Eigenchannels and Current density analysis

Software Advancement Team, ISSP

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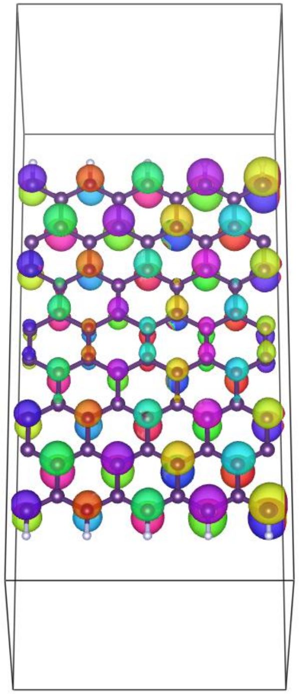
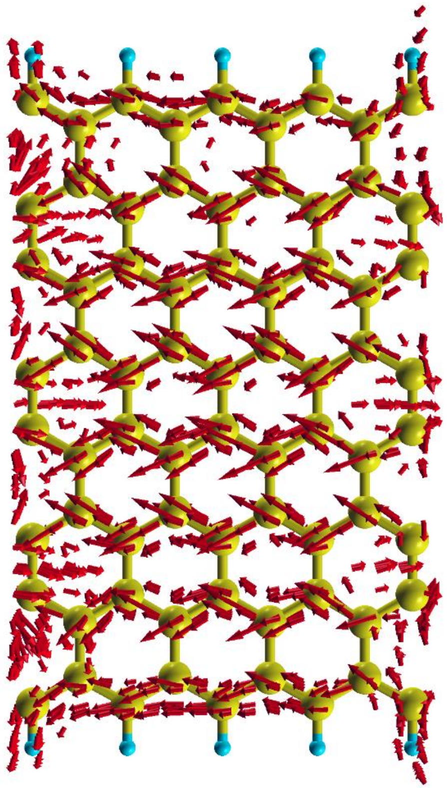
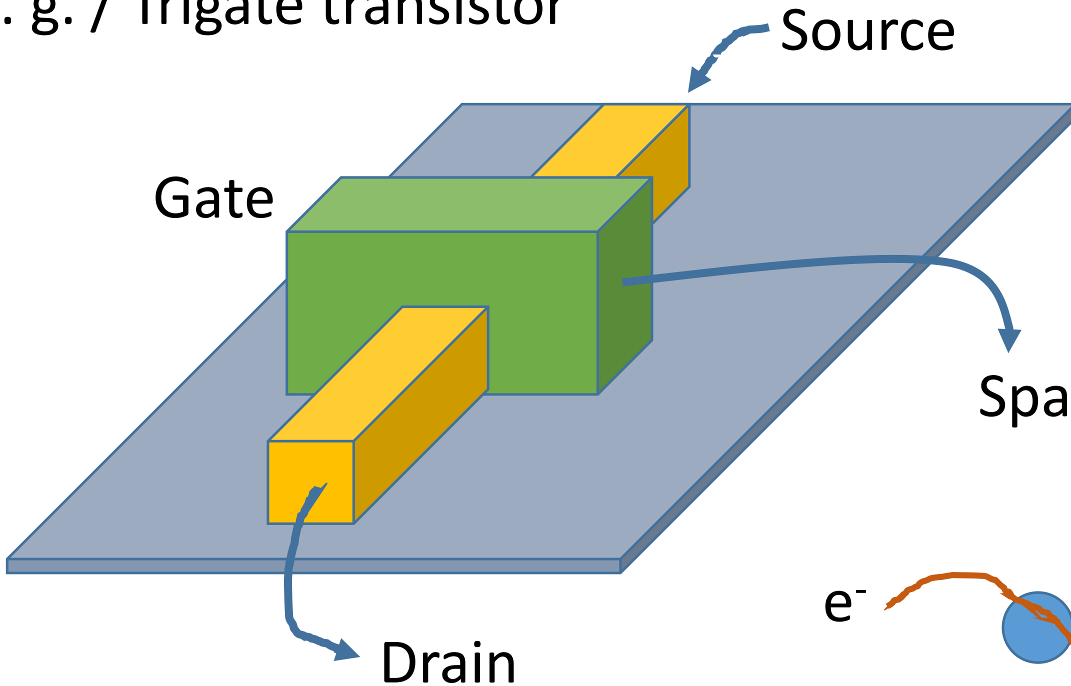




