

Approach:

- Running simulations for different cross-section and length of nanowire on Steele cluster
(<http://www.rcac.purdue.edu/userinfo/resources/steele/>)
- Extracting memory/time estimation for different CPU per energy point(CPP)

Impact:

- Estimate memory/time usage for OMEN Nanowire (<https://www.nanohub.org/resources/5359>) user

Result:

- Memory/time estimation increases linearly to the length of the nanowire (Fig. 1).
- When memory estimation is larger than 2GB, the walltime increases non-linearly (Fig. 2) due to usage of swap memory. (CPP should be increased)
- Memory/time estimation increases quadratically to the cross section of the nanowire (Fig. 3).

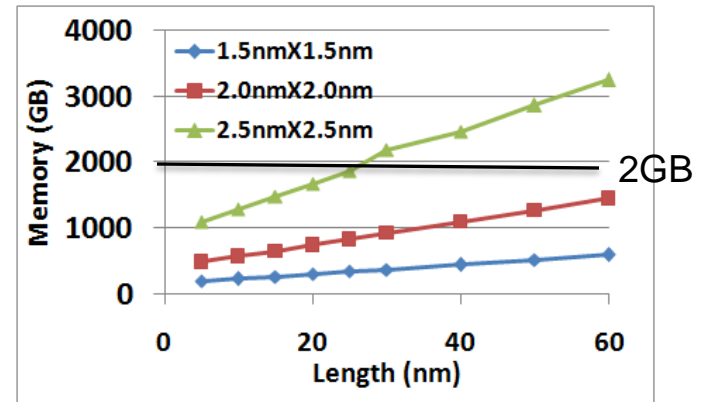


Fig. 1 Memory estimation

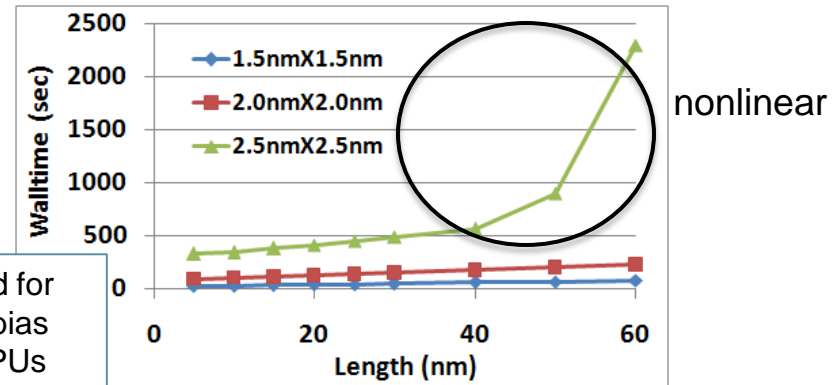


Fig. 2 Simulation time(walltime) estimation

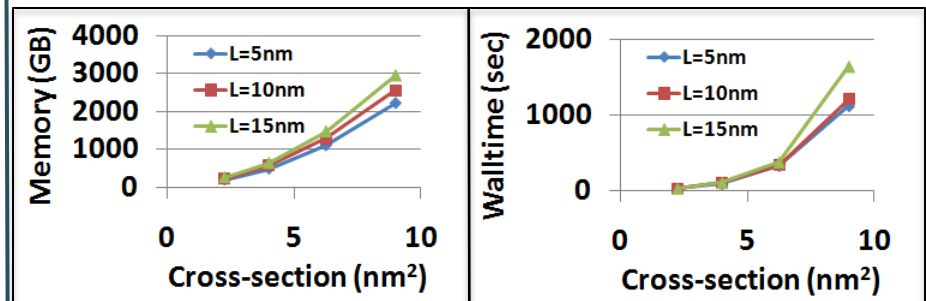


Fig. 3 Memory/time estimation for different cross section