

A differentiable representation of solvent-solute interface

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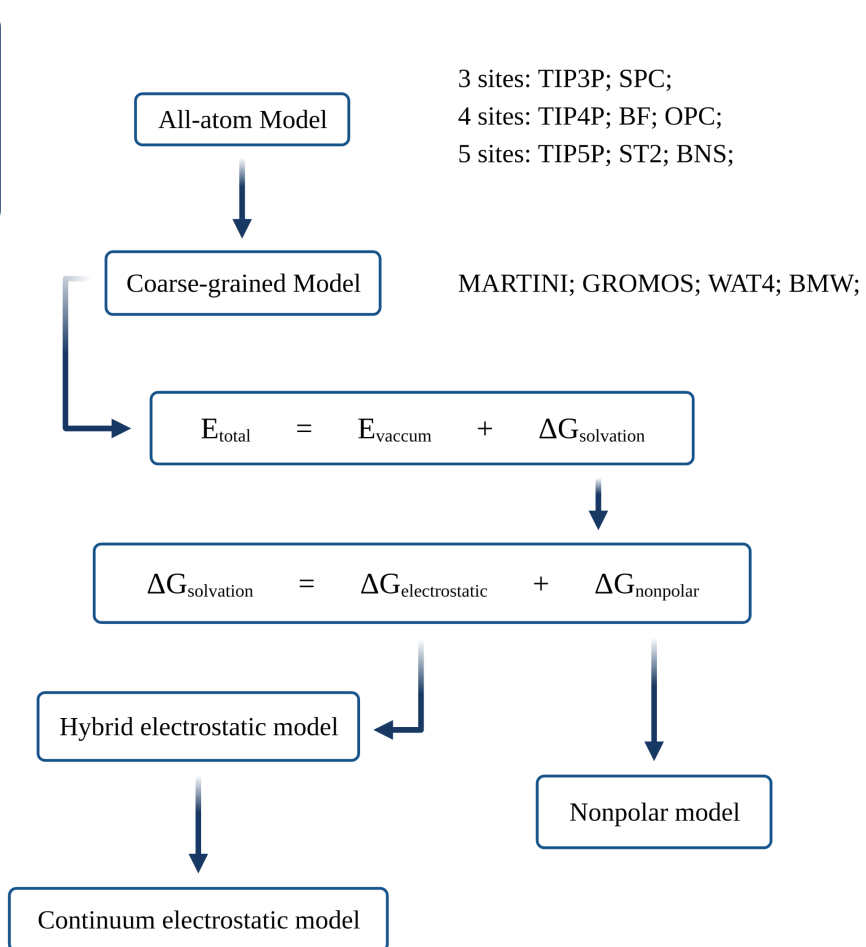
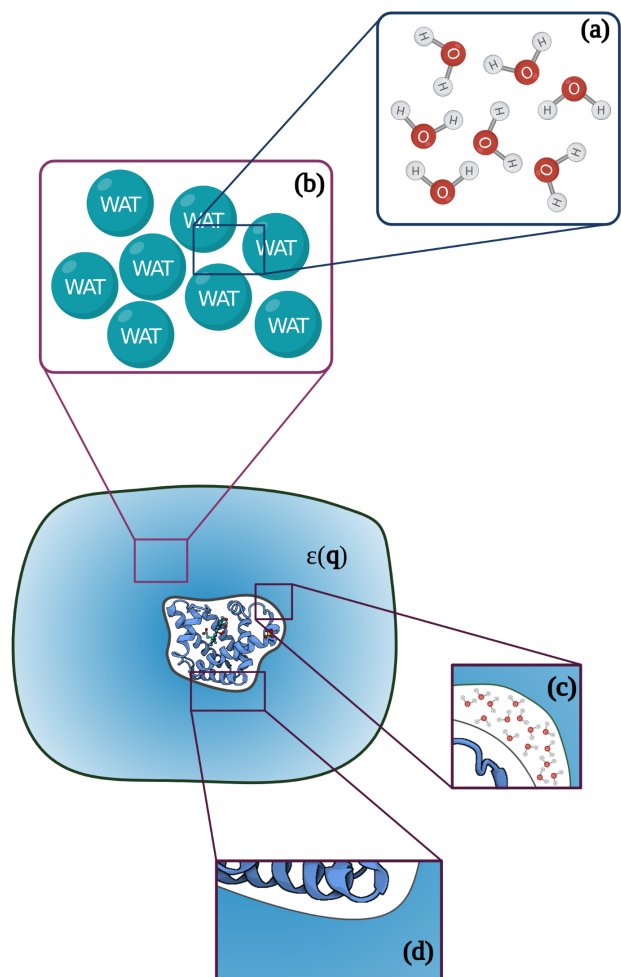
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Inspiration



