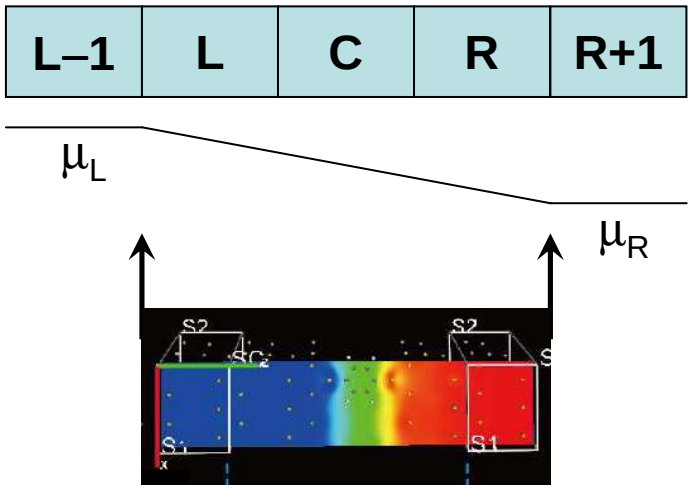
ElectrodeConstraint, commonalities

- Determines the matching between the Hamiltonian **H**, density matrix (**DM**), real-space density $\rho(\mathbf{r})$, and effective potential $V(\mathbf{r})$
  - 1. H $\rightarrow$ DM [Schrödinger]
  - 2. DM $\rightarrow \rho(\mathbf{r})$
  - 3. $\rho(\mathbf{r}) \rightarrow V(\mathbf{r})$ [Poisson]
- Common:
  - **H** in L(R) is always bulk-like (electrode calculation)
  - **DM** in C is always computed from the Green's function
  - The effective potential $V(\mathbf{r})$ is matched at the boundaries of L+C+R to the bulk value
  - Bias is applied over L+C+R
- 3 different constraints, with very different properties

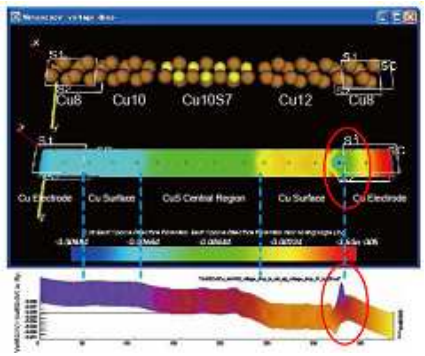


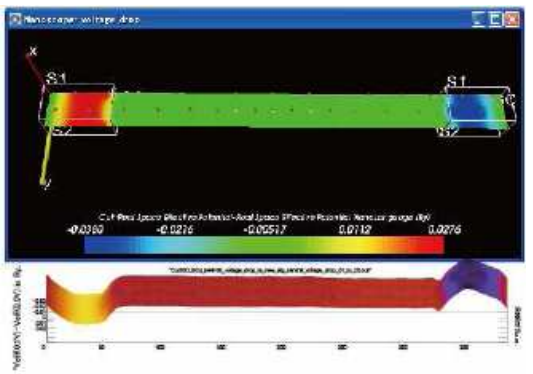
"RealSpaceDensity"

- Original ATK constraint
- ρ(**r**) in L/R is constrained to the bulk density
- **Good**, because this matches **H** in L/R
- **Bad**, DM does not match ρ(**r**) in L/R
- **Worse**, if there is insufficient screening the density can become discontinuous
  - Which in turns leads to other problems...
- **Exactly correct** in the limit of infinitely many screening layers
- Can give bad **voltage drop** → depending on atom positions in the electrode
  - Can be solved by centering the electrode atoms

"Off"

