Distributed parallel non-equilibrium Green's function approach to inelastic charge transport

Sebastian Achilles

RWTH Aachen University

achilles@aices.rwth-aachen.de

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- Paolo Bientinesi.

Motivation

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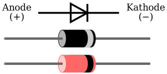

(a) Diodes

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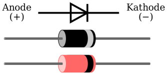

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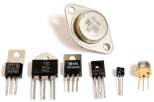

(b) Transistors

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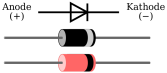

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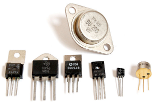

(b) Transistors

(c) LEDs

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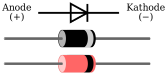

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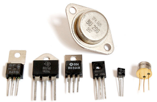


(b) Transistors

(c) LEDs

(d) Solar cells

Motivation

The physical system consists of

- electrons,
- phonons,
- an applied bias through the contacts.

Motivation

- Objective: simulation of microscopic structure where quantum effects are relevant,
- The physical system in question is out of the equilibrium,
- Inelastic quantum transport of paramount importance,

$\Rightarrow$ Semi-classical device simulation no longer valid,

$\Rightarrow$ NEGF formalism allows consistent treatment of inelastic quantum transport in nanostructures and meets all the requirements.

NEGF framework

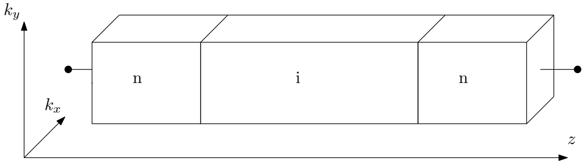
Theoretical challenges and model requirements

- The system has *open boundary conditions* since the diode is coupled to contacts by contact self-energies,
- the *steady state* condition allows Fourier transformation of time difference to energy,
- due to the applied bias the system is *out of equilibrium*,
- the scattering is *non ballistic* due to scattering effects (phonons),
- simulation addresses inelastic *quantum transport* in a consistent and complete way.

NEGF formalism

- quasi 1-D representation for steady-state Green's functions:

$$G(\mathbf{r}, \mathbf{r}', E) \rightarrow G(z, z', \mathbf{k}_{\|}, E)$$



NEGF formalism

- steady state NEGF equations:
  - Computation of G_0^R

$$[E - \mathcal{H}_0(z, \mathbf{k}_\parallel)] G_0^R(z, z', \mathbf{k}_\parallel, E) = \delta(z - z')$$

  - Dyson equation

$$G^R(z, z', \mathbf{k}_\parallel, E) = G_0^R(z, z', \mathbf{k}_\parallel, E) + \int \mathrm{d}z_1 \int \mathrm{d}z_2 \, G_0^R(z, z_1, \mathbf{k}_\parallel, E) \Sigma^R(z_1, z_2, \mathbf{k}_\parallel, E) G^R(z_2, z', \mathbf{k}_\parallel, E)$$

NEGF formalism

- steady state NEGF equations:
  - Keldysh equation

$$G^{\gtrless}(z,z',\mathbf{k}_\parallel,E) = \int \mathrm{d}z_1 \int \mathrm{d}z_2\, G^R(z,z_1,\mathbf{k}_\parallel,E)\Sigma^{\gtrless}(z_1,z_2,\mathbf{k}_\parallel,E) \times G^A(z_2,z',\mathbf{k}_\parallel,E)$$

  - Self-consistent Born approximation for Self-energy

$$\Sigma^{\gtrless}(z,z',\mathbf{k}_\parallel,E) = \sum_{\mathbf{q}_\parallel} F(\mathbf{q}_\parallel,\Delta_{z,z'},k,q_0)\times [N_{LO}\times G^{\gtrless}(z,z',\mathbf{q}_\parallel,E\pm\hbar\omega_{LO}) + (N_{LO}+1)G^{\gtrless}(z,z',\mathbf{q}_\parallel,E\mp\hbar\omega_{LO})]$$

