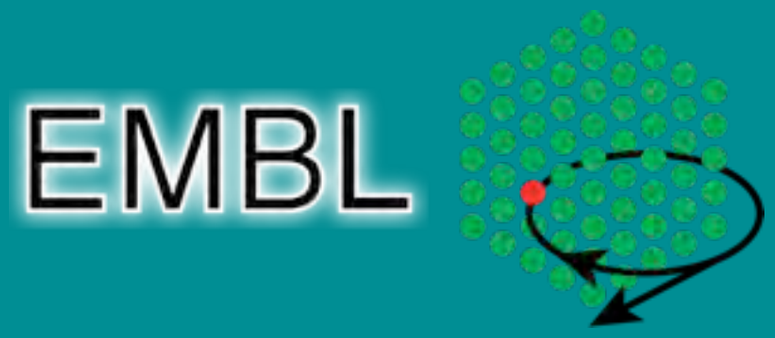
ARP/wARP Tutorial

Ciaran Carolan & Tim Wiegels
Lamzin Group (ARP/wARP), EMBL Hamburg



Where to go...


CCP4 Program Suite 6.1.13 CCP4Interface 2.0.6 running on mac-peter-book.local Project: PROJECT
Change Project
Help
Program List
Acorn
AMoRe
Anisoanl
ArealMol
ARP/wARP
AstexViewer
Balbes
Baverage
Bp3
Buccaneer - autobuild/refine
Buccaneer - fast build only
Cad
Chainsaw
Project Database Job List - currently no jobs
Directories&ProjectDir
View Any File
View Files from Job
Search/Sort Database..
Graphical View of Project
Delete/Archive Files..
Kill Job
ReRun Job..
Edit Job Data
Preferences
System Administration
Mail CCP4
Exit

