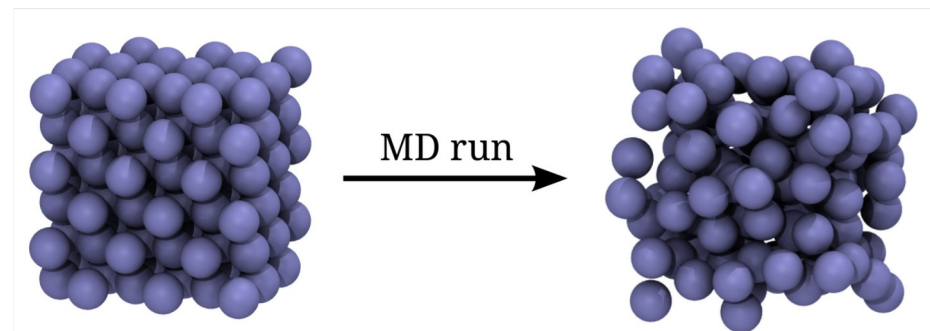


Aula 01 – Introdução ao Python



Prof. Elvis Soares
elvis@peq.coppe.ufrj.br

Infos

Horário de aulas: 3a, 09:00-12:00

Sala de Aula: I224

Calendário: 05/Ago - 09/Dez (~19 encontros)

Professores: Frederico Tavares (tavares@eq.ufrj.br)

Elvis Soares (elvis@peq.coppe.ufrj.br)



<https://github.com/elvissoares/EQE595-SimMol>



<https://elvissoares.com/ensino>

CRITÉRIOS DE AVALIAÇÃO

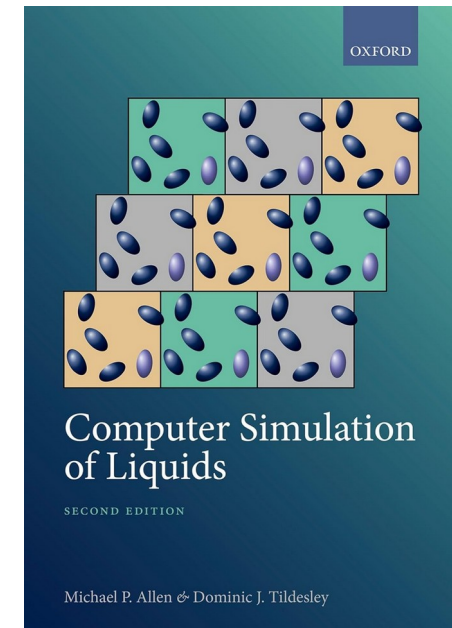
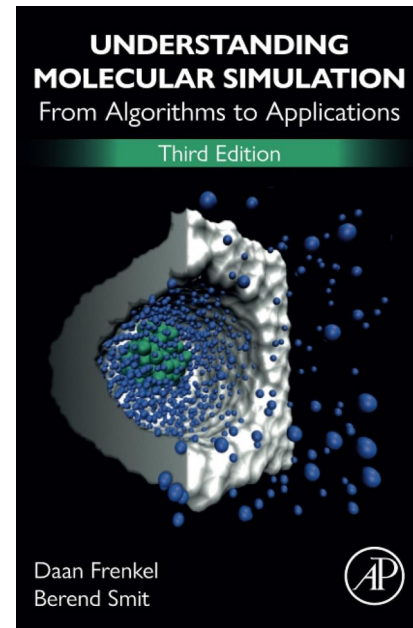
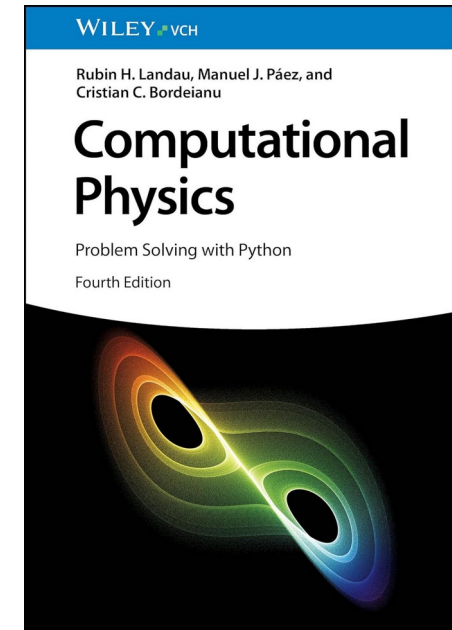
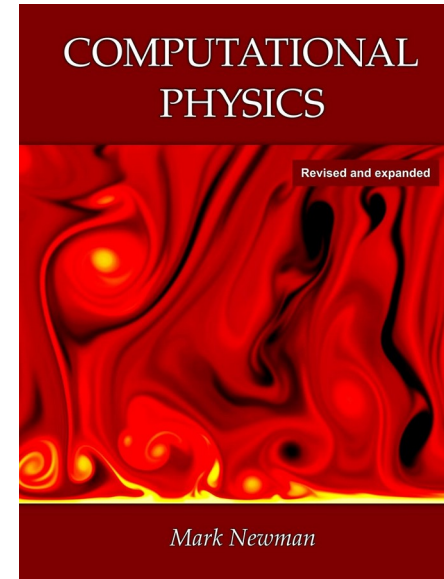
- 20% de Presença e Participação
- 40% de Listas de Exercícios (~10 listas)
- 40% de Projeto Final

