# Analyzing Quantum Many-Body Systems with ITensor and PastaQ

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github.com/mtfishman/ITensorTutorials.jl

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► PhD from Caltech with John Preskill and Steve White (UCI) in 2018.



mtfishman.github.io











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





# SIMONS FOUNDATION

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- Find out more at: julialang.org.



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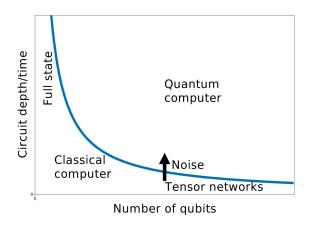


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  - Approximate circuit evolution and optimization with MPS/MPO, etc.
- ► Find out more: github.com/GTorlai/PastaQ.jl

▶ In my opinion, tensor networks are the best general purpose tool we have right now for simulating and analyzing quantum computers.



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  - ► ITensor and PastaQ handle this seamlessly.
  - ► This is not the focus of ITensor and PastaQ at the moment, specialized libraries like Yao.jl may be faster.
- ➤ Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

## What are tensor networks?



Matrix  $M_{ij}$ Order-2 tensor



Tensor  $T_{ijk}$ Order-3 tensor



## What are tensor networks?



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- 2. Launch Julia:
  - 1 \$ julia

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```
1 $ julia
```

3. Type the following commands:

```
julia> using Pkg
julia> Pkg.add("ITensors")
[...]
julia> Pkg.add("PastaQ")
[...]
```

#### Now you can use ITensors and PastaQ:

```
julia> using ITensors

julia> i = Index(2);

julia> A = ITensor(i);
```

Now you can use ITensors and PastaQ:

```
julia> using ITensors
julia> i = Index(2);
julia> A = ITensor(i);
```

```
julia> using PastaQ

julia> gates = [("X", 1), ("CX", (1, 3))];

julia> ψ = runcircuit(gates);
```

```
1 using ITensors
2
3 i = Index(2)
4
5
```

#### Load ITensor

2-dimensional labeled Hilbert space (dim=2|id=510)

```
1 using ITensors
2
3 i = Index(2)
4
5
```



```
1 using ITensors
2
3 i = Index(2)
4
5
```



$$|Z+\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}$$

Construct from a Vector

```
1  using ITensors
2
3  i = Index(2)
4
5

1  Zp = ITensor(i)
2  Zp[i=>1] = 1
3
4  Zp = ITensor([1, 0], i)
```

i

```
 \begin{aligned} & \text{Zp=ITensor}([1,0],\mathbf{i}) \\ & \text{Zm=ITensor}([0,1],\mathbf{i}) \\ & \text{Xp=ITensor}([1,1]/\sqrt{2},\mathbf{i}) \\ & \text{Xm=ITensor}([1,-1]/\sqrt{2},\mathbf{i}) \end{aligned} \qquad |Z+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad |Z-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ & |X+\rangle = \begin{bmatrix} 1 \\ 1 \end{bmatrix} / \sqrt{2}, \quad |X-\rangle = \begin{bmatrix} 1 \\ -1 \end{bmatrix} / \sqrt{2}. \end{aligned}
```

```
i Zp=ITensor([1,0],i)
2 Zm=ITensor([0,1],i)
3 Xp=ITensor([1,1]/\(\frac{1}{2}\),i)
4 Xm=ITensor([1,-1]/\(\frac{1}{2}\),i)

i X+
```

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

2 Zm=ITensor([0,1],i)

3 Xp=ITensor([1,1]/√2,i)

4 Xm=ITensor([1,-1]/√2,i)
```

$$|X+\rangle = (|Z+\rangle + |Z-\rangle)/\sqrt{2}$$

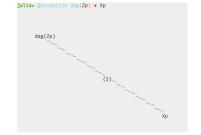
$$\langle Z + | X + \rangle \approx 1/\sqrt{2}$$

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

$$\frac{1}{X+} = \frac{1}{Z+} + \frac{1}{Z-}$$

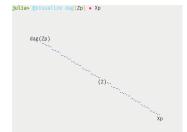
$$Z+$$
  $X+$  =  $1/\sqrt{2}$ 

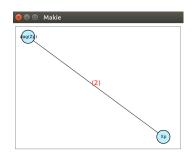
- using ITensorUnicodePlots
- 3 @visualize dag(Zp) \* Xp



- using ITensorUnicodePlots
- @visualize dag(Zp) \* Xp

- using ITensorGLMakie
- @visualize dag(Zp) \* Xp





## Tutorial: One-site states

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

i = Index(2, "S=1
```

```
(dim=2|id=25|"S=1/2")
```

"S=1/2" defines an operator basis

Additionally: "Qubit", "Qudit",

"Electron", ...

#### Tutorial: One-site states

```
1  Zp=state("Zp",i)
2  Zm=state("Zm",i)
3  Xp=state("Xp",i)
4  Xm=state("Xm",i)
```

```
(dim=2|id=25|"S=1/2")

