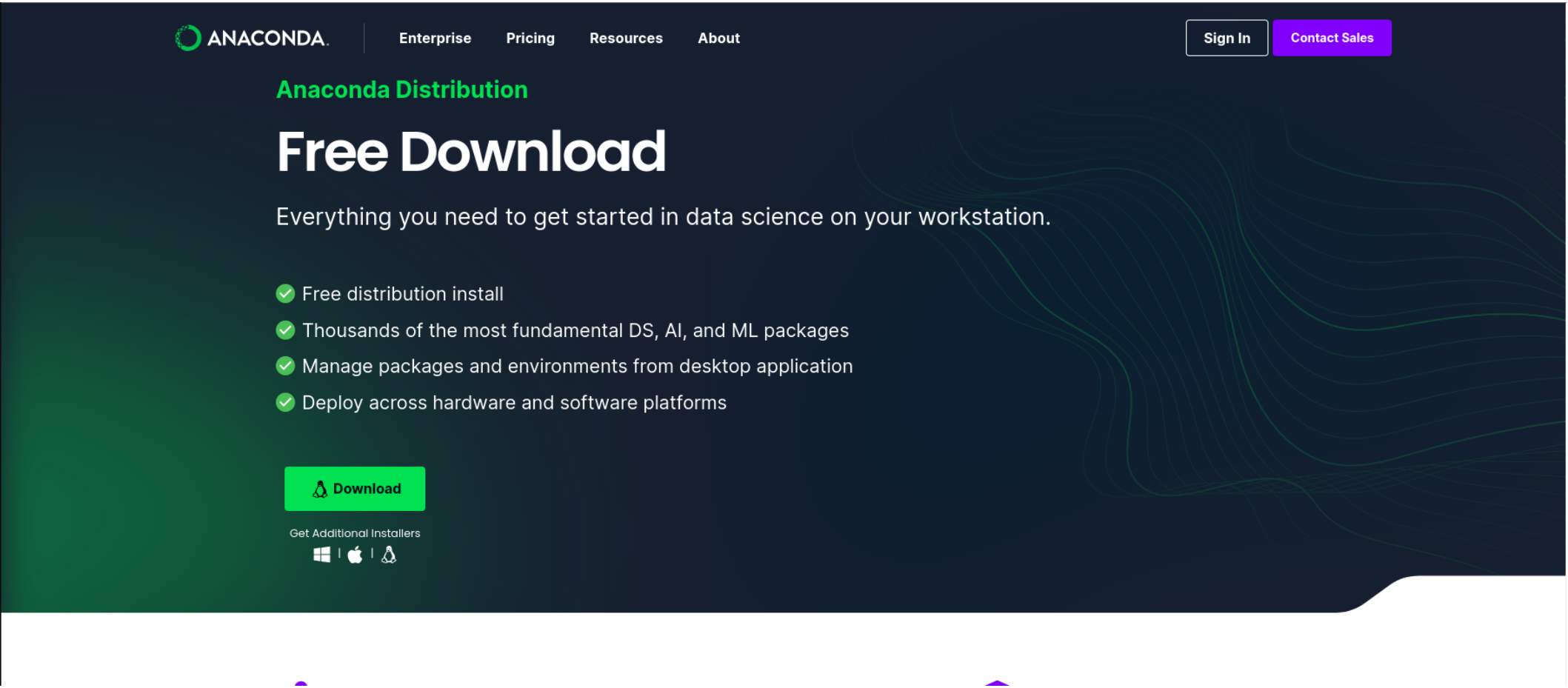
Special Topics in Computational Physics

Special Topics in Computational Physics:

- Preliminary Setup and Configuration
- QuTiP: Quantum Toolbox in Python
- Partial Differential Equations: Laplace and Wave equations

Preliminary Setup and Configuration

Download and install anaconda from https://anaconda.com/download



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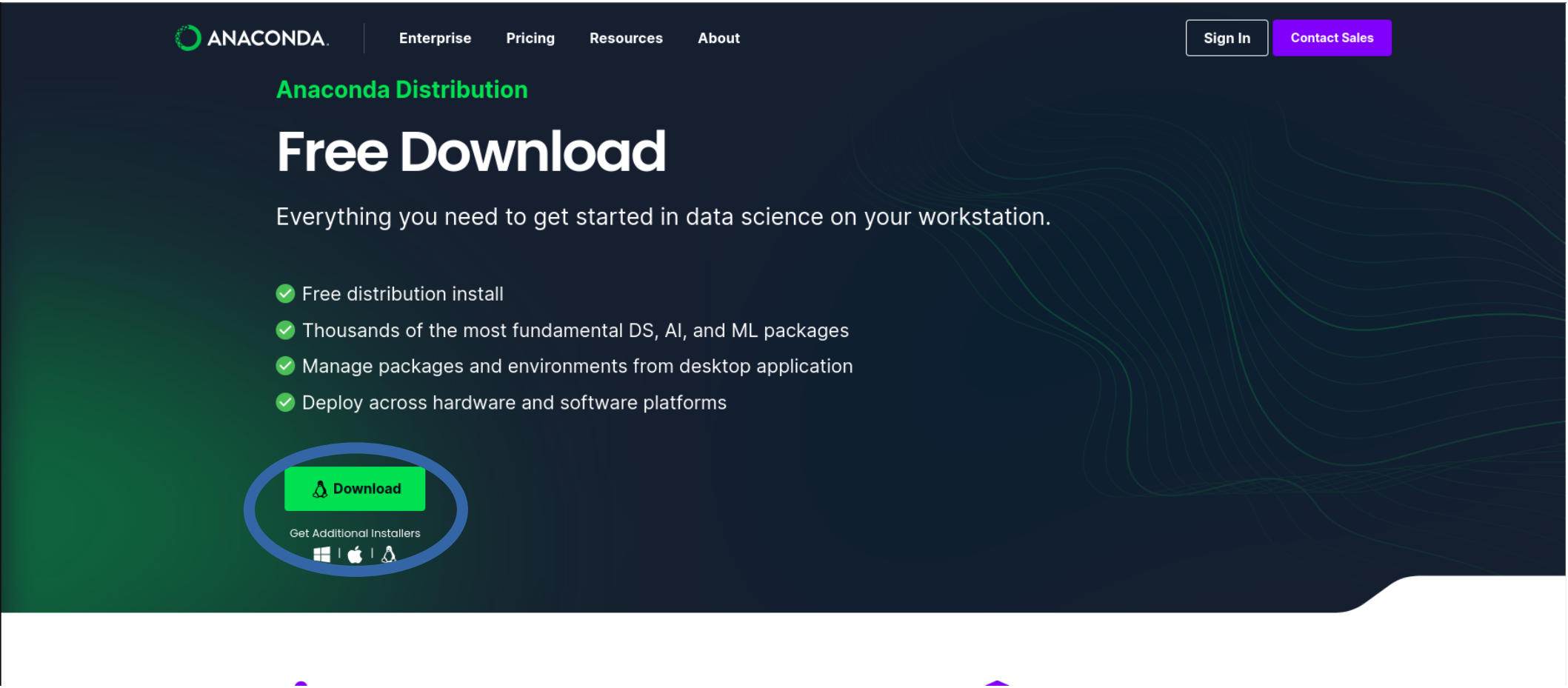
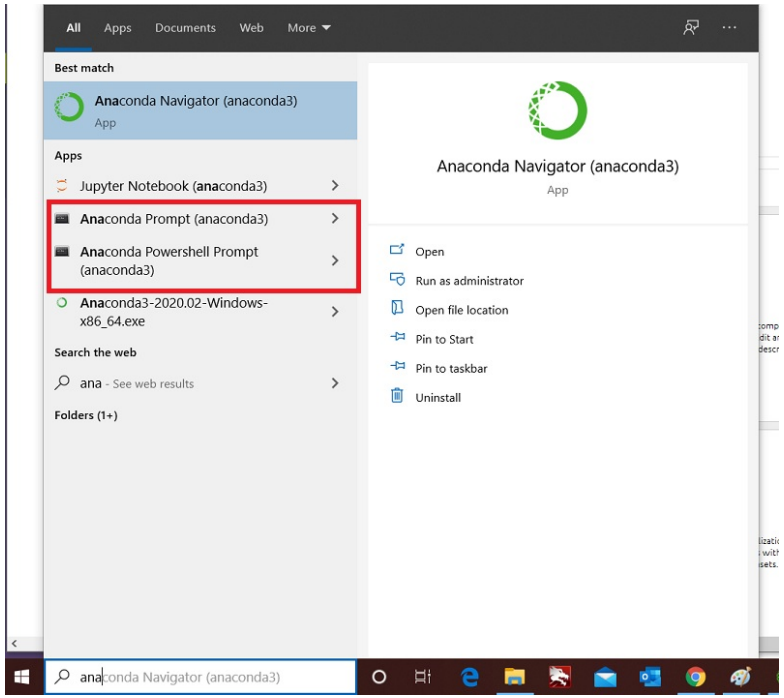


Preliminary Setup and Configuration

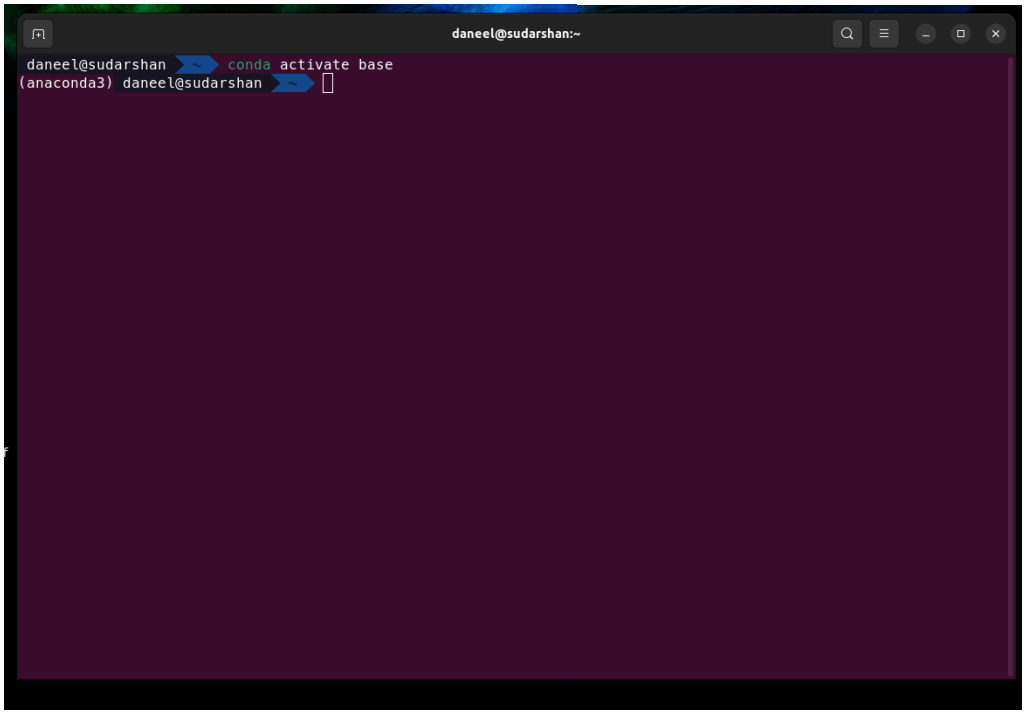
Load a ‘conda shell’ with the base environment activated.

Windows



Linux™

ubuntu®



Preliminary Setup and Configuration

- Use the conda package manager to add the ‘conda-forge’ repository
- After loading the conda shell, create a special conda environment named ‘exercises’, together with the required packages

```
$ conda config --add channels conda-forge
$ conda create -n exercises python=3.11 numpy scipy matplotlib qutip
```

Note that:

1. The conda dependency resolver is a bit slow, so this can take some time to finish.
2. This environment Is named ‘exercises’, but you can use any name that you want.
3. This environment runs a more recent version of python (version 3.11) than the anaconda default.

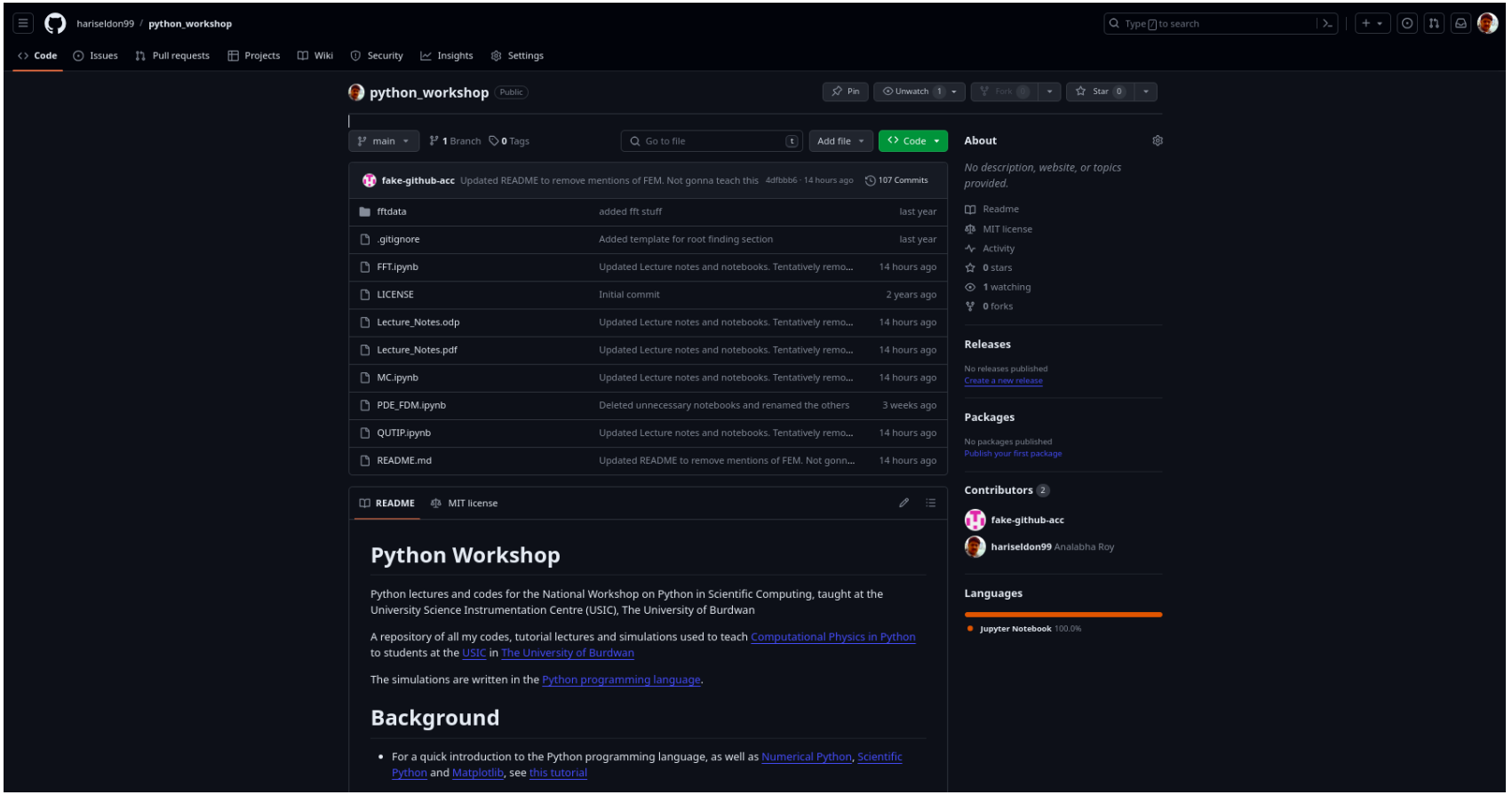
   This is suggested because python versions 3.11 and higher perform better than the default version.