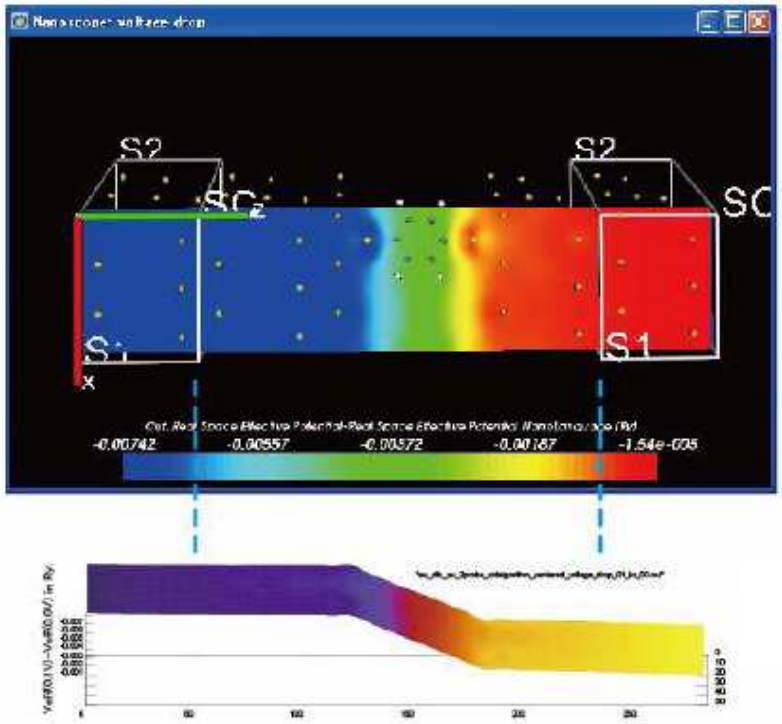
- **Default** since ATK 2008.02
- Allows DM and ρ(**r**) in L/R to vary freely, self-consistently
- Forgiving in cases of few screening layers
- **Good:** Continuous density (and ρ(**r**) matches DM)
- **Bad:** ρ(**r**) and hence *V*(**r**) does not match **H** (and DM is missing some contributions)
- Therefore, "Off" cannot produce a correct **voltage drop**





"DensityMatrix"

- Partially undocumented, introduced in 2008.10
- Not available from VNL
  - » Was initially not 100% tested
- Appears to be the best constraint of all 3
  - » Except some points, see below
- DM in L/R is constrained to bulk values
- ρ(**r**) is computed self-consistently
- Good, because DM matches **H** in L/R
- Even better, the density is continuous
- **Exactly correct** in the limit of infinitely many screening layers
- Less good:
  - » Slower
  - » Less forgiving if screening is insufficient (convergence failure)
- Best: The *only* constraint that consistently can give a good **voltage drop**

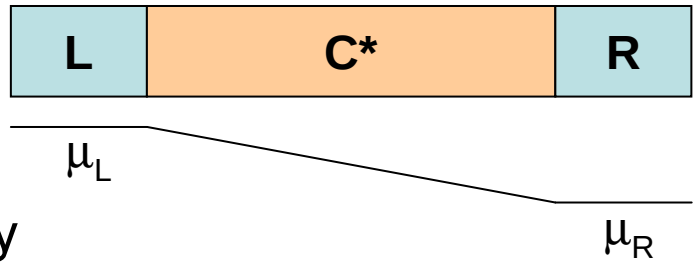


Note

- Transmission spectrum and current appear to be quite insensitive to the constraint
  - Provided the calculation converges...
  - Partly an assumption, not tested in all cases...

Is "DensityMatrix" the end of the story?

- No
- Next version of ATK will use a different separation of L/C/R, which does away with the need for a specified constraint completely
- All quantities, from **H** to $V(\mathbf{r})$, will be treated fully self-consistently in the region over which the bias is applied (C*)
- Effectively this means the user must now include L and R explicitly in C*, thus C*=L+C+R
- Fully consistent approach
  - Continuous density
  - Consistency between **H**, **DM**, $\rho(\mathbf{r})$, and $V(\mathbf{r})$ in C*
  - Correct voltage drop



- "Screening approximation" still necessary
  - Match to bulk at edges of C*