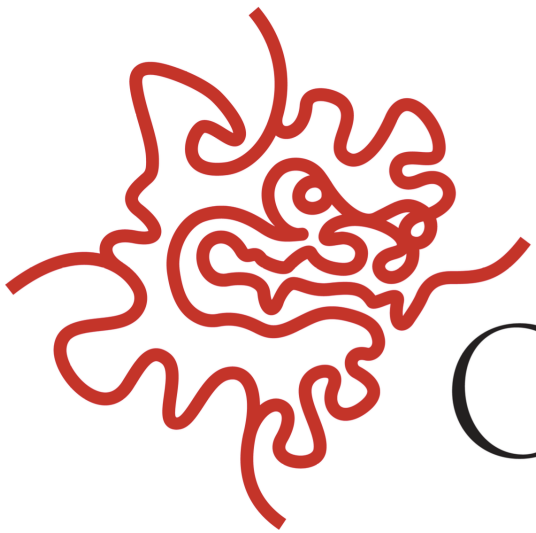
Massively parallel split-step Fourier techniques for simulating quantum systems on graphics processing units

James Schloss

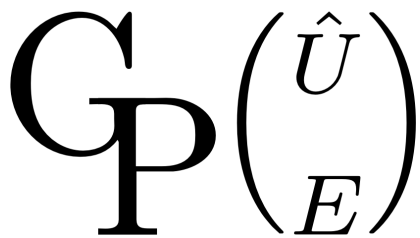
Advisor: **Thomas Busch**
Quantum Systems Unit

December 9, 2019



Overview

This project has created fast, GPU-accelerated software for the simulation of superfluid systems



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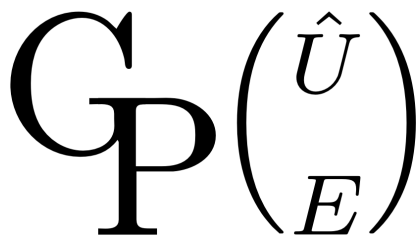

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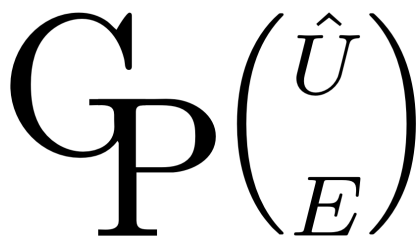

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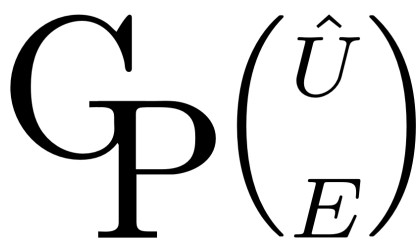

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$$\mathrm{GP}\begin{pmatrix}\hat{U}\\ E\end{pmatrix}$$

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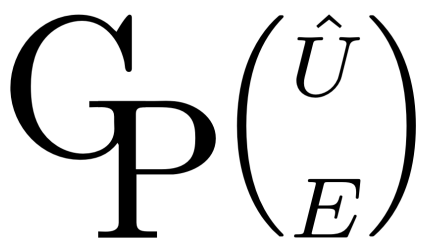
- Vortex rings with artificial magnetic fields
- Conclusions and future directions



The split-step Fourier method

algorithm-archive.org

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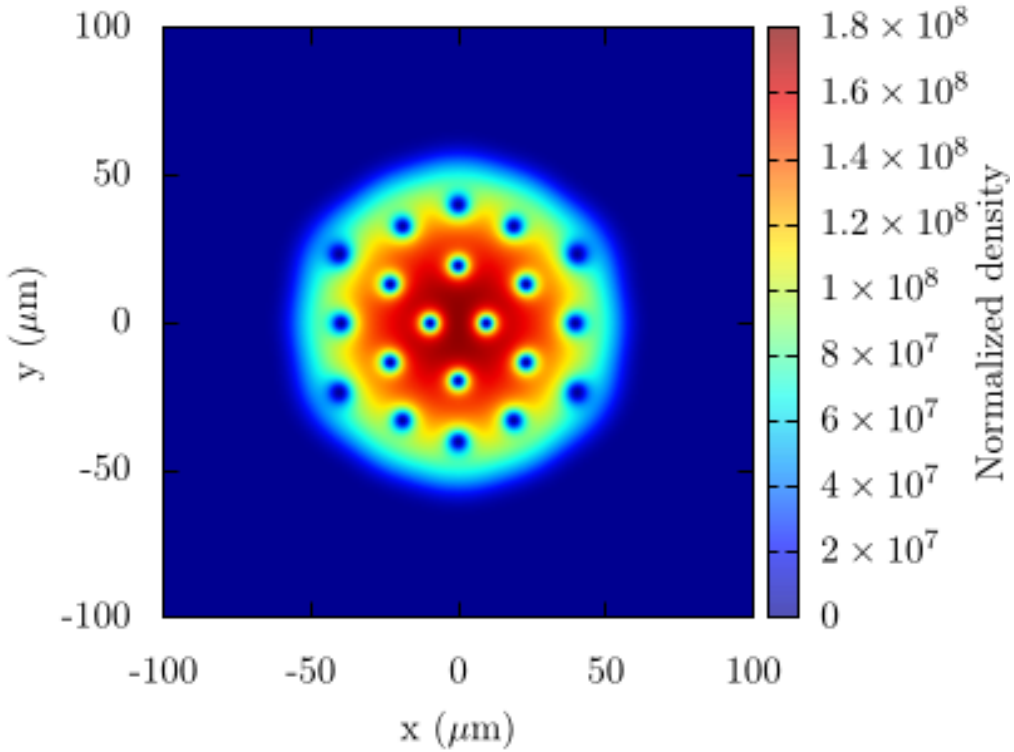

I'll show you how to make this

The Fourier Transform

Fourier Transform:

$$F(\xi) = \int_{-\infty}^{\infty} f(t) e^{-2\pi i t \xi} dt$$

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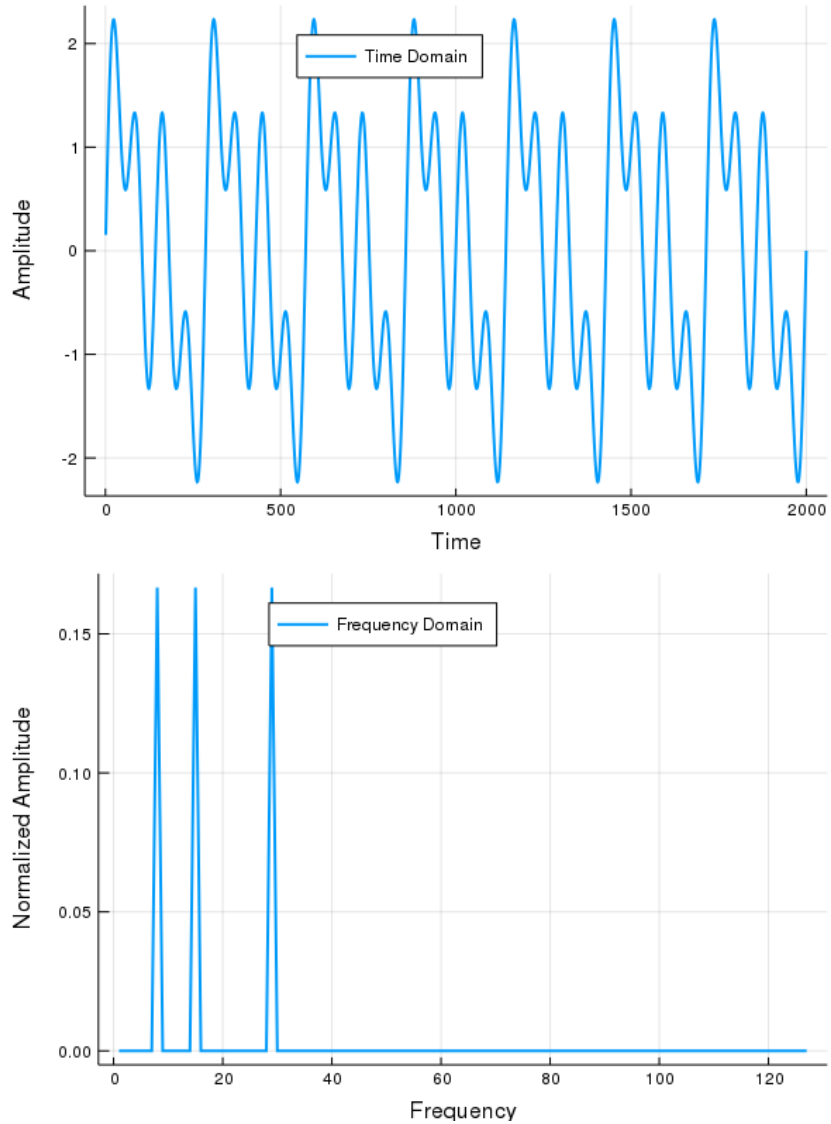

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$$X_k = \sum_{n=0}^{N-1} x_n e^{2\pi i k n / N}$$

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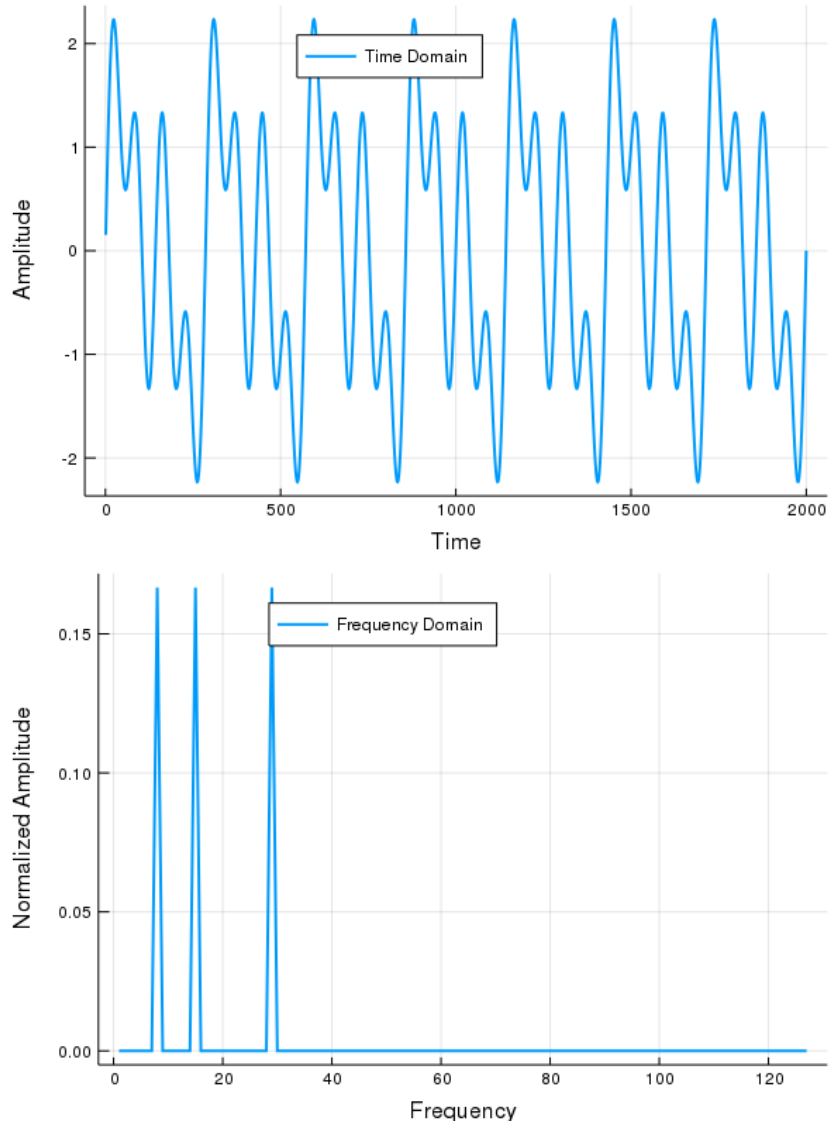

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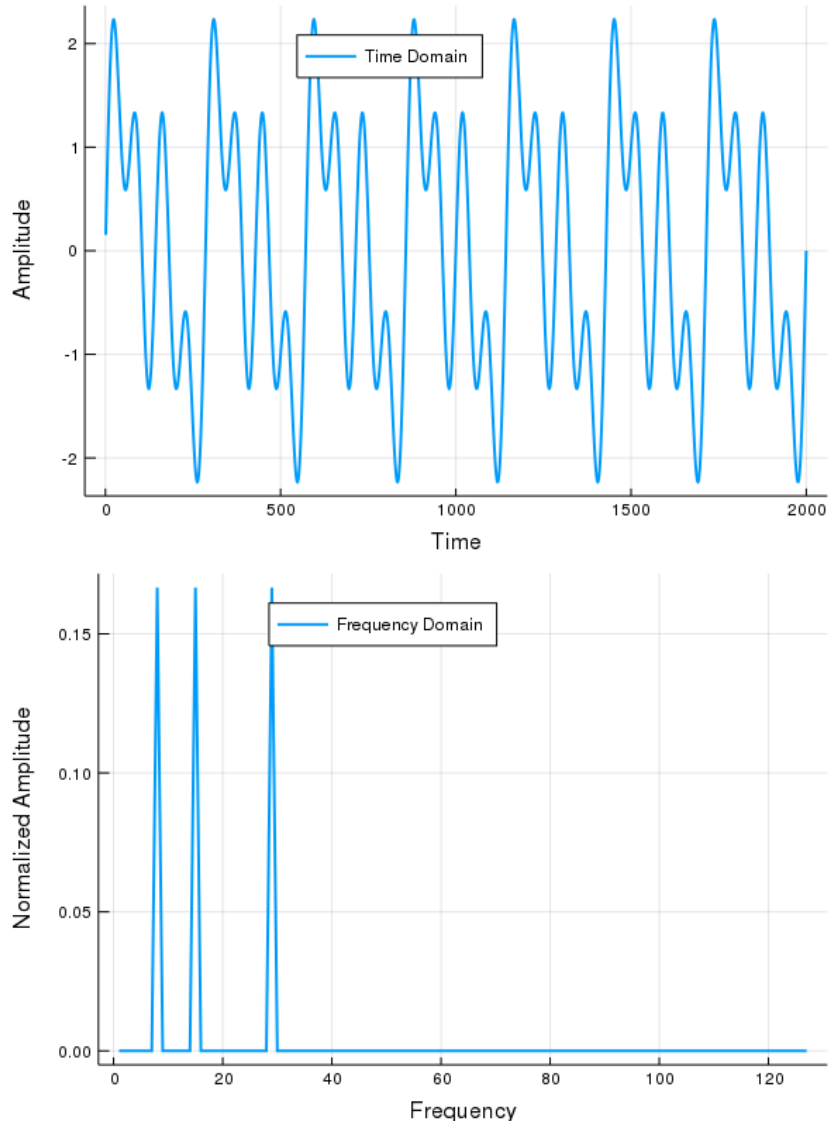
This is a *global* operation requiring matrix multiplications
$\rightarrow$ FFT



Hamiltonian

1D Schrödinger equation:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left(\frac{p^2}{2m} + V_0(x)\right)\Psi(x,t) = \mathcal{H}\Psi(x,t)$$

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Splits into:

$$\mathcal{H}_v = V_0(x) = \frac{1}{2}m\omega^2x^2$$

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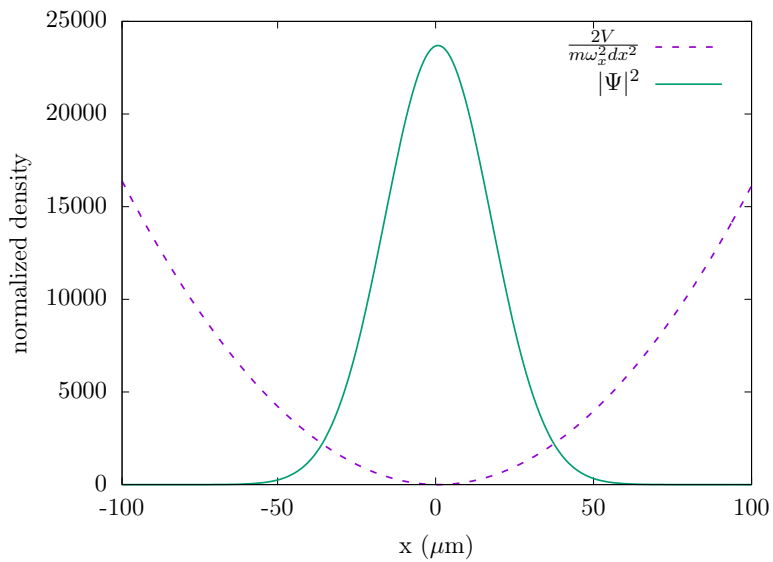