- Activate this environment whenever you want to use it by loading the conda shell and running

```
$ conda activate exercises
$ jupyter notebook
```

Preliminary Setup and Configuration

- All materials for this workshop session are up on my GitHub Repository.
- To view, use a web browser to visit https://github.com/hariseldon99/python_workshop



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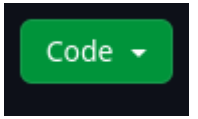
- To download this repository on your local machine, click on 

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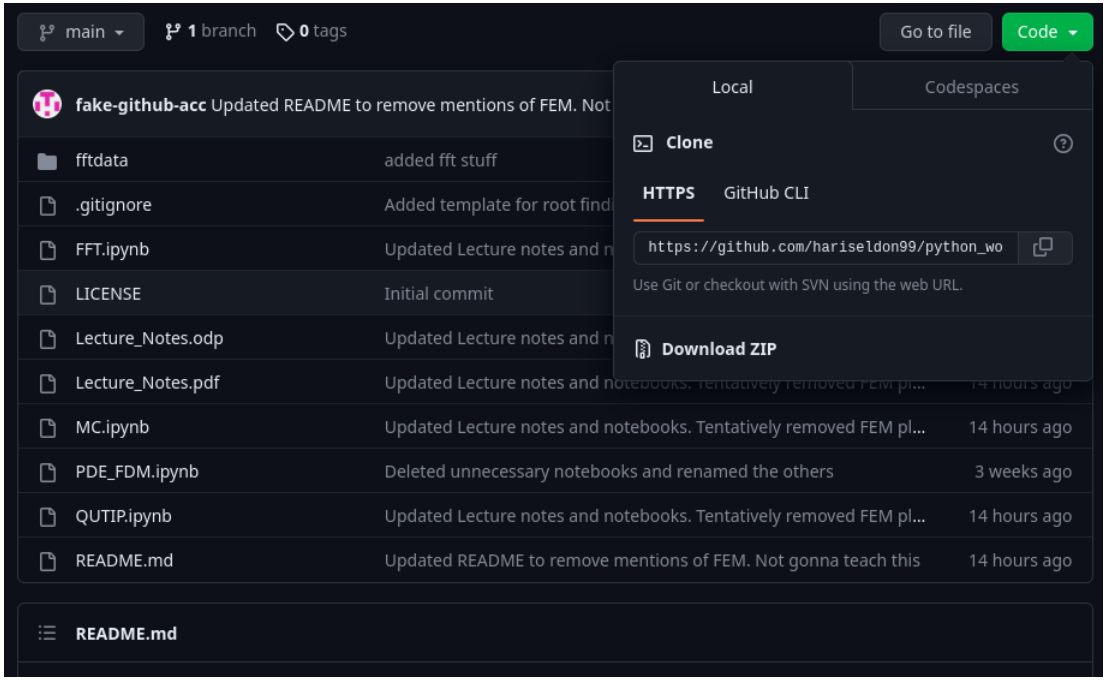

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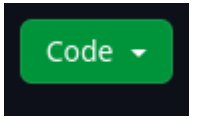
- To download this repository on your local machine, click on 

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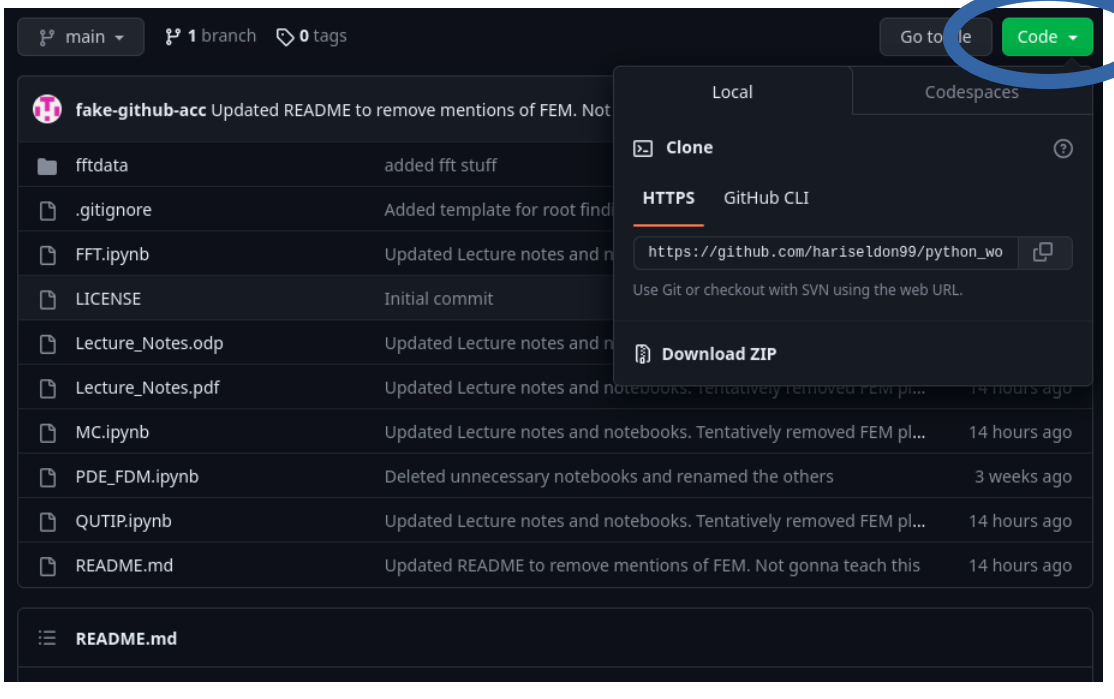

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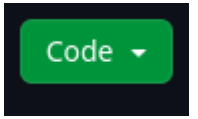
- To download this repository on your local machine, click on 

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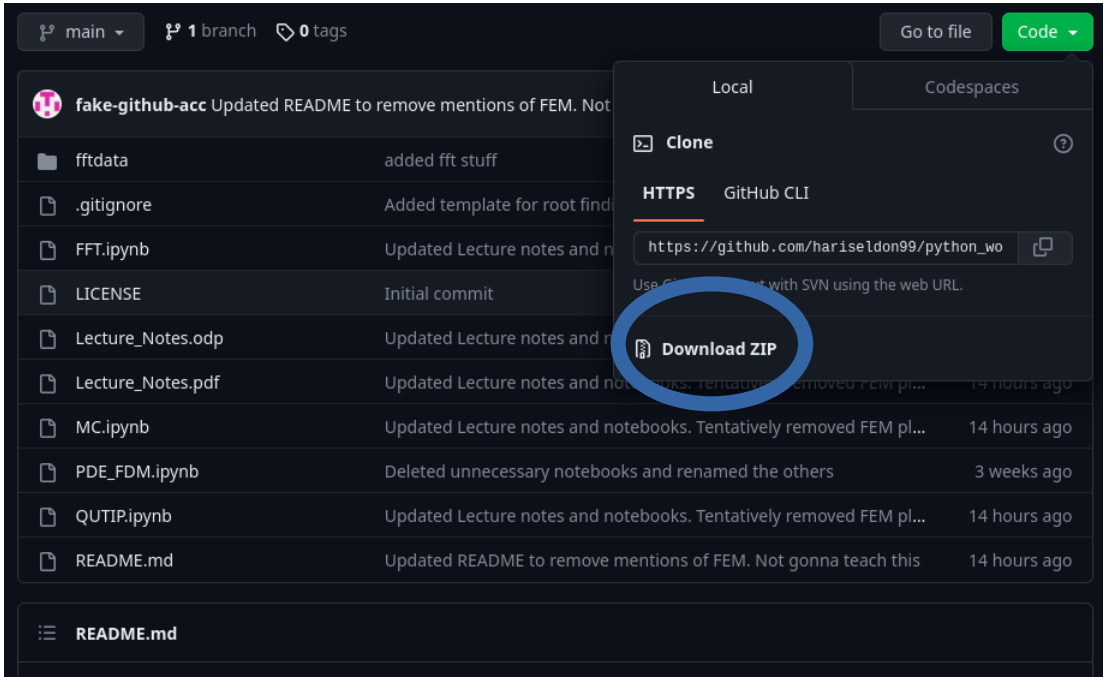


QuTiP: The Quantum Toolbox in Python

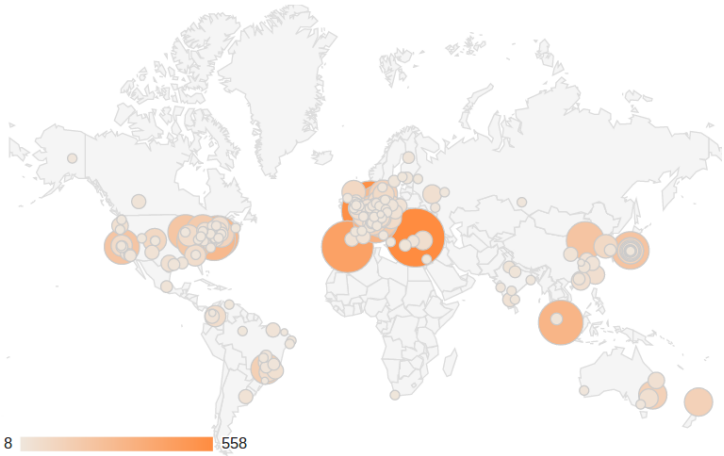
QuTiP: The Quantum Toolbox in Python

- Framework for computational quantum dynamics
  - Efficient and easy to use for quantum physicists
  - Thoroughly tested (100+ unit tests)
  - Well documented (200+ pages, 50+ examples)
  - Quite large number of users (>1000 downloads)
- Suitable for
  - theoretical modeling and simulations
  - modeling experiments
- 100% open source
- Implemented in Python/Cython using SciPy, Numpy, and matplotlib

QuTiP: The Quantum Toolbox in Python

Project information

- Authors: Paul Nation and Robert Johansson
- Web site: http://qutip.org
- License: GPLv3
- Repository: http://github.com/qutip
- Publication: Comp. Phys. Comm. **183**, 1760 (2012)
  arXiv:1211.6518 (2012)



QuTiP: The Quantum Toolbox in Python

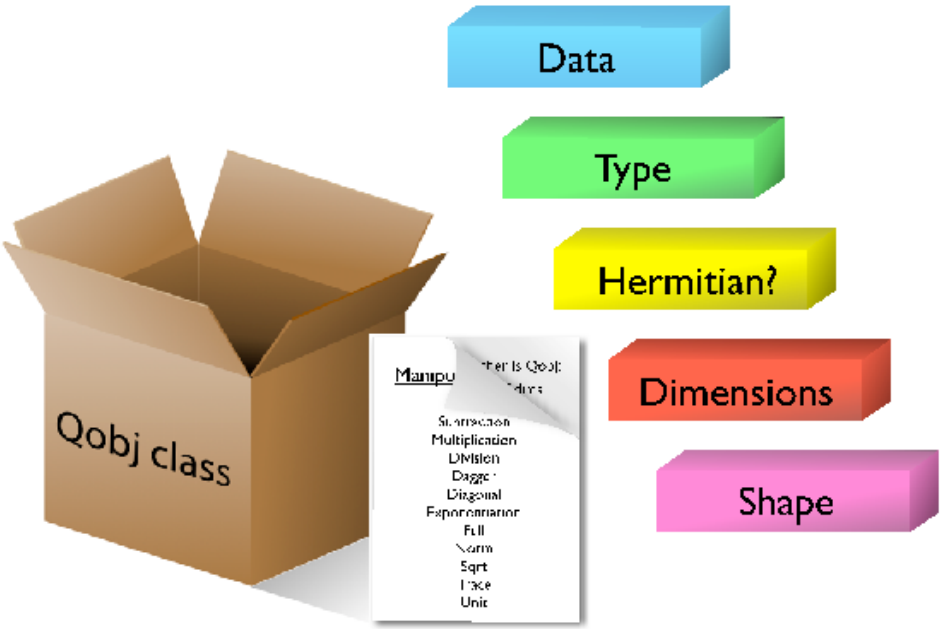
- Objectives

  To provide a powerful framework for quantum mechanics that closely resembles the standard mathematical formulation

  - Efficient and easy to use
  - General framework, able to handle a wide range of different problems

- Design and implementation
  - Object-oriented design
  - Qobj class used to represent quantum objects
    - Operators
    - State vectors
    - Density matrices
  - Library of utility functions that operate on Qobj instances

QuTiP core class:
Qobj

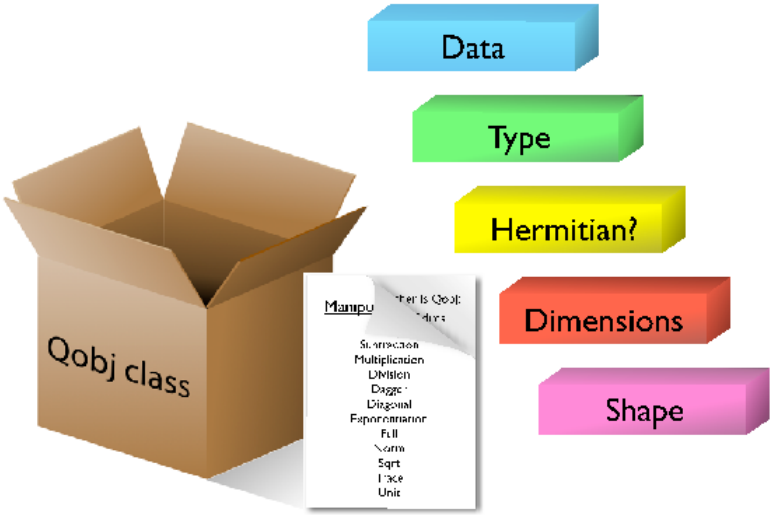


QuTiP: The Quantum Toolbox in Python

Quantum object class: `Qobj`

- Abstract representation of quantum states and operators
  - Matrix representation of the object
  - Structure of the underlaying state space, Hermiticity, type, etc.
  - Methods for performing all common operations on quantum objects:

    `eigs(),dag(),norm(),unit(),expm(),sqrt(),tr(), ...`
  - Operator arithmetic with implementations of: +. -, *, ...



