Doctor I part & Master team   Ensemble Monte Carlo and Classical Simulations

Start code: indoor **MC** simulator
Written in C

Properties:

MONTE CARLO:
single particle, weights,
time duration averages,
robust analytical evolution
of the trajectory via energy ballance;

PHYSICAL:
homogeneous or 1D,
stationary transport
boundary conditions

MATERIAL:
cubic semiconductors:
covalent Si,Ge,
compounds GaAs (polar);
analytical band model
Γ, X, L valleys
nonparabolic,anisotropy;
all scattering models.

End code: VEnsembleMC

Properties:

Many particles , weights,
time step ensemble averages
self-consistency with Poisson eqn.,
numerical evolution of the trajectories
via Newton's eqns,

homogeneous, 1D and 2D
transient & stationary transport
initial & boundary conditions

Semiconductor-light interaction,
Photo-generation, modeling of novel
structures, materials, concepts

add wurtzite semiconductors (GaN),

U valley, scattering between **U** ↔ **X,L,Γ,**
dislocation & piezoelectric scattering

Doctor II part Development of the WIENS union, 2D quantum particles simulations.

WignerENSemble union: theoretical & numerical approaches to quantum transport with dissipation.

State of Art:

THEORETICAL:
Wigner-Boltzmann eqn. for phonons & impurities,
Fokker-Planck eqn. for quantum Brownian motion
Role of scattering for decoherence & localization

ALGORITHMS:
distinguishable vs undistinguishable particles
Affinity, Arizona State Univ., Univ of Paris-Sud
Generation-annihilation, IuE, TU-Wien,

APPLICATIONS: mailnly of the Affinity algorithm
1D: RTD, from resonant to sequential tunneling;
Analysis of de-coherence and localization, Coh. Length
coupling classical & quantum MC regions;
quasi-2D DGMOSFET:
Wigner approach bridges the gap coh./scatt.
CarbonNanotubeFET's
Quantum and classical simulations give close results

Further development of WIENS

2D Wigner-Boltzmann theory, Effect of geometry on coherence and boundary conditions.
Coupling of coherent Greens' & Wigner-Boltzmann eqns.: from boundary → initial condition problem
2D - Calculate G(**x**,**x'**,E) for Δ**x** ~ Coh. Length?

Unification of the two existing approaches,
Novel algorithms
2D Wigner-Boltzmann – bound. cond.
Green's-Wigner-Boltzmann init. cond.;
self-consistency with Poisson equation.

Implementation:
upon the **VEMC** code, parallelization, openMP

Applications: aiming at the rich world between quantum-coherent & scattering–dominated transport processes and phenomena which can be revealed only by intensive simulations.

Conclusions: Rich world with not unique carrier behavior.
No strict barrier between classical & quantum;