Napredne arhitekture neuronskih mreža za učenje interatomskih potencijala

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Uvod

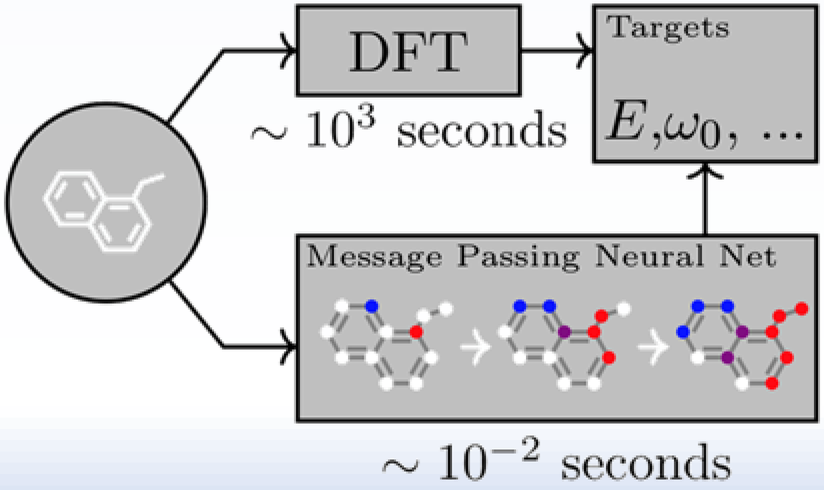
- napredak računalne snage omogućuje nove pristupe u istraživanjima
- simulacije velikih sustava u fizici materijala, kemiji i biologiji

- teorija funkcionala gustoće (DFT)
  - precizno, računalno skupo
  - skaliranje s n^3

- vremenske evolucije sistema Newtonovim jednadžbama
  - kratak vremenski korak

Uvod

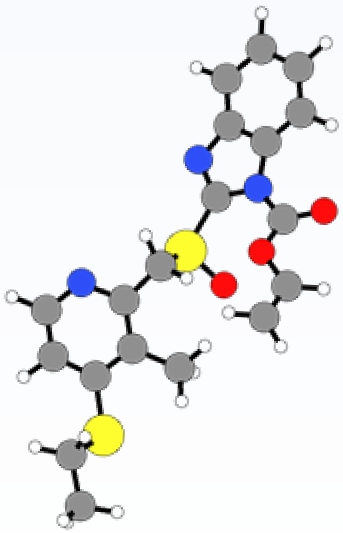
- razvoj strojnog učenja → neuralne mreže
  - učenje interatomskog potencijala
  - skaliranje s n
  - <u>generalizacija</u>
- značajni napredak brzine simulacije
- uključivanje simetrije problema u arhitekturu neuralne mreže

