MPI Parallelization in NEMO 5

- **Objective:**
  - » Provide multi-level parallelization in NEMO 5
  - » Keep parallelization scheme decoupled from physical meaning
  - » Encapsulate parallelization scheme in a class

- **Results / Impact:**
  - » C++ class that makes it easy to parallelize any quantity
  - » Load balancing and relative execution time of each process can be estimated in advance
  - » Proven to work well in quantum transport simulations

- **Approach:**
  - » Organization of levels into hierarchy
  - » Identified 2 different MPI process distribution strategies
  - » Identified conceptual difference between real-space parallelization (→ parallel matrix storage) and others