



WUFI®

Multicore and Batch Calculation with WUFI® 2D

Date: August 2026

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Problem

Core issue:

On newer CPUs with many cores, WUFI 2D can be slower than on older CPUs with up to four cores.

Cause:

- To use multiple cores, the differential equation system to be solved must be split up.
- Information must then be exchanged between the cores used, which takes time (known as synchronization overhead).
- The more cores are used, the greater this overhead becomes and the longer the calculation takes.

Behaviour of WUFI 2D:

- By default, WUFI 2D uses all available CPU cores (including hyperthreading) except one for calculation; the remaining core is used for the user interface.
- Depending on the construction, roughly 4 to 10 cores are usually optimal. If more cores are used, the calculation speed decreases again.
- The number of cores used currently cannot be set directly in WUFI 2D.

Problem

Comparisons with different numbers of cores:

“Bed-Plate” benchmark - calculation over 3 years (26280 h)

CPU	System	Physical Cores	Logical Cores	used	Calculation time
Intel i9-11900K	Win 10	16	32	15	9,5 h
Intel i9-11900K	Win 10	16	32	4	1,6 h
Intel i9-14900	Win 10	24	32	31	6,3 h
Intel i9-14900	Win 10	24	32	8	4,8 h

Solution Approach

Because WUFI 2D currently supports neither directly specifying the number of cores nor automated parallel calculation of multiple simulations, PowerShell-based scripts were developed for this purpose:

- **WUFI2D_BatchCalc:**
Allows one or more prepared WUFI 2D project files to be calculated in batch mode using the optimal number of cores based on a calculation list.
- **WUFI2D_CoreTest:**
Determines the optimal number of cores (threads) for the system and project.
- **WUFI2D_StartGUI:**
Starts the WUFI 2D interface with a user-defined number of cores.
- **WUFI2D_StartGUI_fastlane:**
Starts the WUFI 2D interface directly with the most recently used number of cores.
Can be used for regular program startup.

The latest versions of the scripts, as well as additional information about them, can be found on the WUFI forum: <https://www.wufi-forum.com/viewtopic.php?t=2357>

Using the Scripts

Important files in the WUFI project directory:

- *wufi2d.xml* – project definition^(*)
- *input.dat* – calculation core control file^(*)
- *<project name>.wfd* – result file

^(*) must be present at minimum

Additional files - for information:

- *iter.txt* – calculation sequence
- *input.bak* – backup of input.dat when modified by BatchCalc
- **.bcli* – climate boundary conditions
- *<material>.xml* – material data

Using the Scripts

Preparing the WUFI 2D projects:

- Set up each project in the graphical user interface
- Switch to the “Calculation” tab – this creates the input file (*input.dat*).
- Start the calculation
- Stop the calculation after a few time steps and save the project.
→ All required files are stored in the project folder.

Requirements:

- Operating system: Windows 11, PowerShell 5.1 or higher
- Software: Installation of WUFI 2D 4.x
- Kernel path:
C:\Program Files (x86)\WUFI\WUFI2D-4\kernel\x64\w2dcore-x64.exe

Using the Scripts

Starting the scripts:

1. Extract all files and directories from the ZIP archive into a folder.
2. The shortcuts can be started by double-clicking:
 - *WUFI2D_BatchCalc.Ink*
 - *WUFI2D_CoreTest.Ink*
 - *WUFI2D_StartGUI.Ink*
 - *WUFI2D_StartGUI_fastlane.Ink*

Notes:

- The number of cores is read out and displayed.
- Only one instance of each script can be open at a time.
- The scripts can be cancelled with <Ctrl + C>

Convention:

Calc cores = OMP cores minus 1 (OMP = Windows system variable: Open Multi-Processing)
When prompted in the script interfaces, always enter the cores for the calculation (*calc cores*).

WUFI2D_BatchCalc

This script can automatically calculate one or more WUFI 2D projects sequentially in the background (batch mode).

Core functions:

- Input of the number of cores used for the calculation.
- Multiple projects can be prepared and calculated one after another.
- The calculation settings are saved for each project (*batchcalc.xml*) so that they are available again for later calculations.
- The prepared project list is also saved (*batch-prepare.xml*) and can later be loaded / edited again.
- The calculation period of a project that has already been calculated can be extended (“continue calculation”).

Please note:

As the batch mode directly uses the project directory, write speed also has some influence. The projects for the batch mode should therefore be located on a local disk to achieve optimal speeds.

Start fresh or use project list

If a saved list (*batch-prepare.xml*) exists, the script displays it and asks:

```
[1] Use saved list
```

```
[2] Start fresh
```

```
Select (1/2) [1]:
```

Input	Meaning
1 or Enter	Use saved list
2	Start fresh

Select projects

Please select a WUFI 2D project directory

→ Select the project folder via the Windows dialog.

If the project is already in the list:

Already in queue.

