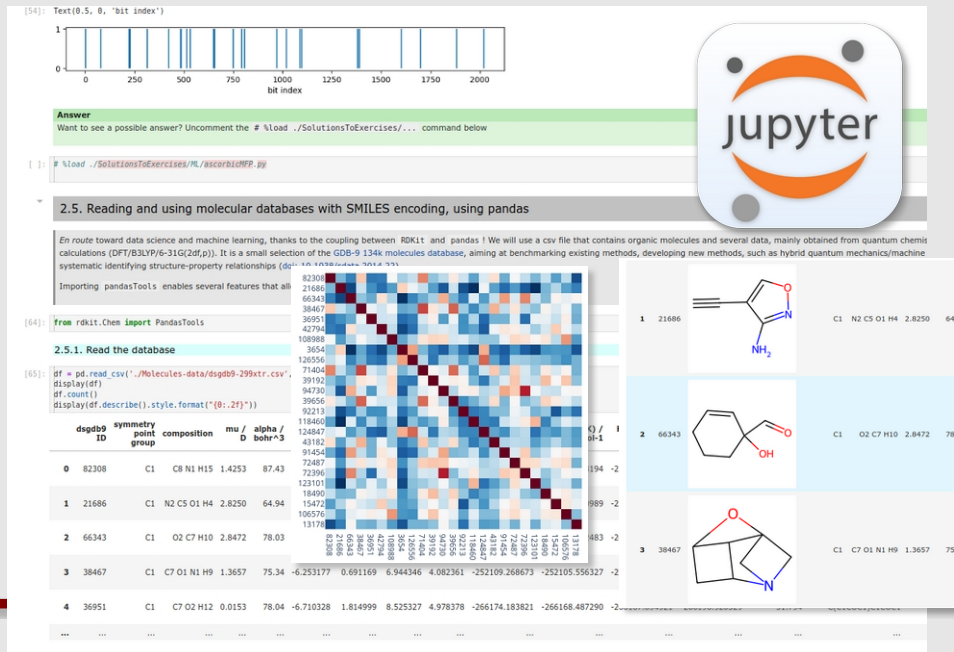
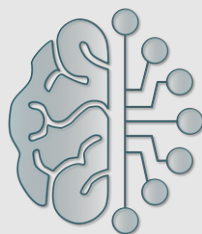


"Talktorials" in physical chemistry and data science

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Python in the Physical Chemistry lab (pyPhysChem) github repository, release v. 1.8.0 (2023), doi: 10.5281/zenodo.8396813



- interactive python
- images / videos
- mathematical equations
- enriched text (markdown)

Motivation

integration of verbal explanations with numerical demonstrations or computer algebra system-based demonstrations proves to be an influential pedagogical tool

let's call them "talktorials"



Python in the
Physical Chemistry Lab



[pyPhysChem]



talktorials specifically tailored for computational
chemistry and data science/machine learning



such mixing not new, but until recently it was restricted to rather simple applications that required a great deal of development effort

What is new is:

- the combination of Python's popularity and libraries
- the interactive nature of Jupyter Notebooks
- personal computers performance; the prevalence of real-world applications that can quite easily be adapted for students thanks to Python libraries available in a lot of domains
- the strong community support
- the ease of reproducibility that makes tutorials more effective, as learners can directly use the code provided to experiment and build upon it

