High Performance Computing using NEMO 5

- **Objective:**
  - » Employ NEMO 5 for large-scale runs on supercomputers
  - » Enable hero simulations
  - » Prove scalability of code

- **Approach:**
  - » Scalability is enabled by PETSc, SLEPc and home-grown multilevel MPI task distribution class
  - » Participation in ORNL's Joule project to test and improve scalability

- **Results / Impact:**
  - » Strong scaling of a ballistic transport simulation in an ultrathin-body transistor up to 1e5 cores
  - » Weak scaling of strain and eigenstates in a quantum dot involving ~1e9 degrees of freedom