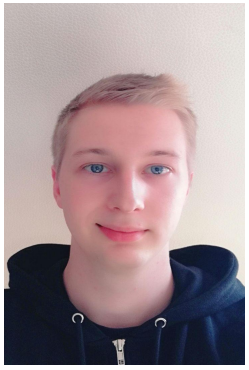
GPU-ISLE

March 13, 2021 | Marcel, Stefan, Johann, Jan-Lukas | JSC, JSC, Uni Bonn, ESS

GPU-ISLE TEAM



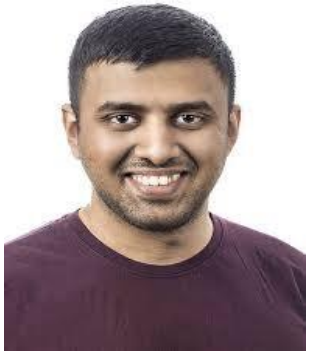
Marcel Rodekamp

Stefan Krieg

Johann Ostmeyer

Jan-Lukas Wynen

Gonzalo Brito



Jayesh Badwaik

JÜLICH Forschungszentrum

SIMULATING CARBON NANO SYSTEMS

- Lattices of carbon atoms
- Various geometries
- High technical interest
  - Improved semiconductors
  - Filtering techniques
- Simulating behaviour: Quantum Field Theory
  1. System description with Energy functional (Hamiltonian)
  2. Generation of many states (Configurations)
  3. Evaluating physical quantities

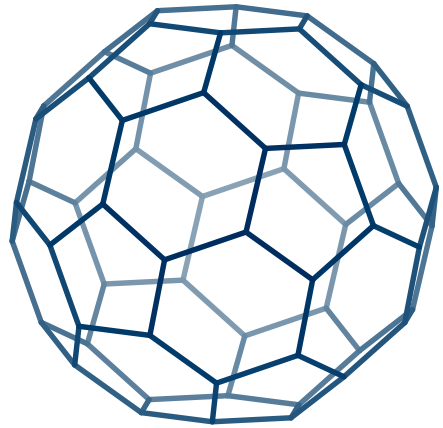


Figure: Graphical representation of a C_{60} (Buckminsterfullerene) system. Each node represents a carbon atom and each edge the bond between two atoms.

SIMULATING CARBON NANO SYSTEMS

- Lattices of carbon atoms
- Various geometries
- High technical interest
  - Improved semiconductors
  - Filtering techniques
- Simulating behaviour: Quantum Field Theory
  1. System description with Energy functional (Hamiltonian)
  2. Generation of many states (Configurations)
  3. Evaluating physical quantities

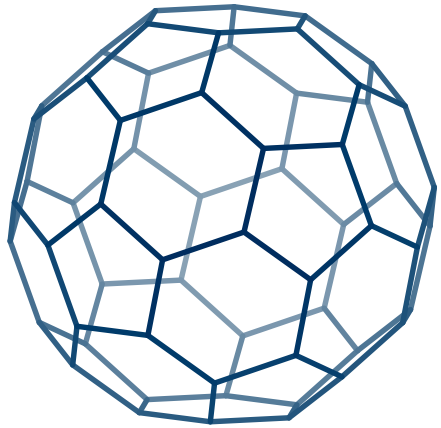
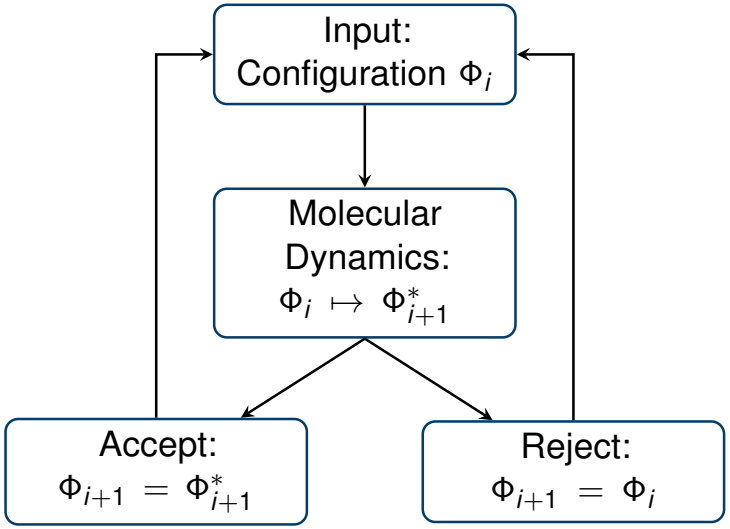


Figure: Graphical representation of a C_{60} (Buckminsterfullerene) system. Each node represents a carbon atom and each edge the bond between two atoms.

THE HYBRID MONTE CARLO ALGORITHM

- Building Markov Chain
- Iteratively updating previous configuration
- Update by Molecular Dynamics
  - Integrate Hamilton equations
    - **Leapfrog**
  - Requires: Matrix inversion
  - Requires: Matrix, vector operations
- Dimension $N_\tau \times \mathcal{O}(N_\sigma)$
  - C_{60} : $N_\tau \times \mathcal{O}(60)$



JÜLICH Forschungszentrum

ISLE

Current State

- C++: Heavy math
- Python: Interface
- Build upon
  - Blaze
  - Lapack

Goal

- Port of Molecular Dynamics
  - Leapfrog
  - Matrix inverter
  - Matrix, vector operations
- Hybridization of Infrastructure (CPU,GPU)
- C++ with CUDA
- Blaze: CUDA Managed Pointer
- Utilize CUDA Math Libraries