"S=1/2" defines an operator basis

Additionally:
"Qubit", "Qudit",
```

```
1 ITensor([1,0],i)
2 ITensor([0,1],i)
3 ITensor([1,1]/\forall2,i)
4 ITensor([1,-1]/\forall2,i)
```

"Electron", ...

#### Tutorial: Custom one-site states

```
import ITensors: state

function state(
::StateName"iXm",
::SiteType"S=1/2")
return [im,-im]/\day
end
```

Overload ITensors.jl behavior

Define a state with the name "iX-"

#### Tutorial: Custom one-site states

```
import ITensors: state

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

```
1    iXm = state("iXm", i)
2
3
4    inner(Zm, iXm)
```

Overload ITensors.jl behavior

Define a state with the name "iX-"

$$|iX-\rangle = i|X-\rangle$$

$$\langle Z - | iX - \rangle = -i/\sqrt{2}$$

#### Tutorial: Custom one-site states

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import ITensors: state

function state(
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return [im,-im]/√2
end
```

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

Overload ITensors.jl behavior

Define a state with the name "iX-"

$$\frac{1}{1}$$
  $IX+ = (\frac{1}{1}X+)*i$ 

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

$$\begin{array}{l} (\mathrm{dim}{=}2|\mathrm{id}{=}837) \\ (\mathrm{dim}{=}2|\mathrm{id}{=}899) \end{array}$$

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

```
1  i = Index(2)
2
3  prime(i) == i'
4
5  i != i'
6  noprime(i') == i
```

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

```
i = Index(2)
prime(i) == i'

i != i'
noprime(i') == i
```

```
1 i = Index(2, "S=1/2")
2 Z = ITensor(i', i)
3 Z[i'=>1, i=>1] = 1
4 Z[i'=>2, i=>2] = -1
```

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

```
1  i = Index(2, "S=1/2")
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3  Z[i'=>1, i=>1] = 1
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```
1 i = Index(2, "S=1/2")

2 Z = ITensor(i', i)

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```

```
1  z = [1 0; 0 -1]
2
3
4
5  Z = ITensor(z, i', i)
6
7
8  Z = op("Z", i)
```



Matrix representation Z

Convert to ITensor

Use predefined definition

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

2 X = op("X", i)

3 X = op("X", i)

4 Zp = state("Zp", i)

5 Zm = state("Zm", i) |Z+>
```

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

2 X = op("X", i)

3 

4 Zp = state("Zp", i)

5 Zm = state("Zm", i)
```

$$X|Z+\rangle = |Z-\rangle$$

```
1  Z = op("Z", i)
2  X = op("X", i)
3
4  Zp = state("Zp", i)
5  Zm = state("Zm", i)
```

$$i'$$
  $X$   $i$   $Z+$   $=$   $i'$   $Z-$ 

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

$$\langle Z - |X|Z + \rangle \approx 1$$

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

$$Z - \frac{i'}{X} X = Z + = 1$$

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

$$Z - X Z + = 1$$

```
1 apply(X, Zp) ==
2 noprime(X * Zp)
3
4
5
6 inner(Zm, apply(X, Zp))
```

$$X|Z+\rangle$$

$$\langle Z - |X|Z + \rangle \approx 1$$

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

```
apply(X, Zp) ==
noprime(X * Zp)

4

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

$$Z - \frac{i'}{X} X = Z + = 1$$

apply 
$$\left(\frac{1}{X}, \frac{1}{X}, \frac{1}{X}, \frac{1}{X}\right)$$

$$= \operatorname{noprime}\left(\frac{1}{X}, \frac{1}{X}, \frac{1}{X}\right)$$

$$= \frac{1}{X}$$

1 import ITensors: op
2
3 function op(
4 ::OpName"iX",

::SiteType"S=1/2")
return [0 im; im 0]

end

Overload ITensors.jl behavior

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import ITensors: op

function op(
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$$\frac{\mathbf{i'} \mathbf{i} \mathbf{X} \cdot \mathbf{i}}{\mathbf{i} \mathbf{X} \mathbf{i}} = \left(\frac{\mathbf{i'} \mathbf{X} \cdot \mathbf{i}}{\mathbf{X} \mathbf{i}}\right) * \mathbf{i}$$

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end
```

```
1 op("iX", i)
```

$$\frac{\mathbf{i}^{\prime} \mathbf{i} \mathbf{X} \cdot \mathbf{i}}{\mathbf{i}} = \left( \frac{\mathbf{i}^{\prime} \mathbf{X} \cdot \mathbf{i}}{\mathbf{X}} \right) * \mathbf{i}$$

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$$\frac{\mathbf{i'} \mathbf{i} \mathbf{X} \cdot \mathbf{i}}{\mathbf{i}} = \left(\frac{\mathbf{i'} \mathbf{X} \cdot \mathbf{i}}{\mathbf{X}}\right) * \mathbf{i}$$

```
1 op("iX", i)
```

```
1 X * im
```