Contents

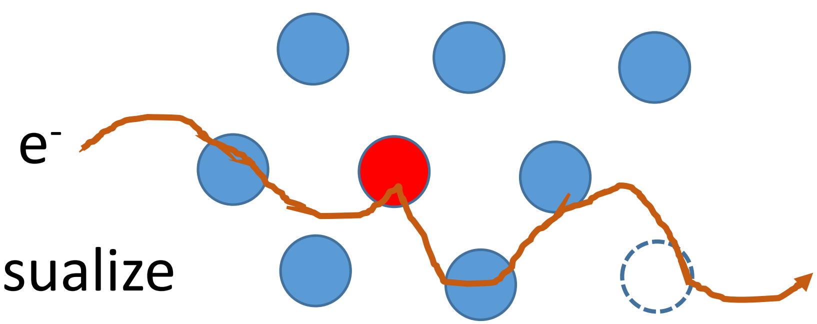
Motivation

E. g. / Trigate transistor



- Transmission
- Total current
- Conductance

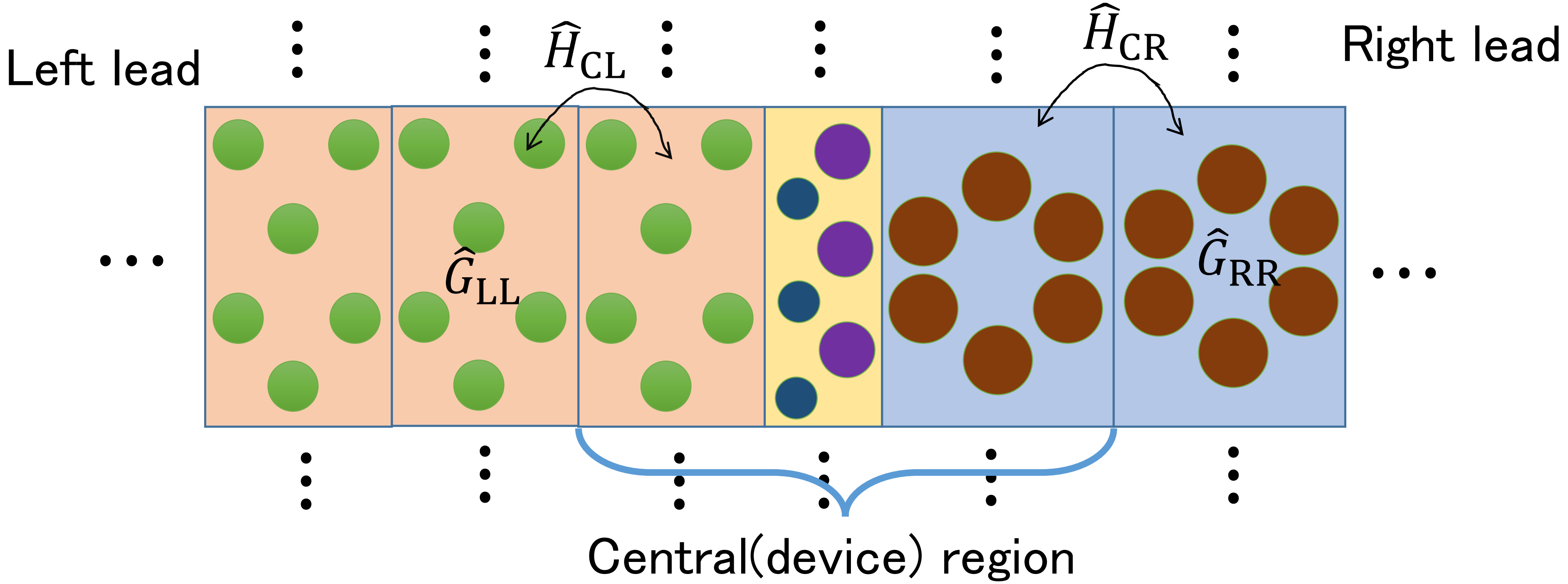
Spatial information



Real-space picture for the conducting phenomena in a nano device

- Eigenchannels
- Real-space current density

[Formalism] System



$$\hat{G}_{\mathrm{C}}(E) = \{E - \hat{H}_{\mathrm{C}} - \hat{\Sigma}_{\mathrm{L}}(E) - \hat{\Sigma}_{\mathrm{R}}(E)\}^{-1}$$

$$\hat{\Sigma}_{L}(E) = \left(E - \hat{H}_{CL}\right)\hat{G}_{LL}\left(E - \hat{H}_{LC}\right)$$

$$J = \int \frac{dE}{2\pi} \mathrm{Tr}\left[\hat{T}(E)\right]\{f(E - \mu_{\mathrm{L}}) - f(E - \mu_{\mathrm{R}})\}$$

$$\hat{T}(E) = \hat{G}_{\mathrm{C}}(E)\hat{\Gamma}_{\mathrm{L}}(E)\hat{G}_{\mathrm{C}}^{\dagger}(E)\hat{\Gamma}_{\mathrm{R}}(E)$$

$$\mathrm{Tr}\left[\hat{T}(E)\right] = \sum_{i} t_i$$

$$\hat{T}(E)|t_i(E)\rangle = t_i(E)|t_i(E)\rangle$$

Two steps for diagonalization

M. Paulsson and M. Brandbyge, PRB 76, 115117 (2007).

$\hat{G}_{\mathrm{C}}\hat{\Gamma}_{\mathrm{L}}\hat{G}_{\mathrm{C}}^{\dagger}$ Spectral function

$$\hat{A}_{\mathrm{L}}\hat{\Gamma}_{\mathrm{R}}|t_i\rangle = t_i|t_i\rangle$$

Hermite

$$\hat{A}_{\mathrm{L}}|a_i\rangle = a_i|a_i\rangle$$

$$\hat{A}_{\mathrm{L}}^{1/2} \equiv (\sqrt{a_1}\,|a_1\rangle, \cdots, \sqrt{a_N}\,|a_N\rangle)$$

$$\hat{A}_{\mathrm{L}}^{1/2}\hat{A}_{\mathrm{L}}^{1/2\dagger}\hat{\Gamma}_{\mathrm{R}}\hat{A}_{\mathrm{L}}^{1/2}\hat{A}_{\mathrm{L}}^{-1/2}|t_i\rangle = t_i\hat{A}_{\mathrm{L}}^{1/2}\hat{A}_{\mathrm{L}}^{-1/2}|t_i\rangle$$

$$\hat{\tilde{\Gamma}}_{\mathrm{R}}|\tilde{t}_i\rangle = t_i|\tilde{t}_i\rangle$$

$$|t_i\rangle = \hat{A}_{\mathrm{L}}^{1/2}|\tilde{t}_i\rangle$$

In the real space

$$t_i(r) = [\chi_1(r), \cdots, \chi_N(r)]|t_i\rangle$$

In OpenMX $\int d^3r\,\chi_i(r)\chi_j(r) \neq \delta_{ij}$

Löwdin orthogonalizations

The Kohn-Shame eqn. in the non-orthogonal basis space

$$\hat{H}|\varphi_i\rangle = \varepsilon_i \hat{S}|\varphi_i\rangle$$

$$S_{ij} \equiv \int d^3r\, \chi_i(r)\chi_j(r)$$

Solve directly Generalized Eigenvalue Problem

Löwdin ort.

$$\hat{H}\hat{S}^{-1/2\dagger}\hat{S}^{1/2\dagger}|\varphi_i\rangle = \varepsilon_i \hat{S}^{1/2}\hat{S}^{1/2\dagger}|\varphi_i\rangle$$

$$\hat{S}|s_i\rangle = s_i|s_i\rangle$$

$$\hat{S}^{1/2} \equiv (\sqrt{s_1}\,|s_1\rangle, \cdots, \sqrt{s_N}\,|s_N\rangle)$$

$$\hat{S}^{-1/2\dagger} \equiv \left(s_1^{-1/2}\,|s_1\rangle, \cdots, s_N^{-1/2}|s_N\rangle\right)$$

$$\hat{\tilde{H}}|\tilde{\varphi}_i\rangle = \varepsilon_i|\tilde{\varphi}_i\rangle$$

$$\hat{\tilde{H}} = \hat{S}^{-1/2}\hat{H}\hat{S}^{-1/2\dagger}$$

$$|\varphi_i\rangle = \hat{S}^{-1/2\dagger}|\tilde{\varphi}_i\rangle$$

Others?

