Data Science Challenges in Computational Chemistry

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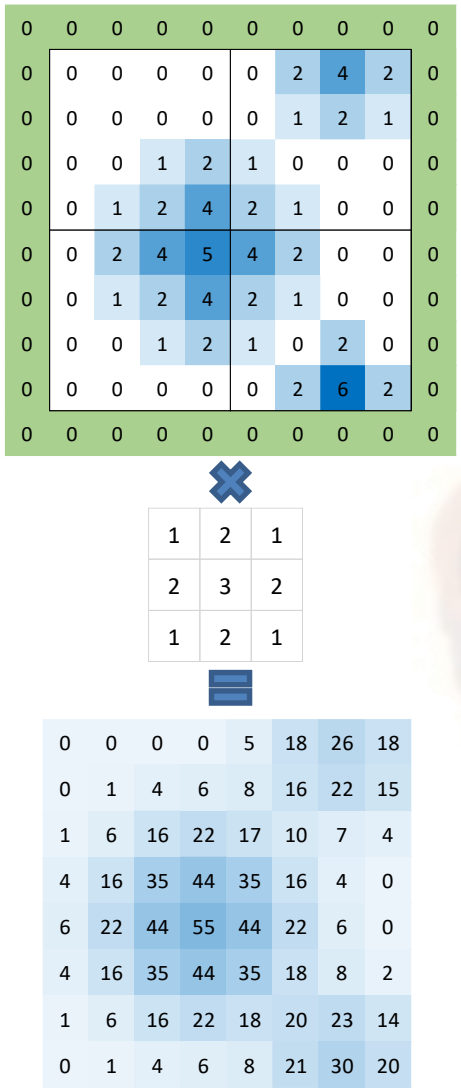
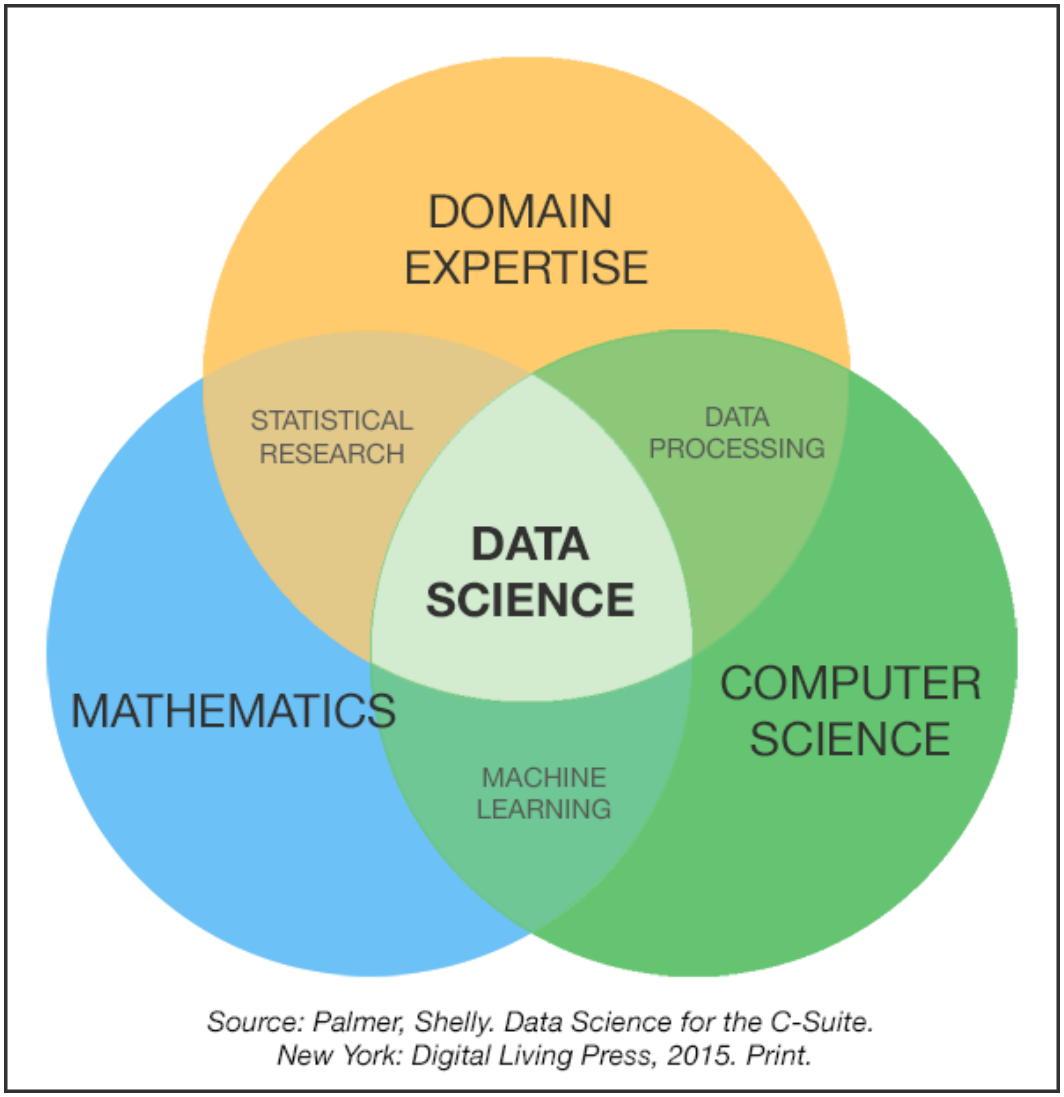
Physikalische Chemie III

