Porting and testing DFTB dynamics to GPU

Science motivation:
- Search for advanced materials
- Modeling molecular devices

Method: quantum dynamics
- DFTB for electrons, classical nuclei
- Forces & energy expensive → weeks!

Quantum dynamics on GPU
- Schroedinger Eq.
- Fine grained parallelism
  ✓ A lot of linear algebra.
  ✓ $F$ – Fock, $P$ – density matrix
  ✓ $F$ and $P$ are dense
  ✓ Good problem size: $1000 < \text{dim}(P) < 10,000$

Hybrid GPU and CPU algorithm:

Promising speedup:
- C1060 vs 8 cores Xeon (MKL)
  - Single precision $\times 20$
  - Double precision $\times 3$