

Motivation

- High time and memory requirements are limiting factor in scattering simulations
- Rank reductions have proven useful in ballistic simulations
- 20-40 times speedup in NEMO5 using Mil'nikov basis

Approach

- Transformation to a position basis so Green's functions regain position information lost in low rank approximation
- Transformation to a common basis is required for inelastic scattering in NEGF

$$P \downarrow MS = T \downarrow MS \uparrow T \downarrow real \downarrow MS \uparrow$$

$$T \downarrow RRS \uparrow = eig(P \downarrow MS)$$

$$\Sigma \downarrow RRS \uparrow R(x, x', k, E) = \int E - \hbar\omega \downarrow D \uparrow E + \hbar\omega \downarrow D \downarrow dE' \downarrow dk' \downarrow U \downarrow q \downarrow T \downarrow RRS \uparrow T \downarrow G \downarrow prev \uparrow R \downarrow T \downarrow RRS \uparrow$$

$$\Sigma \downarrow MS = T \downarrow RRS \uparrow \Sigma \downarrow RRS \downarrow T \downarrow RRS \uparrow T$$

$$G \downarrow new \uparrow R = [EI - H - \Sigma \downarrow c - \Sigma \downarrow MS] \uparrow - 1$$