MALA background
Part of the tutorial on MALA

21.03.2022 // Lenz Fiedler

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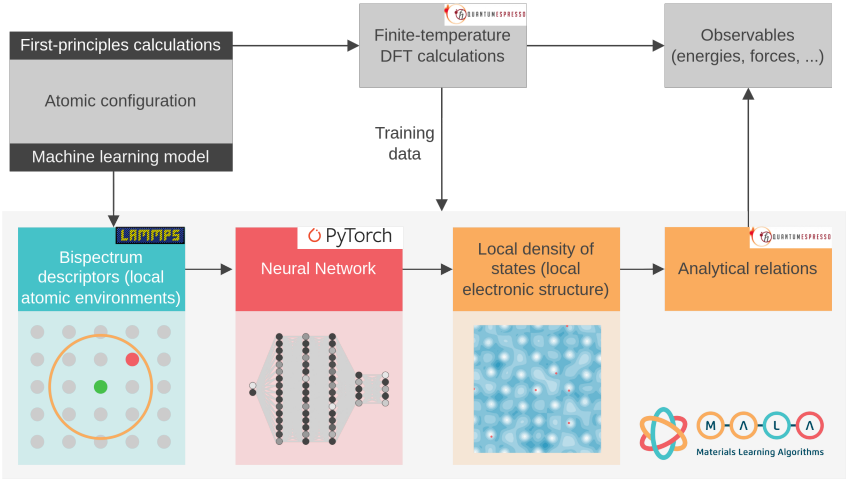
Contents

MALA workflow



Relevant equations

$$\tilde{d}(\epsilon, \boldsymbol{r}) = M(B(J, \boldsymbol{r}))$$

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$$n(\boldsymbol{r}) = \int d\epsilon \, f^{\tau}(\epsilon) d(\epsilon, \boldsymbol{r})$$

$$D(\epsilon) = \int d\boldsymbol{r} \, d(\epsilon, \boldsymbol{r})$$

Relevant equations

$$
\begin{aligned}
\tilde{d}(\epsilon, \boldsymbol{r}) &= M(B(J, \boldsymbol{r})) \\
n(\boldsymbol{r}) &= \int d\epsilon \, f^{\tau}(\epsilon) d(\epsilon, \boldsymbol{r}) \\
D(\epsilon) &= \int d\boldsymbol{r} \, d(\epsilon, \boldsymbol{r}) \\
A[n] = A[n[d], D[d]] &= E_b[D[d]] - k_{\mathrm{B}} \tau S_{\mathrm{S}}[D[d]] - E_{\mathrm{H}}[n[d]] \\
&\quad + E_{\mathrm{XC}} - \int d\boldsymbol{r} v_{\mathrm{XC}}(\boldsymbol{r}) n[d](\boldsymbol{r}) + E_{ii}
\end{aligned}
$$

MALA publications

- Accelerating finite-temperature Kohn-Sham density functional theory with deep neural networks, J. A. Ellis, *et al* 2021 *Phys. Rev. B 104*, 035120

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- Predicting electronic structures at any length scale with machine learning, L. Fiedler *et al*, publication pending, *arXiv:2210.11343*

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- Check MALA out on GitHub: https://github.com/mala-project

MALA cooperation partners

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