Löwdin ort. for $\hat{G}_\mathrm{C}$, $\hat{\Gamma}$, $\hat{T}$, eigenchannels

Hamiltonian $\hat{\tilde{H}} = \hat{S}^{-1/2}\hat{H}\hat{S}^{-1/2\dagger}$

Green's function $\hat{\tilde{G}} = \hat{S}^{1/2\dagger}\hat{G}\hat{S}^{1/2}$

Self energy
Line width $\hat{\tilde{\Gamma}} = \hat{S}^{-1/2}\hat{\Gamma}\hat{S}^{-1/2\dagger}$

Any vectors

$$|\varphi_i\rangle = \hat{S}^{-1/2\dagger}|\tilde{\varphi}_i\rangle$$

Basis set

$$\tilde{\chi}_n(r) = \sum_n \chi_n(r)\left[\hat{S}^{-1/2\dagger}\right]_{n'n}$$

$$\hat{\tilde{T}} = \hat{\tilde{G}}_\mathrm{C}\hat{\tilde{\Gamma}}_\mathrm{L}\hat{\tilde{G}}_\mathrm{C}^\dagger\hat{\tilde{\Gamma}}_\mathrm{R} = \hat{S}^{1/2\dagger}\hat{G}_\mathrm{C}\hat{\Gamma}_\mathrm{L}\hat{G}_\mathrm{C}^\dagger\hat{\Gamma}_\mathrm{R}\hat{S}^{-1/2\dagger}$$

Obtain it in the orthogonal basis space

↓

$$\hat{\tilde{T}}(E)|\tilde{t}_i(E)\rangle = t_i(E)|\tilde{t}_i(E)\rangle$$

Diagonalize in the orthogonal basis space

↓

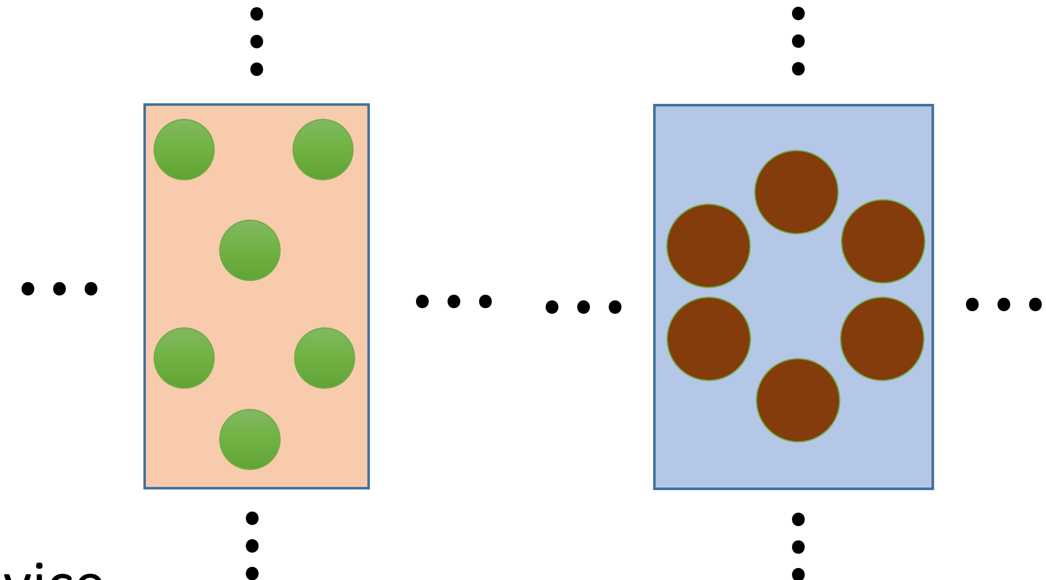
$$|t_i\rangle = \hat{S}^{-1/2\dagger}|\tilde{t}_i\rangle$$

Transform to the non-orthogonal basis space

Overall Procedure

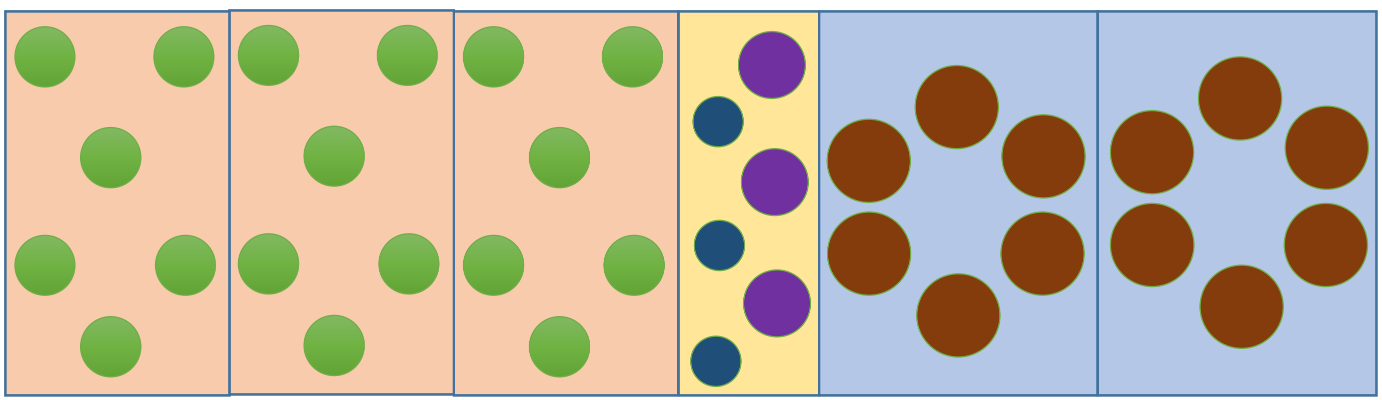
(1) Compute leads
(periodic system)