Example: built-in operator $\hat{\sigma}_x$

```
>>> sigmax()

Quantum object: dims = [[2], [2]], shape = [2, 2],
type = oper, isHerm = True
Qobj data =
[[ 0.  1.]
 [ 1.  0.]]
```

Example: built-in state $|\alpha = 0.5\rangle$

```
>>> coherent(5, 0.5)

Quantum object: dims = [[5], [1]], shape = [5, 1], type = ket
Qobj data =
[[ 0.88249693]
 [ 0.44124785]
 [ 0.15601245]
 [ 0.04496584]
 [ 0.01173405]]
```

Evolution of quantum systems

The main use of QuTiP is quantum evolution. A number of solvers are available.

- Typical simulation workflow:
  i. Define parameters that characterize the system
  ii. Create Qobj instances for operators and states
  iii. Create Hamiltonian, initial state and collapse operators, if any
  iv. Choose a solver and evolve the system
  v. Post-process, visualize the data, etc.

- Available evolution solvers:
  - Unitary evolution: Schrödinger and von Neumann equations
  - Lindblad master equations
  - Monte-Carlo quantum trajectory method
  - Bloch-Redfield master equation
  - Floquet-Markov master equation
  - Propagators

Lindblad master equation

Equation of motion for the density matrix $\rho(t)$ for a quantum system that interacts with its environment:

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H(t), \rho(t)] + \sum_n \frac{1}{2}\left[2c_n\rho(t)c_n^\dagger - \rho(t)c_n^\dagger c_n - c_n^\dagger c_n \rho(t)\right]$$

$H(t) =$ system Hamiltonian

$c_n = \sqrt{\gamma_n}a_n$ describes the effect of the environment on the system

$\gamma_n =$ rate of the environment-system interaction process

How do we solve this equation numerically?

I. Construct the matrix representation of all operators
II. Evolve the ODEs for the unknown elements in the density matrix
III. For example, calculate expectation values for some selected operators for each $\rho(t)$

QuTiP: The Quantum Toolbox in Python

Lindblad master equation

Equation of motion for the density matrix $\rho(t)$ for a quantum system that interacts with its environment:

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H(t), \rho(t)] + \sum_n \frac{1}{2}\left[2c_n\rho(t)c_n^\dagger - \rho(t)c_n^\dagger c_n - c_n^\dagger c_n \rho(t)\right]$$

$$H(t) = \text{system Hamiltonian}$$

$$c_n = \sqrt{\gamma_n}a_n \text{ describes the effect of the environment on the system}$$

$$\gamma_n = \text{rate of the environment-system interaction process}$$

How do we solve this equation numerically in QuTiP?

```
from qutip import *

psi0 = ...              # initial state
H  = ...                # system Hamiltonian
c_op_list = [...]       # collapse operators
e_op_list = [...]       # expectation value operators

tlist = linspace(0, 10, 100)
result = mesolve(H, psi0, tlist, c_op_list, e_op_list)
```

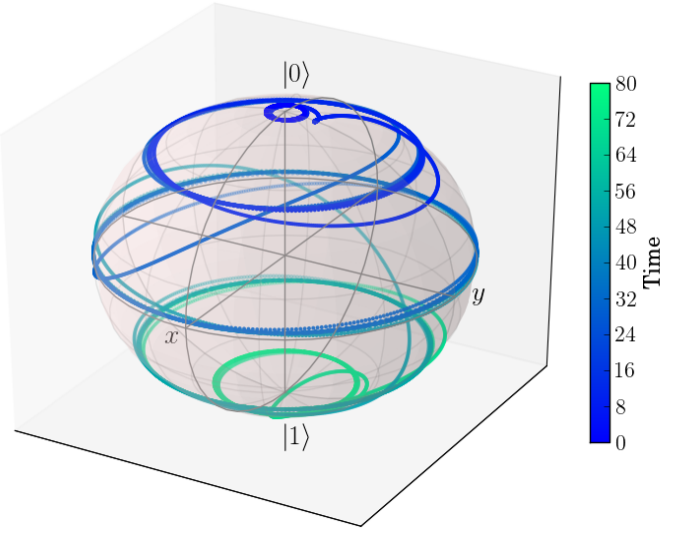
QuTiP: The Quantum Toolbox in Python

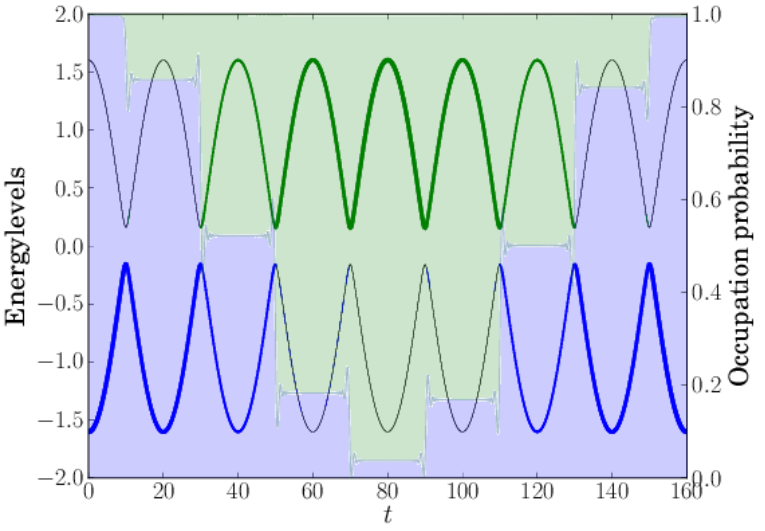
Example: time-dependence

Multiple Landau-Zener transitions

$$\hat{H}(t) = -\frac{\Delta}{2}\hat{\sigma}_z - \frac{\epsilon}{2}\hat{\sigma}_x - A\cos(\omega t)\hat{\sigma}_z$$

```
from qutip import *

# Parameters
epsilon = 0.0
delta = 1.0

# Initial state: start in ground state
psi0 = basis(2,0)

# Hamiltonian
H0 = - delta * sigmaz() - epsilon * sigmax()
H1 = - sigmaz()
h_t = [H0, [H1, 'A * cos(w*t)']]
args = {'A': 10.017, 'w': 0.025*2*pi}

# No dissipation
c_ops = []

# Expectation values
e_ops = [sigmax(), sigmay(), sigmaz()]

# Evolve the system
tlist = linspace(0, 160, 500)
output = mesolve(h_t, psi0, tlist, c_ops, e_ops, args)

# Process and plot result
# ...
```





QuTiP: The Quantum Toolbox in Python

QuTiP: Examples

```
from qutip import *

def evals_multw(w1list, w2, w3, g12, g13):

    # Pre-compute operators for the hamiltonian
    sz1 = tensor(sigmaz(), qeye(2), qeye(2))
    sx1 = tensor(sigmax(), qeye(2), qeye(2))

    sz2 = tensor(qeye(2), sigmaz(), qeye(2))
    sx2 = tensor(qeye(2), sigmax(), qeye(2))

    sz3 = tensor(qeye(2), qeye(2), sigmaz())
    sx3 = tensor(qeye(2), qeye(2), sigmax())

    evals_mat = np.zeros((len(w1list),2**3))
    for idx, w1 in enumerate(w1list):
        # evaluate the Hamiltonian
        H = w1 * sz1 + w2 * sz2 + w3 * sz3 +\
            g12 * sx1 * sx2 + g13 * sx1 * sx3
        # find the energy eigenvalues of the composite system
        evals = H.eigenenergies()
        evals_mat[idx,:] = np.real(evals)

    return evals_mat

w1  = 1.0 * 2 * np.pi   # atom 1 frequency: sweep this one
w2  = 0.9 * 2 * np.pi   # atom 2 frequency
w3  = 1.1 * 2 * np.pi   # atom 3 frequency
g12 = 0.05 * 2 * np.pi   # atom1-atom2 coupling strength
g13 = 0.05 * 2 * np.pi   # atom1-atom3 coupling strength

w1list = np.linspace(0.75, 1.25, 50) * 2 * np.pi # atom 1 frequency
range
evals_mat = evals_multw(w1list, w2, w3, g12, g13)
```

```
import matplotlib.pyplot as plt
plt.rcParams['font.size'] = 20
fig, ax = plt.subplots(figsize=(12,6))

for n in [1,2,3]:
    ax.plot(w1list / (2*np.pi), (evals_mat[:,n]-evals_mat[:,0]) / (2*np.pi), 'b')

ax.set_xlabel('Energy splitting of electron 1')
ax.set_ylabel('Eigenenergies')
ax.set_title('Energy spectrum of three coupled electrons')
plt.show()
```

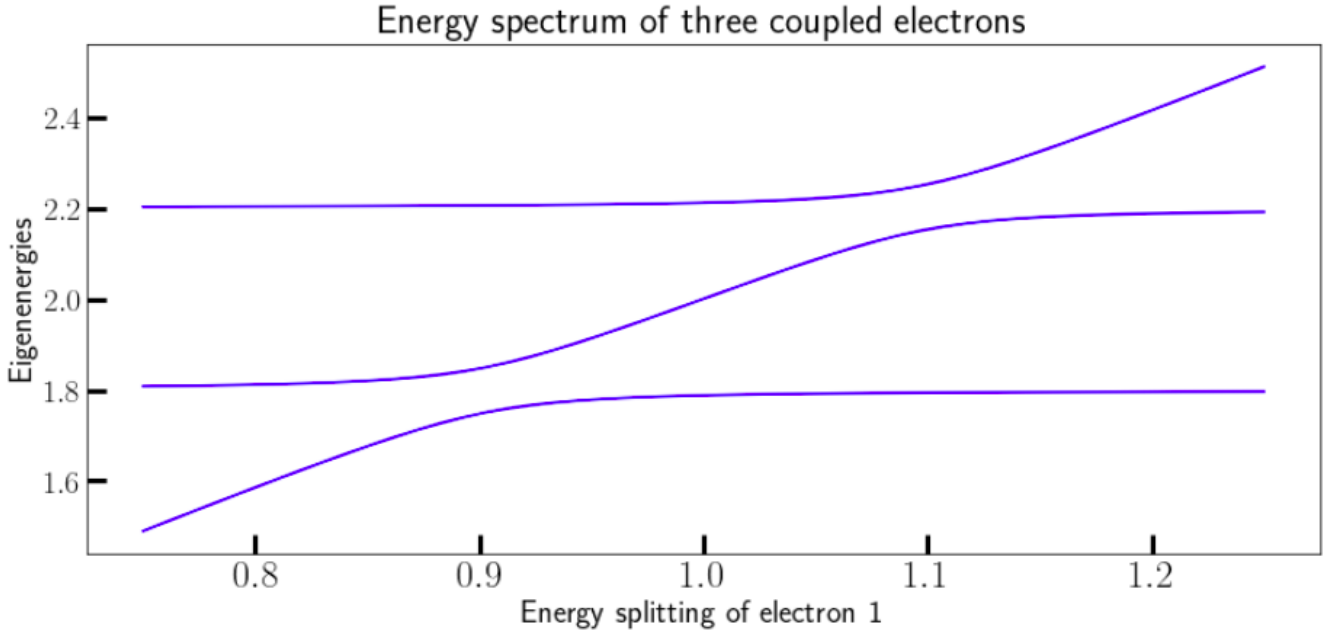
See Jupyter Notebook:
‘QUTIP.ipynb’

$$H = \sum_{i=0}^{N-1} \omega_i \sigma_i^z + g \sum_{i=0}^{N-1} \sigma_i^x \sigma_{i+1}^x$$

QuTiP: The Quantum Toolbox in Python

QuTiP: Examples

$$H = \sum_{i=0}^{N-1} \omega_i \sigma_i^z + g \sum_{i=0}^{N-1} \sigma_i^x \sigma_{i+1}^x$$



See Jupyter Notebook:
'QUTIP.ipynb'

QuTiP: The Quantum Toolbox in Python

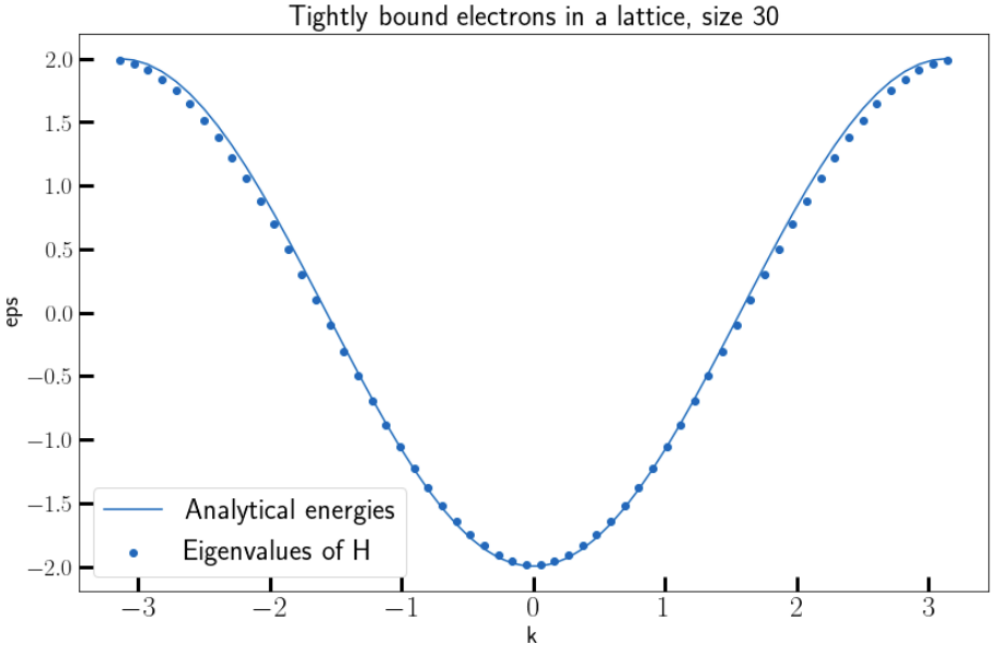
QuTiP: Examples

```
#N = 100
N = 30

H = sum([basis(N,i) * basis(N, i + 1).dag() for i in range(N - 1)]) +\
    sum([basis(N,i) * basis(N, i - 1).dag() for i in range(1, N)])

evals = H.eigenenergies()
# satisfy periodic boundary conditions we need E(-k) = E(k)
numerical = np.concatenate((np.flip(evals, 0), evals), axis=0)


import numpy as np
import matplotlib.pyplot as plt

plt.rcParams['figure.figsize'] = (12,8)
plt.rcParams['font.size'] = 20
k = np.linspace(-np.pi, np.pi, 2*N)

#plt.scatter(k[::3],numerical[::3].real, label='Eigenvalues of H')
plt.scatter(k,numerical.real, label='Eigenvalues of H')

analytical = -2 * np.cos(k)
plt.title(f"Tightly bound electrons in a lattice, size {N}")
plt.plot(k,analytical, label='Analytical energies')
plt.xlabel("k")
plt.ylabel("eps")
plt.legend()
plt.show()
```

