THEORY OF TENSOR-TRAIN QUANTUM DYNAMICS AND OPTIMIZATION

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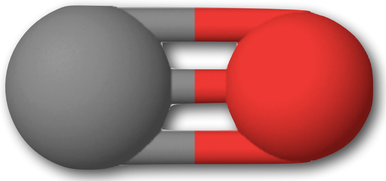
UNIVERSITY OF WISCONSIN-MADISON

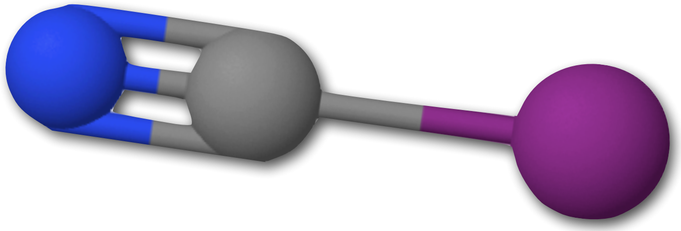
CyberTraining Workshop 2023

COMPUTATIONAL COST OF QUANTUM DYNAMICS AND OPTIMIZATION

Many classical computer approaches to quantum mechanics simulations become computationally intractable for large molecular systems.



2 Atoms:
2 KB



3 Atoms:
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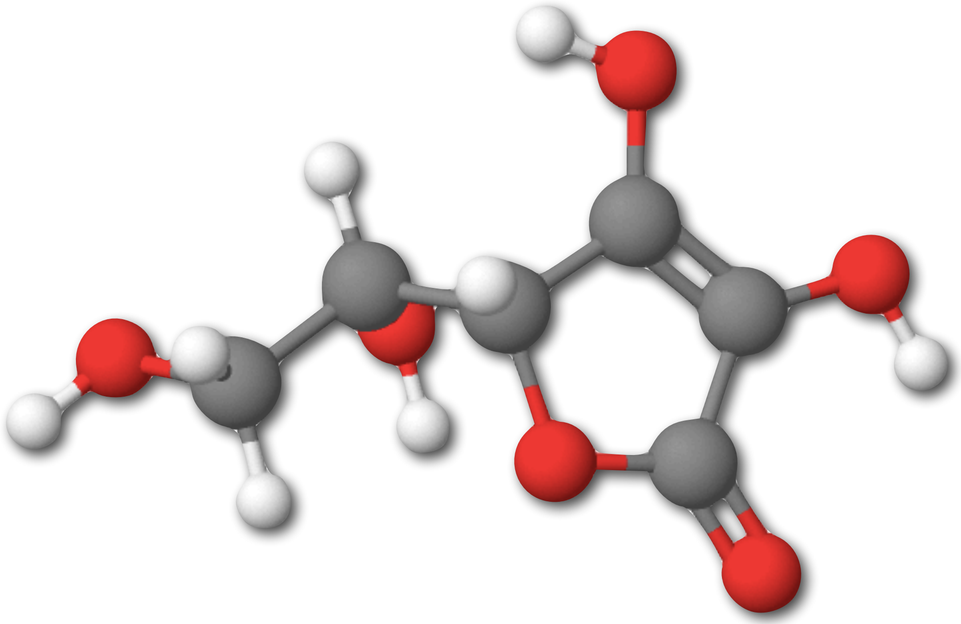

20 Atoms:
10^{119} TB

REDUCING COMPUTATIONAL COST WITH TENSOR TRAINS

Original Image

100%

Tensor Train

15%

N. Lyu*, E. Mulvihill*, **Micheline B. Soley**, E. Geva, V. S. Batista, (2023) JCTC, in press.
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.
Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, J. Phys. Chem. Lett., 13 (2022) 8354.
Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

Y. Wang, E. Mulvihill, Z. Hu, N. Lyu, S. Shivpuje, Y. Liu, **Micheline B. Soley**, E. Geva, V. S. Batista, S. Kais, 2022, arXiv:2209.04956.
N. Lyu, **Micheline B. Soley**, V. S. Batista, JCTC, 18 (2022) 3327.
Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.
B. N. Khoromskij, Constr. Approx. 34 (2011) 257.
I. Oseledets, E. Tyryshnikov, Linear Algebra Appl. 432 (2010) 70.
J. C. Napp, et al. Phys. Rev. X 12 (2022) 021021.

REDUCING COMPUTATIONAL COST WITH TENSOR TRAINS

tt_image.ipynb ☆

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+ Code + Text

Image Compression

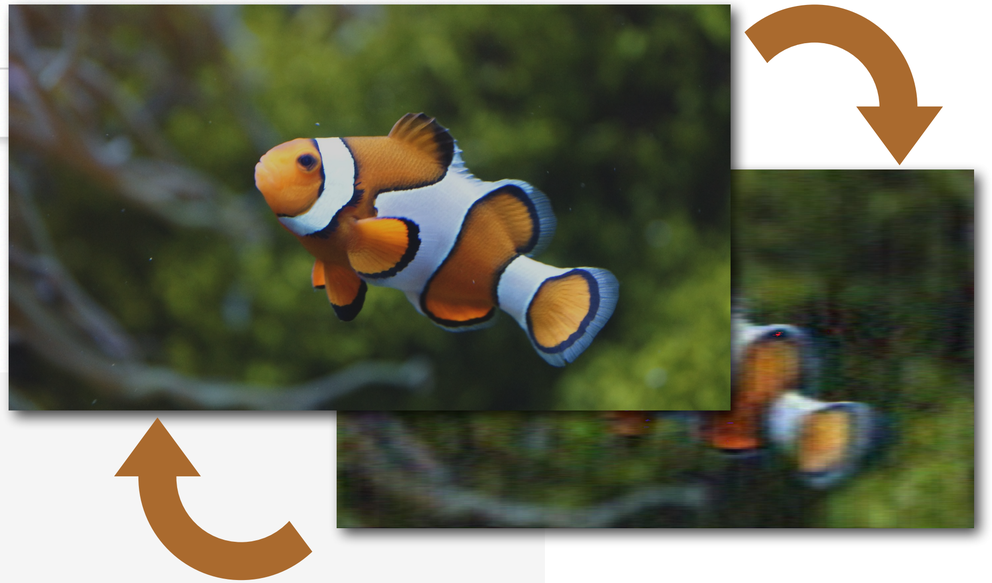
global data global paddedflatdata

```
[ ]  # Parameters, image data
     eps=1e-2
     eps_qttcross=1e-2000
     rma=300# 70 # 300 good for quantics, 70 good for TT
     rma_qttcross=1e100
     rows,columns=img.size
     datasize=rows*columns*3
     print("Original Size: ",datasize)
     img.load()
     data=np.asarray(img).reshape((columns,rows*3))
     flatdata=np.reshape(data,columns*rows*3)
```

```
Original Size:  4320000
```

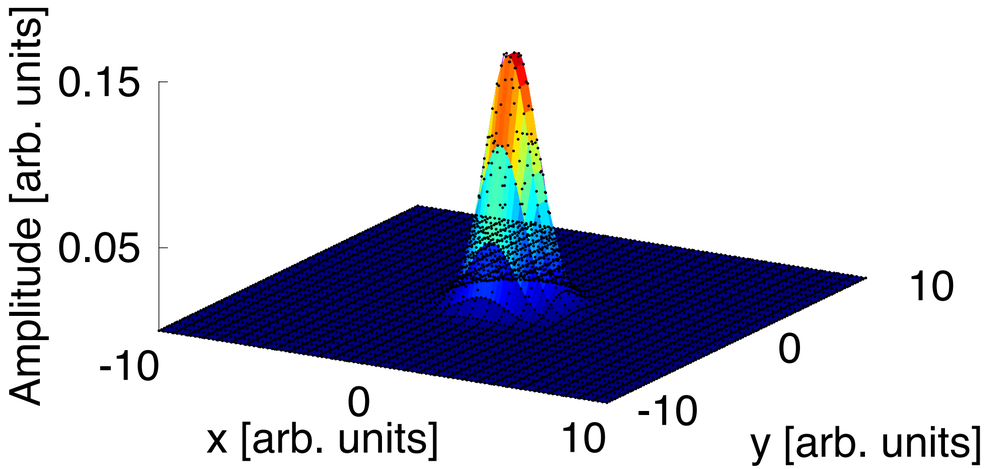
```
[ ]  # TT Image

     tt_data=tt.tensor(data,eps)
     tt_data=tt_data.round(eps,rma)
     ttsize=np.size(tt_data.core)
     tt_reconstructed_data=np.round(tt_data.full()).reshape((columns,rows,3))
     tt_reconstructed_img=Image.fromarray(np.uint8(tt_reconstructed_data))
```

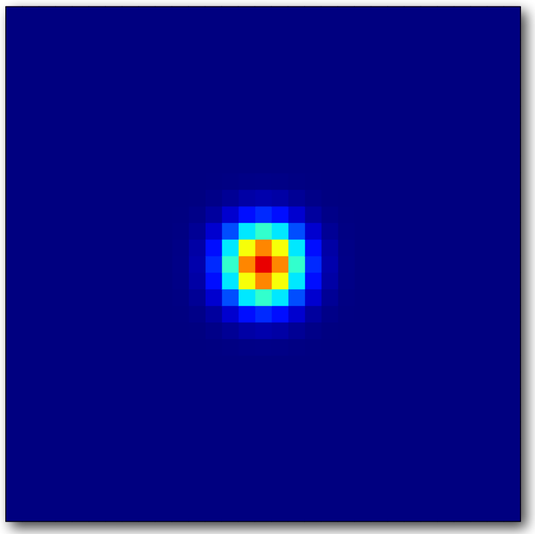


2D TENSOR TRAIN (RANK 1)

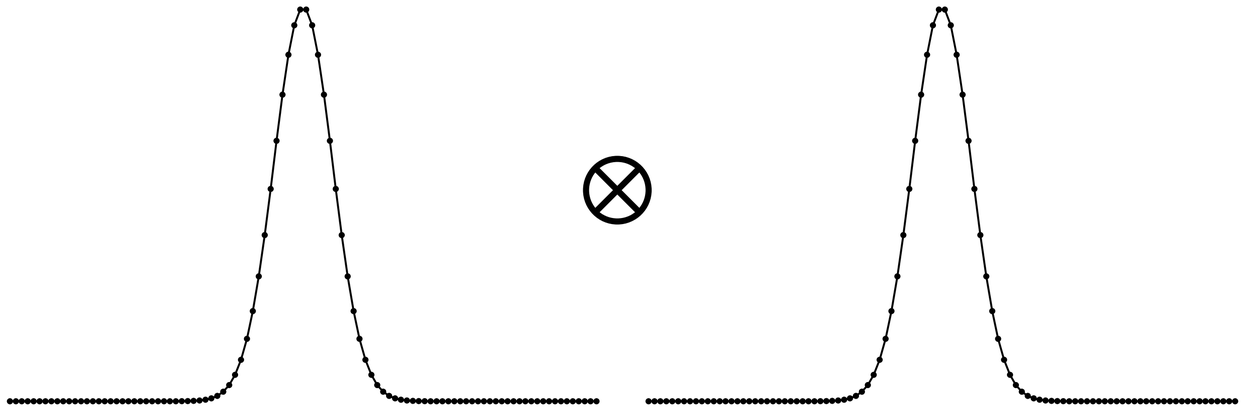
2D Gaussian



$$\Psi(x,y) = \frac{1}{2\pi}\exp\left(-\frac{x^2}{2}-\frac{y^2}{2}\right)$$

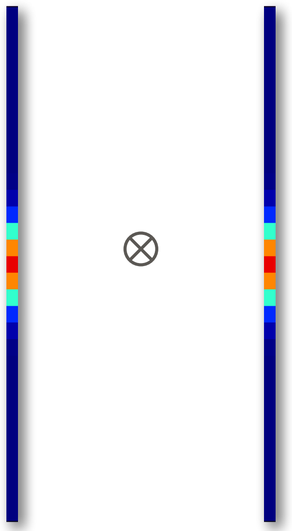


vs.



$$\psi(x)\psi(y) = \left(\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{x^2}{2}\right)\right)\left(\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)\right)$$

$$= \sum_{\alpha=1}^{r} \psi_1(1,x,\alpha)\psi_2(\alpha,y,1)$$

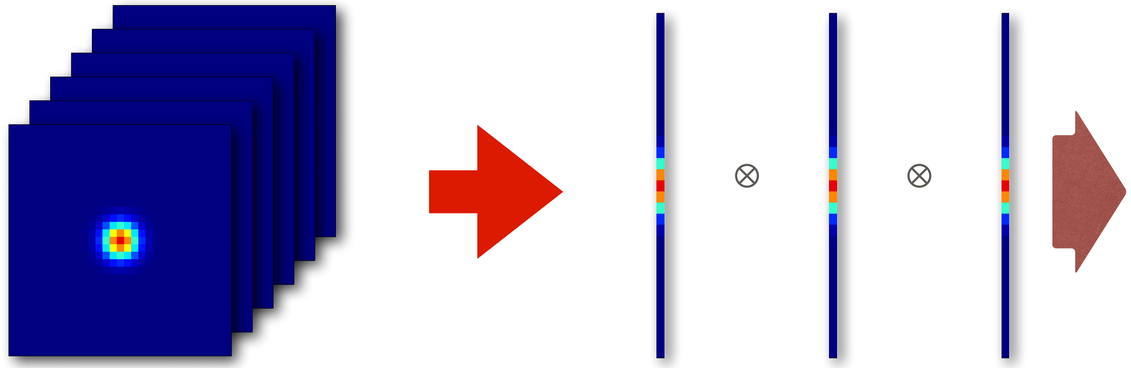


Cost of evaluating reduces to

$$n^2 \rightarrow 2n$$

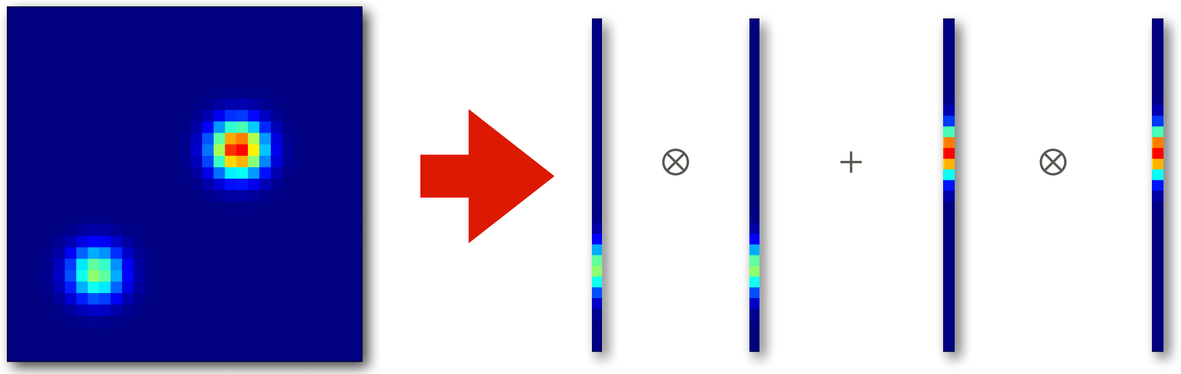
I. V. Oseledets, *SIAM J. Sci Comput.* 33 (2011) 2295

ND TENSOR TRAIN (RANK 1)



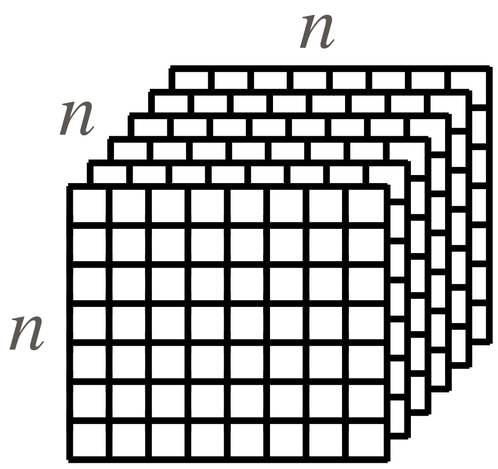
Cost Reduction: $n^3 \rightarrow 3n$

2D TENSOR TRAIN (RANK 2)

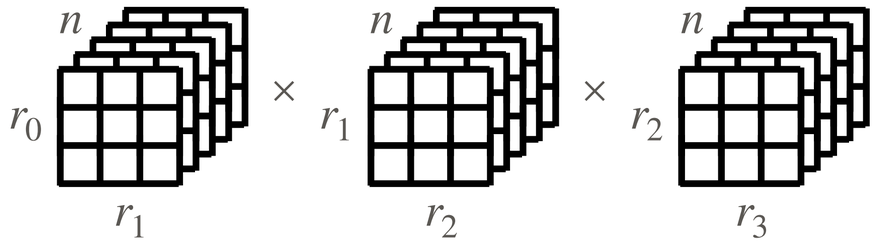


Cost Reduction: $n^2 \rightarrow 2 \times 2n$

ND TENSOR TRAIN (RANK R)



$\Psi(x_1, x_2, \cdots, x_d)$



$$\approx \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_d=1}^{r_d} \psi_1(\alpha_1, x_1, \alpha_2)\psi_2(\alpha_2, x_2, \alpha_3)\cdots\psi_d(\alpha_{d-1}, x_d, \alpha_d)$$

Cost Reduction

$n^d \rightarrow dnr^2$

M.-L. Li, K. S. Candan, M. L. Salino, "GTT: Guiding the tensor train decomposition." International Conference on Similarity Search and Applications. Springer, Cham, 2020.

I. Oseledets, E. Tyryshnikov, Linear Algebra Appl. 432 (2010) 70.

TT-TOOLBOX

tt_tutorial_redux.ipynb ☆

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Table of contents

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Hands-On Tutorial on Tensor Trains

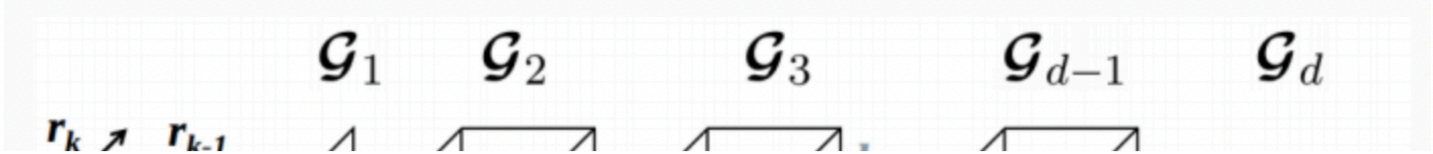
The goal of this tutorial is to get a quick start into the TT-Toolbox for fast multilinear algebra computations. Here, we introduce the basic routines for multidimensional array operations in TT-format with examples, incluiding a presentation based on the quick start document developed by Ivan Oseledets, Sergey Dolgov, Vladimir Kazeev, Olga Lebedeva, Thomas Mach, and developments at Yale by the Batista group.

What is a tensor train?

The TT-format of a tensor **A** is defined, as follows:

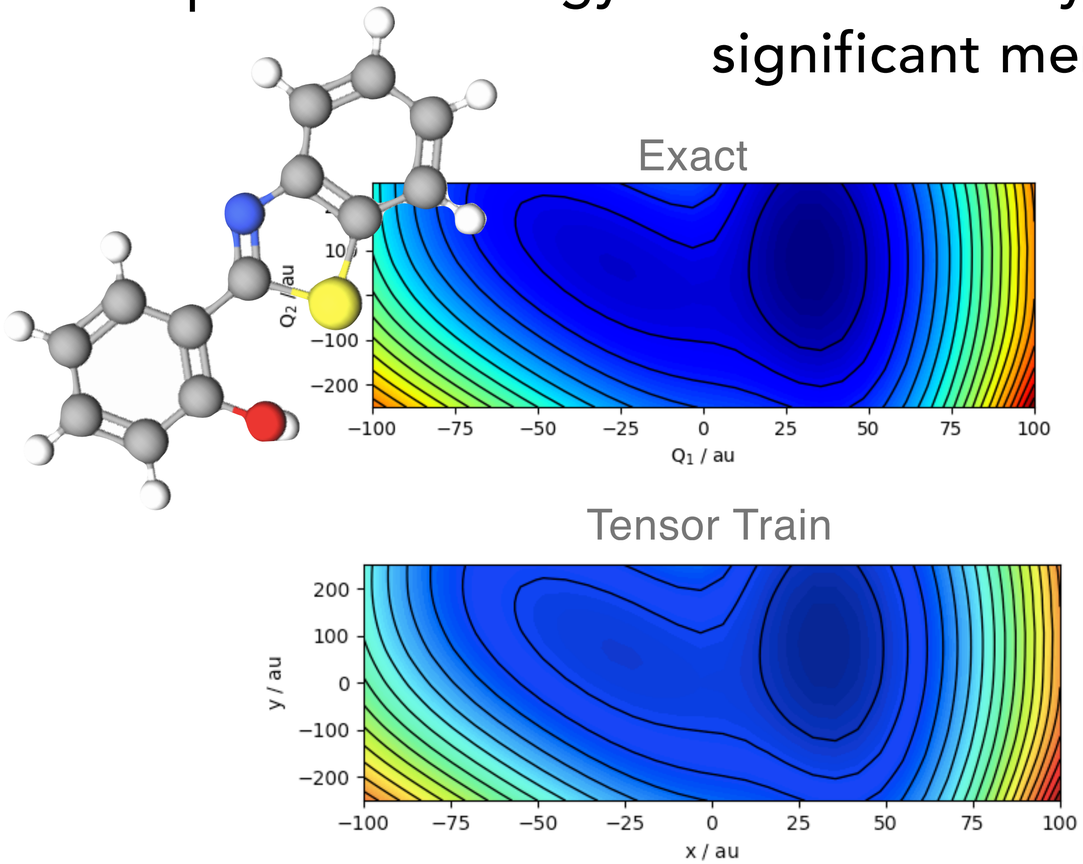
$$A(l_1, l_2, \dots, l_d) = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} G_1(l_1, \alpha_1) G_2(\alpha_1, l_2, \alpha_2) \cdots G_d(\alpha_{d-1}, l_d),$$

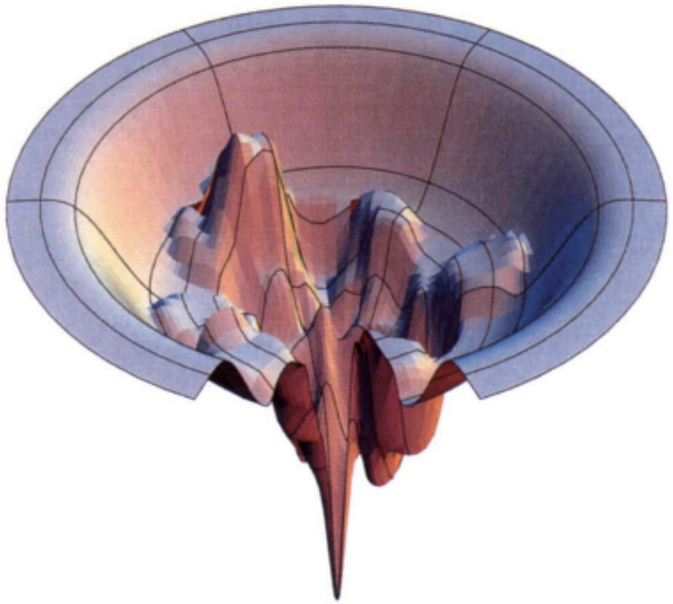
or more concisely $A(l_1, l_2, \dots, l_d) = G_1(l_1) \times G_2(l_2) \times \cdots \times G_d(l_d)$, where $G_k(l_k)$ are $r_{k-1} \times r_k$ matrices, and $r_0 = r_d = 1$, as represented in the following diagram:



TENSOR TRAINS FOR CHEMISTRY

For potential energy surfaces of many chemical systems, tensor trains offer significant memory savings.