Implicit solvent model



Explicit solvent

Implicit solvent

Approximation Level



Poisson-Boltzmann Equation

$$\nabla \varepsilon(\mathbf{r}) \nabla \phi(\mathbf{r}) = -\rho_{mol}(\mathbf{r}) - \lambda(\mathbf{r}) \kappa^2 \sinh \left(-\frac{z_+ e \phi(\mathbf{r})}{kT} \right)$$

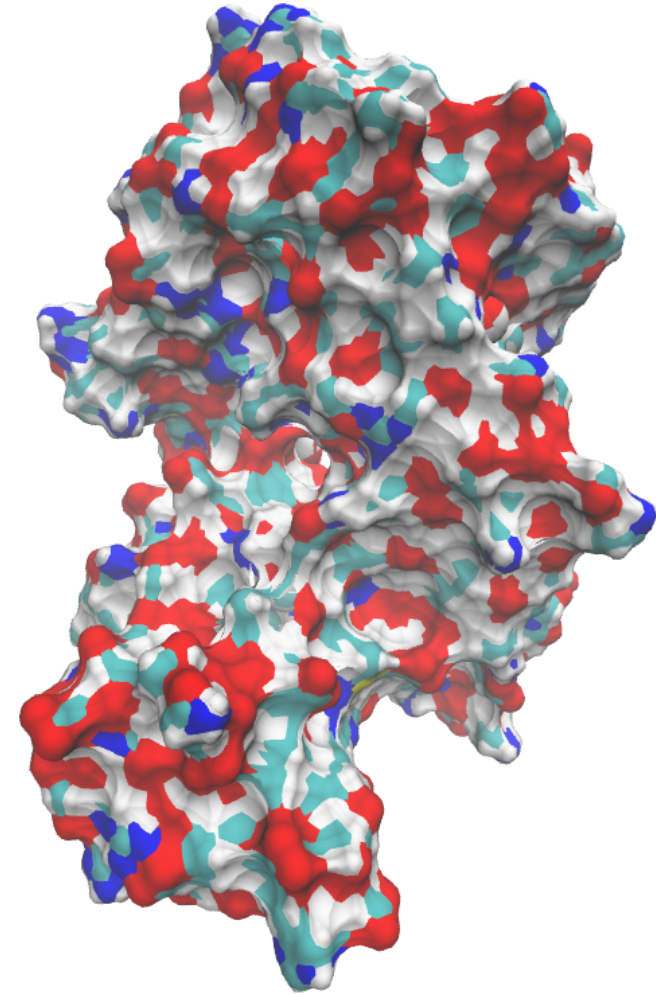
A **differentiable** expression of ε_r is vital for a precise solution of Poisson-Boltzmann Equation (PBE)