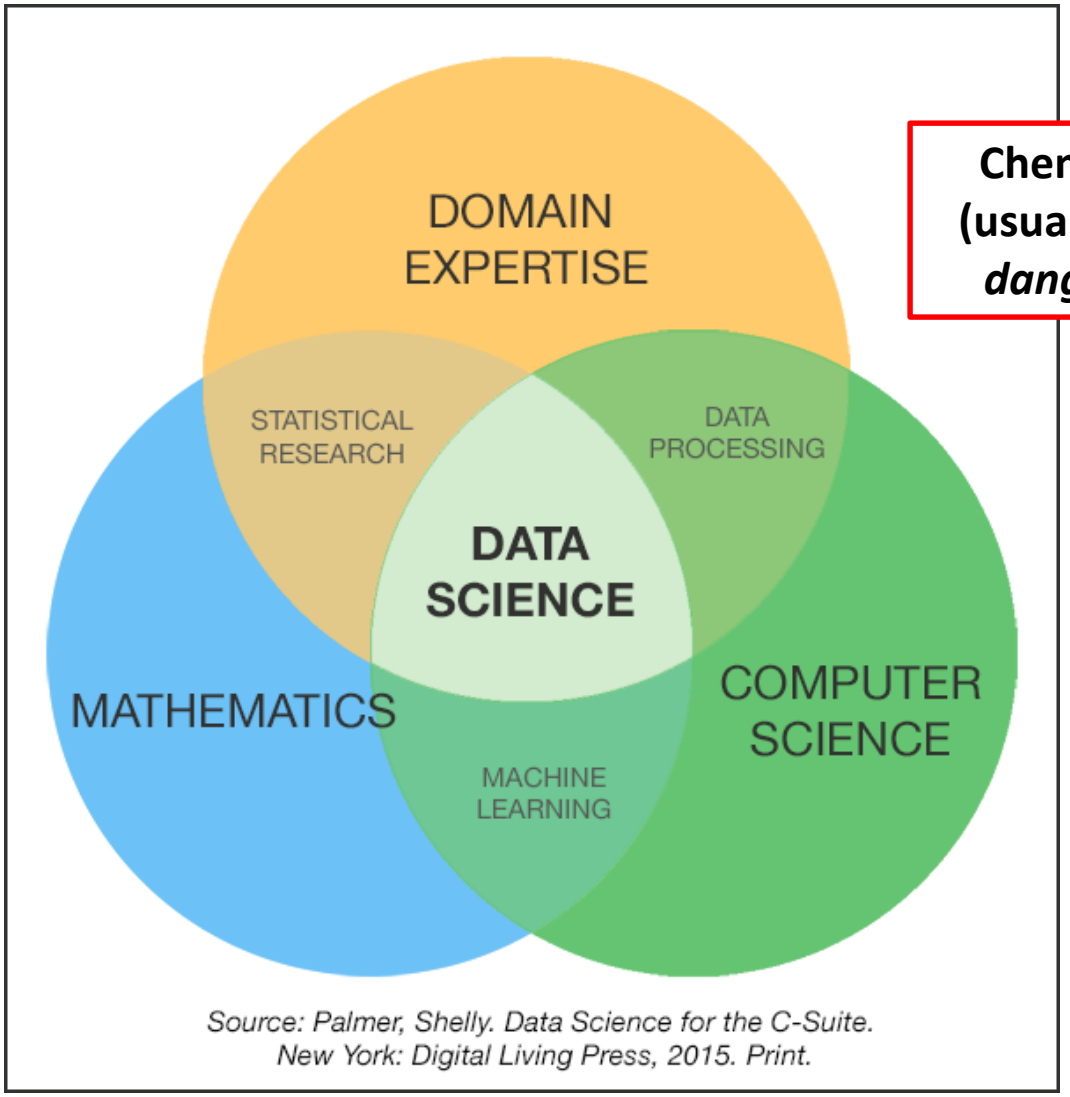


Data & Science in Chemistry



Source: Palmer, Shelly. Data Science for the C-Suite. New York: Digital Living Press, 2015. Print.