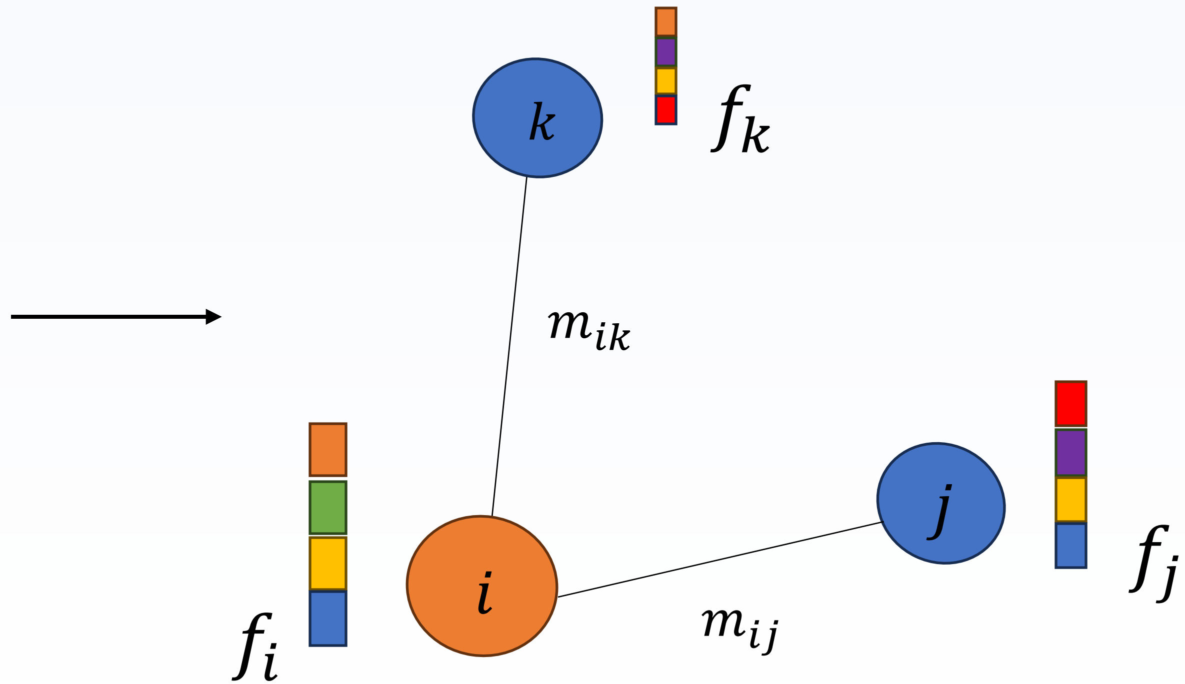


Gilmer, Justin, et al. "Neural message passing for quantum chemistry." *International conference on machine learning*. PMLR, 2017.

SO3krates arhitektura

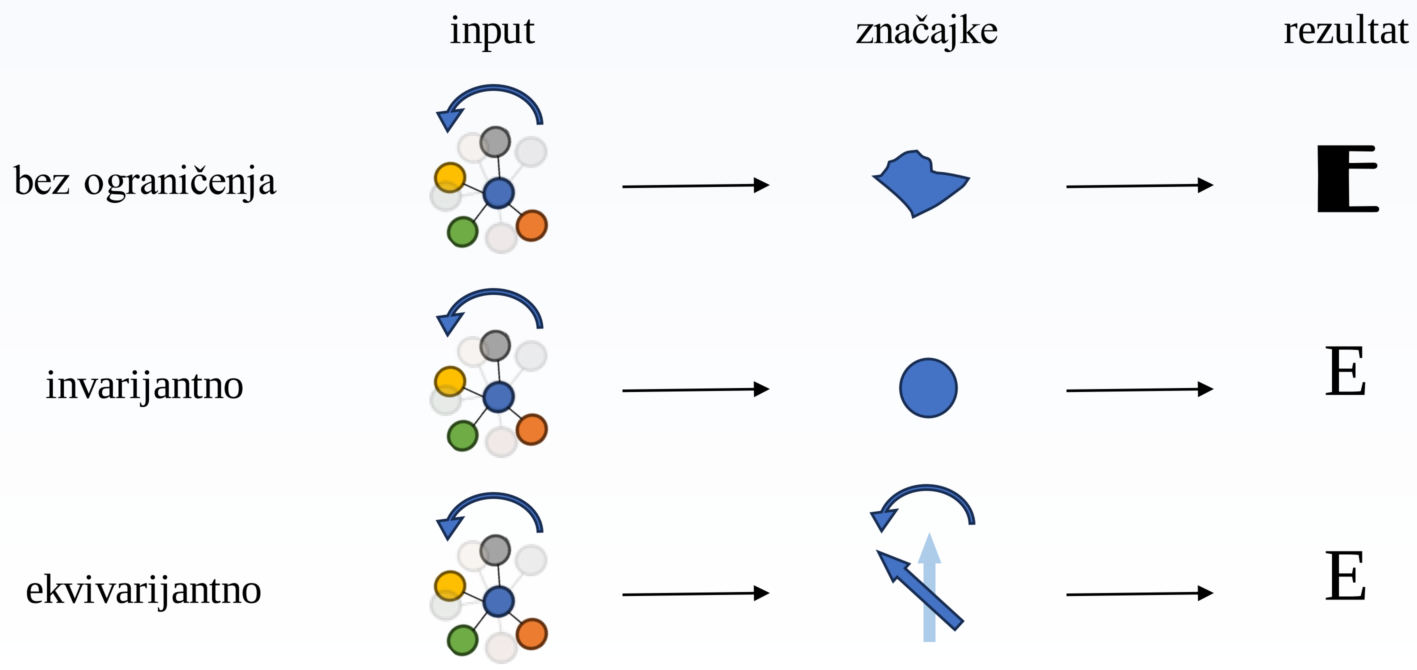
- neuralna mreža sa slanjem poruka (*message passing neural network*)