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

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

3 i1 != i2

6 ZpZm = ITensor(i1, i2)

7 ZpZm[i1=>1, i2=>2] = 1  (dim=2|id=505|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2") (dim=2|id=576|"S=1/2")
```

```
1 i1 = Index(2, "S=1/2,i1")
2 i2 = Index(2, "S=1/2,i2")
3
4 i1 != i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```

```
1  i1 = Index(2, "S=1/2,i1")
2  i2 = Index(2, "S=1/2,i2")
3
4  i1 != i2
5
6  ZpZm = ITensor(i1, i2)
7  ZpZm[i1=>1, i2=>2] = 1
```

```
1  Zp1=state("Zp",i1)
2  Zp2=state("Zp",i2)
3  Zm1=state("Zm",i1)
4  Zm2=state("Zm",i2)
5
6
7  ZpZm = Zp1 * Zm2
```

$$\begin{array}{ccc} \underline{i_1} & \underline{i_2} & Z + \\ \underline{i_2} & Z - \end{array}$$

$$|Z+\rangle_1$$
  
 $|Z+\rangle_2$ 

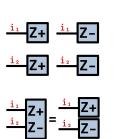
$$|Z-\rangle_1$$
  
 $|Z-\rangle_2$ 

$$|Z+Z-\rangle = |Z+\rangle_1|Z-\rangle_2$$

```
1 i1 = Index(2, "S=1/2,i1")
2 i2 = Index(2, "S=1/2,i2")
3
4 i1 != i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```

```
Typ1=state("Zp",i1)
Zp2=state("Zp",i2)
Zm1=state("Zm",i1)
Zm2=state("Zm",i2)
ZpZm = Zp1 * Zm2
```

$$\begin{array}{ccc} \underline{i_1} & \underline{i_2} & Z + \\ \underline{i_2} & Z - \end{array}$$



```
1 \psi = \text{ITensor}(i1, i2)

2 \psi[i1=>1, i2=>2] = 1/\sqrt{2}

3 \psi[i1=>2, i2=>1] = 1/\sqrt{2}

4 \psi = (\text{Zp1} * \text{Zm2} + \text{Zm1} * \text{Zp2})/\sqrt{2}
```

$$(|Z+\rangle|Z-\rangle + |Z-\rangle|Z+\rangle)/\sqrt{2}$$

From single-site states

```
1 \psi = \text{ITensor}(i1, i2)

2 \psi[i1=>1, i2=>2] = 1/\sqrt{2}

3 \psi[i1=>2, i2=>1] = 1/\sqrt{2}

4 \psi = (\text{Zp1} * \text{Zm2} + \text{Zm1} * \text{Zp2})/\sqrt{2}
```

$$\frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \Psi = \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \sqrt{2}$$

```
1 \psi = ITensor(i1, i2)

2 \psi[i1=>1, i2=>2] = 1/\sqrt{2}

3 \psi[i1=>2, i2=>1] = 1/\sqrt{2}

4

5 \psi = (Zp1 * Zm2 +

2m1 * Zp2)/\sqrt{2}
```

$$\frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \Psi = \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \sqrt{2}$$

$$svd\left(\begin{array}{c|c}i_1&Z+Z-&i_2\\\end{array}\right)$$

$$=\begin{array}{c|c}i_1&U&&S&&V&i_2\\\end{array}$$

$$\begin{array}{c|c}u&S&&&=\begin{bmatrix}1\\0\end{array}$$

```
1 \psi = ITensor(i1, i2)

2 \psi[i1=>1, i2=>2] = 1/\sqrt{2}

3 \psi[i1=>2, i2=>1] = 1/\sqrt{2}

4

5 \psi = (Zp1 * Zm2 +

2m1 * Zp2)/\sqrt{2}
```

$$\frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \Psi = \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} + \sqrt{2}$$

$$svd\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$

$$= \frac{1}{1}, \frac{1}{1}, \frac{1}{2}$$

$$svd\left(\frac{1}{1}, \frac{1}{1}, \frac{1}{2}\right)$$

$$= \frac{1}{1}, \frac{1}{1}, \frac{1}{2}$$

$$= \frac{1}{1}, \frac{1}{2}$$

```
1 H = ITensor(i1', i2',
2 i1, i2)
3 H[i1'=>2, i2'=>1,
4 i1=>2, i2=>1] = -1
5 # ...
```

Make a Hamiltonian: Transverse field Ising (n=2)

$$H = -\sum_{j=1}^{n-1} Z_j Z_{j+1} + h \sum_{j=1}^{n} X_j$$

```
1 H = ITensor(i1', i2',

2 i1, i2)

