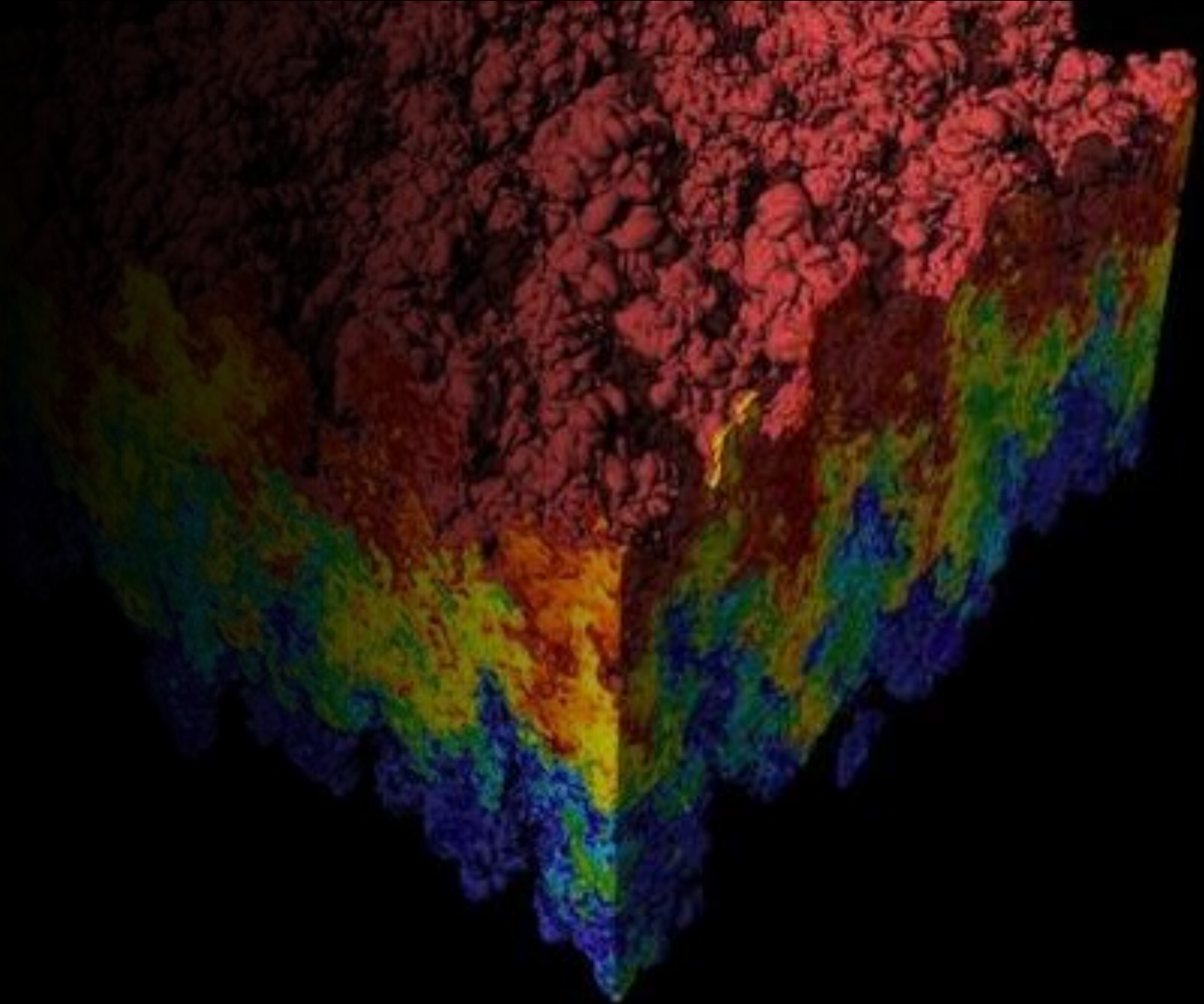