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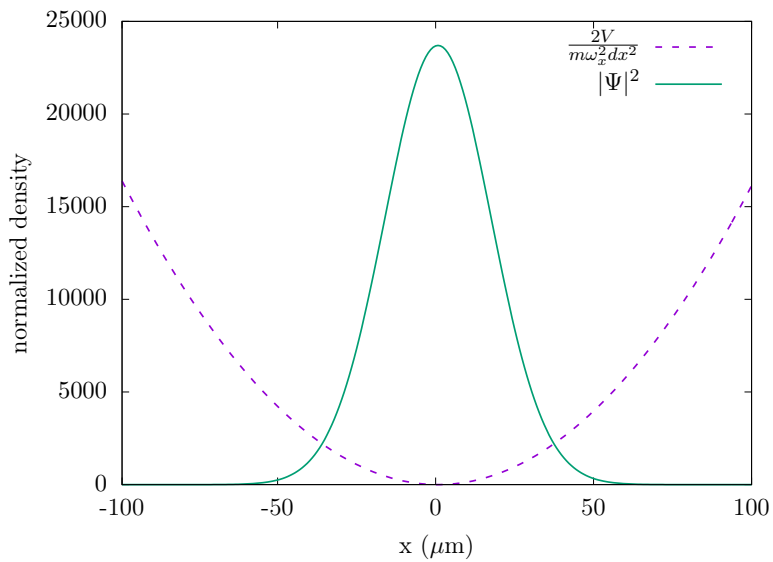


Matrices:

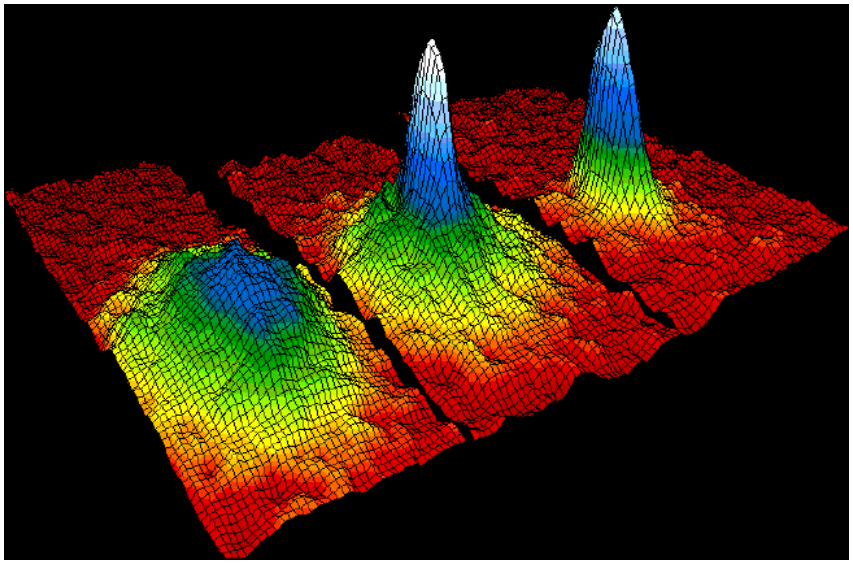
$$U_v = e^{-\frac{i\mathcal{H}_V dt}{\hbar}}$$

$$U_p = e^{-\frac{i\mathcal{H}_p dt}{\hbar}}$$

$$\Psi(\mathbf{r}, t+dt) = \mathcal{F}^{-1}\left[U_v(dt)\mathcal{F}\left[U_r(dt)\Psi(x,t)\right]\right] + \mathcal{O}(dt^2)$$

Bose-Einstein condensation

Bosons condense into a superfluid at roughly 0 Kelvin



NIST/JILA/CU-Boulder

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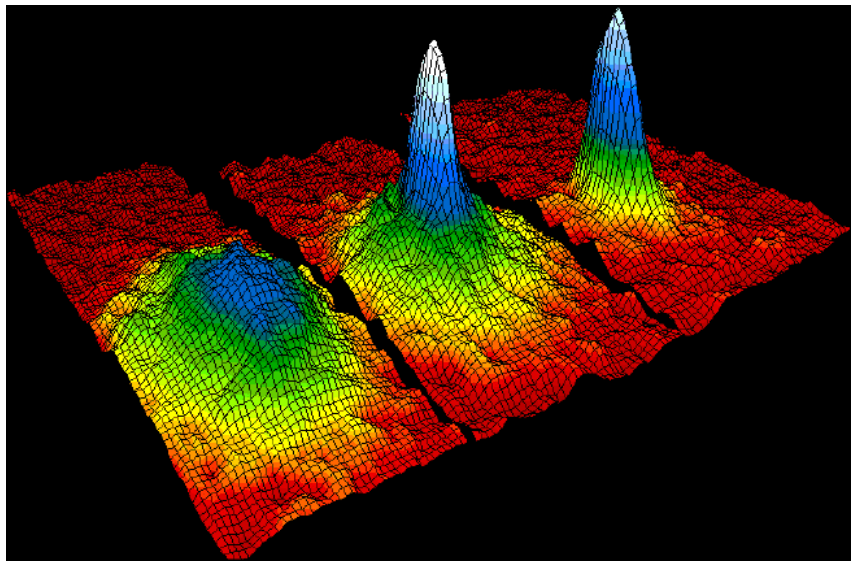


NIST/JILA/CU-Boulder

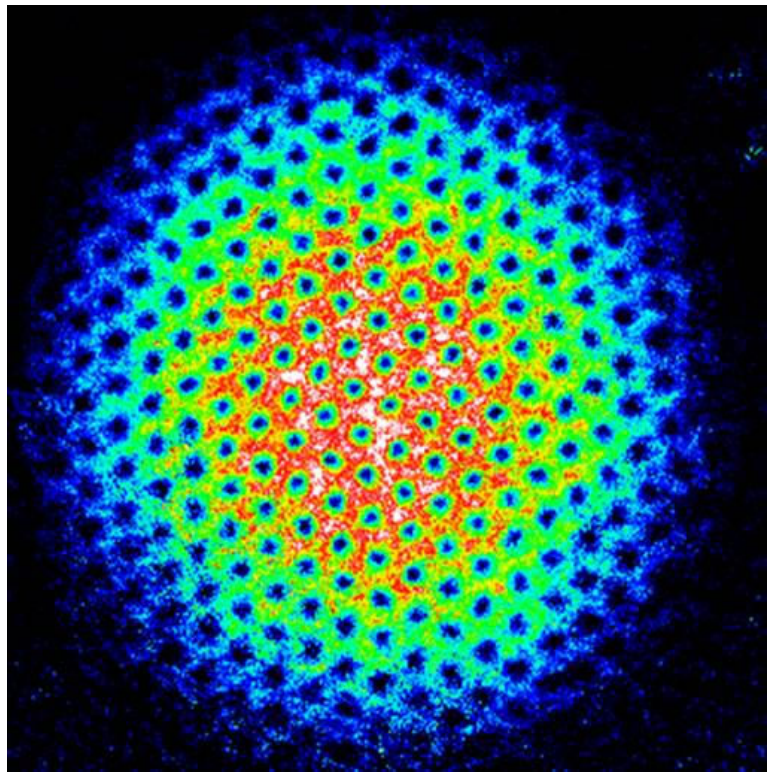
Described by the Gross–Pitaevskii equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2\right)\Psi(\mathbf{r},t)$$

Superfluid rotation

Rotation leads to many vortices along the axis of rotation

Credit: howstuffworks.com



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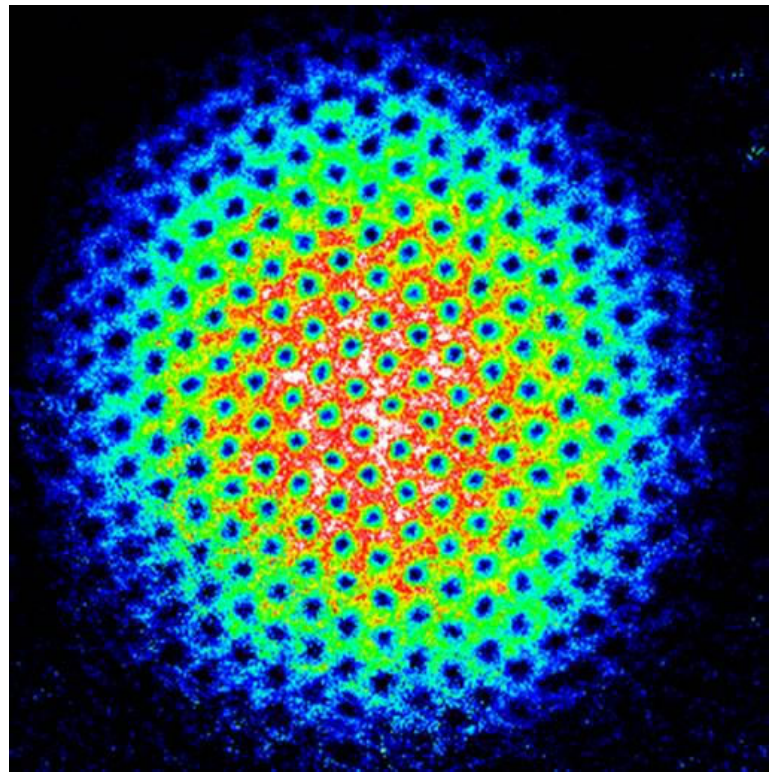
$\longrightarrow$



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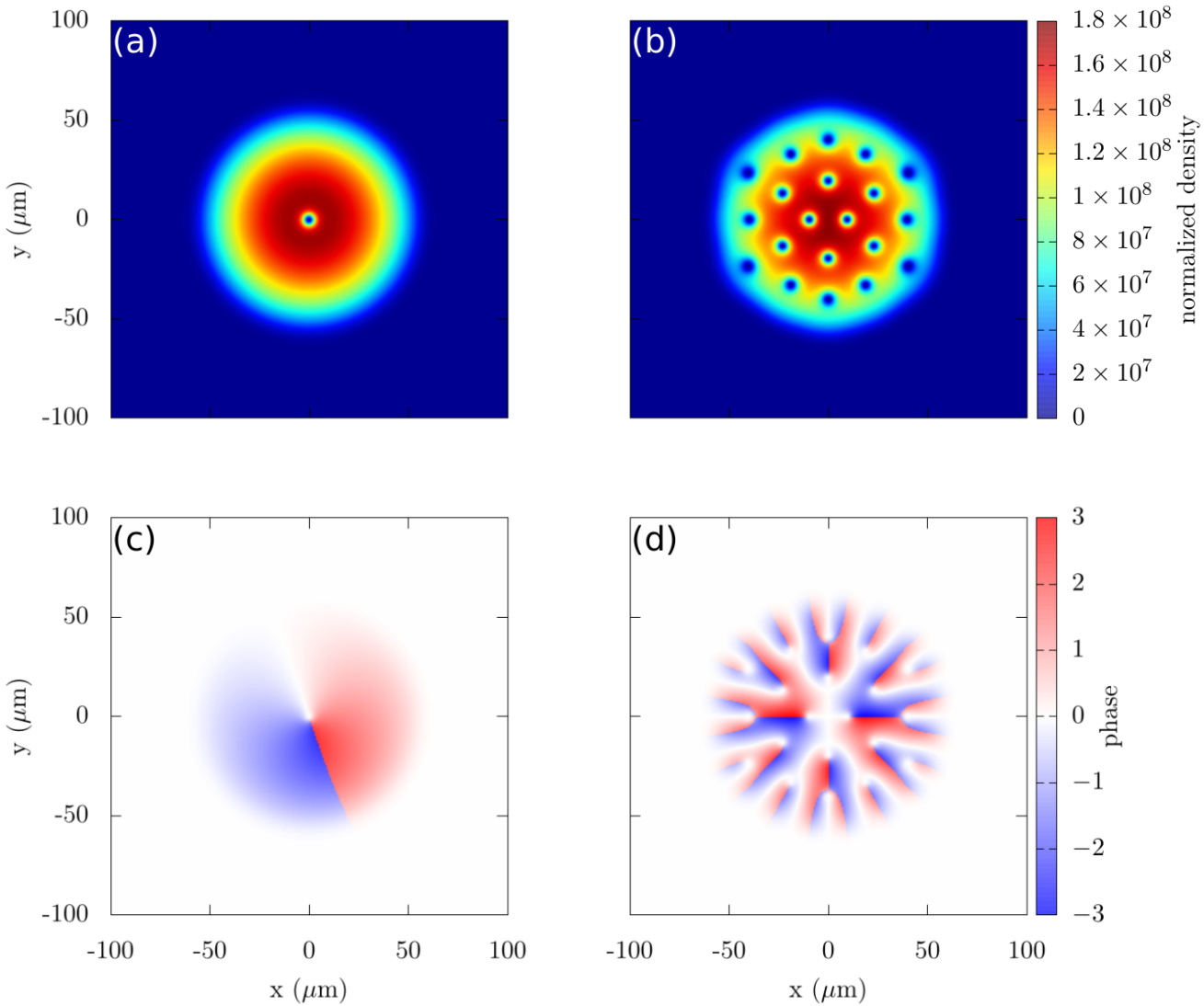
$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2 - \Omega L_z\right)\Psi(\mathbf{r},t)$$

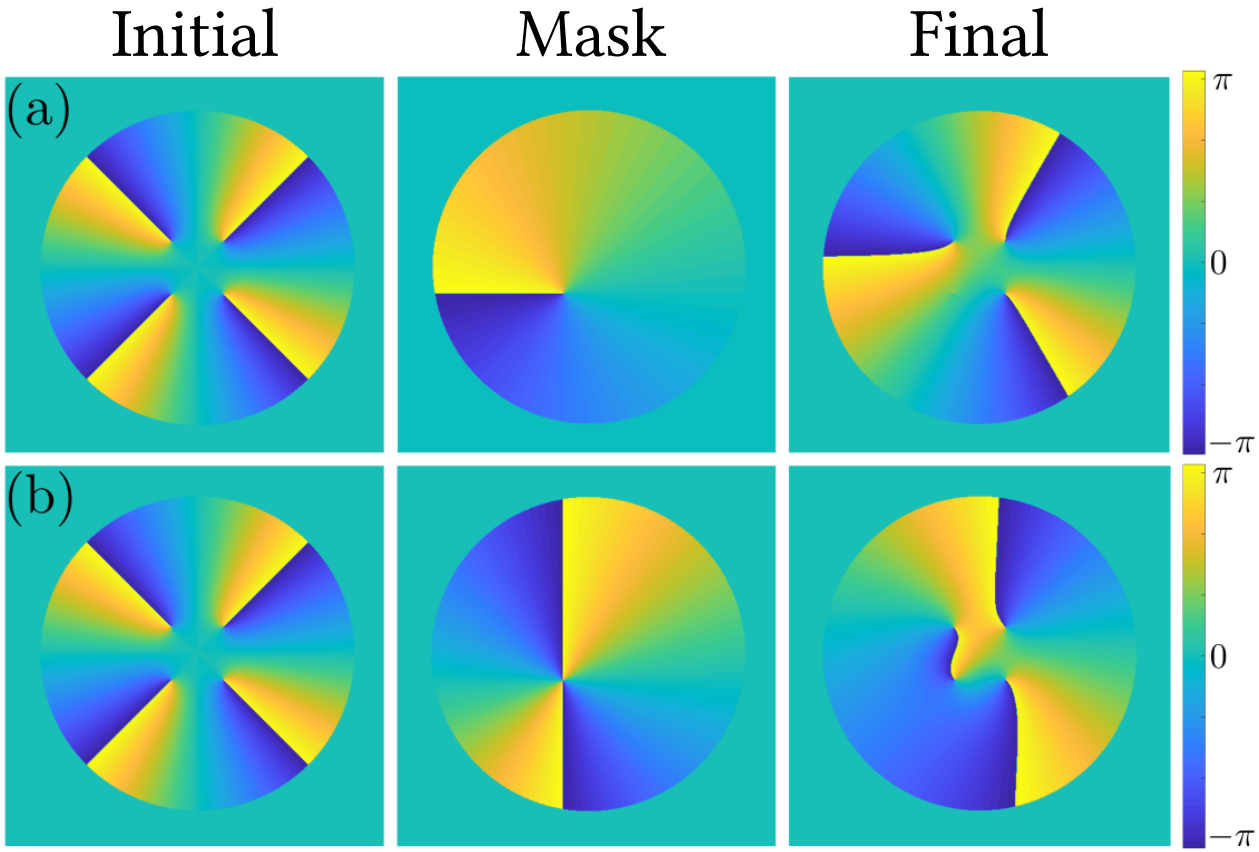
$$L_z = (xp_y - yp_x) = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

Superfluid vortex phase



Each vortex has a 2π complex phase winding

Phase imprinting



Phase masks can induce dynamical vortices

Artificial magnetic fields

Magnetic fields cause rotation in *charged* particles

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- If a two-level atom moves slowly in a tuned light field, *Berry's connection* is

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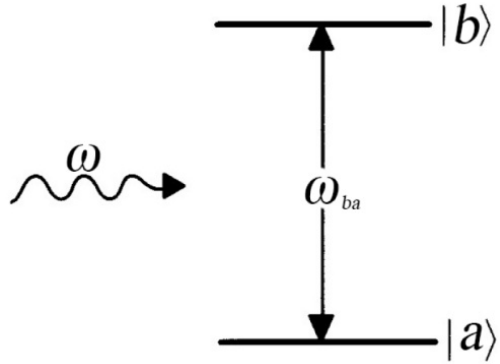
- The magnetic field is

$$\mathbf{B} = \nabla \times \mathbf{A}$$



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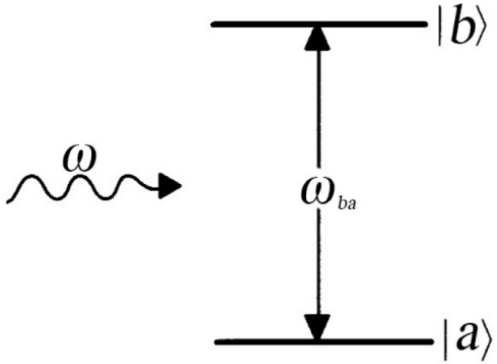

