ANALYZING QUANTUM MANY-BODY SYSTEMS WITH ITENSOR AND PASTAQ

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- Find out more here: `https://mtfishman.github.io/`.

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- We are hiring postdocs, full-time scientists, part-time and full-time software developers, interns, etc.

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- Paper: `https://arxiv.org/abs/2007.14822/`

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When should I use tensor networks?

- Many sites or qubits in your system: linear or log scaling in the system size.

[TODO: "Quantum volume" schematic plot.]

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- If TNs could do everything, we would not need a quantum computer! But in my opinion, it is the best general purpose tool we have right now.
- Perhaps most importantly, tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

[TODO: "Quantum volume" schematic plot.]

What are tensor networks?

[TODO: Show drawings of tensor networks.]

How do I install ITensor/PastaQ?

1. Download Julia.

[TODO: Add links, show code]

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Tutorial: One-site state basics

```julia
using ITensors

i = Index(2)


```

```
# Load ITensor

# 2−dimensional labeled
# Hilbert space
# (dim=2|id=510)
```

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```
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# (dim=2|id=510)
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```
Zp = ITensor(i)
Zp[i=>1] = 1

Zp = ITensor([1 0], i)
```

```
# Z|Z+⟩ = |Z+⟩


# Construct from a Vector
```

Tutorial: One-site state basics

```
Zp = ITensor([1 0], i)
Zm = ITensor([0 1], i)
Xp = ITensor([1 1]/√2, i)
Xm = ITensor([1 -1]/√2, i)
```

```
# Z|Z+⟩ = |Z+⟩
# Z|Z−⟩ = −|Z−⟩
# X|X+⟩ = |X+⟩
# X|X−⟩ = −|X−⟩
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# X|X+⟩ = |X+⟩
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```

```
(Zp + Zm)/√2
(dag(Zp) * Xp)
(dag(Zp) * Xp)[]
inner(Zp, Xp)
norm(Xp)
```

```
# ≈ Xp
# ≈ ITensor(1/√2)
# ≈ 1/√2
# ≈ 1/√2
# ≈ 1
```

Tutorial: One-site state basics

```
using ITensorVisualizationBase: set_backend!
```

Tutorial: One-site state basics

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```
back = "UnicodePlots"
set_backend!(back)

@visualize dag(Zp) * Xp
```

```
# TODO: Add
    UnicodePlots
    visualization.
```

Tutorial: One-site state basics

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using ITensorVisualizationBase: set_backend!
```

```julia
back = "UnicodePlots"
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@visualize dag(Zp) * Xp
```

```julia
# TODO: Add UnicodePlots visualization.
```

```julia
back = "Makie"
set_backend!(back)

@visualize dag(Zp) * Xp
```

[TODO: Add GLMakie visualization.]

Tutorial: One-site state basics

```julia
i = Index(2, "S=1/2")
```

```
# "S=1/2" defines an
# operator basis
#
# Additionally:
# "Qubit", "Qudit",
# "Electron", ...
```

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```

```
# "S=1/2" defines an
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# Additionally:
# "Qubit", "Qudit",
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```

```
Zp = state("Z+", i)
Zm = state("Z-", i)
Xp = state("X+", i)
Xm = state("X-", i)
```

```
# ITensor([1 0], i)
# ITensor([0 1], i)
# (Zp + Zm)/√2
# (Zp - Zm)/√2
```

Tutorial: Custom one-site states

```julia
import ITensors: state


function state(
  ::StateName"iX−",
  ::SiteType"S=1/2"
)
  return [im -im]/√2
end
```

```
# Overload ITensors.jl
# behavior

# Define a state with the
# name "iX−"
```

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  return [im -im]/√2
end
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```
# Overload ITensors.jl
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# Define a state with the
# name "iX−"
```

```
iXm = state("iX−", i)

inner(Zp, iXm)
inner(Zm, iXm)
```

```
# ≈ im ∗ Xm

# ≈ im/√2
# ≈ −im/√2
```

Tutorial: Priming

```
i = Index(2)
j = Index(2)

i == j
```

```
# (dim=2|id=837)
# (dim=2|id=899)

# false
```

Tutorial: Priming

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i = Index(2)
j = Index(2)

i == j
```

```
# (dim=2|id=837)
# (dim=2|id=899)

# false
```

```
i

prime(i)
i'
i == i'
noprime(i')
```

```
# (dim=2|id=837)

# (dim=2|id=837)'
# (dim=2|id=837)'
# false
# (dim=2|id=837)
```

Tutorial: One-site operators

```
Z = ITensor(i', i)
Z[i'=>1, i=>1] = 1
Z[i'=>2, i=>2] = -1
```

```
# TODO: Diagram
# Set elements
```

Tutorial: One-site operators

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```
# TODO: Diagram
# Set elements
```

```
z = [
  1 0
  0 -1
]
Z = ITensor(z, i', dag(i))

Z = op("Z", i)
```

```
# From matrix



# Use predefined definition
```