See Jupyter Notebook:
'QUTIP.ipynb'

$$H = \frac{1}{2}\sum_{i=0}^{N-1}\left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right)$$

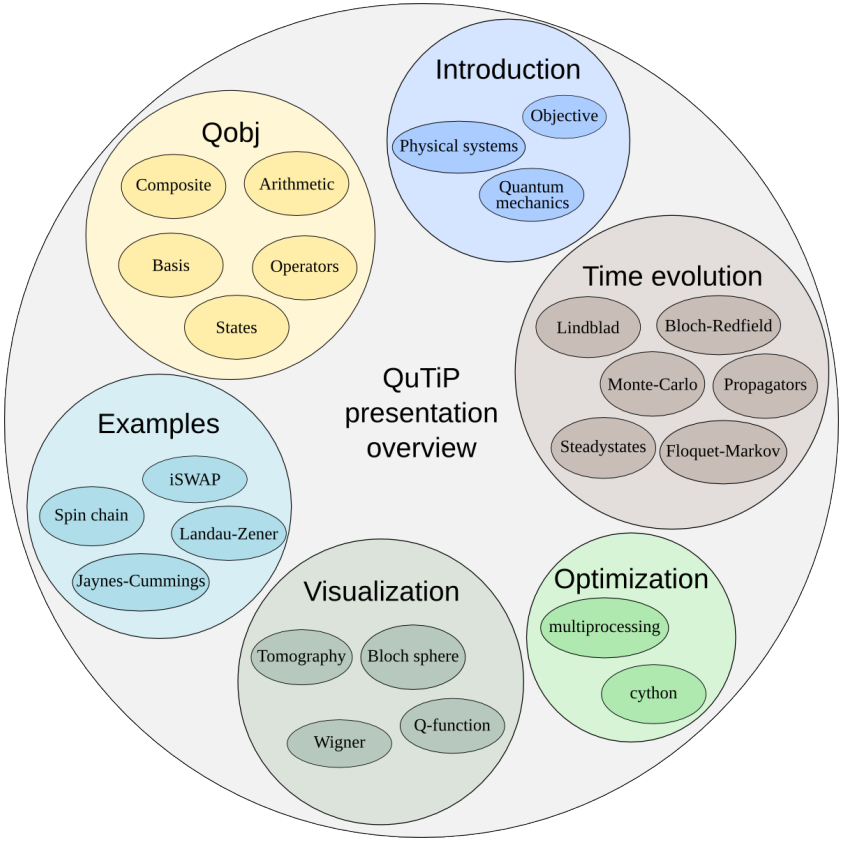
$$c_i^\dagger|0\rangle = |i\rangle \qquad c|i\rangle = |0\rangle \qquad c_i^\dagger|i\rangle = c|0\rangle = 0.$$



QuTiP: The Quantum Toolbox in Python

More information at: http://qutip.org

- QuTiP: framework for numerical simulations of quantum systems
  - Generic framework for representing quantum states and operators
  - Large number of dynamics solvers
- Main strengths:
  - Ease of use: complex quantum systems can programmed rapidly and intuitively
  - Flexibility: Can be used to solve a wide variety of problems
  - Performance: Near C-code performance due to use of Cython for time-critical functions



Partial Differential Equations

PDE: Imposes relations between the various partial derivatives of a multivariable function.

$$f\left(x, y, z \ldots \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z} \ldots \frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial y^2}, \frac{\partial^2 u}{\partial z^2} \ldots\right) = 0$$

Solve for u(x,y,z, ...), subject to **Boundary Conditions**

Partial Differential Equations

PDE: Imposes relations between the various partial derivatives of a multivariable function.

Types of Linear PDE:

1) Parabolic: $\Delta = 0$ $\quad \frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$ Heat Equation

2) Hyperbolic: $\Delta > 0$ $\quad \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$ Wave Equation

3) Elliptic: $\Delta < 0$ $\quad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$ Laplace Equation

$$A\frac{\partial^2}{\partial x^2} + 2B\frac{\partial^2}{\partial x \partial y} + C\frac{\partial^2}{\partial y^2} + \ldots \text{ lower order terms } \cdots = 0$$

$$\Delta \equiv B^2 - AC$$

Partial Differential Equations

PDE: Imposes relations between the various partial derivatives of a multivariable function.

Types of Boundary Conditions in PDE's:

1) Dirichlet: $u(x,y) \; \forall \, (x,y) \in \partial\mathcal{B}$

2) Neumann: $\vec{\nabla} u(x,y) \cdot \hat{n}(x,y) \; \forall \, (x,y) \in \partial\mathcal{B}$

3) Cauchy: Dirichlet + Neumann

$$A\frac{\partial^2}{\partial x^2} + 2B\frac{\partial^2}{\partial x \partial y} + C\frac{\partial^2}{\partial y^2} + \ldots \text{ lower order terms } \cdots = 0$$

$$\text{Domain } \; \mathcal{B} \; \text{ Boundary } \partial\mathcal{B}$$

Partial Differential Equations

PDE: Imposes relations between the various partial derivatives of a multivariable function.

Numerical Methods for PDE's

Finite Difference Methods (FDM):

Approximate the solutions to using finite difference equations to approximate derivatives. Reduce the ODE to a Linear Algebra Equation

Finite Volume Methods (FVM):

Divide the domain into subdomains and use Gauss/Stoke's theorem to reduce PDE to integral equations, solved using quadratures in alegebraic form

Finite Element Methods (FEM):

Divide the domain intosubdomains and use Gauss/Stoke's theorem to reduce PDE to integral equations, weighed by a choice of basis states, discretize them solve as linear eqns.

$$A\frac{\partial^2}{\partial x^2} + 2B\frac{\partial^2}{\partial x \partial y} + C\frac{\partial^2}{\partial y^2} + \ldots \text{ lower order terms } \cdots = 0$$

$$\text{Domain } \mathcal{B} \quad \text{Boundary } \partial\mathcal{B}$$

Partial Differential Equations

PDE: Imposes relations between the various partial derivatives of a multivariable function.

Numerical Methods for PDE's: Unlike ODE's there are no general methods

- Numerical Solutions to PDEs are more complex than ODEs
- Each type of PDE requires its own algorithm
- Algorithms are also dependent on the boundary conditions

$$A\frac{\partial^2}{\partial x^2} + 2B\frac{\partial^2}{\partial x \partial y} + C\frac{\partial^2}{\partial y^2} + \ldots \text{ lower order terms } \cdots = 0$$

$$\text{Domain } \mathcal{B} \quad \text{Boundary } \partial\mathcal{B}$$

Finite Difference Methods: 2D Poisson Equation (Dirichlet)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -4\pi\rho(x, y)$$

1) Divide the 2D Domain into a discrete lattice.

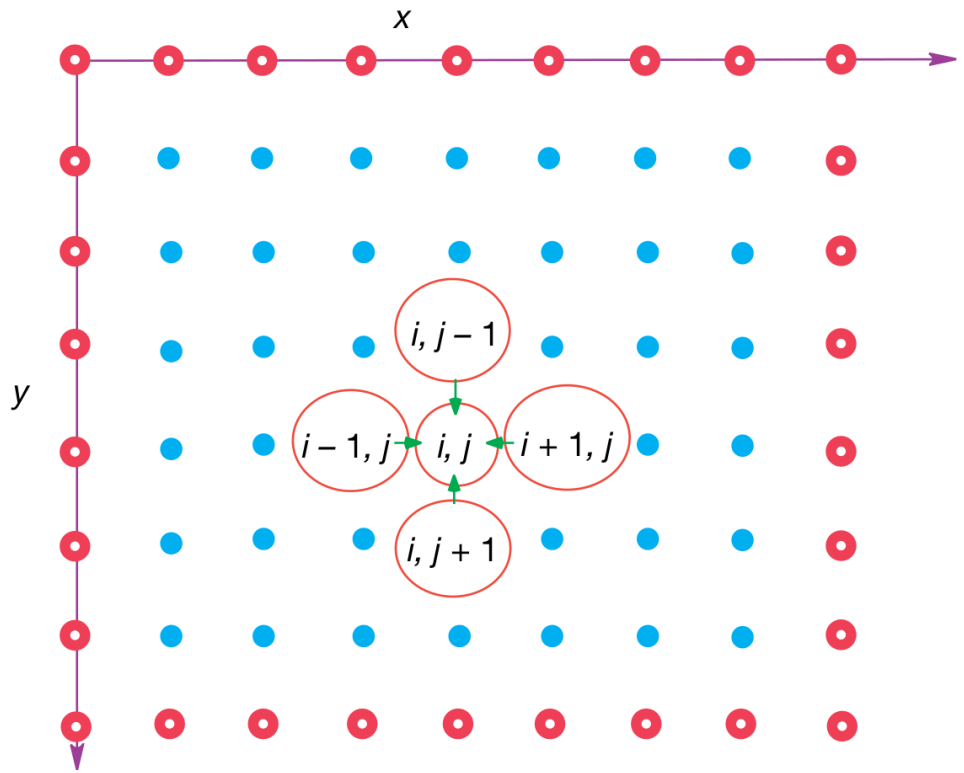
2) Replace the partial derivatives by finite difference approximations evaluated at the lattice points

3) Reduce the PDE to a system of linear algebra equations, with boundary conditions added as extra equations, then solve them (similar to the ‘matrix method’ for ODE’s)

4) Alternatively, reduce the PDE to a system of iterative equations, then update the domain values, starting from the boundary values.

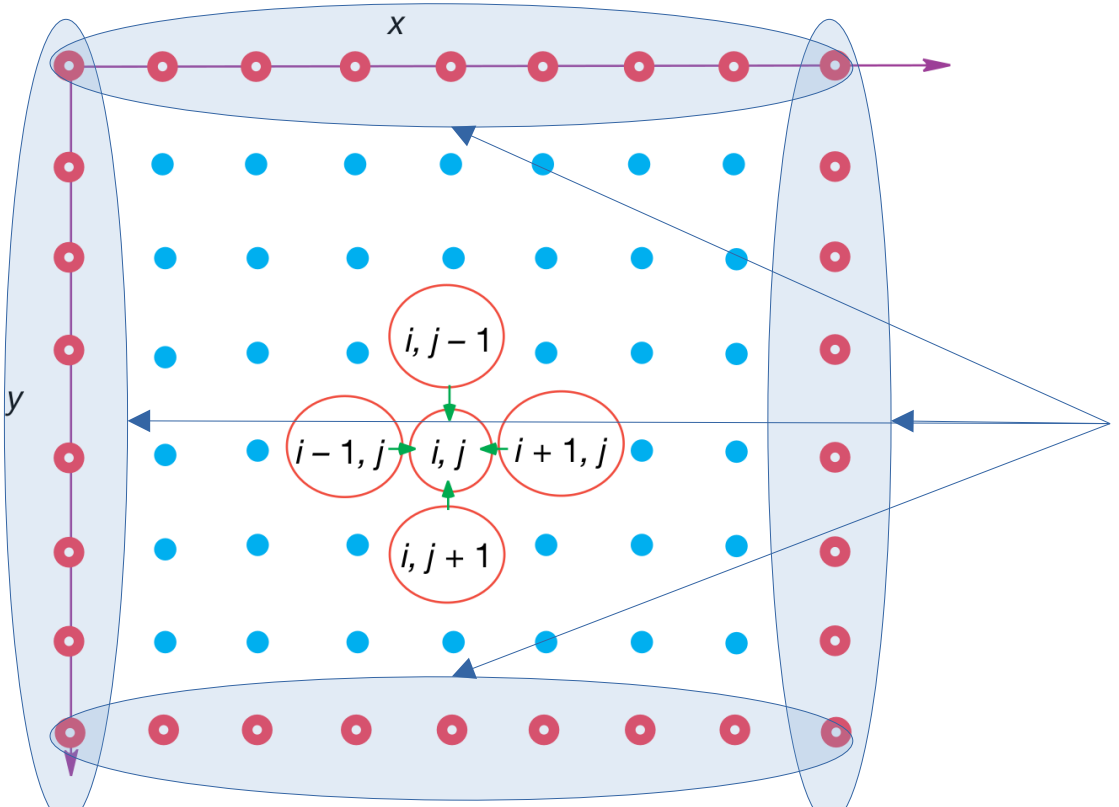
Finite Difference Methods: 2D Poisson Equation (Dirichlet)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -4\pi\rho(x, y)$$



Finite Difference Methods: 2D Poisson Equation (Dirichlet)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -4\pi\rho(x, y)$$



