



Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

NuT

Numerical Toolkit

Program Updates





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NuT 2.0

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1 Updates

In this chapter most recent changes as well as a history of updates are given. This is done as a list of incremental changes from one version to the next one.

1.1 Most recent updates – from 1.0.1 to 2.0

With NuT 2.0 a complete overhaul of the code was done transitioning from Fortran to C/C++. Among other things, see below, this comes with the benefit of a standardized C-interface. A supplementary Fortran interface was developed which is based on Fortran's `bind(c)`-mechanism. Also, internally, PETSc's native C-interface is employed which is more robust and better worked out in detail than its Fortran counterpart.

Important note on compatibility

No backwards-compatibility is given: NuT 2.0 requires an AC²-2021 environment. Likewise, no older versions of NuT are supported by AC²-2021.

1.1.1 Improvements

Scope

- ATHLET/CD may also work in tandem with NuT in the context of coupled computations. Though COCOSYS is not directly supported yet both types of couplings, plugin or driver, may be employed.
- ATHLET's steady state calculations are supported by NuT as well. The same solver preset as for the transient phase applies.
- Each time ATHLET decides to compute a new Jacobian or a partial update of a given one NuT picks the best of three seeding heuristics, namely, the CPR algorithm with largest-first, smallest-last, or incidence-degree ordering.

Software architecture

- The MPI-based communication in AC² is initialized in a uniform and robust way by means of the dedicated library MMA (MPI for Multiple Applications). This holds for all components in AC² that participate in MPI-based communications.
- The library `libnut_core` is now linked statically to the NuT-worker executable. This prevents accidental mixture of different versions.

Output/logging

- Two NuT-related logging files are provided. One focuses on ATHLET's steady state calculations whereas the other provides detailed information about the transient phase. Both, additionally, provide further performance numbers.
- Added an output message when NuT terminates because of no available host applications (e.g. the NuT-worker has been executed without additionally involving a host application).

Manual

- The manual was updated according to above changes. In particular, Chapter 4 provides some new command line invocation pattern for using NuT in the context of coupled computations.

1.1.2 3rd-party related

libpetsc

- Update to PETSc 3.15.5. See [PETSc 3.15 Release](#) and follow the commit history of [PETSc 3.15.5 Tag](#) for details on improvements and fixes. Included is an update of ScaLAPACK to version 2.1.0. See also [Release Notes of ScaLAPACK 2.1.0](#).
- Update to MUMPS 3.5.3. See [MUMP's changelog](#) for details.
- Introduction of [MMA 1.0](#) to handle initialization of MPI-based communication.
- Update to Intel® MPI Library 2021.1.1.
- Update to Intel® Fortran Redist 2021.4.0 (Fortran is still required due to MUMPS).
- Update to Microsoft® Visual C++ 2019 Runtime 14.29.30133.

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- Incremented version number of PETSc, MUMPS, and ScaLAPACK in accordance with the above listed update. Added MMA as well.
- Minor refinements of Markdown formatting.

1.2 Updates from 1.0.0 to 1.0.1

None of the below changes shall have any influence on computational results at all or beyond the impact of finite precision arithmetics.

1.2.1 Improvements

Interface compatibility

- Improved compatibility check between NuT-plugin and NuT-worker.
- Refinement of error output in case of failure of the compatibility check between ATHLET and NuT-plugin. See also Chapter 2 for known issues in case of premature termination of the ATHLET process.

Note: Though it is recommended (and given by default) to use NuT 1.0.1, ATHLET 3.2.1 is also compatible with NuT 1.0.0.

Output/logging

- For solver presets that involve MUMPS: Changed the message type of NuT's output from `NuT Warning` to `NuT Info` in case that MUMPS requires more memory for the numerical decomposition of the shifted Jacobian. No related messages will be printed to standard output anymore. The output to the respective `nut.log` file is still provided with the string prefix changed from `NuT Warning` to `NuT Info`.

Manual

- Refined structure and content of Chapter 4 *Making Use of the Numerical Toolkit*.
- Several additional minor improvements were made to increase clearness and consistency.

1.2.2 Fixes

NuT-worker

- Fixed a rare bug where the `nut.log` file was not written to the intended directory or not written at all. This was due to too small buffer sizes for storing the path of ATHLET's output directory. Note that possible OS limitations may advocate to avoid excessively long pathes in general.

This fix only applies in case that both NuT-plugin and NuT-worker are of version 1.0.1.

- Fixed some ambiguity in number casting during the calculations of the seed matrix.

AC²-GUI

- Plugins that where supposed to be activated via the appropriate `-e` statements in ATHLET's GUI element *Additional parameters* are no longer silently discarded if the Numerical Toolkit is selected as well. This was actually a bug in the GUI-code. But since it affected NuT-related executions, it is additionally listed here.

1.2.3 3rd-party related

libpetsc

- Update to PETSc 3.10.5. See [PETSc 3.10.5 commits](#) for details on fixes and improvements.

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- Added a note regarding the provision of MUMPS's source code on request in compliance with CeCILL-C.
- Incremented version number of PETSc in accordance with the above listed update.
- Added additional copyright notes for METIS.

2 Known issues

Clean termination of NuT-related processes

- If a simulation run is supposed to be executed with activated NuT but the ATHLET-option `-e nut` is missing there will not be an immediate breakdown. Instead, ATHLET resorts to its default numerics and NuT gets stuck in the process of initializing communication.
- If any AC²-related non-NuT process terminates prematurely and before the MPI-based communication is fully established via MMA then the dedicated `nut_worker` process(es) may still be running in the background.

In case of one of the aforementioned scenarios the user is advised to check the general process structure and to kill any remaining corresponding `nut_worker` process(es) manually.