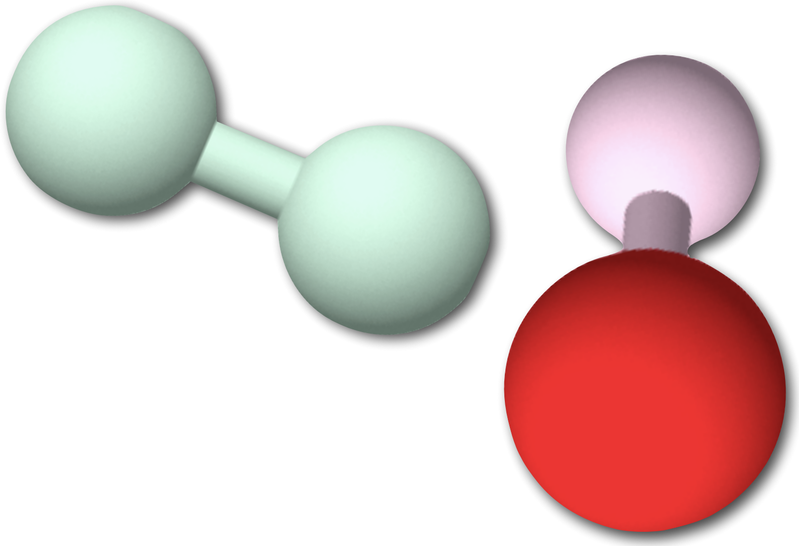


We take advantage of this property for **quantum dynamics** and **global optimization** of molecular systems in high dimensionality.

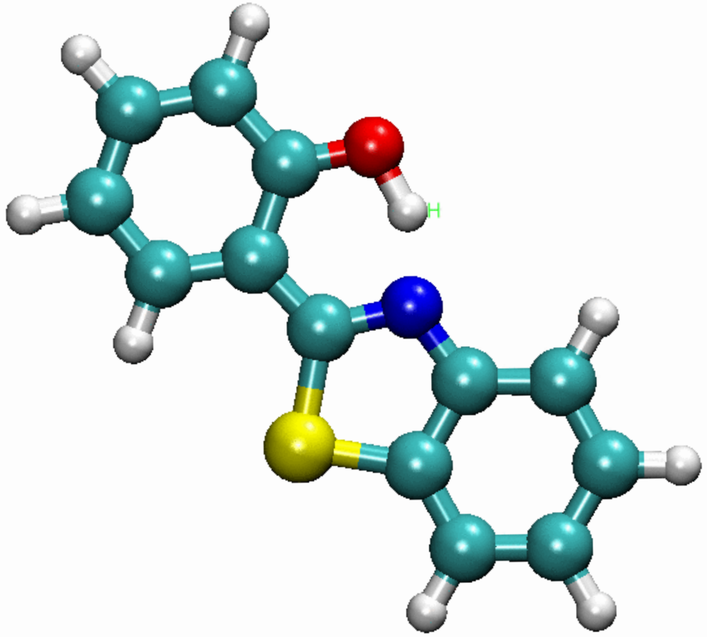
N. Lyu*, E. Mulvihill*, **Micheline B. Soley**, E. Geva, V. S. Batista, JCTC, 19 (2023) 1111.
Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, J. Phys. Chem. Lett., 13 (2022) 8354.
Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.
N. Lyu, **Micheline B. Soley**, V. S. Batista, JCTC, 18 (2022) 3327.
Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.

APPLICATION 1: HIGHLY-MULTIDIMENSIONAL QUANTUM DYNAMICS OF MOLECULES WITH TT-SOFT

Largest System Investigable with Standard Fixed-Grid SOFT Dynamics



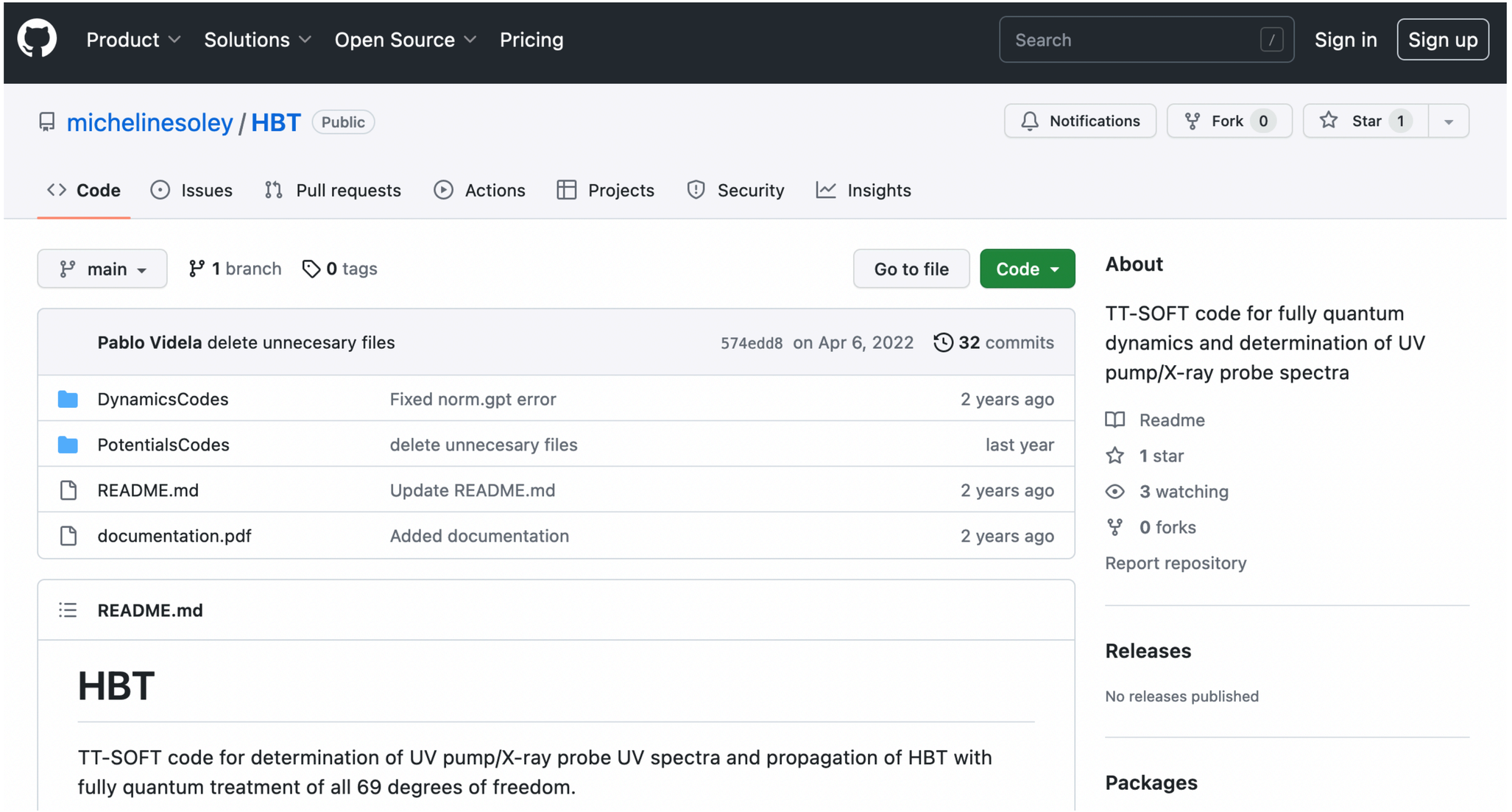
Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Dynamics



J. A. Fleck Jr., A. Steiger, J. Comput. Phys. 47 (1982) 412.
S. M. Greene, V. S. Batista, JCTC 13 (2017) 4034.

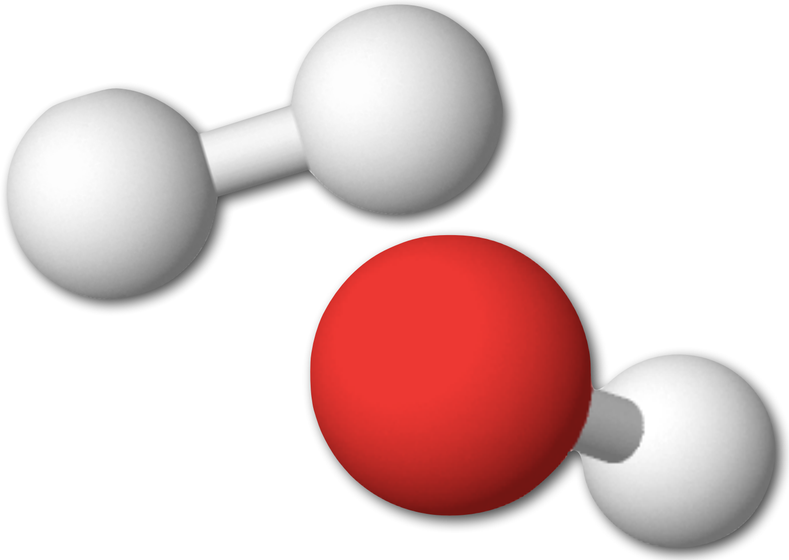
Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.

APPLICATION 1: HIGHLY-MULTIDIMENSIONAL QUANTUM DYNAMICS OF MOLECULES WITH TT-SOFT

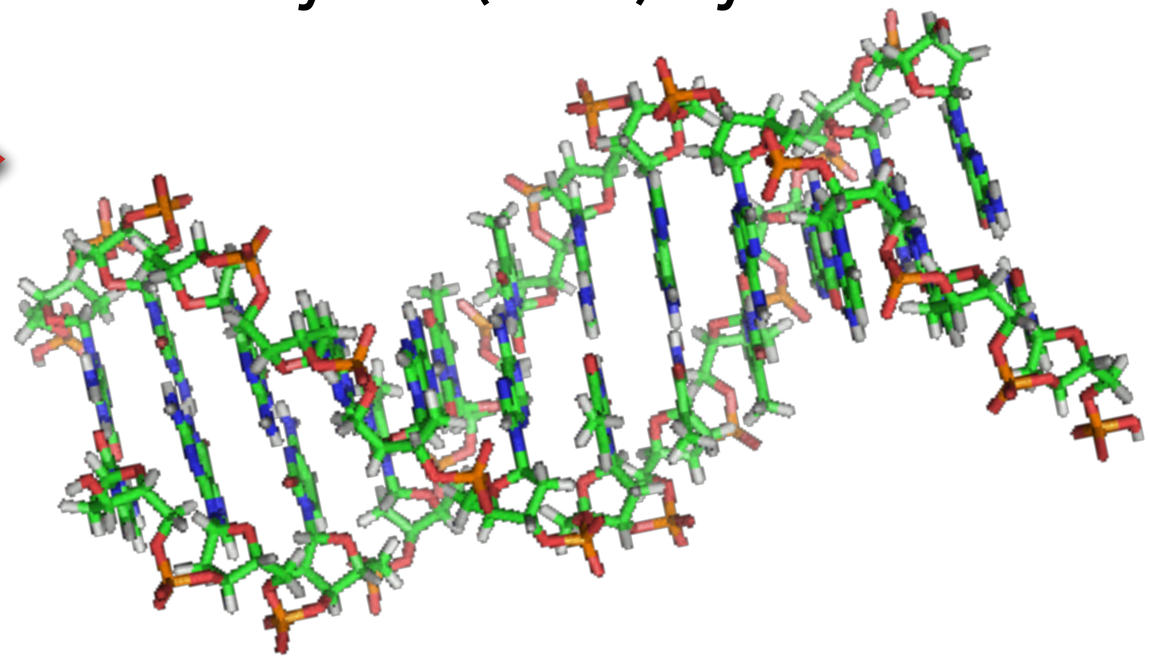


APPLICATION 2: HIGHLY-MULTIDIMENSIONAL QUANTUM DYNAMICS OF MOLECULES WITH TT-CHEBYHSEV

Largest System Investigable with Standard Chebyshev Dynamics



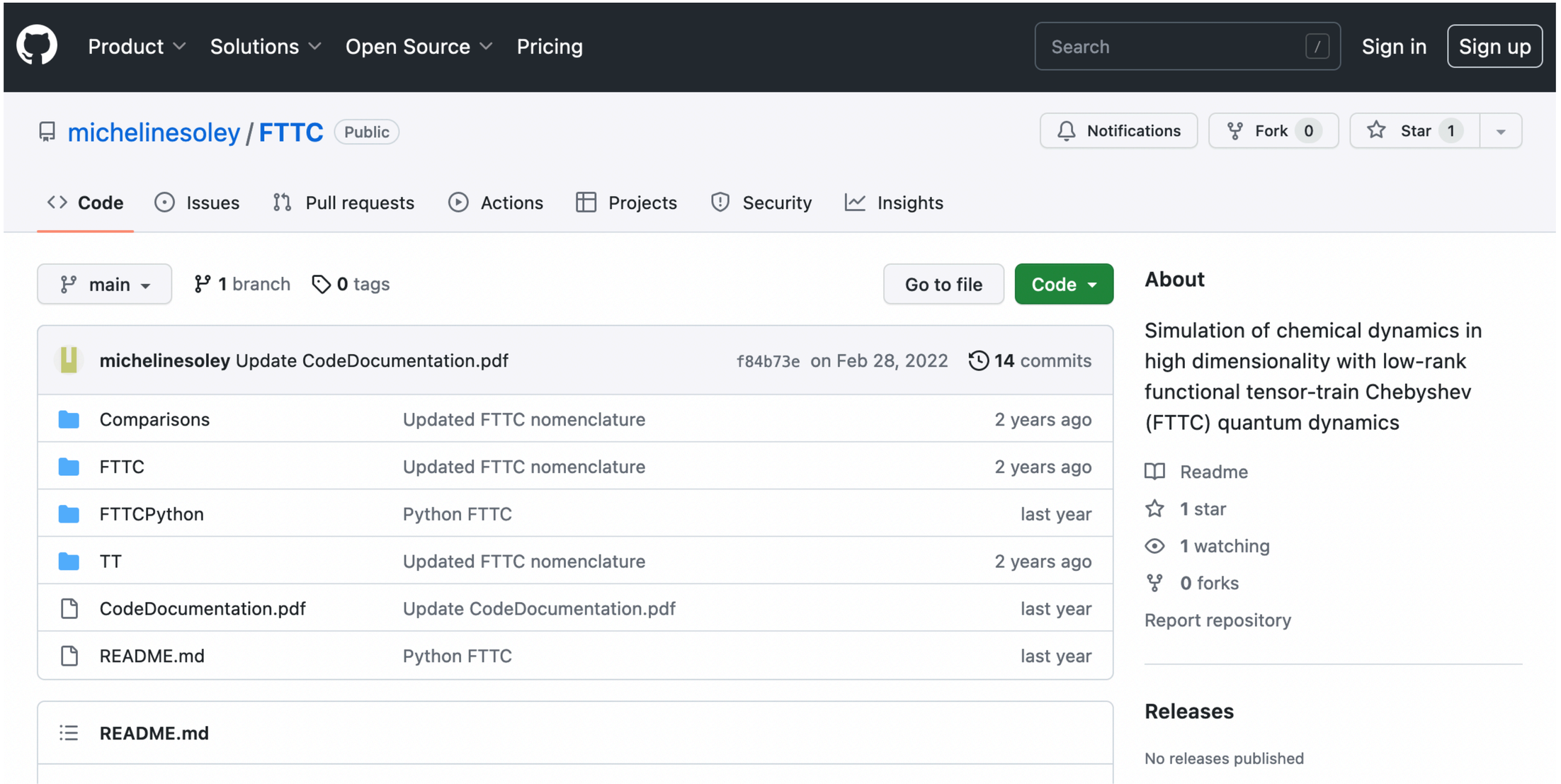
Functional Tensor-Train Chebyshev (FTTC) Dynamics



M. T. Cvitaš, S. C. Althorpe, J. Chem. Phys. 139 (2013) 064307.
E. M. Goldfield, S. K. Gray, J. Chem. Phys. 117 (2002) 1604.
H. Tal-Ezer, R. Kosloff, J. Chem. Phys. 81 (1984) 3967.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

APPLICATION 2: HIGHLY-MULTIDIMENSIONAL QUANTUM DYNAMICS OF MOLECULES WITH TT-CHEBYHSEV

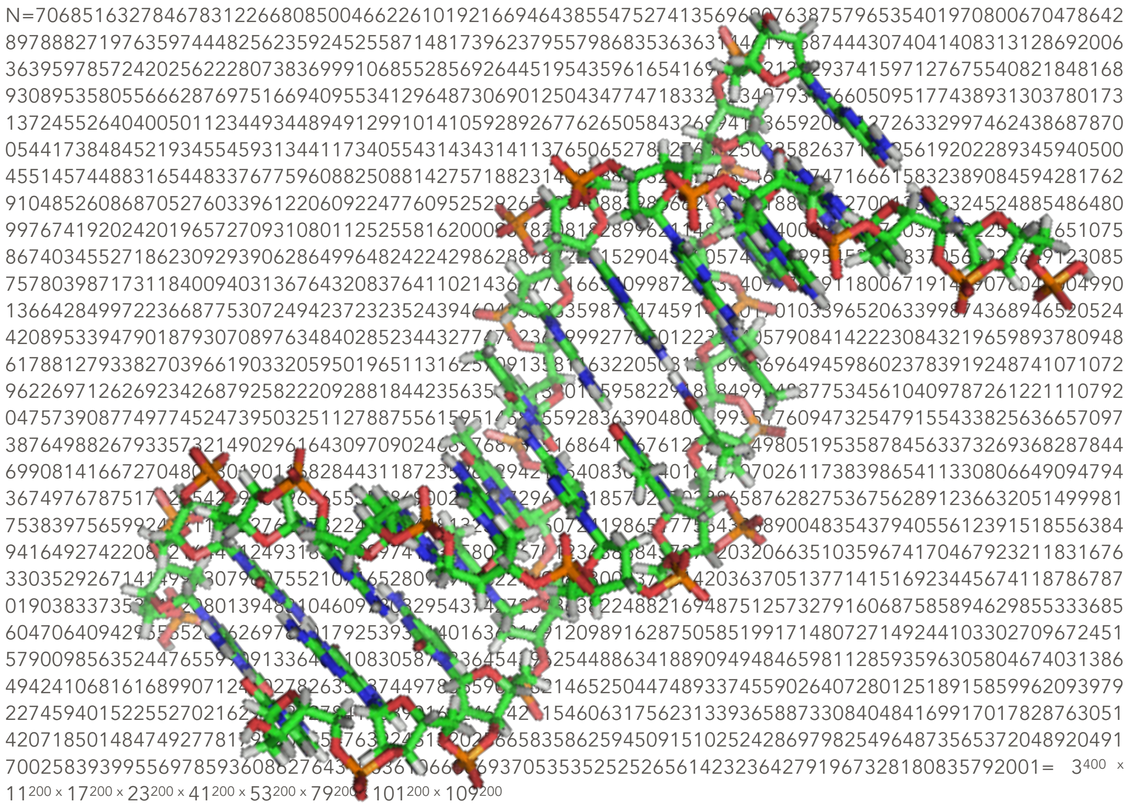


APPLICATION 3: HIGHLY-MULTIDIMENSIONAL OPTIMIZATION FOR MOLECULAR SYSTEMS WITH IPA

Shor's Algorithm in Quantum Computing

$21 = 7 \times 3$

IPA



Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

P. W. Shor, Proceedings 35th Annual Symposium on Foundations of Computer Science, IEEE (1994) 124.

E. Lucero, et al. Nat. Phys. 8 (2012) 719.

APPLICATION 3: HIGHLY-MULTIDIMENSIONAL OPTIMIZATION FOR MOLECULAR SYSTEMS WITH IPA


```
    import numpy as np
    from mpl_toolkits.mplot3d import Axes3D
    from matplotlib import cm
    import matplotlib.pyplot as plt
    import tt

    beta=10
    dim=2
    eps=1.0e-14
    rma=3
    nsteps=30
    d=8
    npts=2**d
    xmin=-1.5
    xmax=2.5

dx=(xmax-xmin)/npts

def gen_1d(mat,e,i,d):
    w=mat
    for j in range(i):
        w=tt.kron(e,w)
    for j in range(d-i-1):
        w=tt.kron(w,e)
    return w

def rhoo(input):
    out=1.+0.*np.sum(input,axis=1)
    return(out);
```

```
import numpy as np
from numpy import zeros,reshape,sqrt,arange,vectorize,extract,int

import matplotlib.pyplot as plt
import tt

import mpmath
from mpmath import mp,mpf,floor,exp,nint

def parameters():
    global dim,eps,num,rmax,nsteps,d,searchspacesize,beta,betaprime
    num=mpf(3*3*11*17*23*41*53*79*101*109)**200
    beta=30
    betaprime=0.5
    dim=1
    eps=1.0e-100
    rmax=100
    nsteps=3
    d=6
    searchspacesize=2**d
    return()

def rhoo(input):
    V=1.0+0*input
    return V

def is_prime(n):
    if n % 2 == 0 and n > 1:
        return False
    return all(n % i for i in range(3,int(sqrt(n))+1,2))

def tto(input, param=None):
    global num,beta
    nevals,dim=input.shape
    out=np.zeros((nevals,))
    for ii in range(nevals):
        a=num-nint(input[ii,0])*floor(num/nint(input[ii,0]))
```

IMPLEMENTATION: TENSOR TRAINS ON GOOGLE COLAB

The low computational cost of these methods allows the codes presented in this session to be run either on personal computers or on a single core on clusters/cloud-based resource. We will run codes today on Google Colaboratory.

Google Colaboratory: https://colab.research.google.com/?utm_source=scs-index#

Colab Python Tutorial: https://colab.research.google.com/github/cs231n/cs231n.github.io/blob/master/python-colab.ipynb

IMPLEMENTATION: TENSOR TRAINS ON GOOGLE COLAB

Welcome To Colaboratory

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Getting started

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Machine learning

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Featured examples

Section

+ Code + Text Copy to Drive Connect

Welcome to Colab!

If you're already familiar with Colab, check out this video to learn about interactive tables, the executed code history view, and the command palette.

What is Colab?