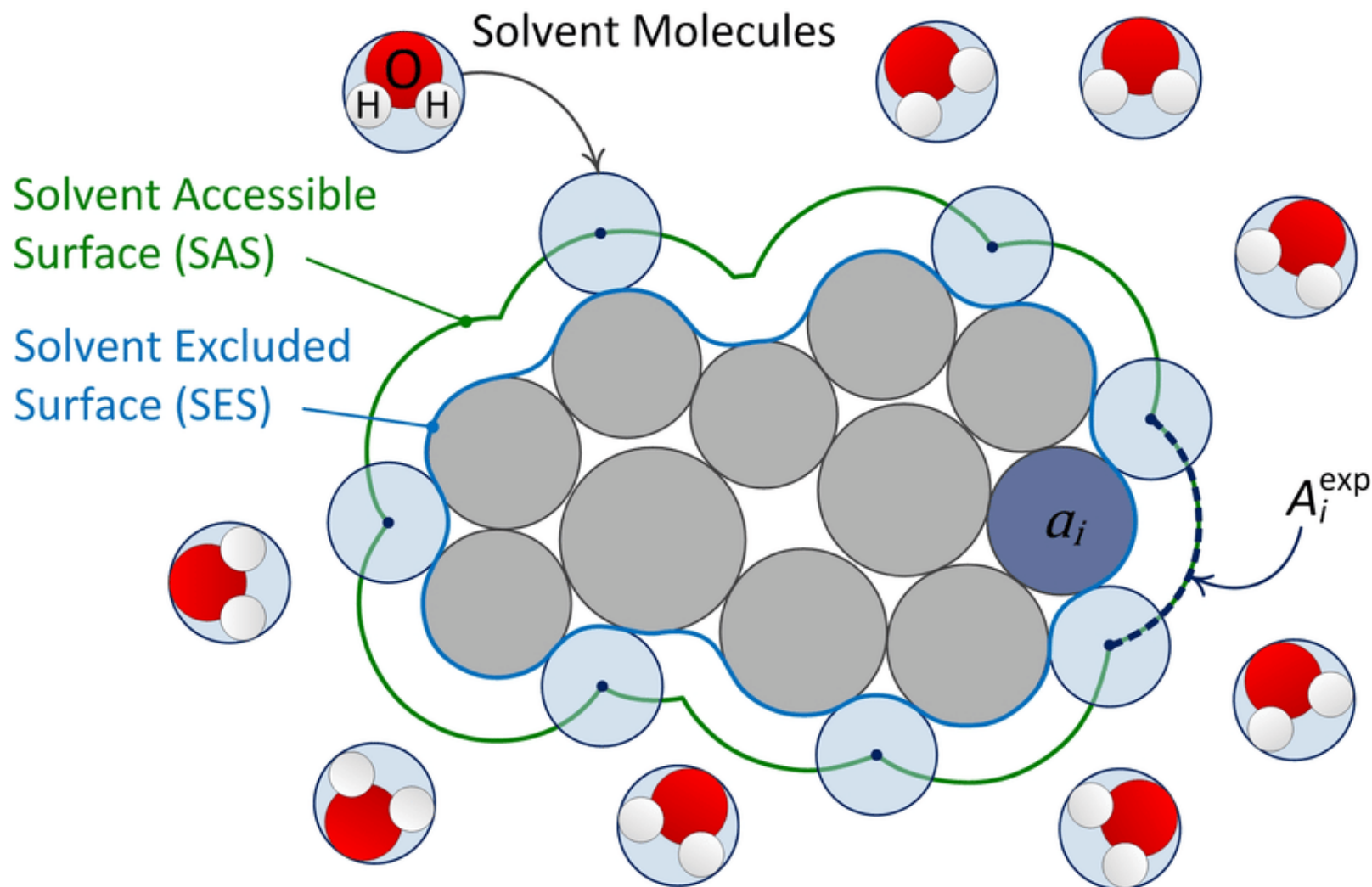
PBE for globular protein

- The surface can be interpreted as a **complex spatial distribution**
- The spatial distribution is highly **non-linear**
- The distribution depends on all of the atom's **position** and **type**

PDB id of protein shown right: 1A1N



Current solution: Van der Waals surface



Current obstacles

- Representation is **not smooth**
- Representation is **not expressed explicitly**
- Representation based on **Hard sphere model**
 - Highly approximated
 - Hyper parameter required

Target

A smooth, differentiable, interface representation for solution of **PBE**



Method



Basic Idea

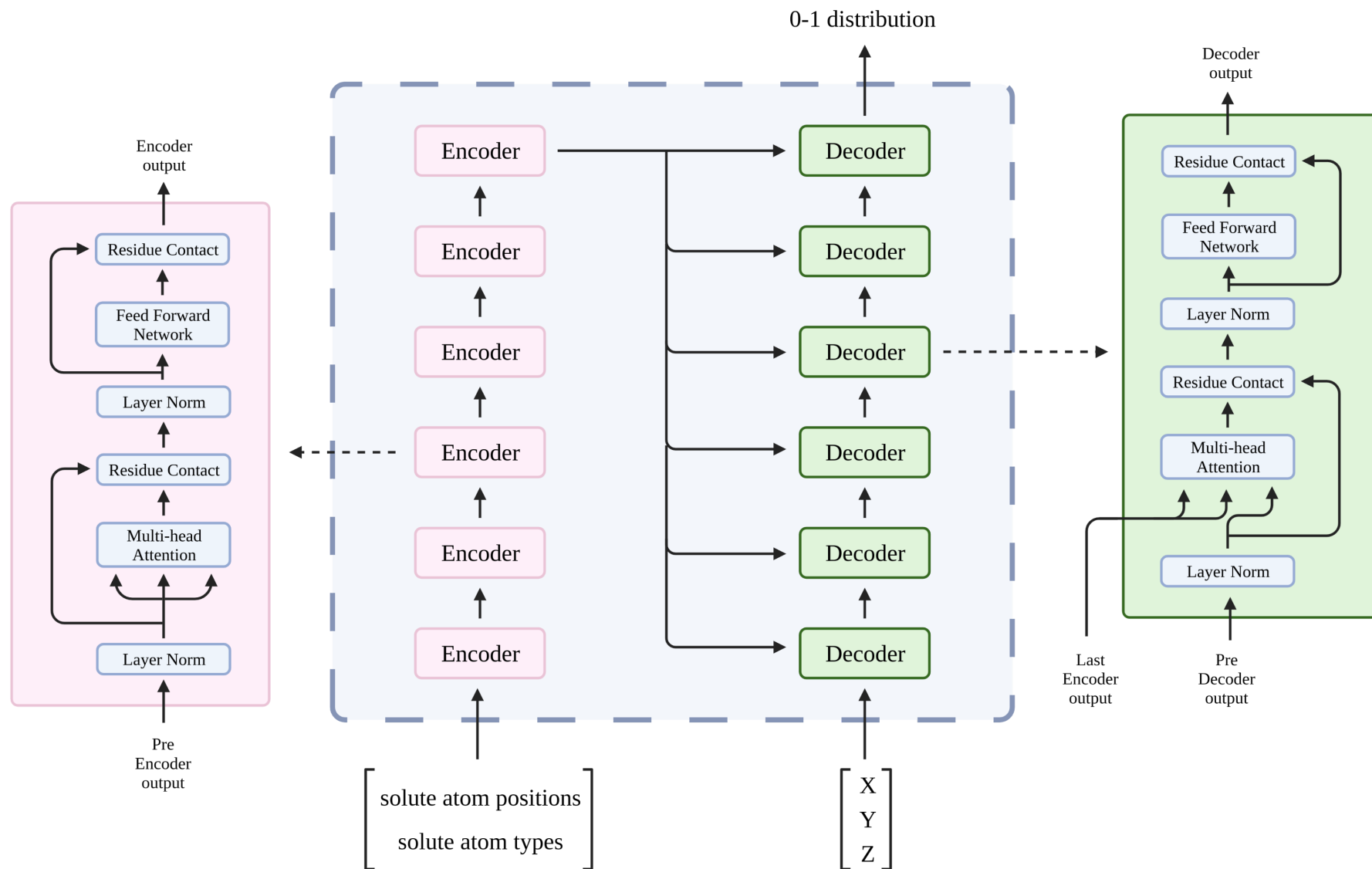
- Using deep neural network to represent the non-linear interface
- Deep neural network are naturally differentiable

