https://gitlab.com/gersonjferreira/computational-quantum-mechanics

Computational Quantum Mechanics

Prof. Gerson J. Ferreira

INFIS/UFU 2020/1

Eigenstates of 2D systems

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2D systems

Now we want to consider a 2D Hamiltonian and solve: $H\psi(x,y) = E\psi(x,y)$

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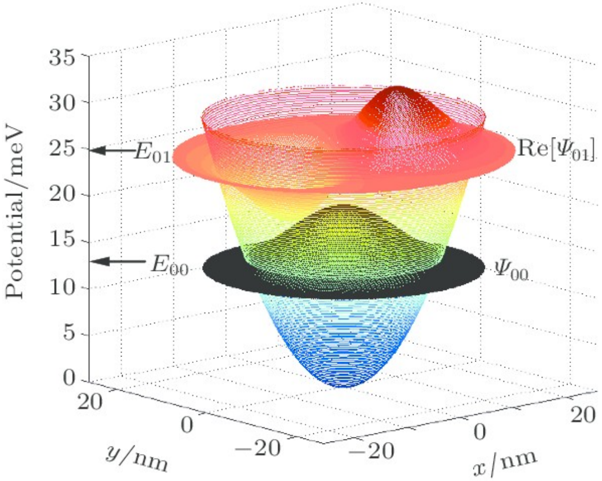

[Edvinsson, R. Soc. Open Sci. 5, 180387 (2018)]

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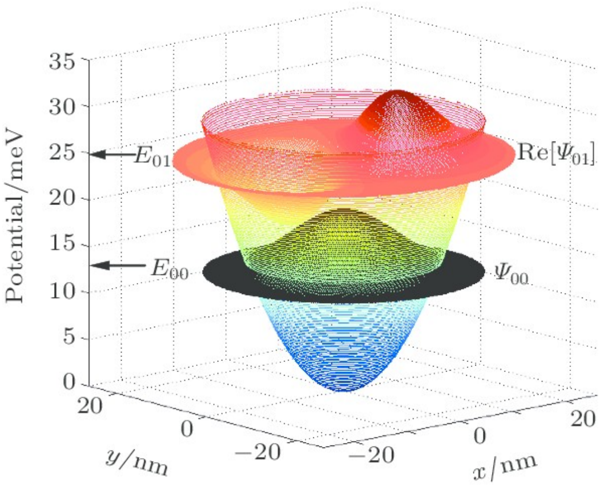
[Song et al. Chinese Phys. B 21, 057302 (2012)]



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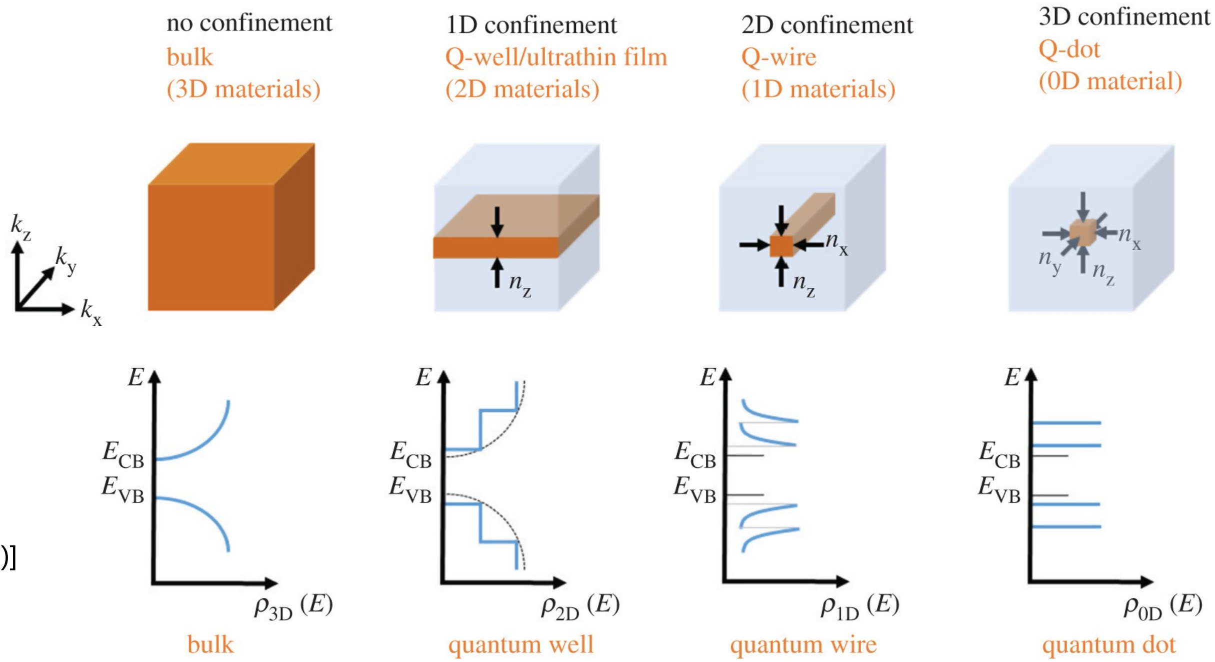

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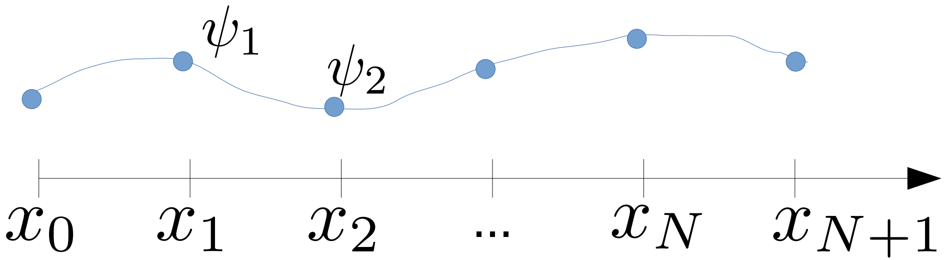

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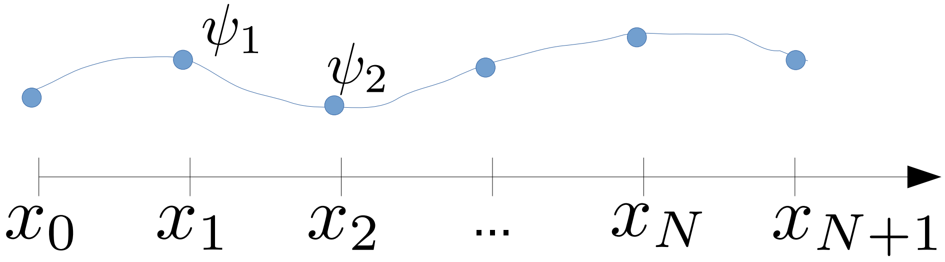

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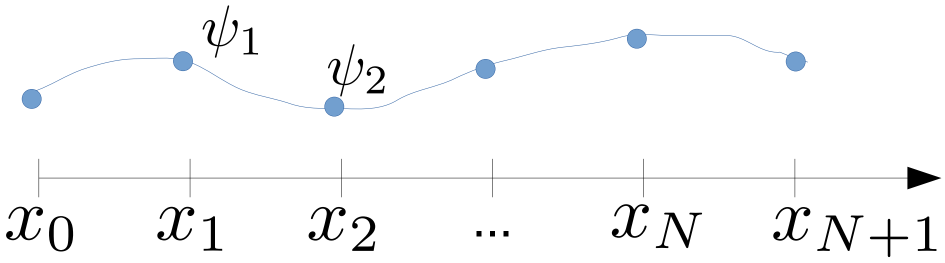

