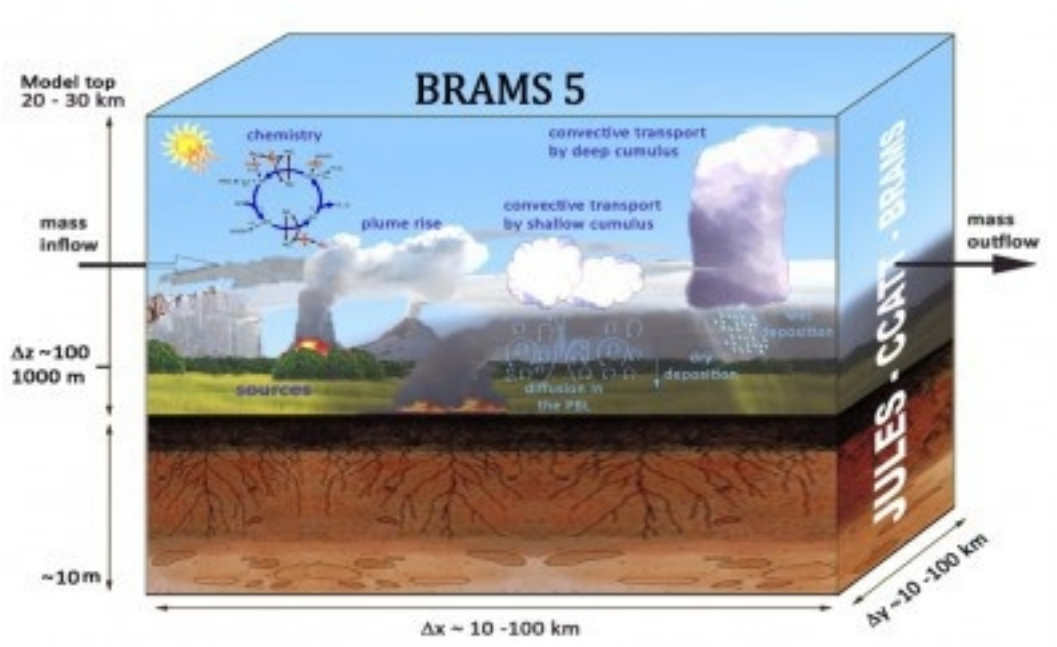

DPREP-CHEM

Users Guide for version 5.1.0

December 2018

Rafael Mello da Fonseca, Denis Eiras

Email: atende.cptec@inpe.br

WEB: http://brams.cptec.inpe.br

meioambiente.cptec.inpe.br

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 Downloads page
http://brams.cptec.inpe.br/downloads.

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

```
→ cd /dados/fontes
→ tar zxvf SPACK-4.3.tar.gz
```

Download DPREP-CHEM-5.0.1.tar.gz from Downloads page http://brams.cptec.inpe.br/downloads.

Copy zipped file DPREP-CHEM-5.0.1.tar.gz to your working local folder.

```
→ cd /dados/fontes
→ cp /download/DPREP-CHEM-5.0.1.tar.gz  ./
```

Unzip it:

```
→ tar zxvf DPREP-CHEM-5.0.1.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-5.0.1/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-5.0.1/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-5.0.1/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-5.0.1/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-5.0.1/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. 0 = disabled. (default) 1 = enabled .
USEGRIB	Enables/disables the GRIB library . 0 = disabled. 1 = enabled. (default)
GRIBLIB	Path and libraries of GRIB-API. Eg: /usr/lib/grib_api -lgrib_api_f90 –lgrib_api
GRIBINC	Include path of GRIB-API. Eg: /usr/lib/grib_api/include
USENETCDF (deprecated)	Enables/disables the NETCDF library. 0 = disabled. (default) 1 = enabled.
USEPARALLEL	Enables/disables the parallelism 0 = disabled. (default) 1 = enabled.
FC	Compiler for the Fortran source code. Ex: /usr/in/ifort
FC_OPTS	Fortran compilation flags. *Caution* some flags are strictly needed for the well working.
FLOADER	Compiler for linking the objects Eg: /usr/in/ifort

Table 1: Variables for configuration and compilation

Appendix B

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

Table 2: Variables for the configuration and execution.