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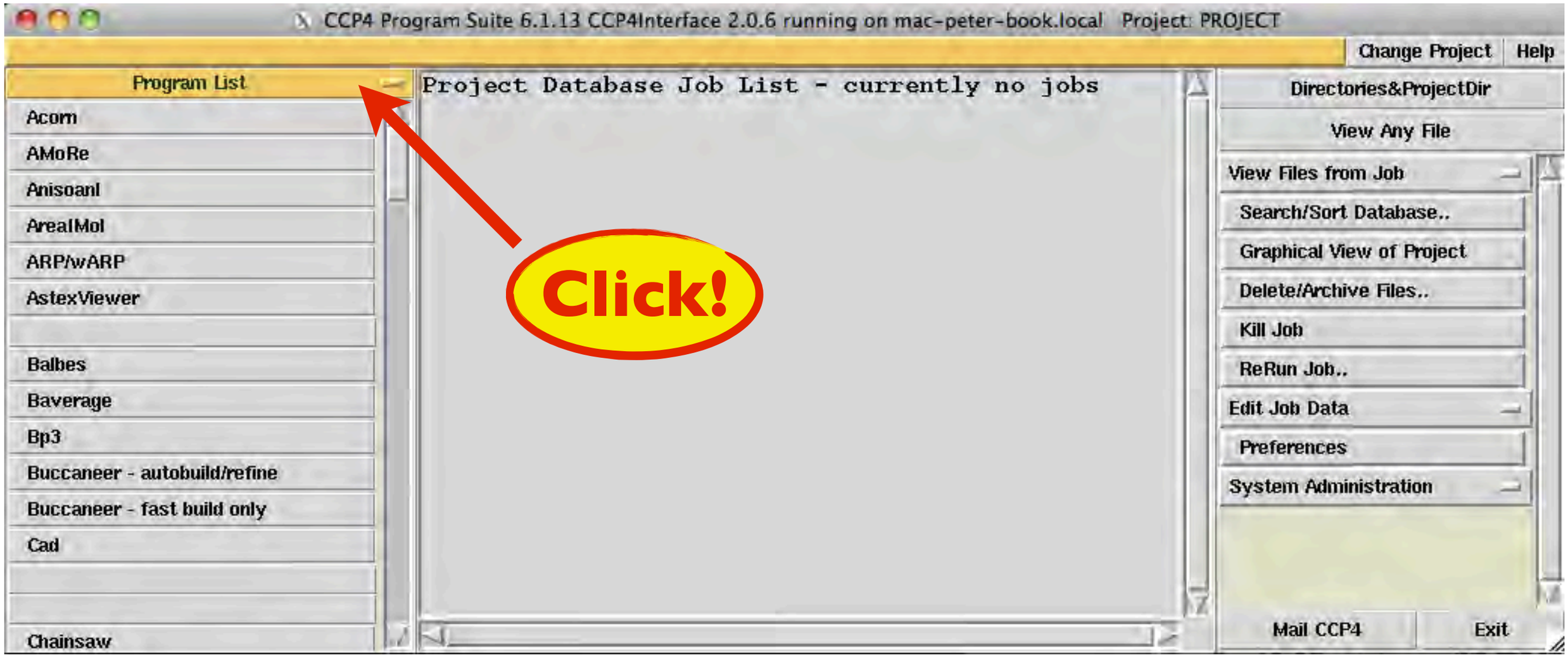
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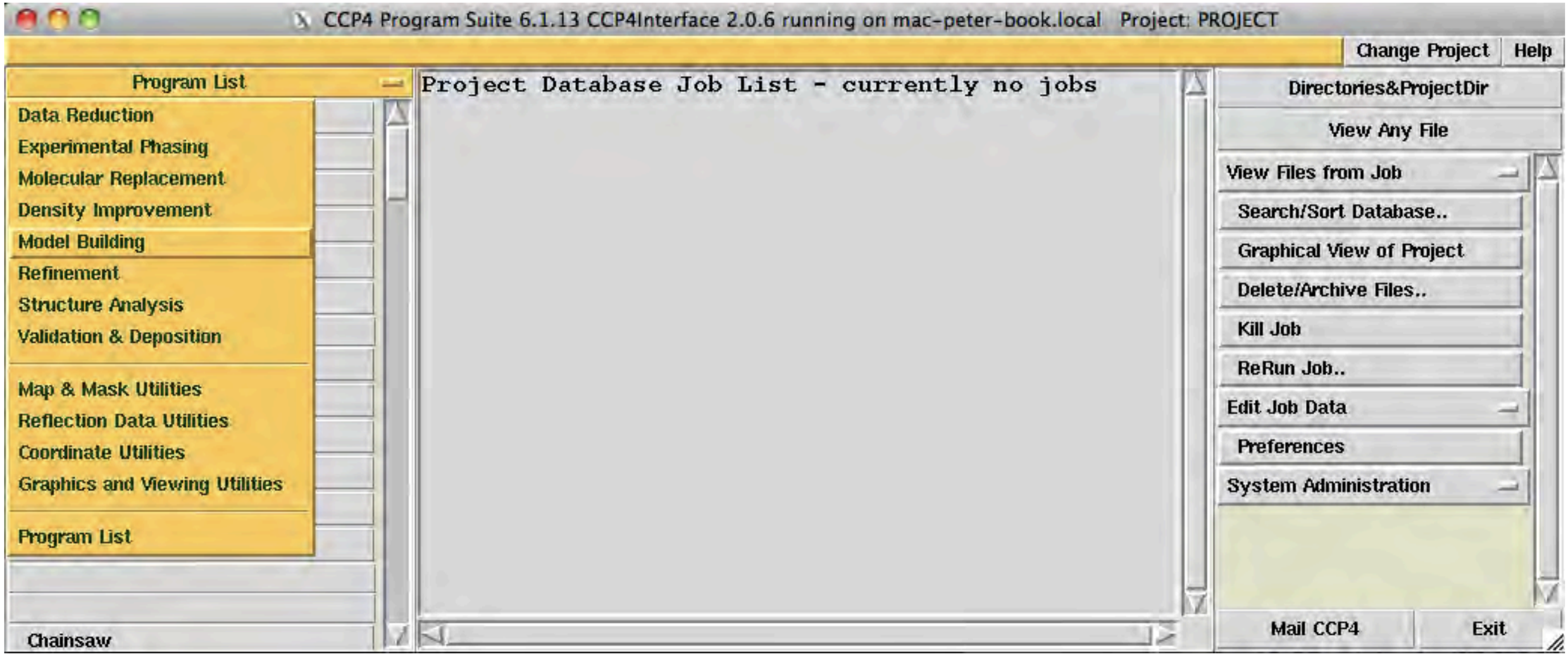
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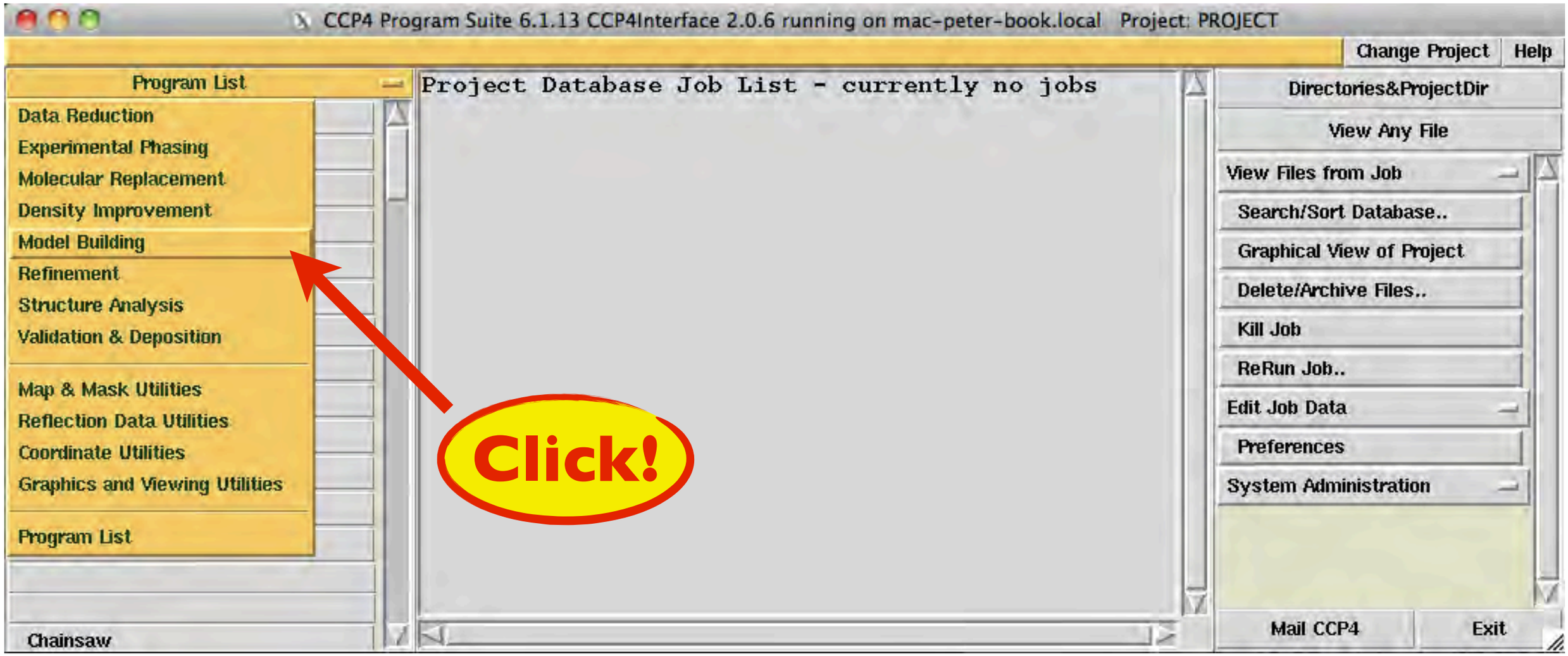
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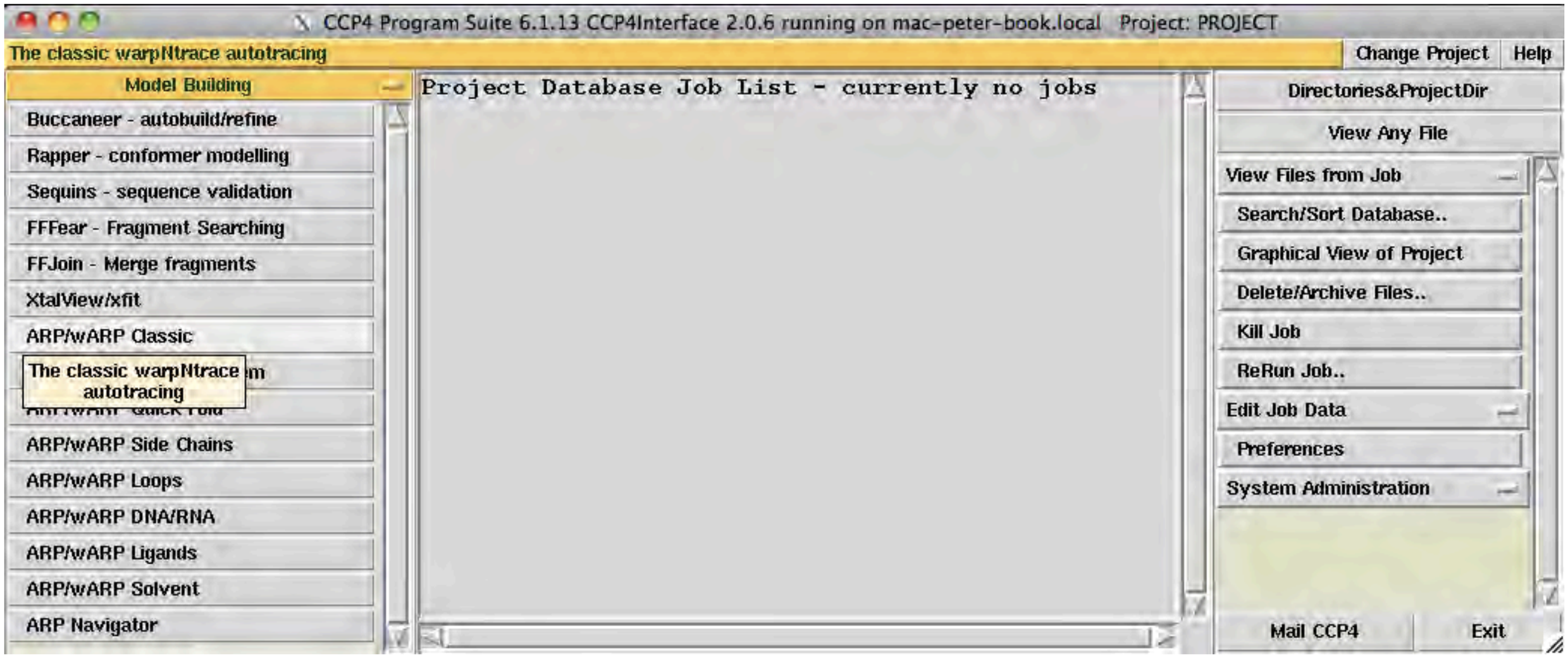
ARP/wARP: Tracing (warp_tracing)