Colab, or "Colaboratory", allows you to write and execute Python in your browser, with

- Zero configuration required
- Access to GPUs free of charge
- Easy sharing

TENSOR TRAINS ON CCR/CLUSTERS

Jupter Notebook Environments:
https://ubccr.freshdesk.com/support/solutions/articles/13000073876-custom-jupyter-notebook-environment-setup

https://ubccr.freshdesk.com/support/solutions/articles/13000063899-configuring-your-environment-and-private-modules-for-use-in-ondemand

TENSOR TRAINS ON PERSONAL COMPUTERS

TT-Toolbox: *https://github.com/oseledets/TT-Toolbox*

Compressed Continuous Computation (C3): *https://github.com/goroda/Compressed-Continuous-Computation*

TENSOR TRAINS ON TT-TOOLBOX WITH M1-CHIP MACS

```
conda activate /Users/*****/opt/anaconda3

conda install numpy
conda install scipy
conda install cython

brew reinstall gcc
brew unlink open-mpi
brew reinstall gfortran
FFLAGS='-fallow-argument-mismatch'
python setup.py install
```

TENSOR-TRAIN DATA COMPRESSION

In order to understand tensor-train data compression, it is essential to understand the **tensors** on which they are based:

$$\mathscr{A} = [A(i_1, i_2, \ldots, i_d)], \quad i_k \in \{1,2,\ldots,n_k\}$$

Dimension D: number of indices

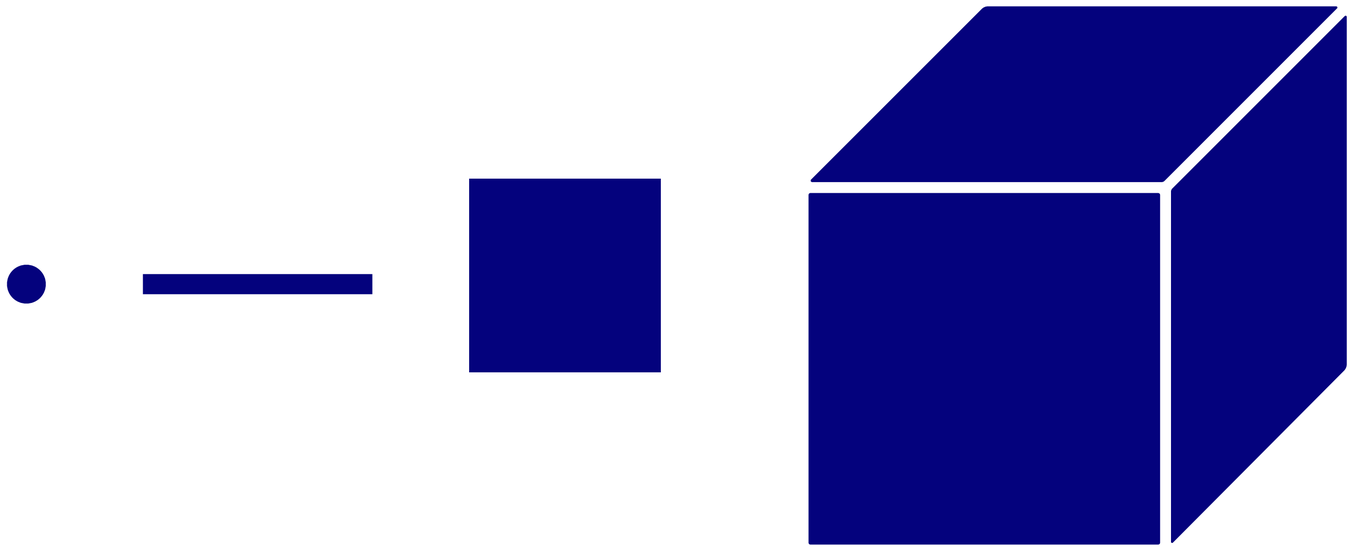
Size: $n_1 \times n_2 \times \cdots \times n_D$.

Zeroth-Order (0D) Tensor: Scalar a

First-Order (1D) Tensor: Vector $\mathbf{a}$

Second-Order (2D) Tensor: Matrix $\mathbf{A}$

Higher-Order (ND) Tensor: Tensor $\mathscr{A}$

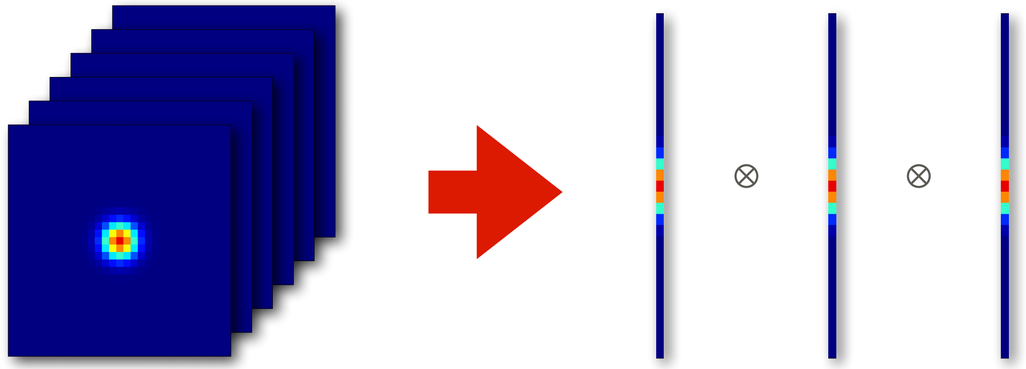


T. G. Kolda, B. W. Bader, SIAM Review, 51 (2009) 455.
C. F. Van Loan, Gene Golub SIAM Summer School, Selva di Fasano, Brindisi, Italy, 2010.

A simple tensor is given by the outer product of vectors

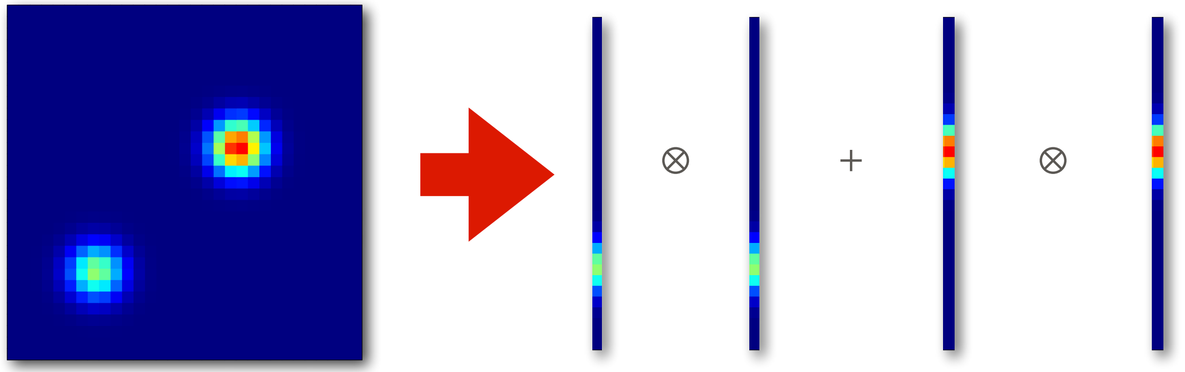
$$\mathscr{A} = \mathbf{a}^{(1)} \otimes \mathbf{a}^{(2)} \otimes \cdots \otimes \mathbf{a}^{(D)}$$

$$a_{i_1 i_2 \cdots i_N} = a^{(1)}_{i_1} a^{(2)}_{i_2} \cdots a^{(D)}_{i_D}$$



and these tensors can be combined to create even more complexity

$$\mathscr{A} = \sum_{k=1}^{r} \mathbf{a}^{(1)}_k \otimes \mathbf{a}^{(2)}_k \otimes \cdots \otimes \mathbf{a}^{(D)}_k$$



In tensor-train terminology, the number of directions is the **dimensionality** and the number of terms in the sum is the **rank**.

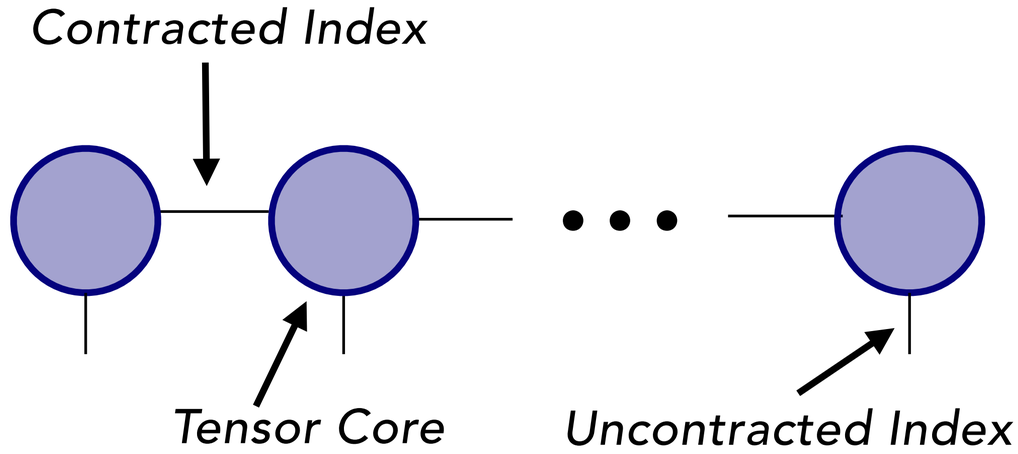
Note: Terminology is reversed in the matrix product state community (rank and bond dimension, respectively)!

LOW-RANK TENSOR-TRAIN (TT) REPRESENTATION

The low-rank TT representation reduces the cost of storing the tensor $\mathscr{A}$ by approximating it by lower rank tensor broken up into tensor cores A_j

$$\begin{aligned}\mathscr{A}\left(i_1,\ldots,i_d\right) &\approx \sum_{\alpha_0,\ldots,\alpha_d} A_1\left(\alpha_0,i_1,\alpha_1\right)A_2\left(\alpha_1,i_2,\alpha_2\right)\cdots A_d\left(\alpha_{d-1},i_d,\alpha_d\right)\\ &= \sum_{\alpha_0,\ldots,\alpha_d} A_1\left(i_1,\alpha_1\right)A_2\left(\alpha_1,i_2,\alpha_2\right)\cdots A_d\left(\alpha_{d-1},i_d\right)\\ &= A_1\left[i_1\right]A_2\left[i_2\right]\cdots A_d\left[i_d\right]\end{aligned}$$

Penrose Notation



α_j: Auxiliary indices for contraction

$A\left(\alpha_{k-1},n_k,\alpha_k\right)$ or $A_j\left[i_j\right]$: Tensor core array of size

$r_{k-1}\times n_k\times r_k$ (expressible as a matrix of size $r_{k-1}\times r_k$)

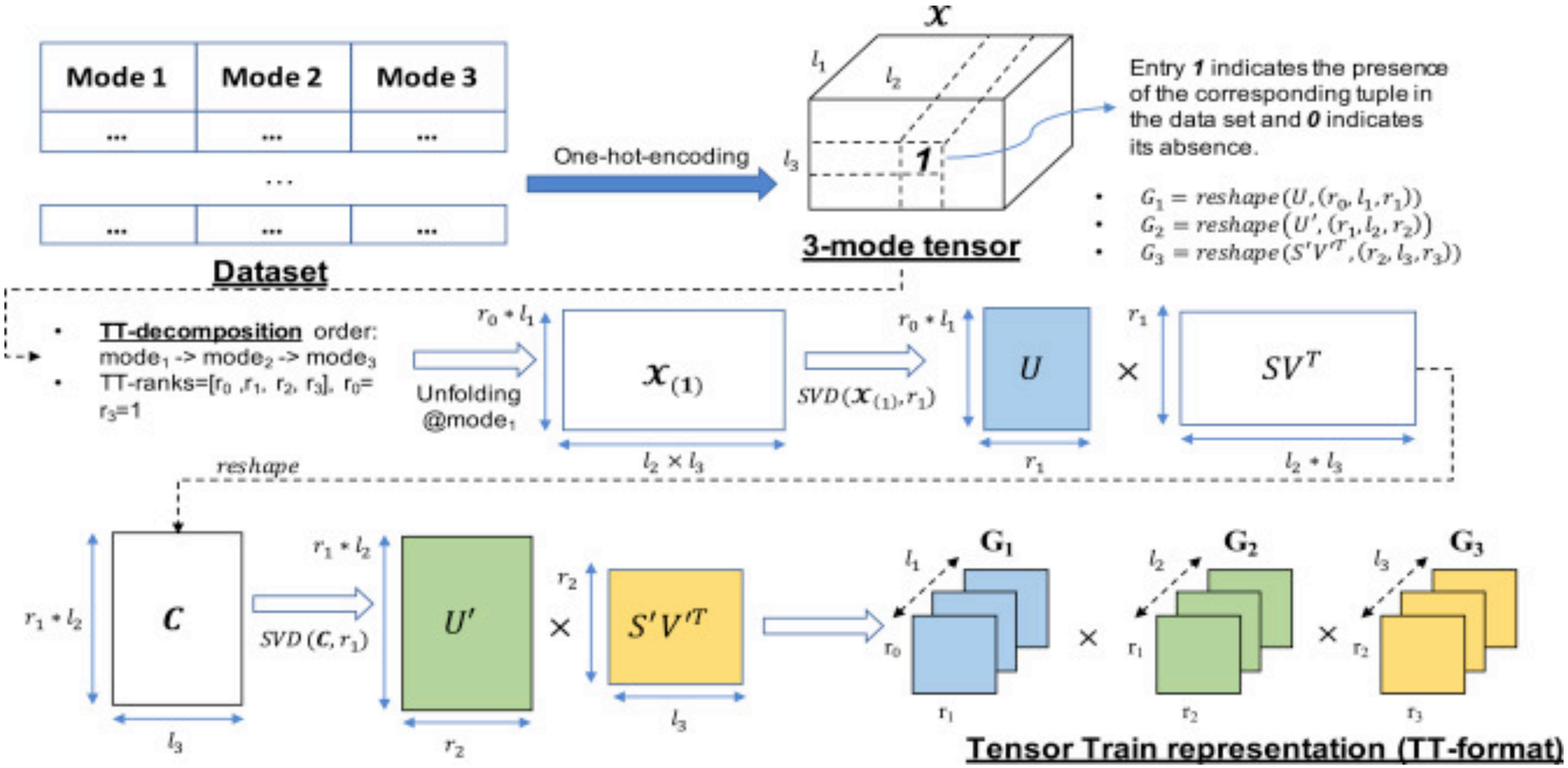
I. V. Oseledets, SIAM J. Sci. Comput. 33 (2011) 2295.

THREE WAYS TO GENERATE TENSOR TRAINS

Method One: Generate from known individual cores.

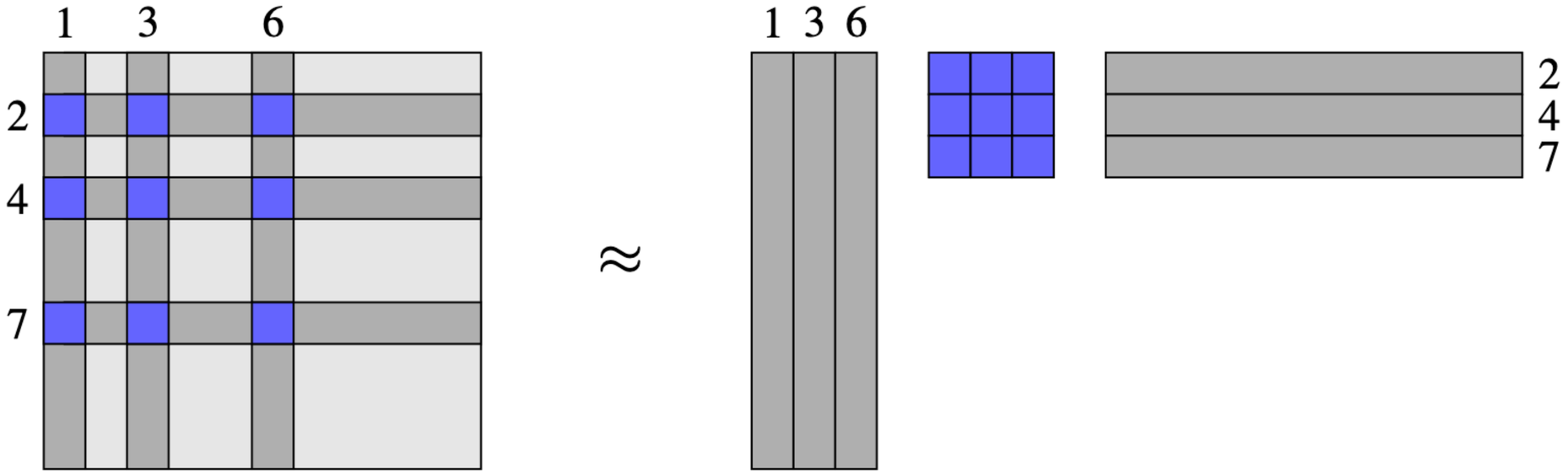
Example: $\mathscr{A}(i_1, \ldots, i_d) = A_1(\alpha_0, i_1, \alpha_1) A_2(\alpha_1, i_2, \alpha_2) \cdots A_d(\alpha_{d-1}, i_d, \alpha_d)$

Method Two: Singular Value Decomposition Method



M.-L. Li, K. Selçuk Candan, M. L. Sabino, Inf. Syst. 108 (2022) 102047.

Method Three: Cross Approximation



Built-In Commands in Oseledets TT-Toolbox

Method One and Two: `tensor` `kron`

Method Two: *`tensor`*

Method Three: *`multifuncrs`* *`multifuncrs2`* *`amen_cross`*

J. Ballani, D. Kressner, "Matrices with Hierarchical Low-Rank Structures," Exploiting Hidden Structure in Matrix Computations: Algorithms and Applications, 2173 (2017) 161.

I. Oseledets, E. Tyrtyshnikov, Linear Algebra Appl. 432 (2010) 70.

I. Oseledets, oseledets/TT-Toolbox (2020) https://www.github.com/oseledets/TT-Toolbox.

KEY: Once data is compressed in tensor-train form, computations can be carried out while staying in the data efficient representation, including:

Addition: $E(i_1, i_2, \ldots, i_d) = A(i_1, i_2, \ldots, i_d) + B(i_1, i_2, \ldots, i_d)$

Subtraction: $E(i_1, i_2, \ldots, i_d) = A(i_1, i_2, \ldots, i_d) - B(i_1, i_2, \ldots, i_d)$

Elementwise Multiplication: $E(i_1, i_2, \ldots, i_d) = A(i_1, i_2, \ldots, i_d)B(i_1, i_2, \ldots, i_d)$

Dot Product: $\sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \cdots \sum_{i_d=1}^{n_d} A^{\star}(i_1, i_2, \ldots, i_d)B(i_1, i_2, \ldots, i_d)$

In particular, tensor-train representations are generated with fast adaptive interpolation of multidimensional arrays in TT-Toolbox, and codes are generated to avoid returning to the full grid-based representation.

The tensor-train approach therefore ensures functions are never evaluated everywhere on the original grid, including:

- Functions of TTs (ex. exponential/propagator $e^{-V(\mathbf{x})}$)
- Operators (ex. Heaviside function/projection $\Theta(\mathbf{x} - \overline{\mathbf{x}})$)
- Integrals (ex. Expectation values $\langle x \rangle$)

Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.
S. M. Greene, V. S. Batista, JCTC 13 (2017) 4034.
I. Oseledets, oseledets/TT-Toolbox (2020) https://www.github.com/oseledets/TT-Toolbox.

This points to a central approach to creation of tensor-train codes for molecular simulations:

Translate codes from linear algebra to multilinear algebra, taking care to remain in tensor-train data compressed format throughout.

This is the core principle of the codes we will discuss today: TT-SOFT, TT-Chebyshev, and IPA.

Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.
S. M. Greene, V. S. Batista, JCTC 13 (2017) 4034.
I. Oseledets, oseledets/TT-Toolbox (2020) https://www.github.com/oseledets/TT-Toolbox.

Table of contents

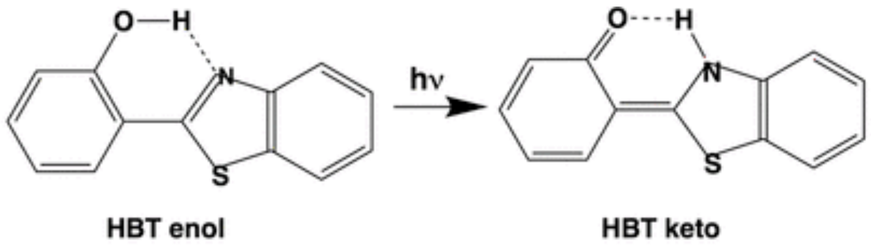
Import Libraries

```
[ ] #!pip install ttpy
    #!pip install git+https://github.com/oseledets/ttpy.git@refs/pull/87/head
    # As soon as #87 is merged you can drop @... suffix and run.
    !pip install git+https://github.com/oseledets/ttpy.git
```

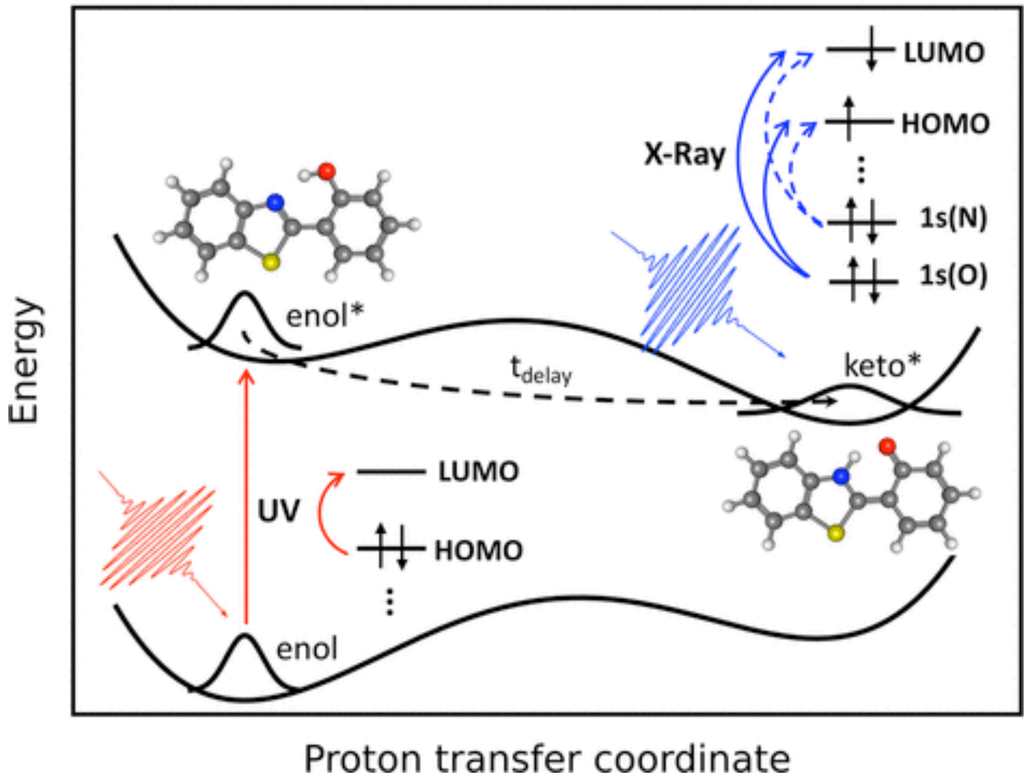
```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple
Collecting git+https://github.com/oseledets/ttpy.git
  Cloning https://github.com/oseledets/ttpy.git to /tmp/pip-req-build-2nh1wbdf
  Running command git clone --filter=blob:none --quiet https://github.com/oseledets/ttpy.git /tmp
  Resolved https://github.com/oseledets/ttpy.git to commit a50d5e0ce2a033a4b1aa703715cb85d715b9b3
  Running command git submodule update --init --recursive -q
  Installing build dependencies ... done
  Getting requirements to build wheel ... done
  Preparing metadata (pyproject.toml) ... done
Building wheels for collected packages: ttpy
  Building wheel for ttpy (pyproject.toml) ... done
  Created wheel for ttpy: filename=ttpy-1.2.0-cp310-cp310-linux_x86_64.whl size=3546003 sha256=dd
  Stored in directory: /tmp/pip-ephem-wheel-cache-605g0su8/wheels/0f/9c/16/16342a640cb36d2dad60b1
Successfully built ttpy
Installing collected packages: ttpy
Successfully installed ttpy-1.2.0
```

TOPIC 1: EXACT QUANTUM DYNAMICS IN HIGH DIMENSIONALITY WITH TT-SOFT

TT-SOFT FOR SIMULATION OF QUANTUM EFFECTS IN COMPLEX CHEMICAL SYSTEMS



HBT enol HBT keto



Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.

