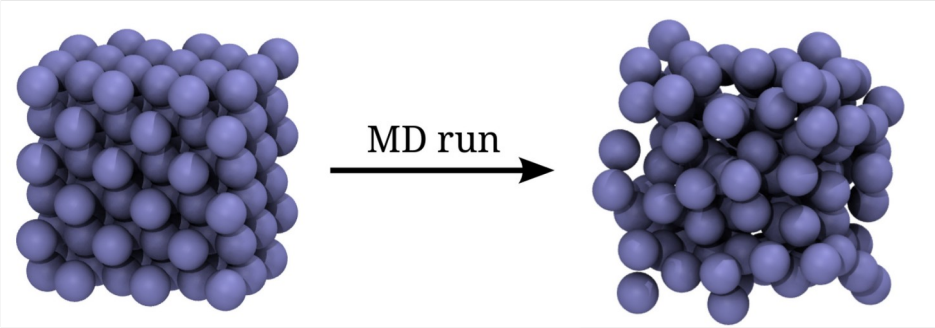
UFRJ
UNIVERSIDADE FEDERAL
DO RIO DE JANEIRO

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

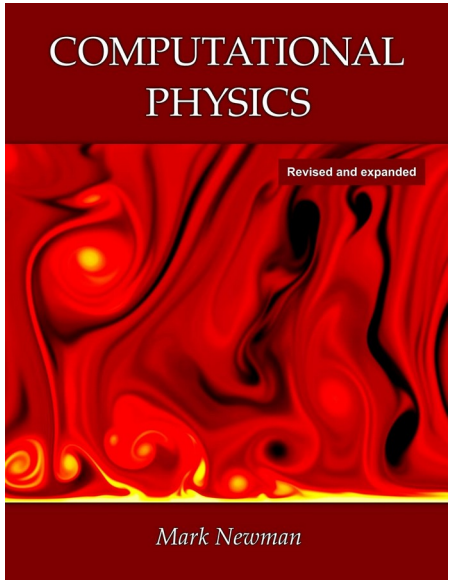
- 20% de Presença e Participação
- 40% de Listas de Exercícios (~10 listas)
- 40% de Projeto Final

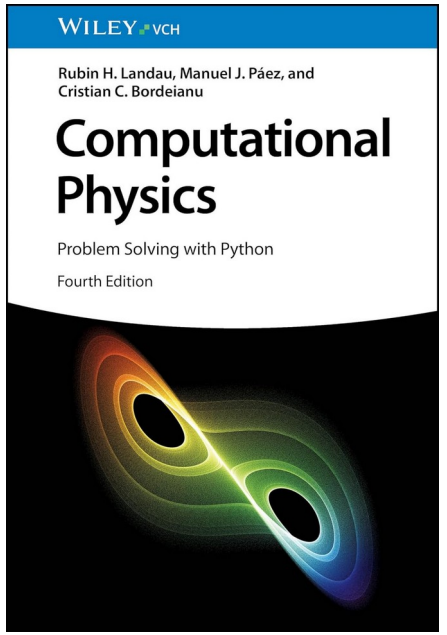
Ementa

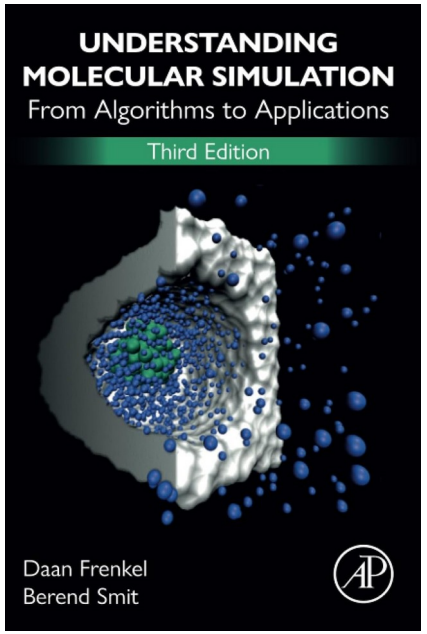
1) Introdução ao Python
2) Ensemble NVE e integrador de Verlet
3) Interação de Lennard-Jones
4) Distribuição de Maxwell-Boltzmann
5) Ensemble NVT e integrador de Langevin
6) Ensemble NPT
7) Água e Campos de Força
8) Soluto e Solvente
9) Integração Termodinâmica