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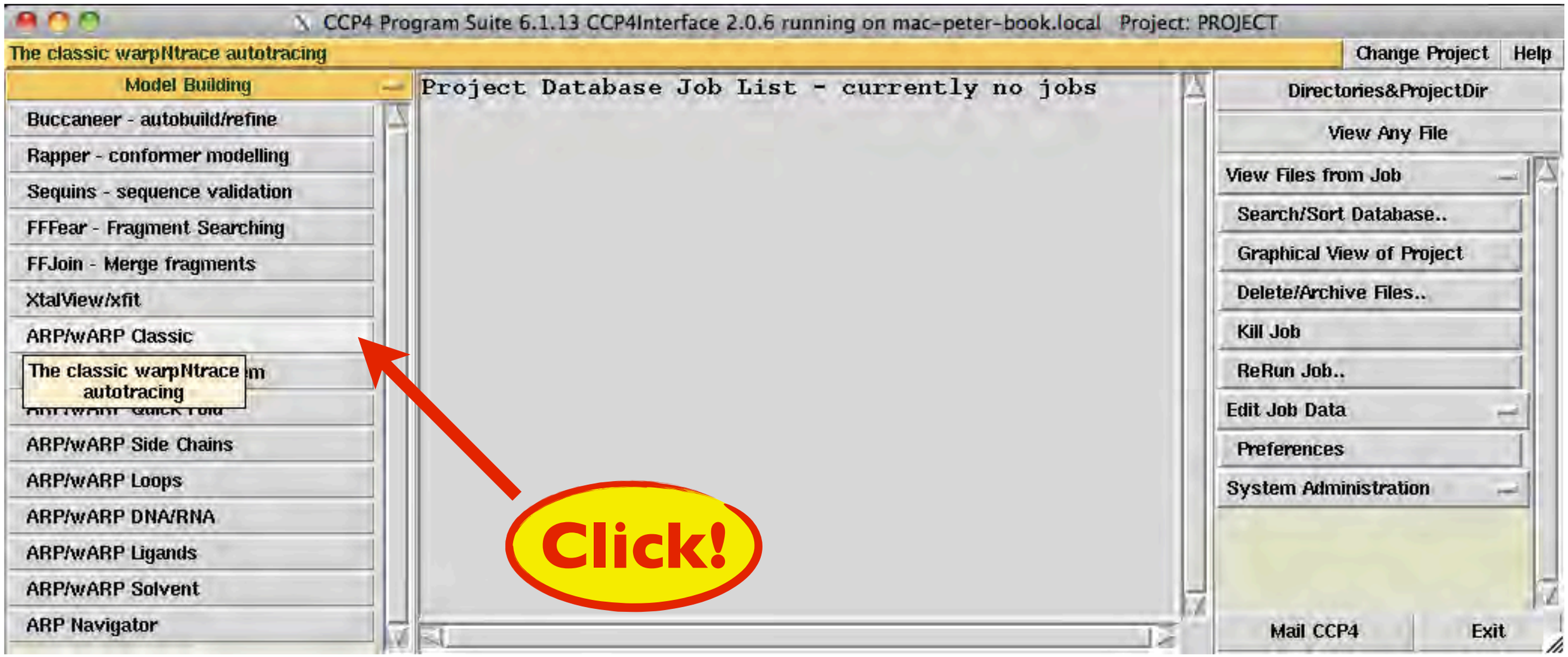