With openmx



SCF.EigenvalueSolver Band
NEGF.filename.hks LLLL.hks

(2) Compute sandwiched device

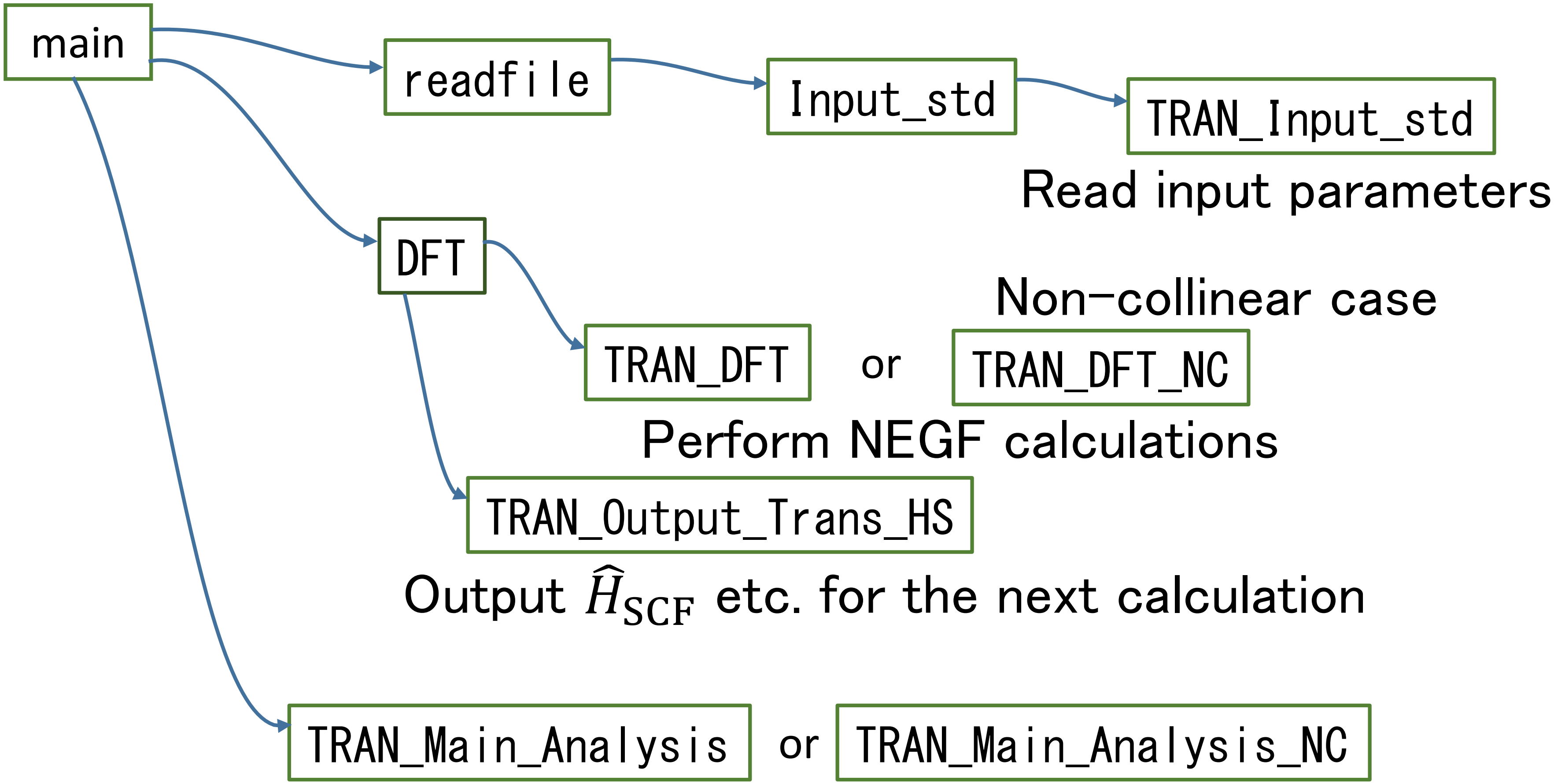


With openmx

scf.EigenvalueSolver NEGF
NEGF.filename.hks.l LLLL.hks
NEGF.filename.hks.r RRRR.hks