BASIS OF THE METHOD: SPLIT-OPERATOR FOURIER TRANSFORM (SOFT) QUANTUM DYNAMICS

Consider the wavefunction $\psi(t)$ in the basis of n equidistant delta functions $\delta(x - x_k)$ in the range $\{x_{\min}, x_{\max}\}$.

The Suzuki-Trotter expansion approximates the propagator as

$$e^{-i\hat{H}\tau} = e^{-i\hat{V}\tau/2} e^{-i\hat{p}^2\tau/(2m)} e^{-i\hat{H}\tau/2}$$

such that the wavefunction is propagated for a short time τ as

$$\psi(t+\tau) = e^{-i\hat{V}\tau/2} \int dp e^{ixp} e^{-i\hat{p}^2\tau/(2m)} \frac{1}{2\pi} \int dx' e^{-ipx'} e^{-i\hat{V}\tau/2} \psi(t).$$

Problem: Grid-based implementation rapidly reaches computational memory limits.

M. D. Feit, J. A. Fleck, A. Steiger, J. Comput. Phys. 47 (1982) 412.
M. Soley, A. Markmann, V. S. Batista, J. Phys. Chem. B, 119 (2015) 715.

ADAPTATION TO TENSOR-TRAIN FORMAT: INITIALIZATION

Initialize the wavepacket as a rank-one tensor train

$$\psi(\mathbf{x}; t_0) = \prod_{j=1}^{d} \psi_j(x_j; t_0)$$

$$\psi\left(x_1, \ldots, x_d; t\right) = \sum_{\alpha_0, \ldots, \alpha_d} \psi_1\left(x_1, \alpha_1; t\right) \psi_2\left(\alpha_1, x_2, \alpha_2; t\right) \cdots \psi_d\left(\alpha_{d-1}, i_d; t\right)$$

Represent potential as tensor train by construction/SVD/cross approximation.

$$V\left(x_1, \ldots, x_d; t\right) = \sum_{\alpha_0, \ldots, \alpha_d} V_1\left(x_1, \alpha_1; t\right) V_2\left(\alpha_1, x_2, \alpha_2; t\right) \cdots V_d\left(\alpha_{d-1}, i_d; t\right)$$

Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.

S. M. Greene, V. S. Batista, JCTC 13 (2017) 4034.

ADAPTATION TO TENSOR-TRAIN FORMAT: PROPAGATOR

Evaluate the potential propagator as truncated power series by construction:

$$e^{-iV\tau/\hbar} = \sum_{n=0}^{N} \frac{\left(-iV\tau/\hbar\right)^n}{n!}$$

Equivalently, the exponential may be generated via the scaling-and-squaring method, cross approximation, etc.

Evaluate the kinetic propagator as a rank-one tensor train:

$$e^{-i\mathbf{p}\cdot\mathbf{m}^{-1}\cdot\mathbf{p}\tau/(2\hbar)} = \prod_{j=1}^{d} e^{-ip_j^2\tau/2m_j\hbar}$$

Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.
S. M. Greene, V. S. Batista, JCTC 13 (2017) 4034.

ADAPTATION TO TENSOR-TRAIN FORMAT: PROPAGATION

Calculate required the FFT/IFFT (built-in):

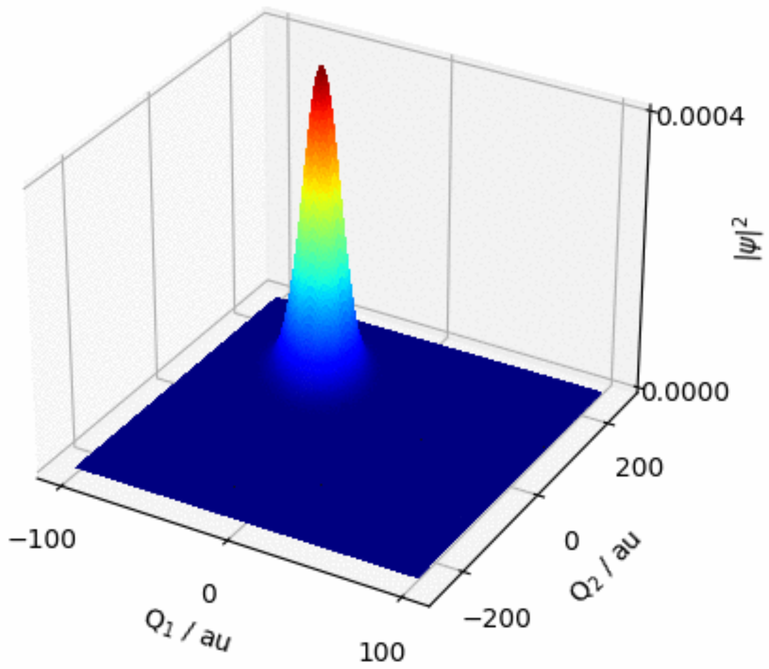
$$\tilde{\psi}(p_1, p_2, \ldots, p_d; t) = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_{d-1}} (2\pi\hbar)^{-d/2} \int \mathrm{d}\mathbf{x}\, \mathrm{e}^{-\mathrm{i}\mathbf{x}\cdot\mathbf{p}/\hbar} \psi_1(x_1, \alpha_1; t)\psi_2(\alpha_1, x_2, \alpha_2; t)\cdots\psi_d(\alpha_{d-1}, x_d; t)$$

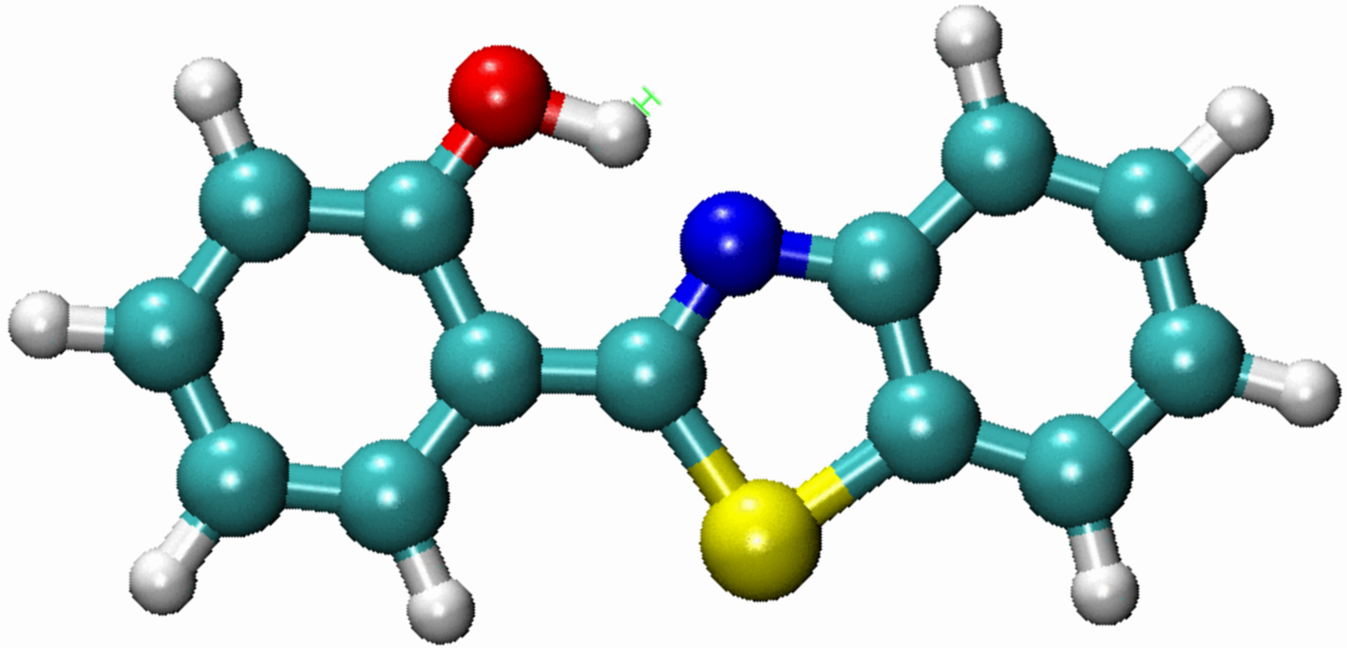
Since the algebraic manipulations in TT-SOFT increase the wavefunction rank during the simulation, the tensor-train rank is rounded after each propagation step.

Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.
S. M. Greene, V. S. Batista, JCTC 13 (2017) 4034.

TT-SOFT RESULTS: QUANTUM DYNAMICS

TT-SOFT propagation in an ab initio potential: https://github.com/michelinesoley/HBT

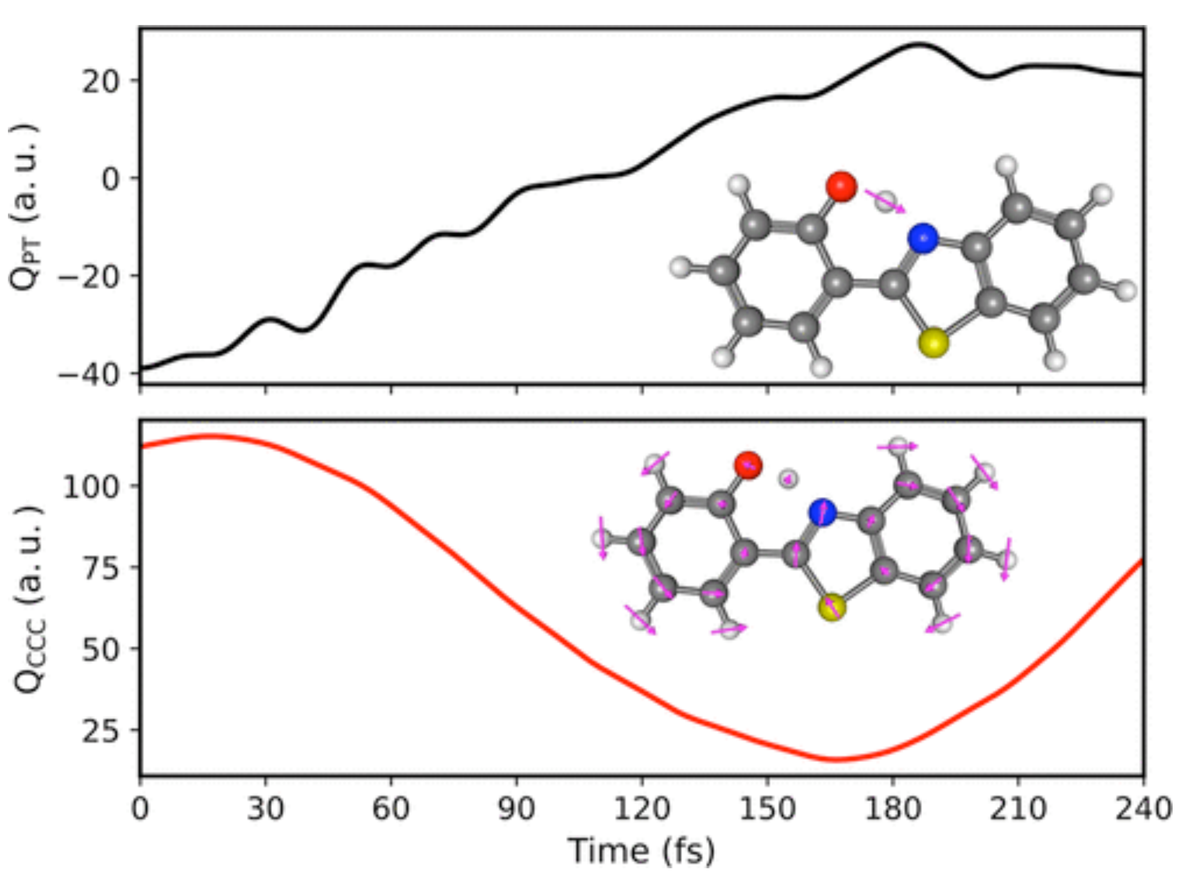


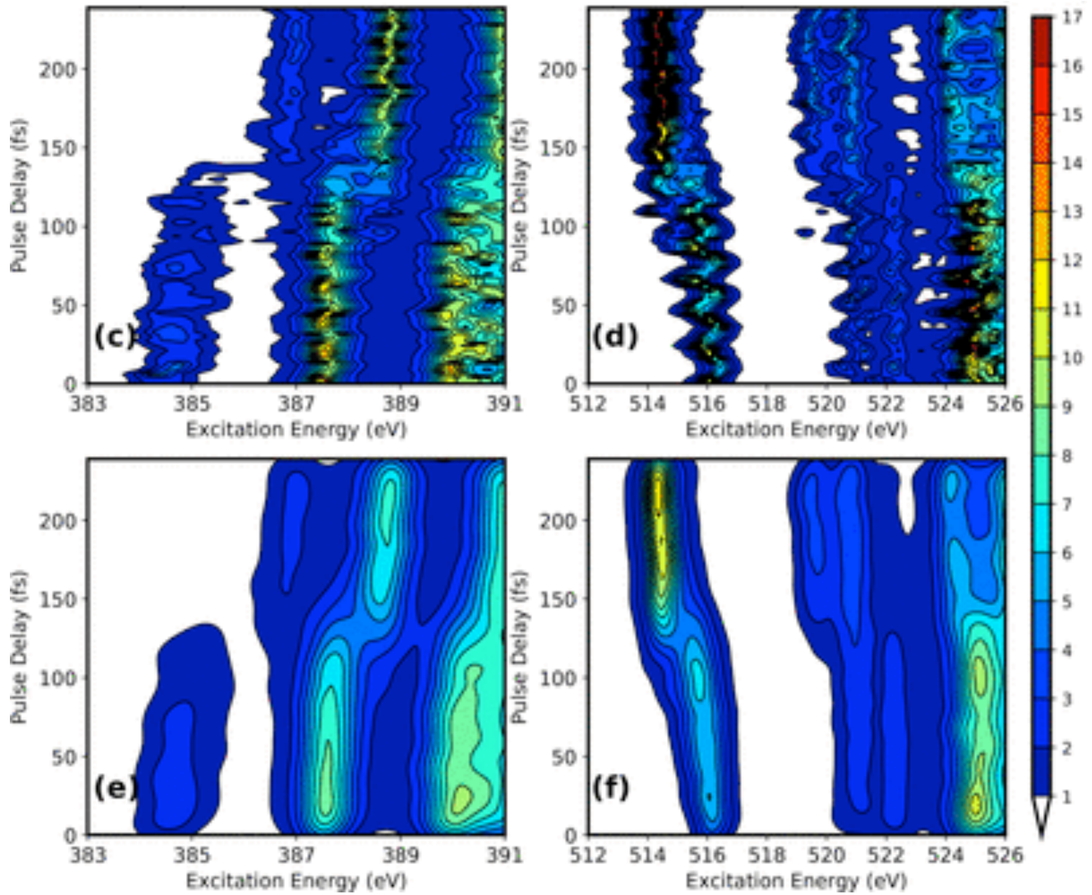


TT-SOFT successfully computes dynamics of a molecular system with **full inclusion of quantum effects in 69D.**

Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.

TT-SOFT RESULTS: PUMP-PROBE SPECTRA



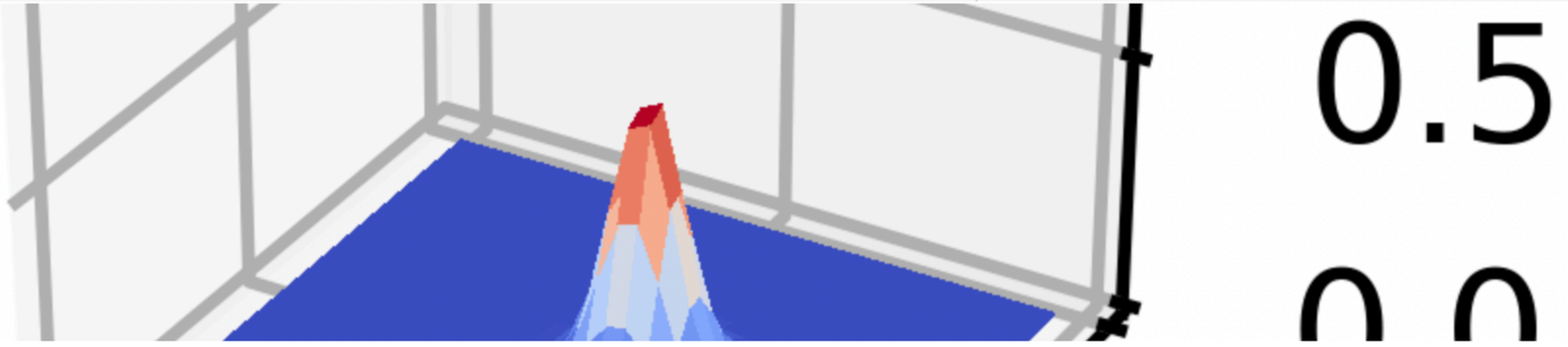


The method thereby enables exact simulation of molecular phenomena beyond reach with standard exact grid-based methods.

Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.

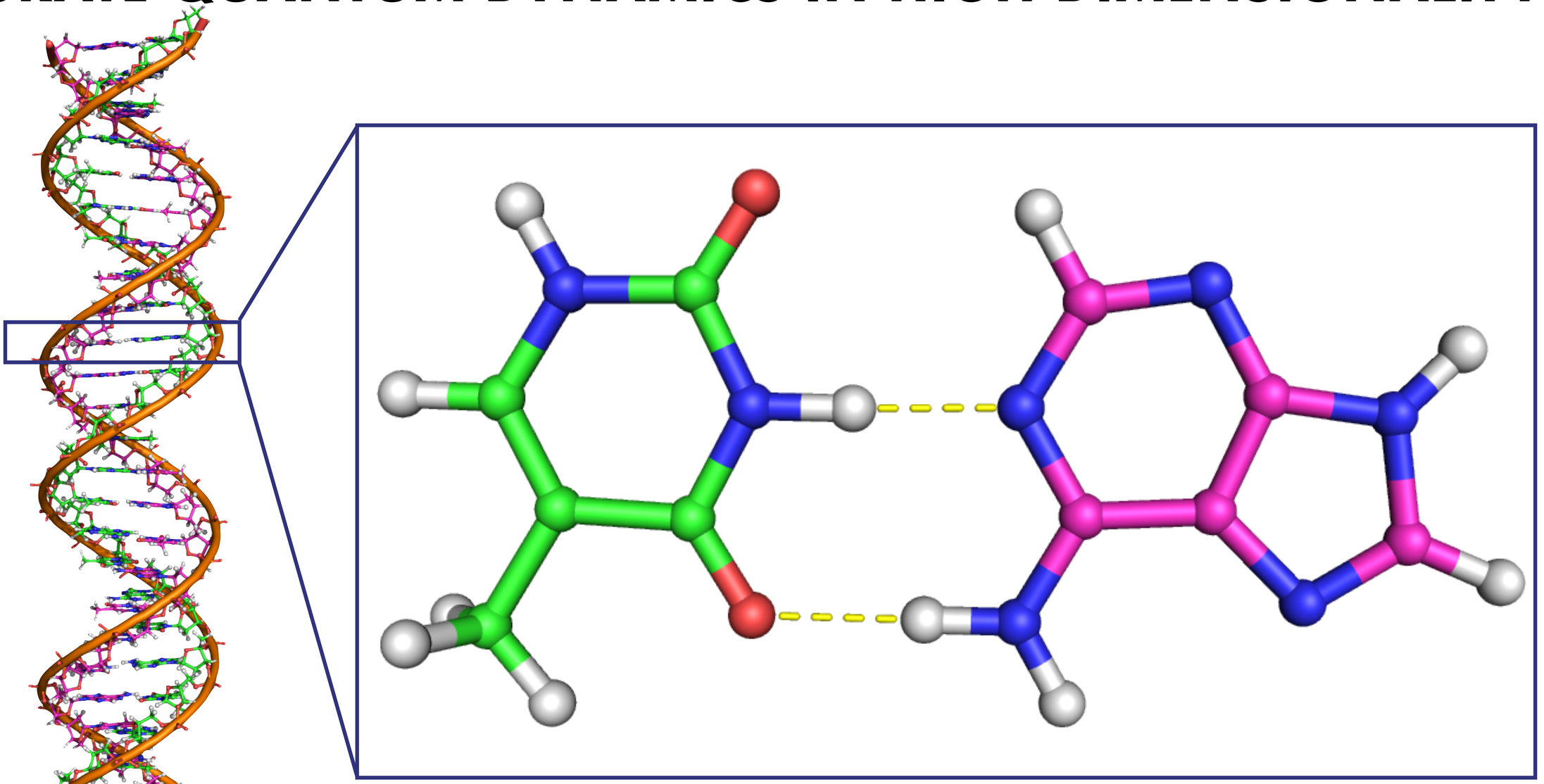
```
[ ]                #print('r0=',tt_psi[0].r)
                # plot wavepacket components
                #if js%1==0:
                    if wfflag == 1: #check param to plot
                        ttpsi1=tt_psi[0].full()
                        ttpsi=np.reshape(ttpsi1,[nx[0]]*dim)
                        plt.figure(dpi=600)
                        ax= plt.subplot(3,2,2, projection='3d')
                        if  qmodes == 0:
                            ax.plot_surface(x, y, np.abs(ttpsi[:,:]), cmap=cm.coolwarm, antialiased=False)
                        if  qmodes == 1:
                            ax.plot_surface(x, y, np.abs(ttpsi2[:,:,nsl]), cmap=cm.coolwarm, antialiased=False)
                        ax.set_zlim3d(0,1)

                        plt.pause(.02)
                        if js < nsc-1:
                            plt.clf()
```



EXACT QUANTUM DYNAMICS IN HIGH DIMENSIONALITY: TT-CHEBYSHEV

ACCURATE QUANTUM DYNAMICS IN HIGH DIMENSIONALITY



Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.
N. Lyu*, E. Mulvihill*, **Micheline B. Soley**, E. Geva, V. S. Batista, JCTC, 19 (2023) 1111.
Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, J. Phys. Chem. Lett., 13 (2022) 8354.
N. Lyu, **Micheline B. Soley**, V. S. Batista, JCTC, 18 (2022) 3327.
Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.