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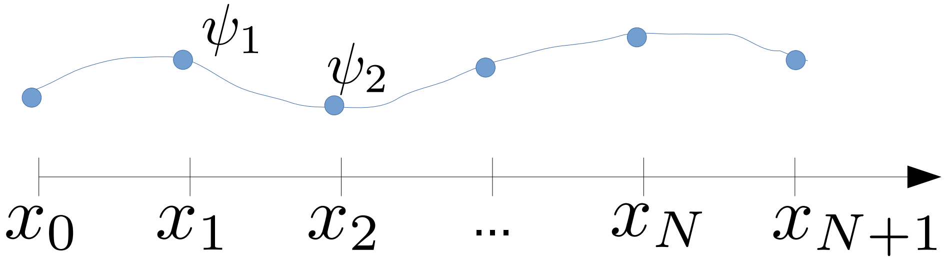

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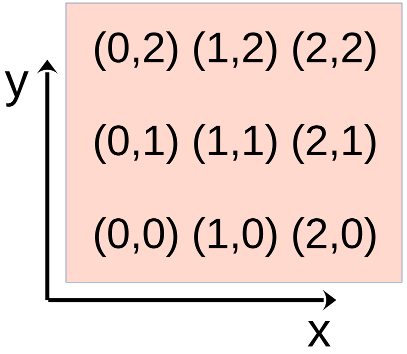

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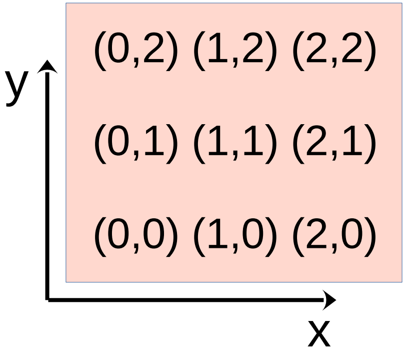

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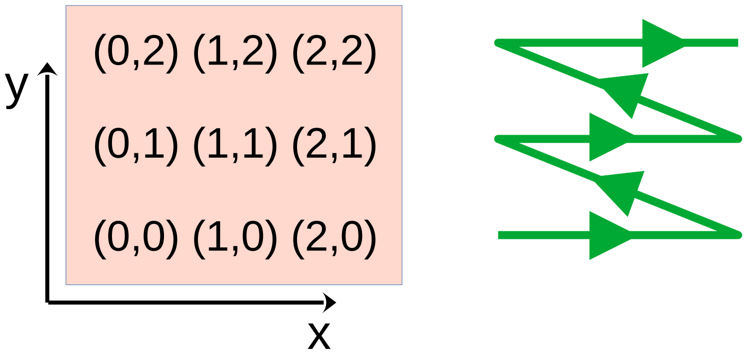

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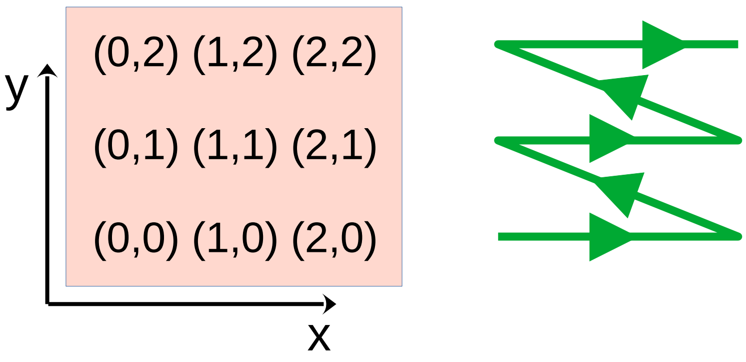

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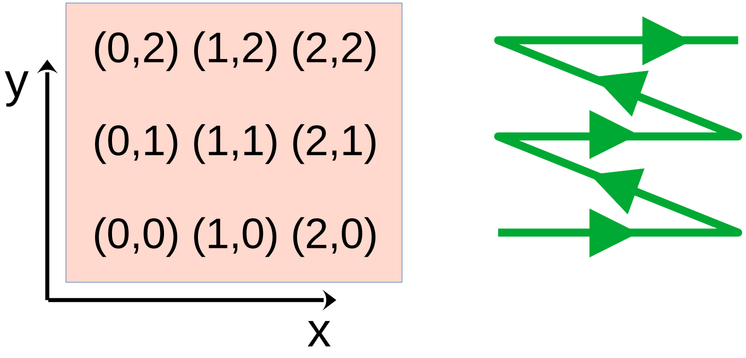

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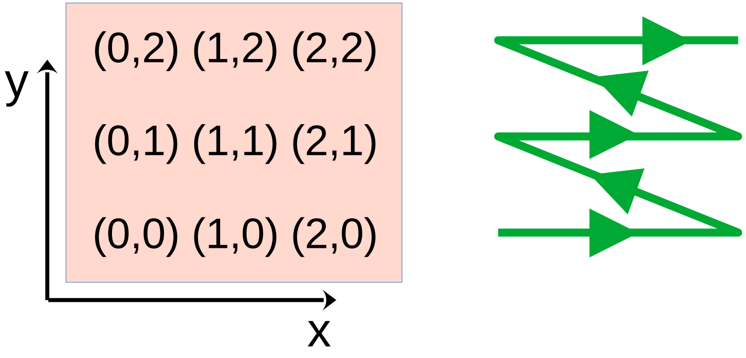

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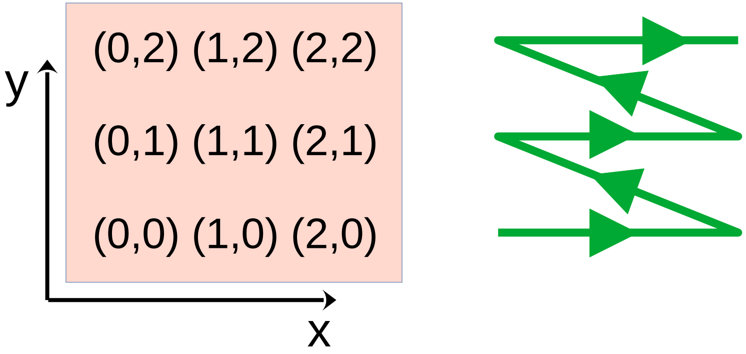

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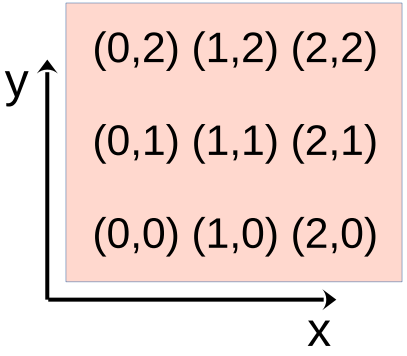

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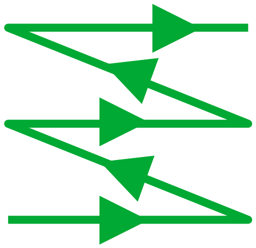