Eigenchannels are computed in the same run

Call graph

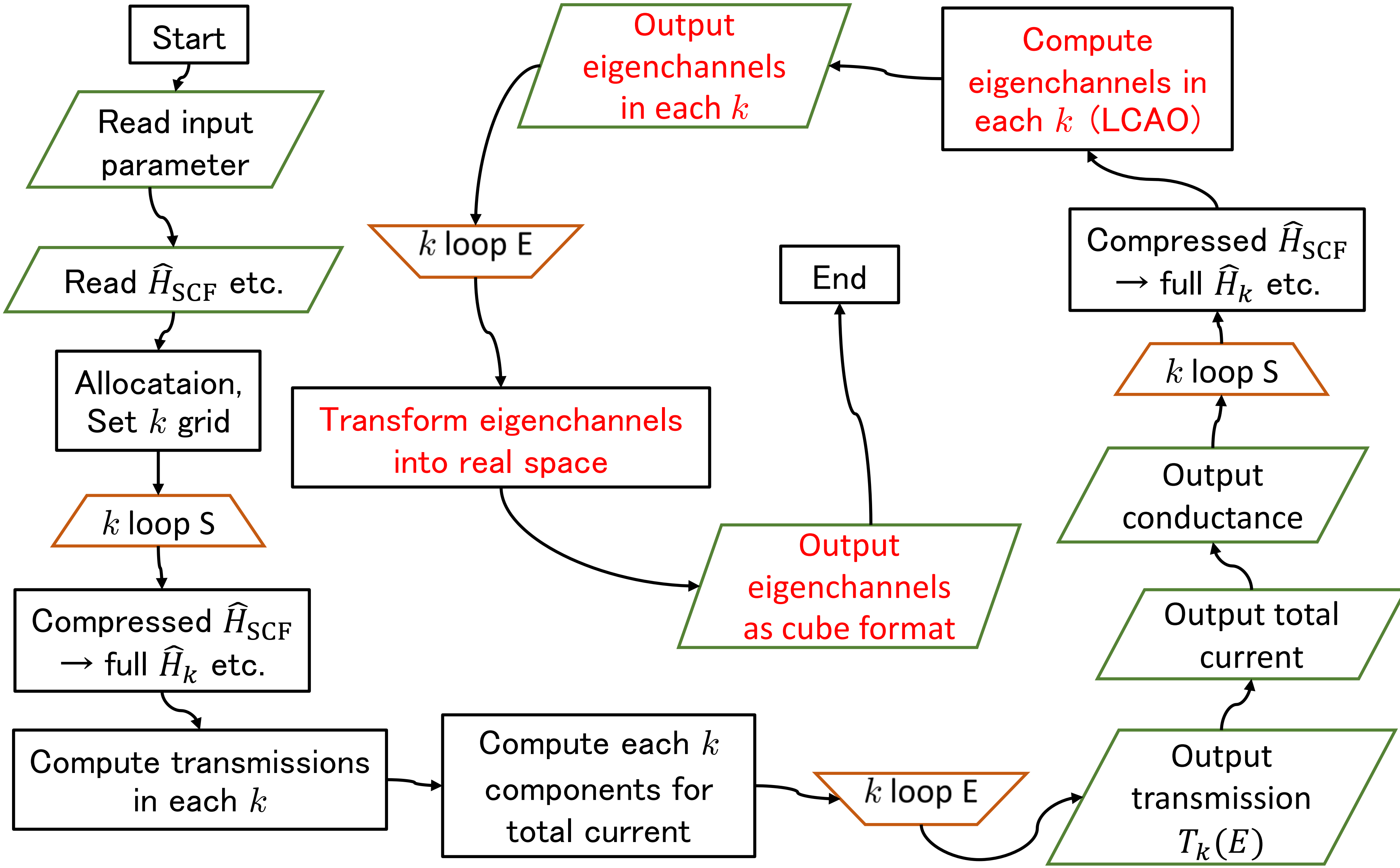


Compute transmission, total current, conductance,
eigenchannels, current density

Independent program TranMain in OpenMX3.7

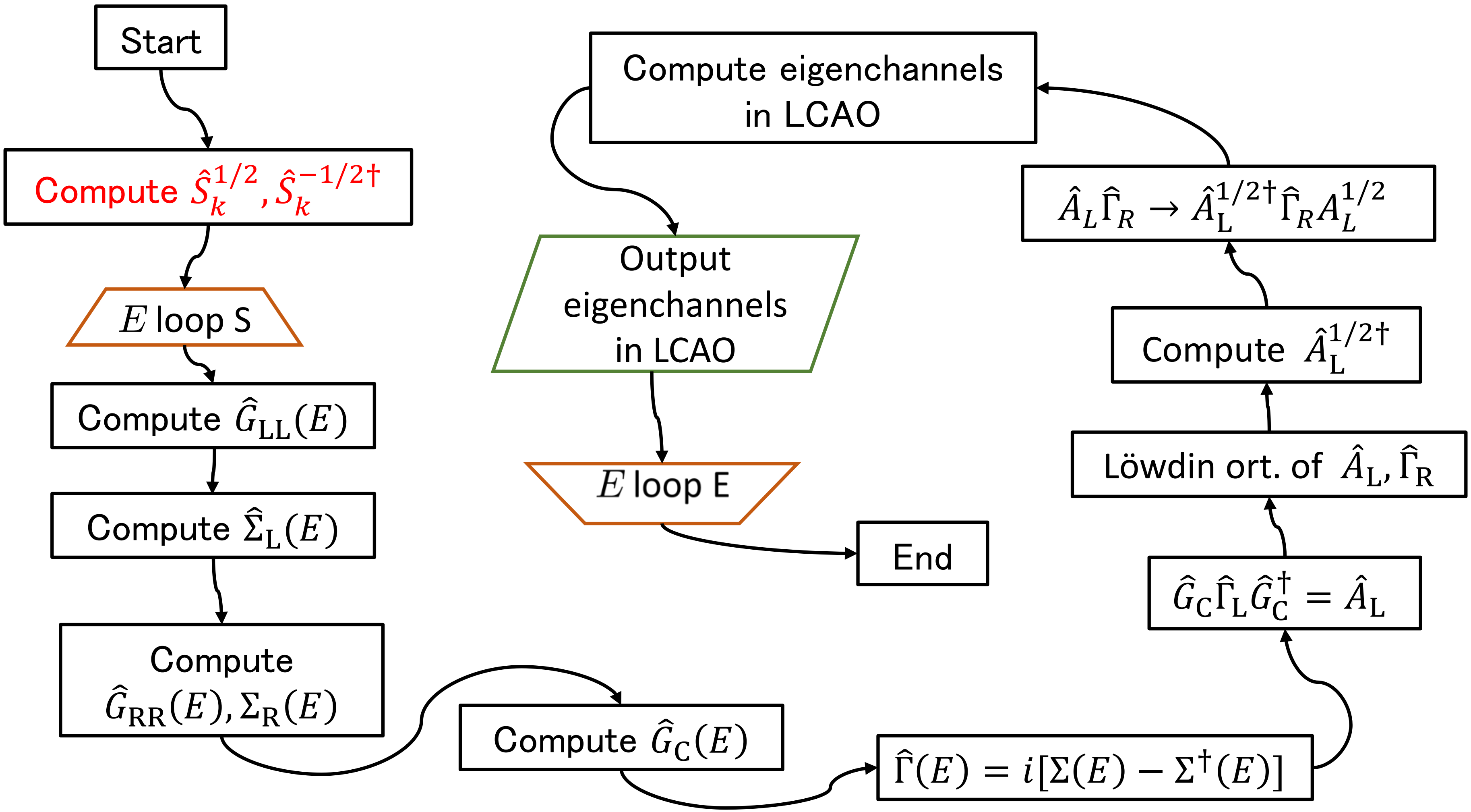
→ Joins into main program

TRAN_Main_Analysis



Detailed flow for eigenchannels

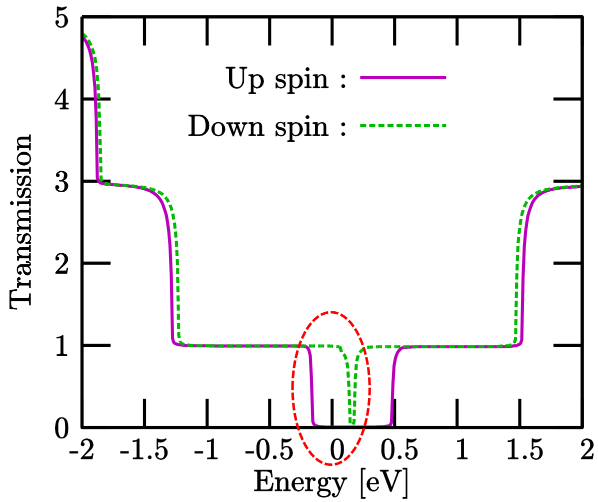
MTRAN_EigenChannel function called by TRAN_Main_Analysis in k loop