Ementa

- 1) Introdução ao Python
- 2) Ensemble NVE e integrador de Verlet
- 3) Interação de Lennard-Jones
- 4) Distribuição de Maxwell-Boltzmann
- 5) Ensemble NVT e integrador de Langevin
- 6) Ensemble NPT
- 7) Água e Campos de Força
- 8) Solute e Solvente
- 9) Integração Termodinâmica

Referências

- Newman, M. (2013). **Computational physics**. CreateSpace Independent Publishing Platform.
- Landau, R. H., Páez, M. J., & Bordeianu, C. C. (2024). **Computational physics: Problem solving with Python, 4th Edition**. John Wiley & Sons.
- Frenkel, D., & Smit, B. (2023). **Understanding molecular simulation: from algorithms to applications, 3rd Edition**. Elsevier.
- Allen, M. P., & Tildesley, D. J. (2017). **Computer simulation of liquids, 2nd Edition**. Oxford university press.



Ferramentas Computacionais



<https://www.anaconda.com/download>



AVOGADRO

Baixando o Notebook

The screenshot shows a web browser displaying a GitHub repository page for 'elvissoares / EQE595-SimMol'. The URL in the address bar is 'github.com/elvissoares/EQE595-SimMol/blob/main/notebooks/1_Introducao_Python.ipynb'. The repository's navigation bar includes links for Code, Issues, Pull requests, Actions, Projects, Wiki, Security, Insights, and Settings. On the left sidebar, the 'Files' section is active, showing a file tree with folders 'aulas', 'listas', and 'notebooks'. The file '1_Introducao_Python.ipynb' is selected and highlighted. The main content area displays the notebook's metadata: 'EQE595-SimMol / notebooks / 1_Introducao_Python.ipynb', the author 'elvissoares', the commit hash '0054cc1', and the time '12 minutes ago'. Below this, there are tabs for 'Preview', 'Code', and 'Blame'. The 'Preview' tab is active, showing the notebook's content. The content includes a title 'Bibliotecas Numpy e Matplotlib', the author 'Prof. Elvis do A. Soares', contact information 'elvis@peq.coppe.ufrj.br', and a section titled 'Numpy: Operações com Arrays e Matrizes'. At the bottom, a code cell is shown with the text 'In [1]: import numpy as np'.

Home x EQE595-SimMol/noteb x +

github.com/elvissoares/EQE595-SimMol/blob/main/notebooks/1_Introducao_Python.ipynb

elvissoares / EQE595-SimMol

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main +

Go to file

aulas

listas

notebooks

1_Introducao_Python.ipynb

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README.md

EQE595-SimMol / notebooks 1_Introducao_Python.ipynb

elvissoares Atualizando Notebook Aula 01 0054cc1 · 12 minutes ago History

Preview Code Blame 2131 lines (2131 loc) · 570 KB

Raw

Bibliotecas Numpy e Matplotlib

Autor: Prof. Elvis do A. Soares

Contato: elvis@peq.coppe.ufrj.br - Programa de Engenharia Química, PEQ/COPPE, UFRJ, Brasil