SO3krates arhitektura

- ekvivarijantna arhitektura – invarijantne i ekvivarijantne značajke



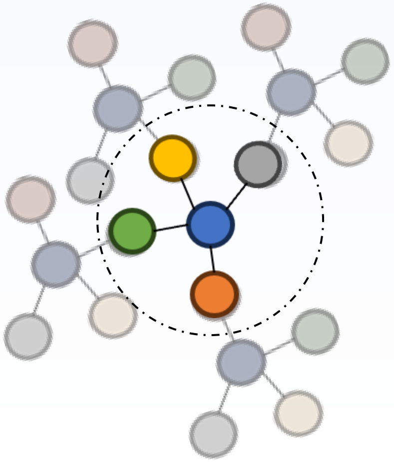
SO3krates arhitektura

- SO(3) konvolucija u funkciji poruke:

$$m_{ij}^{LM} = \sum_{l_1 l_2 m_1 m_2} C_{l_1 m_1 l_2 m_2}^{LM} \phi_{l_1 l_2}^{L}(r_{ij}) Y_{m_1}^{l_1}(\hat{r}_{ij}) f_j^{l_2 m_2}$$

- skaliranje $\mathcal{O}(l_{max}^6 \times F)$

- potrebna preciznost, brzina i stabilnost



SO3krates arhitektura

- konceptualne promjene:

invarijantne značajke $$f_i^{[t=0]} = f_{emb}(Z_i)$$

ekvivarijantne značajke $$x_{iLM} = \frac{1}{\langle \mathcal{N} \rangle} \sum_{j \in \mathcal{N}(i)} \phi_{r_{cut}(r_{ij})} Y_M^L(\hat{r}_{ij})$$

dvije vrste poruka $$m_{ij} = \alpha_{ij} f_j \quad m_{ij}^{LM} = \alpha_{ij}^L Y_M^L(\hat{r}_{ij})$$

funkcija pažnje $$\alpha_{ij} = \alpha \left(f_i, f_j, r_{ij}, \bigoplus_{l=0}^{l_{max}} \mathbf{x}_{ij,l \to 0} \right)$$

J.T. Frank, O.T. Unke and K.-R. Müller, So3krates: Equivariant attention for interactions on arbitrary length-scales in molecular systems, 2023.

J.T. Frank, O.T. Unke, K.-R. Müller and S. Chmiela, From peptides to nanostructures: A euclidean transformer for fast and stable machine learned force fields, 2023.