CHEBYSHEV POLYNOMIALS

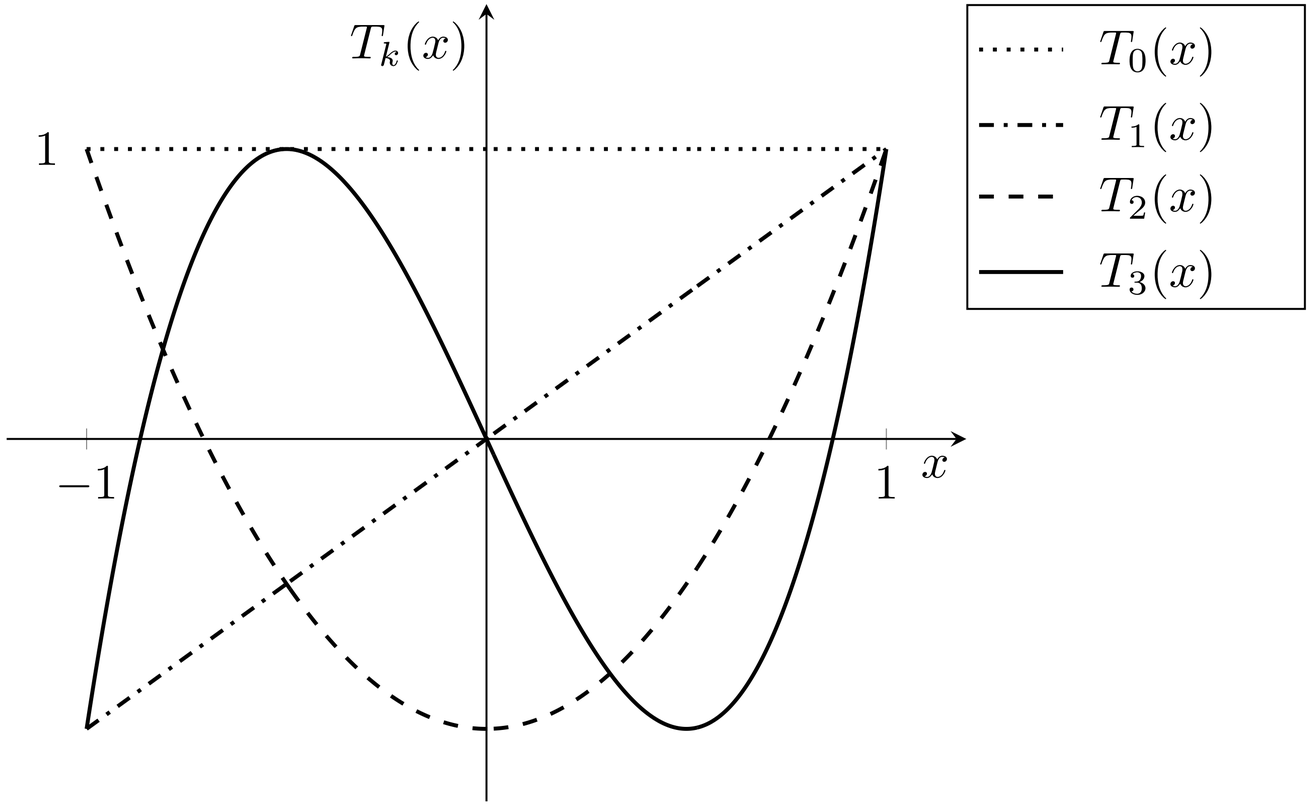
For all integers $k \geq 0$ and all $x \in [-1,1]$, the kth Chebyshev polynomial is defined as

$$T_k(x) = \cos(k \arccos(x))$$

<u>*Recurrence relation:*</u>

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$$

$$T_0(x) = 1,\ T_1(x) = x$$



Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.
L. N. Trefethen, Approximation Theory and Approximation Practice, SIAM: Philadelphia, 2013.
H. Tal-Ezer, R. Kosloff, J. Chem. Phys. 81 (1984) 3967.

CHEBYSHEV EXPANSION OF COMPLEX-VALUED FUNCTIONS

Chebyshev polynomials can be used to approximate a given complex-valued function f via its Fourier series representation

$$g(x) = f(\cos(x))$$

$$g(x) = \sum_{k=0}^{\infty} (2 - \delta_{k,0}) a_k \cos(kx), \quad a_k = \frac{1}{\pi} \int_0^{\pi} g(x) \cos(kx) \mathrm{d}x$$

such that $f(y) = g(\arccos(y))$ can be represented in terms of Chebyshev polynomials for $y \in [-1,1]$

$$f(y) = \sum_{k=0}^{\infty} (2 - \delta_{k,0} c_k T_k(y), \quad c_k = \frac{1}{\pi} \int_{-1} 1 \frac{\mathrm{d}y}{\sqrt{1 - y^2}} f(y) T_k(y)$$

CHEBYSHEV APPROXIMANT OF COMPLEX-VALUED FUNCTIONS

This Chebyshev expansion of f can then be used to approximate f as the linear combination of the first N Chebyshev polynomials

$$f(y) \approx S_N f(y) - \sum_{k=0}^{N-1} (2 - \delta_{k,0}) c_k T_k(y)$$

The resulting Chebyshev approximant $S_N f$ is a polynomial of degree N that is known to be close to the polynomial of the same degree with minimal error in the interval $[-1,1]$.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.
H. Tal-Ezer, R. Kosloff, J. Chem. Phys. 81 (1984) 3967.

CHEBYSHEV PROPAGATION IN DISCRETE REPRESENTATIONS

We obtain an approximation of the propagator as applied to the wavefunction according to the Chebyshev expansion of complex-valued functions:

$$\Psi(t) = e^{-itH}\Psi(0)$$

$$e^{itH} \approx e^{-it^{+}} \sum_{k=0}^{N-1} \left(2 - \delta_{k,0}\right) (-i)^{k} J_{k}(t^{-})\, T_{k}\left(H_{0}\right)$$

$$t^{\pm} = \frac{t}{2}\left(b \pm a\right)$$

$$H_{0} = \frac{2}{b-a}\left(H - \frac{b+a}{2} I_{D}\right)$$

Fast convergence is typically obtained for e^{-ity} since it is a smooth function, with error falling as the N^{th} order in $\left|t^{-}\right|/(2N)$ for sufficiently large N.

M. T. Cvitaš, S. C. Althorpe, J. Chem. Phys. 139 (2013) 064307.
E. M. Goldfield, S. K. Gray, J. Chem. Phys. 117 (2002) 1604.
H. Tal-Ezer, R. Kosloff, J. Chem. Phys. 81 (1984) 3967.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25
H. Tal-Ezer, R. Kosloff, J. Chem. Phys. 81 (1984) 3967.

DISCRETE TENSOR-TRAIN IMPLEMENTATION: HAMILTONIAN

Discrete low-rank TT representations are generated for the wavefunction $\mathscr{W}$ and potential energy operator $\mathscr{V}$, and the action of the kinetic energy operator on the wavefunction $\hat{\mathscr{T}}\mathscr{W}$.

Here, $\hat{\mathscr{T}}\mathscr{W}$ is found in terms of the Laplacian (to take advantage of highly-efficient implementations of multidimensional discrete Fourier transforms of tensor trains to switch between position and momentum space) to generate the Hamiltonian $\hat{\mathscr{H}}$.

he discrete Hamiltonian is then rescaled as in standard Chebyshev propagation

$$\hat{\mathscr{H}}_0 = \frac{2}{E_{\max} - E_{\min}} \left(\hat{\mathscr{H}} - \frac{E_{\max} - E_{\min}}{2} \hat{\mathscr{I}} \right)$$

where $\hat{\mathscr{I}}$ is the identity on the tensor space.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

DISCRETE TENSOR-TRAIN IMPLEMENTATIONL: PROPAGATION

The propagated wavefunction $\Psi(t)$ is then approximated with N Chebyshev polynomials

$$\Psi(t) = e^{-it\hat{H}}\Psi(0) \approx e^{-it^{+}} \sum_{k=0}^{N-1} (2 - \delta_{k,0})(-i)^k J_k(t^{-}) T_k(\hat{\mathscr{H}}_0)\mathscr{W}_0$$

where we employ the Chebyshev Clenshaw algorithm or the recurrence relation

$$T_0(\hat{\mathscr{H}}_0)\mathscr{W}_0 = \mathscr{W}_0$$
$$T_1(\hat{\mathscr{H}}_0)\mathscr{W}_0 = \hat{\mathscr{H}}_0\mathscr{W}_0$$
$$T_{k+1}(\hat{\mathscr{H}}_0)\mathscr{W}_0 = 2\hat{\mathscr{H}}_0 T_k(\hat{\mathscr{H}}_0)\mathscr{W}_0 - T_{k-1}(\hat{\mathscr{H}}_0)\mathscr{W}_0, \quad \text{for } k \geq 1$$

The same Chebyshev propagation scheme can be readily implemented using the continuous analogue **functional tensor-train decomposition**.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

CONTINUOUS ANALOGUE OF THE TENSOR-TRAIN DECOMPOSITION

In place of discrete numerical entries, **functional tensor trains** are composed of univariate functions $f_k^{(ij)}$.

$$f(x_1, x_2, \ldots, x_d) = \sum_{i_0=1}^{r_0} \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} f_1^{(i_0 i_1)}(x_1) f_2^{(i_1 i_2)}(x_2) \cdots f_d^{(i_{d-1} i_d)}(x_d)$$

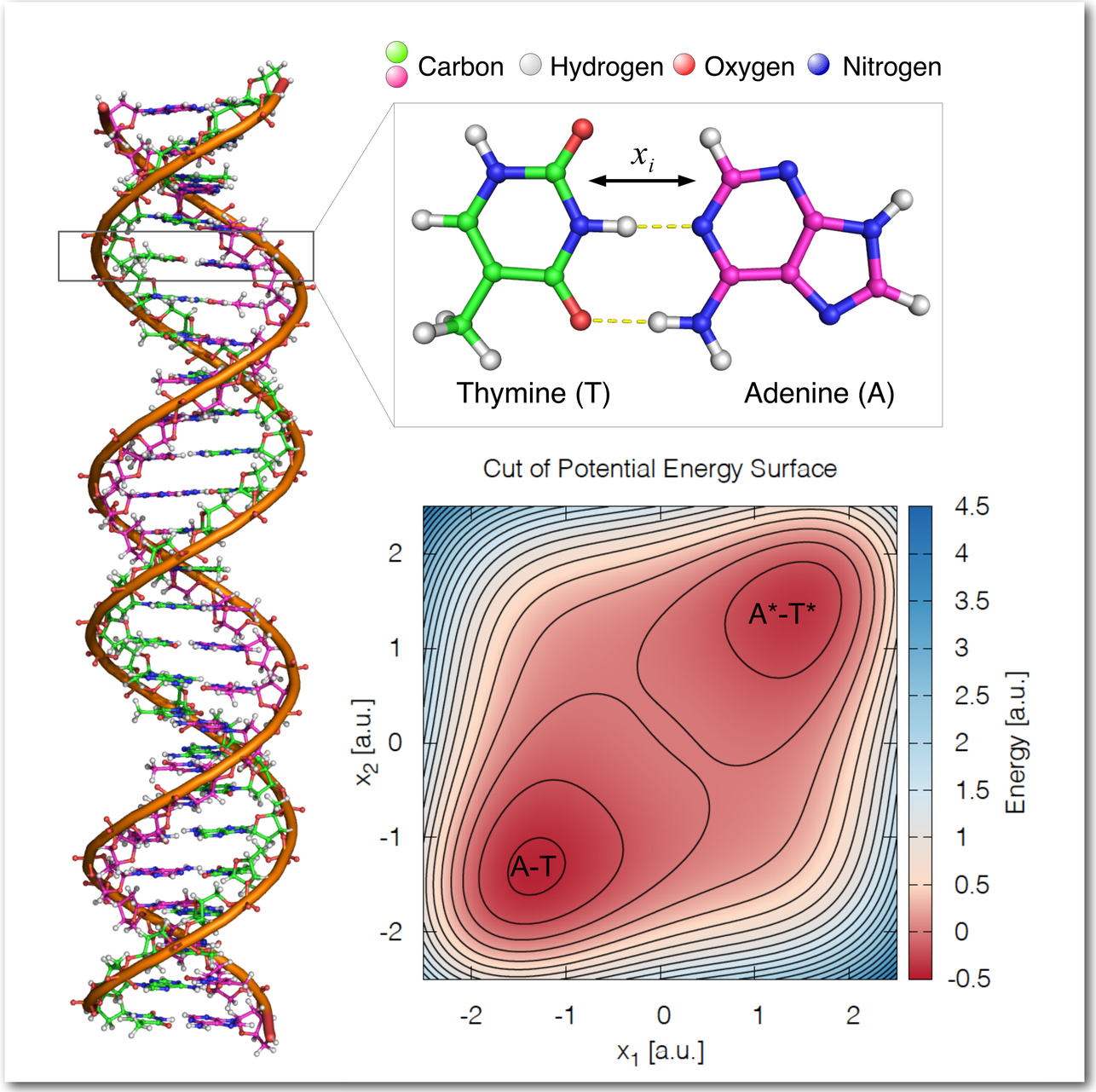
$$f(x_1, x_2, \ldots, x_d) = \mathscr{F}_1(x_1)\mathscr{F}_2(x_2)\cdots\mathscr{F}_d(x_d)$$

$$\mathscr{F}_k = \begin{bmatrix} f_k^{(11)}(x_1) \cdots & f_k^{(1 r_k)}(x_k) \\ \vdots \quad \ddots & \vdots \\ f_k^{(r_{k-1}, 1)}(x_k) \cdots & f_k^{(r_{k-1} r_k)}(x_k) \end{bmatrix}$$

Result: Efficient gradients, integrals, and correlation functions in high dimensionality with likewise ease of calculations

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.
A. Gorodetsky, J. D. Jakeman, J. Comput. Phys. 374 (2018) 1219.
A. Gorodetsky, A. A. Compressed Continuous Computation (C3) Library. https:// github.com/goroda/Compressed-Continuous-Computation.

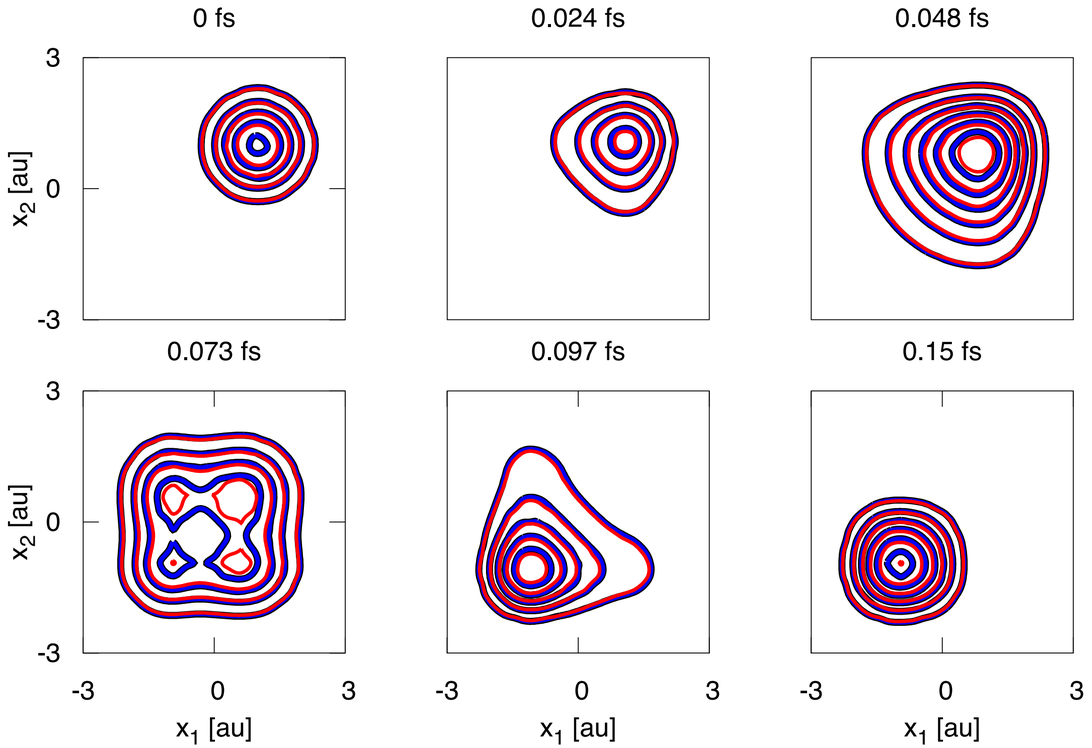
FUNCTIONAL TENSOR TRAIN CHEBYSHEV (FTTC) DYNAMICS RESULTS



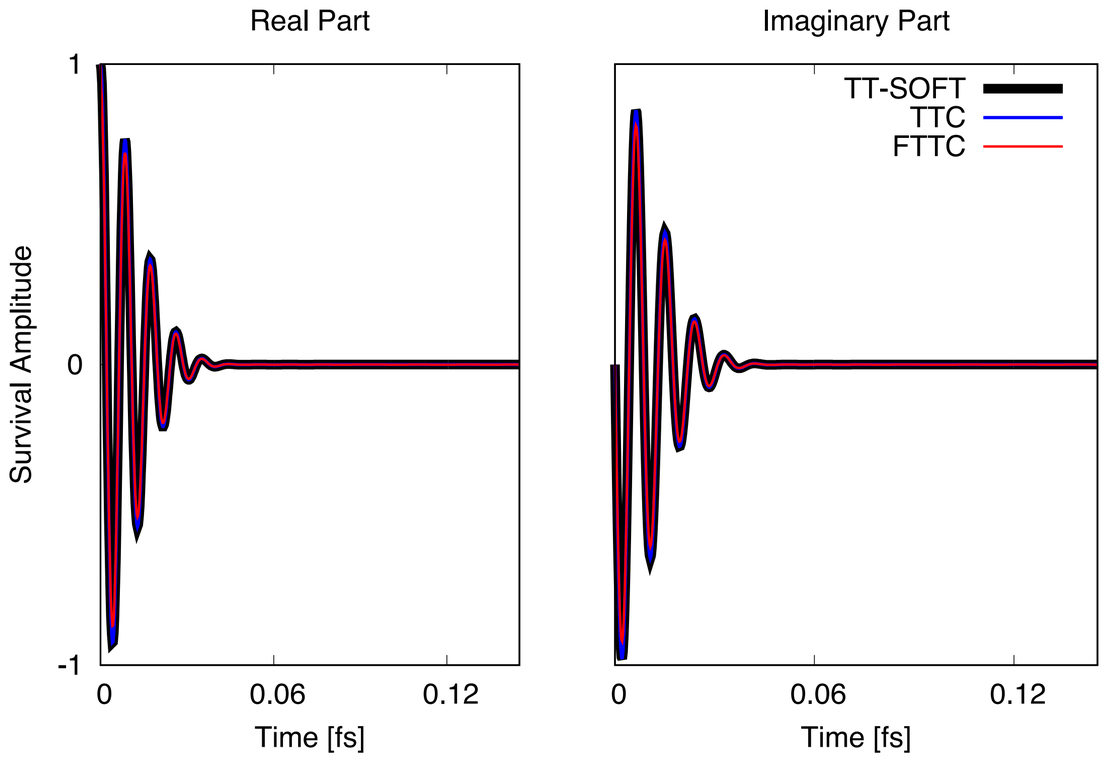
Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

APPLICATION: HYDROGEN BONDING IN DNA

Probability Density Dynamics, Uncoupled Bath



Survival Amplitude

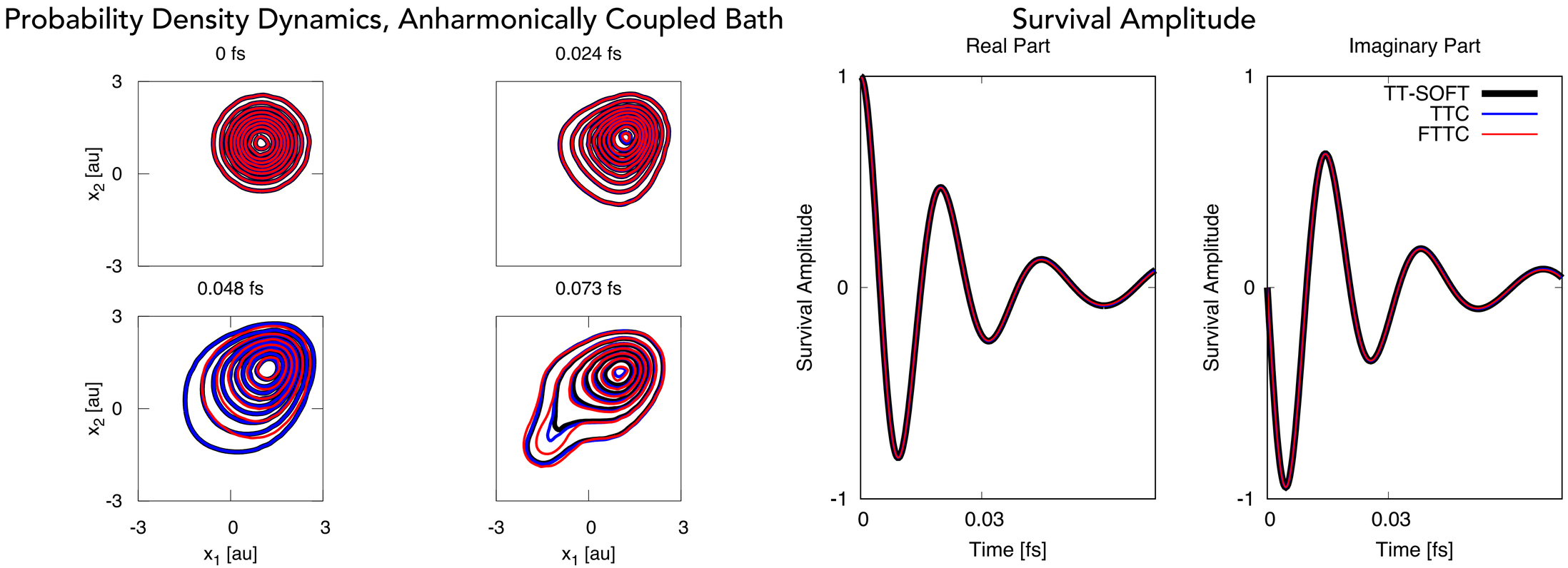


FTTC extends the Chebyshev method from simulation of four-atom systems to molecular systems in

50 dimensions.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

APPLICATION: HYDROGEN BONDING IN DNA



FTTC successfully determines molecular dynamics

even with significant coupling of atomic motion between modes.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

IMPACT OF FTTC

The success of the functional tensor-train decomposition should find wide applicability in studies requiring computations of gradients, integrals, and correlation functions of systems with high dimensionality.