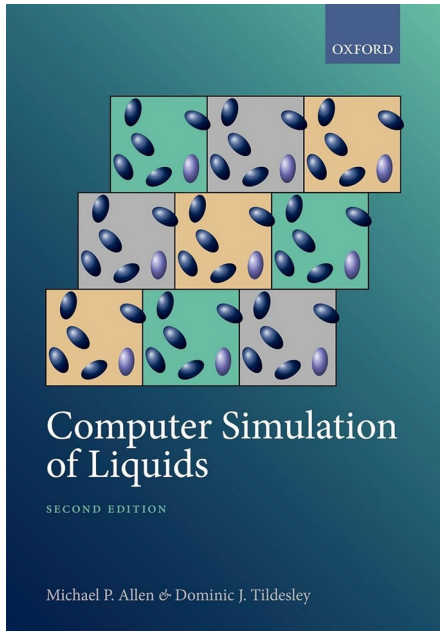
Referências

- 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.







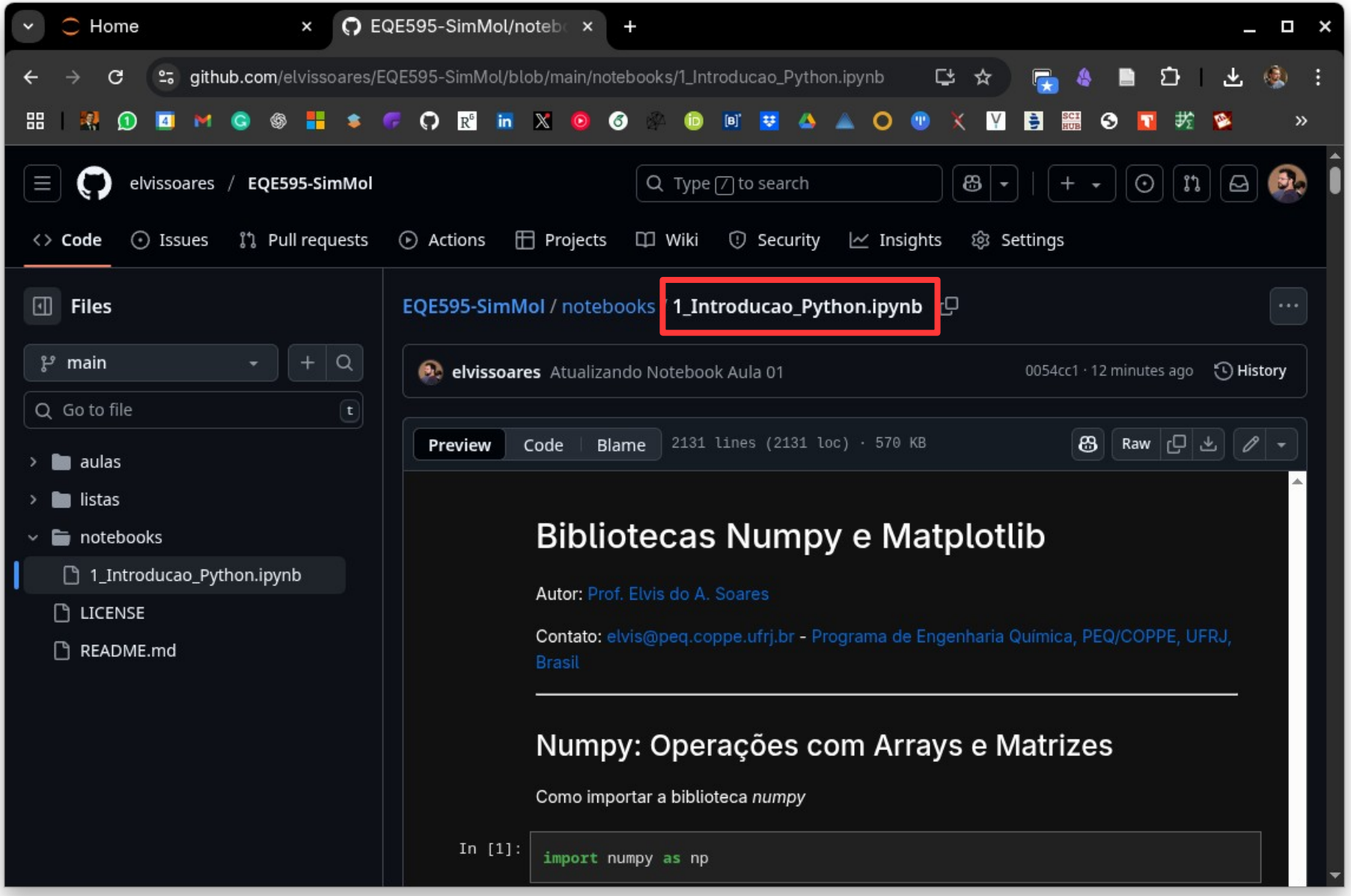