- Vortices follow the magnetic field lines

Modifications to the GPE

With gauge fields, the GPE becomes

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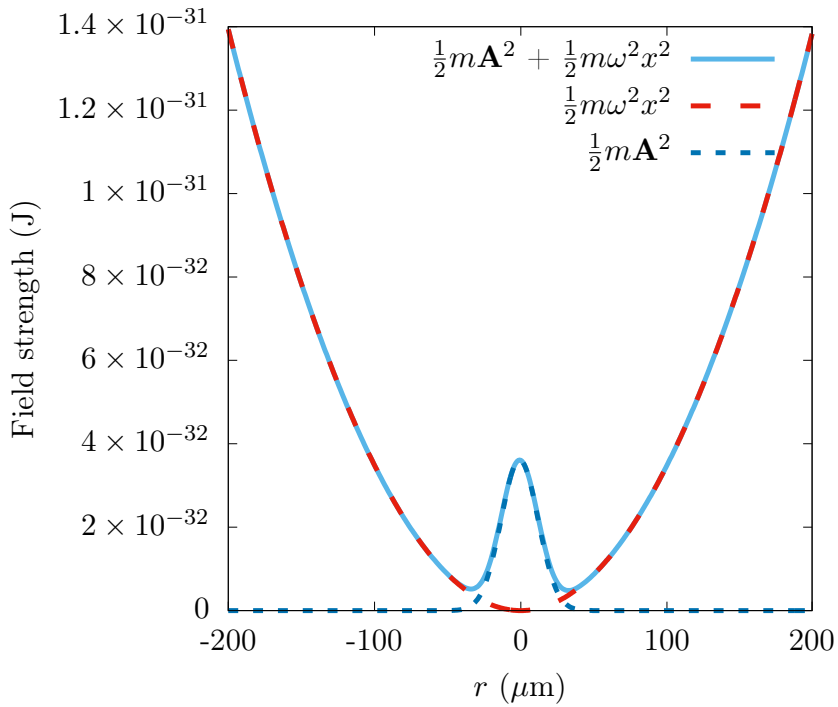

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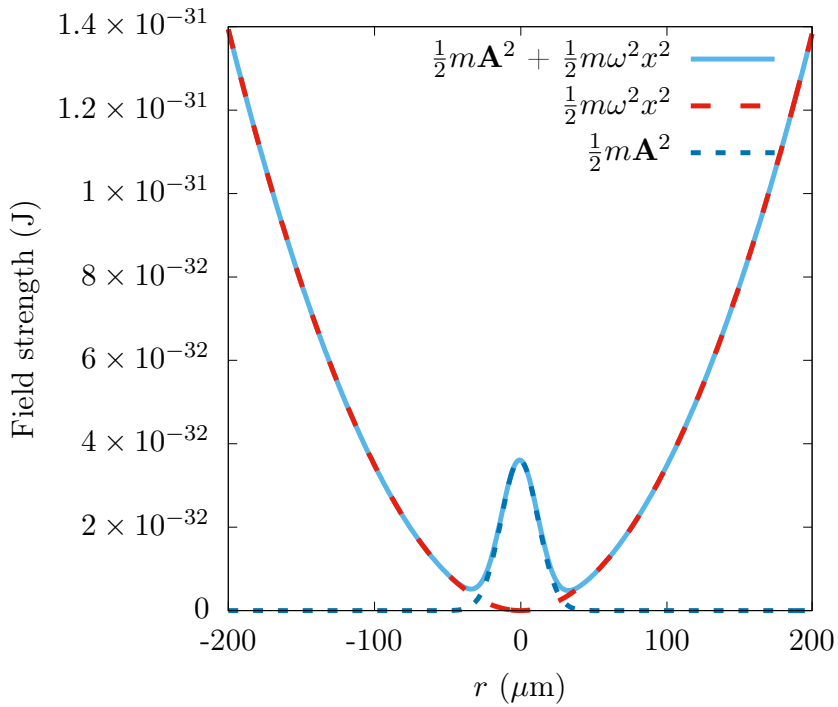
- Components in position and momentum-space, that **require 1D FFT's**

$$-\left(\frac{p\mathbf{A} + \mathbf{A}p}{2}\right)$$



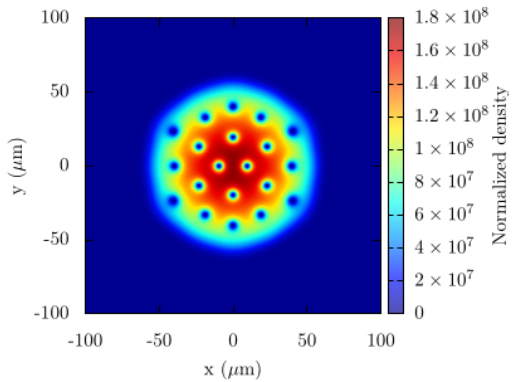
Takeaways

Physics

- Quantized vortices can be formed with rotation, phase imprinting, and artificial magnetic fields
- Quantum state engineering can be used (New Journal of Physics 18 (3), 035012)

Computer Science

- The SSFM requires a large number of FFT's
- This system is a great for testing spectral methods



GPU computing and the GPUE codebase

GPUE: Graphics Processing Unit Gross–Pitaevskii Equation solver
J Schloss, LJ O'Riordan

Journal of Open Source Software 3 (32), 1037

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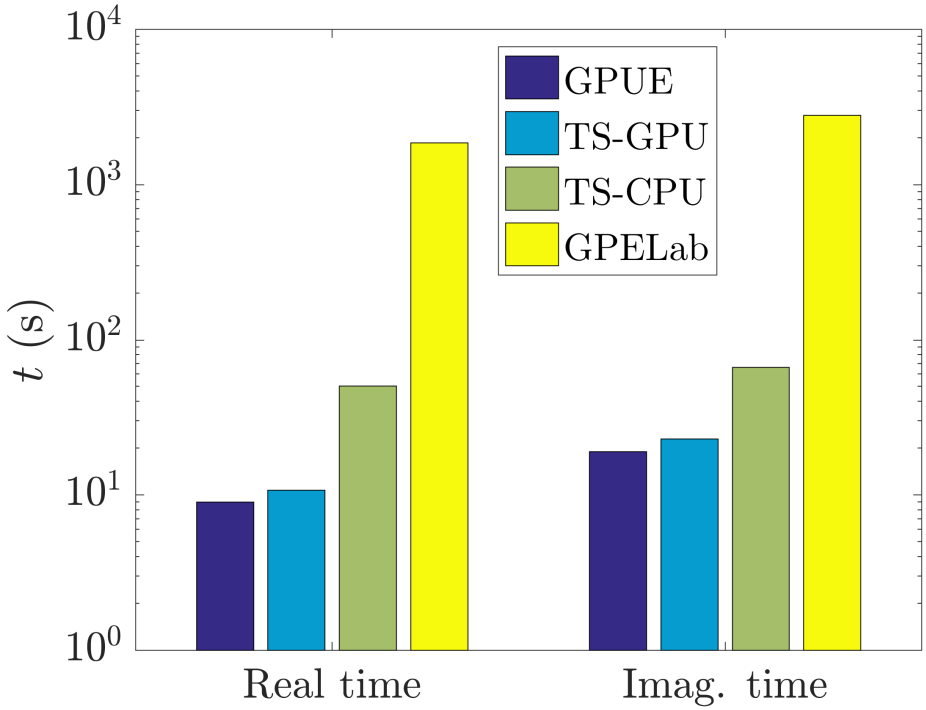

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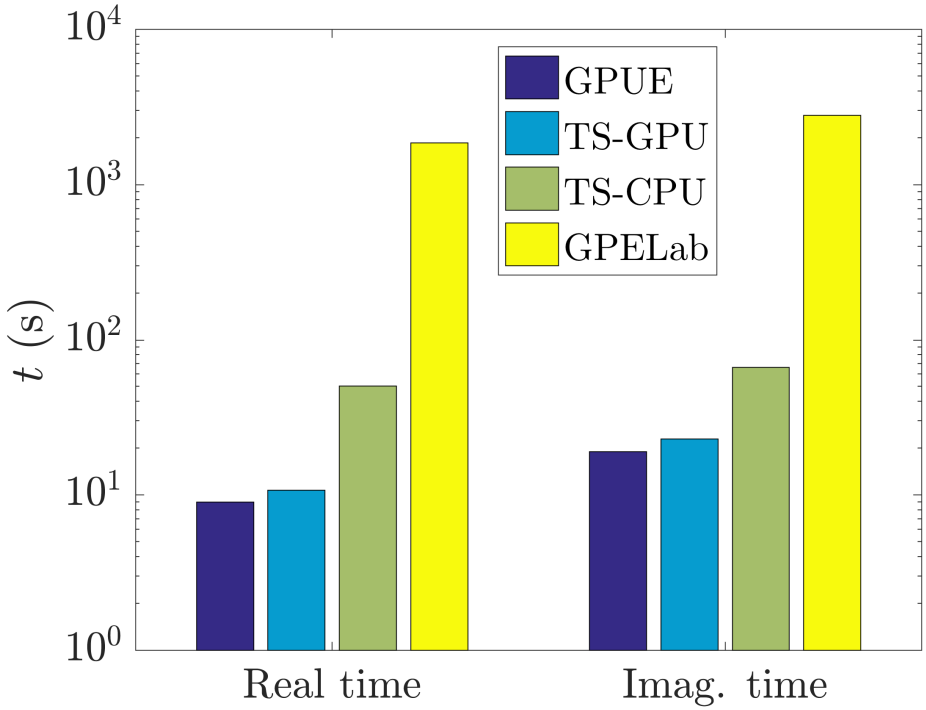
- Summit uses GPUs



GPU memory hierarchy

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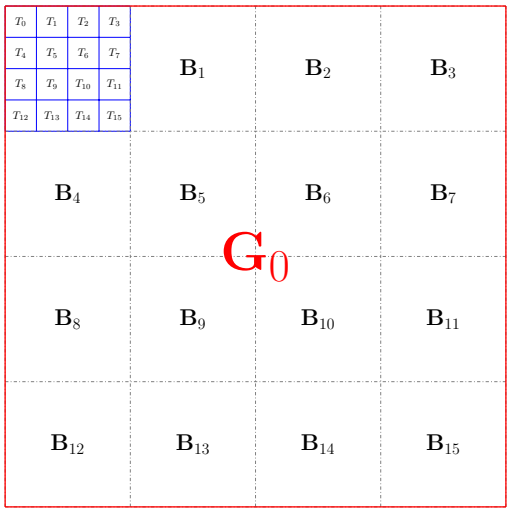
- Computing threads in blocks, blocks in grids



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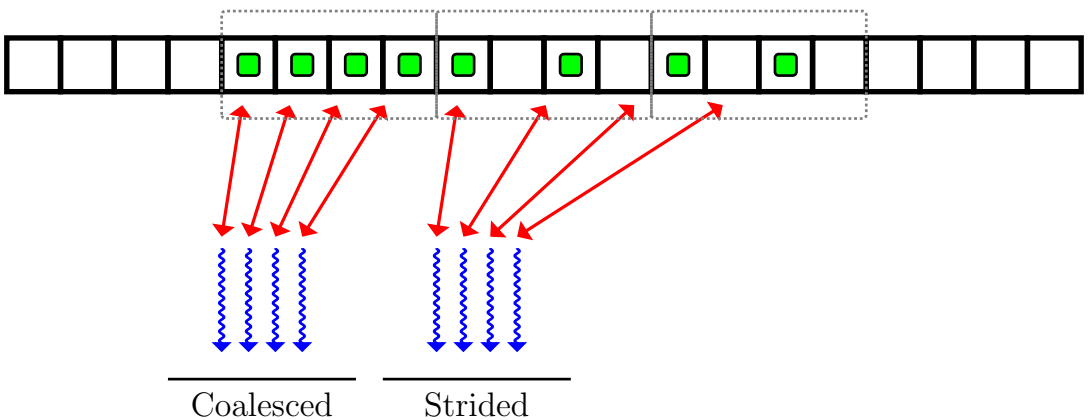

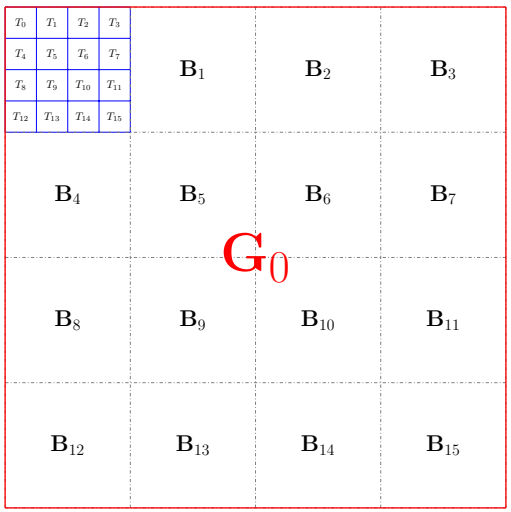

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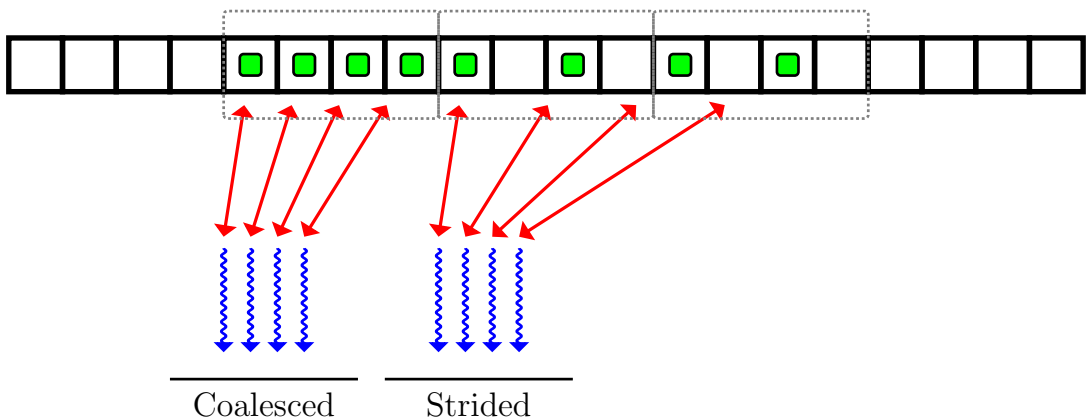
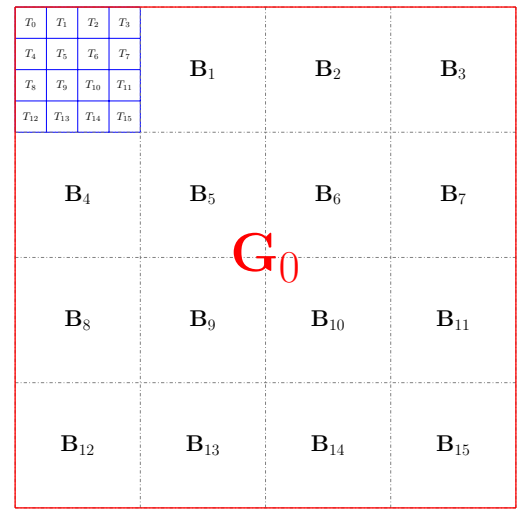
- Data transfer is slow





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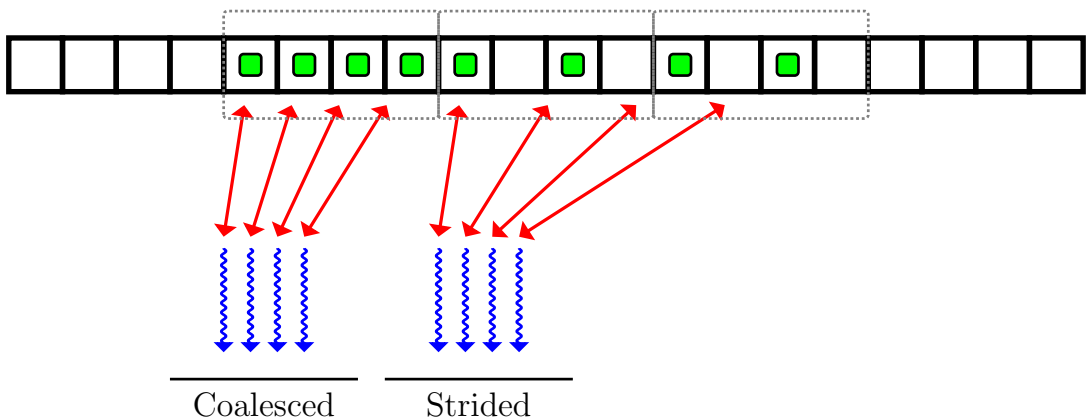
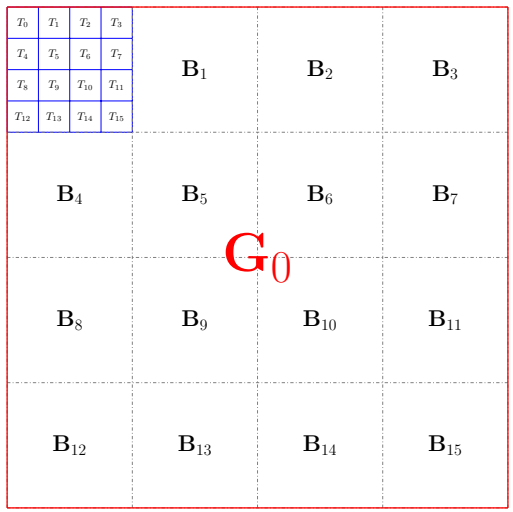
- Recursion and iteration is slow





