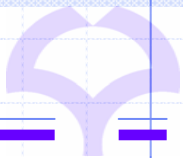


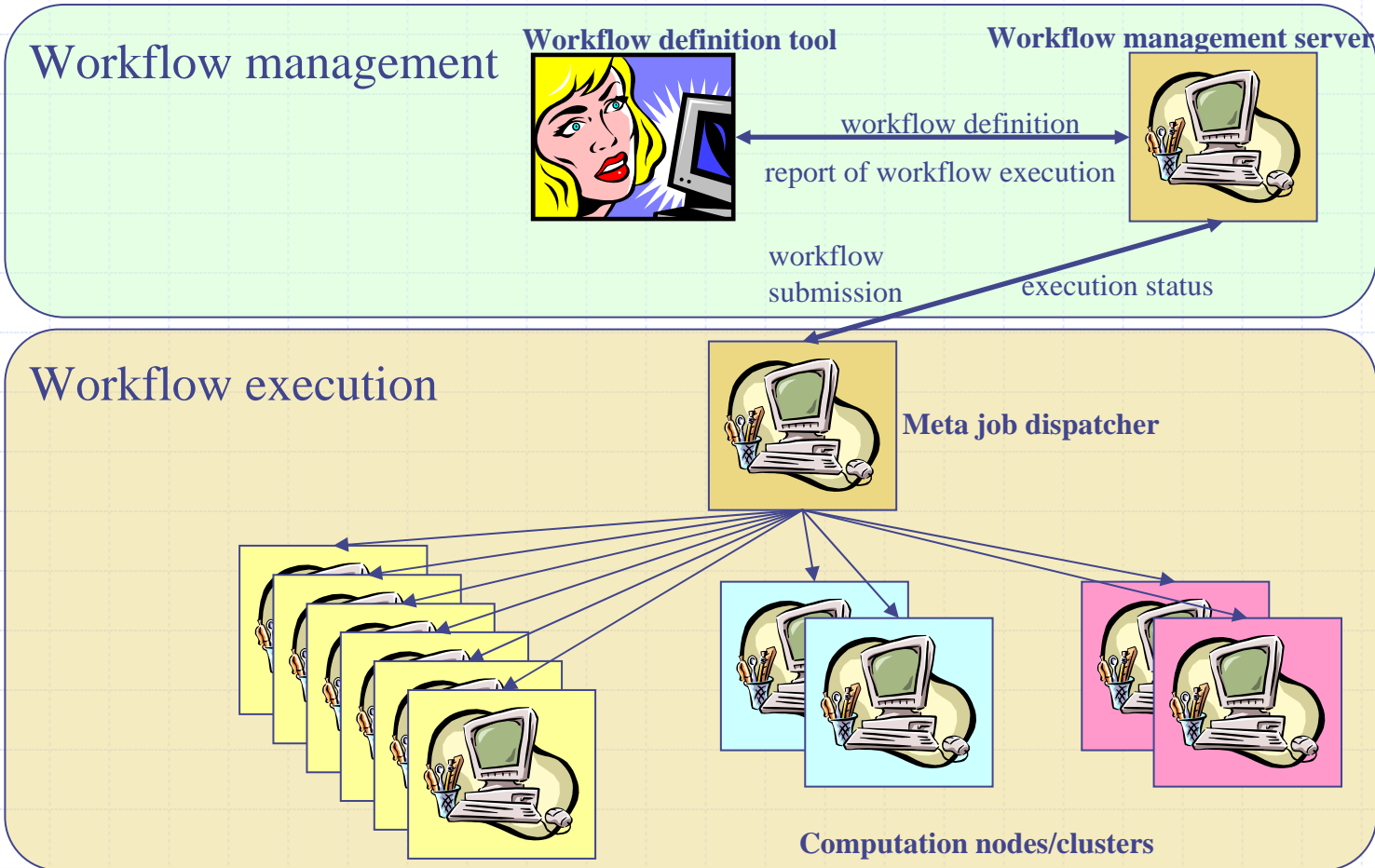


Key concepts of HTC

- ◆ Users can specify the strategy of job/task execution in scientific simulations.
- ◆ Users can dynamically change the strategy during job/task execution according to final/intermediate results.
- ◆ Current target application
 - Protein structure prediction program “ROKKY”



