



# Recording 'namelist' input parameters in HDF5

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**Reproducibility is a key scientific goal.** This requires to know:

- **which code version was used for a particular simulation**
  - more or less okay as we print the release version in the log file
  - this does not catch local source code changes
- **the hard-coded parameters that were used**
  - more or less okay as we print in the log file, but changes not recorded reliably
- **the input parameters that were used**
  - **also how the input parameters changed during a simulation (when restarting)**

The new tool aims to improve the last point.

It will allow to get this information also into IMAS eventually.



## **To allow tracking input parameters in a simulation, we have decided to store all input parameters in the JOREK .h5 restart files**

- This has to be general enough to even work for a simulation restarted with a different code version, as the previous versions don't have necessarily identical sets of input parameters
- The approach is to write out the namelist directly from JOREK, thus **all input parameters are included**, not only those in your input file
- The parameters are then appended in the .h5 restart file
- Each .h5 restart file will contain the entire history, so the parameters for each restart that occurred in the past
- This feature is realized by several scripts/commands



## **Pull request coming up soon**

- The inclusion of the namelist parameters in the .h5 restart files will soon work automatically in the background. Nothing you need to do here yourself.
- There will be an option to extract the input parameters for any time index in the simulation.
- There will be an option to determine exactly how parameters changed during the simulation. This allows to reproduce a complicated simulation with changing parameters (time stepping, numerical parameters, etc.) exactly.

In the following, some technical details are given.



- **store the namelist states for every time a simulation is restarted**
- **store this in the .h5 restart files** (but also in an extra namelist.h5 file for practical reasons)
- **allow to extract the namelist state for any time index**

1) When JOREK starts, we do:

a) if it is a **new simulation** (not a restart):

- delete namelist.h5 file if it exists
- create new namelist.h5 and write the namelist into group "00000" for time index 0

b) else (**restart at time index XXXXX**)

I) if namelist.h5 exists

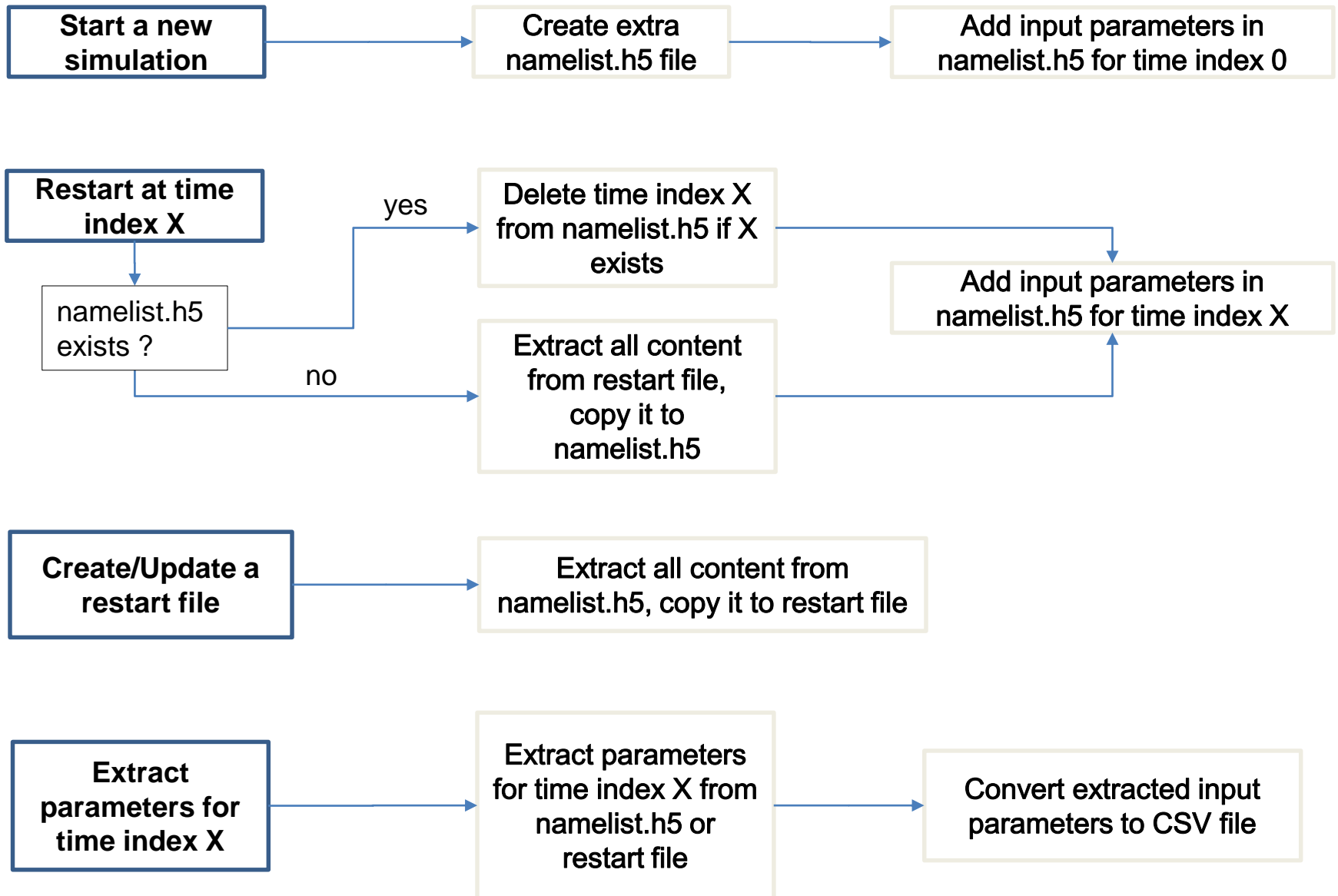
- delete all groups YYYYYY in namelist.h5 for which YYYYYY  $\geq$  XXXXX
- add the namelist parameters into the group XXXXX