GPU memory hierarchy

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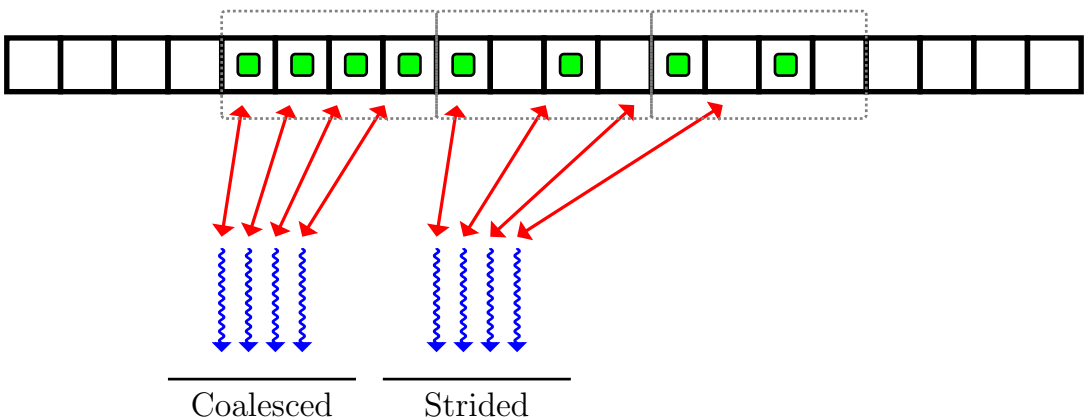
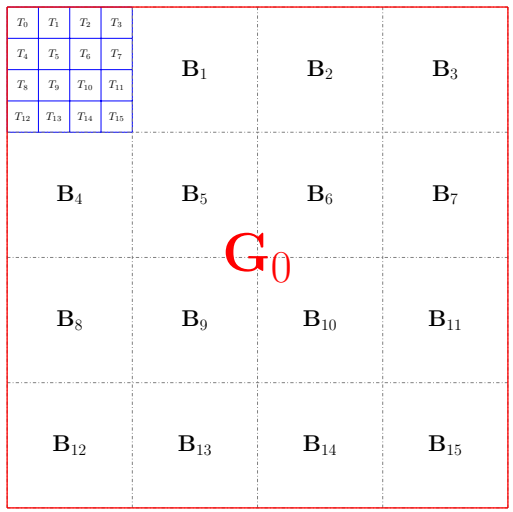
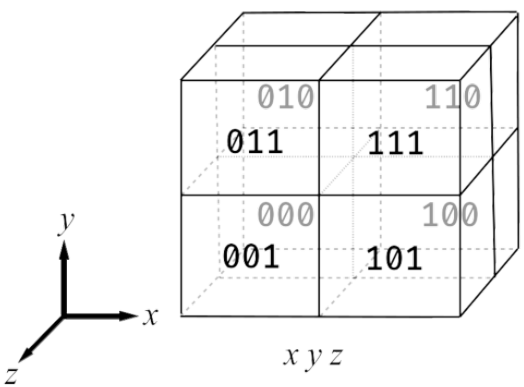
- Data transfer is slow
- Recursion and iteration is slow
- Limited memory

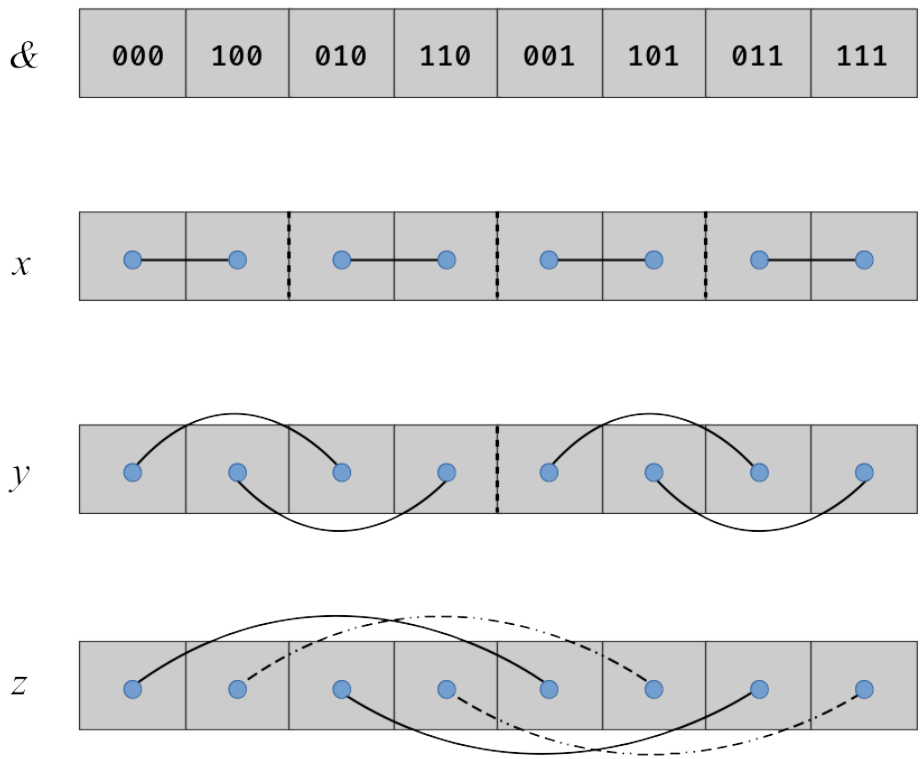




FFT notes

- Global operations
- 1D FFT's are not supported by CuFFT
- Transposes are necessary





Distributed transpose

GPU transpose

- 2D out-of-place transpose $\approx$ copy
  (shared memory, coalescence, bank conflicts)
- In-place transposes are inefficient
- 3D permutations of arrays have 70% efficiency

Distributed transpose

GPU transpose

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- In-place transposes are inefficient
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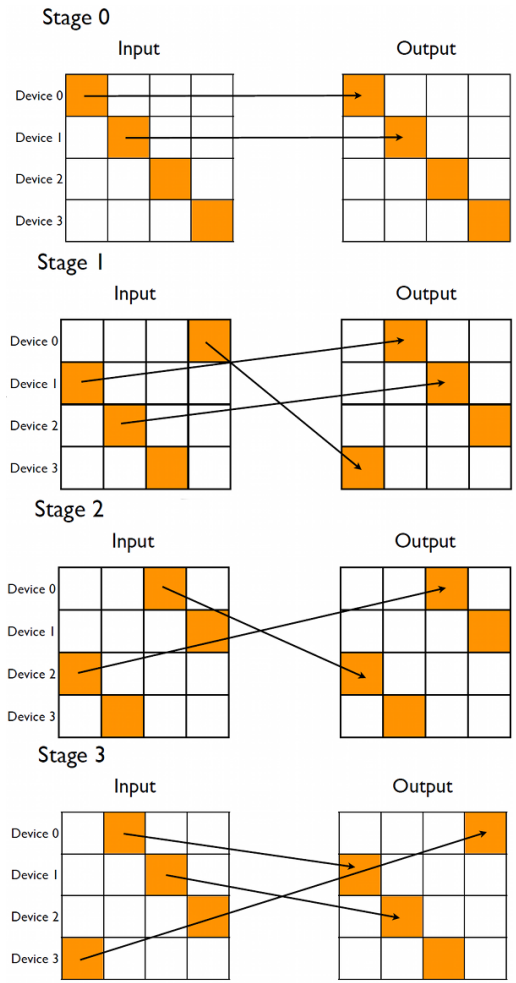
- 2D distributed example



Ruetsch, G. and Fatica, M. 2013

Distributed transpose

GPU transpose

- 2D out-of-place transpose $\approx$ copy
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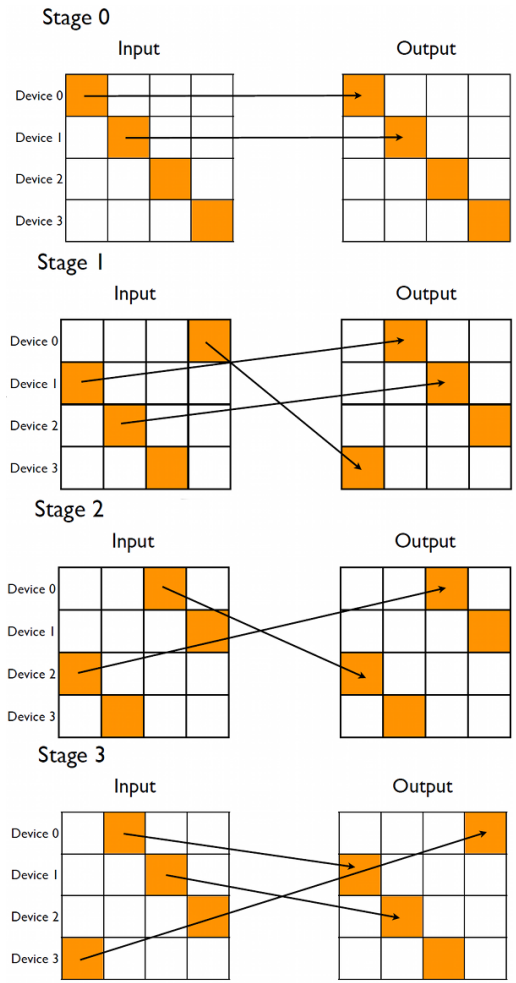
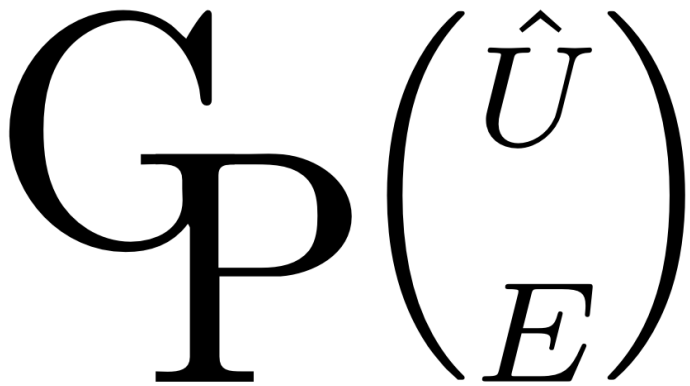
Application in GPUE and CLIMA



Ruetsch, G. and Fatica, M. 2013

Two important features



- Novel features useful for understanding examples
- No discussion of implementation details

Expression trees

Reminders:

- CUDA code is hard to write
- Users want time-dependent fields for state engineering
- GPUs have limited memory

Expression trees

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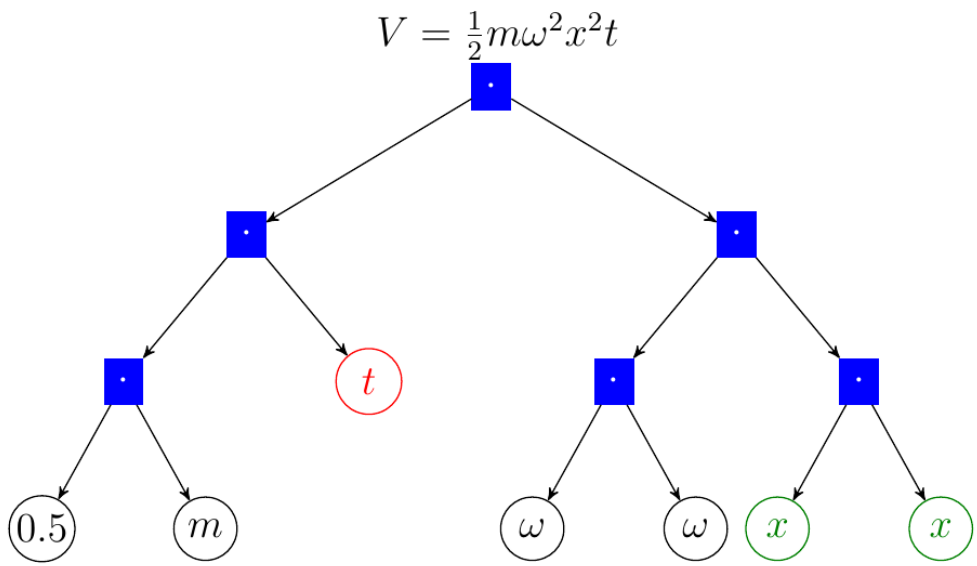
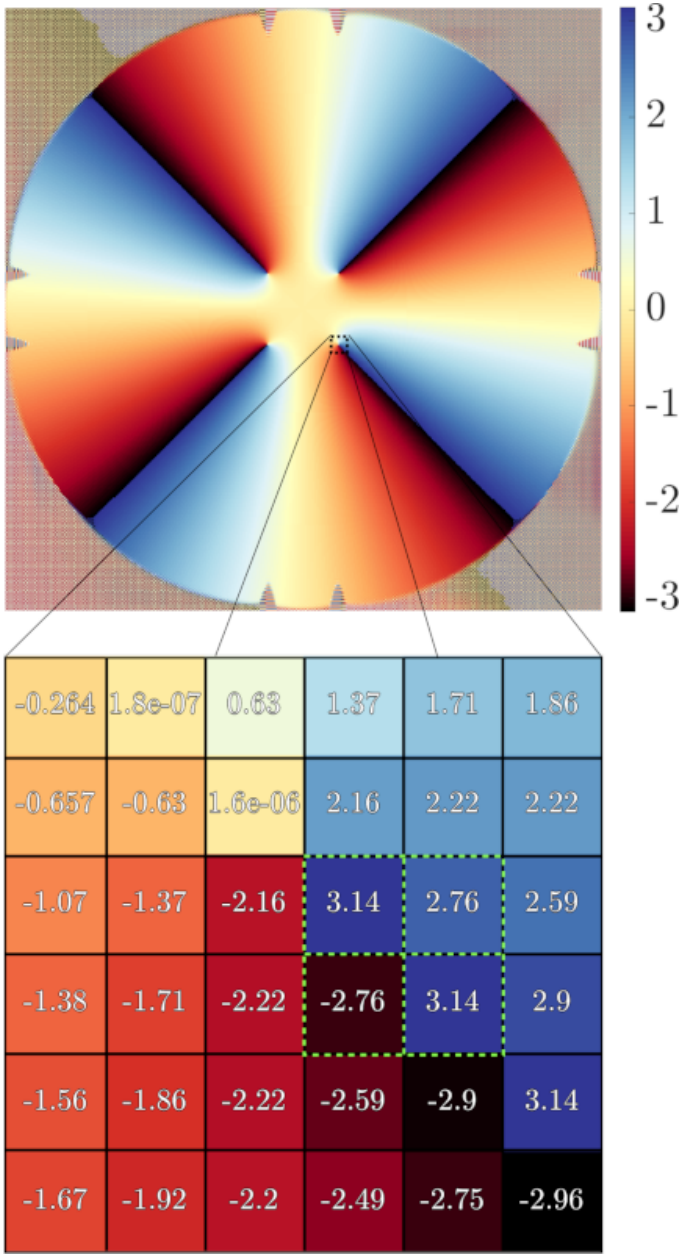


