OMEN Nanowire: Time/memory table

Approach:

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 Running simulations for different crosssection 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 (<u>https://www.nanohub.org/resources/5359</u>) 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-linearily (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).

