN: -2.13" "POSTERIOR MEAN: -1.22"  
793 [3] "POSTERIOR MEAN: -165.12" "POSTERIOR MEAN: 0.9"  
794 [5] "POSTERIOR MEAN: -4.5"  
795  
796 [1] "LEVEL 2.5%: -2.18" "LEVEL 2.5%: -1.23" "LEVEL 2.5%: -205.6"  
797 [4] "LEVEL 2.5%: 0.85" "LEVEL 2.5%: -4.74"  
798  
799 [1] "LEVEL 5%: -2.17" "LEVEL 5%: -1.22" "LEVEL 5%: -200.61"  
800 [4] "LEVEL 5%: 0.85" "LEVEL 5%: -4.71"  
801  
802 [1] "LEVEL 50%: -2.13" "LEVEL 50%: -1.22" "LEVEL 50%: -164.39"  
803 [4] "LEVEL 50%: 0.9" "LEVEL 50%: -4.5"  
804  
805 [1] "LEVEL 95%: -2.1" "LEVEL 95%: -1.22" "LEVEL 95%: -131.19"  
806 [4] "LEVEL 95%: 0.94" "LEVEL 95%: -4.29"  
807  
808 [1] "LEVEL 97.5%: -2.09" "LEVEL 97.5%: -1.21" "LEVEL 97.5%: -127.28"

809 [4] "LEVEL 97.5%: 0.94" "LEVEL 97.5%: -4.27"

810

811 [1] "Phenomenology: 1; Emplacement: 3; Response: 1"

812

813 [1] "POSTERIOR MEAN: -9.53" "POSTERIOR MEAN: -1.16" "POSTERIOR MEAN: -4.47"

814 [4] "POSTERIOR MEAN: 4.95" "POSTERIOR MEAN: 0.34"

815

816 [1] "LEVEL 2.5%: -9.54" "LEVEL 2.5%: -1.16" "LEVEL 2.5%: -4.51"

817 [4] "LEVEL 2.5%: 4.9" "LEVEL 2.5%: 0.31"

818

819 [1] "LEVEL 5%: -9.54" "LEVEL 5%: -1.16" "LEVEL 5%: -4.5" "LEVEL 5%: 4.91"

820 [5] "LEVEL 5%: 0.32"

821

822 [1] "LEVEL 50%: -9.53" "LEVEL 50%: -1.16" "LEVEL 50%: -4.47" "LEVEL 50%: 4.95"

823 [5] "LEVEL 50%: 0.34"

824

825 [1] "LEVEL 95%: -9.51" "LEVEL 95%: -1.16" "LEVEL 95%: -4.43" "LEVEL 95%: 5"

826 [5] "LEVEL 95%: 0.36"

827

828 [1] "LEVEL 97.5%: -9.51" "LEVEL 97.5%: -1.15" "LEVEL 97.5%: -4.42"

829 [4] "LEVEL 97.5%: 5.01" "LEVEL 97.5%: 0.36"

830

831 [1] "Phenomenology: 1; Emplacement: 3; Response: 2"

832

833 [1] "POSTERIOR MEAN: -2.85" "POSTERIOR MEAN: -0.71" "POSTERIOR MEAN: -2.17"

834 [4] "POSTERIOR MEAN: 2.6" "POSTERIOR MEAN: 0.09"

835

836 [1] "LEVEL 2.5%: -2.88" "LEVEL 2.5%: -0.71" "LEVEL 2.5%: -2.38"

837 [4] "LEVEL 2.5%: 2.43" "LEVEL 2.5%: -0.11"

838

839 [1] "LEVEL 5%: -2.87" "LEVEL 5%: -0.71" "LEVEL 5%: -2.34" "LEVEL 5%: 2.45"

840 [5] "LEVEL 5%: -0.07"

841

842 [1] "LEVEL 50%: -2.84" "LEVEL 50%: -0.71" "LEVEL 50%: -2.16" "LEVEL 50%: 2.61"

843 [5] "LEVEL 50%: 0.09"

