

Diffusion Module

Token, Reference Conformer,
MSA, Template features

Step 1 : Condition the pair representations by encoding the relative positions of each token. Condition the single representation by embedding time information.

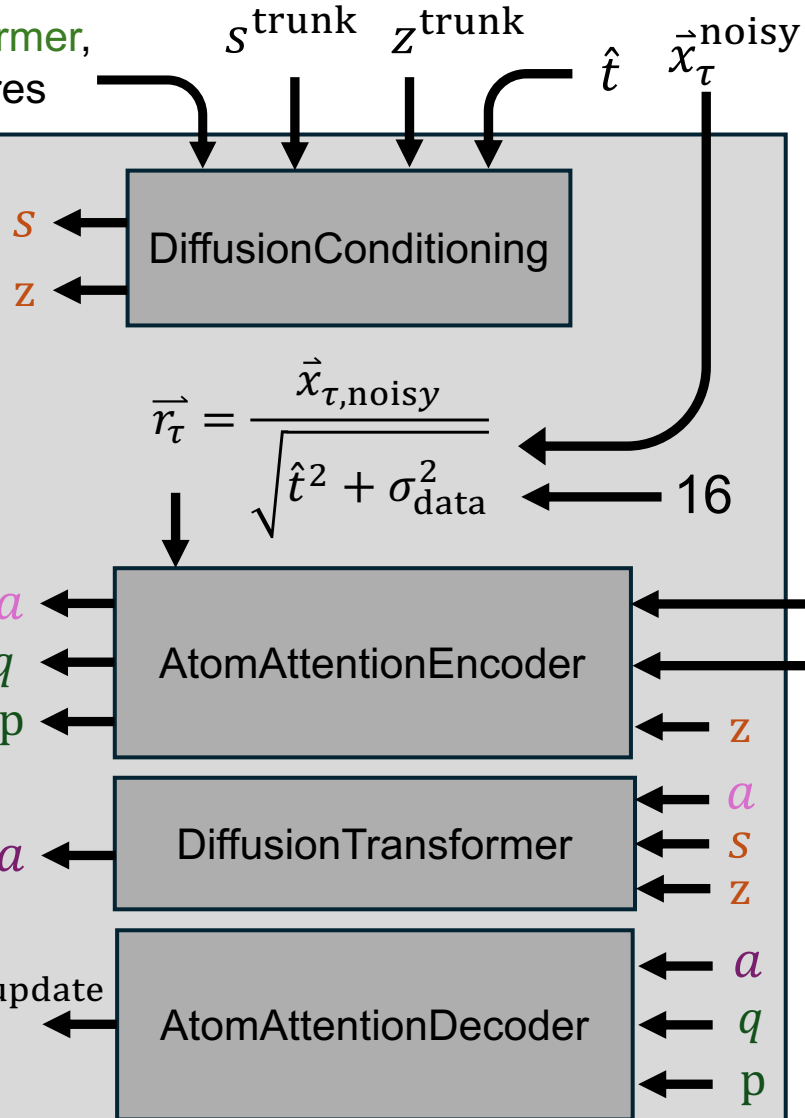
Step 2 : Scale coords to unit variance.

Step 3 : Condition the atom-level single and pair representations.

Step 4 : Perform global reasoning at token-level representation using 24 Transformer Blocks.

Step 5 : Refine q by (1) summing with broadcasted a (2) applying DiffusionTransformer with sparse attention mask (3) mapping to coord. space.

Step 6 : Rescale updates to positions and combine with input positions $\vec{x}_\tau^{\text{noisy}}$ to generate $\vec{x}_\tau^{\text{denoise}}$



Token-level Rep :

s, z

Atom-level Rep :

q, p

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 s^{trunk}

Key points :

- No invariance or equivariance with respect to global rotations or translations if enforced.
- Two level architecture working on atom-level, then token-level then finally atom-level.