Numpy: Operações com Arrays e Matrizes

Como importar a biblioteca *numpy*

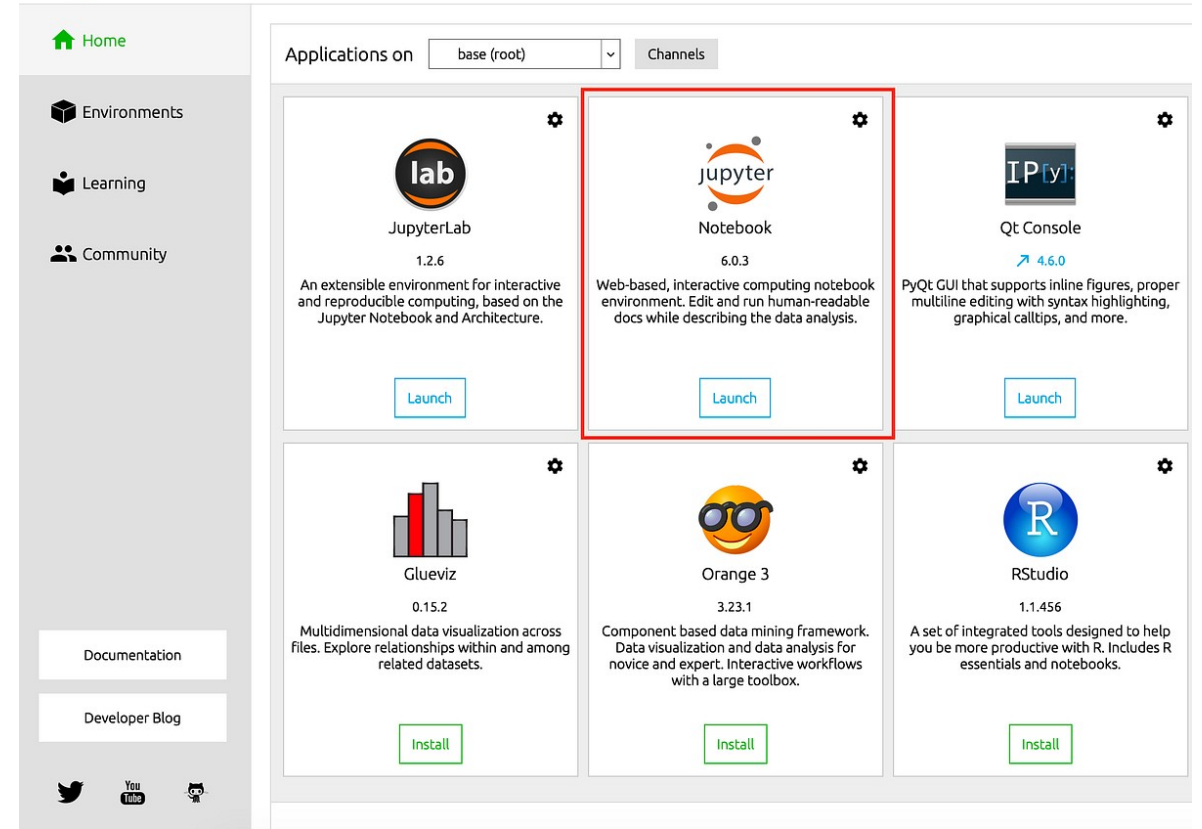
In [1]: `import numpy as np`

Usando Python pelo Anaconda

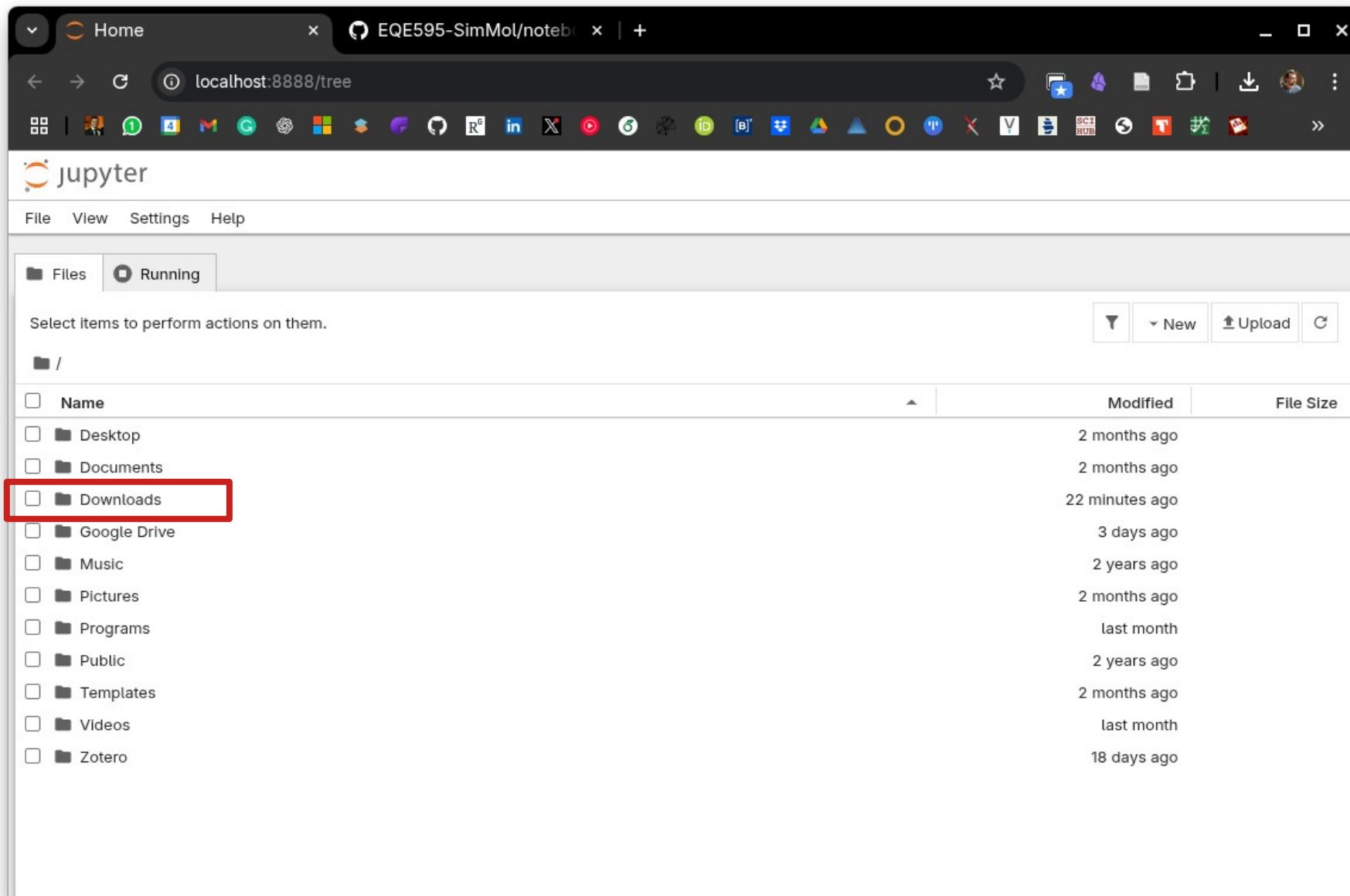


<https://www.anaconda.com/download>

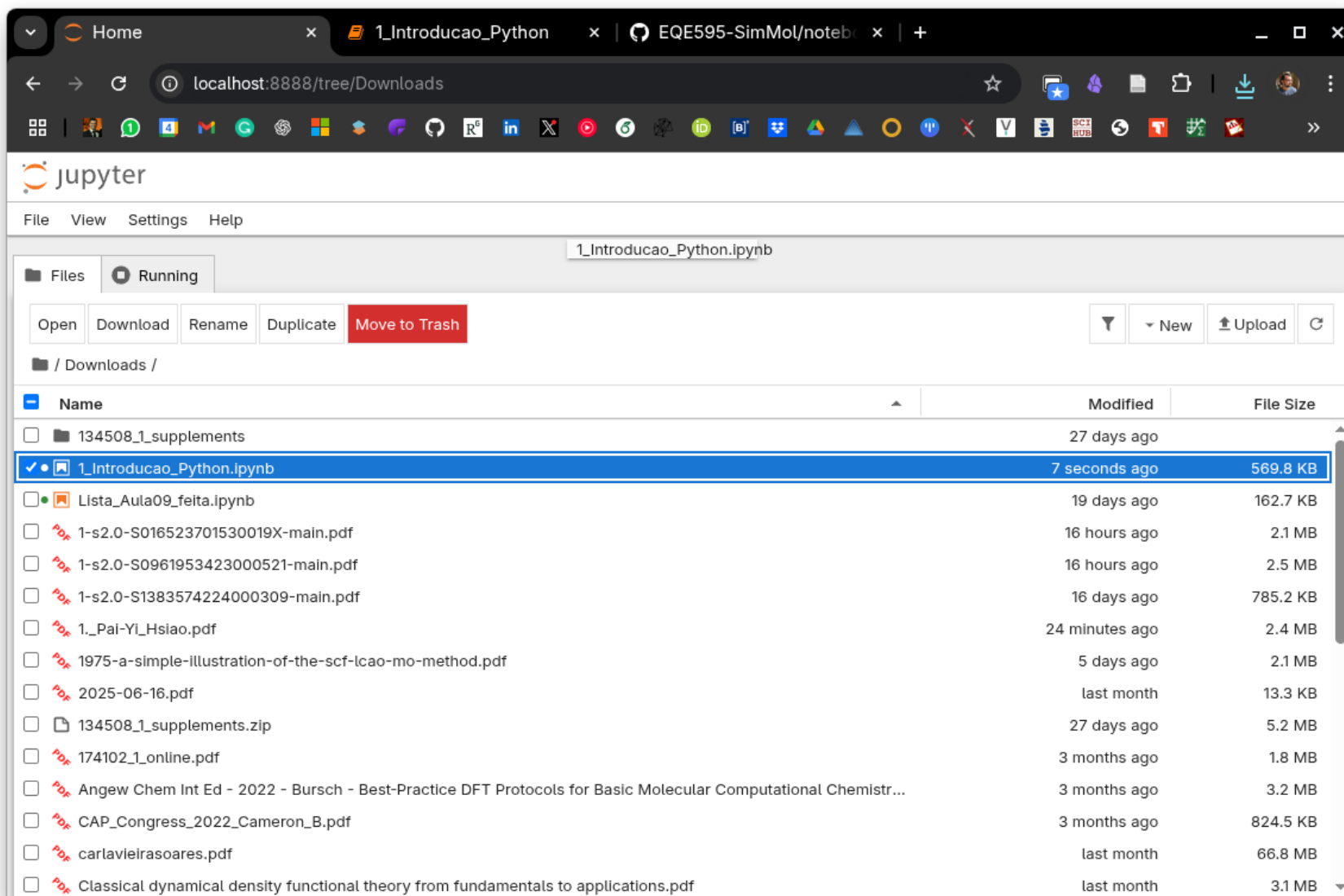
ANACONDA NAVIGATOR



Usando Python pelo Anaconda



Usando Python pelo Anaconda



Usando Python pelo Anaconda

The screenshot shows a web browser window with a JupyterLab interface. The browser tabs include 'Home', '1_Introducao_Python', and 'EQE595-SimMol/noteb...'. The address bar shows 'localhost:8888/notebooks/Downloads/1_Introducao_Python.ipynb'. The JupyterLab header shows the notebook title '1_Introducao_Python' and a 'Last Checkpoint: 38 seconds ago' message. The menu bar includes 'File', 'Edit', 'View', 'Run', 'Kernel', 'Settings', and 'Help'. The toolbar shows various icons for file operations and execution. The notebook content is displayed in a cell with a blue border. It starts with a title 'Bibliotecas Numpy e Matplotlib' and an author 'Prof. Elvis do A. Soares'. Below this, there is a contact information line: 'Contato: elvis@peq.coppe.ufrj.br - Programa de Engenharia Química, PEQ/COPPE, UFRJ, Brasil'. The main section is titled 'Numpy: Operações com Arrays e Matrizes' and contains the text 'Como importar a biblioteca *numpy*'. The code in the notebook is as follows:

```
[1]: import numpy as np
```

Existem diversas funções já definidas na biblioteca, as mais comuns são *sin*, *cos*, *exp*, *sinh*, etc

```
[3]: np.sin(0)
```

```
[3]: 0.0
```

```
[4]: np.cos(0)
```

```
[4]: 1.0
```