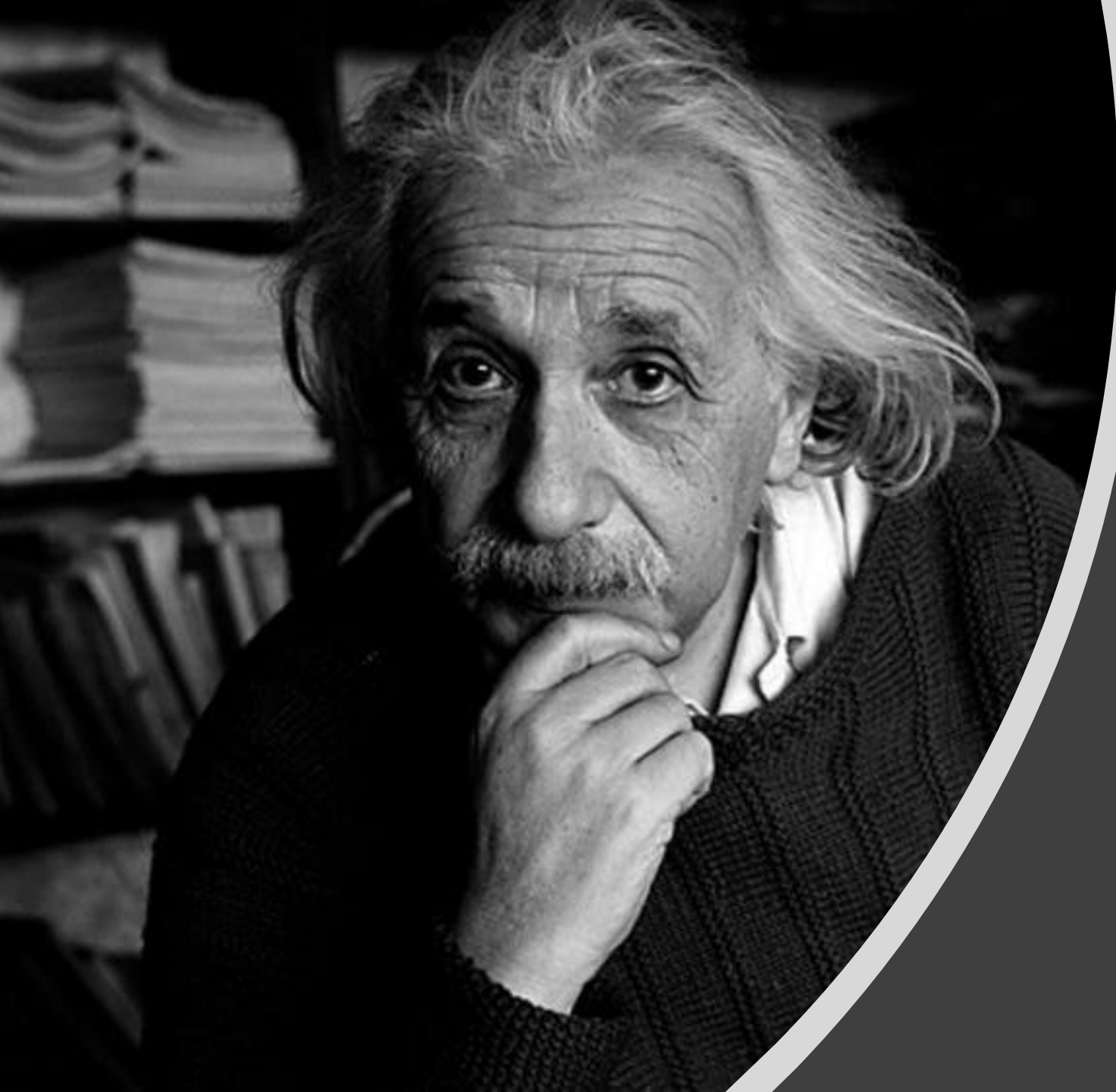