Ferramentas Computacionais

https://www.anaconda.com/download

AVOGADRO

Baixando o Notebook



Usando Python pelo Anaconda

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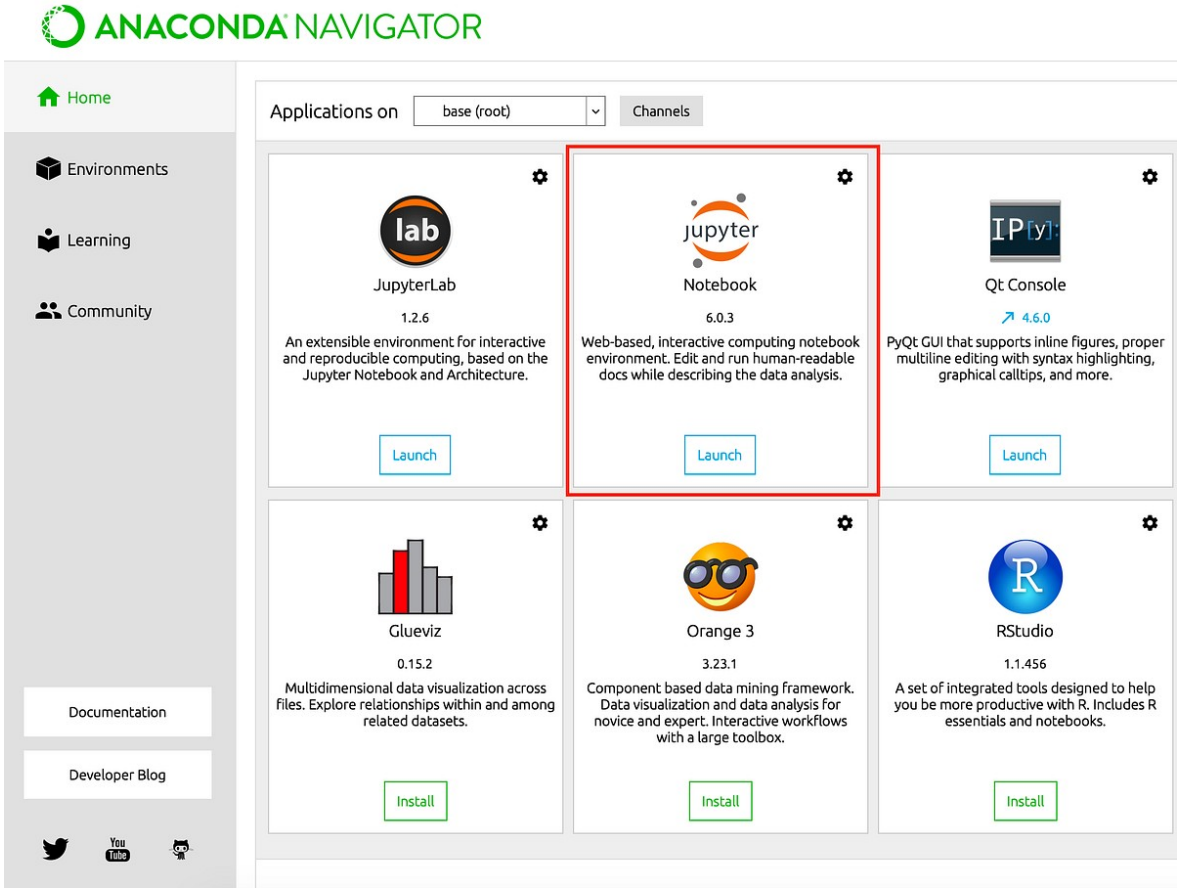
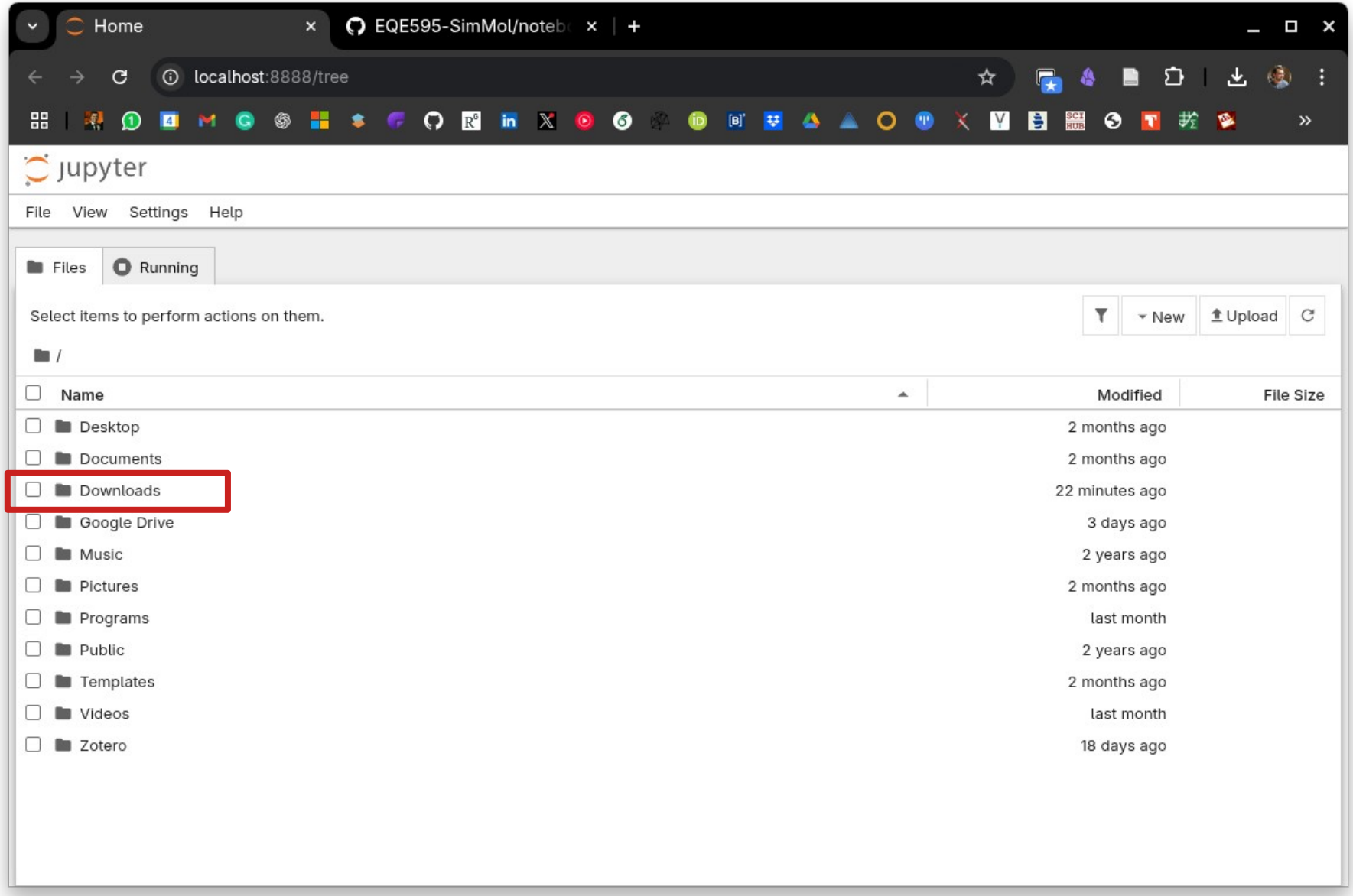