3 H[i1'=>2, i2'=>1,

4 i1=>2, i2=>1] = -1

5 # ...
```

```
1 Id1 = op("Id", i1)
2 Z1 = op("Z", i1)
3 X1 = op("X", i1)
4 Id2 = op("Id", i2)
5 Z2 = op("Z", i2)
6 X2 = op("X", i2)
7
8 ZZ = Z1 * Z2
9 XI = X1 * Id2
10 IX = Id1 * X2
11
12 h = 0.5
13 H = -ZZ + h * (XI + IX)
```

Make a Hamiltonian:

Transverse field Ising (n=2)

$$H = -\sum_{j}^{n-1} Z_j Z_{j+1} + h \sum_{j}^{n} X_j$$

$$\frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{H} \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} = - \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{Z} \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} + \mathbf{h} \left( \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{X} \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} + \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{X} \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \right)$$

```
inner(Zp1' * Zp2', H,
Zp1 * Zp2)
```

$$\langle Z{+}Z{+}|H|Z{+}Z{+}\rangle$$

$$\frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{H} \mathbf{i}_{1} \mathbf{U} \mathbf{U}$$

$$= \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{U} \mathbf{U} \mathbf{D} \mathbf{U}$$

$$= \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}} \mathbf{U} \mathbf{U} \mathbf{D} \mathbf{U}$$

$$= \frac{-\sqrt{2}}{-1}$$

$$1$$

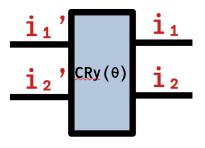
```
import ITensors: op
    function op(
       :: OpName "CRy",
     ::SiteType"S=1/2"; θ)
      c = \cos(\theta/2)
      s = \sin(\theta/2)
 8
      return
        0 0 c -s
        0 0 s c]
13
    end
```

```
Controlled-Ry (CRy) rotation gate
```

 $CRy(\theta)$ 

```
1 import ITensors: op

2
3 function op(
4 ::OpName"CRy",
5 ::SiteType"S=1/2"; θ)
6 c = cos(θ/2)
7 s = sin(θ/2)
8 return [
9 1 0 0 0
10 0 1 0 0
11 0 0 c -s
12 end
```



1 CRy = op("CRy", i1, i2; 
$$\theta = \pi/2$$
)

Controlled-rotation gate  $CRy(\pi/2)$ 

1 CRy = op("CRy", i1, i2; 
$$\theta = \pi/2$$
)



## Tutorial: Custom two-site operators

```
1 CRy = op("CRy", i1, i2; \theta = \pi/2)
```

```
1  Xp1=state("Xp",i1)
2  Xm1=state("Xm",i1)
3  Xp2=state("Xp",i2)
4  Xm2=state("Xm",i2)
5
6  apply(CRy, Zm1 * Zp2) ≈
7  Zm1 * Xp2
```



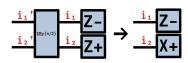
$$\begin{array}{c} \operatorname{CRy}(\pi/2)|\operatorname{Z-Z+}\rangle = \\ |\operatorname{Z-X+}\rangle \end{array}$$

## Tutorial: Custom two-site operators

```
1    Xp1=state("Xp",i1)
2    Xm1=state("Xm",i1)
3    Xp2=state("Xp",i2)
4    Xm2=state("Xm",i2)
5
6    apply(CRy, Zm1 * Zp2) ≈
7    Zm1 * Xp2
```

CRy = op("CRy", i1, i2;  $\theta = \pi/2$ )





```
1 function E(\psi)

2 \psi H \psi = inner(\psi', H, \psi)

3 \psi \psi = inner(\psi, \psi)

4 return \psi H \psi / \psi \psi

5 end
```

$$\mathrm{E}(\psi) = \langle \psi | \mathrm{H} | \psi \rangle / \langle \psi | \psi \rangle$$



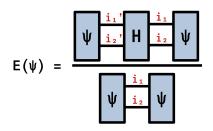
```
1 function E(\psi)

2 \psi H \psi = inner(\psi', H, \psi)

3 \psi \psi = inner(\psi, \psi)

4 return \psi H \psi / \psi \psi

5 end
```



Gradient descent.

f(x): function to minimize.

 $\partial f(x)$ : gradient of f.

 $\gamma$ : step size.

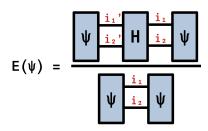
```
1 function E(\psi)

2 \psi H \psi = inner(\psi', H, \psi)

3 \psi \psi = inner(\psi, \psi)

4 return \psi H \psi / \psi \psi

5 end
```



$$_{\psi}^{\text{min}}\mathsf{E}(\psi)$$
  $\partial_{\psi}\mathsf{E}(\psi)$ 

```
1 \psi 0 = (Zp1 * Zp2 + Zm1 * Zm2)/\sqrt{2}

3 E(\psi 0) == -1

6 using Zygote # autodiff

7 \partial E(\psi) = \text{gradient}(E, \psi)[1]