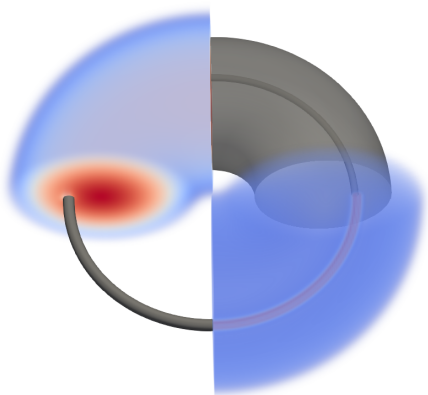
Vortex tracking and highlighting

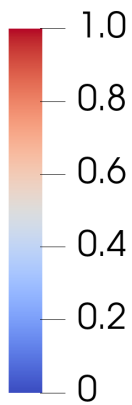
- Phase plaquettes in 2D

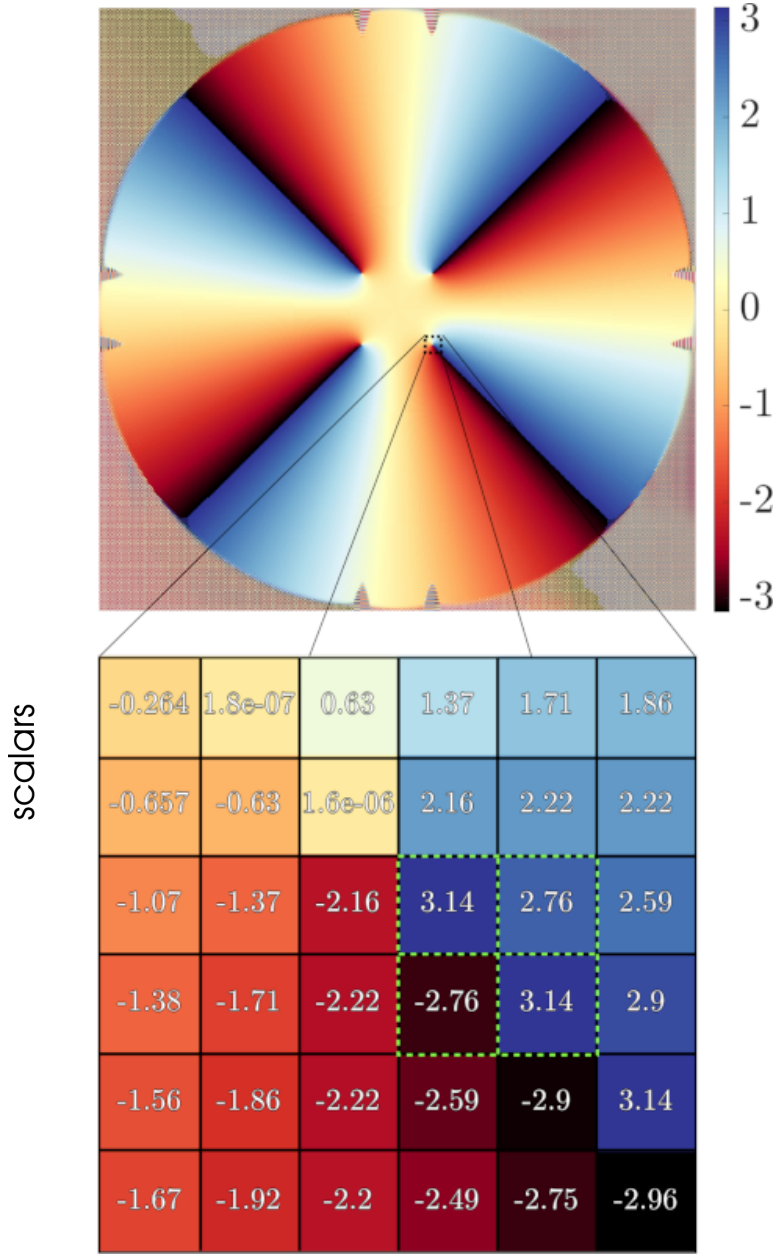


Vortex tracking and highlighting

- Phase plaquettes in 2D
- Vortex highlighting in 3D







Takeaways

Physics

- GPUE is fast, can do dynamic simulations, and vortex detection
- Multi-component simulations and HDF5 have also been implemented

Computer Science

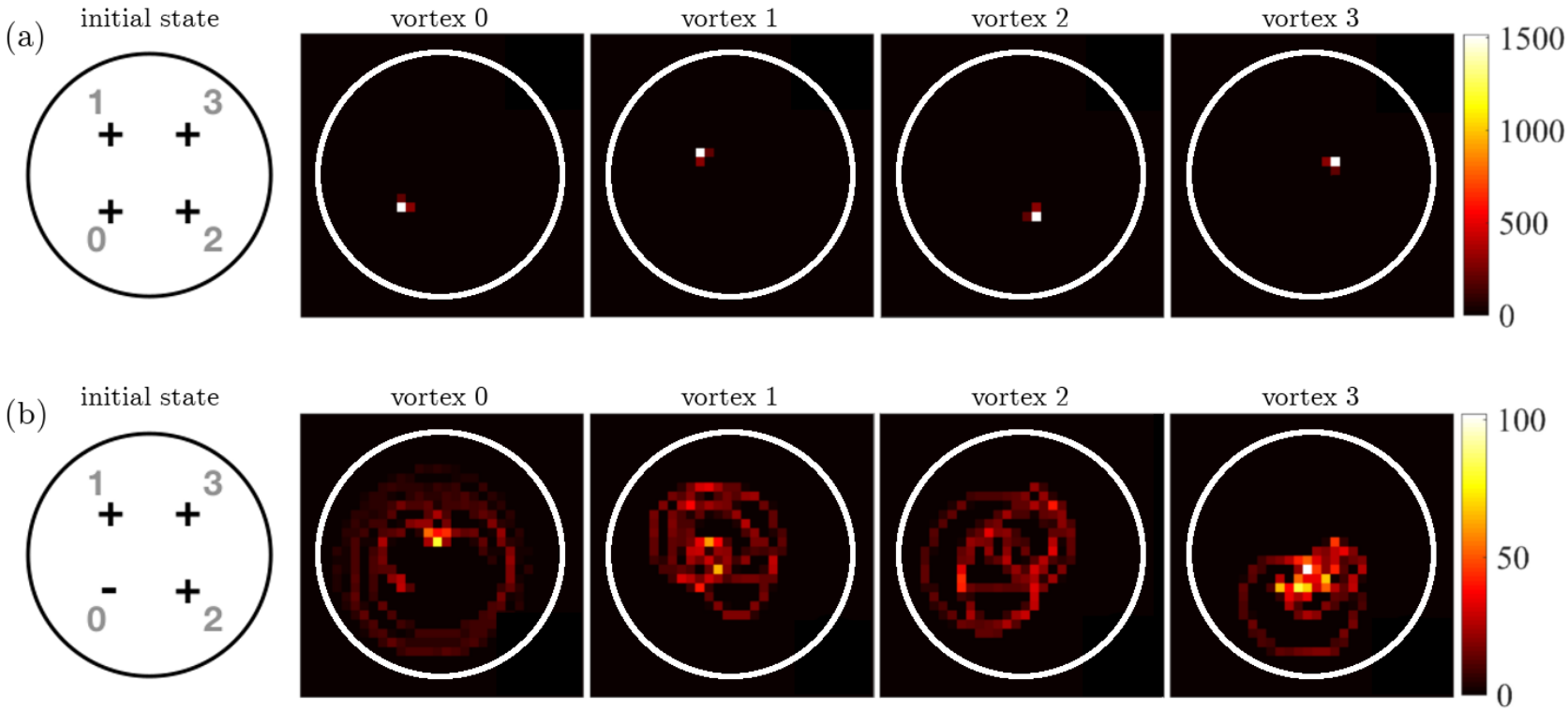
- The distributed transpose is hard
- Expression trees save a lot of GPU memory when usable

Chaotic vortex dynamics in 2D BEC simulations

Chaotic few-body vortex dynamics in rotating Bose-Einstein condensates
T Zhang, J Schloss, A Thomasen, LJ O'Riordan, T Busch, A White

Physical Review Fluids 4 (5), 054701

3 vortex, 1 anti-vortex



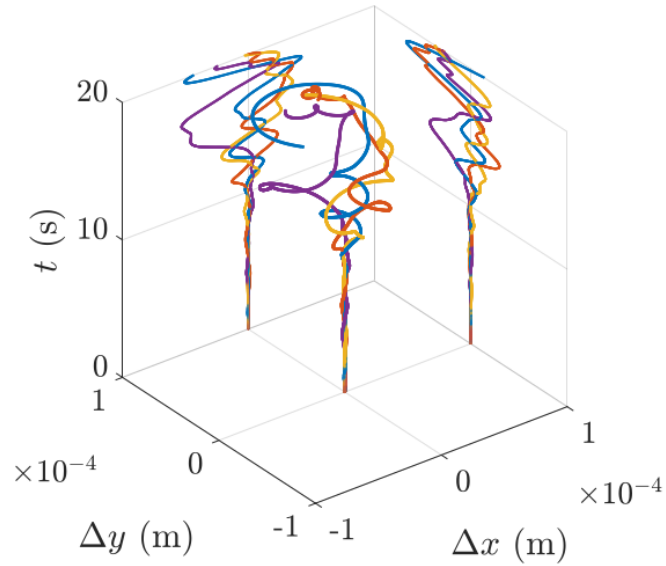
Dynamics

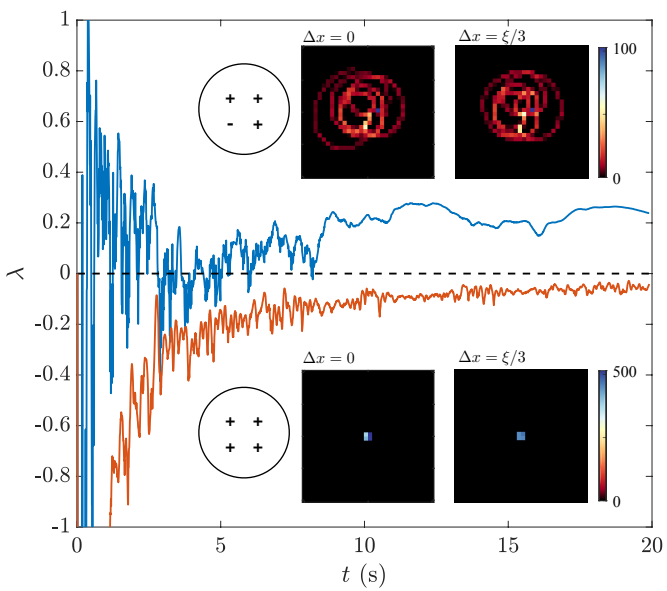
Divergence in trajectories

Divergence in trajectory when Lyapunov exp (λ) becomes positive

$$|\delta \mathbf{P}(t)| \approx e^{\lambda t} |\delta \mathbf{P}_0|$$

$$\lambda = \lim_{t \to \infty} \frac{1}{t} \ln \frac{||\delta \mathbf{P}(t)||}{||\delta \mathbf{P}(0)||}$$





Takeaway

Physics

- Chaotic dynamics of few-vortex systems is accelerated by collisional events

Computer Science

- 50 TB of data
- Reliant on post-processing metrics (Lyapunov exp, Vortex tracking)
- 1 hour per run, infeasible with other software

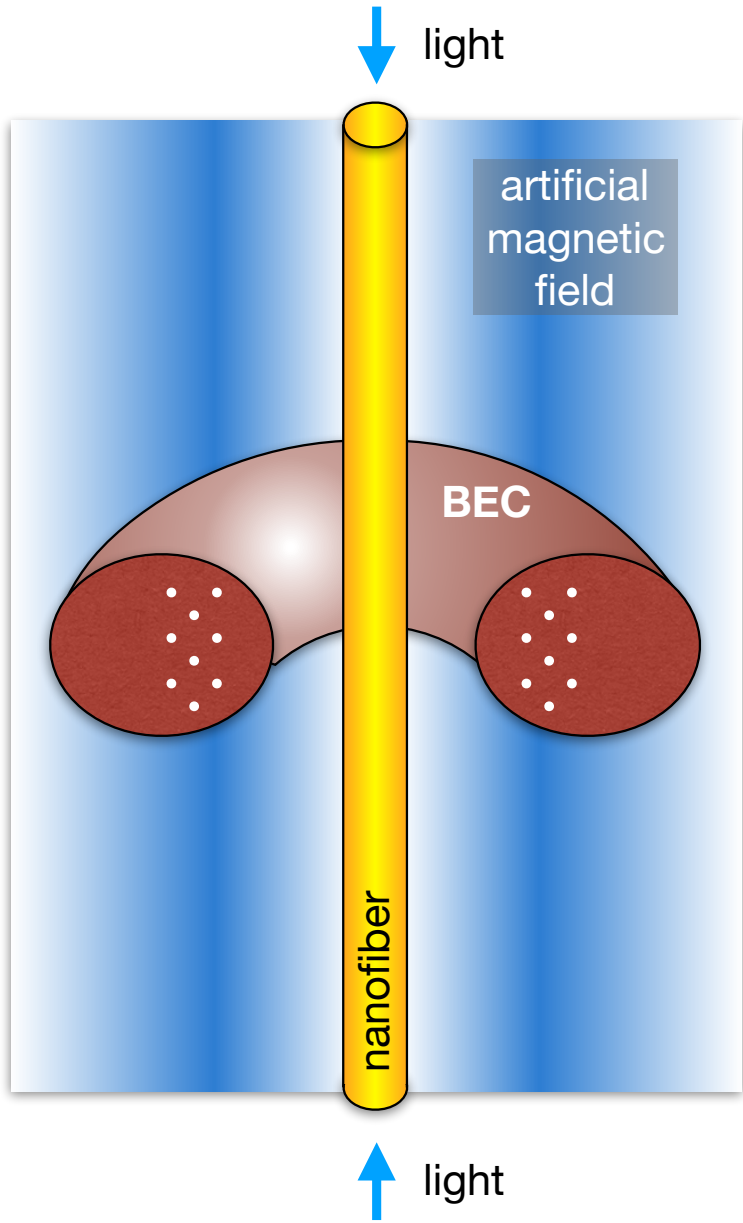
3D vortex ring generation in toroidal BEC systems

Controlled creation of three-dimensional vortex structures in Bose–Einstein condensates using artificial magnetic fields
J Schloss, P Barnett, R Sachdeva, T Busch

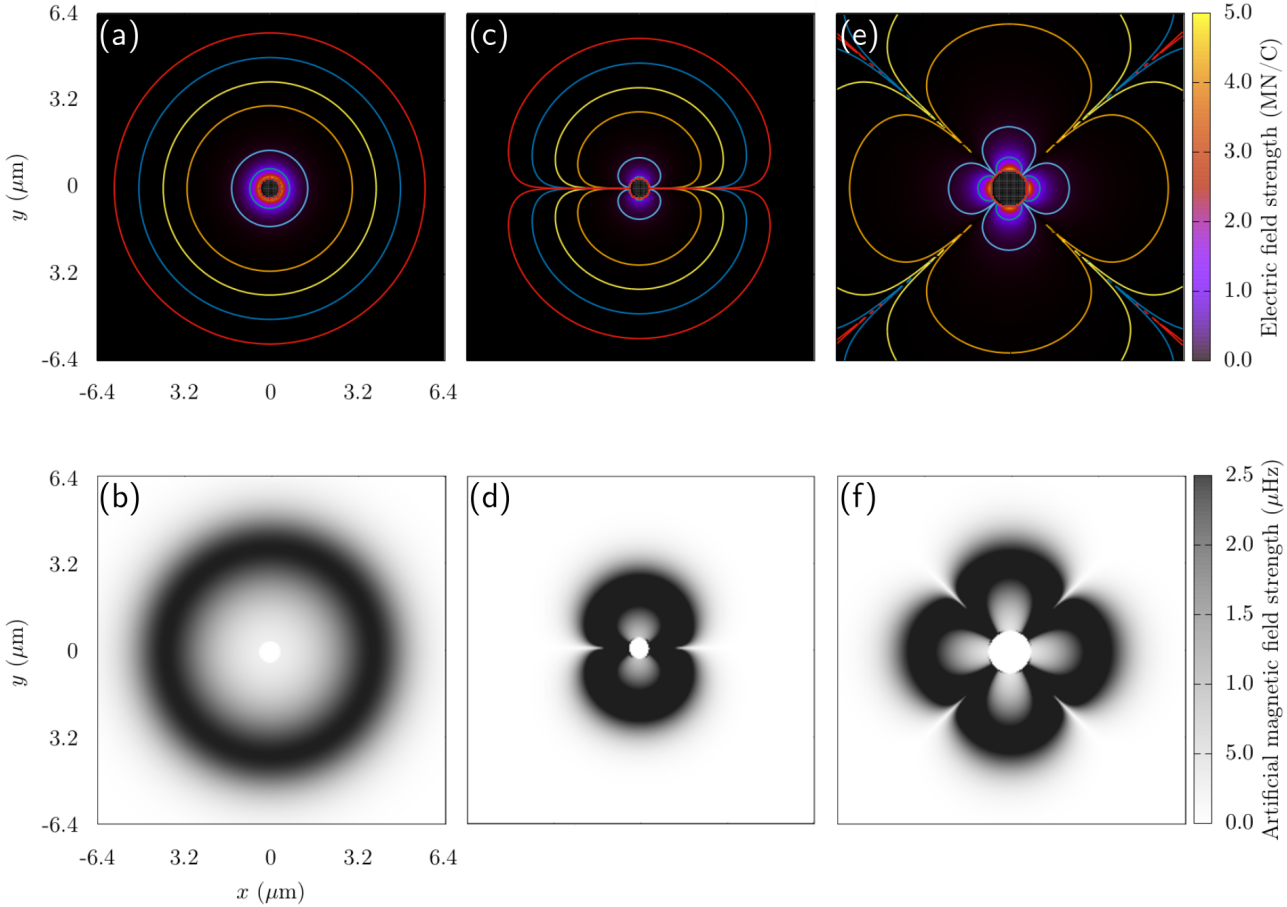
arXiv preprint arXiv:1910.02364

The system

- BEC toroidally trapped around nanofiber
- Nanofiber generates $\mathbf{A}$
- Vortices follow $\mathbf{B} = \nabla \times \mathbf{A}$

