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My current research topicis in the substrate-enzyme docking reactivity interface evalutaiton; I am now a Ph.D. Student, I am using 3DCNN/SE3-transformer neural network; Now I am interesting in adopt structures information from native PDB structures of enzyme and predict the regression enzyme-function related task (interface energy and substrates orientation) ; I am using Super computing at VU – ACCRE; my codes are serial; 54000 protein structure decoys (cooridnates), I am developing my own code but also I will use the community code as benchmark; NoSQL database which stores enzyme structural/sequence related (amino acid sequences, smiles string (substrates) and PDB files)

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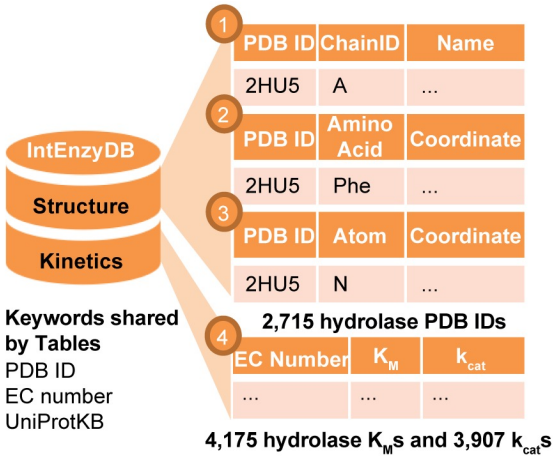
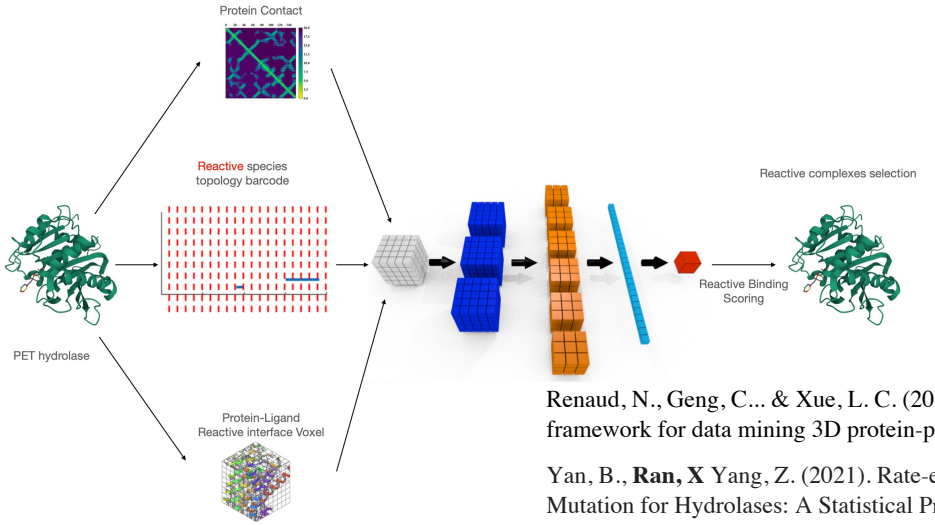
My first problem is how to scale up the voxel sampling process at enzyme-substrate interface in parallelization manner.

My second problem is how to parallelization a 3D neural network. I always run out GPU memory when processing the 3D data in training the SE3-transformer related network. (on ACCRE I usually use 128GB GPU memory)





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