844

845 [1] "LEVEL 95%: -2.82" "LEVEL 95%: -0.7" "LEVEL 95%: -2" "LEVEL 95%: 2.75"

846 [5] "LEVEL 95%: 0.25"

847

848 [1] "LEVEL 97.5%: -2.81" "LEVEL 97.5%: -0.7" "LEVEL 97.5%: -1.97"

849 [4] "LEVEL 97.5%: 2.78" "LEVEL 97.5%: 0.27"

850

851 [1] "Phenomenology: 2; Emplacement: 1; Response: 1"

852

853 [1] "POSTERIOR MEAN: 3.87"

854 [1] "LEVEL 2.5%: 3.85"

855

856 [1] "LEVEL 5%: 3.85"

857

858 [1] "LEVEL 50%: 3.87"

859

860 [1] "LEVEL 95%: 3.89"

861

862 [1] "LEVEL 97.5%: 3.89"

863

864 [1] "Phenomenology: 2; Emplacement: 1; Response: 2"

865

866 [1] "POSTERIOR MEAN: -0.17"

867

868 [1] "LEVEL 2.5%: -0.19"

869

870 [1] "LEVEL 5%: -0.18"

871

872 [1] "LEVEL 50%: -0.17"

873

874 [1] "LEVEL 95%: -0.15"

875

876 [1] "LEVEL 97.5%: -0.14"

877

878 [1] "Phenomenology: 2; Emplacement: 2; Response: 1"

879

880 [1] "POSTERIOR MEAN: 3.11"

881

882 [1] "LEVEL 2.5%: 3.11"

883

884 [1] "LEVEL 5%: 3.11"

885

886 [1] "LEVEL 50%: 3.11"

887

888 [1] "LEVEL 95%: 3.12"

889

890 [1] "LEVEL 97.5%: 3.12"

891

892 [1] "Phenomenology: 2; Emplacement: 2; Response: 2"

893

894 [1] "POSTERIOR MEAN: -0.9"

895

896 [1] "LEVEL 2.5%: -0.95"

897

898



899 [1] "LEVEL 5%: -0.94"

900

901 [1] "LEVEL 50%: -0.9"

902

903 [1] "LEVEL 95%: -0.86"

904

905 [1] "LEVEL 97.5%: -0.85"

906

907 [1] "Phenomenology: 2; Emplacement: 3; Response: 1"

908

909 [1] "POSTERIOR MEAN: 2.16"

910

911 [1] "LEVEL 2.5%: 2.14"

912

913 [1] "LEVEL 5%: 2.14"

914

915 [1] "LEVEL 50%: 2.16"

916

917 [1] "LEVEL 95%: 2.17"

918

919 [1] "LEVEL 97.5%: 2.17"

920

921 [1] "Phenomenology: 2; Emplacement: 3; Response: 2"

922

923 [1] "POSTERIOR MEAN: -0.94"

924

925 [1] "LEVEL 2.5%: -0.99"

926

927 [1] "LEVEL 5%: -0.98"

928

929 [1] "LEVEL 50%: -0.94"

930

931 [1] "LEVEL 95%: -0.91"

932

933 [1] "LEVEL 97.5%: -0.9"

934

935 [1] "LEVEL 1 VARIANCE COMPONENTS"

936

937 [1] "Phenomenology: 1; Response: 1"

938

939 [1] "POSTERIOR MEAN: 0.0012"

940

941 [1] "LEVEL 2.5%: 0.001"

942

943 [1] "LEVEL 5%: 0.001"