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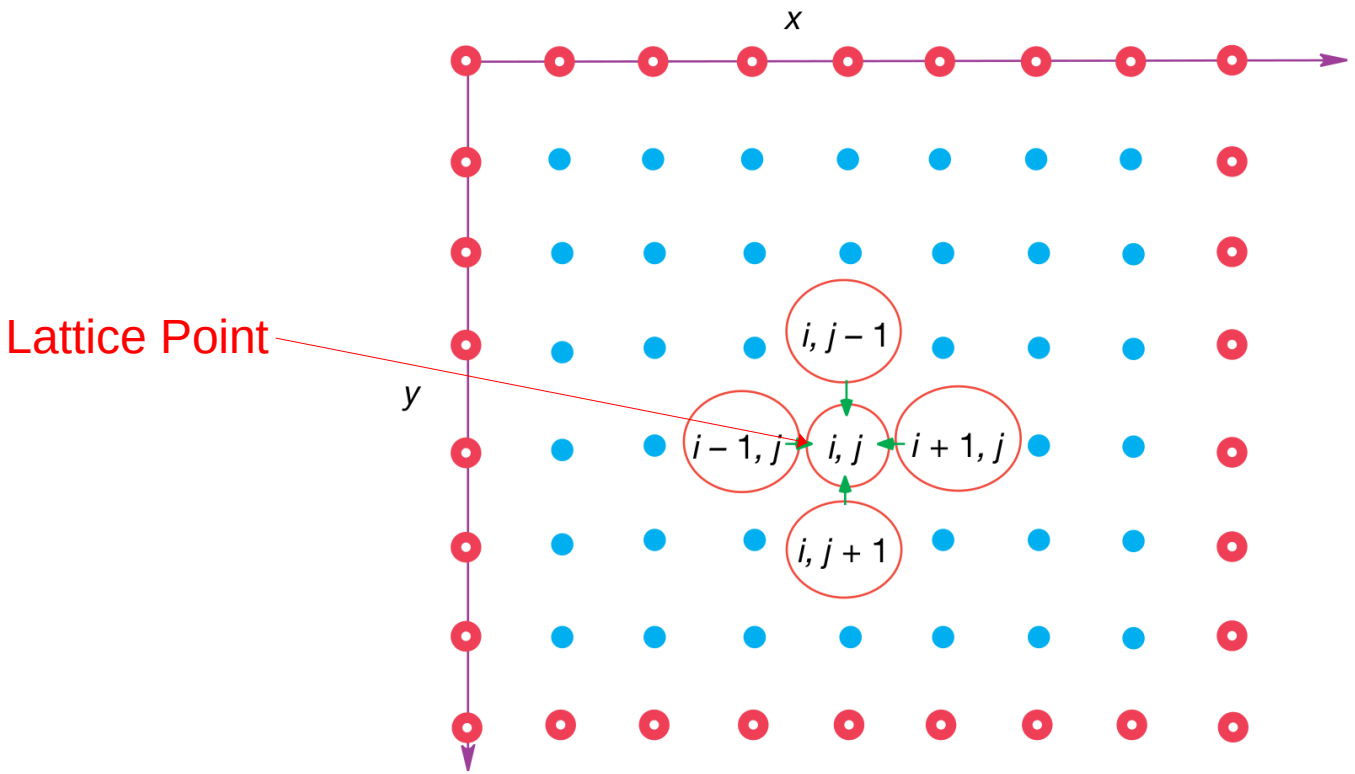

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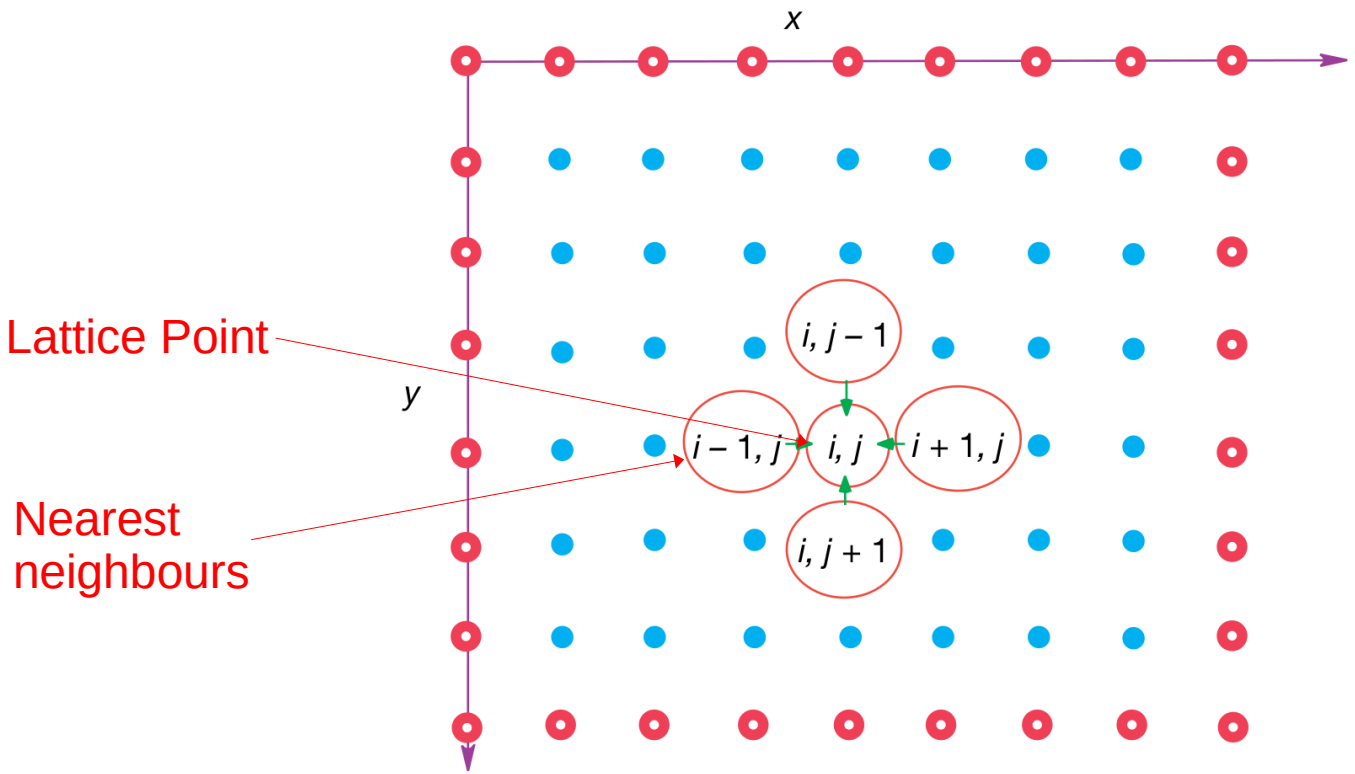

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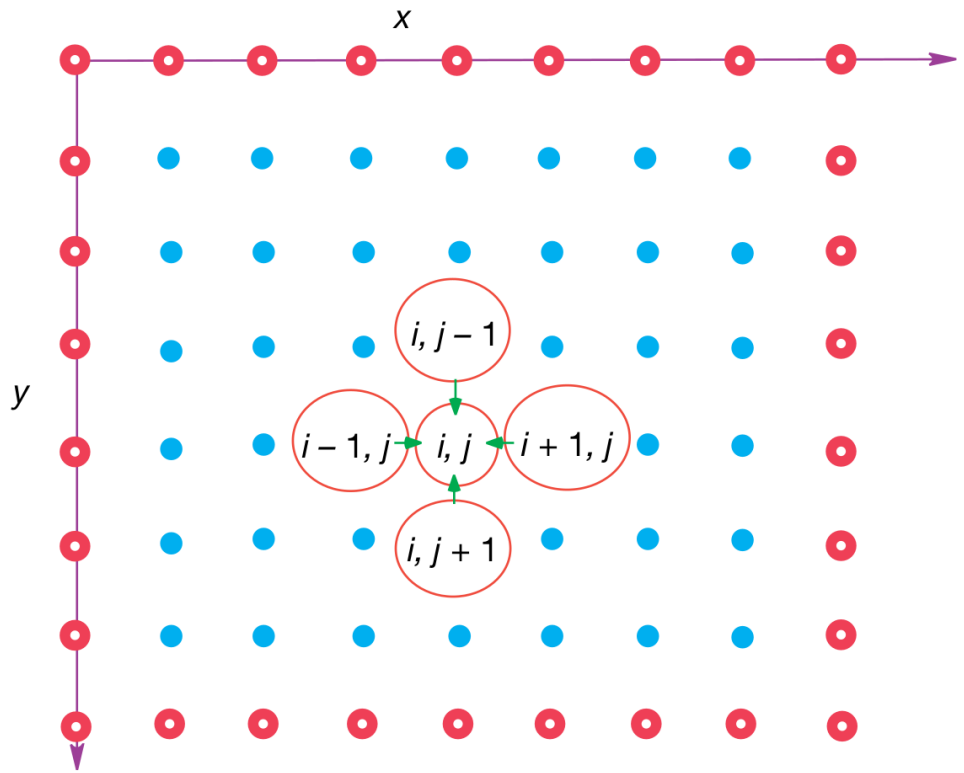

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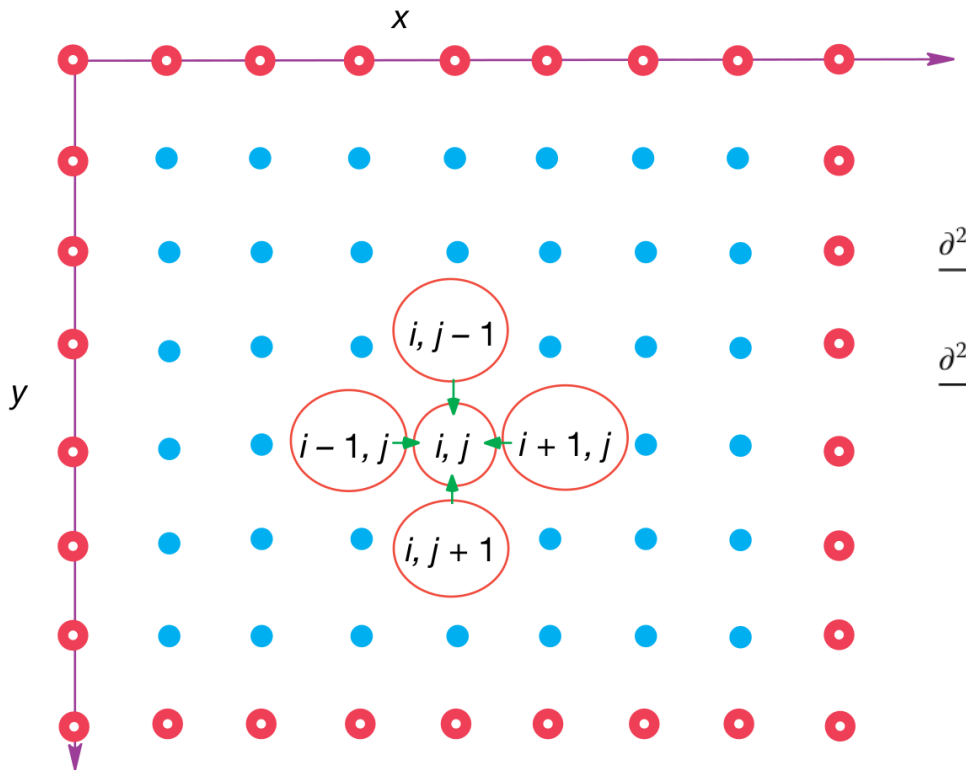


Three point difference formula!

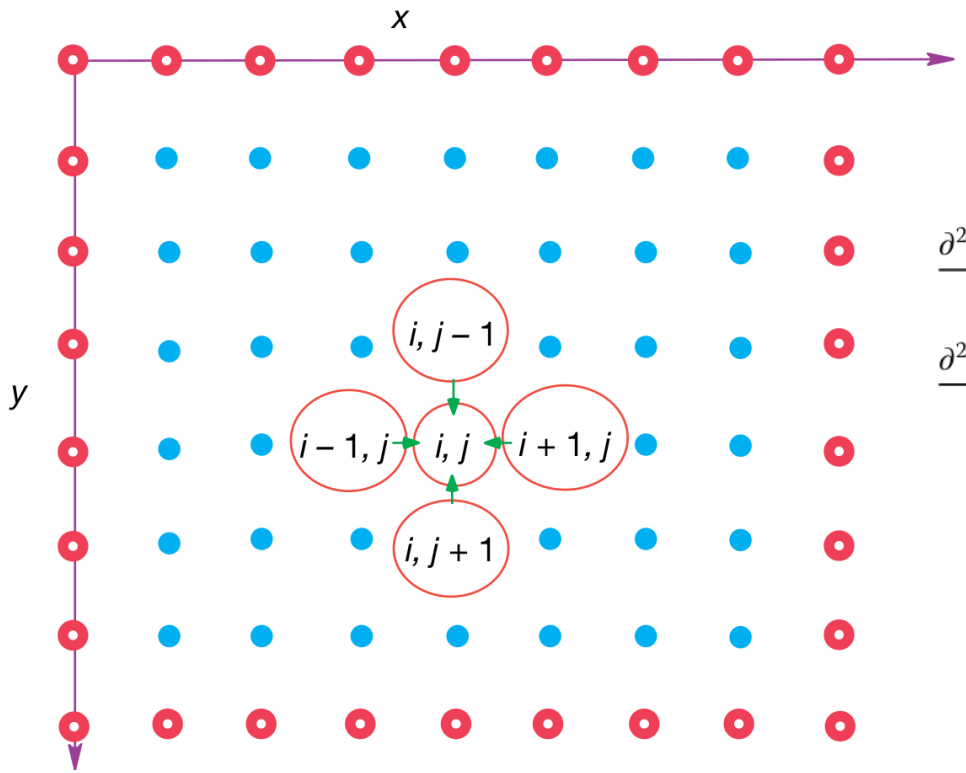
$$\frac{\partial^2 U(x, y)}{\partial x^2} \simeq \frac{U(x + \Delta x, y) + U(x - \Delta x, y) - 2U(x, y)}{(\Delta x)^2},$$

$$\frac{\partial^2 U(x, y)}{\partial y^2} \simeq \frac{U(x, y + \Delta y) + U(x, y - \Delta y) - 2U(x, y)}{(\Delta y)^2}.$$

Finite Difference Methods: 2D Poisson Equation (Dirichlet)

$$\frac{U(x+\Delta x, y)+U(x-\Delta x, y)-2U(x, y)}{(\Delta x)^2}$$

$$+\frac{U(x, y+\Delta y)+U(x, y-\Delta y)-2U(x, y)}{(\Delta y)^2}=-4\pi\rho\ .$$



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Finite Difference Methods: 2D Poisson Equation (Dirichlet)

