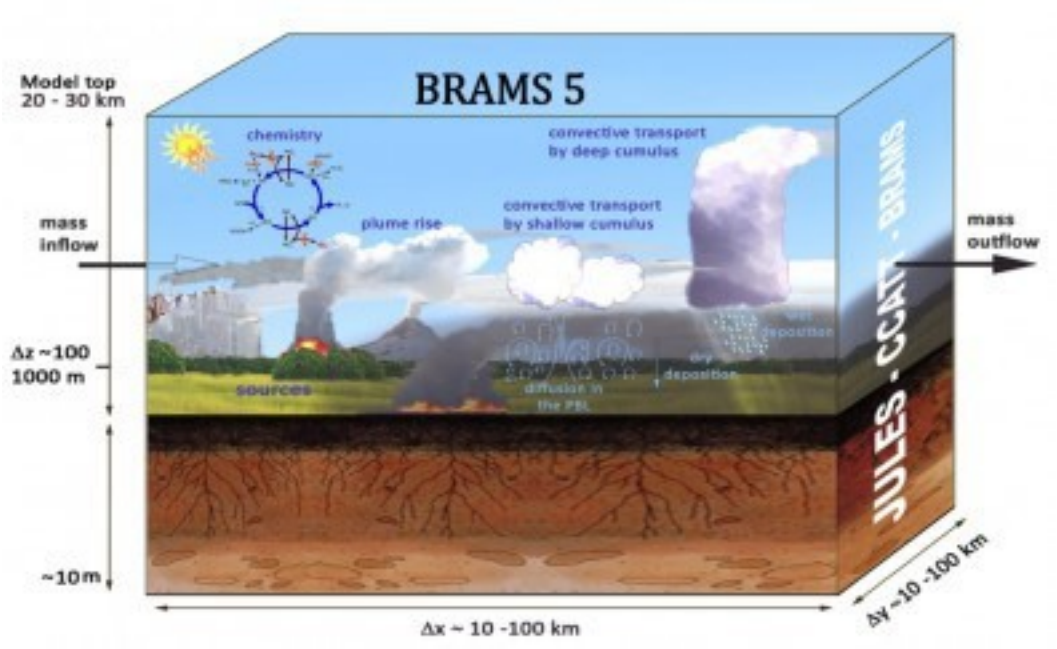


# DPREP-CHEM

Users Guide for version 5.0

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## 1. Introduction:

DPREP-CHEM is a tool used to include chemical species to initial and atmospheric boundary conditions in the format required by the model. It depends on an input file named dprep.inp , which must be set according to the domain, simulation data and input file types. This guide aims to present the process of installing and running.

## 2. Structure:

DREP-CHEM is organized in the follow structure:

a) bin – Input configuration files and binary file.
b) bin/build – Configuration files related to the tool compilation.
c) src - Fortran90 source code.

## 3. Installation and configuration instructions:

a) PHASE I – Environment and compilation.

**DPREP-CHEM compilation is only compatible to PGI and Intel compilers. The gfortran version will be available in the future.**

The examples below are considering a build with Intel compiler.

Download the SPACK in Chemical section of
http://brams.cptec.inpe.br/input-data/.

Unzip the source code file on your desktop , eg /dados/fontes:

```
→ cd /dados/fontes

→ tar zxvf SPACK-4.3.tar.gz
```

Download DPREP-CHEM-5.0.tar.gz from http://brams.cptec.inpe.br/input-data/, in the Chemical Section.

Copy zipped file DPREP-CHEM-5.0.tar.gz to your working local folder.

```
→ cd /dados/fontes

→ cp /download/DPREP-CHEM-5.0.tar.gz  ./
```

Unzip it:

```
→ tar zxvf DPREP-CHEM-5.0.tar.gz
```

Create an symbolic link to the desired chemical mechanism, eg “RELACS”:

```
→ cd ./src

→ ln -fs /dados/fontes/SPACK-4.3/Mechanism/RELACS
```

The DPREP -CHEM also needs the GRIB API installation. Please refer to the site https://software.ecmwf.int/wiki/display/GRIB/GRIB+API+CMake+installation For more information about the installation.

Download GRIB API from:
https://software.ecmwf.int/wiki/display/GRIB/Releases

Choose a folder to copy the GRIB API:

```
→ mkdir -p /dados/source/
```

Unzip the GRIB API file in that folder:

```
→ cd /dados/source/

→ tar -xzvf grib_api-1.14.7-Source.tar.gz
```

Create a folder to install the GRIB API:

```
→ mkdir -p /dados/libs/grib_api-1.14.7-intel
```

Create a temporary folder to the build of the GRIB API:

```
→ mkdir -p /dados/libs/build-intel
```

Execute the cmake command inside the build folder, pointing to the source code and the and GRIB API installation folder.

Before running cmake, check whether the libopenjpeg-dev library is already installed. If not, install it:

```
→ apt-get install libopenjpeg-dev
```

Execute the following cmake command:

```
→ cd /dados/libs/build-intel

→ CC=icc FC=ifort cmake /dados/source/grib_api-1.14.7-Source
-DCMAKE_INSTALL_PREFIX=/dados/libs/grib_api-1.14.7-intel
-DENABLE_FORTRAN=ON -DENABLE_JPG=ON -DBUILD_SHARED_LIBS=ON
```

Check if the command result has enabled the features like the example:

```
-- The following features have been enabled:

* FORTRAN , build the GRIB_API Fortran interface

* JPG , support for JPG decoding/encoding
```

Make it. If you prefer more than one compiler, use the -j option (-j  <number of processors>):

```
→ make -j8
```

Install it. If you prefer more than one compiler, use the -j option (-j <number of processors>:

```
→ make install -j8
```

If for any reason there are errors in cmake , compilation or installation, remove all files fom the build and installation folder before retrace the steps.