HTC environment



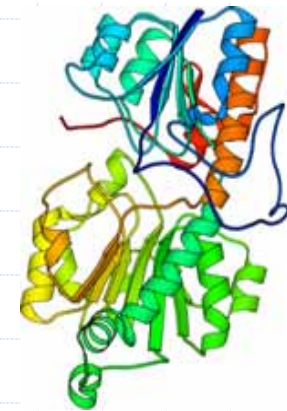
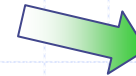


Structure Prediction:

A key challenge in post-genome sequencing era

Given
amino acid sequence:

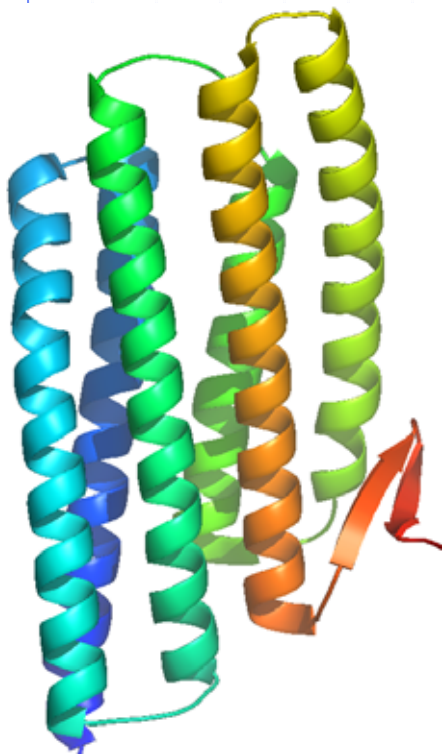
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KTVEEVNALKNEILKAHATIDQWLLKNAKEDAIAE  
LKKAGITSDFYFNAINKAKTVEEVNALKNEILKAH  
ATIDQWLLKNAKEDAIAELKKAGITSDFYFNAINK  
AKTVEEVNALKNEILKAHATIDQWLLKNAKEDAIA  
ELKKAGITSDFYFNAINKAKTVEEVNALKNEILKA  
HA
```



Functional Annotation
Drug design



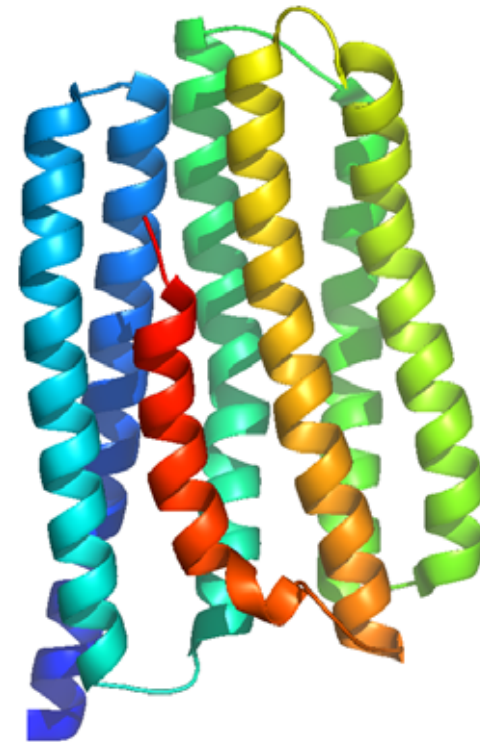
Full automation vs Human intervention



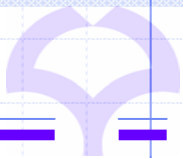
Answer



By full automation



By human intervention



Sample workflow for ROKKY