[1] Reconfigure

[2] Keep

(1/2) [2]:

Input	Meaning
1	Reconfigure
2 or Enter	Keep existing setting

Set calculation hours

The calculation period can be changed again here, if desired:

Calculation hours (Enter = keep <value> h):

Input	Meaning
Enter	Keep current number of hours
Number	Set new number of hours

Set number of cores

Case A – saved information available
(*core-test.xml* or *batchcalc.xml*)

```
core-test.xml: Calc cores: X (OMP=X+1)
```

```
Use these calc cores? (Enter = X, or enter value, max <max>):
```

Input	Meaning
Enter	Apply saved calculation cores
Number	Set custom calculation core count

Set number of cores

Case B – no saved information available or generated on another computer.

First, the script asks whether a core test should be run:

```
No core-test.xml found.  
(or: core-test.xml from different CPU!)  
Run CoreTest now? (Y/N) [Y]:
```

Input	Meaning
Enter or Y	Core test is run now
N	No core test → continue to manual input (see next slide)

Set number of cores

If no core test is run – manual input:

```
CPU: <name> (max <maxCalc> calc cores)
```

```
Enter calc cores (1-<maxCalc>):
```

Input	Meaning
Number 1 ... maxCalc	Set calculation cores
Number > maxCalc	Core count is limited to the maximum

Calculation mode (restart)

Appears only if the following conditions are met:

- a result file (*.wfd*) already exists and
- the new number of hours selected is greater than the one stored in the project

```
Result file found: <file>
```

```
[1] Run full calculation (<new> hours)
```

```
[2] Resume calculation (from hour <old> to hour <new>)
```

```
Mode (1/2) [1]:
```

Input	Meaning
1 (or Enter)	Full recalculation over the complete number of hours
2	Resume from the last hour (from hour <old> to hour <new>)

Rename result file

In case of batch calculation, the result file is not automatically named like the project.

```
The result filename will be 'wufi2dresult.wfd' (WUFI default).  
Rename result file to '<project name>.wfd' after calculation?  
Rename? (Y/N) [Y]:
```

Input	Meaning
Enter or Y	Result file is renamed to <i><project name>.wfd</i> after calculation
N	Default name <i>wufi2dresult.wfd</i> is retained

Action menu

BATCH PREPARATION STATUS

[1] Start calculation (all prepared projects)

[2] Add another project

[3] Edit project settings -> reconfiguration

[4] Delete a project from list

[5] Delete project list

[6] Exit without calculating

Select (1-6) [1]:

Input	Meaning
1 or Enter	Start calculation of all projects
2	Add another project
3	Edit project settings
4	Delete project from list
5	Delete entire project list
6	Exit without calculation

Calculation running

- Projects are calculated one after another
- Progress display: Time step X / Y (Z%) | Elapsed: hh:mm:ss

```
Batch calculation (2 project(s))
Project 1 of 2 : Variante7_Start0kt
[
Calculating: Variante7_Start0kt
Time step 6705 / 43800 (15%) | Elapsed: 00:14:09
[ooooooooooooooooooooo
```

Summary

After all calculations are complete, a summary is displayed

```
=====
ALL CALCULATIONS COMPLETED
Total: hh:mm:ss
=====
[OK]    <project>
        Wallclock: hh:mm:ss | CPU: <s>s | Calc cores: X (OMP=Y)
[??]    <project>
        Wallclock: ... | CPU: ... | Calc cores: X (OMP=Y)
[FAIL]  <project>: <error message>
Summary: <n> OK, <m> failed
```

Symbol	Meaning
[OK]	Calculation completed successfully
[??]	Calculation completed, no response from calculation core
[FAIL]	Calculation failed (error message is displayed)

Summary

The following prompt appears only if no project has failed:

```
Delete batch-prepare.xml? (Y/N) [Y]:
```

Input	Meaning
Enter or Y	<i>batch-prepare.xml</i> is deleted
N	List is retained and can be loaded again later

WUFI2D_CoreTest

The script automatically determines the optimal number of cores for a WUFI 2D calculation. To do this, the same calculation case is repeated with different numbers of cores until the optimum is determined.

Notes:

- The calculation period for the test can be specified (recommended: 730 h).
- The start month can be set (recommended: coldest month).
- The result is saved in the project directory (*core-test.xml*).

Please note:

As the batch mode writes directly to the project directory, write speed also has an influence. Therefore, projects for core test should be located on a local disk to achieve optimal speeds.