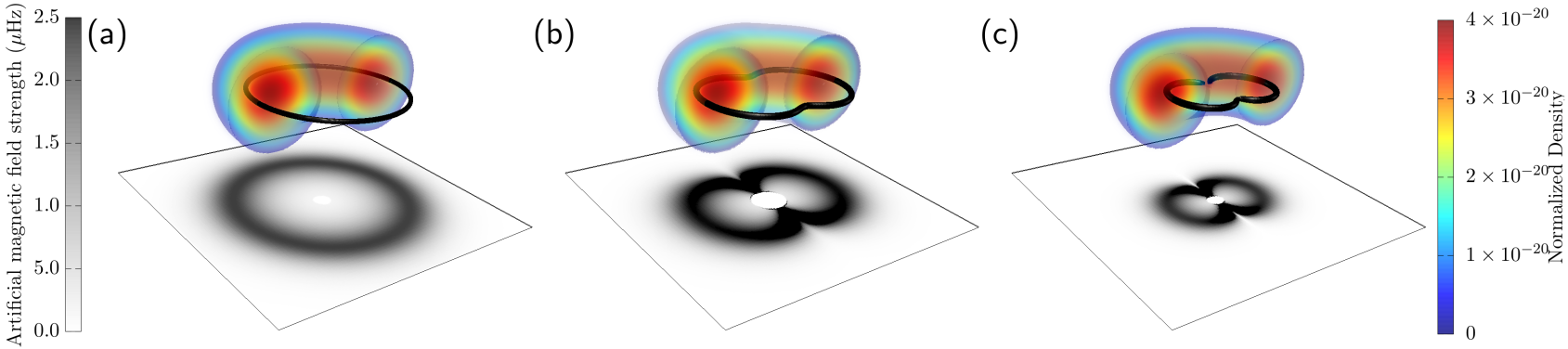


Optical nanofiber

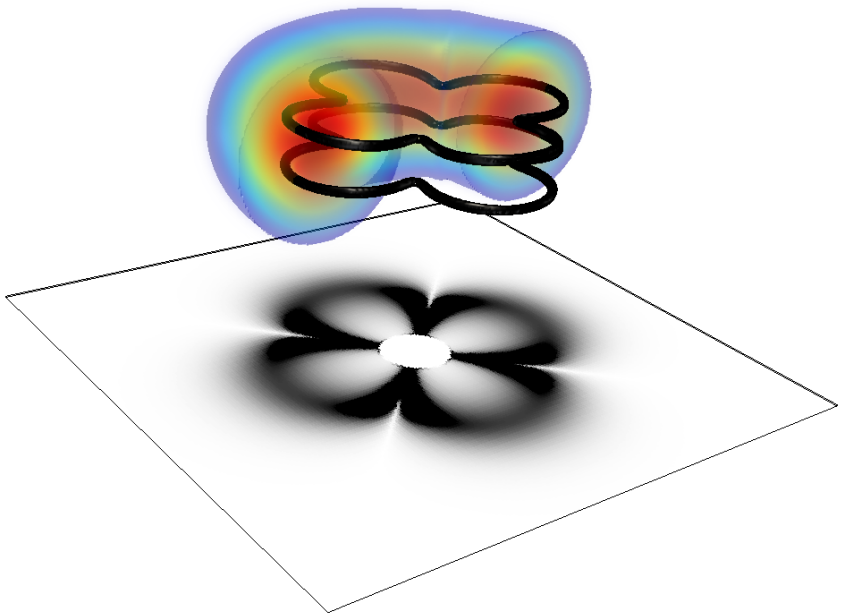


$$\mathbf{A} = \hat{z}\hbar\kappa_0(n_1+1)\tilde{s}\left[\frac{|d_r E_r + d_\phi E_\phi + d_z E_z|^2}{1+\tilde{s}^2|d_r E_r + d_\phi E_\phi + d_z E_z|^2}\right]$$

Vortex structures

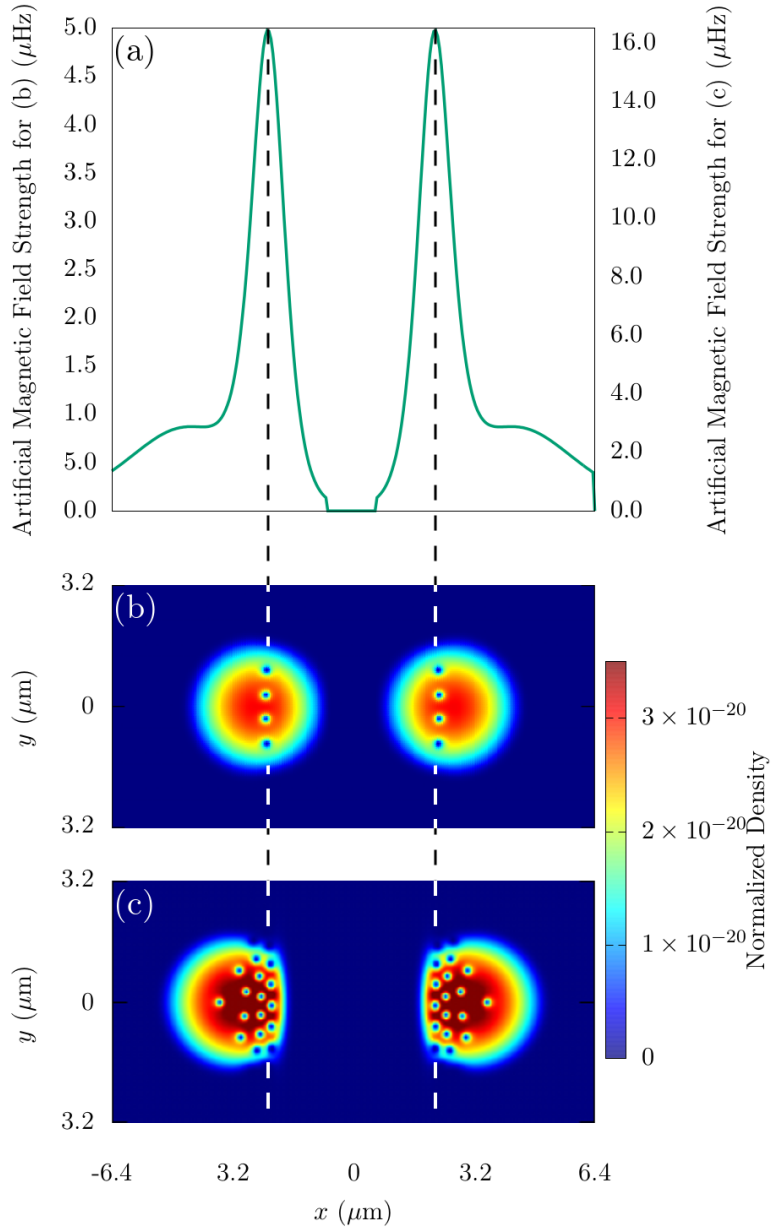


- Transition with linear polarization
- Vortex structures align with **B**



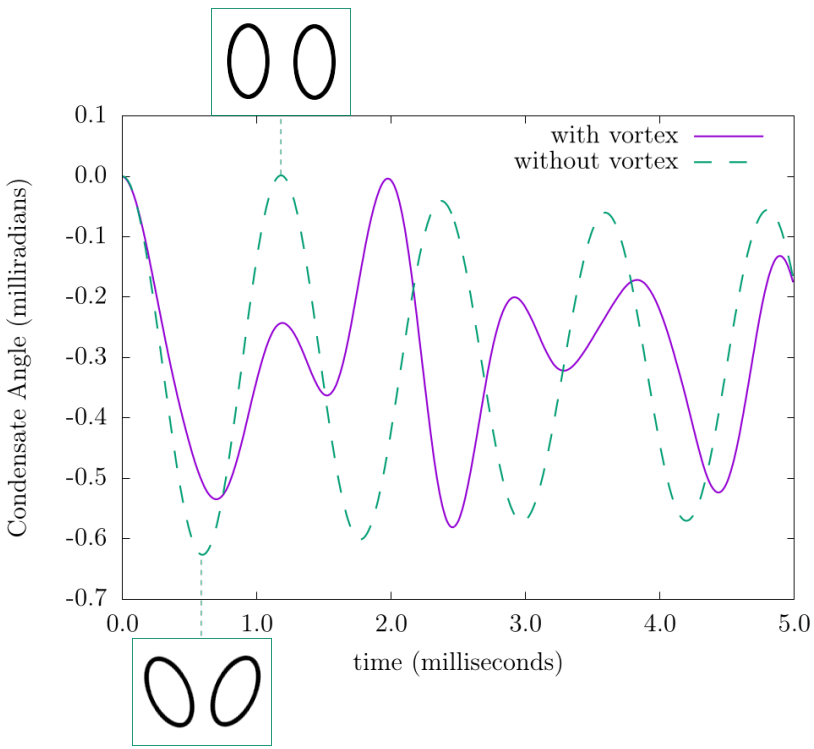
Interesting notes

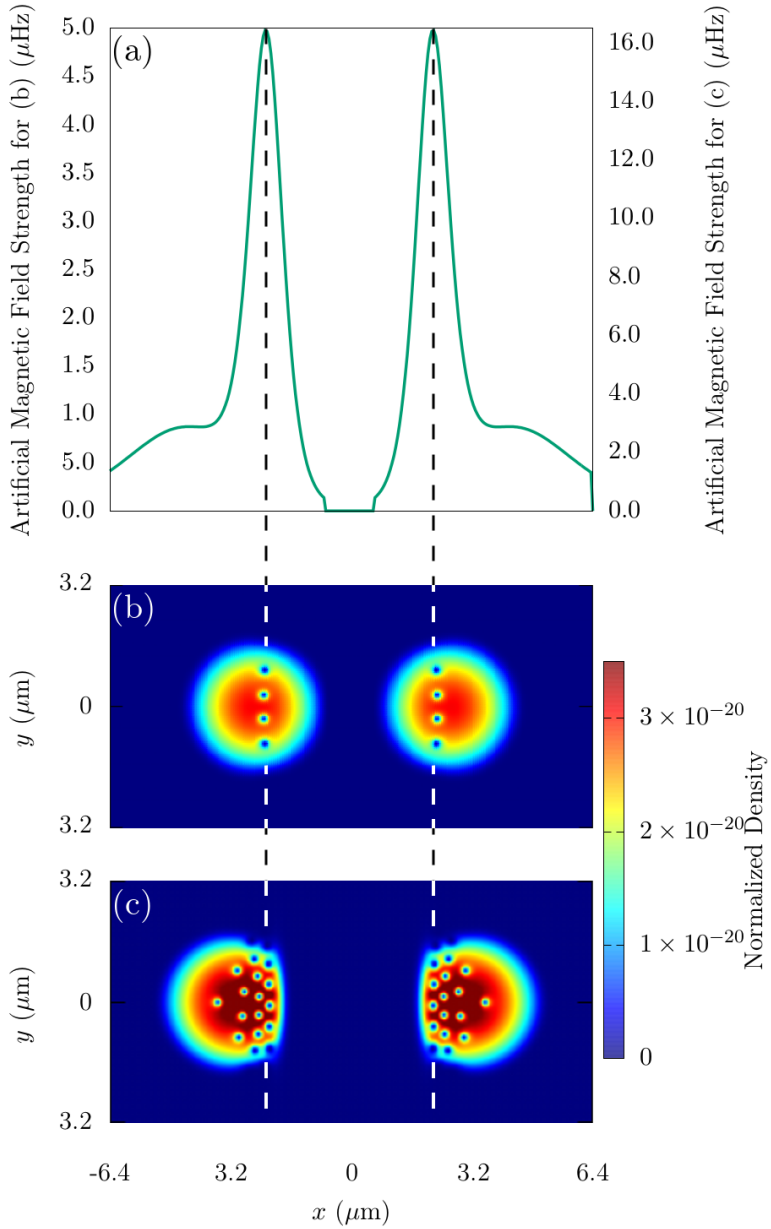
- A vortex ring lattice can be generated with high **B**



Interesting notes

- A vortex ring lattice can be generated with high **B**
- Scissors modes can be used to detect vortices





Takeaway

Physics

- We can generate, control, and detect vortex structures in a BEC around a nanofiber
- Dynamic simulations are underway!

Computer Science

- Dynamic simulations require a large amount of fileIO
- Scaling to a larger grid requires multiple GPU's

Overall conclusions

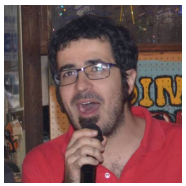
Overall conclusions

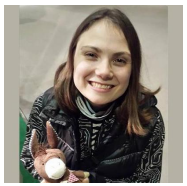
- The SSFM is nice
- GPU computing is fast
- We can create chaos
- We can create not-chaos

Future directions

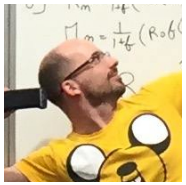
- Distributed Transpose
- GPUE.jl
- General-purpose Hamiltonian solver
- Full vortex tracking
- Octree-based gridding for SSFM

People












Organizations:

Conclusions

Quantum state engineering

Quantum optimal control

Overall goal: optimize cost function by twiddling control parameters

Quantum optimal control

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- Many known methods, such as **gradient descent**, **genetic algorithms**, and **machine learning**

Quantum optimal control

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- For quantum systems, cost function is often the fidelity:

$$\mathcal{F} = |\langle\psi|\phi\rangle|^2$$

which required re-simulation every time a control parameter is changed

Quantum optimal control

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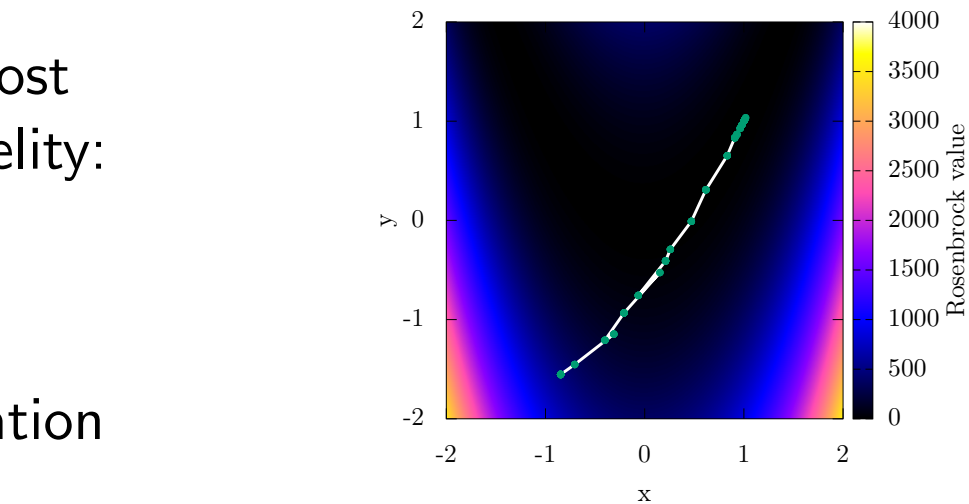
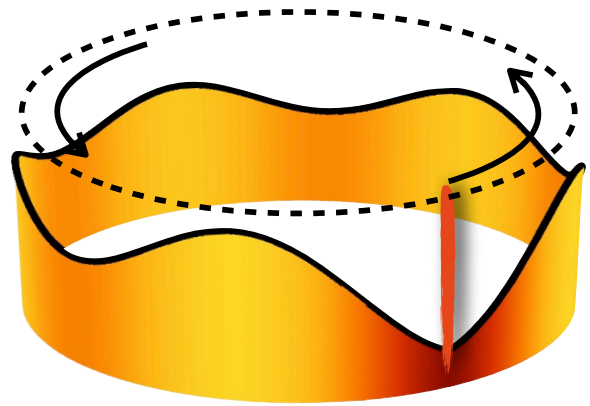
Nelder–Mead



Example Tonks–Girardeau gas system

- NOON state: $|N, 0\rangle + |0, N\rangle$
- Tonks–Girardeau Gas:
  $g \to \infty$