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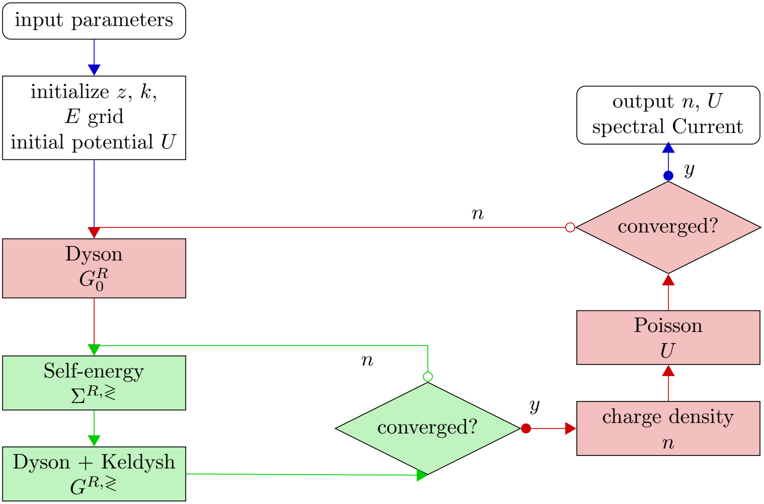
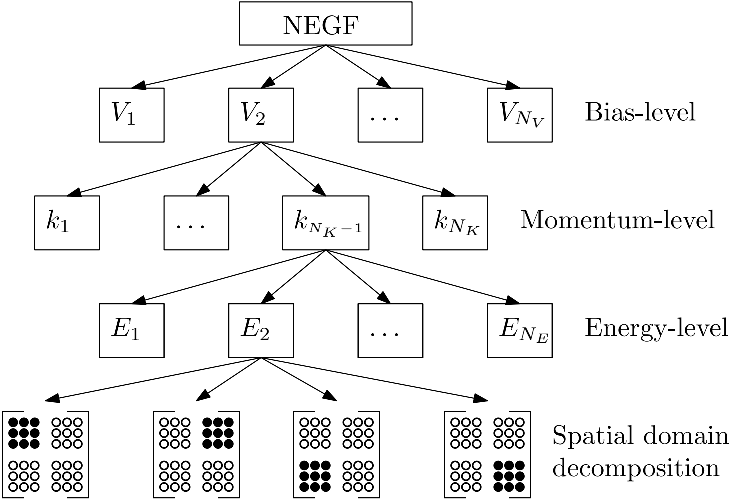
$\rightarrow$ Self-energy needs to be solved self-consistently.

Flowchart of NEGF



Parallelization

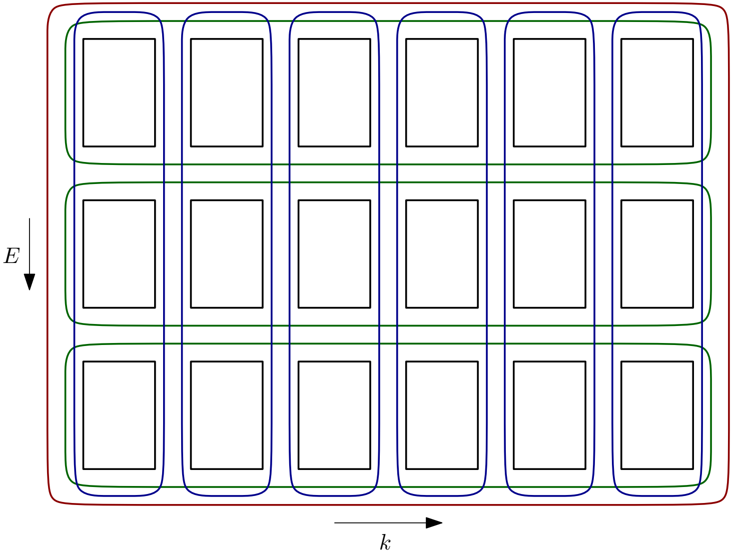
Parallelization levels



Momentum and energy distribution

$K = 0, 1$ $E = 0, 1, 2$	$K = 2, 3$ $E = 0, 1, 2$	$K = 4, 5$ $E = 0, 1, 2$	$K = 6, 7$ $E = 0, 1, 2$	$K = 8, 9$ $E = 0, 1, 2$
$K = 0, 1$ $E = 3, 4, 5$	$K = 2, 3$ $E = 3, 4, 5$	$K = 4, 5$ $E = 3, 4, 5$	$K = 6, 7$ $E = 3, 4, 5$	$K = 8, 9$ $E = 3, 4, 5$
$K = 0, 1$ $E = 6, 7, 8$	$K = 2, 3$ $E = 6, 7, 8$	$K = 4, 5$ $E = 6, 7, 8$	$K = 6, 7$ $E = 6, 7, 8$	$K = 8, 9$ $E = 6, 7, 8$
$K = 0, 1$ $E = 9, 10, 11$	$K = 2, 3$ $E = 9, 10, 11$	$K = 4, 5$ $E = 9, 10, 11$	$K = 6, 7$ $E = 9, 10, 11$	$K = 8, 9$ $E = 9, 10, 11$