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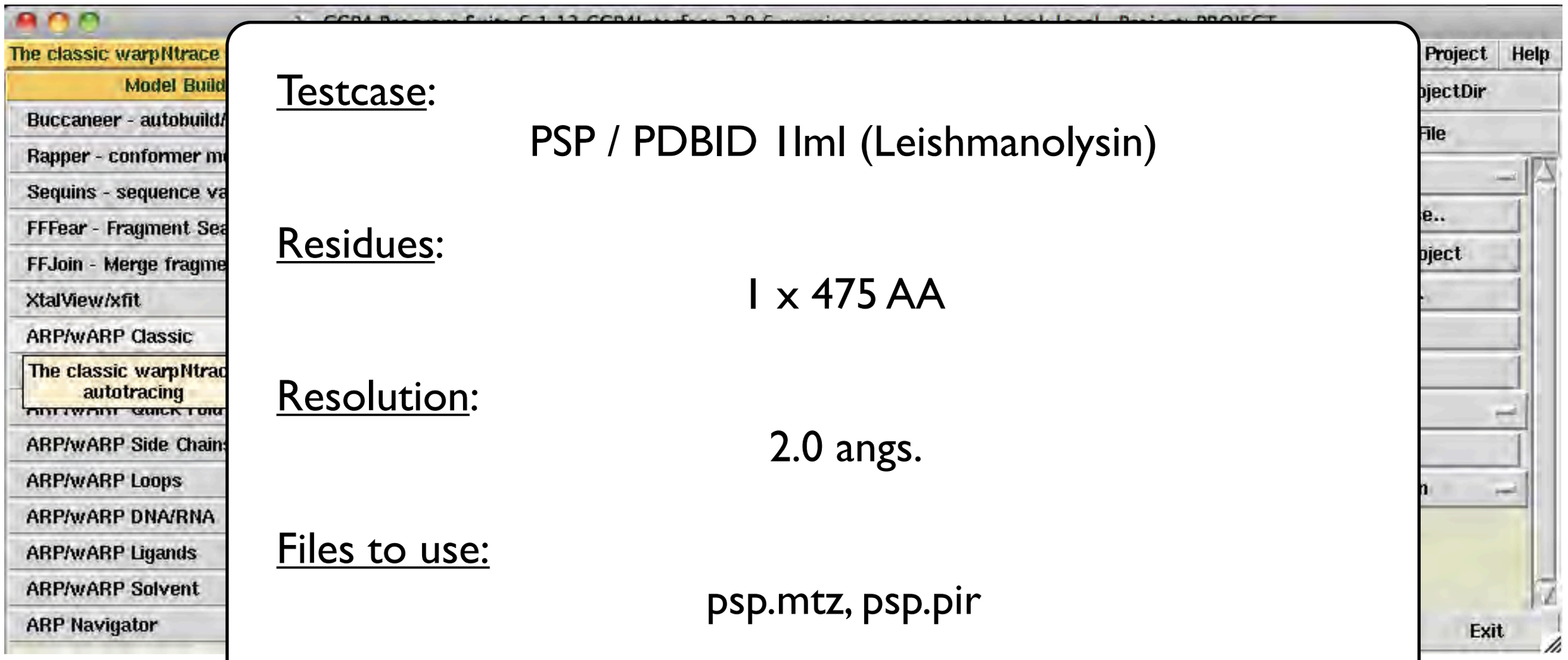
PSP



Testcase:

PSP / PDBID 1lml (Leishmanolysin)

Residues:

1 x 475 AA

Resolution:

2.0 angs.

Files to use:

psp.mtz, psp.pir

MTS labels to use:

FP, SIGFP, PHIDM, FOMDM

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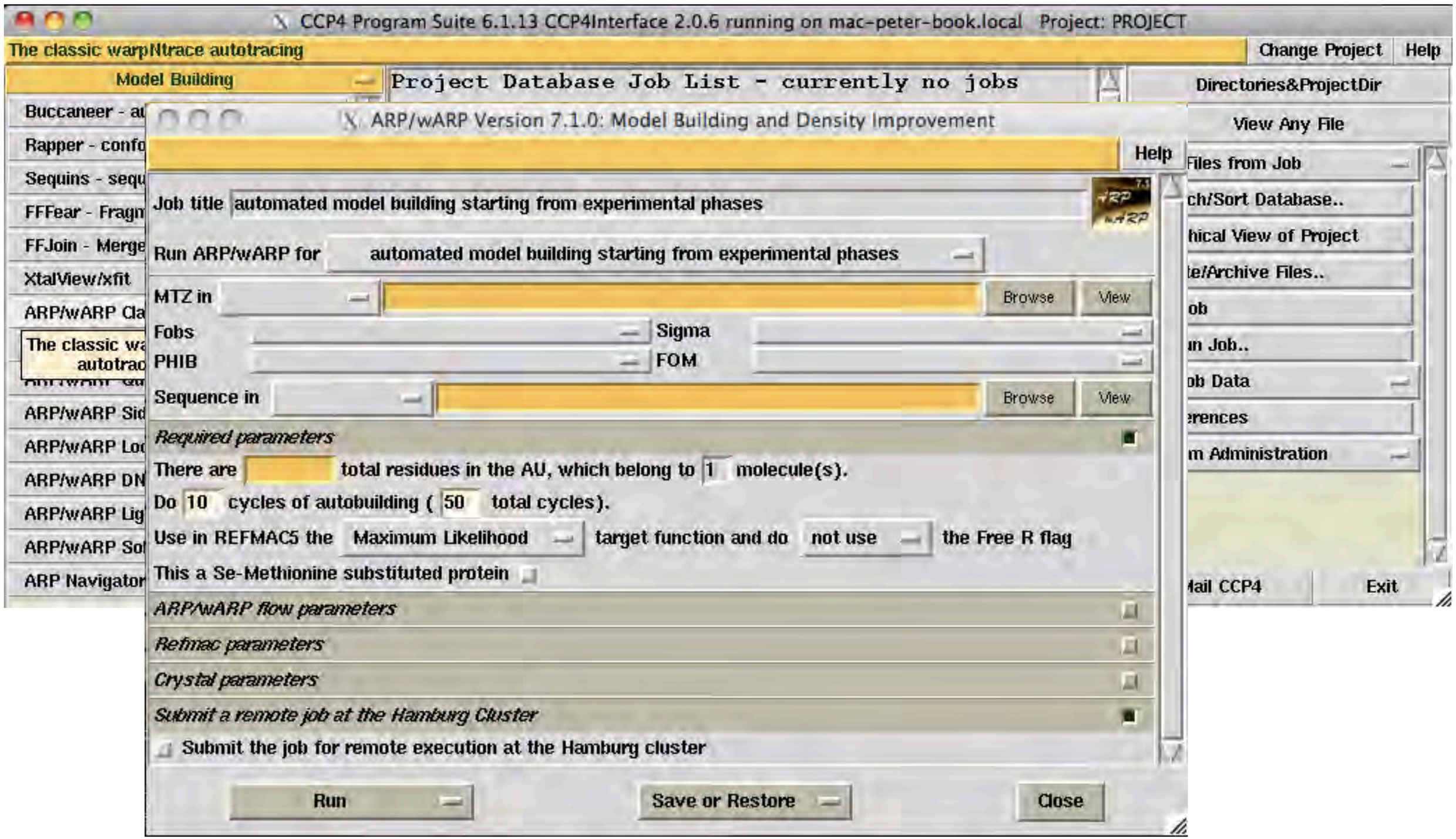
PSP