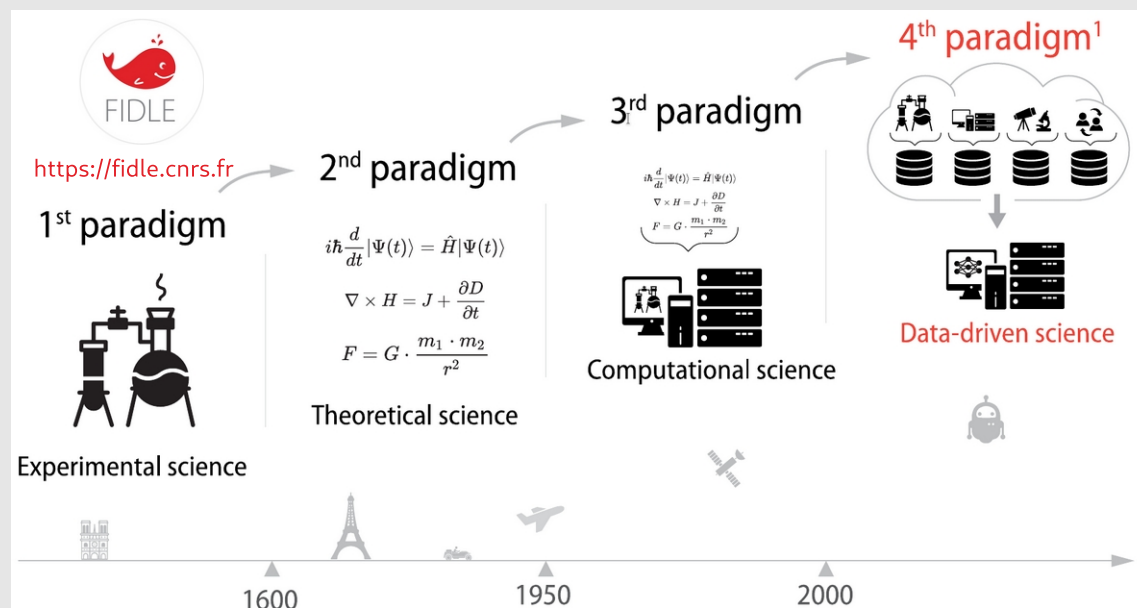


Motivation

The emergence of such innovative approaches in the realm of computational chemistry is truly encouraging

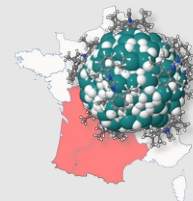
It not only enables learners to grasp theoretical concepts but also offers a practical perspective on their application

For students specialising in computational chemistry who develop their own scripts, they acquire a **dual skill set that could be sought after in various areas of research and industry**



Which students (so far...)?

masters' (graduate) degrees



Réseau Français de
Chimie Théorique

bachelor degree

all chemistry students, 2nd year



Traitement statistique de données
(data science pour débutants)

*Statistical treatment of data
(data science for beginners)*

Lecture et analyse de la base de données "iris" par la bibliothèque pandas

Reading and analysis of the "iris" database with the pandas library

Ce sujet exploite une base de données souvent utilisée pour l'apprentissage de méthodes statistiques, la base **IRIS** :

- elle regroupe les caractéristiques de trois espèces de fleurs d'Iris : Setosa, Versicolor et Virginica
- la base regroupe 50 observations par espèce (soit 150 **individus**)
- chaque observation repose sur 4 caractéristiques (c'est-à-dire 4 **variables**) : longueur et largeur de sépales ainsi que longueur et largeur de pétales

Un [article wikipedia](#) porte sur ce dataset, qui contient à la fois des données numériques (longueur & largeur de pétales et sépales) et descriptives (types d'iris).



This subject uses a database often used for the training of statistical methods, the **IRIS** database:



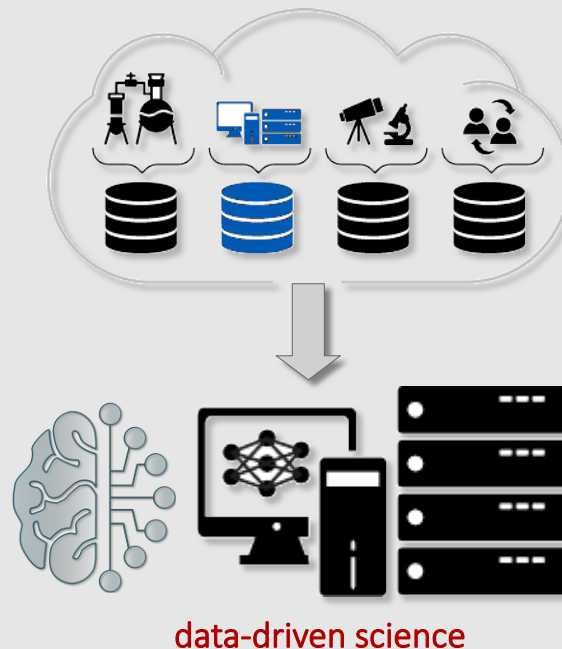


<https://github.com/rpoteau/pyPhysChem>

10.5281/zenodo.8396813

- python for physicists and chemists in a nutshell
- Computer Algebra System
- Physical chemistry (incl. quantum chemistry)
- coding and use of representations of molecular structures and related data
- Data science and ML

can we expect a strong convergence between **quantum and computational chemistry**, data science and machine learning?



increase in the number of students in the master's programmes in theoretical and computational chemistry?

... unless we do not really give them a **dual skill set that could be sought after in various areas of research and industry**