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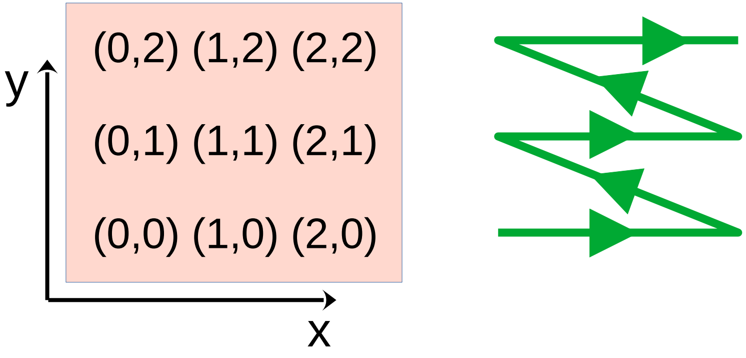

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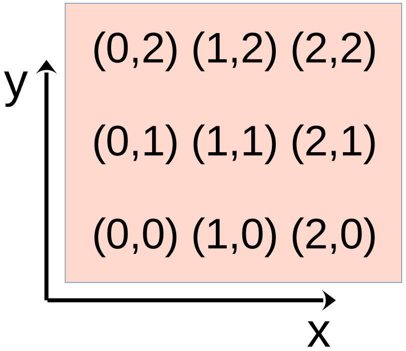
How these python commands work? meshgrid and flatten

meshgrid: convert vectors x, y into coordinate matrices
flatten: collapses the array into one dimension



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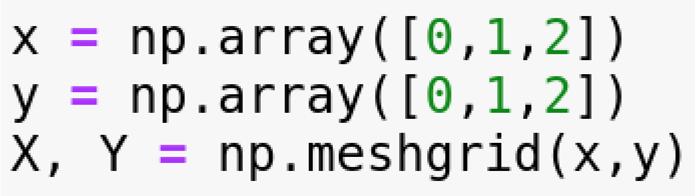

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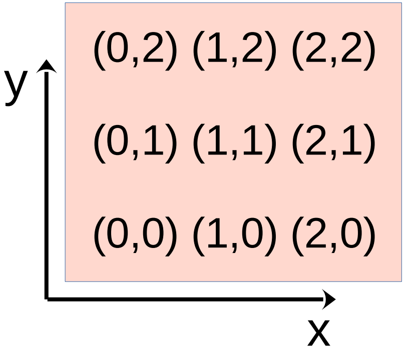

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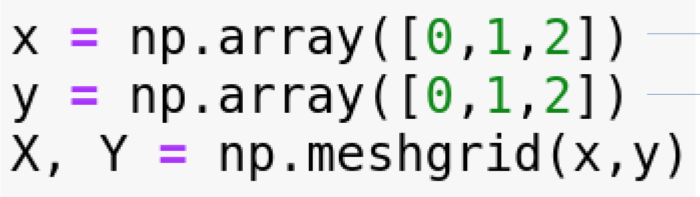

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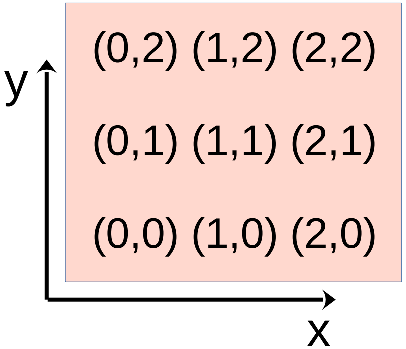

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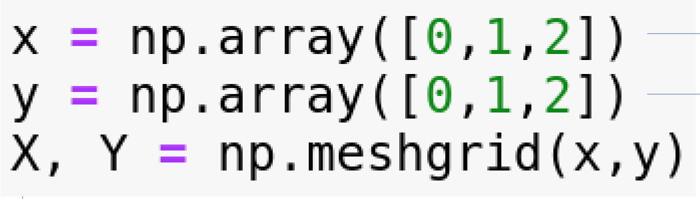

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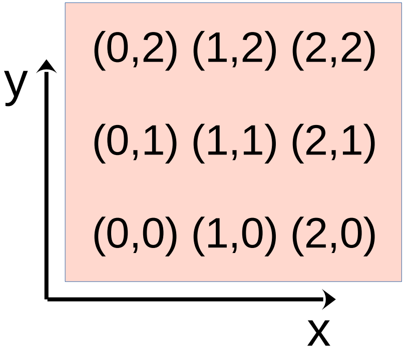

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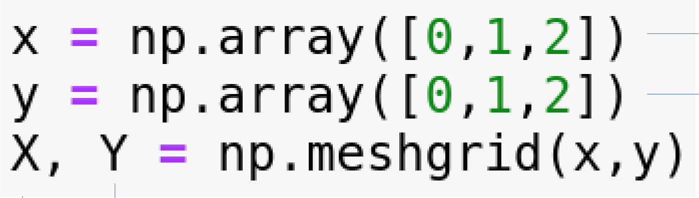

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Matrix:
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|2,2,2|
↑ ↑ ↑
y y y

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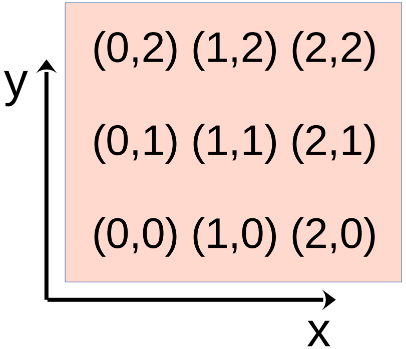

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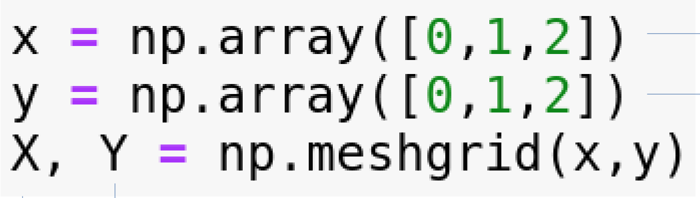

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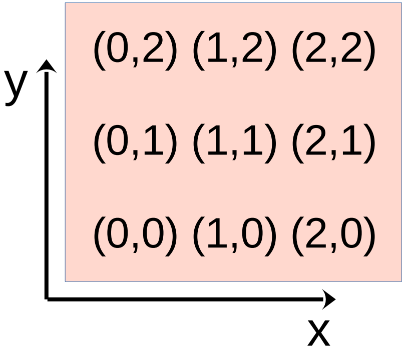
The matrix elements form the pairs $p_n = (x_n, y_n)$



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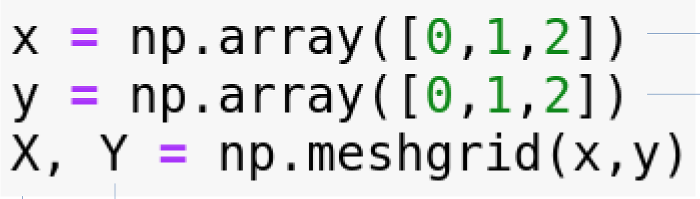

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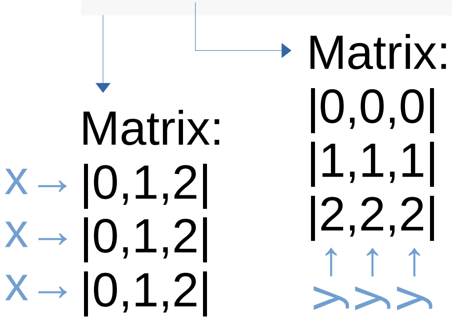

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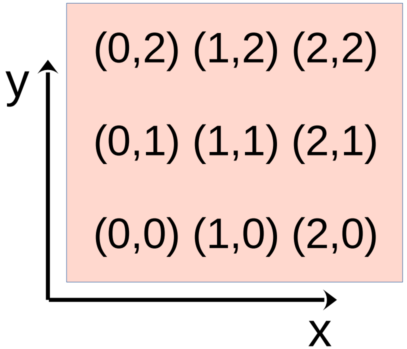
To linearize into vectors, use .flatten()