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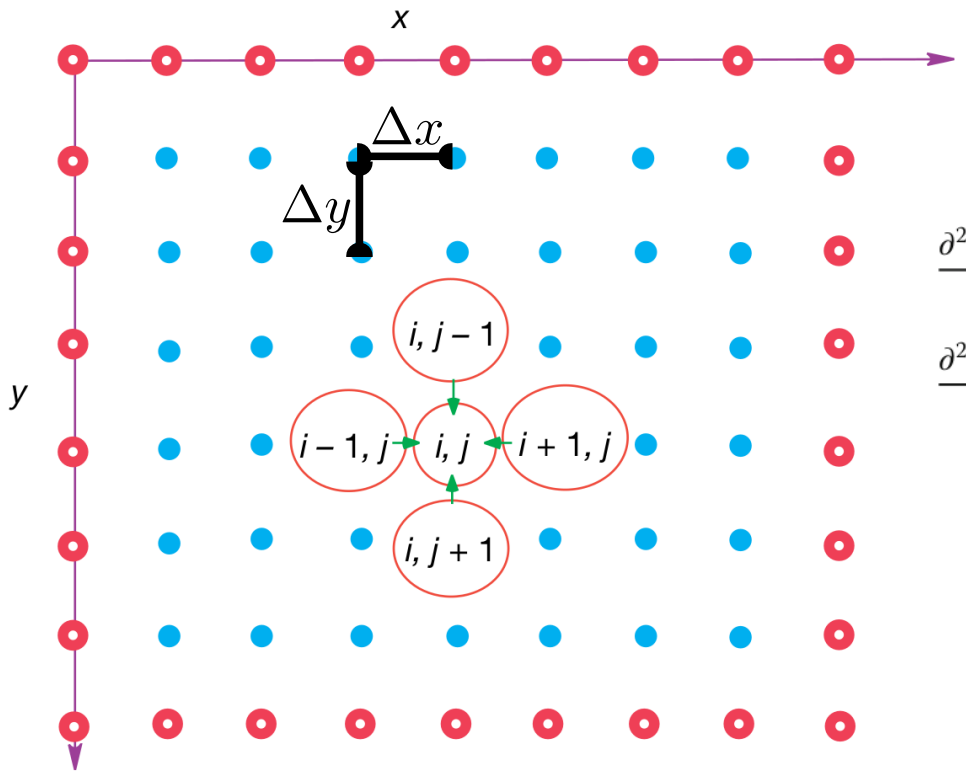

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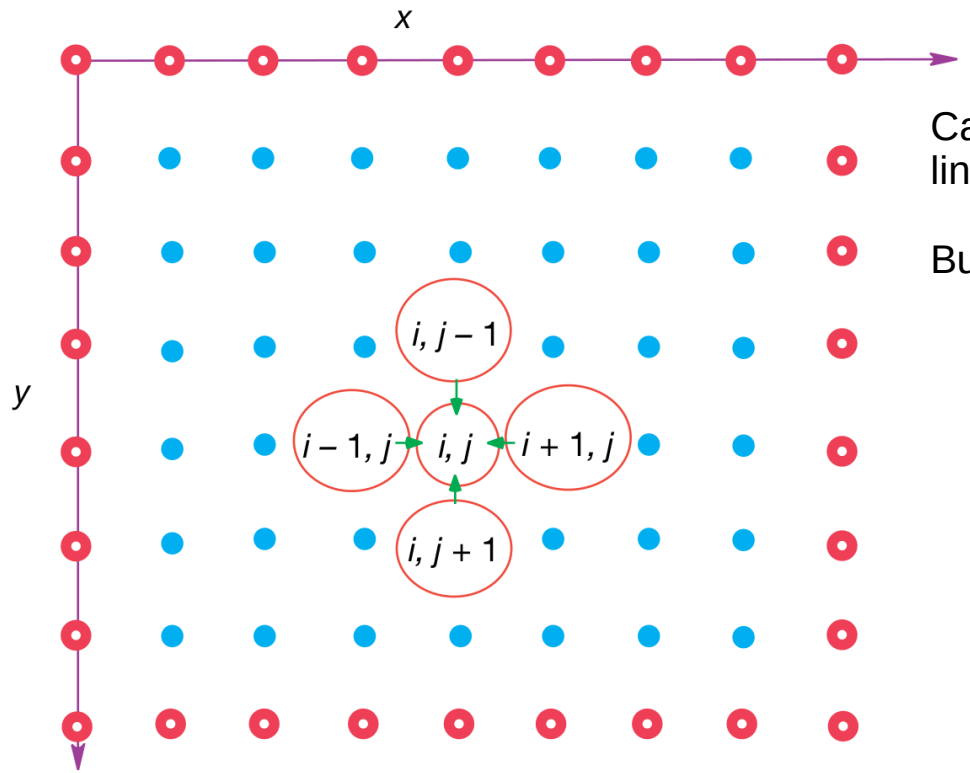
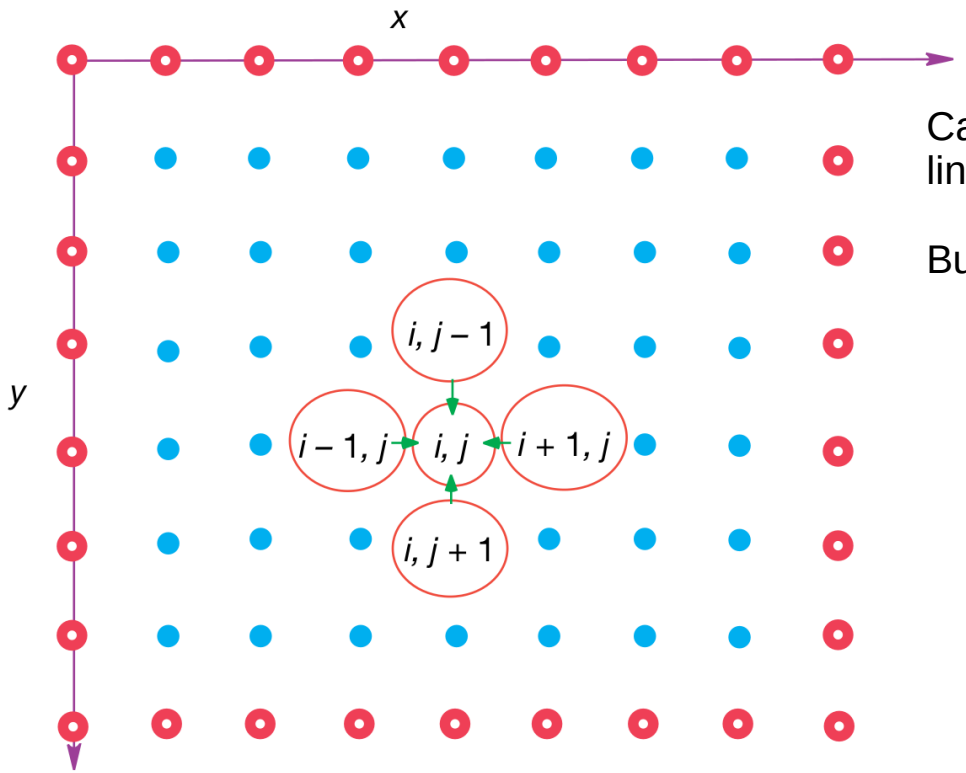


Can solve these equations numerically using linear algebra methods

But, there is a better way (less memory)

Finite Difference Methods: 2D Poisson Equation (Dirichlet)

$$U_{i,j} = \frac{1}{4}\left[U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}\right] + \pi\rho(i\Delta, j\Delta)\Delta^2$$



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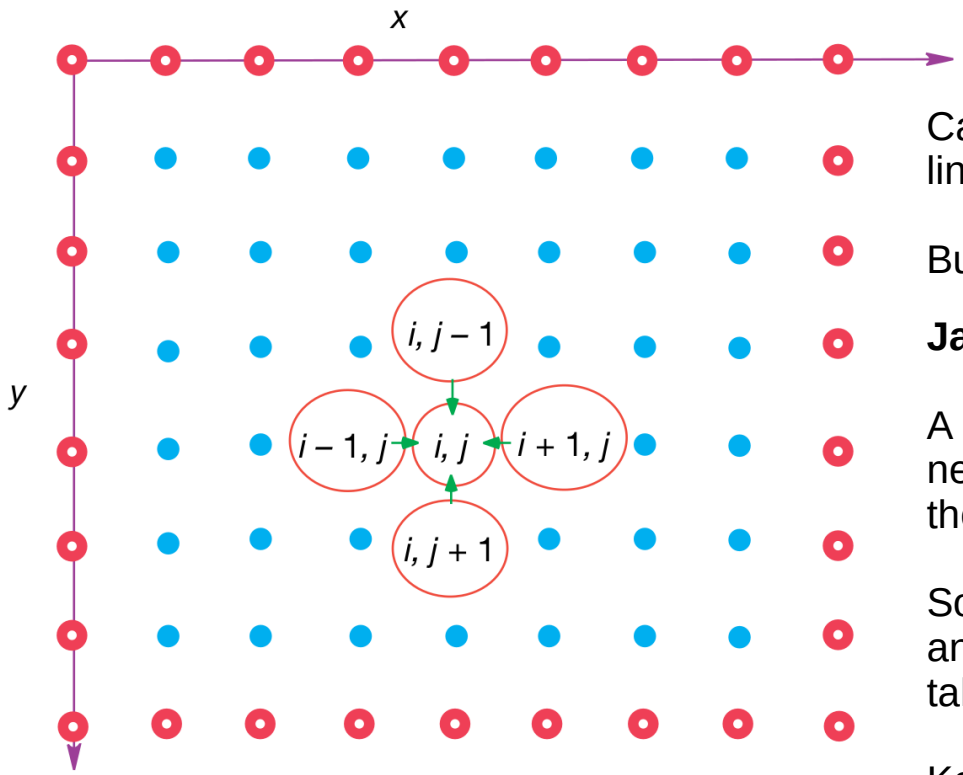

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Jacobi Update:

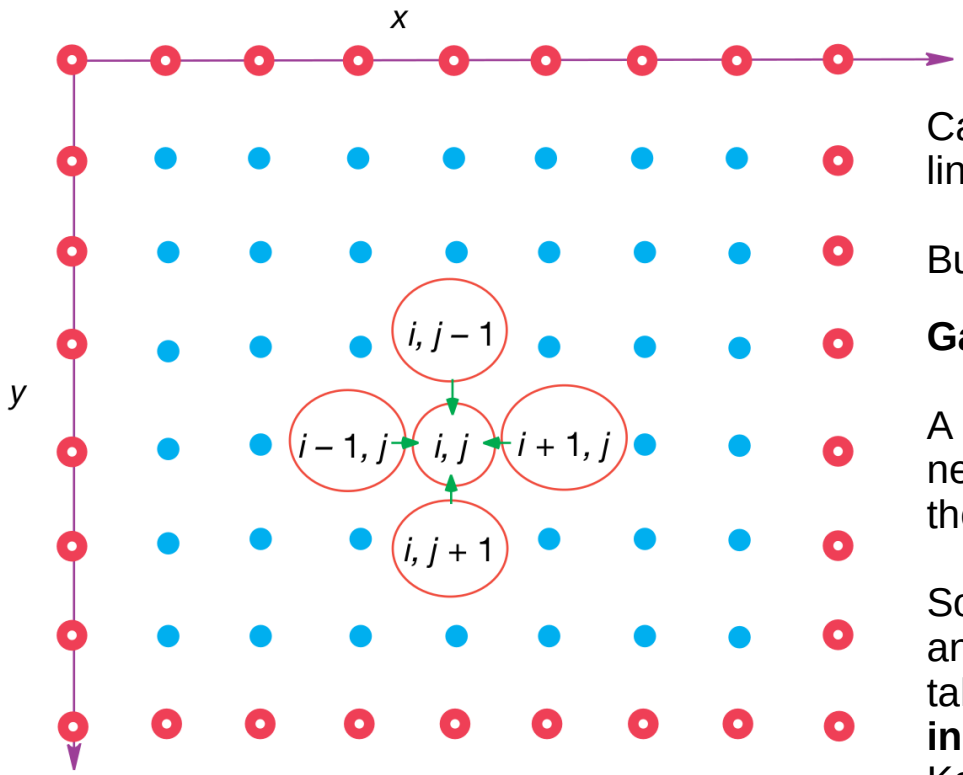
A proper solution will be the **average** of the nearest neighbors plus a contribution from the charge density

So, start with an initial guess for the potential and improve it by striding through the lattice taking the average over nearest neighbors

Keep doing this until solution converges

Finite Difference Methods: 2D Poisson Equation (Dirichlet)

$$U_{i,j}^{(\text{new})} = \frac{1}{4}\left[U_{i+1,j}^{(\text{old})} + U_{i-1,j}^{(\text{new})} + U_{i,j+1}^{(\text{old})} + U_{i,j-1}^{(\text{new})}\right]$$



Can solve these equations numerically using linear algebra methods

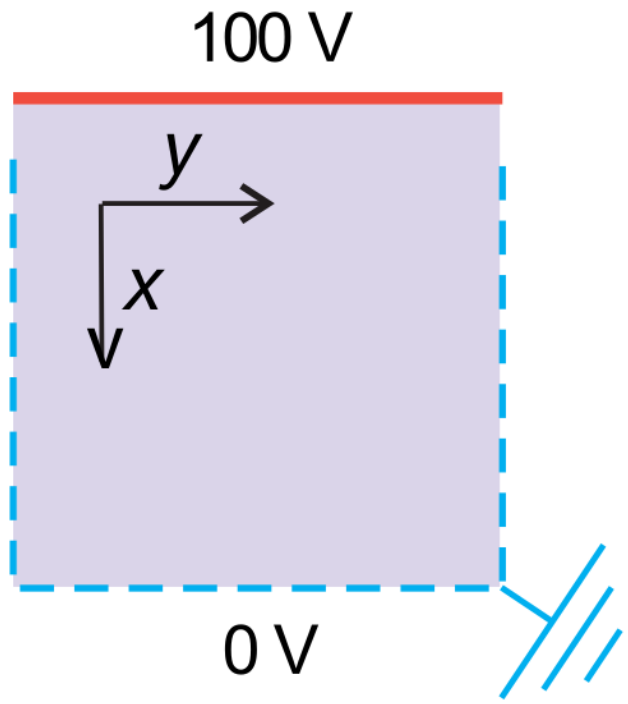
But, there is a better way (less memory)

Gauss-Seidel Update:

A proper solution will be the **average** of the nearest neighbors plus a contribution from the charge density

So, start with an initial guess for the potential and improve it by striding through the lattice taking the average over nearest neighbors **in real time.**
Keep doing this until solution converges

Finite Difference Methods: 2D Poisson Equation (Dirichlet)