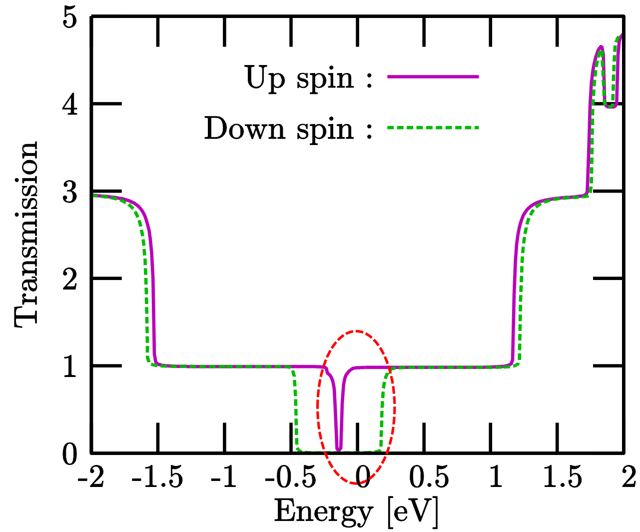


[Examples] 8-Zigzag Graphene Nano Ribbon

T. Ozaki, *et al.*, PRB 81, 075422 (2010).

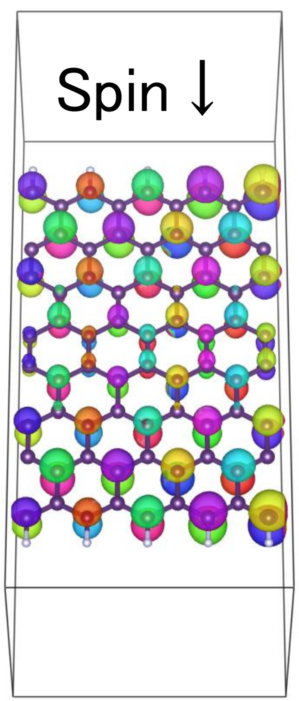
0.3 V bias



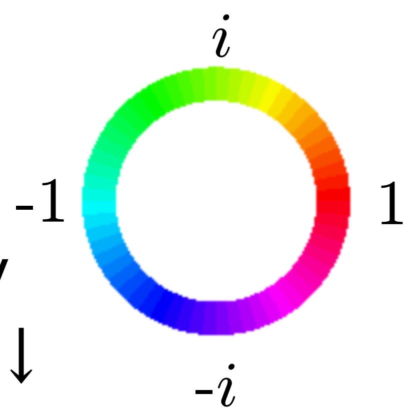


−0.3 V bias

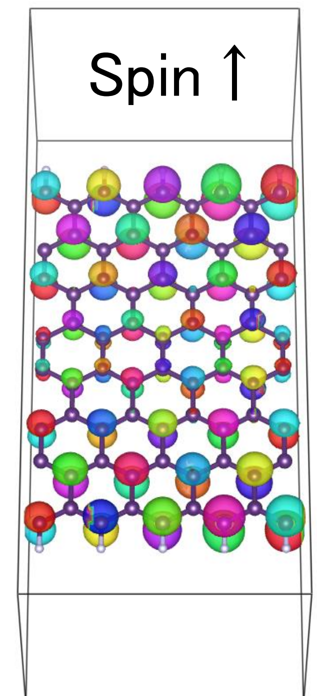
0.3 V Spin ↑



0 V Spin ↓



−0.3 V Spin ↑



0 V Spin ↓

- Large intensity in edges
- k=X orbitals contribute

Formalism for the current density

$$\boldsymbol{J}_{\mathrm{Loc}}(r,t) = \frac{i}{2}[\psi(r,t)\nabla\psi^*(r,t) - \psi^*(r,t)\nabla\psi(r,t)]$$

Without non-local potential ← Hybrid functional

← Pseudopotentails

With non-local potential

C. Li, L. Wan, Y. Wei, and J. Wang, Nanotechnology 19, 155401 (2008).

$$i\frac{\partial\psi(r,t)}{\partial t} = \frac{-\nabla^2}{2}\psi(r,t) + \int d^3r'\, V(r,r')\psi(r',t) \quad (1)$$

$$\psi^*(r,t)\times(1) - \psi(r,t)\times(1)^*$$

$$-\frac{\partial\rho(r,t)}{\partial t} = \nabla\cdot\boldsymbol{J}_{\mathrm{Loc}}(r,t) + \rho_{\mathrm{NLoc}}(r,t)$$

$$\rho_{\mathrm{NLoc}}(r,t) \equiv \int d^3r'\, V(r,r')\psi(r',t)\psi^*(r,t) + \mathrm{c.c.}$$

$$\boldsymbol{J}_{\mathrm{NLoc}}(r,t) \equiv \nabla\cdot\varphi_{NLoc}(r,t)$$

$$\nabla^2\varphi_{\mathrm{NLoc}}(r,t) = \rho_{\mathrm{NLoc}}(r,t)$$

$$-\frac{\partial\rho(r,t)}{\partial t} = \nabla\cdot[\boldsymbol{J}_{\mathrm{Loc}}(r,t) + \boldsymbol{J}_{\mathrm{NLoc}}(r,t)]$$

NEGF + Current density

Replace

$$\psi(r,t)\psi^*(r',t)\cdots \to \int dE \frac{-i}{2\pi} G^<(r,r',E)\cdots$$

$$\hat{G}^< \equiv \hat{G}_C i[\hat{\Gamma}_L f(E-\mu_L) + \hat{\Gamma}_R f(E-\mu_R)]\hat{G}_C^\dagger$$

$$\boldsymbol{J}_{\mathrm{Loc}}(r) = \int \frac{dE}{2\pi}[i(\nabla_r - \nabla_{r'})D_{\mathrm{R}}(r,r',E)]_{r'=r}[f(E-\mu_L) - f(E-\mu_R)]$$

$$\hat{D}_{\mathrm{R}} \equiv \hat{G}_C \hat{\Gamma}_R \hat{G}_C^\dagger$$

$$\sum_{ij} D_{R\,ij}[\chi_j(r)\nabla\chi_i(r) - \chi_i(r)\nabla\chi_j(r)]$$

$$\rho_{\mathrm{NLoc}}(r) = -\int \frac{dE}{2\pi} 2\mathrm{Im}[V(r,r')D_{\mathrm{R}}(r,r',E)][f(E-\mu_L) - f(E-\mu_R)]$$