SO3krates arhitektura

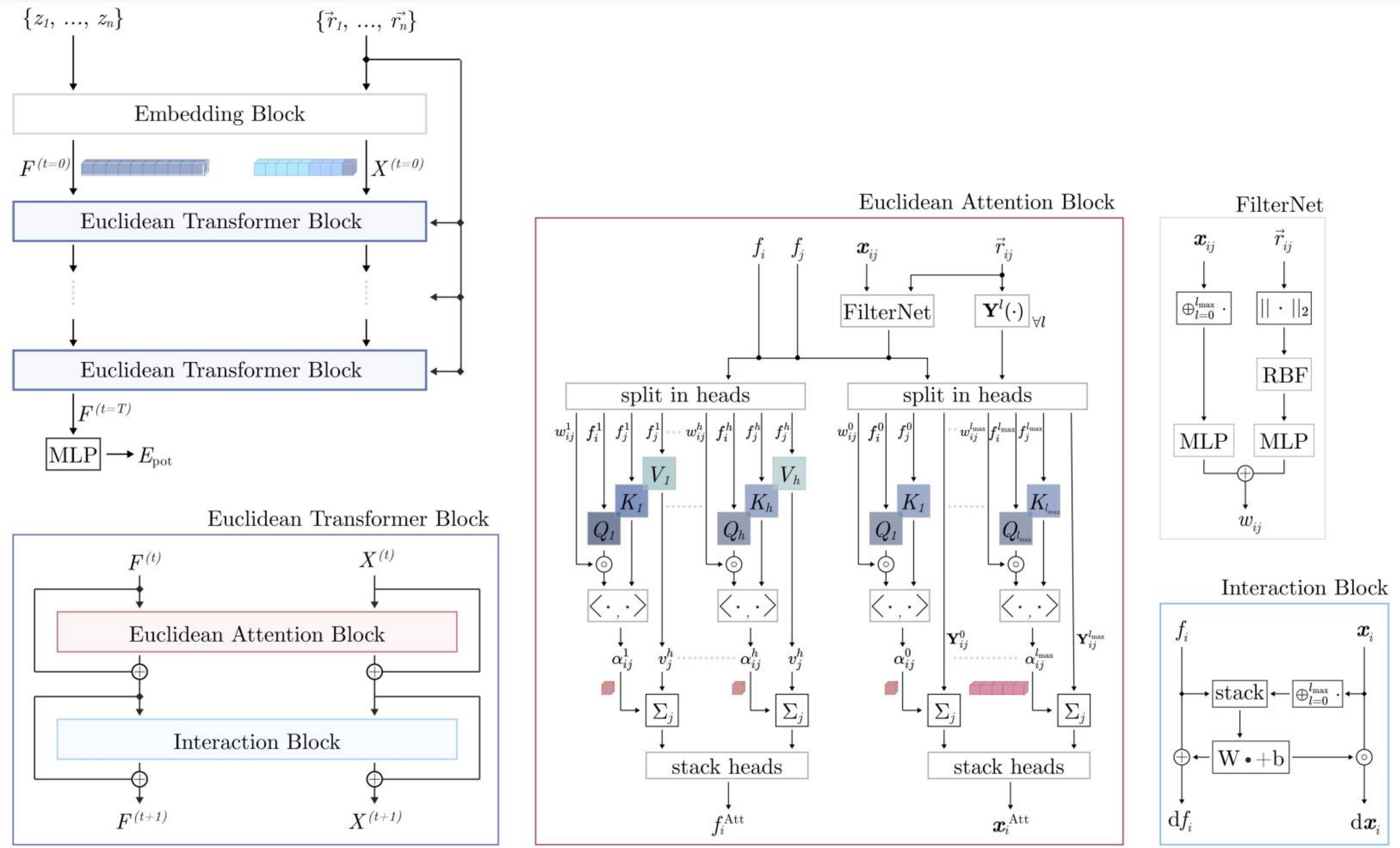
ažuriranje značajki

$$f_i^{[t+1]} = f_i^{[t]} + \sum_{j \in \mathcal{N}(i)} m_{ij}$$

$$x_{iLM}^{[t+1]} = x_{iLM}^{[t]} + \sum_{j \in \mathcal{N}(i)} m_{ij}^{LM}$$

$$[\mathbf{f}_i^{[t+1]}, \mathbf{x}_i^{[t+1]}] = \text{ETBlok}\left[\left\{\mathbf{f}_j^{[t]}, \mathbf{x}_j^{[t]}, \vec{r}_{ij}\right\}_{j \in \mathcal{N}(i)}\right]$$

SO3krates arhitektura



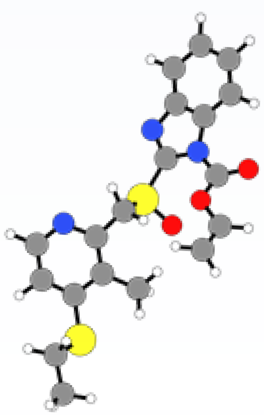
J.T. Frank, O.T. Unke, K.-R. Müller and S. Chmiela, From peptides to nanostructures: A euclidean transformer for fast and stable machine learned force fields, 2023.

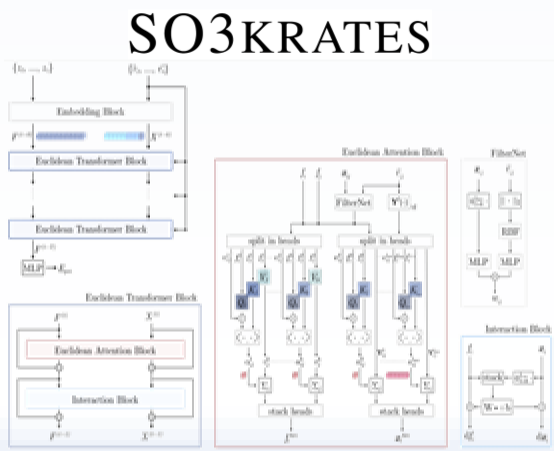
SO3krates arhitektura

- iz konačnih značajki atoma nakon T koraka slanja poruka računaju se energija i sila