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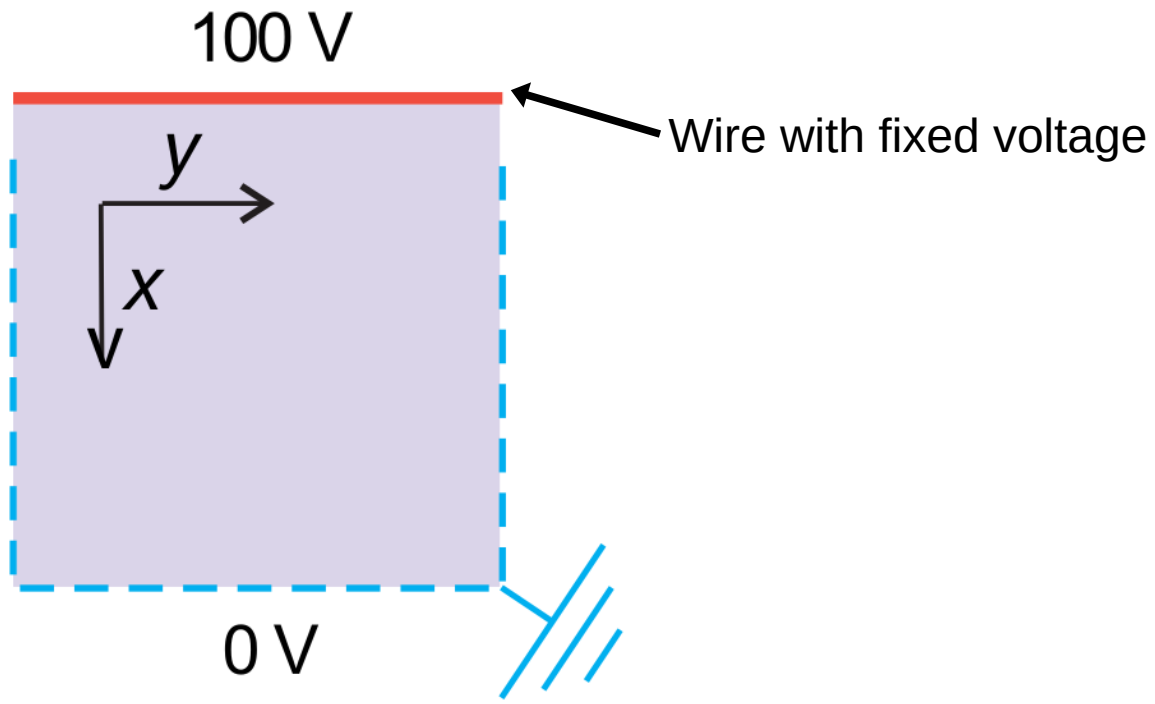

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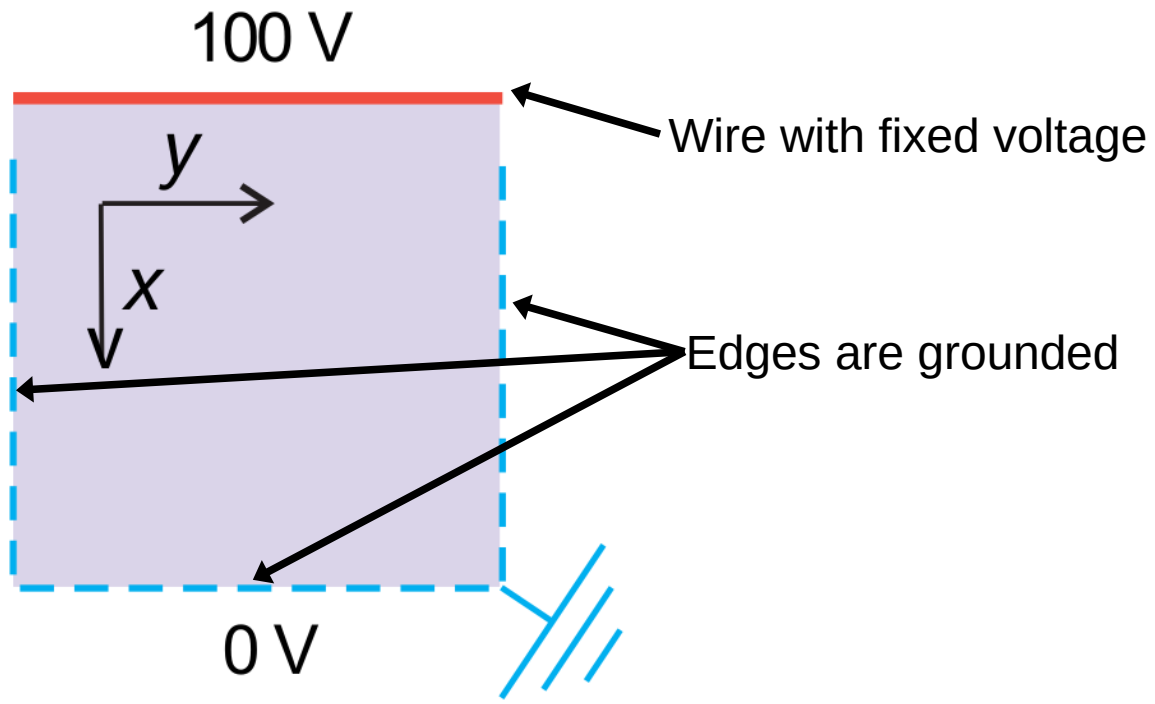

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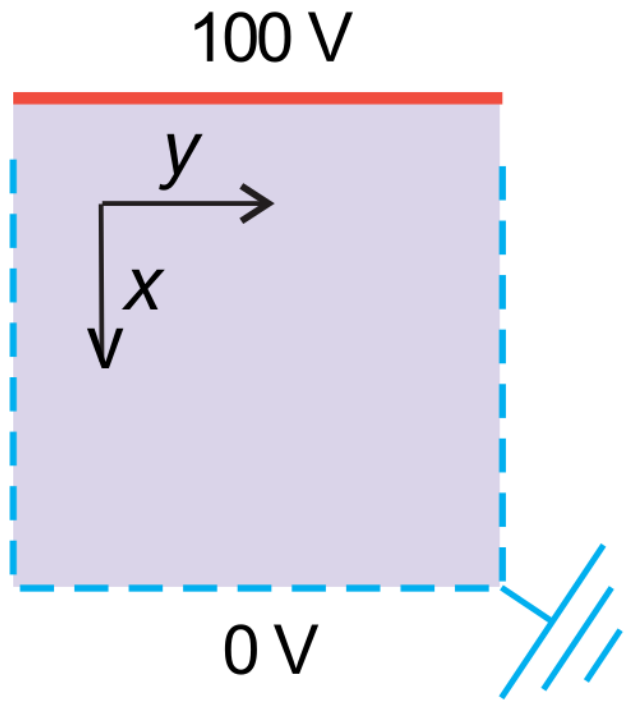

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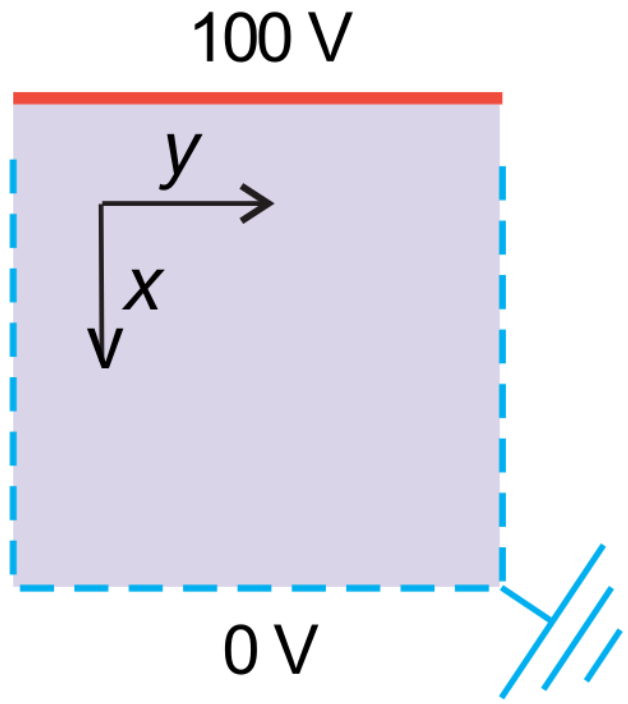
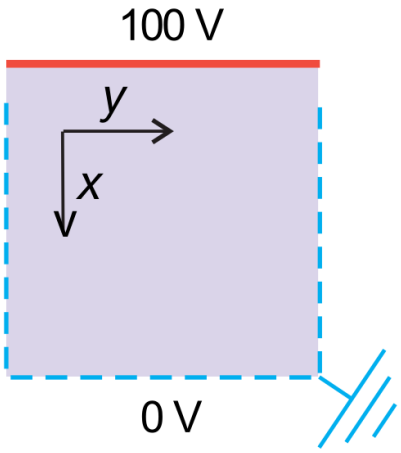



```
import numpy as np
import matplotlib.pyplot as plt

plt.rcParams['figure.figsize'] = (12,8)
plt.rcParams['font.size'] = 20


Nmax = 100
V_wire = 100

V = np.zeros((Nmax, Nmax))
V[:,0] = V_wire                                  # Line at V_wire volts

print ("Running the Jacobi Update Solver ...")

def jacobi_update(V, Niter=70):
    Nmax = V.shape[0]
    for iter in range(Niter):
        for i in range(1, Nmax-2):
            for j in range(1,Nmax-2):
                V[i,j] = 0.25*(V[i+1,j]+V[i-1,j]+V[i,j+1]+V[i,j-1])
    return V

V = jacobi_update(V)
x = np.arange(0, Nmax-1, 2);  y = np.arange(0, 50, 2)
X, Y = np.meshgrid(x,y)

def functz(V):                                   # V(x, y)
    z = V[X,Y]
    return z

Z = functz(V)
ax = plt.figure().add_subplot(projection='3d')
ax.plot_wireframe(X, Y, Z, color = 'r')          # Red wireframe
ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_zlabel('Potential')
ax.view_init(30, 140)                            #Perspective
plt.show()                                       # Show fig
```

Partial Differential Equations

Finite Difference Methods: 2D Poisson Equation (Dirichlet)



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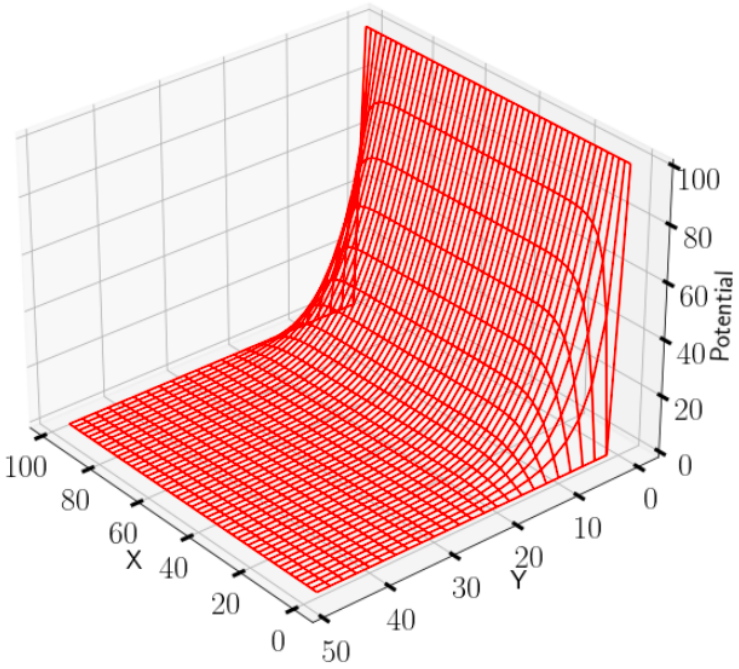

See Jupyter notebook: “PDE_FDM.ipynb”

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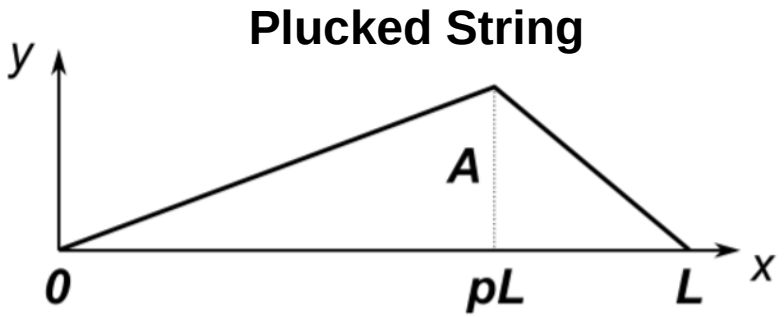
Finite Difference Methods: 1D Wave Equation (Dirichlet)

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$



Time-Stepping (Leapfrog Method):

1) Divide the space-time domain into a discrete lattice

2) Replace the partial derivatives by finite difference approximations evaluated at the lattice points

3) Reduce the PDE to a system of linear algebra equations, with initial/boundary conditions added as extra equations

4) Jacobi-update one time-step at a time, updating space-steps from the previous time

5) Repeat for all times

Finite Difference Methods: 1D Wave Equation (Dirichlet)

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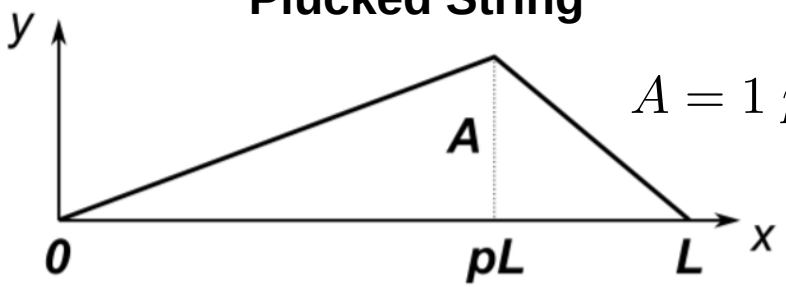
Plucked String



$A = 1 \; p = 0.8$

Time-Stepping (Leapfrog Method):

$$y(x, t=0) = \begin{cases} 1.25x/L\,, & x \le 0.8L\,, \\ (5 - 5x/L)\,, & x > 0.8L\,, \end{cases}$$

$$\frac{\partial y}{\partial t}(x, t=0) = 0$$

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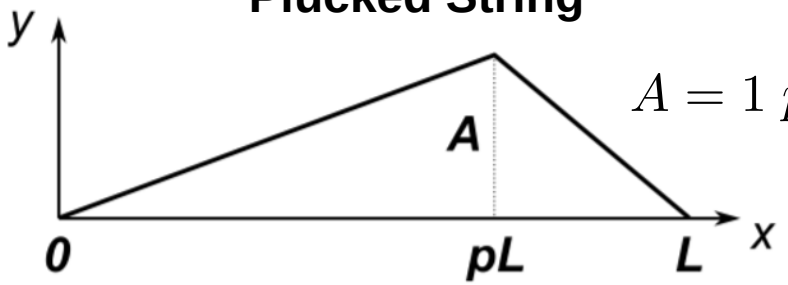