9 \text{norm}(\partial E(\psi 0)) == 2
```

$$E(\psi) = \frac{\begin{array}{c} \downarrow \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \downarrow \end{array}}{\begin{array}{c} \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \end{array}} \psi$$

$$\partial_{\psi} E(\psi)$$

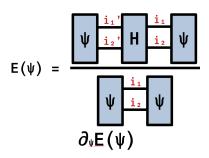
```
1 \psi 0 = (Zp1 * Zp2 + Zm1 * Zm2)/\sqrt{2}

3 E(\psi 0) == -1

6 using Zygote # autodiff

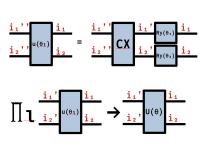
7 \partial E(\psi) = \text{gradient}(E, \psi)[1]

9 \text{norm}(\partial E(\psi 0)) == 2
```



$$\min_{\psi} E(\psi) = \min_{\psi} \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$$

```
1 # Circuit as a vector of gates:
2 U(θ, i1, i2) = [
3 op("Ry", i1; θ=θ[1]),
4 op("Ry", i2; θ=θ[2]),
5 op("CX", i1, i2),
6 op("Ry", i1; θ=θ[3]),
7 op("Ry", i2; θ=θ[4]),
8 ]
9
10
11
```



```
1 # PastaQ notation:

2 u(θ) = [

3 ("Ry", 1, (; θ=θ[1])),

4 ("Ry", 2, (; θ=θ[2])),

5 ("CNOT", 1, 2),

6 ("Ry", 1, (; θ=θ[3])),

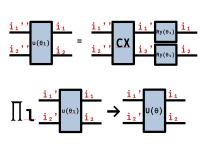
7 ("Ry", 2, (; θ=θ[4])),

8 ]

9

10 U(θ, i1, i2) =

buildcircuit(u(θ), [i1, i2])
```



```
1 \psi0 = Zp1 * Zp2

2 3 4 function E(\theta)

5 \psi_{\theta} = apply(U(\theta, i1, i2), \psi

0)

6 return inner(\psi_{\theta}', H, \psi_{\theta})

7 end
```

```
References state:

|0\rangle = |Z+Z+\rangle

\min_{\theta} E(\theta)

= \min_{\theta} \langle 0|U(\theta)^{\dagger} H U(\theta)|0\rangle

= \min_{\theta} \langle \theta|H|\theta\rangle
```

```
1 \psi0 = Zp1 * Zp2

2 3

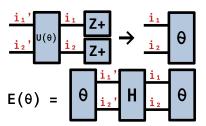
4 function E(\theta)

5 \psi_{\theta} = apply(U(\theta, i1, i2), \psi

0)

6 return inner(\psi_{\theta}', H, \psi_{\theta})

7 end
```



```
1 \psi0 = Zp1 * Zp2

2 3 4 function E(\theta)

5 \psi_{\theta} = apply(U(\theta, i1, i2), \psi

0)

6 return inner(\psi_{\theta}', H, \psi_{\theta})

7 end
```

```
1 \theta_0 = [0, 0, 0, 0]

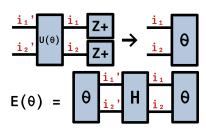
2 \partial E(\theta) = \text{gradient}(E, \theta)[1]

3 \theta = \text{minimize}(E, \partial E, \theta_0;

4 \text{nsteps=40}, \gamma=0.5)

6 E(\theta_0) == -1

7 E(\theta) == -1.4142077 \approx -\sqrt{2}
```



$$\frac{\min}{\Theta} E(\Theta) \qquad \partial_{\theta} E(\Theta)$$

## Tutorial: Two-site fidelity optimization

```
1 \psi0 = Zp1 * Zp2

2 \psi = (ZpZp + ZmZm) / \sqrt{2}

3 4

5 6 function F(\theta)

7 \psi_{\theta} = apply(U(\theta, i1, i2), \psi

0)

8 return -abs(inner(\psi, \psi_{\theta}))

^2 end
```

Reference state: 
$$\begin{aligned} |0\rangle &= |\mathbf{Z} + \mathbf{Z} + \rangle \\ \text{Target state:} \\ |\psi\rangle &= (|\mathbf{Z} + \mathbf{Z} + \rangle + |\mathbf{Z} - \mathbf{Z} - \rangle)/\sqrt{2} \\ \min_{\theta} & \mathbf{F}(\theta) = \\ & \min_{\theta} & -|\langle \psi | \mathbf{U}(\theta) | \mathbf{0} \rangle|^2 \end{aligned}$$

# Tutorial: Two-site fidelity optimization

```
1 \psi0 = Zp1 * Zp2

2 \psi = (ZpZp + ZmZm) / \sqrt{2}

3 4

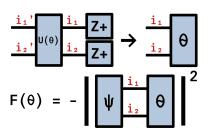
5 6 function F(\theta)

7 \psi_{\theta} = apply(U(\theta, i1, i2), \psi

0)

8 return -abs(inner(\psi, \psi_{\theta}))

^2 end
```



# Tutorial: Two-site fidelity optimization

```
1 \psi0 = Zp1 * Zp2

2 \psi = (ZpZp + ZmZm) / \sqrt{2}

3

4

5

6 function F(\theta)