And, the success of FTTC invites its use for other not only for simulations of quantum reaction dynamics in general, but also as a general method to obtain numerical solutions of linear systems in high dimensionality.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

```
[ ]  ax.contour3D(xmesh, ymesh, v_ft_psim, 100, cmap='binary')
     ax.set_xlabel('x [au]')
     ax.set_ylabel('y [au]')
     ax.set_zlabel('Density [arb. u.]');
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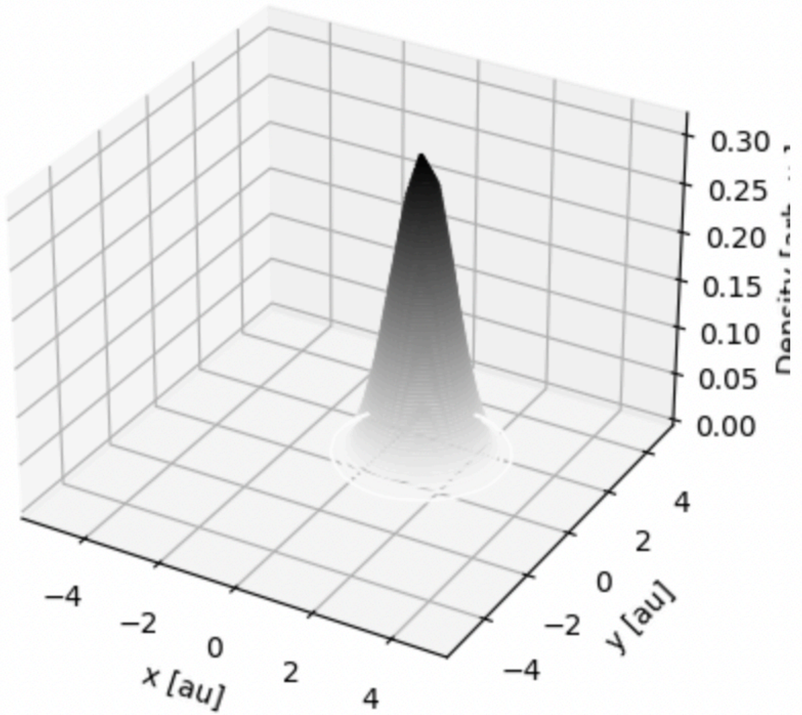
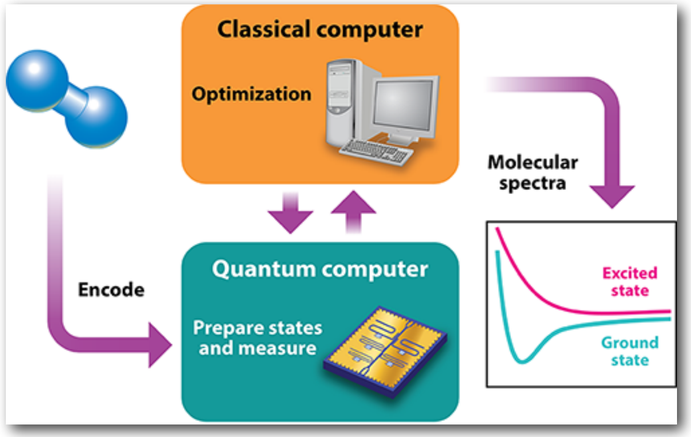


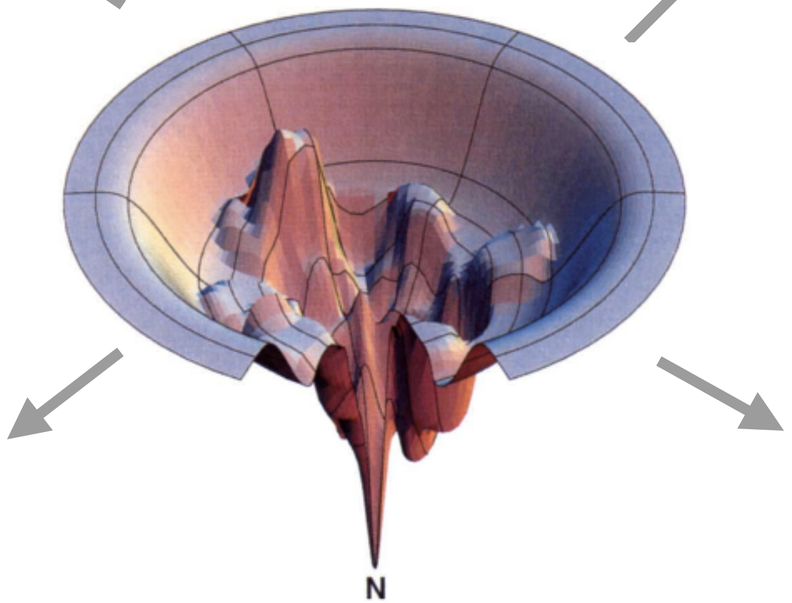
GLOBAL OPTIMIZATION WITH THE ITERATIVE POWER ALGORITHM

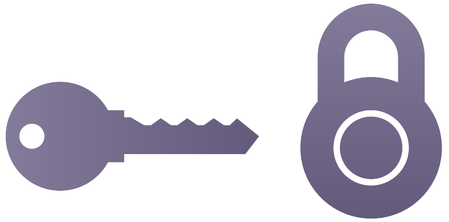
GLOBAL OPTIMIZATION

$$\arg\min_{x\in\mathbb{R}} V(x) = \left\{x^\star \in \mathbb{R} \,|\, V(x) \geq V(x^\star) \text{ for all } x \in \mathbb{R}\right\}$$

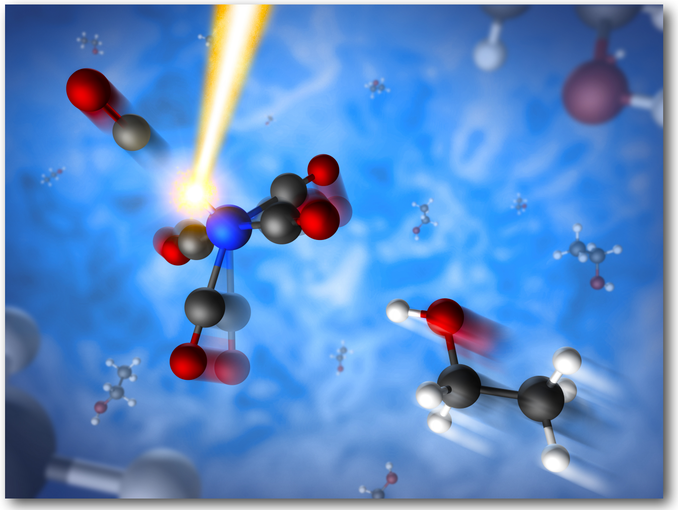
$$V(\mathbf{x}) = \min! \qquad V : \mathbb{R}^n \to \mathbb{R}$$

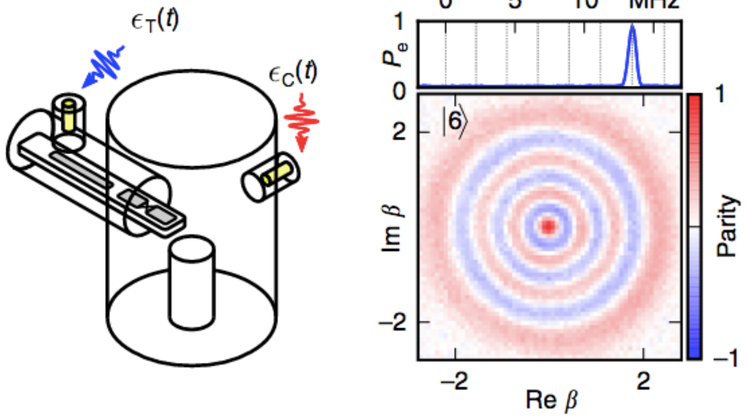






21 = 3 x 7





S. Sim, J. Romero, P. D. Johnson, A. Aspuru-Guzik, Physics 11 (2018) 14.
R. W. Heeres et al., Nature Comm. 8 (2017) 94.
K. A. Dill, H. S. Chan, Nat. Struct. Diol. 4 (1997) 10.
SLAC National Accelerator Laboratory.

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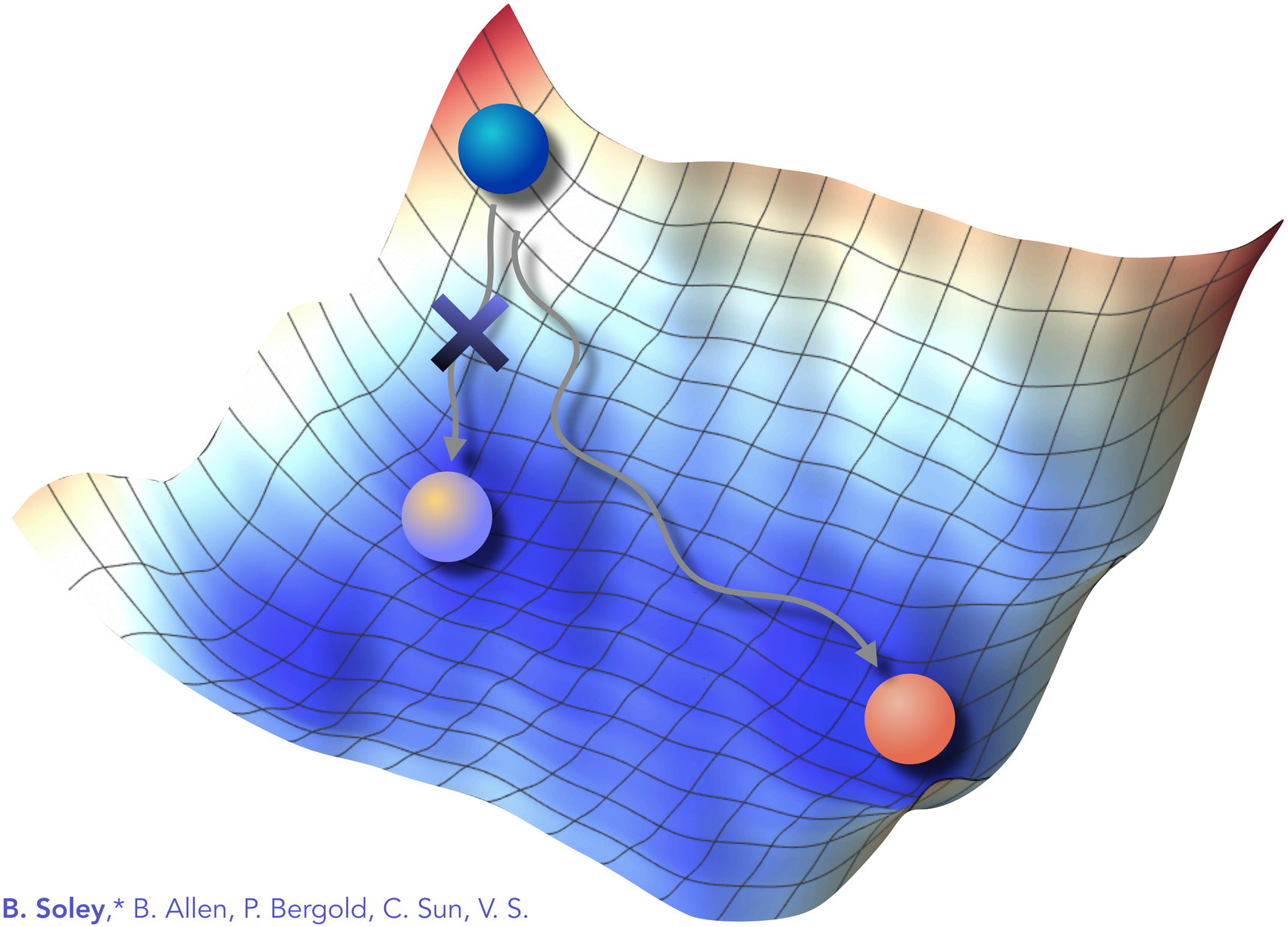
M. B. Soley, A. Markmann, V. S. Batista, JCTC, 14 (2018) 3351.
M. Soley, A. Markmann, V. S. Batista, J. Phys. Chem. B, 119 (2015) 715.
K. A. Dill, J. L. MacCallum, Science 338 (2012) 1042.

LOCAL MINIMUM TRAPS

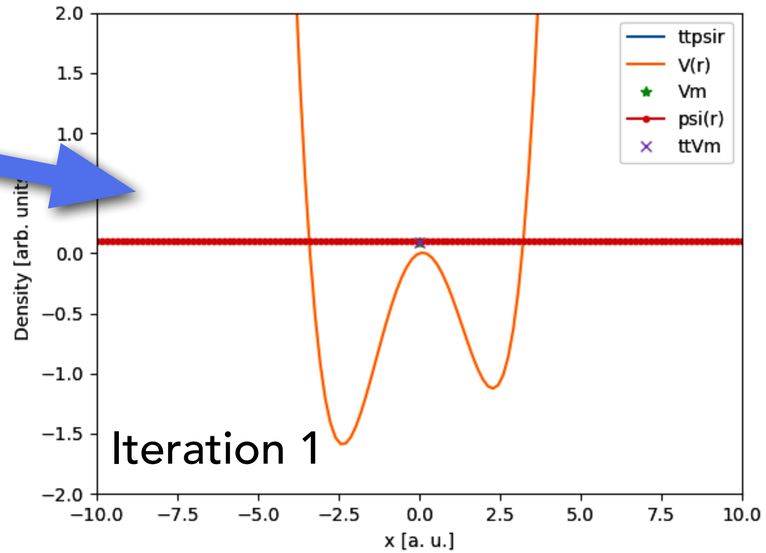


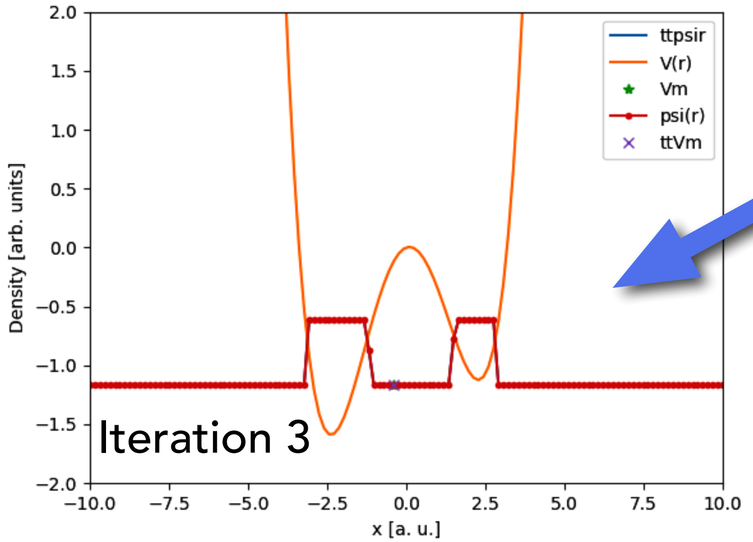
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.
M. B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.

M. B. Soley, A. Markmann, V. S. Batista, JCTC, 14 (2018) 3351.
M. Soley, A. Markmann, V. S. Batista, J. Phys. Chem. B, 119 (2015) 715.

We introduce the **iterative power algorithm (IPA)** that bypasses local minimum traps to converge to the global minima.

Initialize ρ and V as Tensor Trains

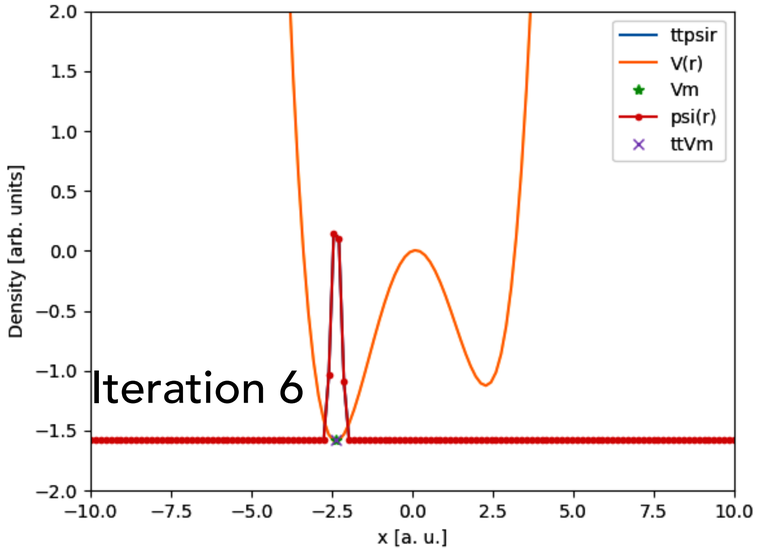


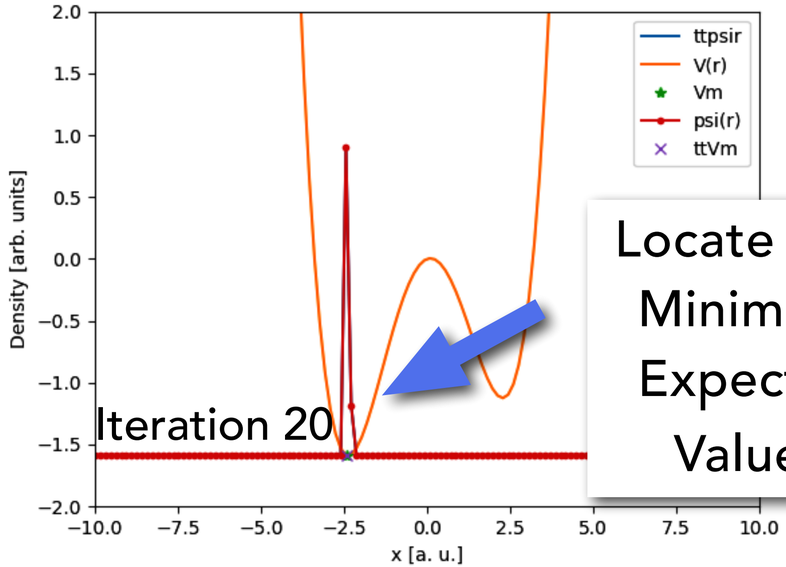


Iteratively Apply Oracle

$$\rho(x) \rightarrow \mathcal{N}U(x)\rho(x)$$

$$U(x) = e^{-cV(x)}$$



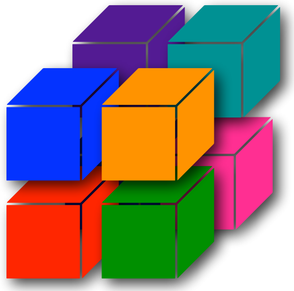


Locate Global Minimum as Expectation Value $\langle x \rangle$

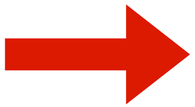
Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.

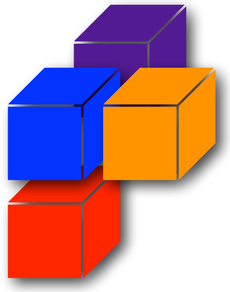
IPA can efficiently find the global minimum of low-rank high-dimensional potential energy surfaces by approximating $\rho(\mathbf{x})$ and $V(\mathbf{x})$ in D physical dimensions in the form of **quantics tensor trains** (QTTs) in n reshaped dimensions.

2^d-element array (length 2^d grid in one dimension)



$2_1 \times 2_2 \times \cdots \times 2_d$ tensor





QTT

$$\approx \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} A_1(1,i_1,\alpha_1)A_2(\alpha_1,i_2,\alpha_2)\cdots A_d(\alpha_{d-1},i_d,1)$$

Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.
B. N. Khoromskij, Constr. Approx. 34 (2011) 257.

THE IPA METHOD

INITIALIZATION: UNIFORM SUPERPOSITION

- Consider the cost function as a potential surface $V(\mathbf{x})$ with global minimum at $\mathbf{x} = \mathbf{x}^\star$
- Initialize a probability distribution $\rho_0(\mathbf{x})$ in the potential as a quantics tensor train

$$\rho_0 : \mathbb{R} \rightarrow [0,\infty)$$

$$\|\rho_0\|_{L^1} = \int_{\mathbb{R}} \mathrm{d}x \rho_0(x) = 1$$

