

May 2014 - ELS

TOUGHREACT V3-OMP Documentation

Documentation for TOUGHREACT V3-OMP now consists of four documents:

1. TOUGHREACT_V3_OMP_QuickRef.pdf
2. TOUGHREACT_V3-OMP_RefManual.pdf
3. TOUGHREACT_V3-OMP_SampleProblems&Tutorial
4. TOUGHREACT V3-OMP_Readme. Doc (this file)

The documents provided here are in draft form. The most current versions of the documents can be found on the TOUGH Software website:

<http://esd.lbl.gov/research/projects/tough/documentation/manuals.html>

Using OpenMP and Optimizing TOUGHREACT V3-OMP Performance

The speed of codes using parallel processing can increase with the number of cores (or threads), reach a maximum, and then decline as the number of cores increase further. This is expected for all parallel codes, since at some point each core is fast enough to solve more calculations than it takes to spread them out over many cores. For TOUGHREACT V3-OMP, the larger the chemical system, and the greater the number of grid blocks, the more likely the problem will keep increasing in speed (decreasing in time) as the maximum number of cores is reached. The relation depends on several factors, in particular the speed of each core (thread), the memory available, the problem size, the workload distribution, and the time spent for the multiphase flow calculation.

It is advisable to determine how fast the problem runs using the full number of cores on the computer, and also with about half that number for comparison. For those problems running only flow, the number of threads should be set to one, because the primary flow routines are not parallelized and increasing the number of threads will just increase the computational overhead. Setting the number of threads is also useful if you want to run more than one job on your machine and then they won't compete for resources.

Setting the number of threads:

If you don't know how many threads are on your machine, and you don't set the number of threads, the maximum will be used and displayed on the screen.

For the PC on the command line (according to Microsoft):

```
set OMP_NUM_THREADS=6
```

For Linux or Mac OS X using the default bash shell:

```
export OMP_NUM_THREADS=6
```

Under tcsh:

```
setenv OMP_NUM_THREADS 6
```