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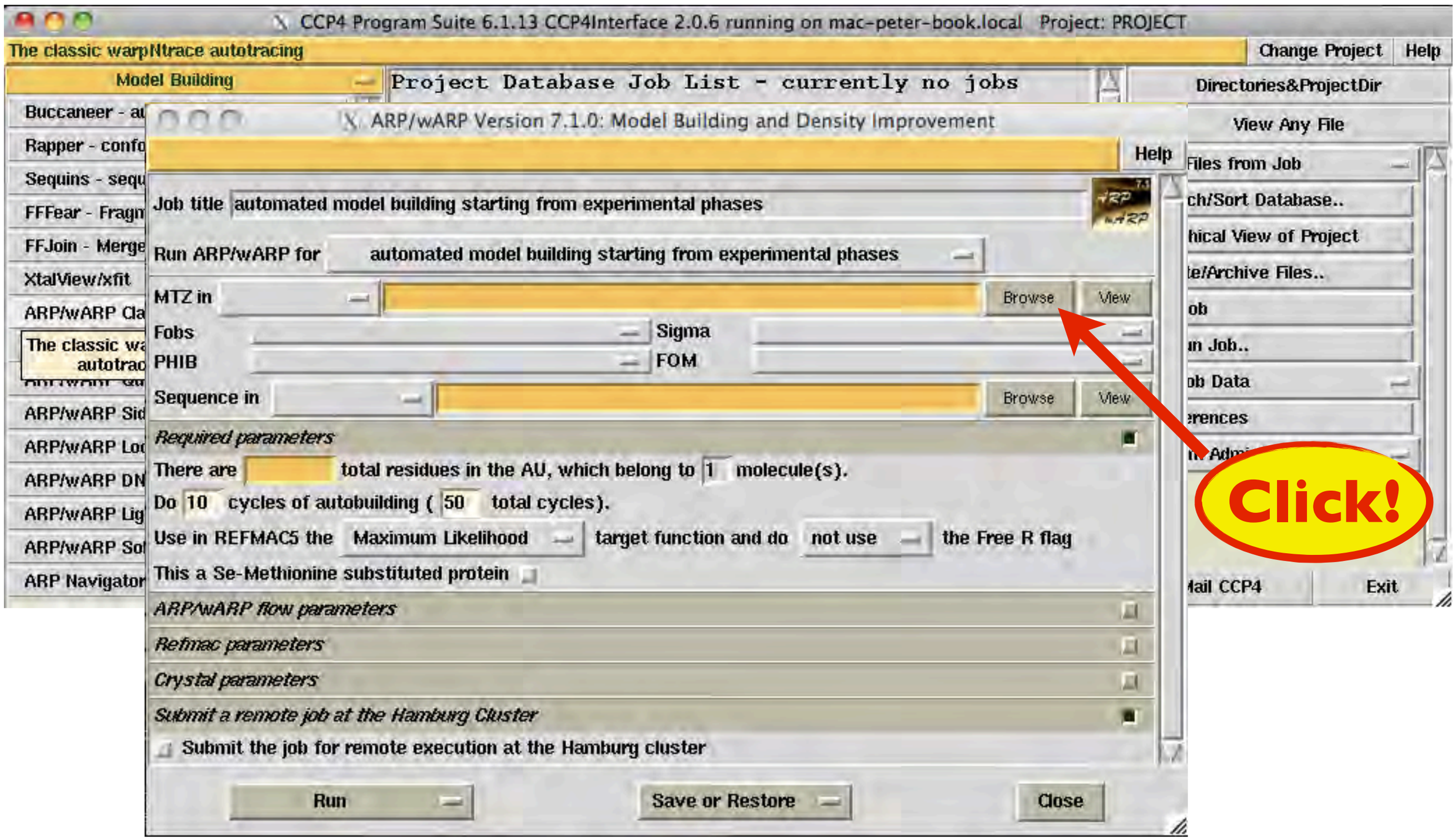