$$\int_{x^\star - r}^{x^\star + r} \mathrm{d}x \rho_0(x) > 0 \quad \text{where } r > 0$$

MBS, P. Bergold, V. S. Batista, JCTC (2021) in press, arXiv:2101.03377.

EVOLUTION: AMPLITUDE AMPLIFICATION

DEFINE $U(x)$

(i) a continuous and strictly positive function maximized at the global minima of $V(x)$

$$\arg\max_{x\in\mathbb{R}} U(x) = \arg\min_{x\in\mathbb{R}} V(x)$$

(ii) an integrable function ($U(x) \in L^1(\mathbb{R})$)

EXAMPLE

$U(x) = e^{-\beta V(x)}$ for fixed scaling parameter $\beta > 0$

MBS, P. Bergold, V. S. Batista, JCTC (2021) in press, arXiv:2101.03377.

ITERATIVELY APPLY RECURRENCE RELATION

for $k = 1,2,\ldots$

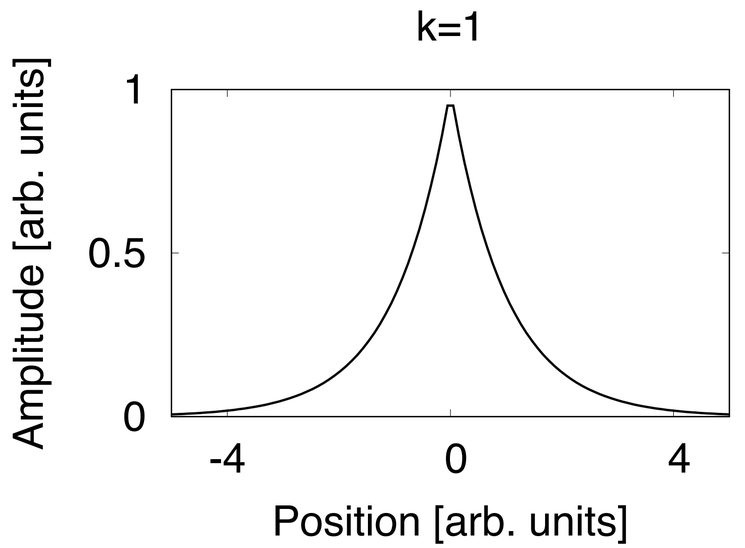
$$\eta_k = \|U\rho_{k-1}\|_{L^1} = \int_{\mathbb{R}} \mathrm{d}x U(x)\rho_{k-1}(x);$$

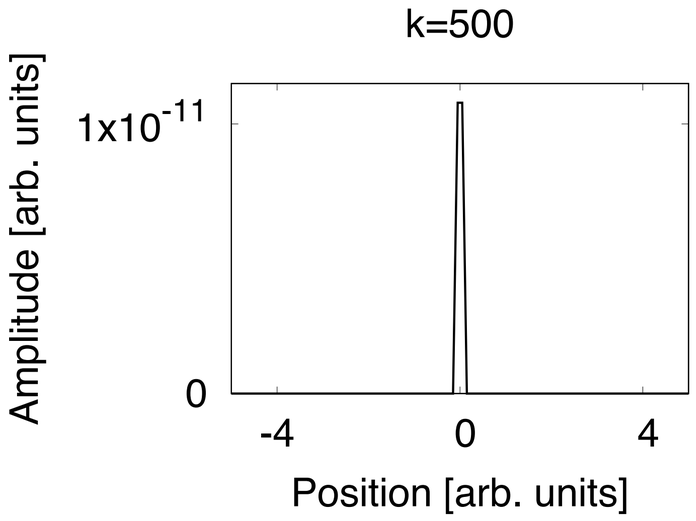
$$\rho_k(x) = \frac{U(x)\rho_{k-1}(x)}{\eta_k} = \frac{(U(x))^k\rho_0(x)}{\|U^k\rho_0\|_{L^1}};$$

end

$$\rho_{\text{final}}(x) = \lim_{k\to\infty} \rho_k(x) = \sum_{j=1}^{s} \delta(x - x_j^\star)$$

U^k **for** $U = e^{-V(x)}$ **with** $V(x) = |x|$





MBS, P. Bergold, V. S. Batista, JCTC (2021) in press, arXiv:2101.03377.

RESOLUTION OF GLOBAL MINIMA: MEASUREMENT

OBTAIN THE GLOBAL MINIMUM POSITION

(i) Single global minimum

$$x^\star = \langle x \rangle_{\rho_{\text{final}}} = \int_{\mathbb{R}} \mathrm{d}x \, x \rho_{\text{final}}(x)$$

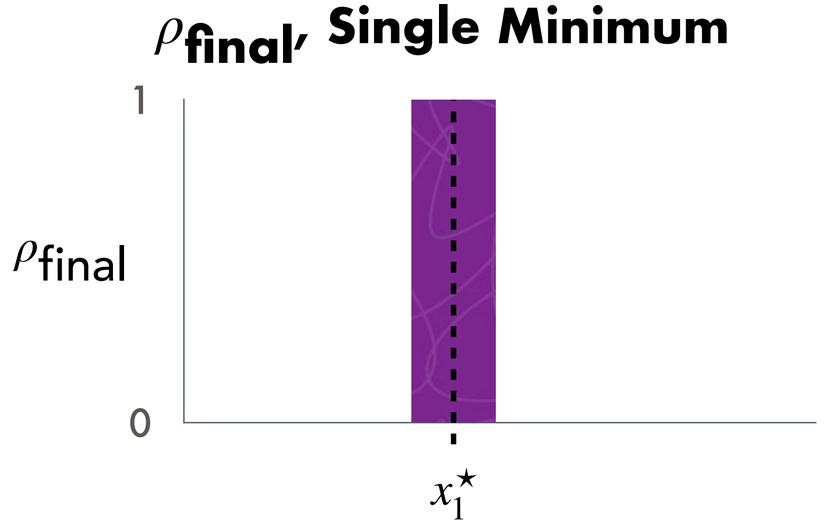
(ii) Two degenerate global minima

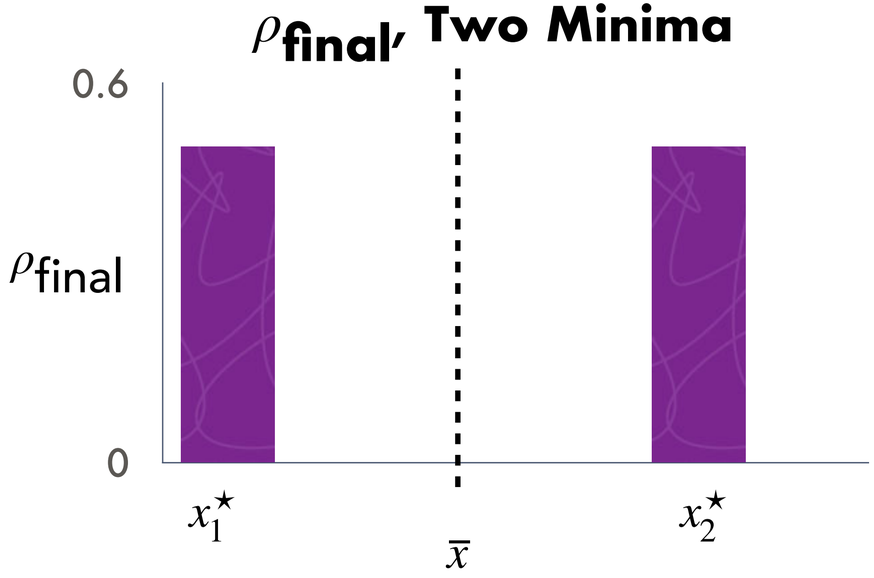
$$\bar{x} = \langle x \rangle_{\rho_{\text{final}}}$$

$$\Theta(x - \bar{x}) = \begin{cases} 0, & \text{if } x \leq \bar{x} \\ 1, & \text{if } x > \bar{x} \end{cases}$$

$$x_1^\star = \langle x \rangle_{\rho_{\text{final}}}(x)\Theta(x - \bar{x})$$

$$x_2^\star = \langle x \rangle_{\rho_{\text{final}}}(x)(1 - \Theta(x - \bar{x}))$$

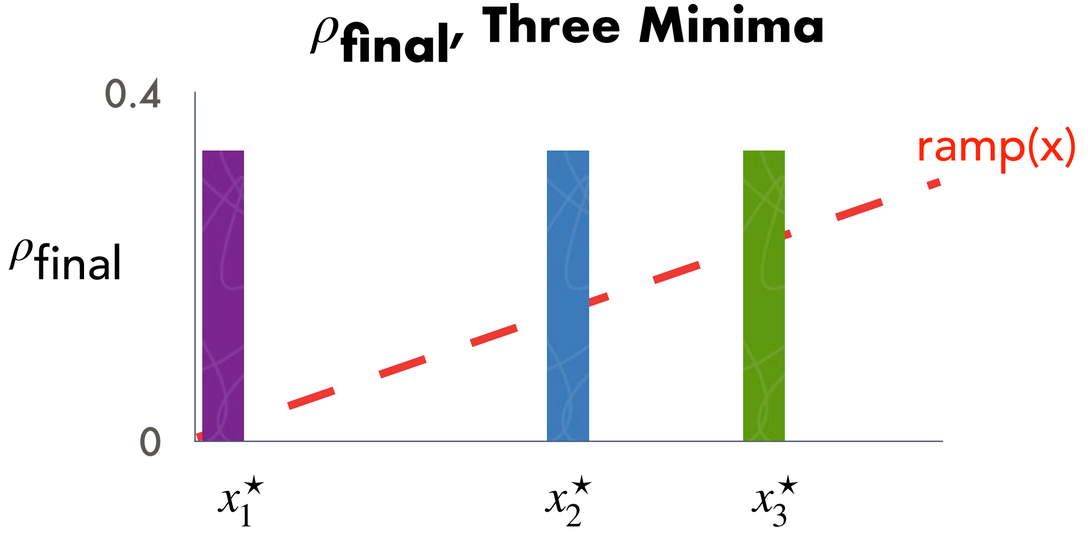




MBS, P. Bergold, V. S. Batista, JCTC (2021) in press, arXiv:2101.03377.

(iii) Unknown number of global minima

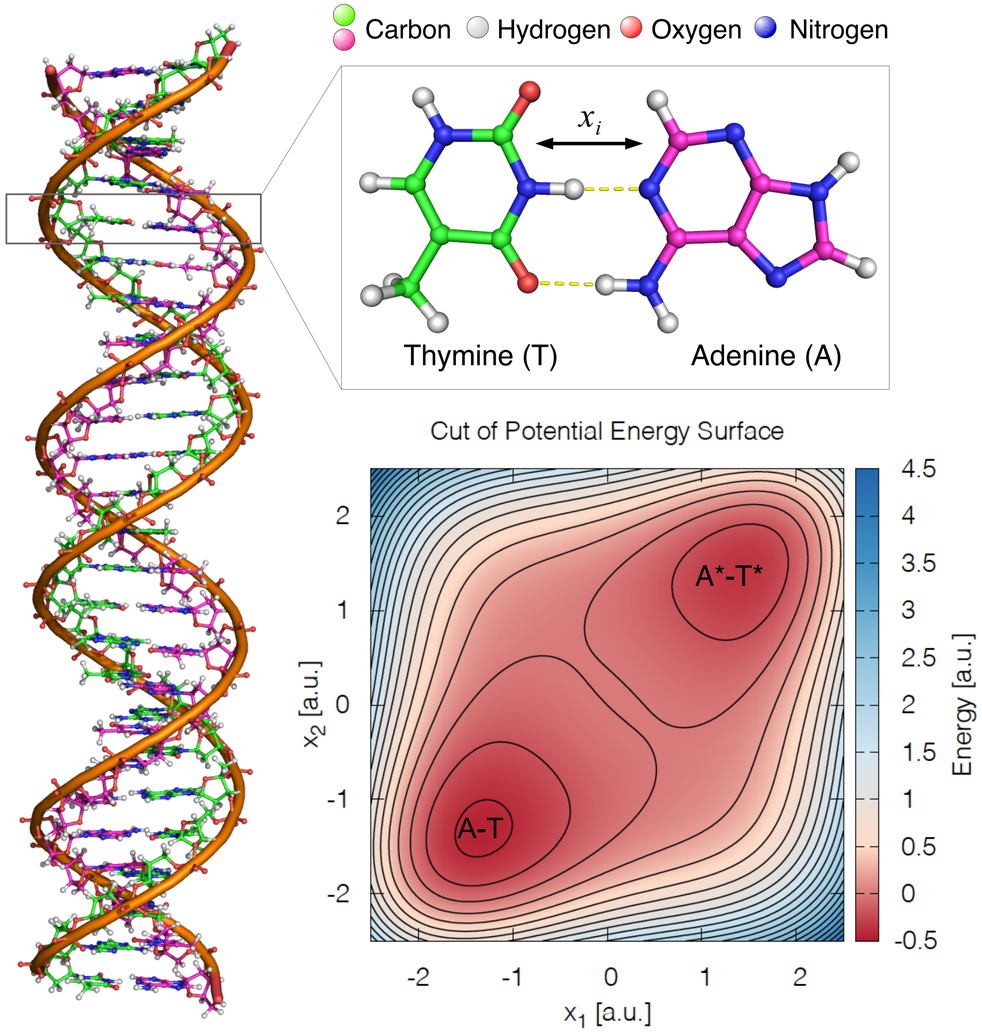
- Obtain ρ_{final} using IPA
- Reinitialize $\rho_0 \propto \rho_{\text{final}}$

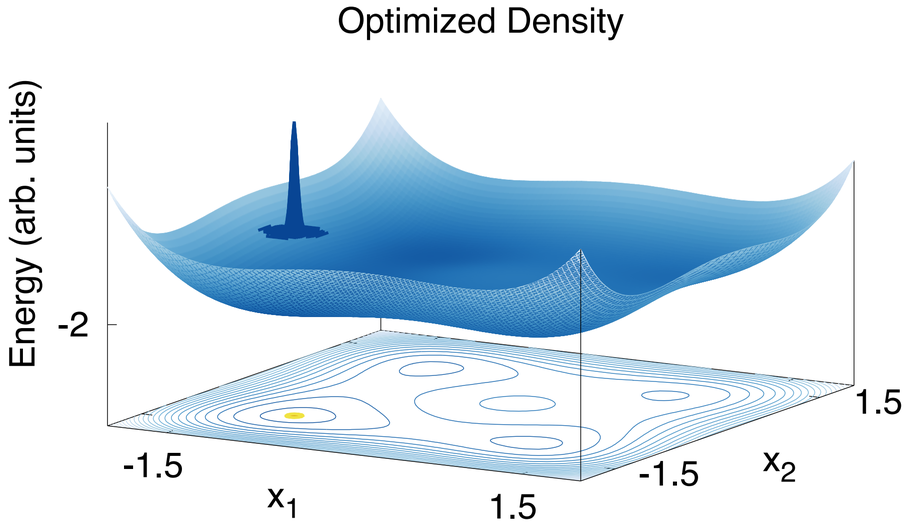


- Isolate first component $x_1^\star$ of Dirac comb with a second use of IPA using a **"ramp potential"** (*e.g.* $\text{ramp}(x) = x$)
- Multiply ρ_{final} by the Heaviside function $\Theta(x - x_1^\star)$
- Repeat process to identify the remaining components $x_i^\star$ until all global minima are resolved

MBS, P. Bergold, V. S. Batista, JCTC (2021) in press, arXiv:2101.03377.

IPA FOR HYDROGEN BOND CONFIGURATIONS





IPA successfully identifies global optimization of functions with up to 2^{50} **local minima**, beyond the capabilities of a straightforward enumeration approach.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 17 (2021) 3280.

IPA CONVERGENCE

Number of iterations required to reach optimal result with 50% certainty (á la Grover's algorithm):

$$U = \text{diag}(\lambda_2, \ldots, \lambda_2, \lambda_1, \lambda_2, \ldots, \lambda_2) \in \mathbb{R}^{n\times n}, \quad 0 < \lambda_2 < \lambda_1$$

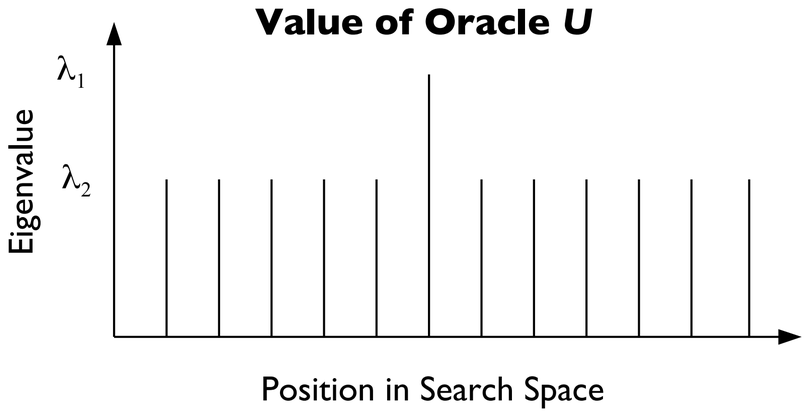
$$\rho_0 = \frac{1}{n}(1,\ldots,1) \in \mathbb{R}^n$$

$$\rho_k = \frac{\mathbf{U}^k\rho_0}{|\mathbf{U}^k\rho_0\|_1} \qquad \frac{\rho_{k,\min}}{\rho_{k,\max}} = \left(\frac{\lambda_2}{\lambda_1}\right)^k$$

$$1 = \|\rho_k\| = \rho_{k,\max} + (n-1)\rho_{k,\min}$$

$$\rho_{k,\max} = \frac{1}{1 + (n-1)\cdot(\lambda_2/\lambda_1)^k}$$