$$E(\overrightarrow{r_1}, \dots, \overrightarrow{r_2}) = \sum_{i=1}^{n} E_i$$

$$\vec{F}_i = -\nabla_i E_{pot}$$

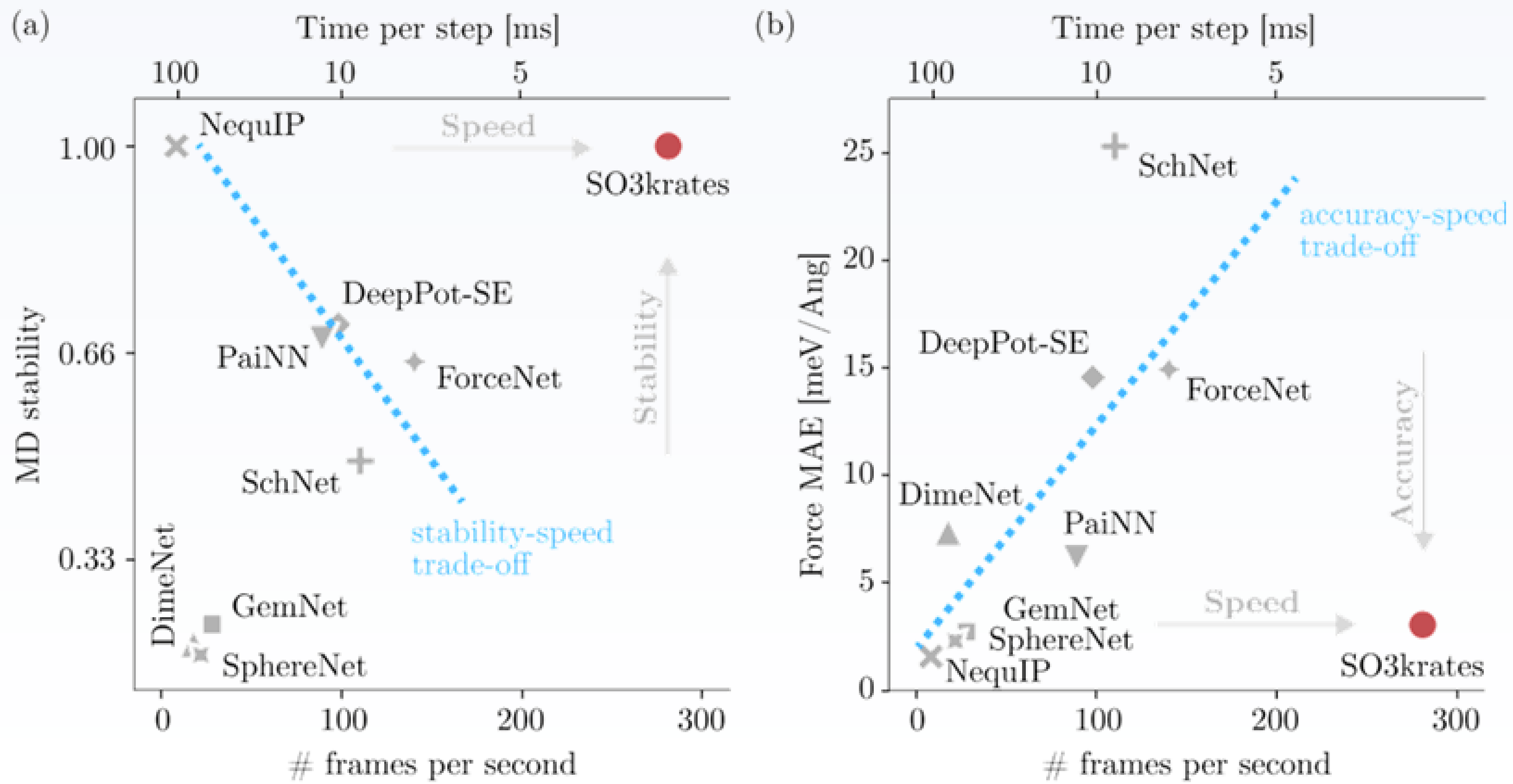




$E, \vec{F}$

SO3krates arhitektura

- konačno skaliranje $\mathcal{O}(n \times \langle \mathcal{N} \rangle \times (l_{\max}^2 + F))$



J.T. Frank, O.T. Unke, K.-R. Müller and S. Chmiela, From peptides to nanostructures: A euclidean transformer for fast and stable machine learned force fields, 2023.