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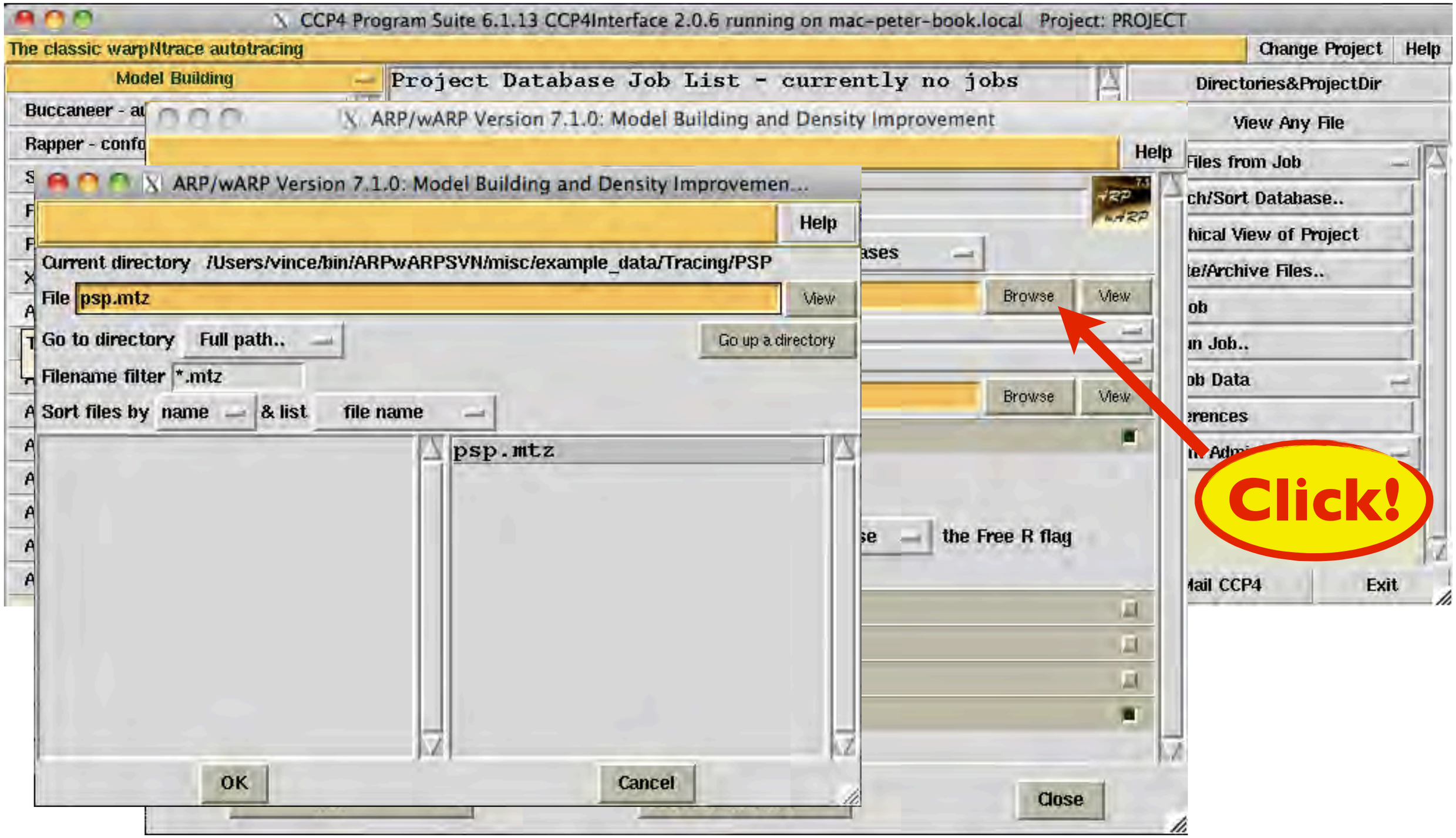

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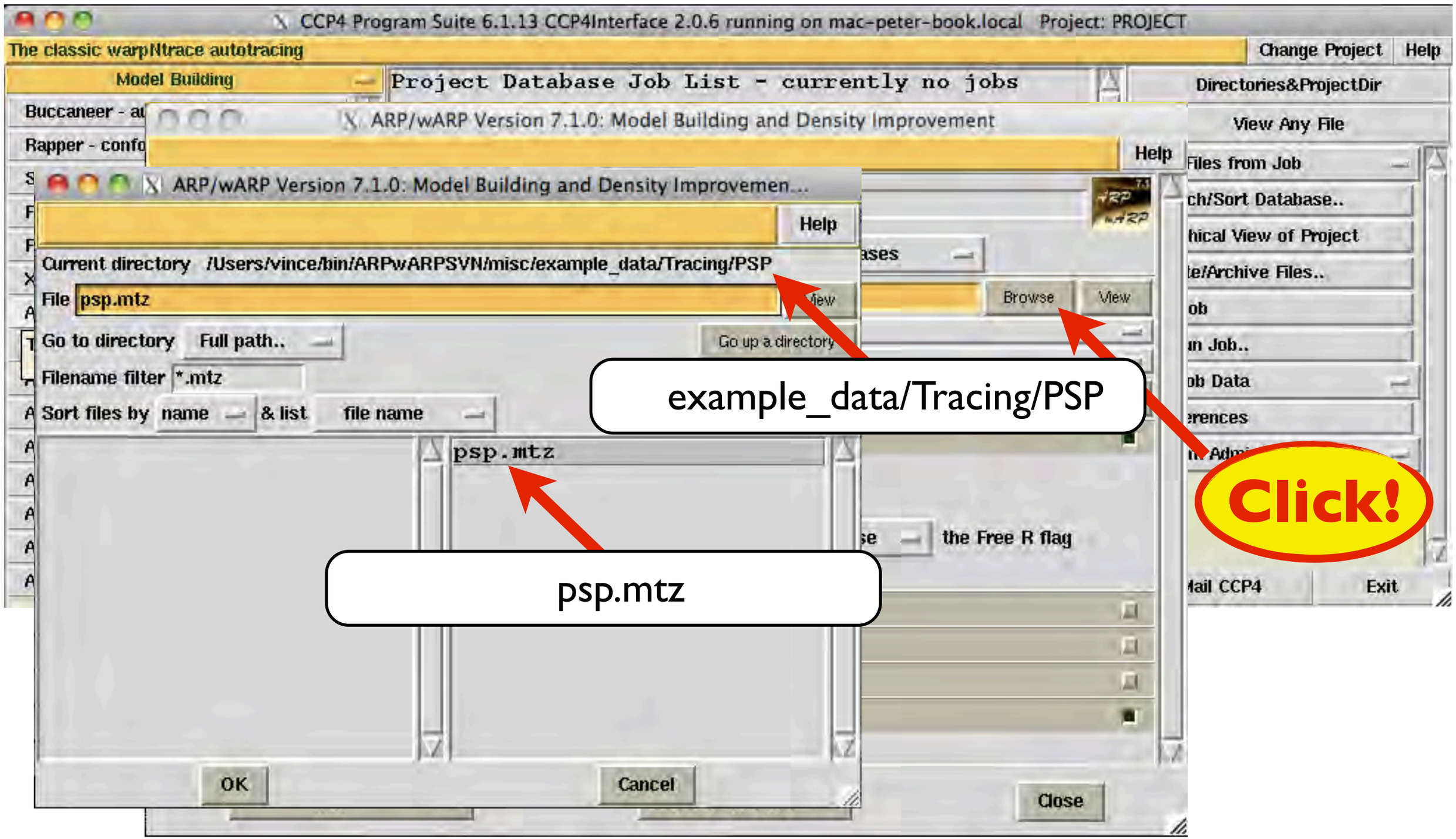