7 \psi_{\theta} = apply(U(\theta, i1, i2), \psi

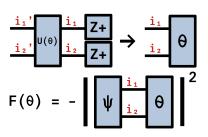
0)

8 return -abs(inner(\psi, \psi_{\theta}))

^2

9 end
```

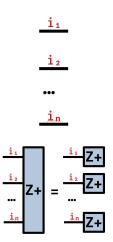
1 
$$\theta_0 = [0, 0, 0, 0]$$
  
2  $\partial F(\theta) = \text{gradient}(F, \theta)[1]$   
3  $\theta = \text{minimize}(F, \partial F, \theta_0;$   
4  $\text{nsteps=50}, \gamma=0.1)$   
5  $F(\theta_0) == -0.5$   
7  $F(\theta) == -0.9938992 \approx -1$ 



$$\frac{\min}{\theta} F(\theta) \qquad \partial_{\theta} E(\theta)$$

n-site state

$$|Z+Z+\ldots Z+\rangle$$



```
1 \psi = (Zp + Zm)/\sqrt{2}

2 3 4 maxlinkdim(\psi) == 2 # entangled state
```

$$(|Z+Z+...Z+\rangle+$$
  
 $|Z-Z-...Z-\rangle)/\sqrt{2}$ 

```
1 \psi = (Zp + Zm)/\sqrt{2}

2 3

4 \max \lim_{\phi \to \infty} (\psi) == 2 \#

entangled state
```

$$\frac{\frac{1}{1}}{\frac{1}{1}} \psi = \frac{\frac{1}{1}}{\frac{1}{1}} \frac{\mathbb{Z}}{\mathbb{Z}} + \frac{\frac{1}{1}}{1}} \frac{\mathbb{Z}}{\mathbb{Z}} = \frac{\frac{1}{1}}{\frac{1}{1}} \frac{\psi_1}{\psi_1} + \frac{2}{1} \frac{\psi_2}{\psi_1}$$

1 
$$\psi = (Zp + Zm)/\sqrt{2}$$
  
2 3  
4  $\max \lim(\psi) == 2 \#$   
entangled state

inner(Zp, Zp) == 1
$$\begin{array}{ccc}
1 & inner(Zp, Zp) == 1 \\
2 & & \\
3 & & \\
4 & inner(Zp, \psi) == 1/\sqrt{2}
\end{array}$$

$$\langle Z + | Z + \rangle = 1$$

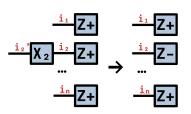
$$\langle Z + | \psi \rangle = 1/\sqrt{2}$$

1 
$$\psi = (Zp + Zm)/\sqrt{2}$$
  
2 3 4 maxlinkdim( $\psi$ ) == 2 # entangled state

inner(Zp, Zp) == 1  
inner(Zp, 
$$\psi$$
) == 1/ $\sqrt{2}$ 

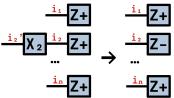
$$X_j|Z+Z+\ldots Z+\rangle = |Z+Z+\ldots Z-\ldots Z+\rangle$$

$$|Z+Z+\ldots Z-\ldots Z+\rangle$$



 $\max \min (X_j Zp) == 1$ inner(Zp,  $X_i Zp$ ) == 0

```
in 1:n]
X_{j}Zp = MPS(i, state)
```



# Tutorial: n-site operators with MPO

```
function ising(n; h)
2
3
4
5
6
7
8
9
      H = OpSum()
     for j in 1:(n - 1)
        H = "Z", j, "Z", j + 1
     end
     for j in 1:n
        H += h, "X", j
      end
      return H
10
    end
    h = 0.5 \# field
13
    H = MPO(ising(n; h), i)
    maxlinkdim(H) == 3
14
```

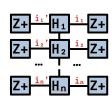
$$n$$
 sites 
$$H = -\sum_{j}^{n-1} Z_{j} Z_{j+1} + h \sum_{j}^{n} X_{j}$$

# Tutorial: n-site operators with MPO

```
function ising(n; h)
 2 3 4 5 6 7 8 9
       H = OpSum()
      for j in 1:(n - 1)
        H = "Z", j, "Z", j + 1
      end
      for j in 1:n
         H += h, "X", j
      end
      return H
10
    end
    h = 0.5 \# field
13
    H = MPO(ising(n; h), i)
    maxlinkdim(H) == 3
14
```

# Tutorial: n-site operators with MPO

```
function ising(n; h)
23456789
      H = OpSum()
     for j in 1:(n - 1)
        H = "Z", j, "Z", j + 1
     end
     for j in 1:n
        H += h, "X", j
     end
    return H
    end
    h = 0.5 \# field
    H = MPO(ising(n; h), i)
    maxlinkdim(H) == 3
14
```



```
1 function E(\psi)

2 \psi H \psi = inner(\psi', H, \psi)