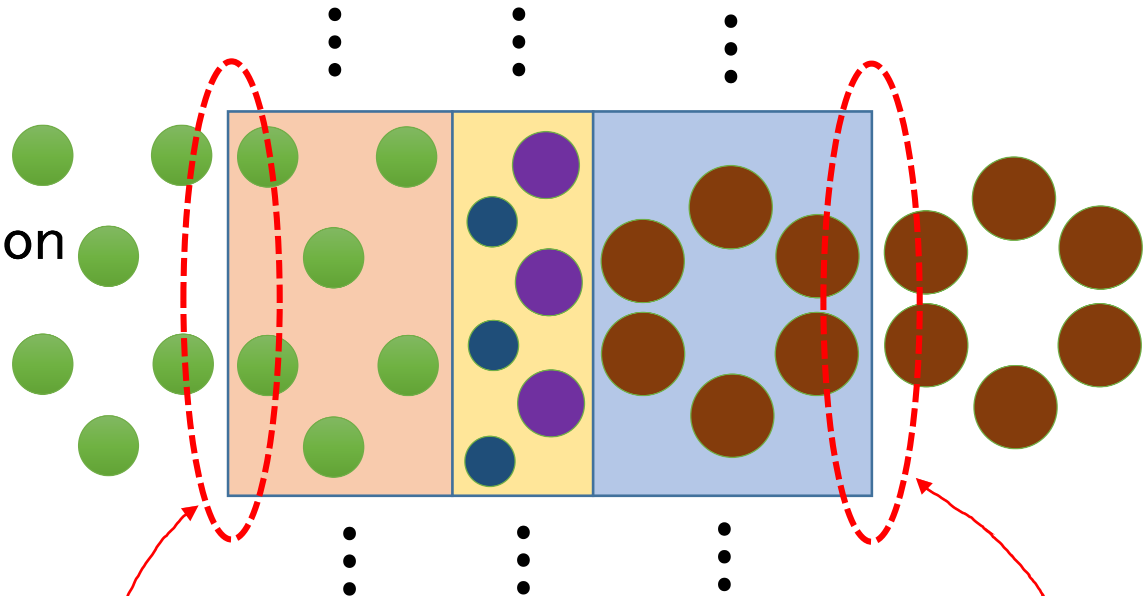
$$[\hat{S}^{-1}\hat{V}\hat{D}_R]_{ij}\chi_i(r)\chi_j(r)$$

Poisson's eq. for the non-local current

$\nabla^2 \varphi_{\mathrm{NLoc}}(r) = \rho_{\mathrm{NLoc}}(r)$ Boundary conditions are required.

Periodic b.c.

No information of φ_{NLoc}



No information of φ_{NLoc}

Periodic b.c.

$$\nabla \varphi_{\mathrm{NLoc}}(r_L)\Big|_{\parallel} = J(r_L) - J_{\mathrm{Loc}}(r_L)$$

$$\nabla \varphi_{\mathrm{NLoc}}(r_R)\Big|_{\parallel} = J(r_R) - J_{\mathrm{NLoc}}(r_R)$$

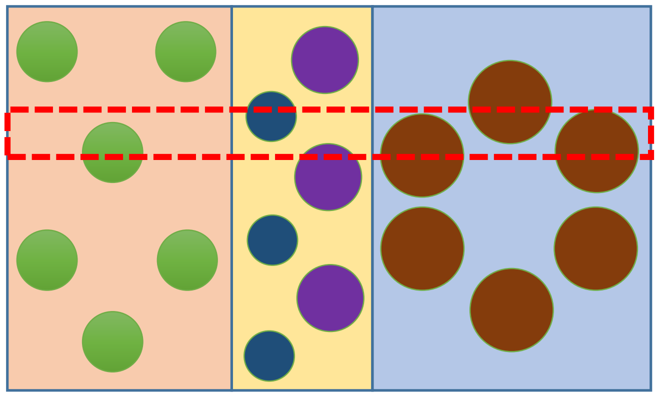
How can we obtain them ?

Approximation for the boundary current

Obtain $J(r_L)$ with a different way

$$\int_{LB} d^3r\, J_{\parallel}(r) = \int \frac{dE}{2\pi}\{f(E-\mu_{\mathrm{L}}) - f(E-\mu_{\mathrm{R}})\}\mathrm{Tr}\left[\hat{T}(E)\right]$$

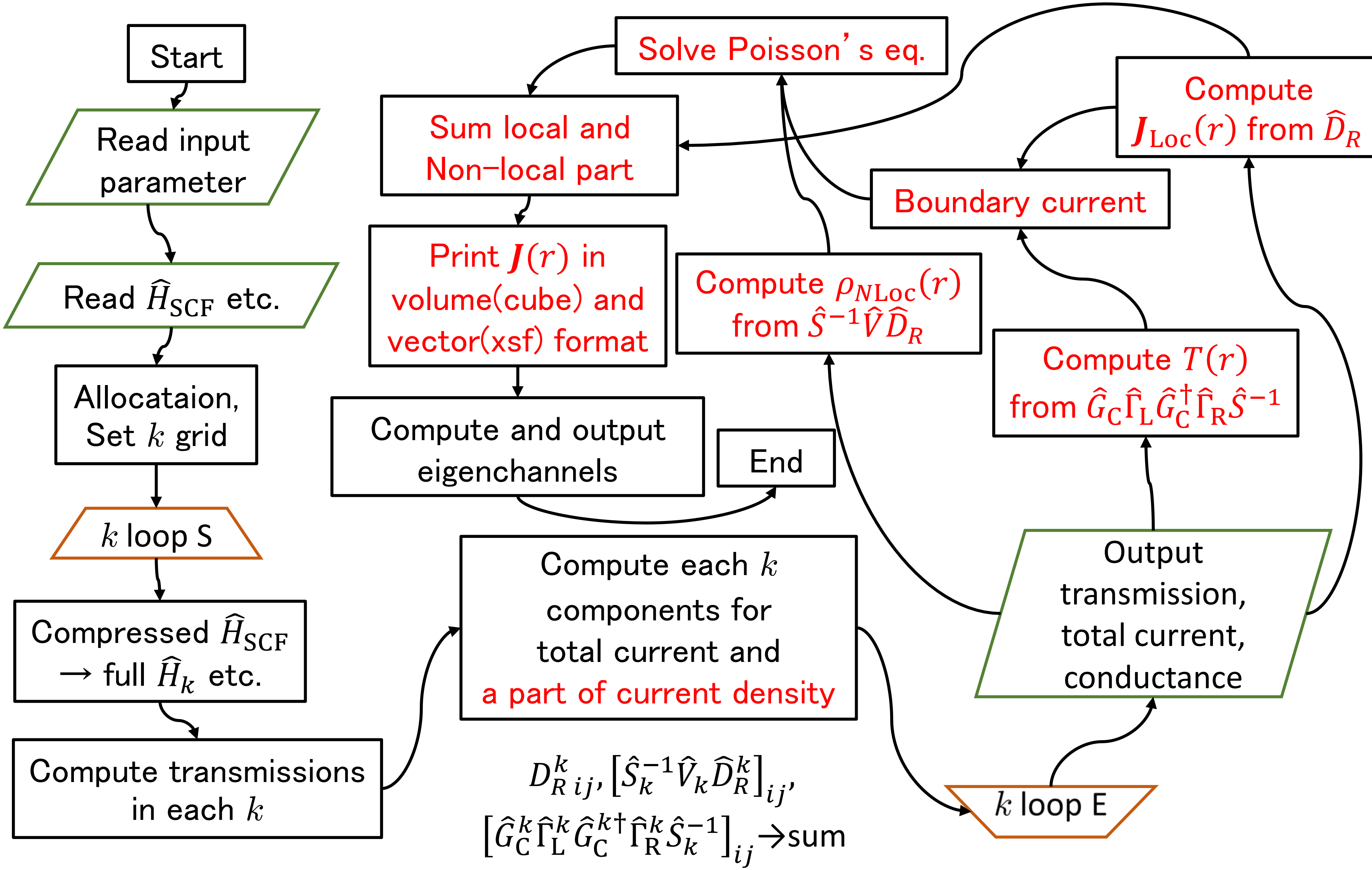
$$J_{\parallel}(r) \approx \int \frac{dE}{2\pi}\{f(E-\mu_{\mathrm{L}}) - f(E-\mu_{\mathrm{R}})\} \int dr_{\parallel}\, T(r_{\parallel}, \mathrm{r}_{\perp})$$