944  
945 [1] "LEVEL 50%: 0.0012"  
946  
947 [1] "LEVEL 95%: 0.0014"  
948  
949 [1] "LEVEL 97.5%: 0.0014"  
950  
951 [1] "Phenomenology: 1; Response: 2"  
952  
953 [1] "POSTERIOR MEAN: 0.0017"  
954  
955 [1] "LEVEL 2.5%: 0.0014"  
956  
957 [1] "LEVEL 5%: 0.0014"  
958  
959 [1] "LEVEL 50%: 0.0017"  
960  
961 [1] "LEVEL 95%: 0.002"  
962  
963 [1] "LEVEL 97.5%: 0.0021"  
964  
965 [1] "Phenomenology: 2; Response: 1"  
966  
967 [1] "POSTERIOR MEAN: 0.0038"  
968  
969 [1] "LEVEL 2.5%: 0.0034"  
970  
971 [1] "LEVEL 5%: 0.0034"  
972  
973 [1] "LEVEL 50%: 0.0038"  
974  
975 [1] "LEVEL 95%: 0.0043"  
976  
977 [1] "LEVEL 97.5%: 0.0044"  
978  
979 [1] "Phenomenology: 2; Response: 2"  
980  
981 [1] "POSTERIOR MEAN: 0.0016"  
982  
983 [1] "LEVEL 2.5%: 0.0014"  
984  
985 [1] "LEVEL 5%: 0.0014"  
986  
987 [1] "LEVEL 50%: 0.0016"  
988

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989 [1] "LEVEL 95%: 0.0018"
990
991 [1] "LEVEL 97.5%: 0.0019"
992
993 [1] "LEVEL 2 VARIANCE COMPONENTS"
994
995 [1] "Phenomenology: 1; Response: 1"
996
997 [1] "POSTERIOR MEAN: 0.001"
998
999 [1] "LEVEL 2.5%: 9e-04"
1000
1001 [1] "LEVEL 5%: 9e-04"
1002
1003 [1] "LEVEL 50%: 0.001"
1004
1005 [1] "LEVEL 95%: 0.0011"
1006
1007 [1] "LEVEL 97.5%: 0.0012"
1008
1009 [1] "Phenomenology: 1; Response: 2"
1010
1011 [1] "POSTERIOR MEAN: 0.001"
1012
1013 [1] "LEVEL 2.5%: 9e-04"
1014
1015 [1] "LEVEL 5%: 9e-04"
1016
1017 [1] "LEVEL 50%: 0.001"
1018
1019 [1] "LEVEL 95%: 0.001"
1020
1021 [1] "LEVEL 97.5%: 0.001"
1022
1023 [1] "OBSERVATIONAL ERROR COVARIANCE PARAMETERS"
1024
1025 [1] "Phenomenology 1"
1026
1027 [1] "POSTERIOR MEAN:"
1028
1029 [1] "Variances"
1030
1031 [1] 0.0021 0.0034
1032
1033 [1] "Correlations"

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1034
1035 [,1] [,2]
1036 [1,] 1 0.27
1037 [2,] 0 1.00
1038
1039 [1] "Variances"
1040
1041 [1] "LEVEL 2.5%: 0.002" "LEVEL 2.5%: 0.0033"
1042
1043 [1] "Correlations"
1044
1045 [1] "LEVEL 2.5%:"
1046 [,1] [,2]
1047 [1,] 1 0.26
1048 [2,] 0 1.00
1049
1050 [1] "Variances"
1051
1052 [1] "LEVEL 5%: 0.002" "LEVEL 5%: 0.0033"
1053
1054 [1] "Correlations"
1055
1056 [1] "LEVEL 5%:"
1057 [,1] [,2]
1058 [1,] 1 0.26
1059 [2,] 0 1.00
1060
1061 [1] "Variances"
1062
1063 [1] "LEVEL 50%: 0.0021" "LEVEL 50%: 0.0034"
1064
1065 [1] "Correlations"
1066
1067 [1] "LEVEL 50%:"
1068 [,1] [,2]
1069 [1,] 1 0.27
1070 [2,] 0 1.00
1071
1072 [1] "Variances"
1073
1074 [1] "LEVEL 95%: 0.0021" "LEVEL 95%: 0.0035"
1075
1076 [1] "Correlations"
1077
1078 [1] "LEVEL 95%:"

