



GPU-ISLE

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GPU-ISLE TEAM



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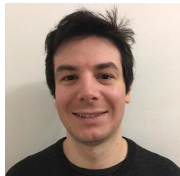
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SIMULATING CARBON NANO SYSTEMS

- 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

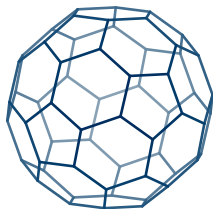


Figure: Graphical representation of a C_{60} (Buckminsterfullerene) system. Each node represents a carbon atom and each edge the bond between two atoms.

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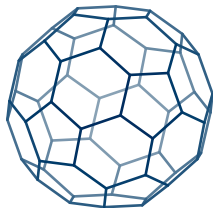
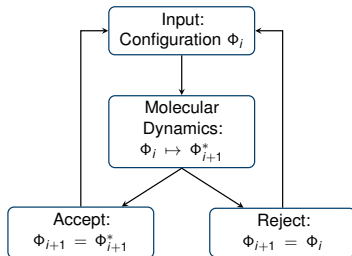


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THE HYBRID MONTE CARLO ALGORITHM

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



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