Gesellschaft für Anlagen-
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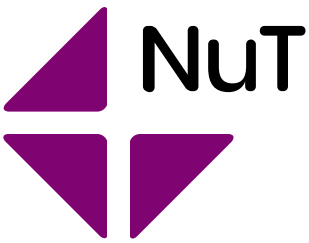
(GRS) gGmbH

NuT

Numerical Toolkit

Program Updates



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Rev. 4

Gesellschaft für Anlagen-
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NuT 2.0.2

Numerical Toolkit

Program Updates

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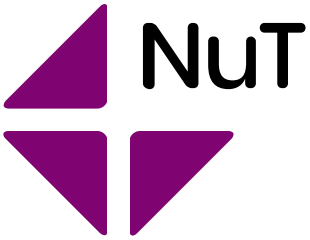

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Contents

1 Most recent updates – from 2.0.1 to 2.0.2

With Patch 2.0.2 NuT-support for linear algebra tasks in COCOSYS's THY-module Ramain is introduced. That support can be made use of during stand-alone computations of COCOSYS as well as during coupled computations with ATHLET/CD.

Furthermore, some general improvements and fixes were made as listed below.

As a reminder on compatibility

NuT 2.0 requires at least an AC^2-2021 environment. To make use of support for Ramain's linear alegbra NuT 2.0.2 as well as AC^2-2023 are required. No older versions of NuT than 2.0 are supported by AC^2-2021 or AC^2-2023.

1.1 Improvements

Scope

- Linear algebra support for COCOSYS's THY-module Ramain added.
- Update of the AC^2-GUI to allow for easy handling of NuT supporting ATHLET/CD and/or Ramain.

NuT-worker

- Add support for CPU affinity. This is done via the shared environment variable `AC2_CPU_AFFINITY`. See AC^2's user manual for details.
- Improve efficiency of vector handling while solving linear systems.
- Make NuT's logging capabilities more flexible. Also, add information about cpu-affinity to log files.
- Apply several tweaks and refinements to further improve interfaces and type signatures.

Output/logging

- Include identifier of host application in log file suffix.

1.2 Fixes

NuT-worker

- Ensure that finalization cannot be missed and avoid getting stuck in case of unhandled exceptions.

Note that these fixes will not prevent the situation that the NuT-worker waits for ATHLET/CD to initiate communication but waits indefinitely if ATHLET/CD forgets to load the NuT-plugin. That behavior is intended since NuT cannot know how long it takes a host to come to a point where communication might be considered.

1.3 3rd-party related

libpetsc

- Update to PETSc 3.19.4. See PETSc Releases for details on changes.
- Update to MUMPS 5.5.1. See MUMP's changelog for details on changes.
- Update to Intel® Fortran Redist 2023.1.0
- Instead of netlib's LAPACK and (Sca)LAPACK use Intel® oneMKL, version 2023.1.0, to provide basic linear algebra routines.

MPI runtime

- Update to Intel® MPI Library 2021.9.0.

3rd-party license files

- Complete overhaul of the 3rd-party license processing:
  - separated license files for Linux-based systems and Microsoft® Windows,
  - stand-alone NuT-related 3rd-party license files or subsumed under AC^2's 3rd-party license files,
  - format of 3rd-party licenses as given by the respective 3rd-party sources.

2 Updates from 2.0.0 to 2.0.1

Patch 2.0.1 mainly introduces a couple of tweaks and refinements of NuT's code in order to improve performance. Neither the handling of NuT nor numerical results are affected by these changes. Details are shown below.

As a reminder on compatibility
No backwards-compatibility is given: NuT 2.0 requires an AC^2-2021 environment. Likewise, no older versions of NuT are supported by AC^2-2021.

2.1 Improvements

Solver presets that utilize an iterative method

- Avoid a redundant application of the preconditioner on the RHS, i.e. Pb, per linear system to solve.

  Redundancy is introduced on the part of PETSc when using the default convergence test combined with activating the so-called Knoll trick to compute an initial guess for the iterative method via Pb. Providing a carefully designed custom convergence test avoids the double computation of Pb without any further divergence from the default procedure. No PETSc code was changed. Numerical results stay the same.

  The solver presets that benefit from the modifications are as follows:

  – `lu-gmres` (default preset if the number of NuT-processes equals one),
  – `ilu_k-gmres`,
  – `mumps-gmres`.

NuT-worker

- Several tweaks and refinements were introduced w.r.t. when and how numerical objects are assembled in libnut_core. This includes an optimized treatment of the case that NuT runs in sequential mode (number of NuT-processes equals one).
- The worker now only checks for termination if suitable.

Documentation

- Restructuring of the updates document to allow for better navigation.
- Couple of minor rephrasings in the manual to improve clearness.

- Several under-the-hood tweaks to the overall typesetting approach to improve robustness.
- Instead of the file name the document title is now displayed in pdf-viewers.
- Section numbers are now part of the bookmarks of the pdf-documents.

2.2 Fixes

NuT-worker

- Fixed a rare bug where certain exceptions thrown by MUMPS were falsely answered by increasing the memory MUMPS is allowed to use for its numerical factorizations.

NuT Fortran interface

- Use nested if statements instead of relying on the principle of short-circuit evaluation if invocations of `allocated` are involved.

Manual

- Fixed some out-of-bounds issues for certain bibliography entries.

2.3 3rd-party related

NuT_3rd-party_licenses.html

- Regarding MUMPS and in accordance with CeCILL-C 1.0, some notice w.r.t. warranty and liability were added.

3 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 AC^2-2021 environment. Likewise, no older versions of NuT are supported by AC^2-2021.

3.1 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 AC^2 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 AC^2 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.

3.2 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.

NuT_3rd-party_licenses.html

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

4 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.

4.1 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 5 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.

4.2 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.

AC^2-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.

4.3 3rd-party related

libpetsc

- Update to PETSc 3.10.5. See PETSc 3.10.5 commits for details on fixes and improvements.

NuT_3rd-party_licenses.html

- 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.

5 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 AC^2-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.