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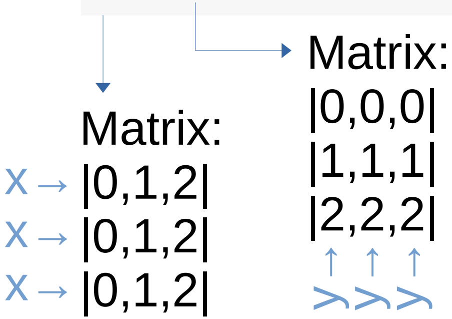
meshgrid: convert vectors x, y into coordinate matrices
flatten: collapses the array into one dimension

```
x = np.array([0,1,2])
y = np.array([0,1,2])
X, Y = np.meshgrid(x,y)
```

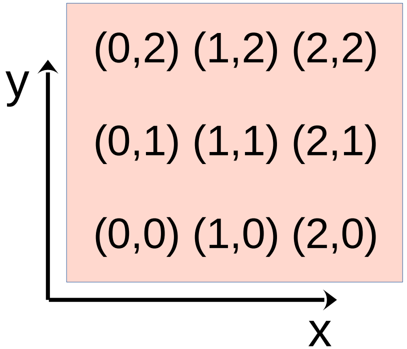
vectors [0, 1, 2]



The matrix elements form the pairs $p_n = (x_n, y_n)$

To linearize into vectors, use .flatten()

```
X = X.flatten()
Y = Y.flatten()
```



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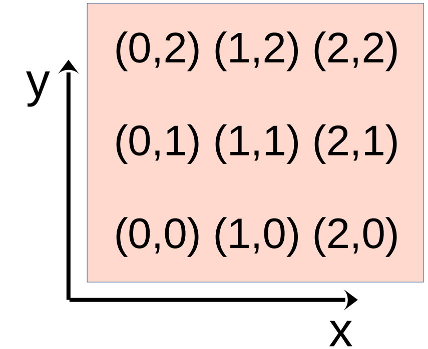
```

vectors [0, 1, 2]

Matrix:
x → |0,1,2|
x → |0,1,2|
x → |0,1,2|

Matrix:
|0,0,0|
|1,1,1|
|2,2,2|
↑ ↑ ↑
y y y



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```

0
1
2
0
1
2
0
1
2

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Matrix:

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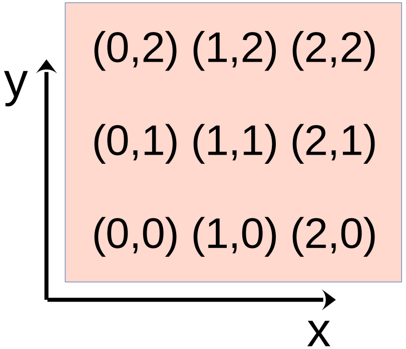

(0,2) (1,2) (2,2)

(0,1) (1,1) (2,1)

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0 0
1 0
2 0
0 1
1 1
2 1
0 2
1 2
2 2

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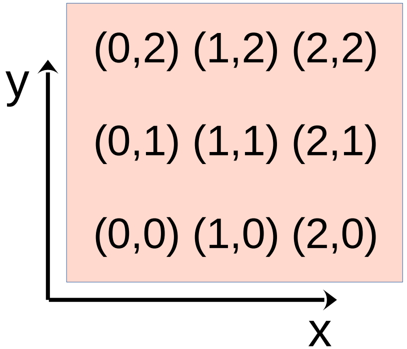

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X	Y	$p_n = (x_n, y_n)$
0	0	(0, 0)
1	0	(1, 0)
2	0	(2, 0)
0	1	(0, 1)
1	1	(1, 1)
2	1	(2, 1)
0	2	(0, 2)
1	2	(1, 2)
2	2	(2, 2)

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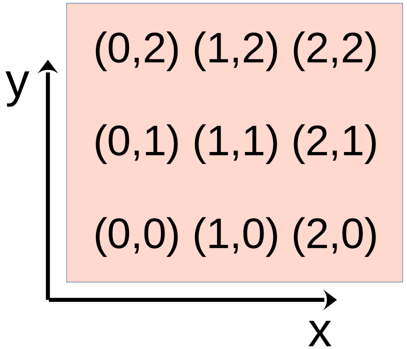

(0,2) (1,2) (2,2)
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(0,0) (1,0) (2,0)

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```

		$p_n = (x_n, y_n)$
0	0	(0, 0)
1	0	(1, 0)
2	0	(2, 0)
0	1	(0, 1)
1	1	(1, 1)
2	1	(2, 1)
0	2	(0, 2)
1	2	(1, 2)
2	2	(2, 2)

Now check this:

```
V = 0.5*(X**2 + Y**2)
```

→ is this useful? ;-)

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meshgrid: convert vectors x, y into coordinate matrices
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```

→ vectors [0, 1, 2]

You can also use kron! see next slides

Matrix:
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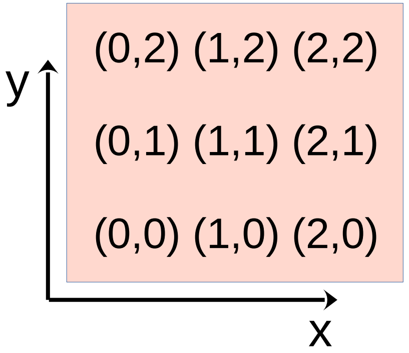
Matrix:
|0,0,0|
|1,1,1|
|2,2,2|
↑ ↑ ↑
y y y



(0,2)	(1,2)	(2,2)
(0,1)	(1,1)	(2,1)
(0,0)	(1,0)	(2,0)

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```

X	Y	$p_n = (x_n, y_n)$
0	0	(0, 0)
1	0	(1, 0)
2	0	(2, 0)
0	1	(0, 1)
1	1	(1, 1)
2	1	(2, 1)
0	2	(0, 2)
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How these python commands work? kron

kron: is the Kronecker product, or the direct product → ⊗

$p_n = (x_n, y_n)$

(0, 0)
(1, 0)
(2, 0)
(0, 1)
(1, 1)
(2, 1)
(0, 2)
(1, 2)
(2, 2)

How these python commands work? kron

kron: is the Kronecker product, or the direct product → ⊗

If A and B are matrices:

$p_n = (x_n, y_n)$

(0, 0)
(1, 0)
(2, 0)
(0, 1)
(1, 1)
(2, 1)
(0, 2)
(1, 2)
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How these python commands work? kron

kron: is the Kronecker product, or the direct product → ⊗

If A and B are matrices:

$$A = \begin{pmatrix} a_{0,0} & a_{0,1} \\ a_{1,0} & a_{1,1} \end{pmatrix} \rightarrow A \otimes B = \begin{pmatrix} a_{0,0}B & a_{0,1}B \\ a_{1,0}B & a_{1,1}B \end{pmatrix}$$

$p_n = (x_n, y_n)$

(0, 0)
(1, 0)
(2, 0)
(0, 1)
(1, 1)
(2, 1)
(0, 2)
(1, 2)
(2, 2)

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Consider now the 1D matrix representations for these operators

$p_n = (x_n, y_n)$
(0, 0)
(1, 0)
(2, 0)
(0, 1)
(1, 1)
(2, 1)
(0, 2)
(1, 2)
(2, 2)

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Consider now the 1D matrix representations for these operators (see previous classes)

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(0, 1)
(1, 1)
(2, 1)
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(1, 2)
(2, 2)

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$$D_x = \partial_x^2$$

$$I_x = \text{ identity } N_x \times N_x$$

$p_n = (x_n, y_n)$

(0, 0)
(1, 0)
(2, 0)
(0, 1)
(1, 1)
(2, 1)
(0, 2)
(1, 2)
(2, 2)

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kron: is the Kronecker product, or the direct product → ⊗

If A and B are matrices:

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Consider now the 1D matrix representations for these operators (see previous classes)

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$$I_x = \text{ identity } N_x \times N_x$$

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$$I_y = \text{ identity } N_y \times N_y$$

$p_n = (x_n, y_n)$
(0, 0)
(1, 0)
(2, 0)
(0, 1)
(1, 1)
(2, 1)
(0, 2)
(1, 2)
(2, 2)

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The 2D version becomes:

$p_n = (x_n, y_n)$
(0, 0)
(1, 0)
(2, 0)
(0, 1)
(1, 1)
(2, 1)
(0, 2)
(1, 2)
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(1, 2)
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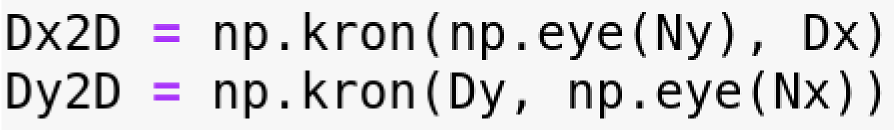