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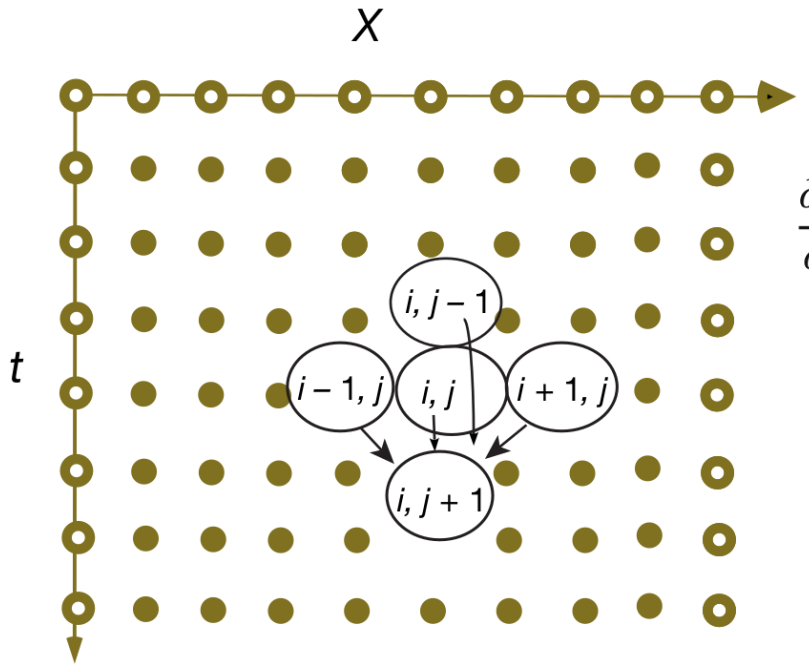

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$$\frac{\partial^2 y}{\partial t^2} \simeq \frac{y_{i,j+1} + y_{i,j-1} - 2y_{i,j}}{(\Delta t)^2}\,, \qquad \frac{\partial^2 y}{\partial x^2} \simeq \frac{y_{i+1,j} + y_{i-1,j} - 2y_{i,j}}{(\Delta x)^2}$$

$$\frac{y_{i,j+1} + y_{i,j-1} - 2y_{i,j}}{c^2(\Delta t)^2} = \frac{y_{i+1,j} + y_{i-1,j} - 2y_{i,j}}{(\Delta x)^2}$$

Contains three time values:

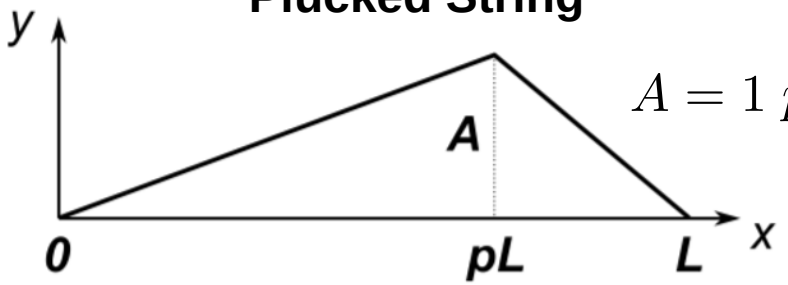
- j + 1 = the future,
- j = the present,
- j − 1 = the past

Predict the future solution from the present and past solutions

Finite Difference Methods: 1D Wave Equation (Dirichlet)

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$

Plucked String



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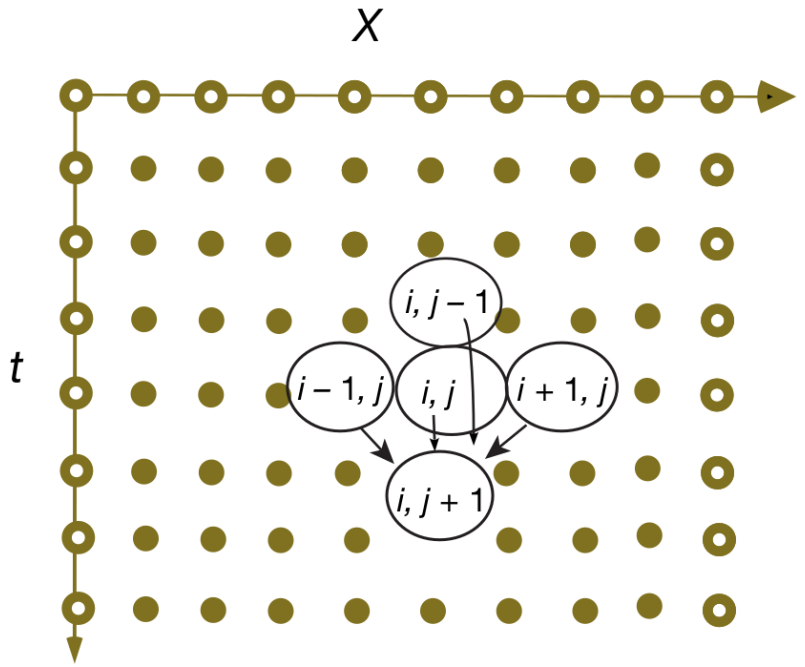


$$y(x, t=0) = \begin{cases} 1.25x/L\,, & x \le 0.8L\,, \\ (5 - 5x/L)\,, & x > 0.8L\,, \end{cases}$$

$$\frac{\partial y}{\partial t}(x, t=0) = 0$$

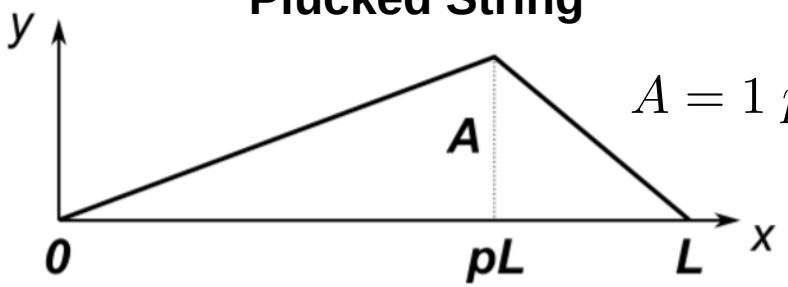
$$\frac{y_{i,j+1} + y_{i,j-1} - 2y_{i,j}}{c^2(\Delta t)^2} = \frac{y_{i+1,j} + y_{i-1,j} - 2y_{i,j}}{(\Delta x)^2}$$

$$y_{i,j+1} = 2y_{i,j} - y_{i,j-1} + \frac{c^2}{c'^2}\left[y_{i+1,j} + y_{i-1,j} - 2y_{i,j}\right]\,, \quad c' \overset{\text{def}}{=} \frac{\Delta x}{\Delta t}$$

Finite Difference Methods: 1D Wave Equation (Dirichlet)

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$

Plucked String



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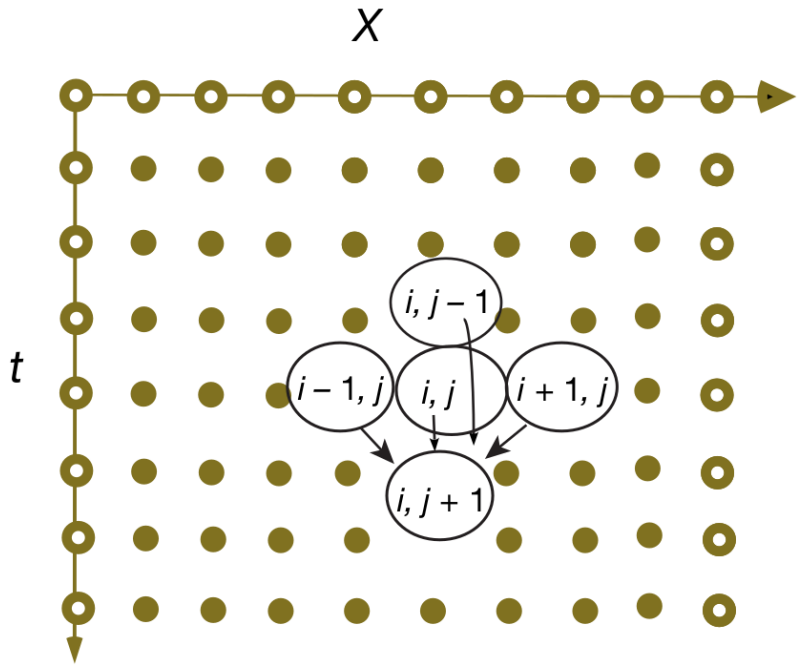

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Von-Neumann Stability Analysis
Ensures that the eigenfuncs don't blow up

$$c \le c' = \frac{\Delta x}{\Delta t}$$ **Courant condition**

Solution gets better with smaller time steps
But gets worse for smaller space steps

Finite Difference Methods: 1D Wave Equation (Dirichlet)

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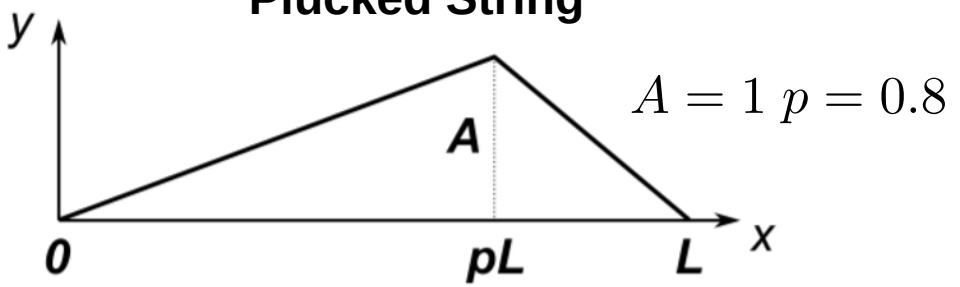
Plucked String



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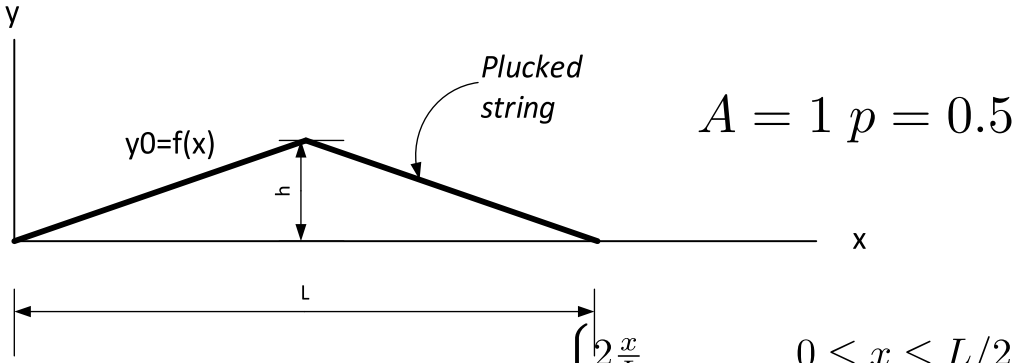
Homework: See if you can change the code to pluck the string in the middle

See Jupyter notebook: “PDE_FDM.ipynb”

Finite Difference Methods: 1D Wave Equation (Dirichlet)

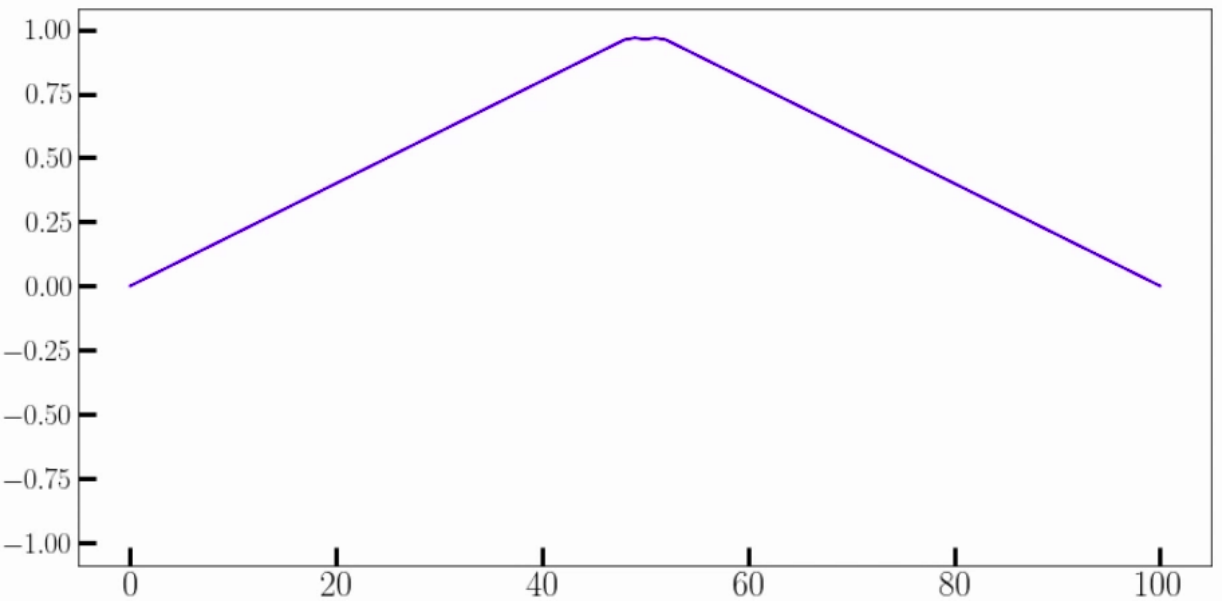
$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$



$$A = 1 \; p = 0.5$$

Time-Stepping (Leapfrog Method):

$$y(x, t=0) = \begin{cases} 2\frac{x}{L} & 0 \le x \le L/2 \\ 2\left(1 - \frac{x}{L}\right) & L/2 \le x \le L \end{cases}$$



Homework: See if you can change the code to pluck the string in the middle

See Jupyter notebook: “PDE_FDM.ipynb”

Finite Element Methods: 2D Poisson Equation (Dirichlet)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -4\pi\rho(x, y)$$

1) Reduce the PDE to an integral equation using Gauss/Stoke's theorem on the boundary

2) Divide the domain into a discrete mesh

3) Choose basis functions, usually polynomials, corresponding spatially to each mesh element

4) Write the RHS as a (known) linear superposition of these basis functions, and the LHS as a superposition with unknown coefficients

5) Substitute into the Integral equation and reduce it to a system of linear equations

6) Solve using BLAS or whatever.

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