II) else (namelist.h5 does not exist)

- extract all contents from namelist/ in the JOREK restart file into namelist.h5
- add the namelist parameters into the group XXXXX

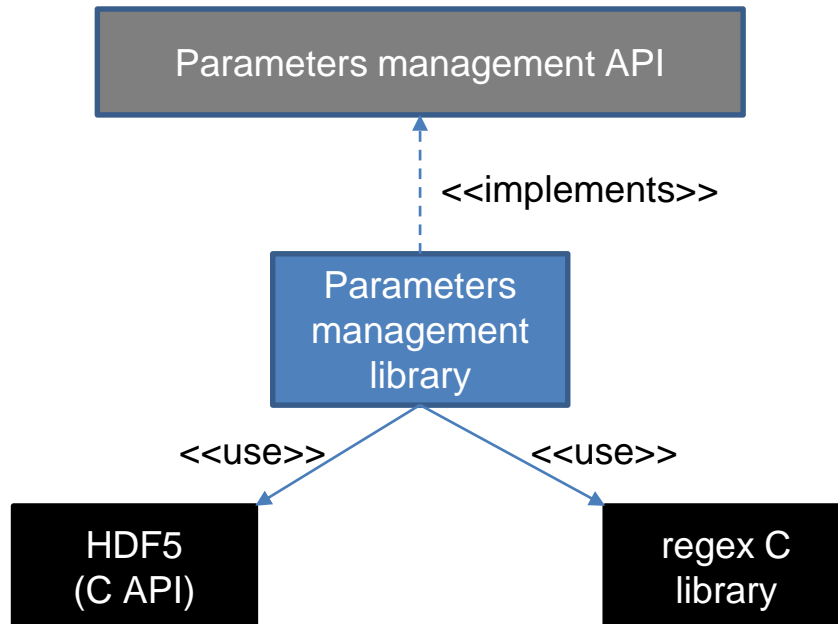
2) When we **write out an hdf5 restart file** in JOREK, we add the full content of namelist.h5 into that restart file in the subgroup namelist/, i.e., the namelist for all (restart) time indices

3) For the hdf5-to-namelist script, we add a parameter ZZZZZ which specifies the time index during the simulation for which we want to extract the namelist. The script will find the group XXXXX where XXXXX is the largest existing number smaller or equal to ZZZZZ and **extract the namelist from group XXXXX**. The script should be able to work both on the namelist.h5 file or on a JOREK restart file.





```
//Parameters management C API -----  
int new_simulation(const char* h5_namelist_folder, const char* nml_file_name);  
int restart(const char* h5_namelist_folder, const char* nml_file_name, const char*  
jorek_restart_file_name, const char* time_index);  
int write_restart_file (const char* h5_namelist_folder, const char* jorek_restart_file);  
int extract_from_h5_namelist (const char* h5_namelist_folder, const char* nml_file, const char*  
time_index);  
int extract_from_jorek_restart_file (const char* h5_namelist_folder, const char*  
jorek_restart_file_name, const char* nml_file_name, const char* time_index);  
//-----
```