Data & Science in Chemistry



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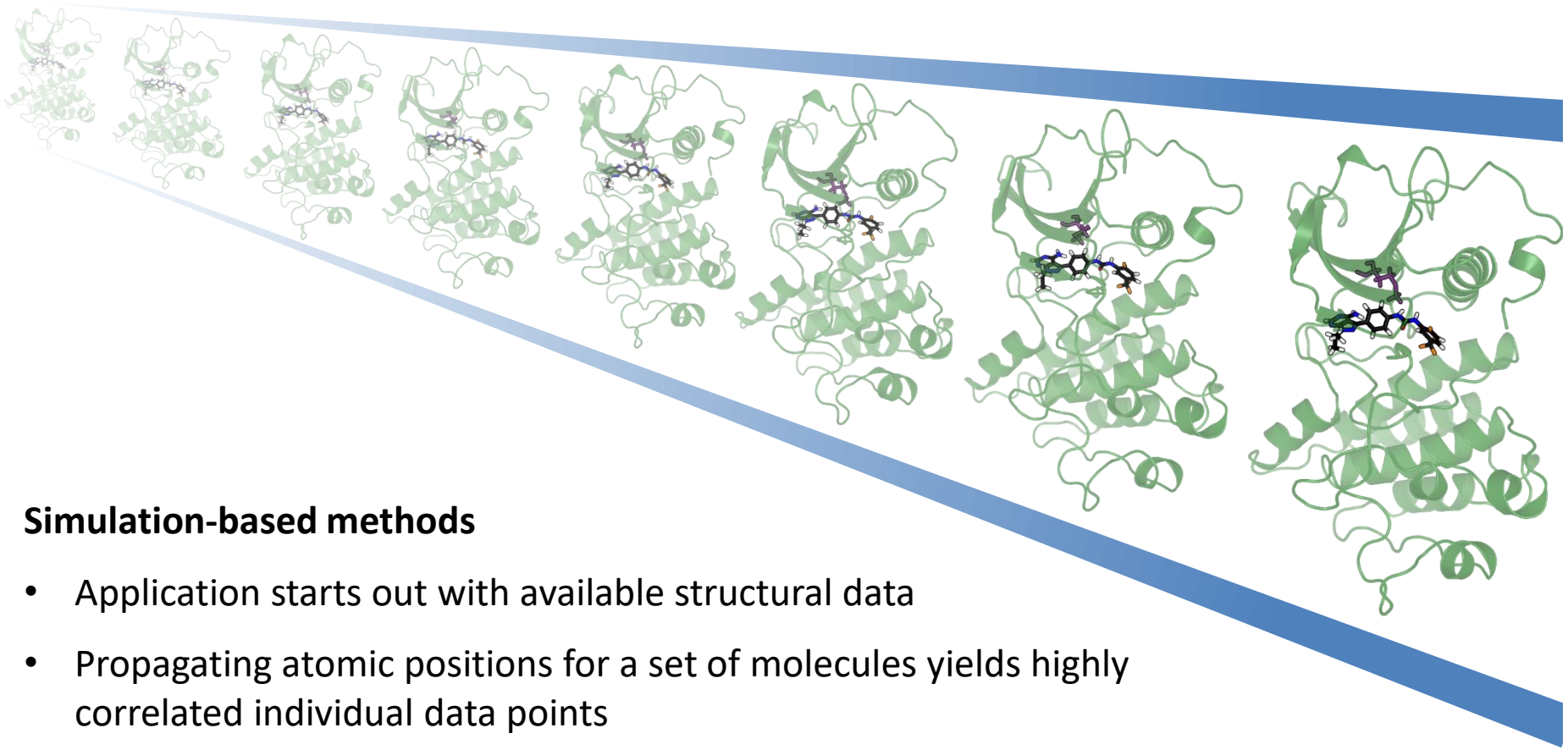
Chemists are (usually) in the *danger zone*