Usando Python pelo Anaconda



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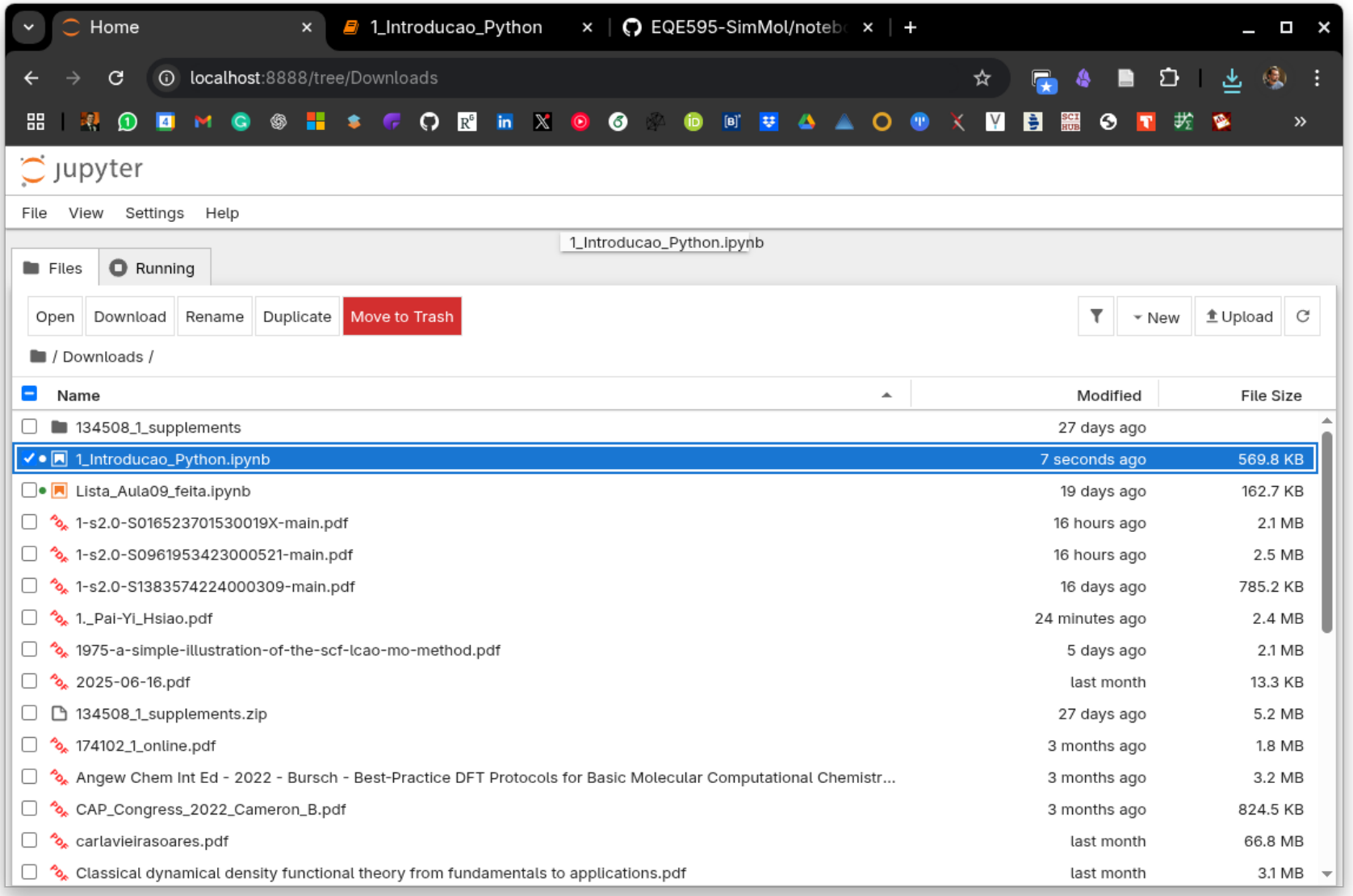

Usando Python pelo Anaconda