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1079 [,1] [,2]
1080 [1,] 1 0.29
1081 [2,] 0 1.00
1082
1083 [1] "Variances"
1084
1085 [1] "LEVEL 97.5%: 0.0021" "LEVEL 97.5%: 0.0035"
1086
1087 [1] "Correlations"
1088
1089 [1] "LEVEL 97.5%:"
1090 [,1] [,2]
1091 [1,] 1 0.29
1092 [2,] 0 1.00
1093
1094 [1] "Phenomenology 2"
1095
1096 [1] "POSTERIOR MEAN:"
1097
1098 [1] "Variances"
1099
1100 [1] 1e-03 3e-04
1101
1102 [1] "Correlations"
1103
1104 [,1] [,2]
1105 [1,] 1 -0.25
1106 [2,] 0 1.00
1107
1108 [1] "Variances"
1109
1110 [1] "LEVEL 2.5%: 0.001" "LEVEL 2.5%: 3e-04"
1111
1112 [1] "Correlations"
1113
1114 [1] "LEVEL 2.5%:"
1115 [,1] [,2]
1116 [1,] 1 -0.29
1117 [2,] 0 1.00
1118
1119 [1] "Variances"
1120
1121 [1] "LEVEL 5%: 0.001" "LEVEL 5%: 3e-04"
1122
1123 [1] "Correlations"

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1124
1125 [1] "LEVEL 5%:"
1126 [,1] [,2]
1127 [1,] 1 -0.28
1128 [2,] 0 1.00
1129
1130 [1] "Variances"
1131
1132 [1] "LEVEL 50%: 0.001" "LEVEL 50%: 3e-04"
1133
1134 [1] "Correlations"
1135
1136 [1] "LEVEL 50%:"
1137 [,1] [,2]
1138 [1,] 1 -0.26
1139 [2,] 0 1.00
1140
1141 [1] "Variances"
1142
1143 [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 3e-04"
1144
1145 [1] "Correlations"
1146
1147 [1] "LEVEL 95%:"
1148 [,1] [,2]
1149 [1,] 1 -0.22
1150 [2,] 0 1.00
1151
1152 [1] "Variances"
1153
1154 [1] "LEVEL 97.5%: 0.0011" "LEVEL 97.5%: 3e-04"
1155
1156 [1] "Correlations"
1157
1158 [1] "LEVEL 97.5%:"
1159 [,1] [,2]
1160 [1,] 1 -0.22
1161 [2,] 0 1.00
1162
1163 [1] "Phenomenology 3"
1164
1165 [1] "POSTERIOR MEAN:"
1166
1167 [1] "Variances"
1168

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1169 [1] 9e-04 9e-04
1170
1171 [1] "Correlations"
1172
1173 [,1] [,2]
1174 [1,] 1 0.91
1175 [2,] 0 1.00
1176
1177 [1] "Variances"
1178
1179 [1] "LEVEL 2.5%: 8e-04" "LEVEL 2.5%: 7e-04"
1180
1181 [1] "Correlations"
1182
1183 [1] "LEVEL 2.5%:"
1184 [,1] [,2]
1185 [1,] 1 0.89
1186 [2,] 0 1.00
1187
1188 [1] "Variances"
1189
1190 [1] "LEVEL 5%: 8e-04" "LEVEL 5%: 8e-04"
1191
1192 [1] "Correlations"
1193
1194 [1] "LEVEL 5%:"
1195 [,1] [,2]
1196 [1,] 1 0.89
1197 [2,] 0 1.00
1198
1199 [1] "Variances"
1200
1201 [1] "LEVEL 50%: 9e-04" "LEVEL 50%: 9e-04"
1202
1203 [1] "Correlations"
1204
1205 [1] "LEVEL 50%:"
1206 [,1] [,2]
1207 [1,] 1 0.92
1208 [2,] 0 1.00
1209
1210 [1] "Variances"
1211
1212 [1] "LEVEL 95%: 0.0011" "LEVEL 95%: 0.001"
1213