Molecular Simulations



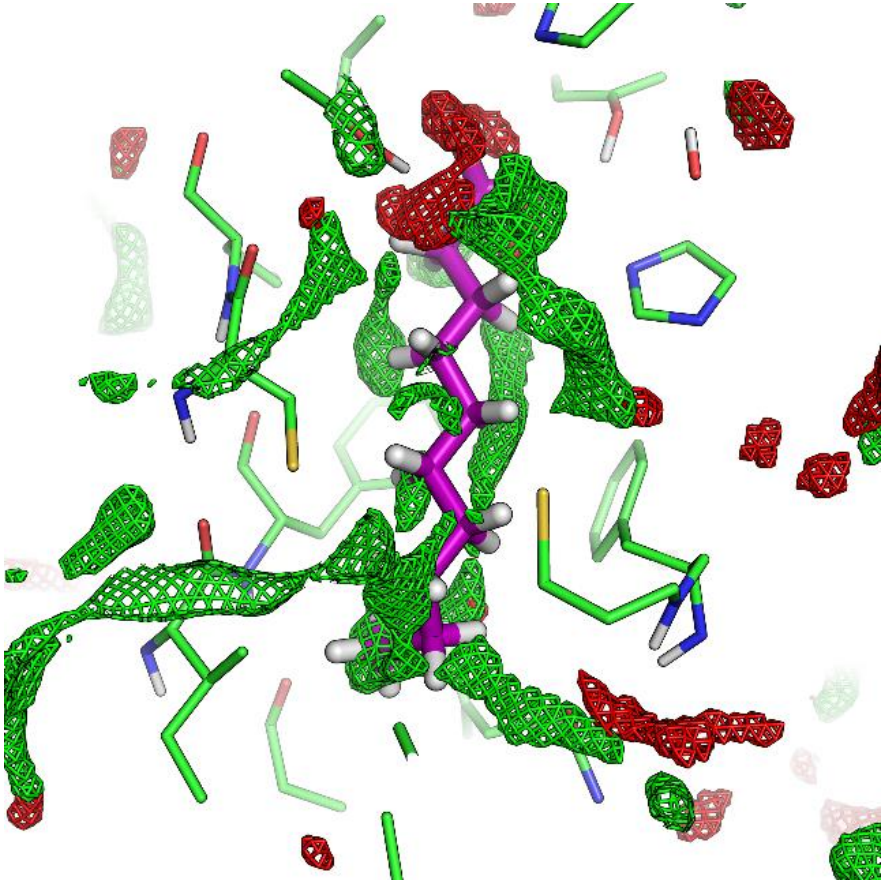
Simulation-based methods

- Application starts out with available structural data
- Propagating atomic positions for a set of molecules yields highly correlated individual data points
- Millions of snapshots (results have to be extracted from trajectory)
- Tools for analysis often originate from statistics (Markov chain models, correlation analysis)

Molecular Simulations – Volumetric Data

Data structures

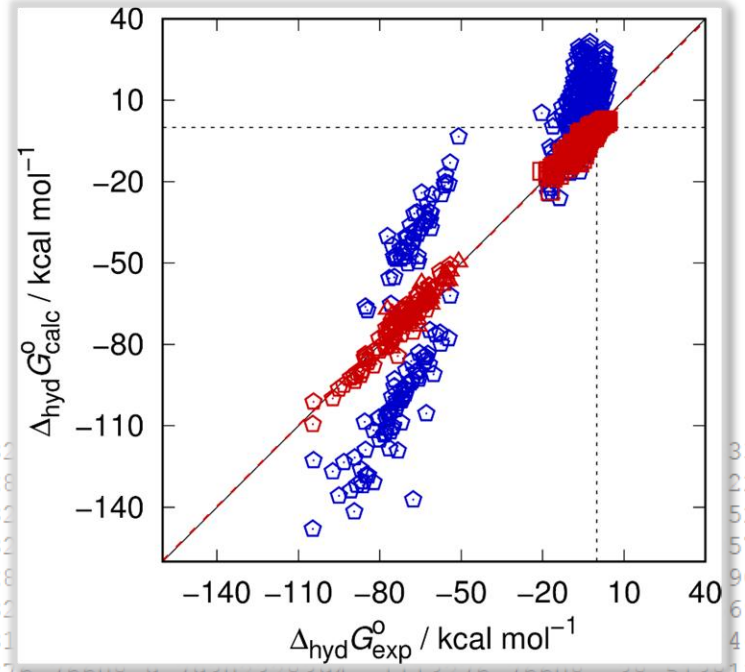
- Distribution of solvent around a solute
- Volumetric data on 3D grids (density or energy value at each point)
- Large files → storage problem
- Volumetric data collapsed to scalars
- Both data types can be used for machine learning