SPICE set podataka

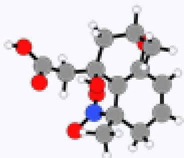
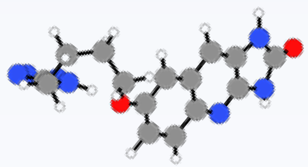
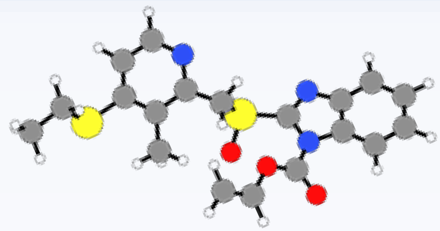
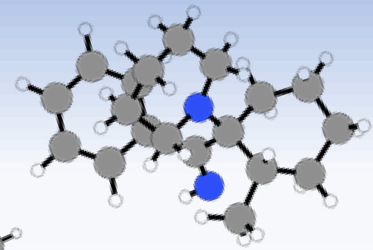
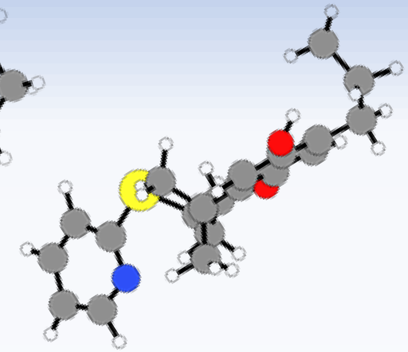
- nedovoljno kvallitetnih setova podataka
- računanje DFT-om

- Small molecule/Protein Interaction Chemical Energies (SPICE)
- raznolik set 1.1 milijuna konformacija

- potrebni: položaji atoma, sile na atome, energija molekule, atomski brojevi

P. Eastman, P.K. Behara, D.L. Dotson, R. Galvelis, J.E. Herr, J.T. Horton et al., Spice, a dataset of drug-like molecules and peptides for training machine learning potentials, 2022.

SPICE set podataka

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28
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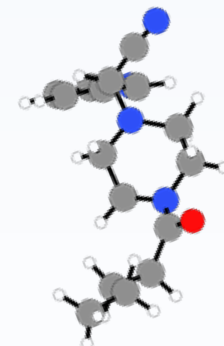
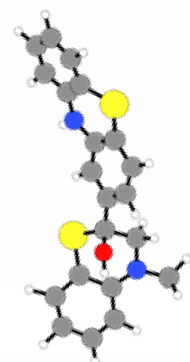



Metoda

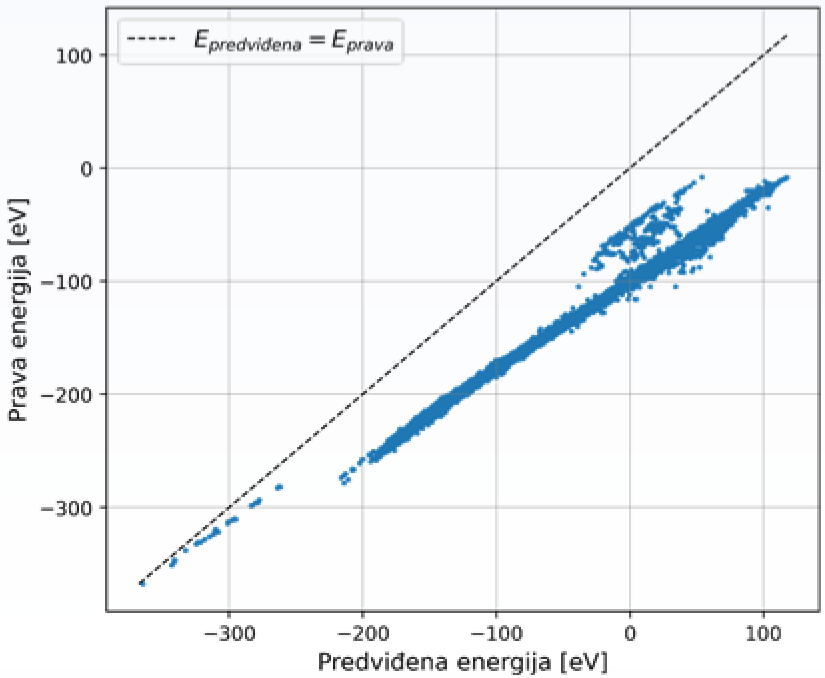
- testirati arhitekturu na SPICE podacima
- treniranje na jednoj Nvidia A100 GPU