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1214 [1] "Correlations"
1215
1216 [1] "LEVEL 95%:"
1217 [,1] [,2]
1218 [1,] 1 0.93
1219 [2,] 0 1.00
1220
1221 [1] "Variances"
1222
1223 [1] "LEVEL 97.5%: 0.0011" "LEVEL 97.5%: 0.001"
1224
1225 [1] "Correlations"
1226
1227 [1] "LEVEL 97.5%:"
1228 [,1] [,2]
1229 [1,] 1 0.93
1230 [2,] 0 1.00
1231
1232 [1] "Phenomenology 4"
1233
1234 [1] "POSTERIOR MEAN:"
1235
1236 [1] "Variances"
1237
1238 [1] 0.0201 0.0071
1239
1240 [1] "Correlations"
1241
1242 [,1] [,2]
1243 [1,] 1 0.53
1244 [2,] 0 1.00
1245
1246 [1] "Variances"
1247
1248 [1] "LEVEL 2.5%: 0.0156" "LEVEL 2.5%: 0.0056"
1249
1250 [1] "Correlations"
1251
1252 [1] "LEVEL 2.5%:"
1253 [,1] [,2]
1254 [1,] 1 0.4
1255 [2,] 0 1.0
1256
1257 [1] "Variances"
1258

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1259 [1] "LEVEL 5%: 0.0162" "LEVEL 5%: 0.0058"
1260
1261 [1] "Correlations"
1262
1263 [1] "LEVEL 5%:"
1264 [,1] [,2]
1265 [1,] 1 0.42
1266 [2,] 0 1.00
1267
1268 [1] "Variances"
1269
1270 [1] "LEVEL 50%: 0.02" "LEVEL 50%: 0.0071"
1271
1272 [1] "Correlations"
1273
1274 [1] "LEVEL 50%:"
1275 [,1] [,2]
1276 [1,] 1 0.53
1277 [2,] 0 1.00
1278
1279 [1] "Variances"
1280
1281 [1] "LEVEL 95%: 0.0244" "LEVEL 95%: 0.0086"
1282
1283 [1] "Correlations"
1284
1285 [1] "LEVEL 95%:"
1286 [,1] [,2]
1287 [1,] 1 0.63
1288 [2,] 0 1.00
1289
1290 [1] "Variances"
1291
1292 [1] "LEVEL 97.5%: 0.0253" "LEVEL 97.5%: 0.0088"
1293
1294 [1] "Correlations"
1295
1296 [1] "LEVEL 97.5%:"
1297 [,1] [,2]
1298 [1,] 1 0.65
1299 [2,] 0 1.00
1300
1301 [1] "FGSN PRIOR PARAMETERS"
1302
1303 [1] "POSTERIOR MEAN:"

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1304
1305 [1] "Alpha = 17.32"
1306 [1] "Lambda squared = 8.03"
1307 [1] "Omega = -1.68" "Omega = 0.57"
1308
1309 [1] "Alpha:"
1310 [1] "LEVEL 2.5%: 17.25"
1311
1312 [1] "LEVEL 5%: 17.26"
1313
1314 [1] "LEVEL 50%: 17.32"
1315
1316 [1] "LEVEL 95%: 17.38"
1317
1318 [1] "LEVEL 97.5%: 17.39"
1319
1320 [1] "Lambda squared:"
1321 [1] "LEVEL 2.5%: 7.4"
1322
1323 [1] "LEVEL 5%: 7.51"
1324
1325 [1] "LEVEL 50%: 8.01"
1326
1327 [1] "LEVEL 95%: 8.57"
1328
1329 [1] "LEVEL 97.5%: 8.68"
1330
1331 [1] "Omega:"
1332 [1] "LEVEL 2.5%: -1.93" "LEVEL 2.5%: 0.48"
1333
1334 [1] "LEVEL 5%: -1.9" "LEVEL 5%: 0.49"
1335
1336 [1] "LEVEL 50%: -1.68" "LEVEL 50%: 0.57"
1337
1338 [1] "LEVEL 95%: -1.46" "LEVEL 95%: 0.65"
1339
1340 [1] "LEVEL 97.5%: -1.41" "LEVEL 97.5%: 0.66"
1341
1342 [1] "DIC = -6086.65"
1343
1344 [1] "PIC = -6080.32"

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