```
Dx2D = np.kron(np.eye(Ny), Dx)
Dy2D = np.kron(Dy, np.eye(Nx))
```

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(2, 1)
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The 2D version becomes:

```
Dx2D = np.kron(np.eye(Ny), Dx)
Dy2D = np.kron(Dy, np.eye(Nx))
```

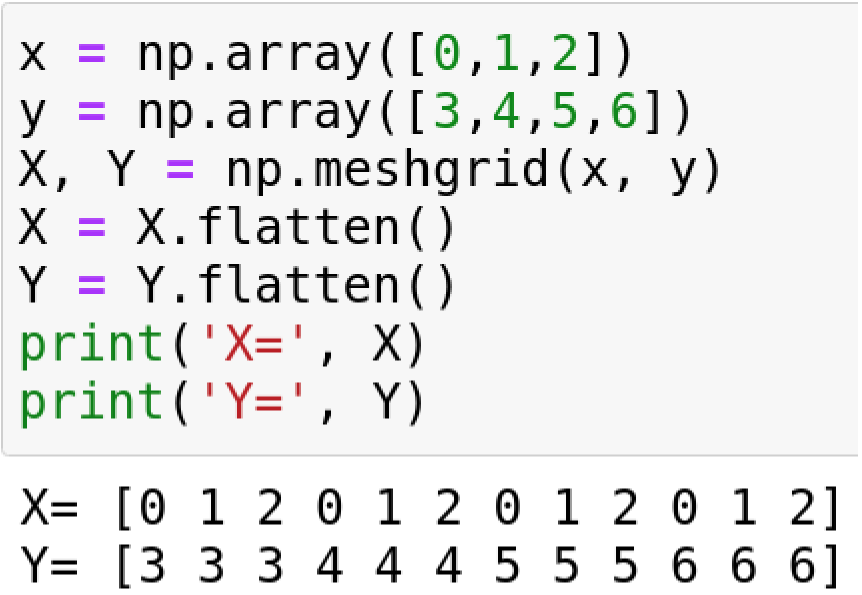
So we get:

```
H = -0.5*(Dx2D + Dy2D) + V
```

Using kron instead of meshgrid and flatten

Check that these codes return the same vectors:

Using meshgrid/flatten



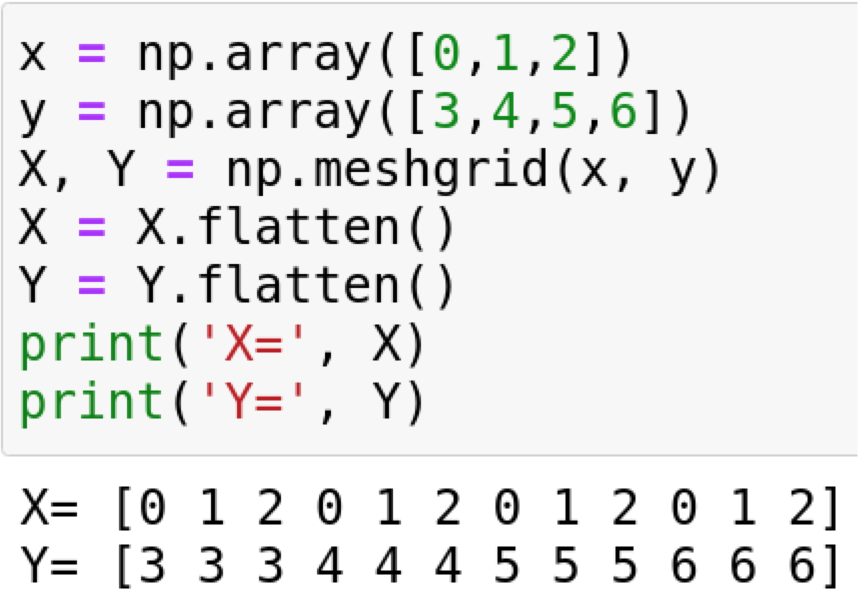
```
x = np.array([0,1,2])
y = np.array([3,4,5,6])
X, Y = np.meshgrid(x, y)
X = X.flatten()
Y = Y.flatten()
print('X=', X)
print('Y=', Y)
```

```
X= [0 1 2 0 1 2 0 1 2 0 1 2]
Y= [3 3 3 4 4 4 5 5 5 6 6 6]
```

Using kron instead of meshgrid and flatten

Check that these codes return the same vectors:

Using meshgrid/flatten



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```
X= [0 1 2 0 1 2 0 1 2 0 1 2]
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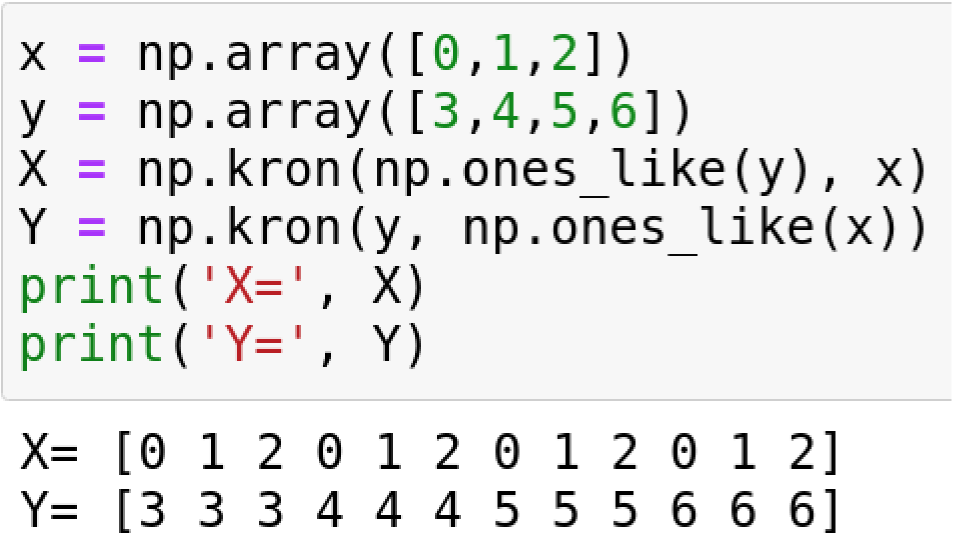
```