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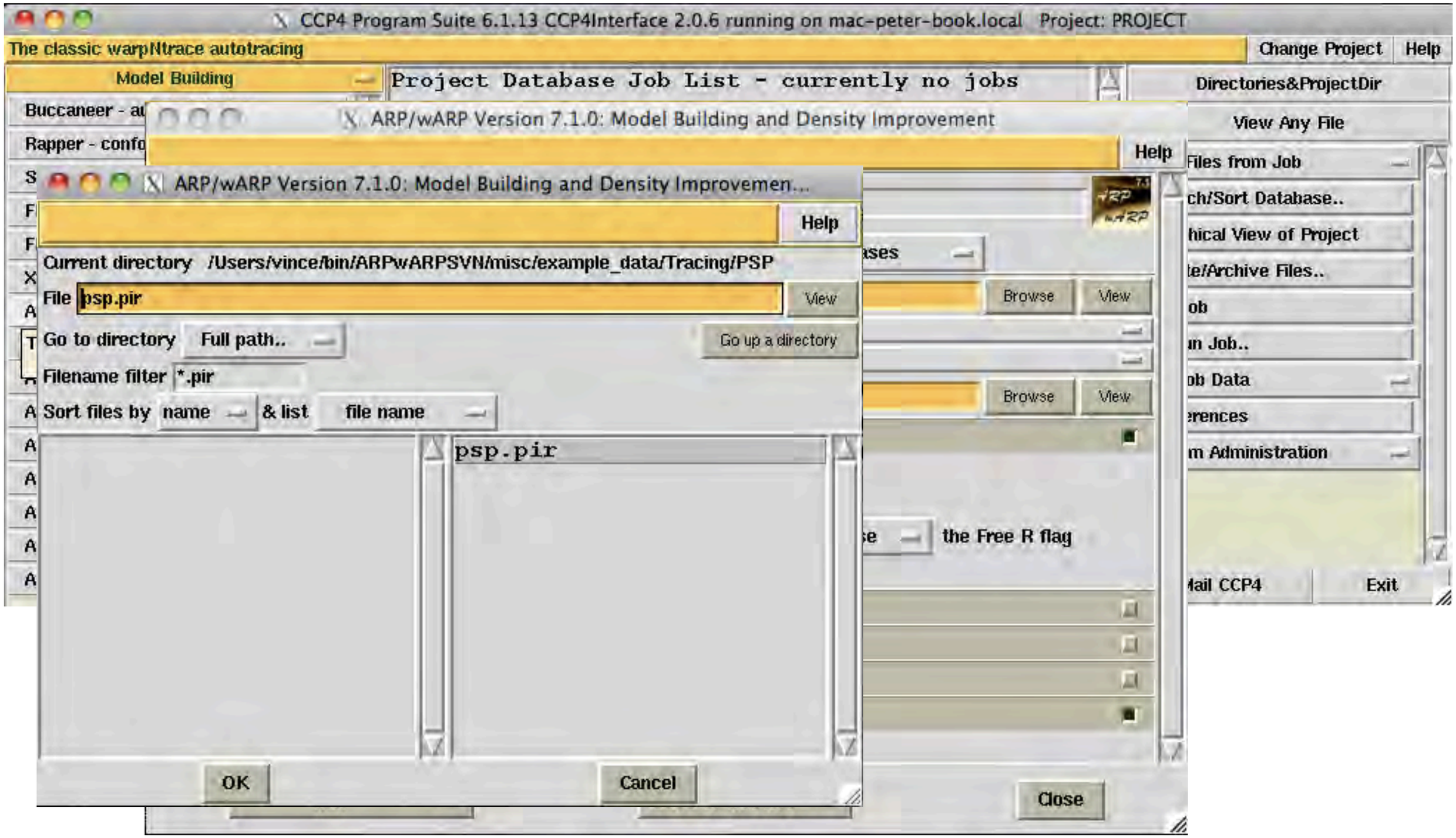

