

MALA background

DPG Meeting 2023

27.03.2022 // Lenz Fiedler



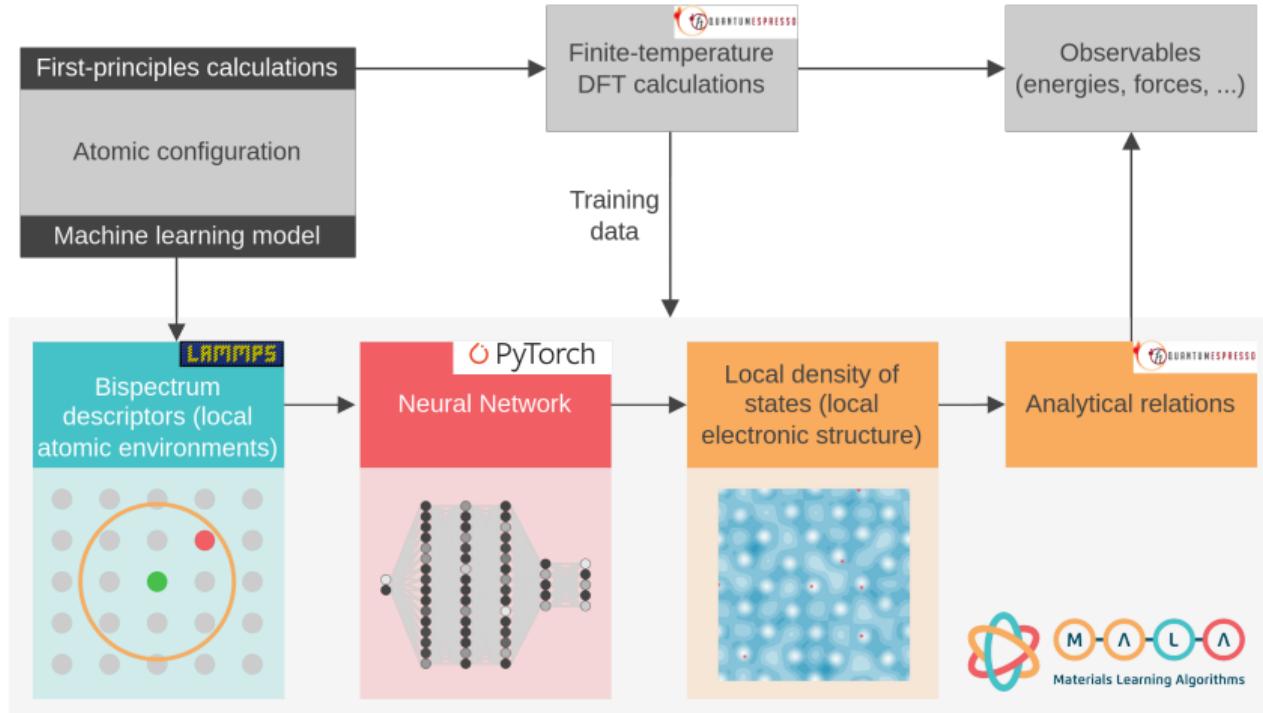
```
mirror_object_to_mirror
mirror_mod.mirror_object
operation == "MIRROR_X":
    mirror_mod.use_x = True
    mirror_mod.use_y = False
    mirror_mod.use_z = False
operation == "MIRROR_Y"
    mirror_mod.use_x = False
    mirror_mod.use_y = True
    mirror_mod.use_z = False
operation == "MIRROR_Z"
    mirror_mod.use_x = False
    mirror_mod.use_y = False
    mirror_mod.use_z = True
```



Contents



MALA workflow



Relevant equations

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

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$$\begin{aligned} A[n] = A[n[d], D[d]] &= E_b[D[d]] - k_B \tau S_S[D[d]] - E_H[n[d]] \\ &\quad + E_{XC} - \int d\mathbf{r} v_{XC}(\mathbf{r}) n[d](\mathbf{r}) + E_{ii} \end{aligned}$$

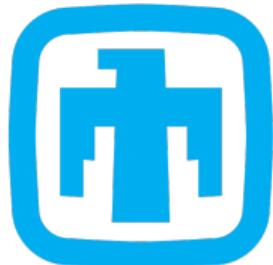
- Accelerating finite-temperature Kohn-Sham density functional theory with deep neural networks, J. A. Ellis, *et al* 2021 *Phys. Rev. B* 104, 035120

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

MALA cooperation partners



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