Using kron



```
x = np.array([0,1,2])
y = np.array([3,4,5,6])
X = np.kron(np.ones_like(y), x)
Y = np.kron(y, np.ones_like(x))
print('X=', X)
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```
X= [0 1 2 0 1 2 0 1 2 0 1 2]
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```

Results for 2D atoms or molecules

Atomic potential = inverse Gaussian

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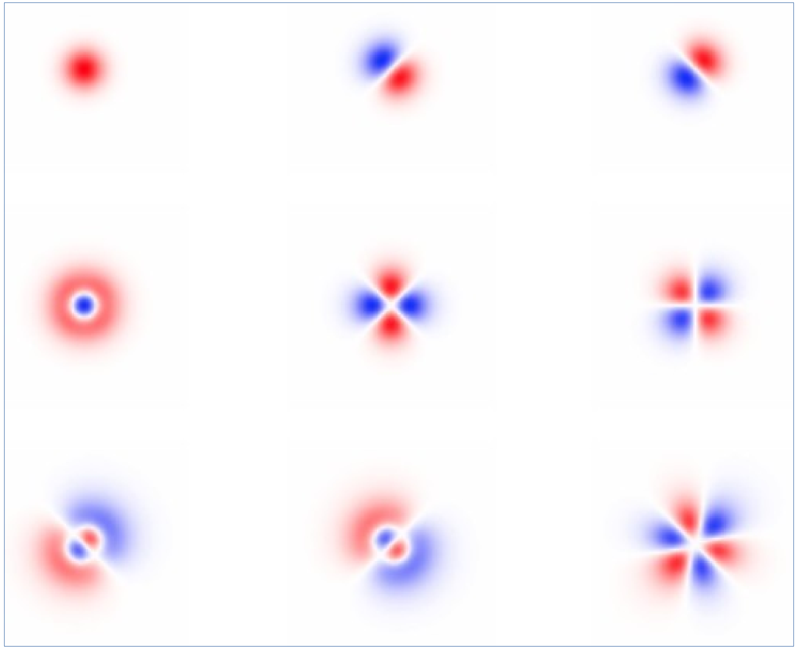
Atomic potential = inverse Gaussian

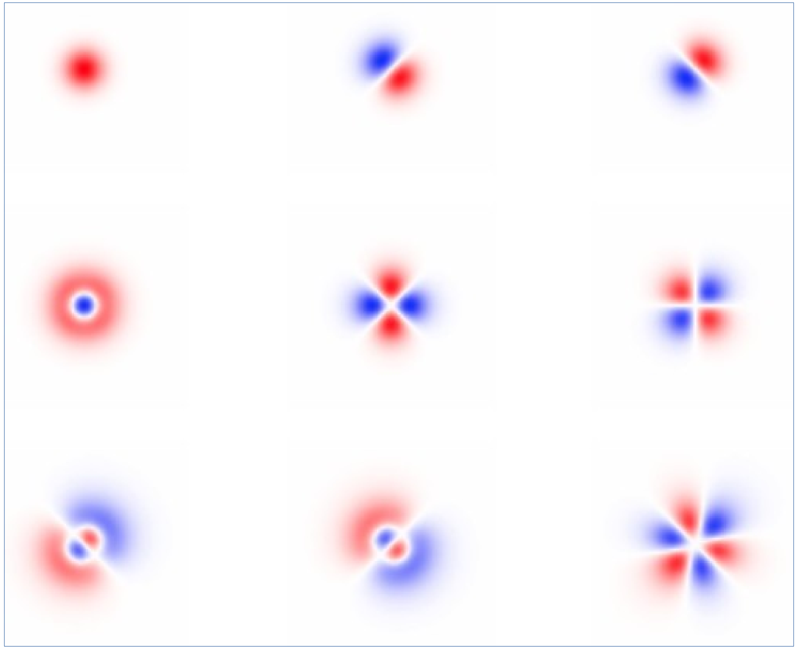
1 atom



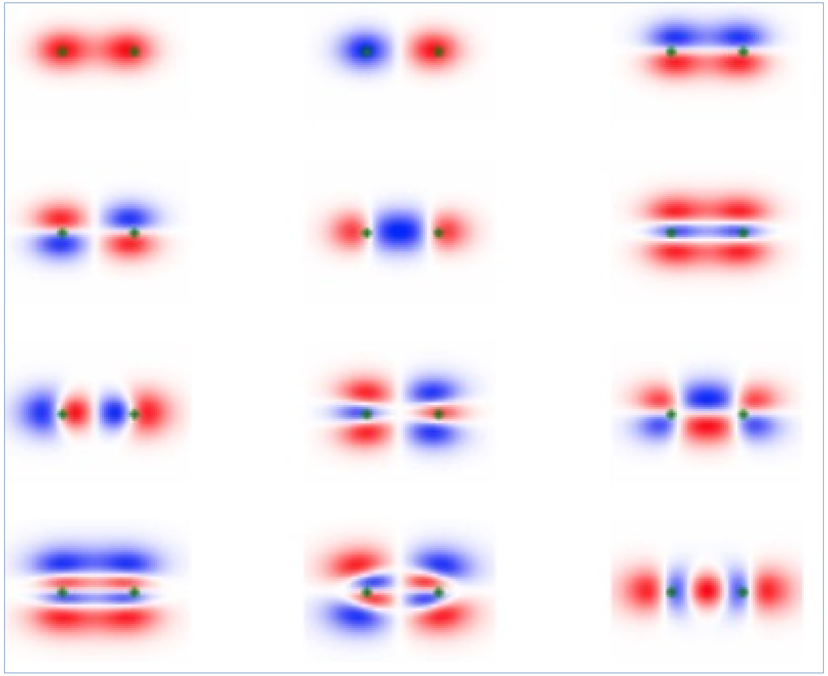
Results for 2D atoms or molecules

Atomic potential = inverse Gaussian

1 atom

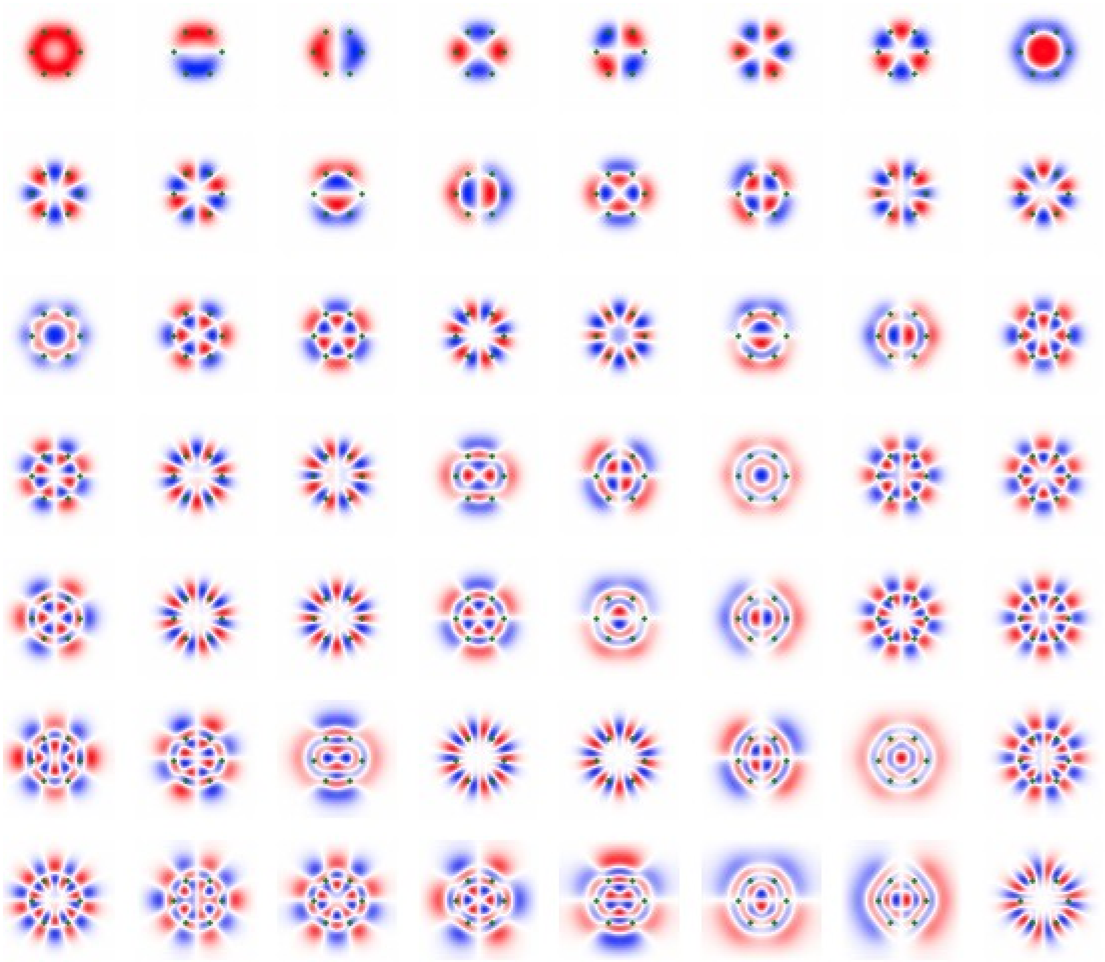


2 atoms



Results for 2D atoms or molecules

6 atoms
hexagon



How to improve? For large matrices: use scipy sparse matrices

