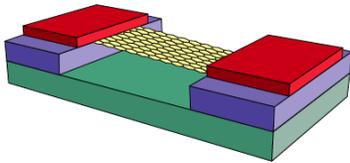


Porting and testing DFTB dynamics to GPU

Quantum dynamics on GPU

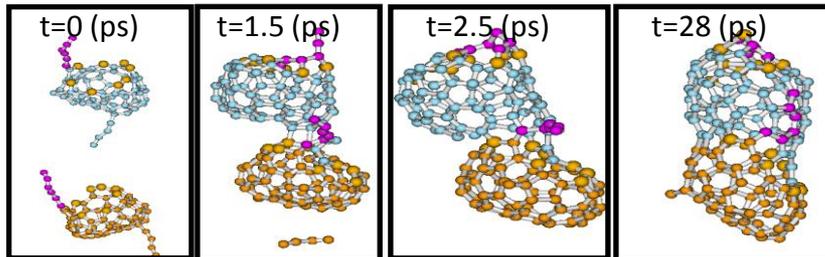
Science motivation:

- Search for advanced materials
- Modeling molecular devices



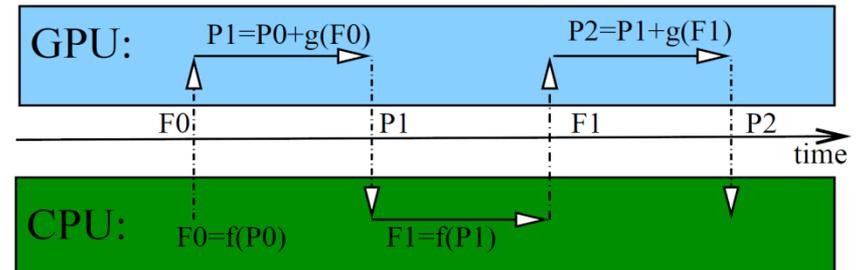
Method: quantum dynamics

- DFTB for electrons, classical nuclei
- Forces & energy expensive → weeks!



2 min/1MD step → 2 weeks /10k steps
Speedup needed!

- Schroedinger Eq. $i\hbar \frac{dP(t)}{dt} = [P(t), F(t)]$
- Fine grained parallelism
 - ✓ A lot of linear algebra.
Matrices: F –Fock , P –density matrix
 - ✓ F and P are dense
 - ✓ Good problem size: $1000 < \dim(P) < 10,000$
- Hybrid GPU and CPU algorithm:



- Promising speedup:
 - C1060 vs 8 cores Xeon (MKL)
 - single precision x20
 - double precision x 3
- Jakowski, “GPU computing Gems”,ch.5,2011