Summary 1st day

Model building

Objective

To **construct 3D atomic models** of biomolecules (typically proteins) based on experimental or predicted data, enabling insights into their **function**.

1st step: Map Preprocessing.- enhance map sharpness

One effective approach is local filtering (LocalDeblur), which adaptively enhance features based on local resolution.

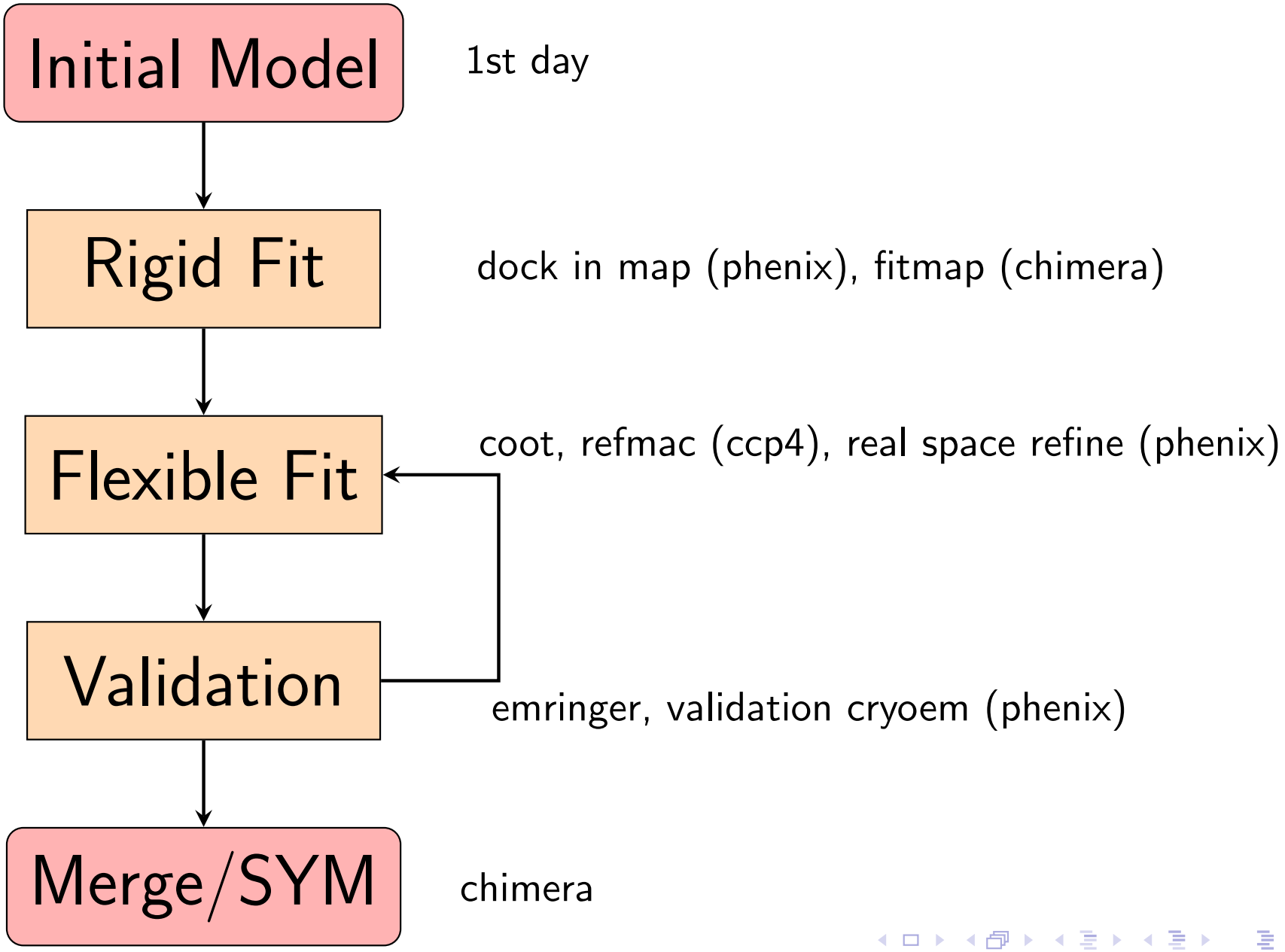
2nd step: Initial Model

- Alphafold
  - Highly accurate, especially for single-chain proteins (5000)
  - No experimental structure is used
  - Main input sequences
  - Relies on coevolution
- ModelAngelo
  - Integrates structural constraints (3D maps)
  - Works better at resolution less than 3.5 Å
- Modeller (Sequence Homology Modeling)
  - Builds models based on known structures of similar sequences
  - Relies on evolutionary conservation
  - Effective when homologous templates are available

Summary 2nd day

Model building

Workflow


Initial Model
1st day
Rigid Fit
dock in map (phenix), fitmap (chimera)
Flexible Fit
coot, refmac (ccp4), real space refine (phenix)
Validation
emringer, validation cryoem (phenix)
Merge/SYM
chimera