Quantum-Mechanical Data

Compensating for physical approximations

- Clean data but errors caused by physical approximations
- Complexity unaccounted for by high level data fitted through regression models
- Expensive and slow (larger systems can be unfeasible due to exponential scaling)

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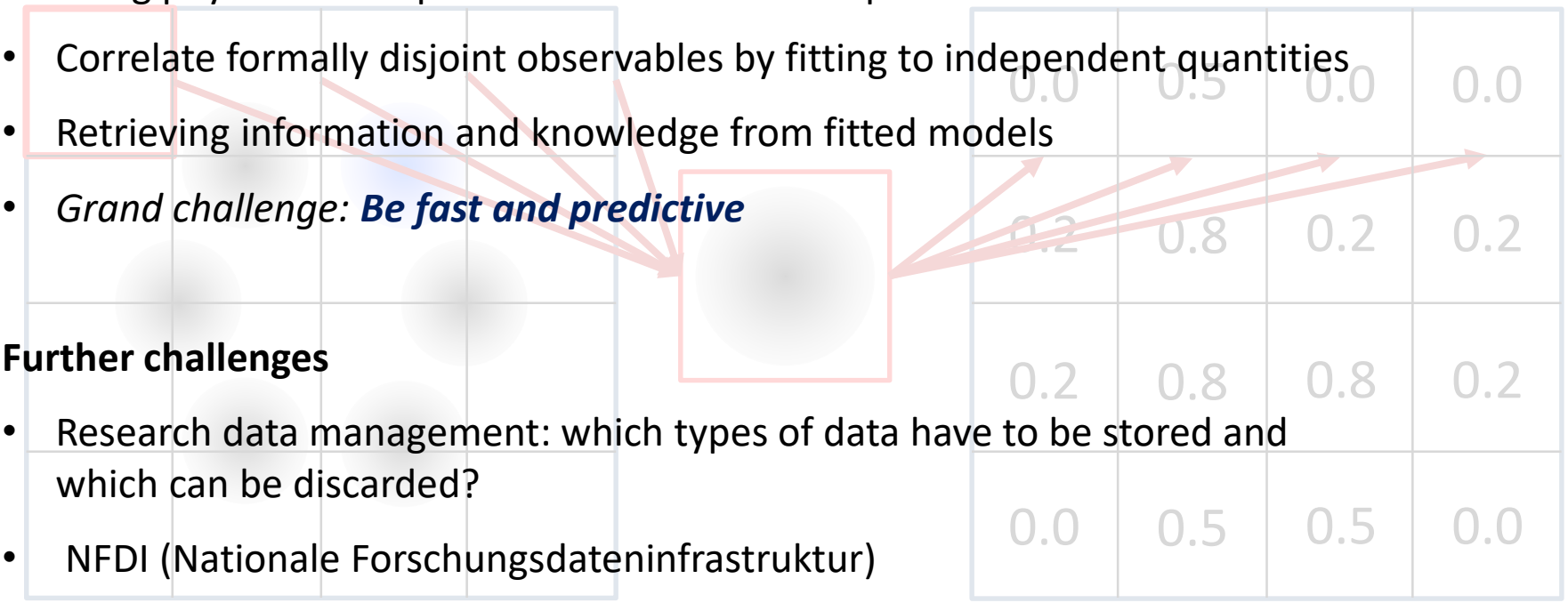
Regression Models on Synthetic Data

Practical applications of Data Science

- Correcting errors within the data generated using physics-based methods by training low level models
- Using physics to compensate for insufficient experimental data sources
- Correlate formally disjoint observables by fitting to independent quantities
- Retrieving information and knowledge from fitted models
- *Grand challenge:* ***Be fast and predictive***



Further challenges

- Research data management: which types of data have to be stored and which can be discarded?
- NFDI (Nationale Forschungsdateninfrastruktur)
- Integration of Data Science in curricula