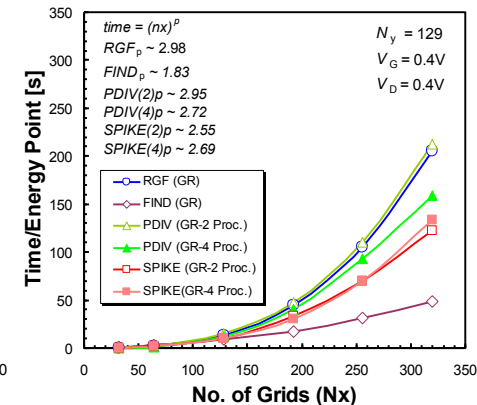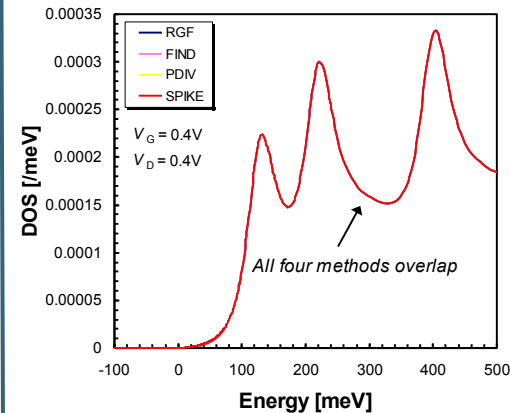## Objective:

• Collaborated with several groups to develop and implement novel algorithms for the calculations of charge densities from large and sparse NEGF matrices related to nanoscale devices.

Approach:

• **FIND algorithm** (*Song Li and Eric Darve, Stanford University; Shaikh Ahmed, Purdue University*)

• **The Divide and Conquer Approach** (*Stephen Cauley and Jitesh Jain, Balakrishnan-Kok group, Purdue University*)

• **SPIKE** (*Eric Polizzi and Ahmed Sameh, Purdue University*)

• SPIKE and PDIV are parallelized with MPI. RGF is an intrinsically serial algorithm. FIND is a serial algorithm at this stage.

Impact:

• Demonstrated validity and scaling properties of novel algorithms

• Faster algorithms will accelerate the discovery of new devices

$V_G = 0.4V$
$V_D = 0.4V$

All four methods overlap

RGF, FIND, PDIV, SPIKE

DOS [/meV] vs Energy [meV]

$time = (nx)^p$
$RGF_p \sim 2.98$
$FIND_p \sim 1.83$
$PDIV(2)p \sim 2.95$
$PDIV(4)p \sim 2.72$
$SPIKE(2)p \sim 2.55$
$SPIKE(4)p \sim 2.69$

$N_y = 129$
$V_G = 0.4V$
$V_D = 0.4V$

RGF (GR)
FIND (GR)
PDIV (GR-2 Proc.)
PDIV (GR-4 Proc.)
SPIKE (GR-2 Proc.)
SPIKE(GR-4 Proc.)

Time/Energy Point [s] vs No. of Grids (Nx)

Result:

• Integrated the three new algorithms into the nanoFET code

• Verified that the new codes provide exactly the same numerical answers as the original state-of-the-art RGF algorithm (see the DOS figure on the left).

• Figure on the right compares the scaling of all algorithms against N_x, the nanoFET cross section, for a nominally short channel with $N_y=129$.

• FIND outperforms all algorithms on a single CPU.

Shaikh S. Ahmed