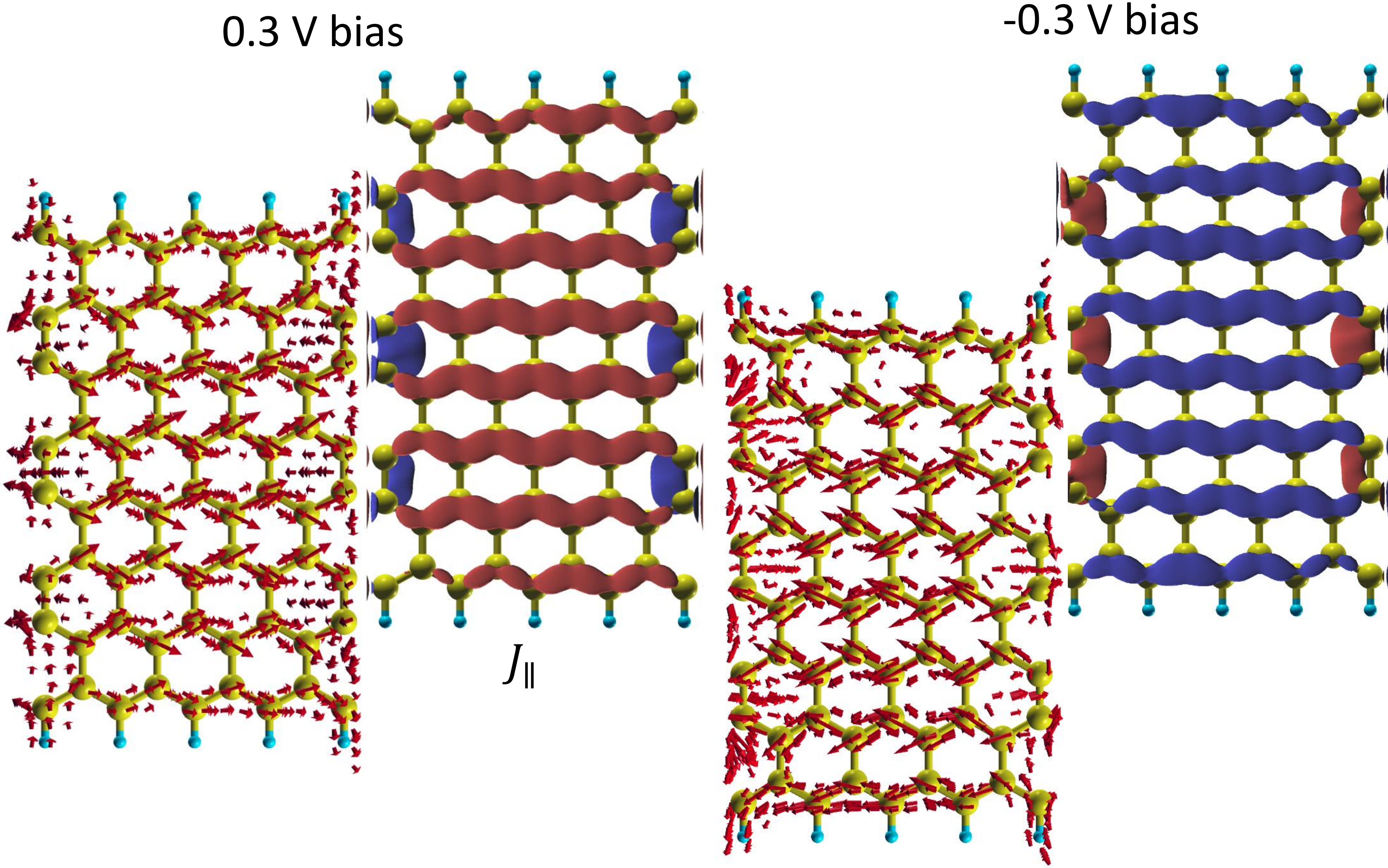
Integrate in this region

$$T(r) = \sum_{ij} \left[\hat{G}_{\mathrm{C}}\hat{\Gamma}_{\mathrm{L}}\hat{G}_{\mathrm{C}}^{\dagger}\hat{\Gamma}_{\mathrm{R}}\hat{S}^{-1}\right]_{ij}\chi_i(r)\chi_j(r)$$

Implementation in TRAN_Main_Analysis



[Example] Zigzag Graphene Nano Ribbon



Summary

- Implement Eigenchannel analysis and current density in OpenMX to study microscopic, spartial description of any conducting phenomena.
- The are performed as a post-processes of OpenMX-NEGF calculations
- Targets
  - Tunnel (Anisotropic) Magnet-Resistance devices
  - Graphen Nano Ribbon
  - Scanning Tunneling Spectroscopy
  - Etc…