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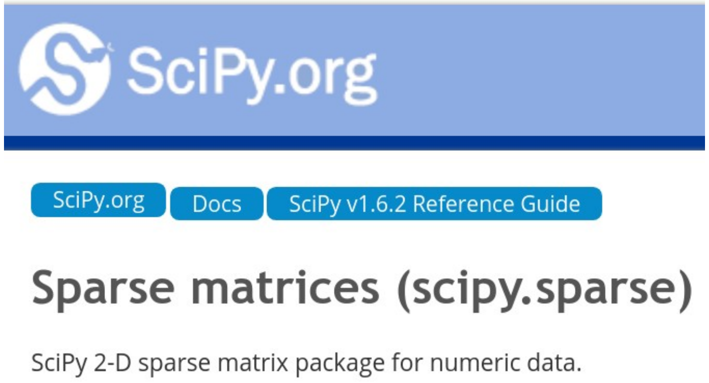
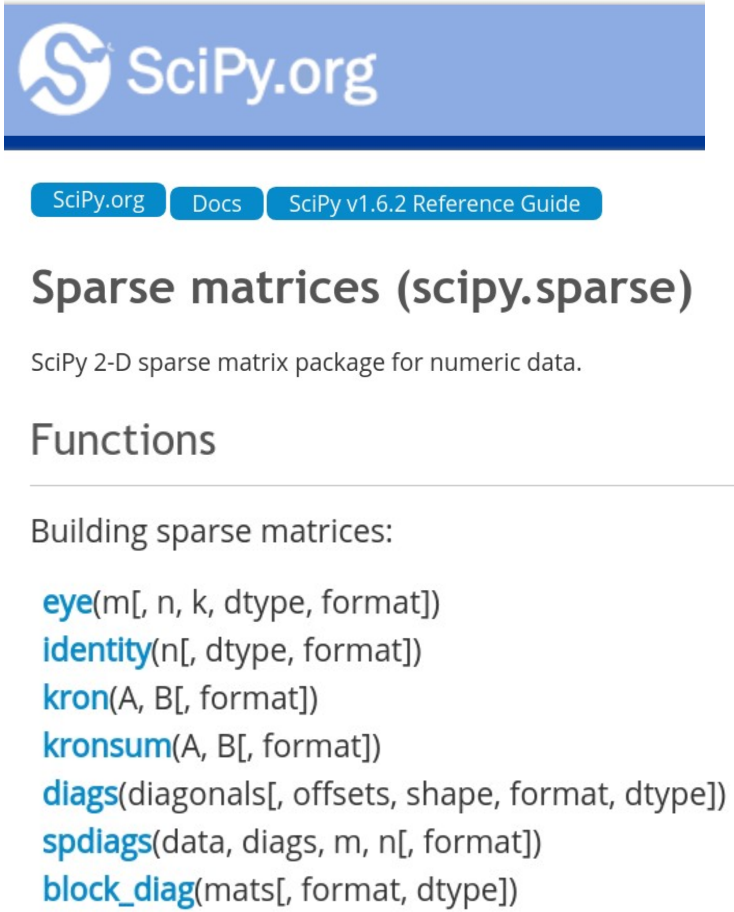


Sparse matrices (scipy.sparse)

SciPy 2-D sparse matrix package for numeric data.

How to improve? For large matrices: use scipy sparse matrices



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Sparse matrices (scipy.sparse)

SciPy 2-D sparse matrix package for numeric data.

Functions

Building sparse matrices:

- eye(m[, n, k, dtype, format])
- identity(n[, dtype, format])
- kron(A, B[, format])
- kronsum(A, B[, format])
- diags(diagonals[, offsets, shape, format, dtype])
- spdiags(data, diags, m, n[, format])
- block_diag(mats[, format, dtype])

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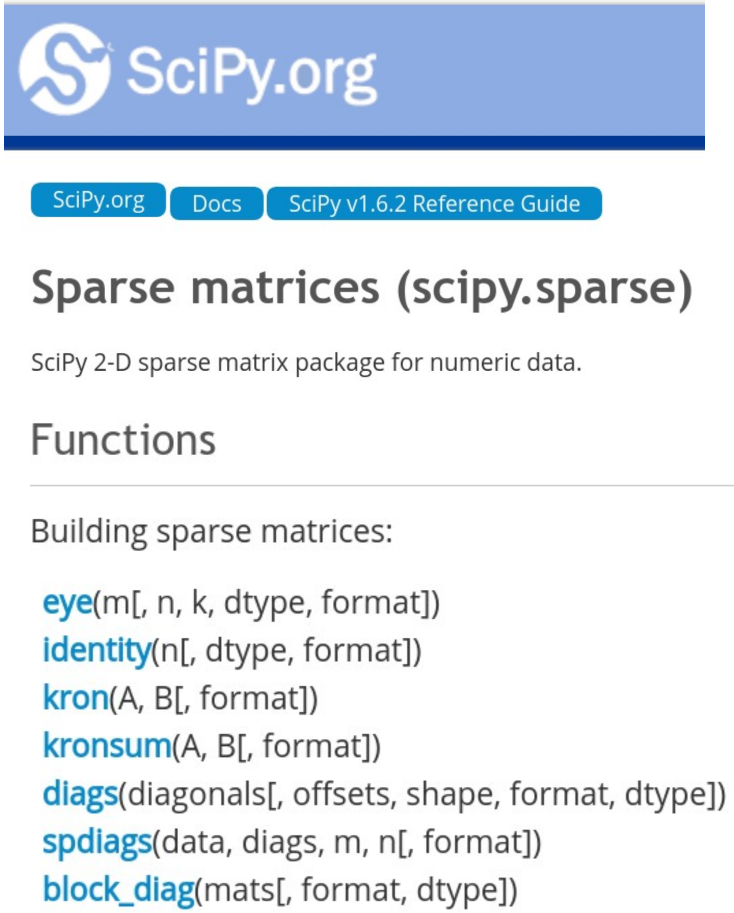
How to improve? For large matrices: use scipy sparse matrices