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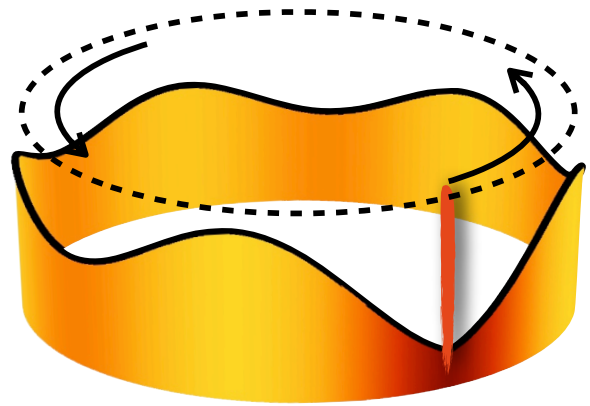
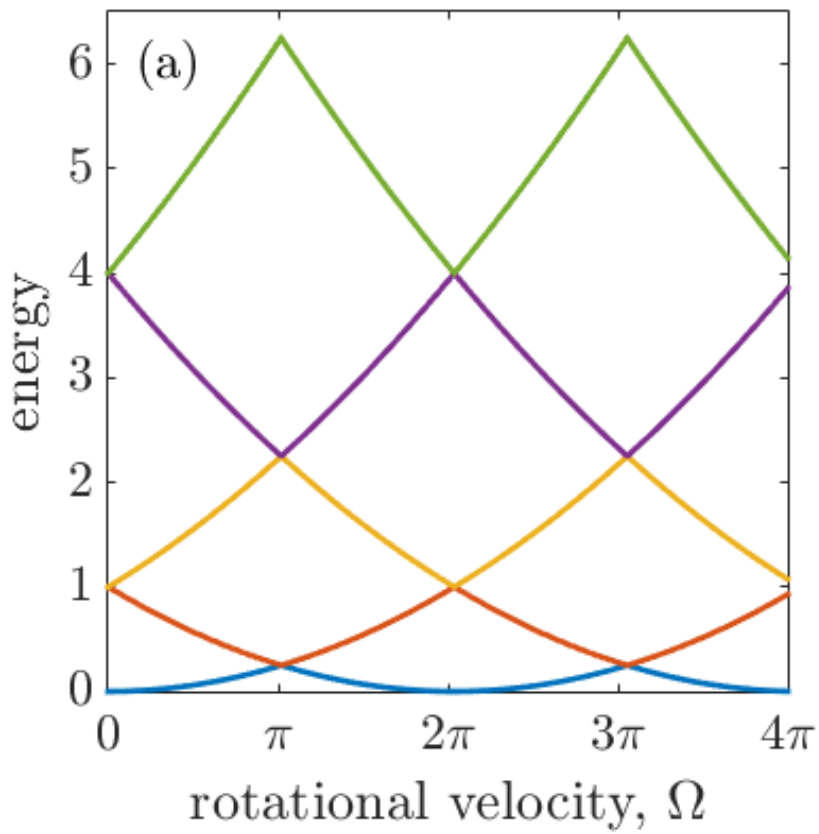
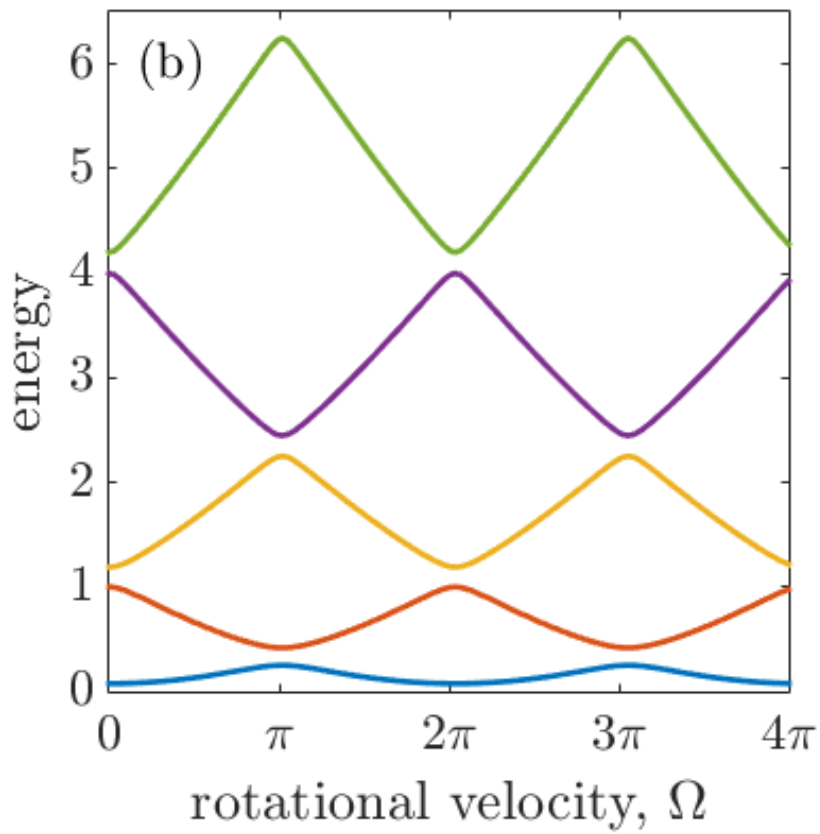






CRAB method

An example protocol is the Chopped RAndom Basis (CRAB) optimal control method where...

- A control parameter is modified with

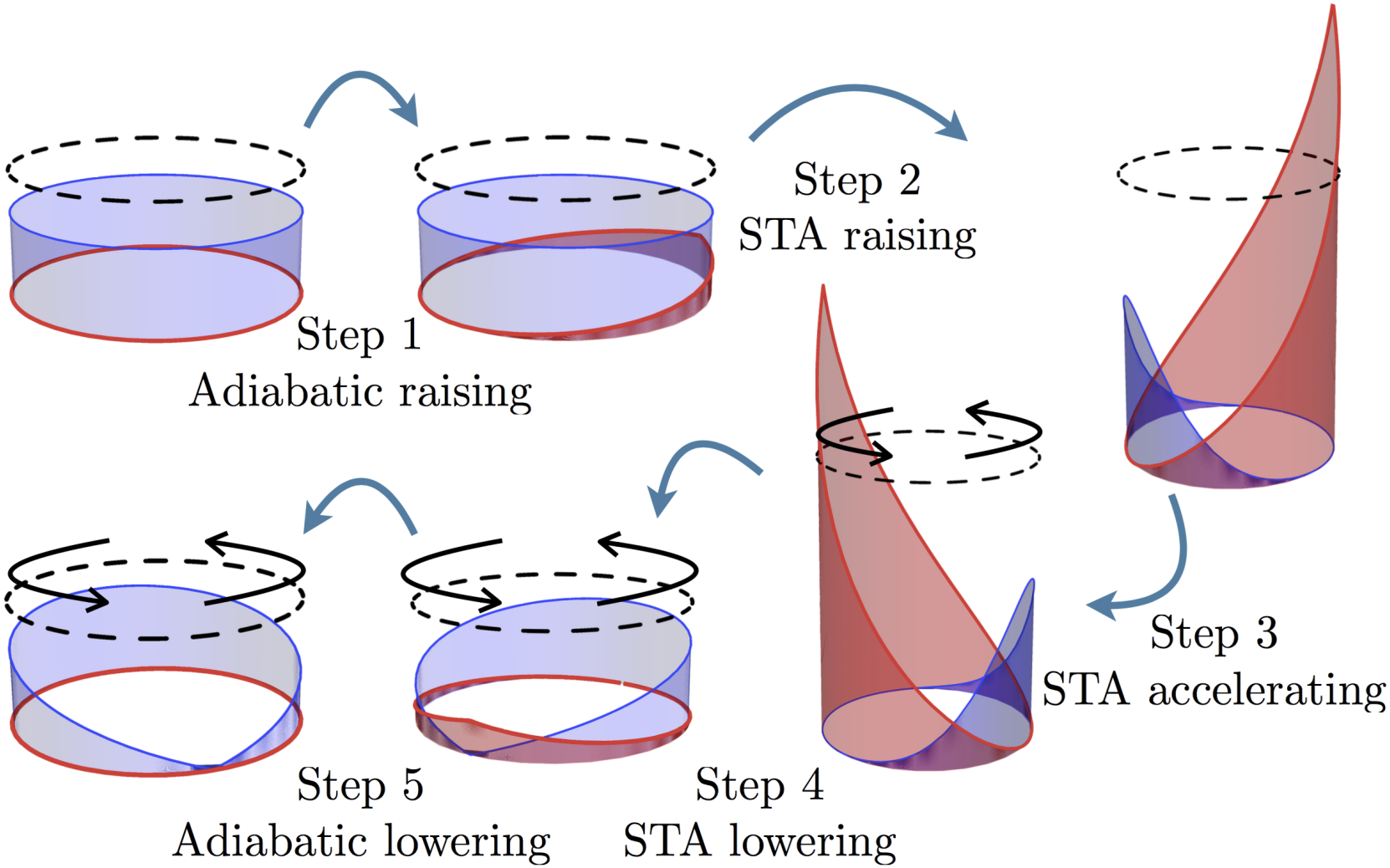
$$\Gamma^{\mathrm{CRAB}}(t) = \Gamma^{0}(t)\gamma(t)$$

  where

$$\gamma(t) = 1 + \frac{1}{\lambda(t)} \sum_{j=1}^{J} (A_j \sin(\nu_j t) + B_j \cos(\nu_j t))$$

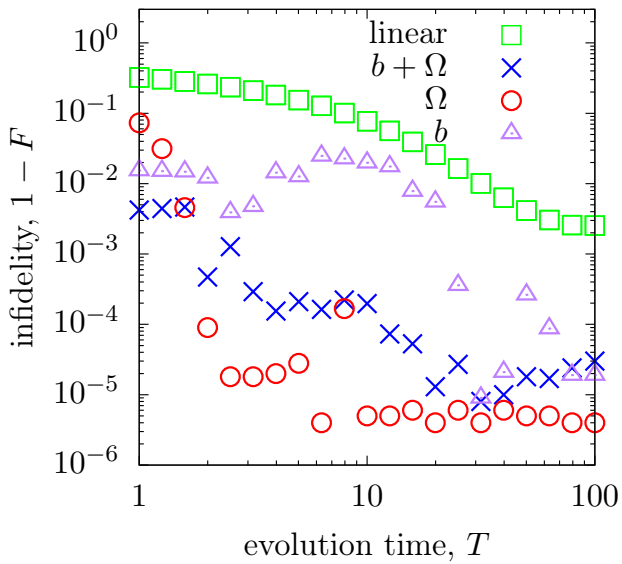
- Works if $\lim_{t\to 0} \lambda(t) = \lim_{t\to T} \lambda(t) = \infty$
- Creates a $3J$-dimensional space to optimize (A, B, ν)

STA protocol

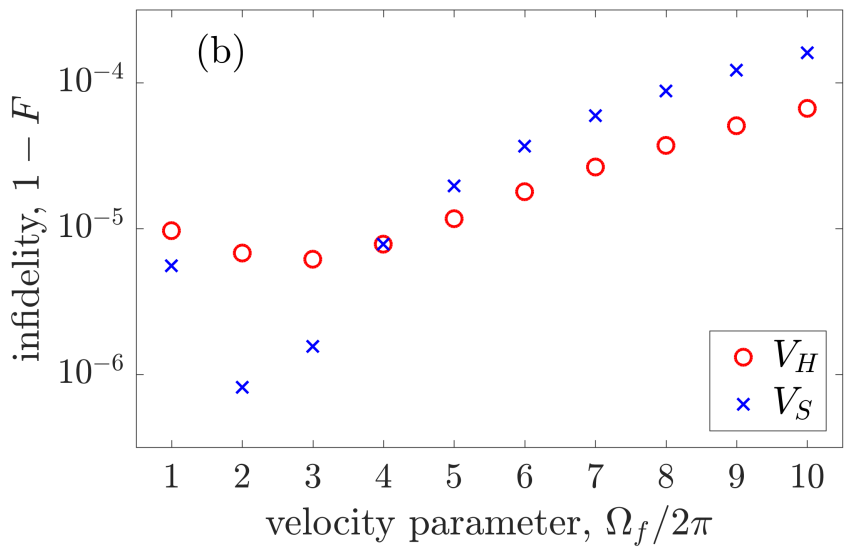


NOON optimization

Optimal control



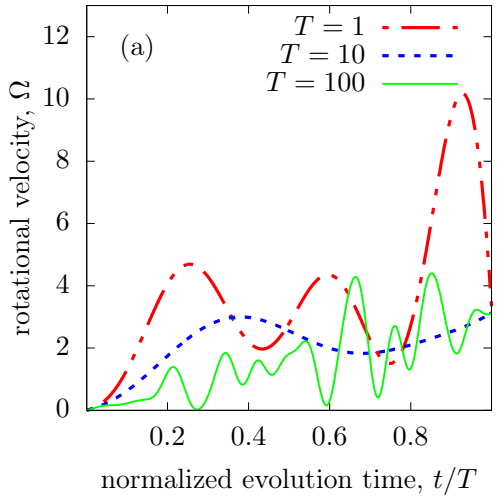
STA



Please ask questions at the end!

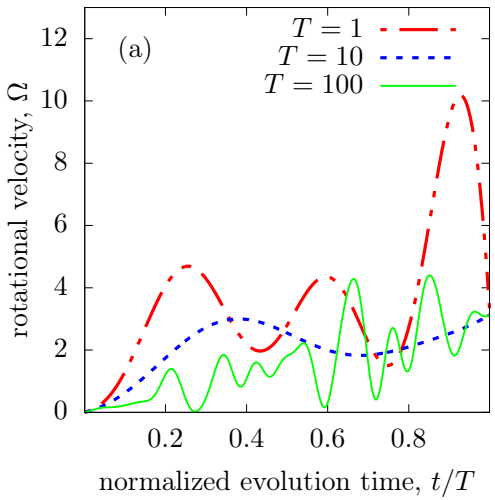
Fidelities with optimal control

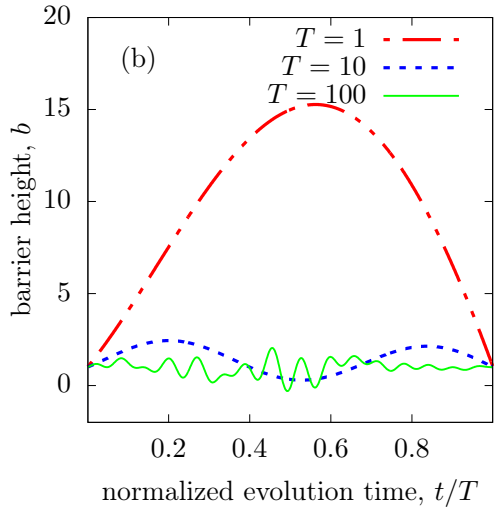
- Rotation ($\Omega(t)$)



Fidelities with optimal control

- Rotation ($\Omega(t)$)
- Barrier height ($b(t)$)





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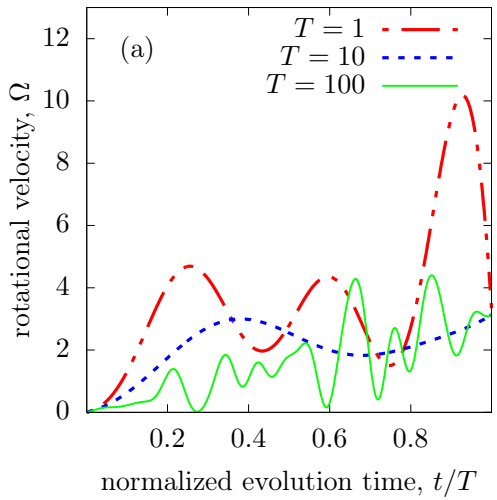