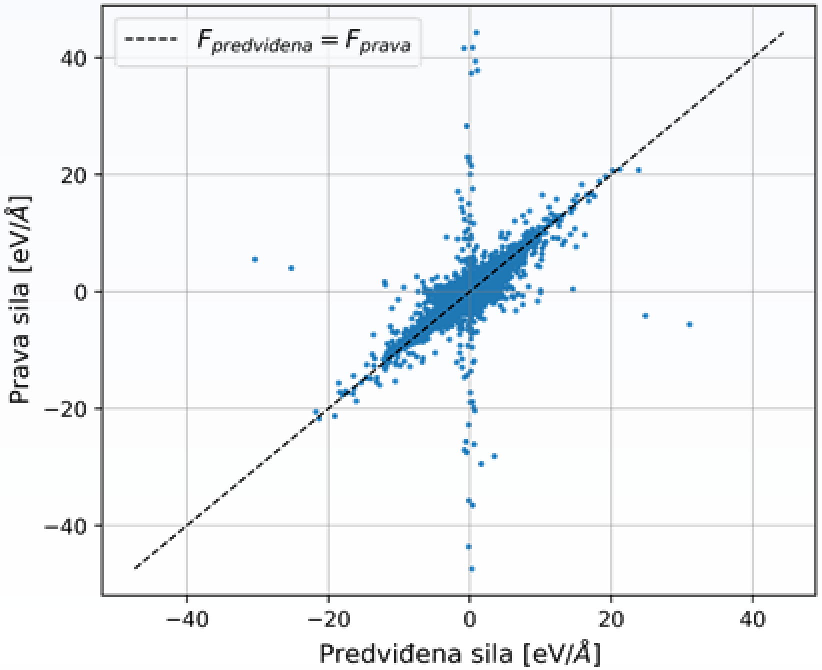
- SPICE → C, H, N, O, S ~ 680 000 podataka
  - 100 000 za trening
  - 20 000 za validaciju
  - 20 000 za testiranje

- hiperparametri $r_{cut}, F,\ l,\ T,\ \beta$

Metoda

- sa zadanim hiperparametrima:
  - MAE: 90 eV za energiju, 0.17 eV/Å za silu





Metoda

- funkcija gubitka:

$$\mathcal{L} = (1-\beta)(E-\tilde{E})^2 + \frac{\beta}{3N}\sum_{k=1}^{n}\sum_{i=1}^{3}(F_k^i - \tilde{F}_k^i)^2$$

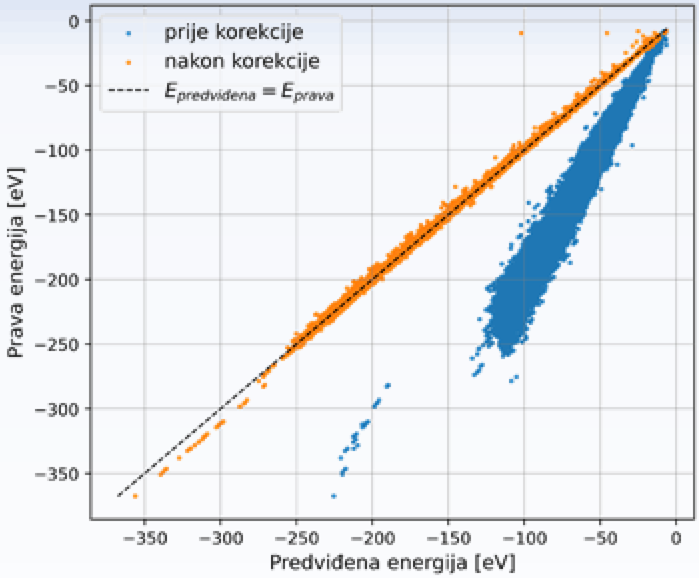
- treniranje samo na silama:
  - MAE: 64 eV za energiju, 0.047 eV/Å za silu

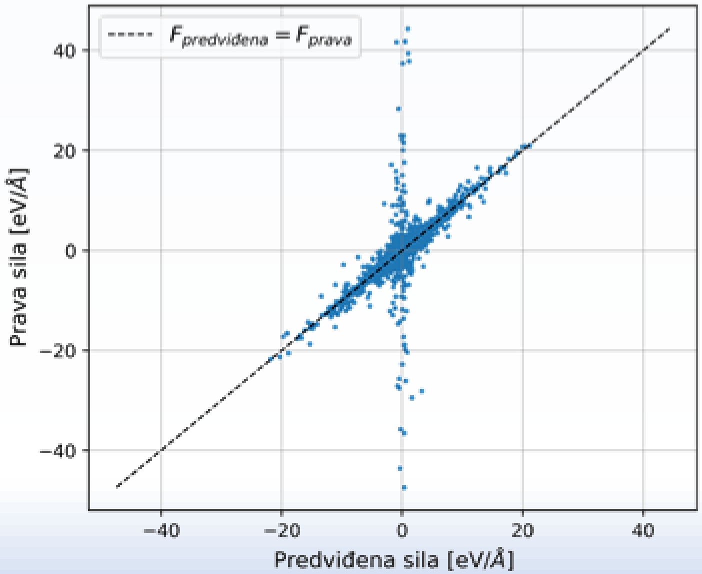
- korigiranje energija prilagodbom linearne funkcije broja atomskih elemenata u molekuli na energiju

$$E(n_H, n_C, n_N, n_O, n_S) = E_H n_H + E_C n_C + E_N n_N + E_O n_O + E_S n_S + c$$