Edit the configuration file ( file include.mk.intel for intel ):

```
→ gedit /dados/fontes/DPREP-CHEM-5.0/Bin/build/include.mk.intel
```

Change the path of the GRIB API installation folder and the compiler folder ( intel ) . See Appendix A :

```
FC = /opt/Intel/Bin/ifort

GRIBLIB=-L/dados/libs/grib_api-1.14.7-intel/lib -lgrib_api_f90 -lgrib_api

GRIBINC=-I/dados/libs/grib_api-1.14.7-intel/include

FLOADER = /opt/Intel/Bin/ifort
```

Edit paths.mk file, which points to the chemical variables used ind BRAMS:

```
→ gedit /dados/fontes/DPREP-CHEM-5.0/bin/build/paths.mk
```

Change the value of the following variable, pointing it to the root BRAMS folder:

```
# USER RELATED

RAMS_ROOT=/dados/fontes/BRAMS-5.2
```

Compile the code. The OPT=intel option includes the include.mk.intel file during the make command, and the CHEM option selects the chemistry used in BRAMS :

```
→ cd /dados/curso/fontes/DPREP-CHEM-5.0/bin/build

→ make OPT=intel CHEM=RELACS_TUV
```

b) PHASE II – Execution

Before you start the application you must configure your input options :

```
→ gedit /dados/cursos/fontes/DPREP-CHEM-5.0/bin/dprep.inp
```

Change the following variables. Please refer to the Appendix B.

```
$ARGS_INPUT

!!!!! DATE !!!!!

init_year  = 2016,

init_month = 04,

init_day   = 11,

init_hour  = 12,

!!!!! TIME STEP !!!!!!!

step  = 6,

times = 4,

!!!!! ATMOS !!!!!

atmos_type   = 0,

atmos_prefix ='dp',

atmos_sufix  ='00',

atmos_idir   ='./dp/',

!!!!! CHEM !!!!!!

!10 shadoz, 11 binary clim, 12 oper mocage

chem_type     = 11,

chem_merge    = .TRUE.,

chem_interp   = 1,

chem_ppbmconv = .TRUE.,

chem_idir  = './climatology/',

!!!!! OUTPUT !!!!!

out_type   = 1,

out_prefix = 'dp-chem-relacs-',

out_sufix  = '00',

out_dir    = './',


$END,
```

Execute the DPREP binary:

```
→ cd ./DPREP-CHEM-5.0/bin/

→ ./dprep_RELACS.x
```

At the end of the run it can be seen that the result consist of files for evaluation ( ctl and gra ) and files that will be used for model input ( vfm ).

Input files:

- Boundary and initial condition atmospheric files:

Boundary and initial condition atmospheric files are converted files from Global GFS to the required format for DPREP-CHEM. The conversion of files is done by GeraDP program, which is also available in BRAMS site, in the Input Data / Atmospheric section.

- Chemical files:

It contains chemical species to be included in the initial conditions and atmospheric boundary in the specific format for the template.

The files are available in BRAMS site , at Input Data / Chemical section.

## Appendix A

| Variables | Description and comments |
|---|---|
| USEHDF4 (deprecated) | enable/disable HDF4 lybrary.<br>0 = disabled. (default)<br>1 = enabled . |
| USEGRIB | Enables/disables the GRIB library .<br>0 = disabled.<br>1 = enabled. (default) |
| GRIBLIB | Path and libraries of GRIB-API.<br>Eg: /usr/lib/grib_api -lgrib_api_f90 –lgrib_api |
| GRIBINC | Include path of GRIB-API.<br>Eg: /usr/lib/grib_api/include |
| USENETCDF (deprecated) | Enables/disables the NETCDF library.<br>0 = disabled. (default)<br>1 = enabled. |
| USEPARALLEL | Enables/disables the parallelism<br>0 = disabled. (default)<br>1 = enabled. |
| FC | Compiler for the Fortran source code.<br>Ex: /usr/in/ifort |
| FC_OPTS | Fortran compilation flags.<br>*Caution* some flags are strictly needed for the well working. |
| FLOADER | Compiler for linking the objects<br>Eg: /usr/in/ifort |

Table 1: Variables for configuration and compilation

**Appendix B**

| Variables | Description and comments |
|---|---|
| init_year | Start year<br>Integer type |
| init_month | Start Month<br>Integer type |
| init_day | Start day<br>Integer type |
| init_hour | Start hour<br>Integer type |
| Step | Time step in hour for conditions to be processed.<br>Ex: 6 |
| Times | Amount of conditions to be generated.<br>Integer type |
| atmos_type | Atmospheric input file type<br>0 = DP asc default CPTEC. |
| atmos_prefix | Atmospheric input file prefix<br>Eg=’dp’ |
| atmos_sufix | Atmospheric input file suffix.<br>Eg=’00’ |
| atmos_idir | Atmospheric input file folder |
| chem_type | Chemical input file type<br>10 = vertical profile<br>11 = binary climatology<br>12 = operacional mocage. |
| chem_merge (obsoleto) | Controls whether the files should be concatenated.<br>.true. or .false. |
| chem_interp | Interpolation type for chemical data.<br>1 = bilinear. |
| chem_ppbmconv | Convert the output in ppbm.<br>.true. or .false. |
| chem_idir | Folder of the chemical files. |
| out_type | Output file type<br>1 = vfm |
| out_prefix | Output file type prefix.<br>Eg = dp-chem-cb07 |
| out_sufix | Output file type suffix.<br>Eg = 00 |
| out_dir | Output folder<br>Ex = . |

Table 2: Variables for the configuration and execution.