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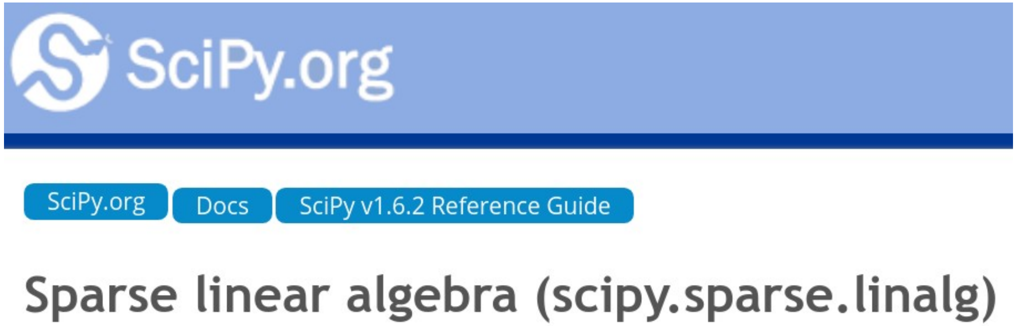
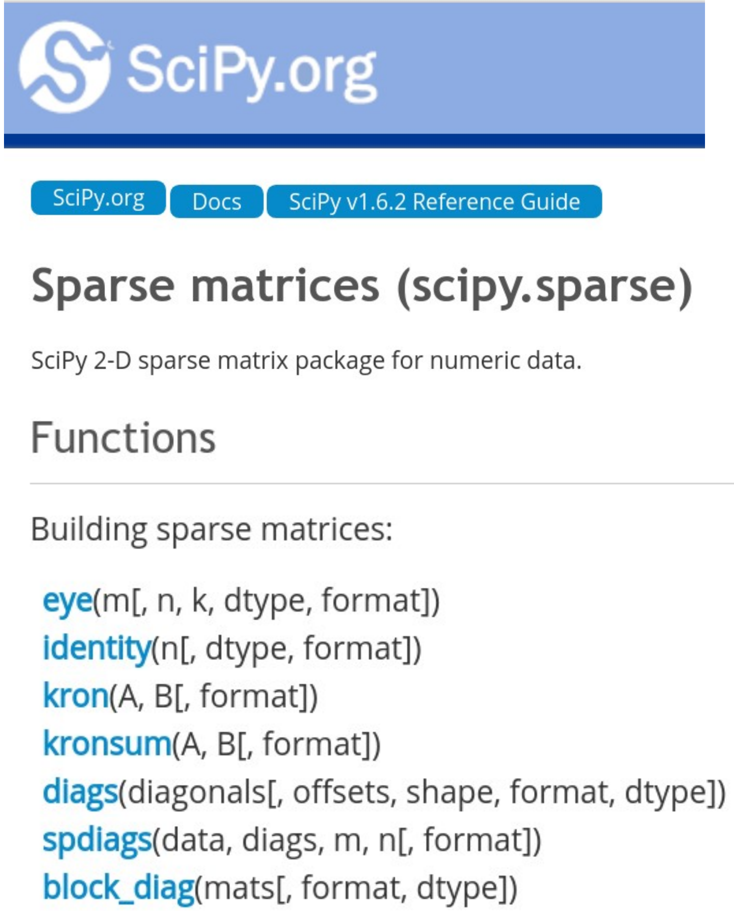
- **kronsum**(A, B[, format])
- **diags**(diagonals[, offsets, shape, format, dtype])
- **spdiags**(data, diags, m, n[, format])
- **block_diag**(mats[, format, dtype])



Sparse linear algebra (scipy.sparse.linalg)

How to improve? For large matrices: use scipy sparse matrices



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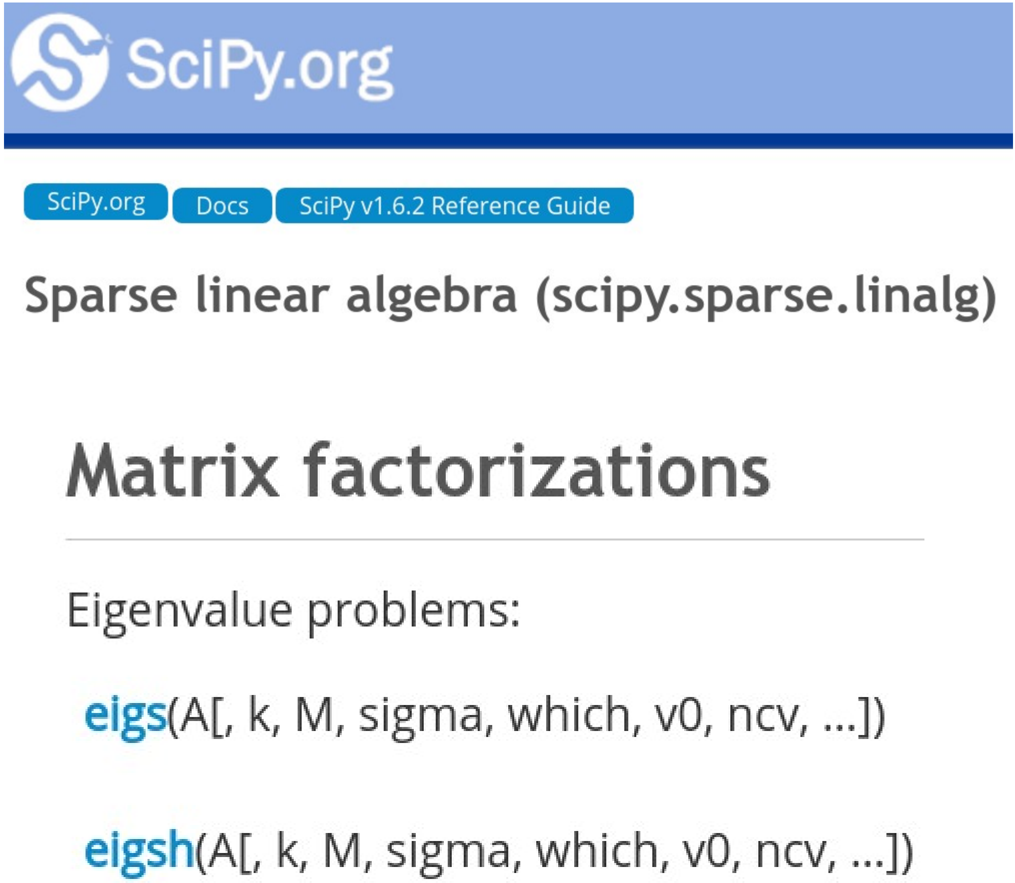
- diags(diagonals[, offsets, shape, format, dtype])
- spdiags(data, diags, m, n[, format])
- block_diag(mats[, format, dtype])



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Sparse linear algebra (scipy.sparse.linalg)

Matrix factorizations

Eigenvalue problems:

- eigs(A[, k, M, sigma, which, v0, ncv, ...])
- eigsh(A[, k, M, sigma, which, v0, ncv, ...])