Rezultati

- SPICE set podataka
- srednja apsolutna greška:
  - 0.053 eV/atom
  - 0.047 eV/Å
- 50 puta lošiji rezultat sličnog istraživanja
- mogući razlozi:
  - <u>pogrešno predviđanje energija</u>
  - treniranje samo na silama
  - greške u setu podataka

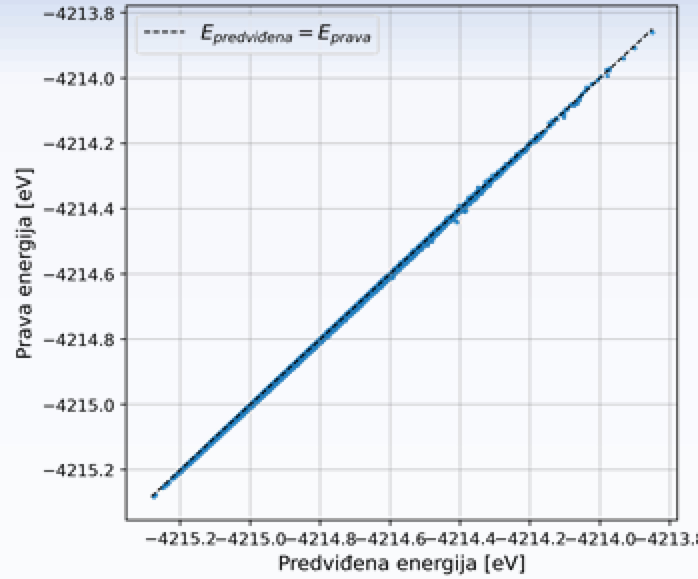


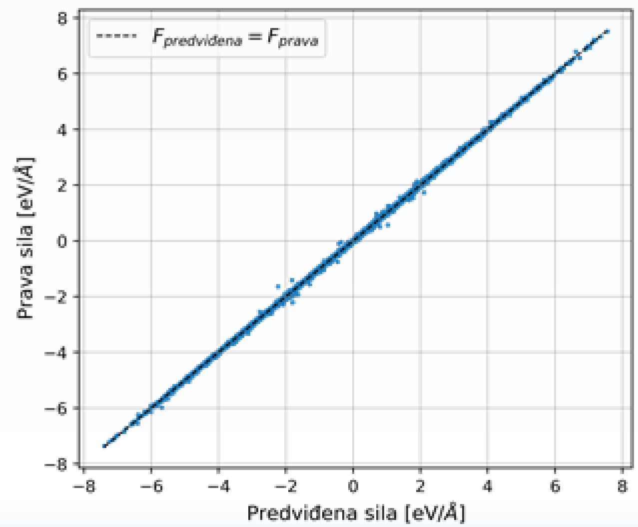


D.P. Kovacs, J.H. Moore, N.J. Browning, I. Batatia, J.T. Horton, V. Kapil et al., Mace-off23: Transferable machine learning force fields for organic molecules, 2023.

Rezultati

- etanol iz MD17 seta podataka
- srednje apsolutne greške:
  - 0.11 kcal/mol (4.96 meV)
  - 0.12 kcal/mol/Å (5.01 meV/Å)
- referentne vrijednosti:
  - 0.052 kcal/mol
  - 0.096 kcal/mol/Å
- korigiranje → 0.052 kcal/mol





A.S. Christensen and A.V. lilienfeld, Revised MD17 dataset (rMD17) (7, 2020),

Zaključak

- veliki doprinosi strojnog učenja u simulacijama
- digitalna budućnost traženja novih materijala

- rezultati lošiji od očekivanog
- neuspješno reproduciranje rezultata
- problemi:
  - pogrešno predviđanje energija
  - trening samo na silama
  - greške u podacima
- vjerojatno izolirani slučaj

Hvala na pažnji!

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