

Objective:

- Physics-based simulations of nanoelectronic devices with an atomistic resolution and a sustained performance > 1 Pflop/s

Approach:

- Multi-Level parallelism
- Dynamic load balancing in double integral
- Computational interleaving
- Development of new direct solver (block cyclic reduction)

Result:

- Highly efficient parallel algorithm, stressing the most advanced resources available today

Impact:

- Move from nano-science to nanodevice engineering in minutes
- Unprecedented insight into atomistic device simulation
- One of the few codes with sustained performances at the peta-scale on Jaguar @ ORNL