Cartesian topology



Self-energy

$$\Sigma^{\gtrless}(z, z', \mathbf{k}_{||}, E) = \sum_{\mathbf{q}_{||}} F(\mathbf{q}_{||}, \Delta_{z,z'}, \mathbf{k}_{||}, q_0) \times$$
$$[N_{LO} \times G^{\gtrless}(z, z', \mathbf{q}_{||}, E \pm \hbar\omega_{LO})$$
$$+ (N_{LO} + 1) G^{\gtrless}(z, z', \mathbf{q}_{||}, E \mp \hbar\omega_{LO})]$$

Self-energy

1. Communication across energy:
   - $G_{+}(q, E) = G(q, E + \hbar\omega)$
   - $G_{-}(q, E) = G(q, E - \hbar\omega)$

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   - $G_+(q, E) = G(q, E + \hbar\omega)$
   - $G_-(q, E) = G(q, E - \hbar\omega)$
2. Build H + Update local
   - $H(q, E) = \alpha G_+(q, E) + \beta G_-(q, E)$
   - $\Sigma(k, E) = \Sigma(k, E) + c(q, k) H_{local}(q, E)$

Self-energy

1. Communication across energy:
   - $G_{+}(q, E) = G(q, E + \hbar\omega)$
   - $G_{-}(q, E) = G(q, E - \hbar\omega)$
2. Build H + Update local
   - $H(q, E) = \alpha G_{+}(q, E) + \beta G_{-}(q, E)$
   - $\Sigma(k, E) = \Sigma(k, E) + c(q, k) H_{local}(q, E)$
3. Communication across momentum + remote update
   - exchange H across the momentum level
   - $\Sigma(k, E) = \Sigma(k, E) + c(q, k) H_{remote}(q, E)$

Results

Speedup on Juqueen

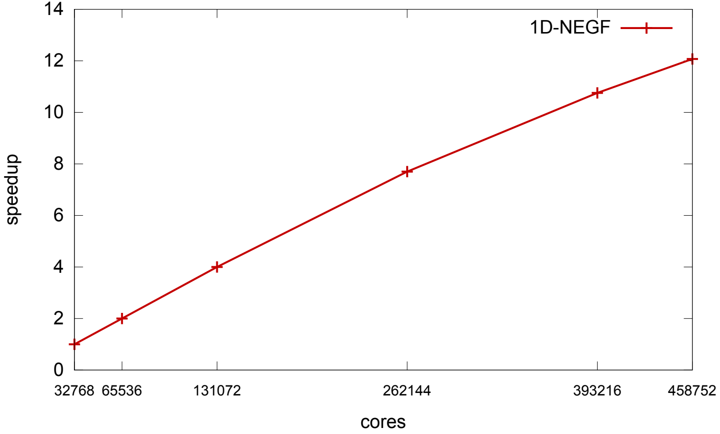

Figure : Hybrid scaling for a system with $N_K = 2048$, $N_E = 5376$, and $N_P = 100$.

Efficiency on Juqueen

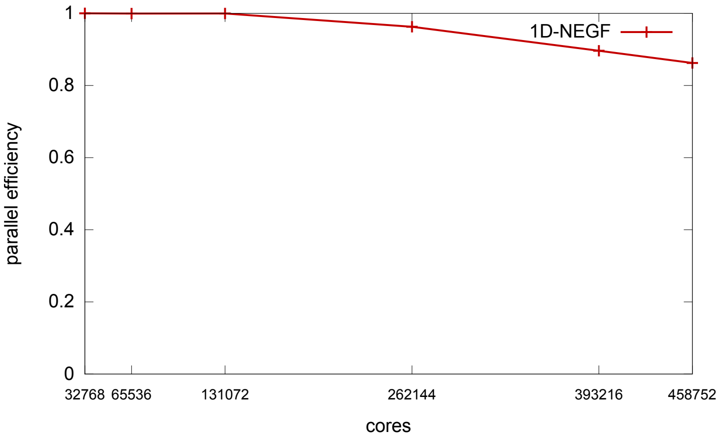

Figure : Hybrid scaling for a system with $N_K = 2048$, $N_E = 5376$, and $N_P = 100$.

Conclusion

- A efficient parallelization approach was presented,
- the approach can use MPI, OpenMP, or both,
- scaling up to 458.762 cores on JUQUEEN.

Outlook

- Using the parallelization approach in PVnegf,
- implementation of advanced mixing schemes and preconditioner,
- adaptive mesh and adaptive integration.

The End