Step 1: Select project directory

If the current folder is not a valid WUFI project, a selection dialog opens:

```
Current directory is NOT a WUFI 2D project directory.  
Please select the WUFI 2D project directory...
```

If the selection is invalid:

```
Selected directory is NOT valid!  
Try again? [Y/N] (Default: Y):
```

Input	Meaning
Enter or Y	Select a directory again
N	Cancel the script

Step 2: Check existing result

If saved information exists (*core-test.xml*), the script displays its contents and asks:

Case A – core test was run on the same CPU:

```
Run a new test? [Y] Yes / [N] No, keep existing result  
(Default: N):
```

Input	Meaning
Enter or N	Keep existing result, script exits
Y	Start a new test

Step 2: Check existing result

If saved information exists (*core-test.xml*), the script displays its contents and asks:

Case B – core test was run on a different CPU:

```
The existing result was calculated on a different CPU.  
Run a new test? [Y] Yes (recommended) / [N] No, keep existing  
result (Default: Y):
```

Input	Meaning
Enter or Y	Start a new test (recommended)
N	Keep existing result

Step 3: Test physical or logical cores

CPU cores detected:

[1] Physical cores: <n>

[2] Logical cores: <m> (incl. Hyper-Threading)

Which cores should be tested? [1] Physical / [2] Logical
(Default: 2):

Input	Meaning
Enter or 2	Test logical cores (recommended)
1	Test physical cores

Step 4: Set start month

Current start date in file: 1.10.1991_0.00

Recommendation: choose the coldest month of the year.
Enter 'K' to keep the start date from input.dat.

Which start month? (1-12, [K] keep from input.dat, Default: 1 = January):

Input	Meaning
Enter	Use default value 1 (= January)
Number 1 to 12	Corresponds to the month to which the start date should be set. The start day is always set to day 1.
K	Use start date from <i>input.dat</i>

Step 5: Set number of test hours

Recommended: 730 hours for test.

How many hours for the test? (Default: 730):

Input	Meaning
Enter	Use default value 730 h
Number > 0	Set custom number of test hours

Step 6: Start test

Press Enter to start the core test

Input	Meaning
Enter	Start test runs

The test then runs automatically:

- Progress bar per time step:

```
WUFI 2D Core Test
OMP=8 (calc cores: 7)...
[ooooooooooooooooooooo
Calculating: OMP=8 (calc cores: 7)
Time step 360 / 730 (49%) | Elapsed: 00:00:57
[ooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooo
```

- Automatic termination after two consecutive calculation runs without improvement

Step 7: Result and saving

After completion, the script displays a results table:

CalcCores	OMP	CPU Time (s)	Wallclock (s)	Note
-----	---	-----	-----	----
...				
★ Optimal: Calc cores: X (OMP_NUM_THREADS=X+1)				

- The optimum value is marked with << optimal.

```
Results:
=====
Project: C:\DATEN\WUFI2D\BedPlate_Benchmark
Grid: 152 * 202 | Test: 730 h | Original: 26280 h

CalcCores  OMP  CPU Time (s)  Wallclock (s)  Note
-----
7          8    203.4        217.1
8          9    151.0        166.0
9         10    144.1        158.2
10        11    141.9        156.1      << optimal
11        12    145.9        160.3
12        13    145.7        160.4

★ Optimal: Calc cores: 10 (OMP_NUM_THREADS=11)

Total duration: 00:17:00
Results saved:
C:\DATEN\WUFI2D\BedPlate_Benchmark\core-test.xml
```

- The result is automatically saved in *core-test.xml*.

Step 8: Test another project

Do you want to test another project? [Y] Yes / [N] No
(Default: N):

Input	Meaning
Enter or N	Exit script
Y	Test another project (back to step 1)

WUFI2D_StartGUI

This script starts the WUFI 2D user interface with a specified number of cores.

Functions:

- The number of cores can be specified.
- Results from a core test can be loaded from a project directory.
- The specified number of cores is saved and suggested again when reopened.
- Directly opens WUFI 2D using the saved cores without further prompts (*WUFI2D_StartGUI_fastlane*).

Options for specifying / loading the number of cores

The script offers various options for setting the number of cores:

Situation	Behaviour
Manual input	Direct input of the core count
Saved value	Saved value from the last call is offered
Load from a project	Selection of a project directory

Manual input / use saved value

If a saved configuration exists, it is displayed. Otherwise, only manual input or loading from a project directory is available.

```
Use X calc cores? [Enter]
Enter new number of calc cores (2-<max>)
load from a WUFI 2D project [P]
[Enter] / (2-<max>) / [P]
```

Input	Meaning
Enter	Uses the saved value
Number 4 - <max>	Manually set new number of cores
P	Load core count from a WUFI 2D project

Select project directory (with option [P])

Allows a core test to be loaded from a WUFI 2D project directory.

```
Please select a project directory containing a previous  
core-test.xml...
```

Input	Meaning
Choose folder	Reads the <i>CoreTest data</i> from the selected directory
Cancel	Cancels the selection

After loading, the number of cores is displayed:

```
Use X calc cores? [Enter] = Yes / or enter number of calc cores  
(4-<max>)
```

Input	Meaning
Enter	Uses the value loaded from the project
Number 4 - <max>	Set custom value

Start WUFI 2D

The script checks the selected number of cores and sets it for starting WUFI 2D:

```
=====
Starting WUFI 2D with <X> calculation cores...
(OMP_NUM_THREADS=<X+1>)
=====
```

WUFI 2D is started and the script exits.