3 \psi \psi = inner(\psi, \psi)

4 return \psi H \psi / \psi \psi

5 end
```

```
E(\psi) = \frac{\psi_1 \frac{i_1'}{H_1} \frac{i_1}{\Psi_1}}{\psi_2 \frac{i_2'}{H_2} \frac{H_2}{H_2} \frac{i_2}{\Psi_2}} 
\psi_1 \frac{i_1'}{H_1} \frac{H_2}{H_2} \frac{i_2}{\Psi_2}
\psi_2 \frac{i_2'}{H_2} \frac{H_2}{H_2} \frac{i_2}{\Psi_2}
\psi_1 \frac{i_1'}{H_1} \frac{H_1}{H_1} \frac{i_1}{\Psi_1} \frac{\Psi_1}{\Psi_2}
\langle \psi | \psi \rangle
\psi_1 \frac{i_1'}{H_1} \frac{H_1}{H_2} \frac{i_2}{\Psi_2} \frac{\Psi_2}{H_2}
\langle \psi | \psi \rangle
\psi_1 \frac{i_1'}{H_1} \frac{H_1}{H_1} \frac{i_1}{\Psi_1} \frac{\Psi_1}{\Psi_2}
\psi_2 \frac{i_2'}{H_2} \frac{H_2}{H_2} \frac{i_2}{\Psi_2} \frac{\Psi_2}{H_2}
\psi_1 \frac{i_1'}{H_1} \frac{H_1}{H_1} \frac{i_1}{\Psi_1} \frac{\Psi_2}{H_2}
\psi_2 \frac{i_1'}{H_2} \frac{H_2}{H_2} \frac{i_2}{H_2} \frac{\Psi_2}{H_2}
\psi_1 \frac{i_1'}{H_1} \frac{H_1}{H_1} \frac{i_1}{\Psi_1} \frac{\Psi_2}{H_2} \frac{H_2}{H_2} \frac{H
```

```
1 function E(\psi)

2 \psi H \psi = inner(\psi', H, \psi)

3 \psi \psi = inner(\psi, \psi)

4 return \psi H \psi / \psi \psi

5 end
```

```
1 \psi0 = MPS(i, "Zp")

2 \psi = minimize(E, \partialE, \psi0;

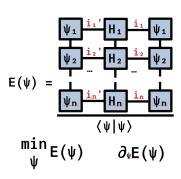
4 nsteps=50, \gamma=0.1,

5 maxdim=10, cutoff=1e-5)

6 E_{dmrg}, \psi_{dmrg} = dmrg(H, \psi0;

6 nsweeps=10,

7 maxdim=10, cutoff=1e-5)
```



```
function E(\psi)
\psi H \psi = inner(\psi', H, \psi)
\psi \psi = inner(\psi, \psi)
\tau eturn \psi H \psi / \psi \psi
end
```

```
1 \psi0 = MPS(i, "Zp")

2 \psi = minimize(E, \partialE, \psi0;

4 nsteps=50, \gamma=0.1,

5 maxdim=10, cutoff=1e-5)

6 \psi = minimize(E, \psi0;

6 nsteps=50, \psi0;

7 \psi0;

8 nsweeps=10,

9 maxdim=10, cutoff=1e-5)
```

```
E(\psi) = \frac{\psi_{1} \frac{i_{1}'}{H_{1}} \frac{i_{1}}{\psi_{2}}}{\frac{i_{2}'}{H_{2}} \frac{i_{2}}{u}} \psi_{2}}
\psi_{1} \frac{i_{1}'}{H_{1}} \frac{i_{1}}{\psi_{1}} \psi_{1}}{\langle \psi | \psi \rangle}
\min_{\psi} E(\psi) \qquad \partial_{\psi} E(\psi)
```

```
1 \max \lim \dim(\psi 0) == 1

2 \max \lim \dim(\psi) == 3

3 \max \lim \dim(\psi_{dmrg}) == 3

4 E(\psi 0) == -29

5 E(\psi) == -31.0317917

6 E(\psi_{dmrg}) == -31.0356110
```

```
1 Ry_layer(θ, i) = [op("Ry", i[j]; θ=θ[j]) for j in 1:n]
2 CX_layer(i) = [op("CX", i[j], i[j+1]) for j in 1:2:(n-1)]
```

```
1 Ry_layer(\theta, i) = [op("Ry", i[j]; \theta=\theta[j]) for j in 1:n]
2 CX_layer(i) = [op("CX", i[j], i[j+1]) for j in 1:2:(n-1)]
```

```
1  function U(θ, i; nlayers)
2  n = length(i)
3  for l in 1:(nlayers - 1)
4  θ<sub>l</sub> = θ[(1:n) .+ l * n]
5  Uθ = [Uθ; Ry_layer(θl, i)]
6  Uθ = [Uθ; CX_layer(i)]
7  end
8  return Uθ
9  end
```

