



Learn Git and GitHub without any code!

Using the Hello World guide, you'll start a branch, write comments, and open a pull request.

Read the guide

ITensor / ITensor

WIP: parallelize over block sparse contractions #325

Merged emstoudenmire merged 14 commits into v3 from parallelcontract on Feb 14

Conversation 5

Commits 14

Checks 0

Files changed 4

+210 -18



mtfishman commented on Feb 4 • edited ▾

Contributor

Here is a work in progress for parallelizing over block sparse contractions. There is a failing test so there may be a bug in the implementation, but initial timings are very promising.

v3 branch, exthubbard sample code:

```
vN Entropy at center bond b=10 = 1.579681649110
Eigs at center bond b=10: 0.2774 0.2770 0.2050 0.2050 0.0033 0.0033 0.0025 0.0025 0.
Largest link dim during sweep 6/6 was 628
Largest truncation error: 6.82202e-13
Energy after sweep 6/6 is -17.435415741677
Sweep 6/6 CPU time = 1m, 5.7s (Wall time = 5.660s)
```

This branch, exthubbard sample code:

```
vN Entropy at center bond b=10 = 1.579681455638
Eigs at center bond b=10: 0.2774 0.2770 0.2050 0.2050 0.0033 0.0033 0.0025 0.0025 0.
Largest link dim during sweep 6/6 was 628
Largest truncation error: 6.88866e-13
Energy after sweep 6/6 is -17.435415742191
Sweep 6/6 CPU time = 19.35s (Wall time = 2.137s)
```

This was run by adding `-fopenmp` to CCCOM in options.mk and setting `export OMP_NUM_THREADS=10` and `export MKL_NUM_THREADS=1`.

Thanks to Nils for his help with openmp and suggesting the parallelization strategy for avoiding race conditions!

👍 1

Reviewers

emstoudenmire

✓

Assignees

No one assigned

Labels

None yet

Projects

None yet

Milestone

No milestone

Linked issues

Successfully merging this pull request may close these issues.

None yet

3 participants

mtfishman and others added 9 commits on Feb 4

- Parallelize block sparse contraction

873b4f8
- Remove print statement, add comment

ed5bda9
- Fix issue with empty output tensor

f600c15
- Revert changes to set ITensor element

69fd8bc
- Add some debug checks to parallel contraction code

8f27a64
- parallelized getContractedOffsets

8741d98
- parallelized getContractedOffsets

0f85585
- merged

48003d9
- Code cleanup

94fd78b



mtfishman commented on Feb 6

Author

Contributor

Alex and I worked on parallelizing `getContractedOffsets`, which analyzes the blocks of A and B to determine the list of contractions and the blocks of C. The following are results for the 2D Hubbard model with DMRG with momentum conservation.

ITensor v3 (no parallelization):

```
vN Entropy at center bond b=8 = 3.019814122626
Eigs at center bond b=8: 0.1677 0.1677 0.1597 0.1597 0.0138 0.0138 0.0138 0.0138
0.0096 0.0096
Largest link dim during sweep 5/5 was 7341
Largest truncation error: 4.5789e-09
```