$$\frac{1}{2} \leq \frac{1}{1 + (n-1)\cdot(\lambda_2/\lambda_1)^k}$$



$$k \geq \frac{\log(n-1)}{\log(\lambda_1/\lambda_2)}$$

IPA requires fewer iterations than foremost quantum approach.

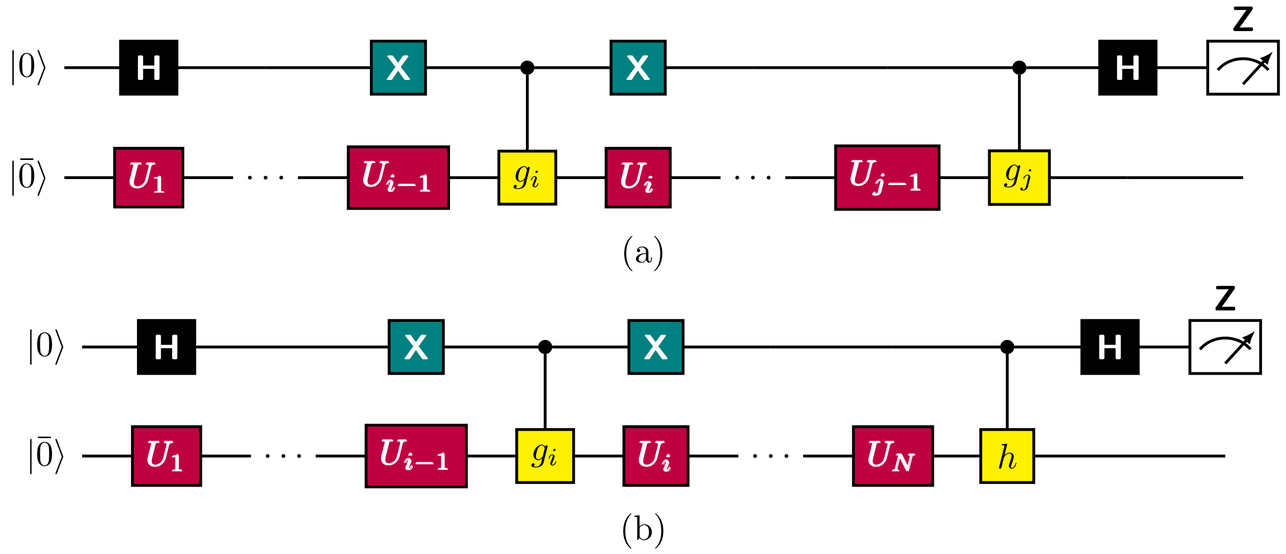
Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.

L. K. Grover, Proceedings, 28th Annual ACM Symposium on the Theory of Computing, May 1996, 212.

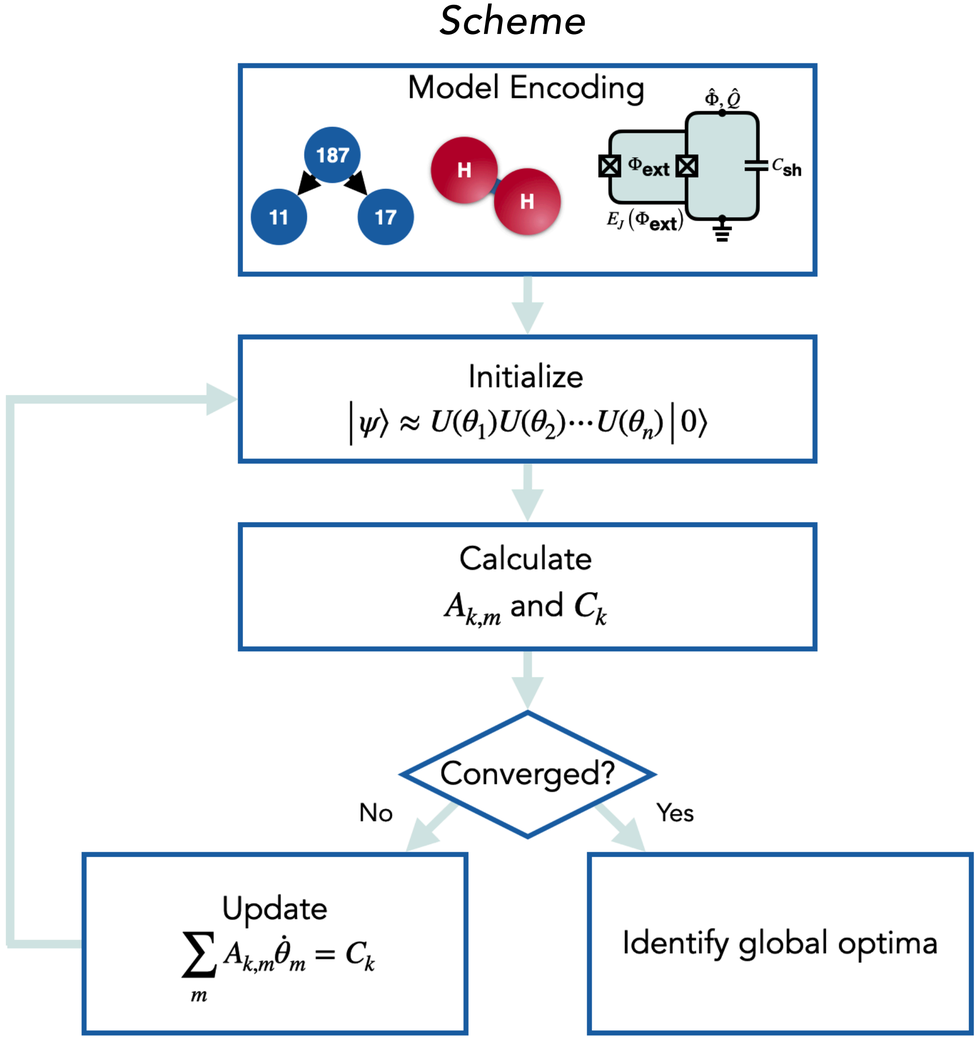
QUANTUM ITERATIVE POWER ALGORITHM (QIPA)

The McLachlan variational principle enables IPA to be also performed as a hybrid quantum-classical algorithm.

Quantum Circuits for $A_{k,m}$ and C_k



Scheme



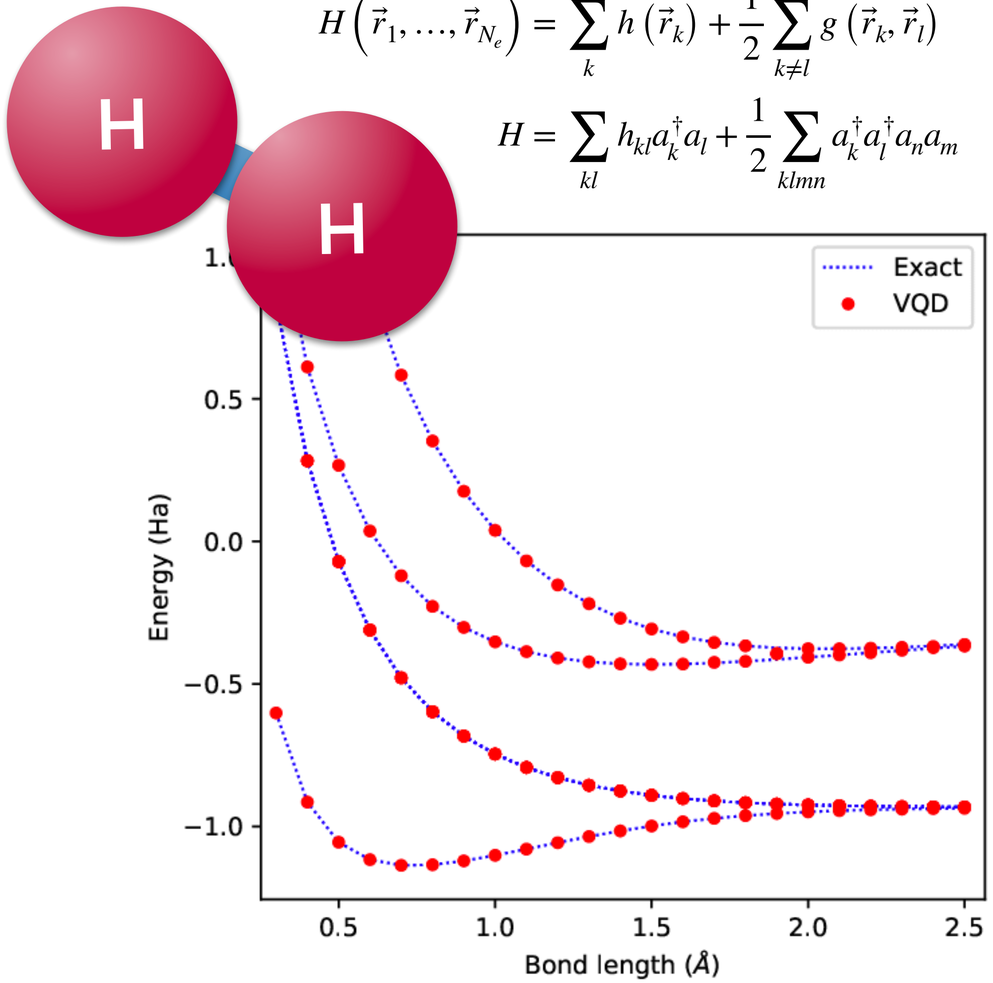
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

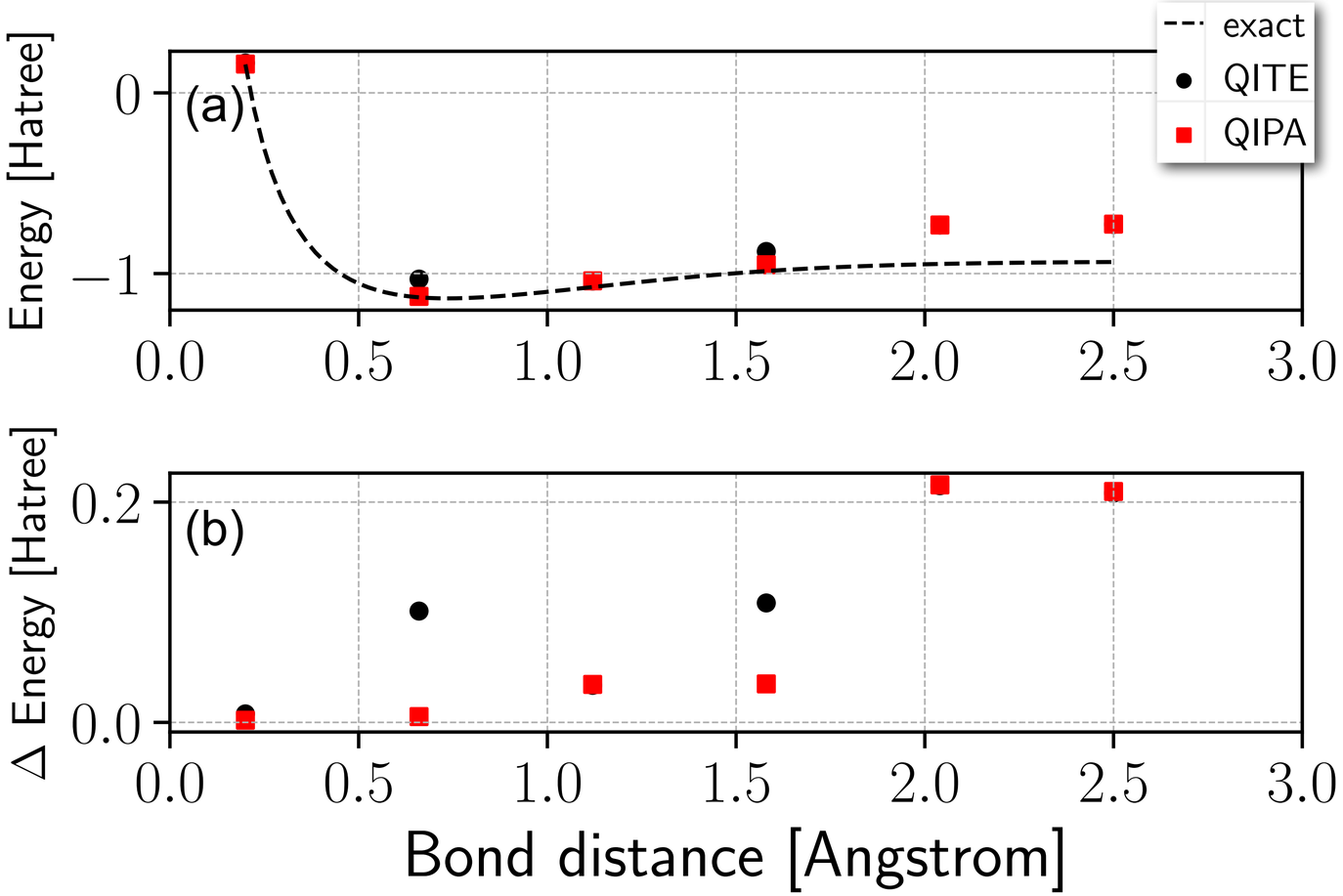
QIPA FOR ELECTRONIC STRUCTURE THEORY

QIPA **successfully** identifies the ground state energies of H_2 to high accuracy

$$H\left(\vec{r}_1,\ldots,\vec{r}_{N_e}\right)=\sum_{k}^{N_e}h\left(\vec{r}_k\right)+\frac{1}{2}\sum_{k\neq l}^{N_e}g\left(\vec{r}_k,\vec{r}_l\right)$$

$$H=\sum_{kl}h_{kl}a_k^\dagger a_l+\frac{1}{2}\sum_{klmn}a_k^\dagger a_l^\dagger a_n a_m$$

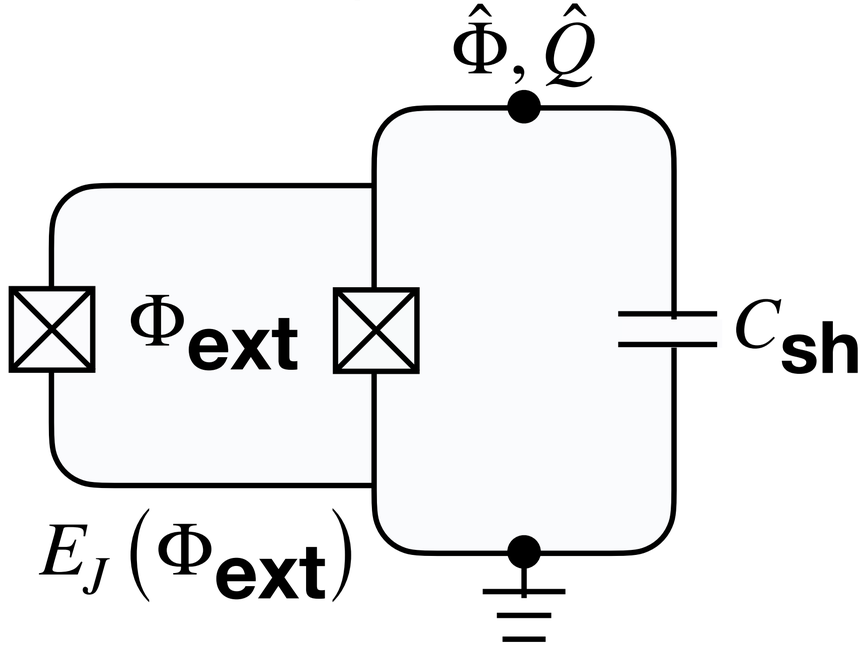




T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

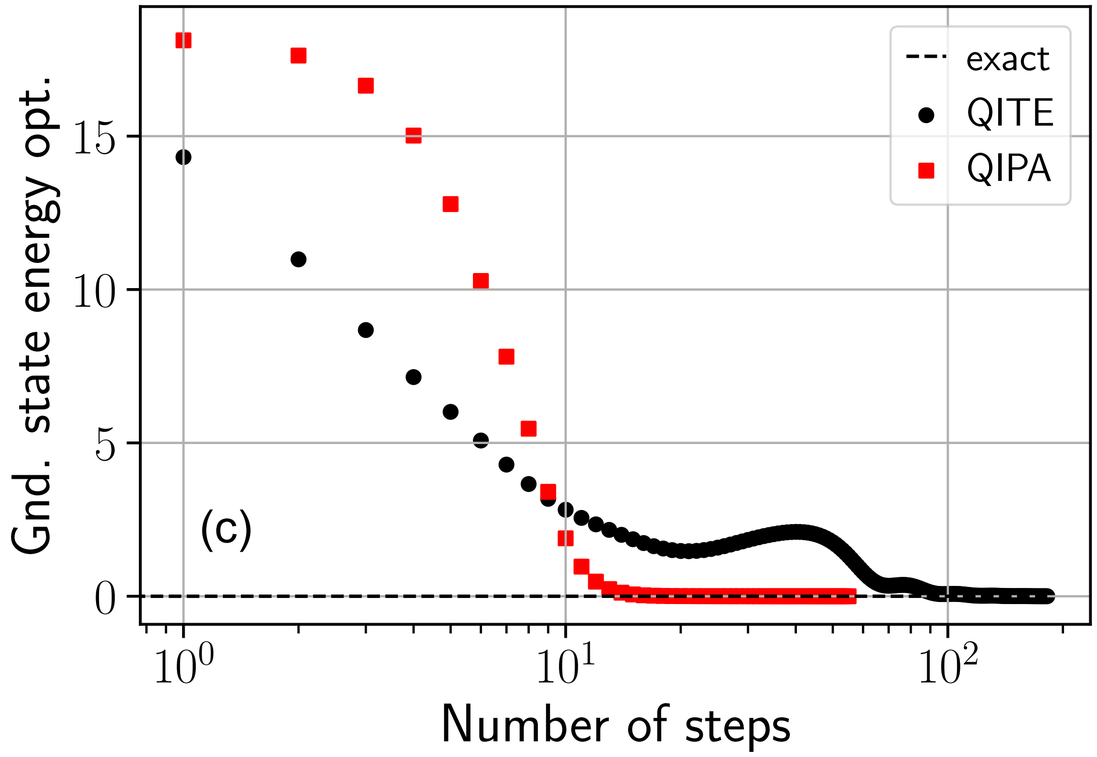
QIPA FOR QUANTUM COMPUTER DESIGN

First dynamical optimization of quantum processor design via quantum computing



$$\hat{H}_{M\text{–transmon}} = 2e^2 \sum_{i,j=1}^{M} \left(\mathbf{C}^{-1}\right)_{ij} \hat{N}_i \hat{N}_j$$

$$-2\sum_{i=1}^{M} E_{J,i} \left|\cos\left(2\pi f_i\right)\right| \cos\hat{\varphi}_i$$



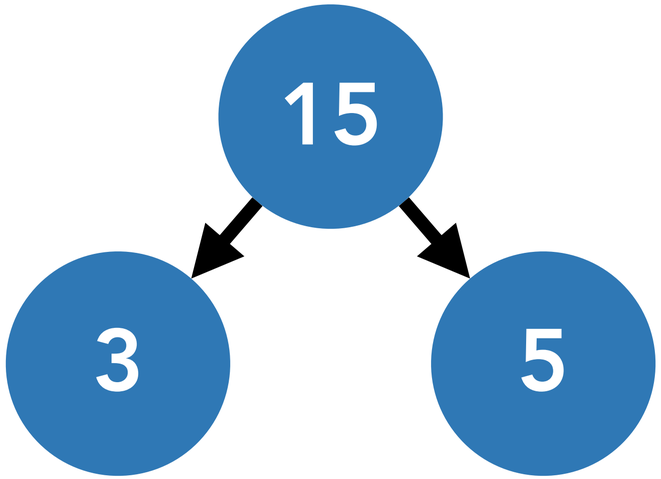
Advantage of QIPA over QITE for early steps over a broad parameter range

T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

T. H. Kyaw,* Ti. Menke,* et al. (2021) arXiv:2006.03070v3.

QIPA FOR PRIME FACTORIZATION (CYBERSECURITY)

QIPA converges **faster than QITE** for all integers factored.

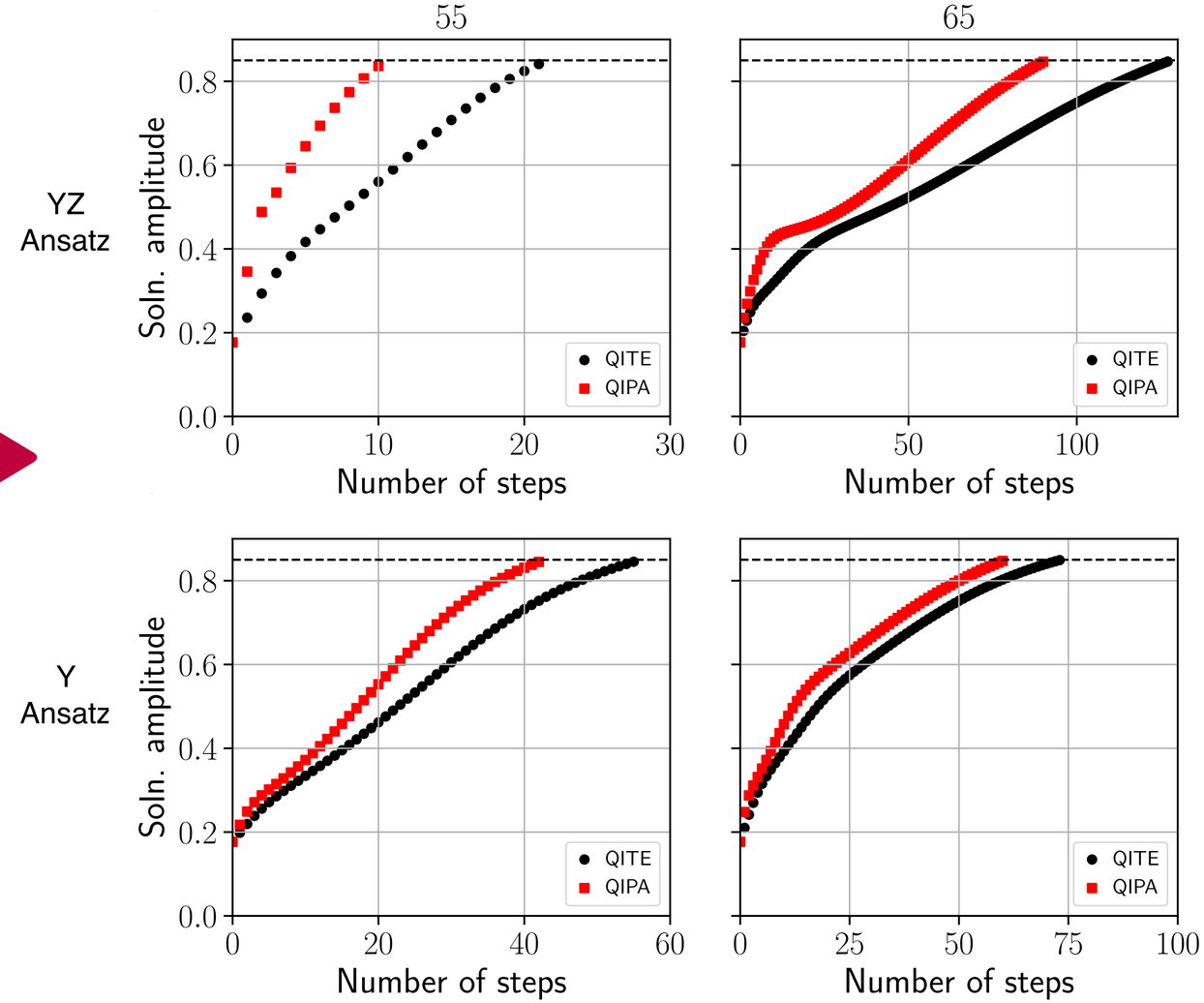


$$N = p \times q$$

$$p = H_N(q,p) = d(N;q,p)^2, \quad d(N;q,p) = N - q \times p$$

$$d\left(N,\vec{x}\right) = N - \left(1 + \sum_{j=1}^{L} x_j 2^j\right) \times \left(1 + \sum_{k=1}^{L} x_{L+k} 2^k\right)$$

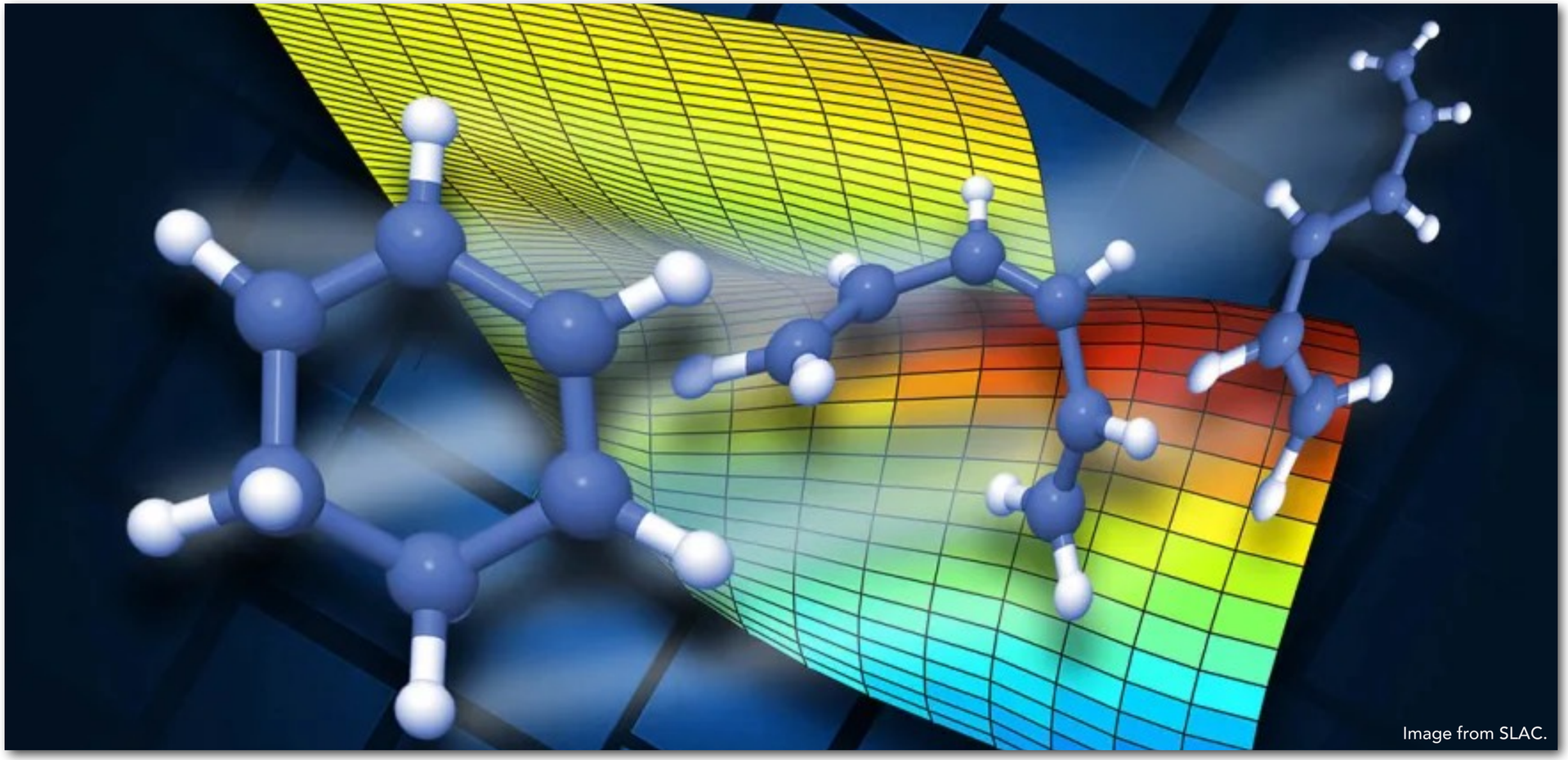
$$d\left(N;\vec{s}\right) = N - \left(2^L + \sum_{j=1}^{L} s_j 2^{j-1}\right) \times \left(2^L + \sum_{k=1}^{L} s_{L+k} 2^{k-1}\right)$$



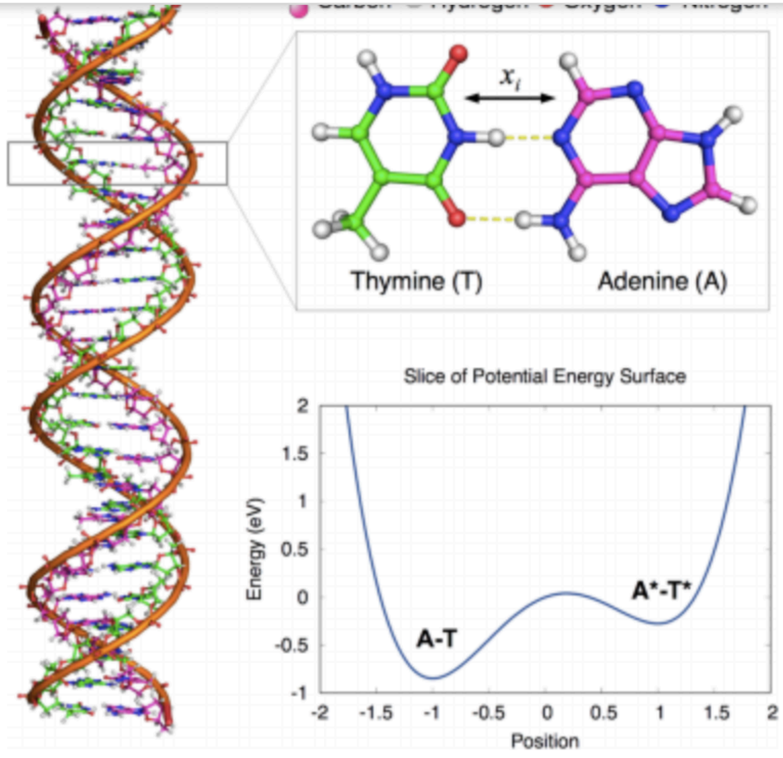
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

OUTLOOK

IPA's efficiency and ability to avoid local minima to converge deterministically to global optima makes the method well-suited to a wide range of global optimization problems in chemistry beyond reach with standard grid-based methods.



T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.
Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.



Above: DNA chain (left) of D = 50 hydrogen bonds corresponding to 25 hydrogen-bonded adenine–thymine base pairs (inset, top right), with hydrogen bonds shown as dashed yellow lines. Each hydrogen bonded proton attaches to either base, with energy represented by the double-well potential (bottom right).

```
[ ]  beta=10
     dim=2
     eps=1.0e-14
```

ACKNOWLEDGEMENTS

University of Wisconsin-Madison Office of the Vice Chancellor for Research and Graduate Education

BLUE WATERS

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NERSC

YQI Postdoctoral Fellowship

Y|CRC

Yale High Performance Computing Center

Harvard GSAS Merit/Graduate Society Fellowship