Simulating thermodynamical properties of noble gases using molecular dynamics

Arne Kristian Kramprud Hjelt
Under veiledning av Raffaella Cabriolu





← That guy again...

«Gedankenexperiment»

- Imagine an experimental setup
- Do the experiment mentally by applying the physics you know
- Evaluate

Benefits

- You can do big experiments that would be expensive or impossible to do in real life
- You can get interesting results that push your understanding further

Challenges

- Systems with many individual elements that cant be approximated to a few big entities can get to complex to keep track of
- Complex systems might generate a lot of data which can be labour intensive to analyze



Molecular Dynamics

- The computer-age extension of the thought experiment

No longer any problem to make many calculations on complex systems

Cheap compared to doing the actual physical experiments

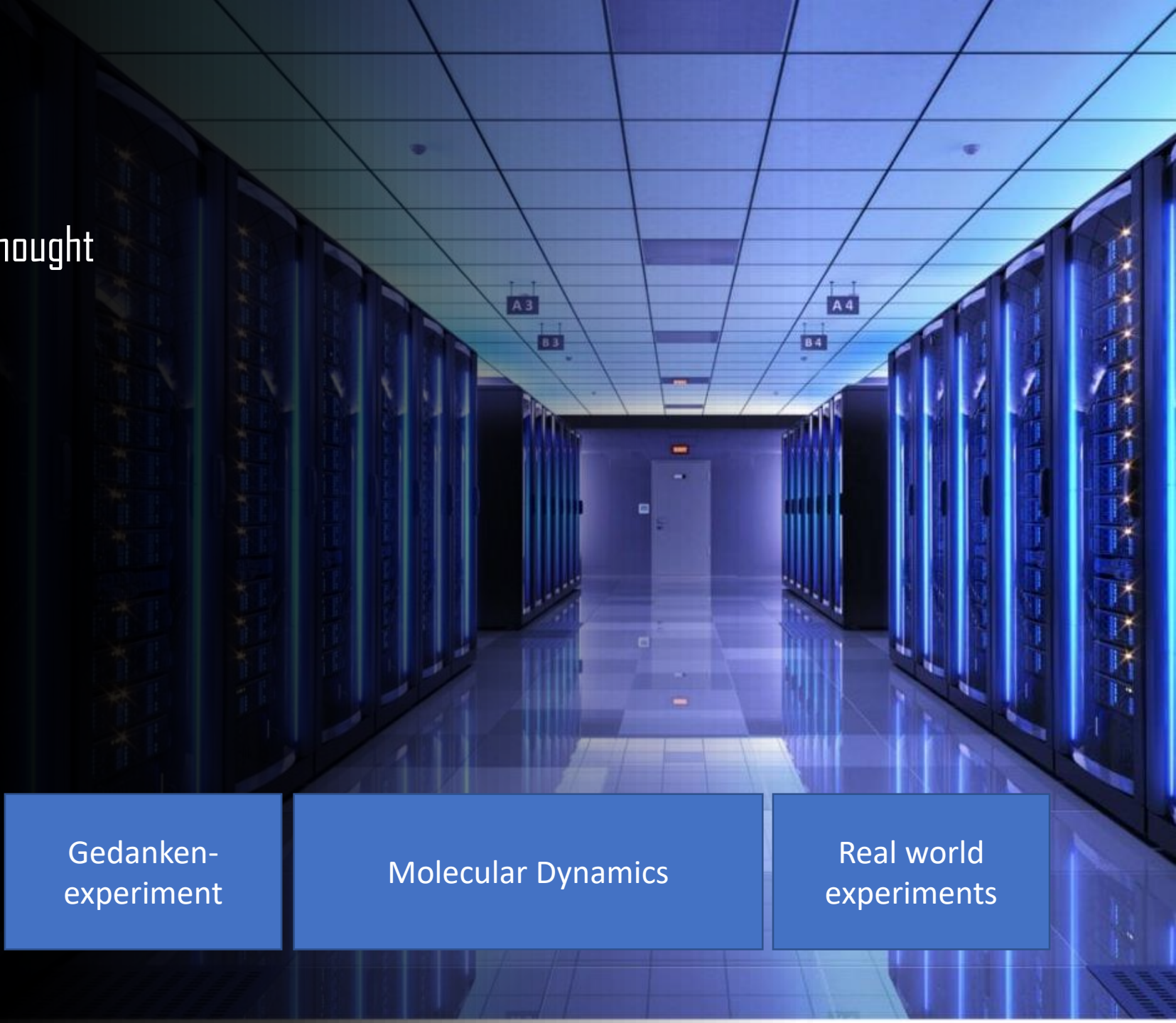
Can analyze vast amounts of data quickly

Results can be graphically represented

Gedanken-
experiment

Molecular Dynamics

Real world
experiments



Simulation of a
4,47 km/s diamond Nano-
Astroid Impacting a Graphene
Sheet

HPC (High Performance
Computing)

LAMMPS

Lennard-Jones potential