Tutorial: One-site operators

```
Z = op("Z", i)
X = op("X", i)

Zp = state("Z+", i)
Zm = state("Z-", i)
```

```
# Z
# X

# |Z+⟩
# |Z-⟩
```

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X = op("X", i)

Zp = state("Z+", i)
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```

```
# Z
# X

# |Z+⟩
# |Z−⟩
```

```
XZp = X * Zp
XZp == Zm
XZp == Zm'
noprime(XZp) == Zm
```

```
# X|Z+⟩ = |Z−⟩
# false
# true
# true
```

Tutorial: One-site operators

[TODO: Add visualization of inner product]

```
XZp = X * Zp                # X|Z+⟩ = |Z−⟩

inner(Zm, XZp)              # error: not a scalar value

inner(Zm', XZp)             # ≈ 1
inner(Zp', XZp)             # ≈ 0
```

Tutorial: One-site operators

[TODO: Add visualization of inner product]

```
XZp = X * Zp

inner(Zm, XZp)

inner(Zm', XZp)
inner(Zp', XZp)
```

```
# X|Z+⟩ = |Z−⟩

# error: not a scalar value

# ≈ 1
# ≈ 0
```

```
apply(X, Zp) == Zm

(dag(Zm)' * X * Zp)[]
inner(Zm', X, Zp)
```

```
# false

# ≈ 1
# ≈ 1
```

Tutorial: Custom one-site operators

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function op(
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  return [
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end
```

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```

```julia
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# behavior
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```julia
op("iX", i)
```

```julia
# im * X
```

Tutorial: Two-site states

```
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 == i2

ZpZm = ITensor(i1, i2)
ZpZm[i1=>1, i2=>2] = 1
```

```
# (dim=2|id=505|"S=1/2")
# (dim=2|id=576|"S=1/2")

# false

# |Z+⟩₁|Z−⟩₂ = |Z+Z−⟩
```

Tutorial: Two-site states

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```
# (dim=2|id=505|“S=1/2”)
# (dim=2|id=576|“S=1/2”)

# false

# |Z+⟩_1|Z−⟩_2 = |Z+Z−⟩
```

```
Zp1 = state("Z+", i1)
Zp2 = state("Z+", i2)

Zm1 = state("Z−", i1)
Zm2 = state("Z−", i2)

ZpZm = Zp1 * Zm2
ZmZp = Zm1 * Zp2
```

```
# |Z+⟩_1
# |Z+⟩_2

# |Z−⟩_1
# |Z−⟩_2

# |Z+Z−⟩ = |Z+⟩_1|Z−⟩_2
# |Z−Z+⟩ = |Z−⟩_1|Z+⟩_2
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Future directions

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- More general built-in tensor networks beyond MPS/MPO
- More HPC with multithreaded and multiprocessor parallelism and GPUs
- Many ongoing projects and directions: quantum chemistry (for example UCC), real space parallel DMRG, TDVP, and TEBD, MPO compression tools, general approximate contraction techniques for unstructured networks, contracting and optimizing general tensor networks with AD, infinite MPS and tensor network tools like VUMPS and TDVP, trying out different network topologies for noisy circuit tomography, simulation and optimization.

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- Building general tools, looking for people with problems and code to contribute.

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- More general built-in tensor networks beyond MPS/MPO
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- Many ongoing projects and directions: quantum chemistry (for example UCC), real space parallel DMRG, TDVP, and TEBD, MPO compression tools, general approximate contraction techniques for unstructured networks, contracting and optimizing general tensor networks with AD, infinite MPS and tensor network tools like VUMPS and TDVP, trying out different network topologies for noisy circuit tomography, simulation and optimization.
- Building general tools, looking for people with problems and code to contribute.

Future directions

- More AD, make ITensor fully differentiable (have some work to do, like tensor decompositions and general network contractions, more MPS/MPO functions. You will find bugs!).
- More general built-in tensor networks beyond MPS/MPO
- More HPC with multithreaded and multiprocessor parallelism and GPUs
- Many ongoing projects and directions: quantum chemistry (for example UCC), real space parallel DMRG, TDVP, and TEBD, MPO compression tools, general approximate contraction techniques for unstructured networks, contracting and optimizing general tensor networks with AD, infinite MPS and tensor network tools like VUMPS and TDVP, trying out different network topologies for noisy circuit tomography, simulation and optimization.
- Building general tools, looking for people with problems and code to contribute.