Input parameters are exported from Jorek in CSV text file



The input parameters are read from the file and store to the namelist.h5 file

```
h5dump namelist.h5 |less
```

```
HDF5 "namelist.h5" {  
  GROUP "/" {  
    GROUP "00000" {  
      DATASET "ADAPTIVE_TIME" {  
        DATATYPE H5T_STRING {  
          STRSIZE H5T_VARIABLE;  
          STRPAD H5T_STR_NULLTERM;  
          CSET H5T_CSET_ASCII;  
          CTYPE H5T_C_S1;  
        }  
        DATASPACE SCALAR  
        DATA {  
          (0): "F"  
        }  
      }  
    }  
    DATASET "AKI_NEO_CONST" {  
      DATATYPE H5T_IEEE_F64LE  
      DATASPACE SCALAR  
      DATA {  
        (0): 0  
      }  
    }  
  }  
}
```

**First simulation**

```
DATASET "CORNER_BLOCK" {  
  DATATYPE H5T_STD_I32LE  
  DATASPACE SIMPLE { ( 30 ) / ( H5S_UNLIMITED ) }  
  DATA {  
    (0): 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,  
    (21): 0, 0, 0, 0, 0, 0, 0, 0, 0  
  }  
}  
DATASET "DELTA_PSI_GS" {  
  DATATYPE H5T_IEEE_F64LE  
  DATASPACE SCALAR  
  DATA {  
    (0): 10000  
  }  
}  
DATASET "DIAG_COILS[]%CURRENT" {  
  DATATYPE H5T_IEEE_F64LE  
  DATASPACE SIMPLE { ( 299, 1 ) / ( H5S_UNLIMITED, H5S_UNLIMITED ) }  
  DATA {  
    (0,0): 0,  
    (1,0): 0,  
    (2,0): 0,  
    ...  
  }  
}
```





Restoring namelist.h5  
from restart file if it does  
not exist

Input parameters are  
exported from Jorek in  
CSV text file

The input parameters are  
read from the file and store  
to the namelist.h5 file

```
h5ls -r namelist.h5
```

```
/          Group
/00000    Group
/00000/ADAPTIVE_TIME Dataset {SCALAR}
/00000/AKI_NEO_CONST Dataset {SCALAR}
/00000/AMIN  Dataset {SCALAR}
/00000/AMIX  Dataset {SCALAR}
```

The new time index is added as a new HDF5 group

```
...
/00001    Group
/00001/ADAPTIVE_TIME Dataset {SCALAR}
/00001/AKI_NEO_CONST Dataset {SCALAR}
/00001/AMIN  Dataset {SCALAR}
/00001/AMIX  Dataset {SCALAR}
...
/00001/Z_LIMITER Dataset {1000/Inf}
```



→ Using the 'write\_restart\_file' API command, a restart file can be created/updated from an existing namelist.h5 file

```
h5ls -r jorek_restart.h5
```

```
/          Group
/namelist  Group
/namelist/00000  Group
/namelist/00000/ADAPTIVE_TIME Dataset {SCALAR}
/namelist/00000/AKI_NEO_CONST Dataset {SCALAR}
/namelist/00000/AMIN  Dataset {SCALAR}
/namelist/00000/AMIX  Dataset {SCALAR}
...
/namelist/00001  Group
/namelist/00001/ADAPTIVE_TIME Dataset {SCALAR}
/namelist/00001/AKI_NEO_CONST Dataset {SCALAR}
/namelist/00001/AMIN  Dataset {SCALAR}
/namelist/00001/AMIX  Dataset {SCALAR}
...
/namelist/00001/Z_LIMITER Dataset {1000/Inf}
```



→ **Parameters for a specific time index can be extracted from an existing restart file and converted to a CSV text file readable by Jorek**

```
$ ./namelist_api extract_from_jorek_restart_file /Home/LF218007/jorek jorek_restart.h5 params.nml 00001
```

```
more params.nml
```

```
&IN1  
ADAPTIVE_TIME = F  
,  
AKI_NEO_CONST = 0.000000e+00,  
AMIN = 1.000000e+00,  
AMIX = 0.000000e+00,  
AMIX_FREEB = 8.500000e-01,  
AMU_NEO_CONST = 0.000000e+00,  
AUTODISTRIBUTE_MODES = T  
,  
...
```



Thank you