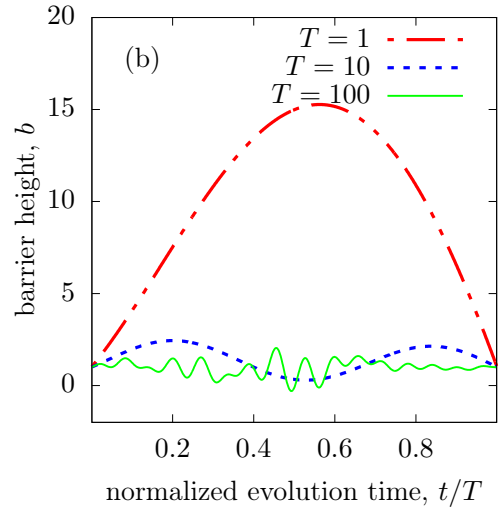

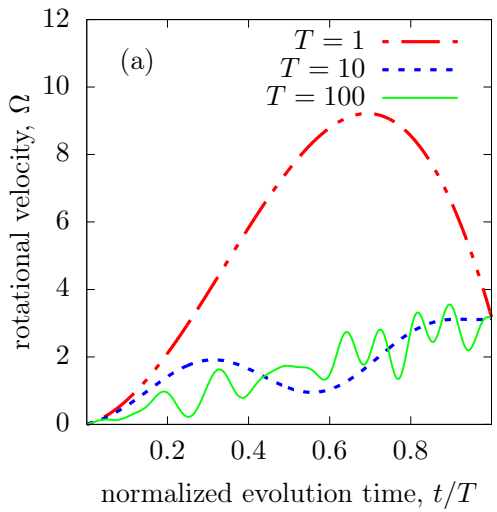

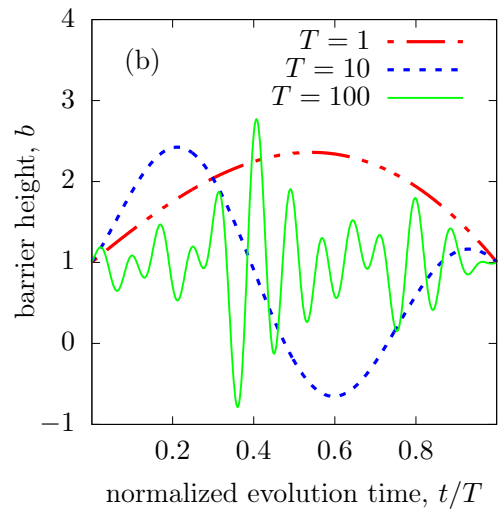

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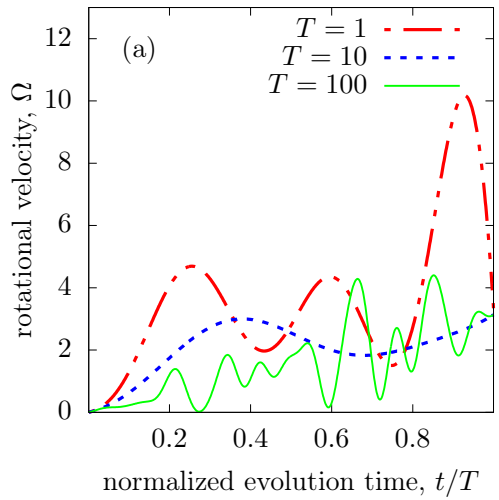
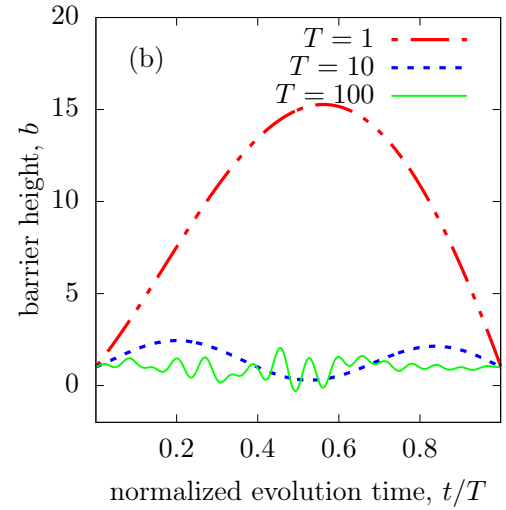
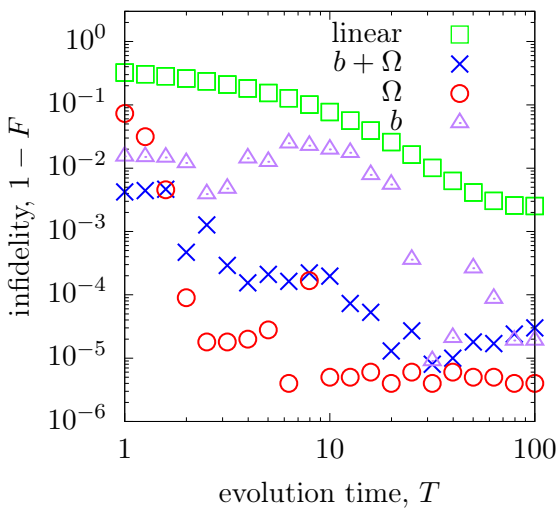
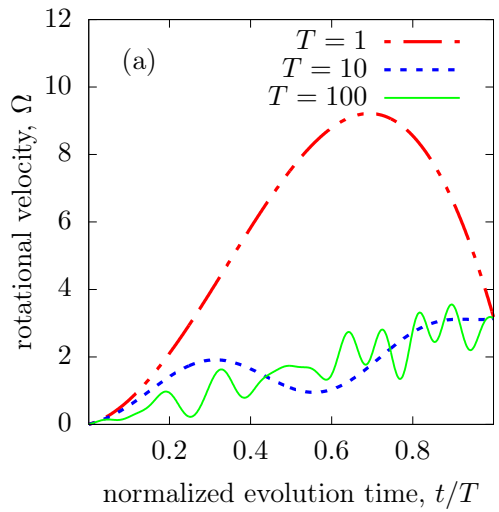
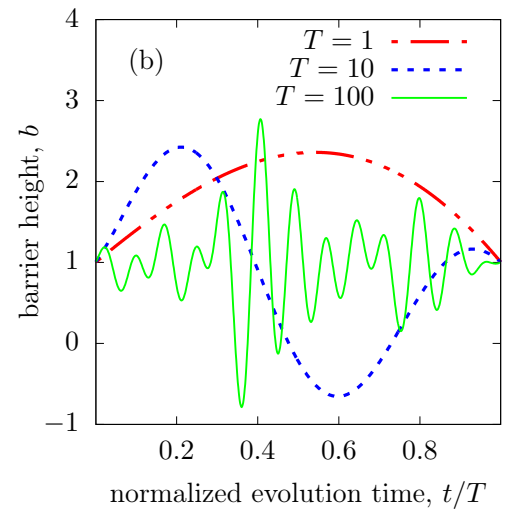




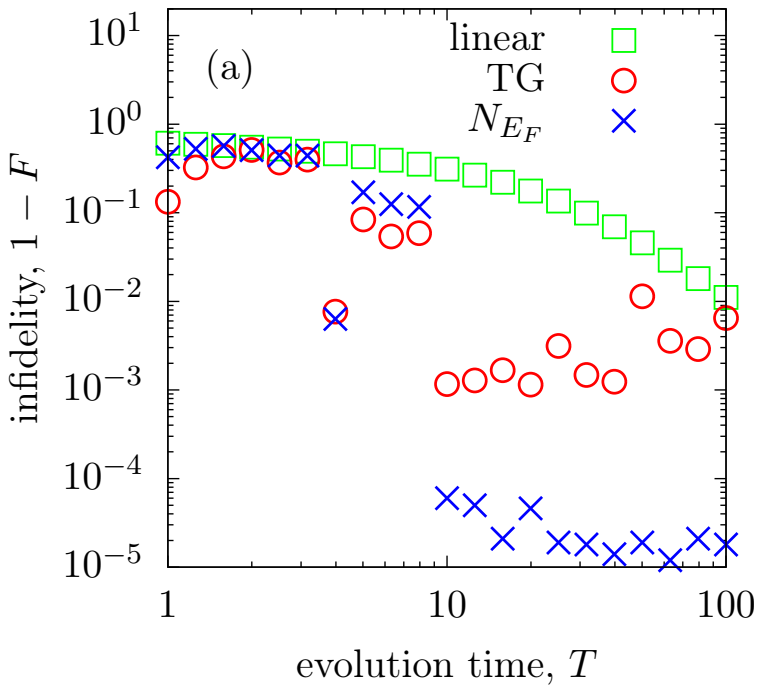


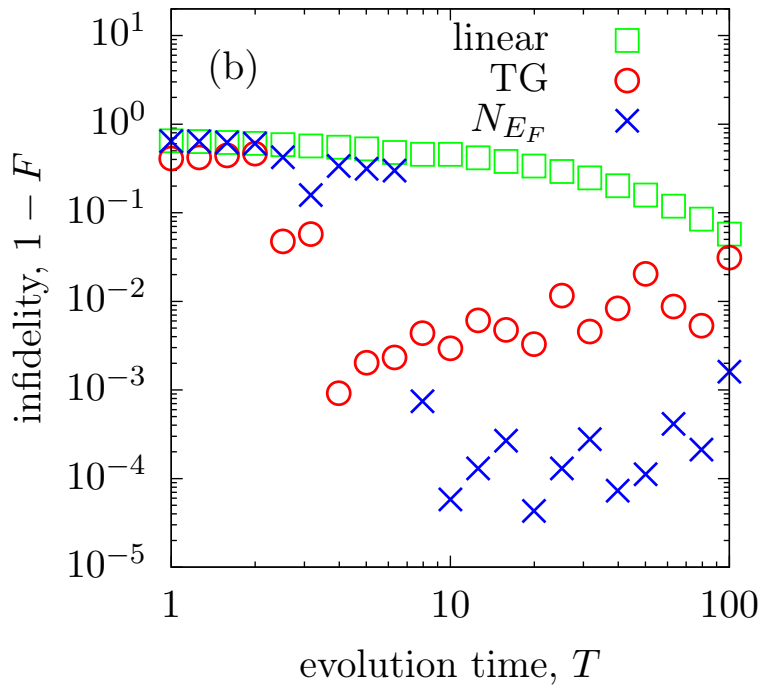




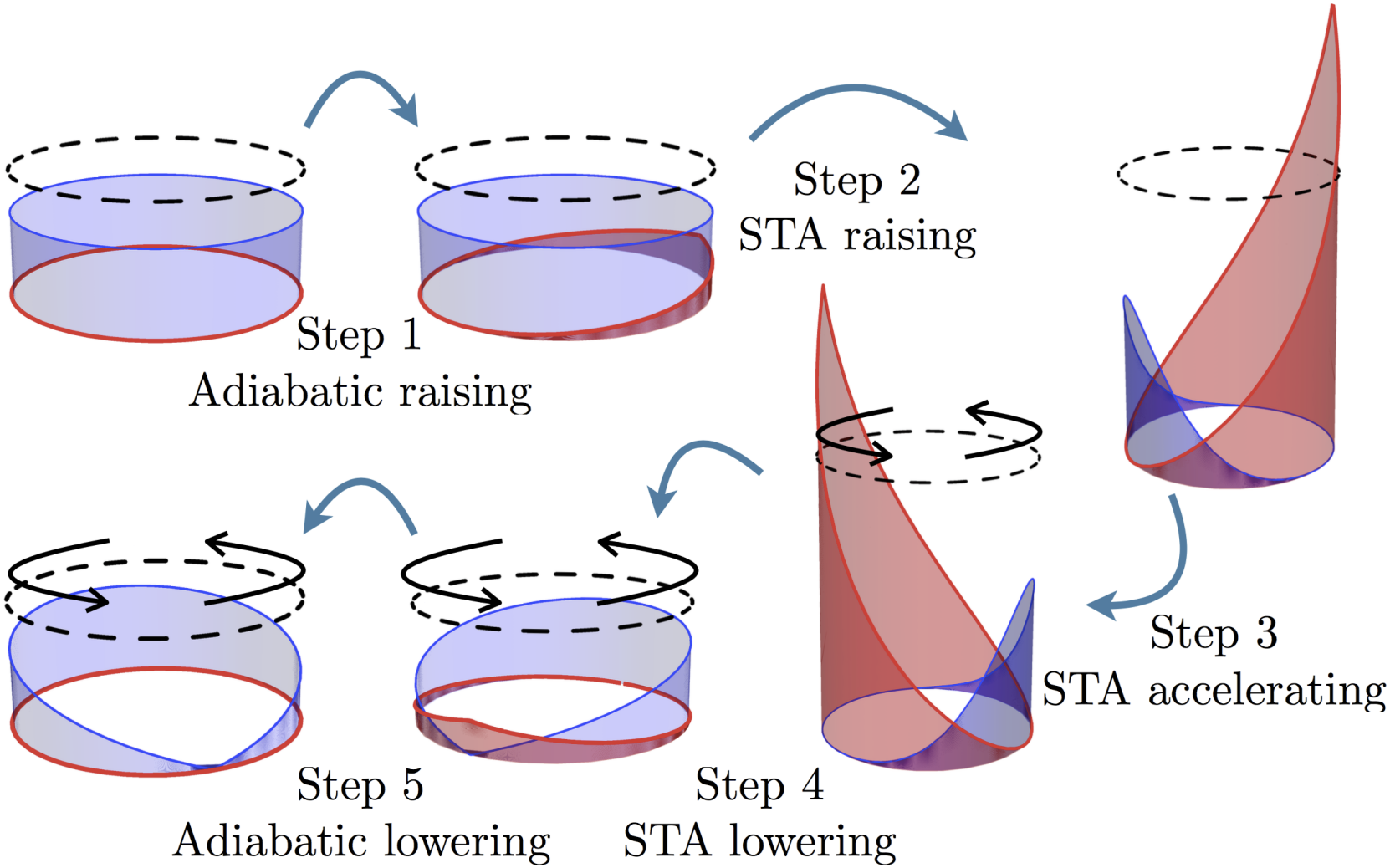
NOON Optimization

Optimizations of NOON state generation with 3 and 5 particles



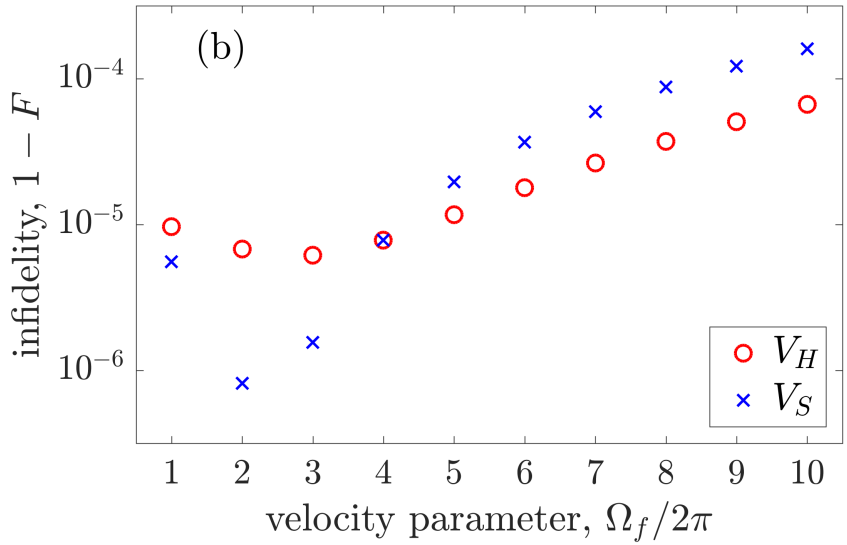


STA protocol



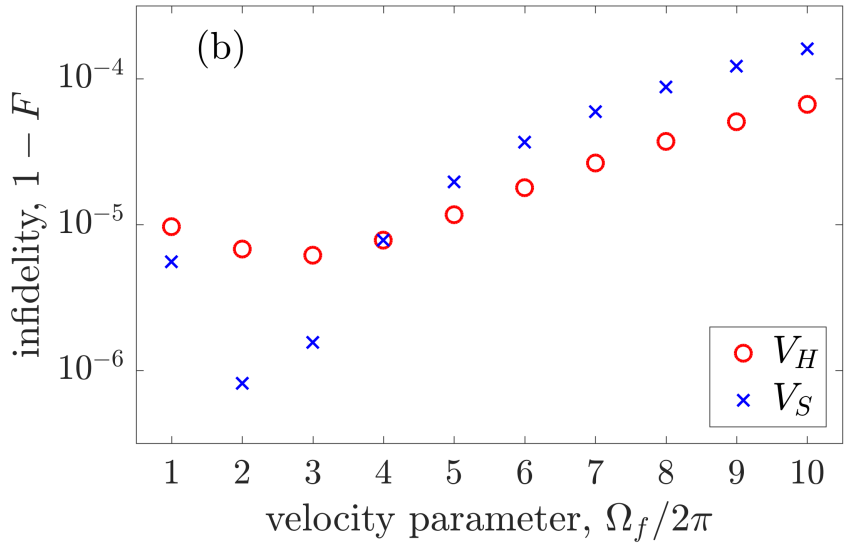
STA fidelities

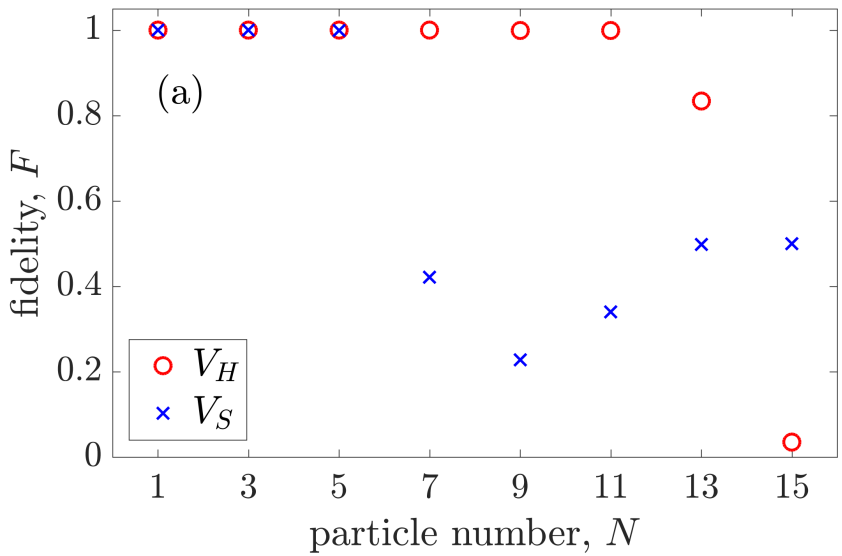
- Fidelities with rotation

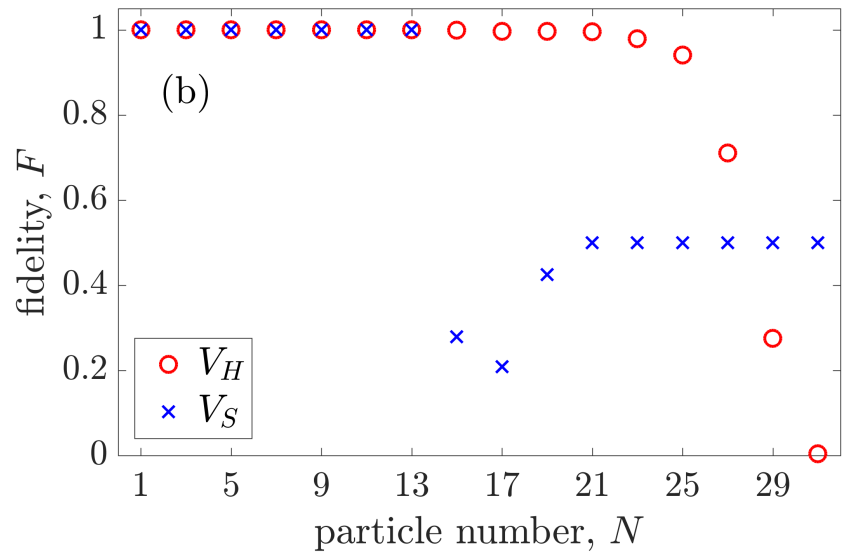


STA fidelities

- Fidelities with rotation
- Fidelities with rotation of 100, 200 and higher particle number







Cooley-Tukey

- Recursively subdivides DFT into simple sums with twiddle factors
- Many known libraries, like FFTW, and CuFFT
- Hard to parallelize (note for later)