Obstacle

- Handling length-varied input: the positions and types of protein's atom



Architecture



Dataset

- Downloaded **12748** structures from PDB website
- Patched and solvated **10962** structures in $60 \times 60 \times 60$ Å box
- Currently, sampled **4458** structures
 - Label solution atom as 1
 - Label solvent atom as 0

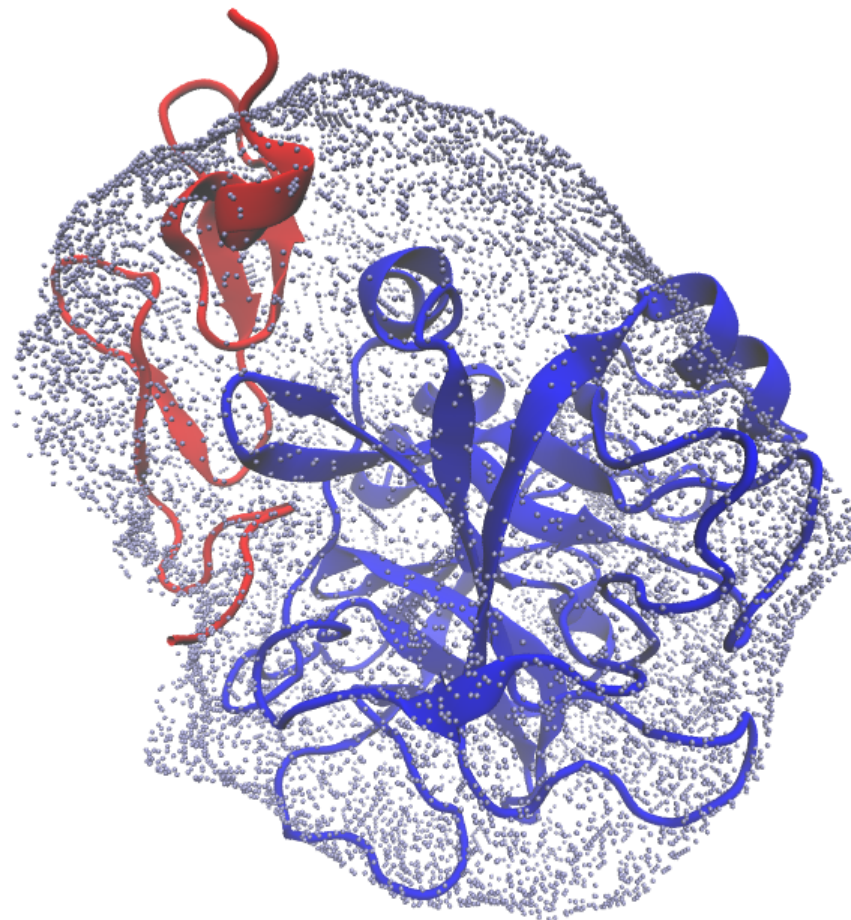


Result and discussion



Feasibility test

- Train network on tiny dataset
 - 28 protein structures
 - Each with 25 samples
- Average accuracy: 92%
- Isosurface with output value of TSSIR between $[0.495, 0.505]$



PDB id of protein shown right: 1IQG



Thanks for your attention

Q & A