```
U(\theta) = Ry_1(\theta_1) \dots Ry_n(\theta_n)
* CX_{1,2} \dots CX_{n-1,n}
* Ry_1(\theta_{n+1}) \dots Ry_n(\theta_{2n})
* ...
```

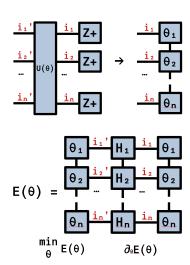
```
Ry_{layer}(\theta, i) = [op("Ry", i[j]; \theta = \theta[j]) \text{ for } j \text{ in } 1:n]
CX_{layer}(i) = [op("CX", i[j], i[j+1]) \text{ for } j \text{ in } 1:2:(n-1)]
```

```
function U(\theta, i; nlayers)
   n = length(i)
   for l in 1:(nlayers - 1)
      \theta_l = \theta \lceil (1:n) \cdot + l * n \rceil
      U_{\theta} = [U_{\theta}; Ry\_layer(\theta_{l}, i)]
      U_{\theta} = [U_{\theta}; CX_{layer}(i)]
   end
   return U<sub>0</sub>
end
```

$$\frac{\mathbf{i}_{1}''}{\mathbf{i}_{2}''} = \frac{\mathbf{i}_{1}''}{\mathbf{i}_{2}} CX = \frac{\mathbf{i}_{1}'}{\mathbf{i}_{2}'} CX = \frac{\mathbf{i}_{1}}{\mathbf{i}_{2}'} CX = \frac{\mathbf{i}_{2}'}{\mathbf{i}_{2}'} CX = \frac{\mathbf{i}_{2}'}{\mathbf{$$

$$\Pi_1 \ \mathsf{u}(\theta_1) \to \mathsf{U}(\theta)$$

```
1  ψ0 = MPS(i, "Zp")
2  nlayers = 6
3  function E(θ)
4  ψθ = apply(U(θ, i; nlayers), ψ0)
5  return inner(ψθ', H, ψθ)
6  end
7
8  θ0 = zeros(nlayers * n)
9  θ = minimize(E, ∂E, θ0; nsteps=20, γ=0.1)
```



```
1 \psi 0 = MPS(i, "Zp")

2 nlayers = 6

3 function E(\theta)

4 \psi_{\theta} = apply(U(\theta, i; nlayers), \psi 0)

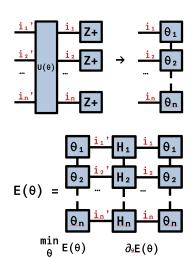
5 return inner(\psi_{\theta}', H, \psi_{\theta})

6 end

7 \theta_{\theta} = zeros(nlayers * n)

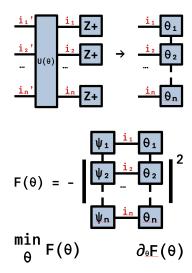
9 \theta = minimize(E, \partial E, \theta_{0}; nsteps=20, \gamma=0.1)
```

```
1 \max \text{linkdim}(\psi 0) = 1
2 \max \text{linkdim}(\psi_{\theta}) = 3
3 E(\theta_0) == -29
4 E(\theta) == -31.017062
```



#### Tutorial: n-site states with MPS

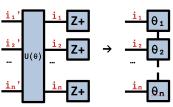
```
1  ψ0 = MPS(i, "Zp")
2  nlayers = 6
3  function F(θ)
4  ψθ = apply(U(θ, i; nlayers), ψ0)
5  return -abs(inner(ψ', ψθ))^2 end
7
8  θ0 = zeros(nlayers * n)
9  θ = minimize(F, ∂F, θ0; nsteps=20, γ=0.1)
```

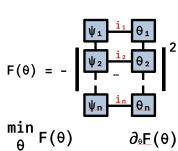


#### Tutorial: n-site states with MPS

```
\psi0 = MPS(i, "Zp")
     nlayers = 6
     function F(\theta)
         \psi_{\theta} = \operatorname{apply}(\mathsf{U}(\theta, i; \mathsf{nlayers}),
        return -abs(inner(\psi', \psi_{\theta}))^2
      end
      \theta_0 = zeros(nlayers * n)
      \theta = \min imize(F, \partial F, \theta_0;
                nsteps=20, \gamma=0.1)
10
```

```
1 \max \text{linkdim}(\psi 0) == 1
2 \max \text{linkdim}(\psi_{\theta}) == 2
3 F(\theta_0) == -0.556066
4 F(\theta) == -0.995230
```





► Noisy state and process simulation (PastaQ). AD/optimization support in progress.

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- ► Conserved quantities with multithreaded block sparse tensors (ITensor/PastaQ).
- ▶ More that I am probably forgetting... Ask Giacomo and me for more details.



▶ 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, please contribute gradient definitions!).

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- ► Improved gradient optimization: higher order derivatives, preconditioners, isometrically constrained gradient optimization, etc.

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- ▶ I'm interested in building general tools and algorithms, and I'm looking for people with problems to solve. Also, we need help, code to contributions are welcome!