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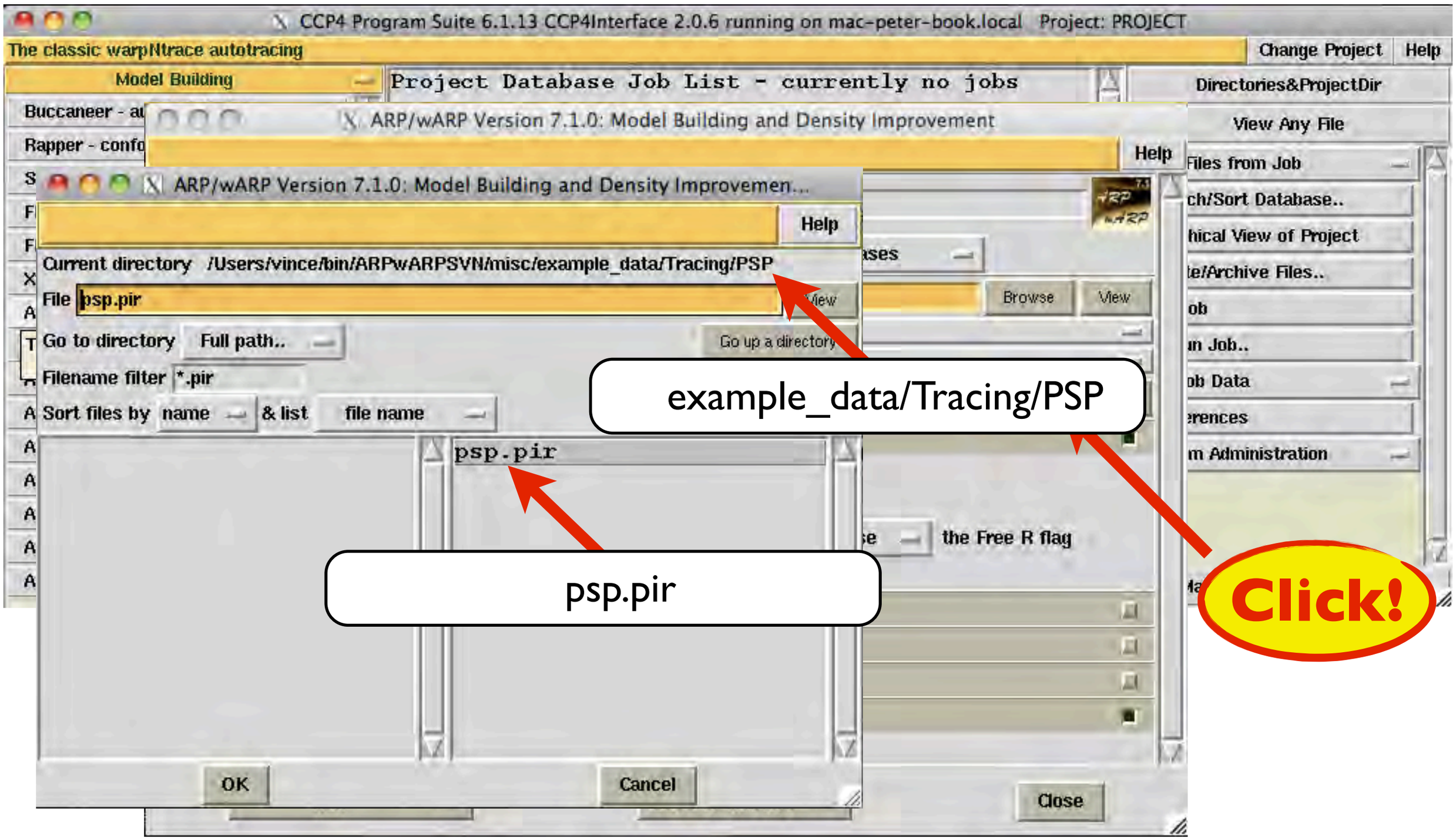

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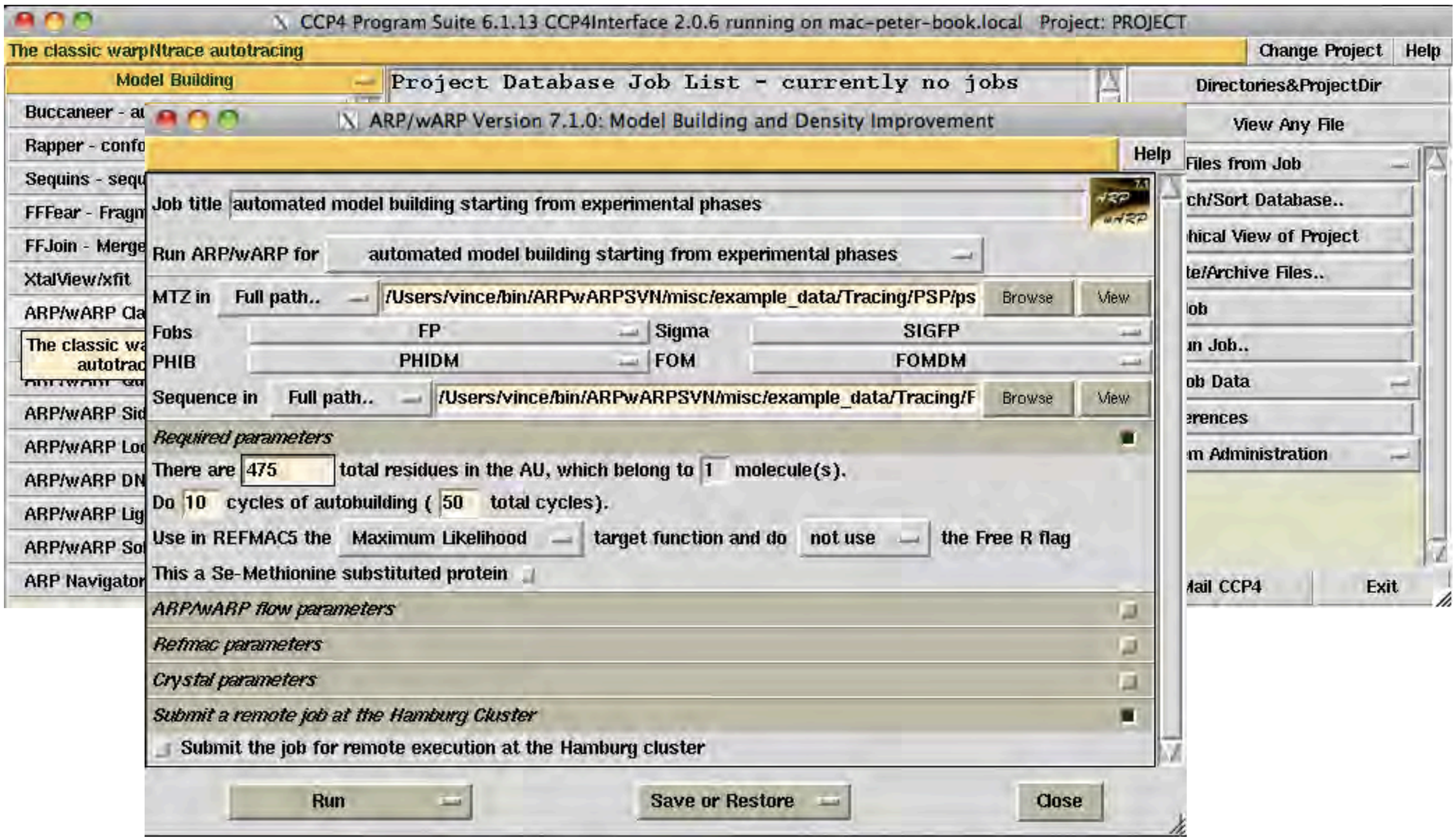

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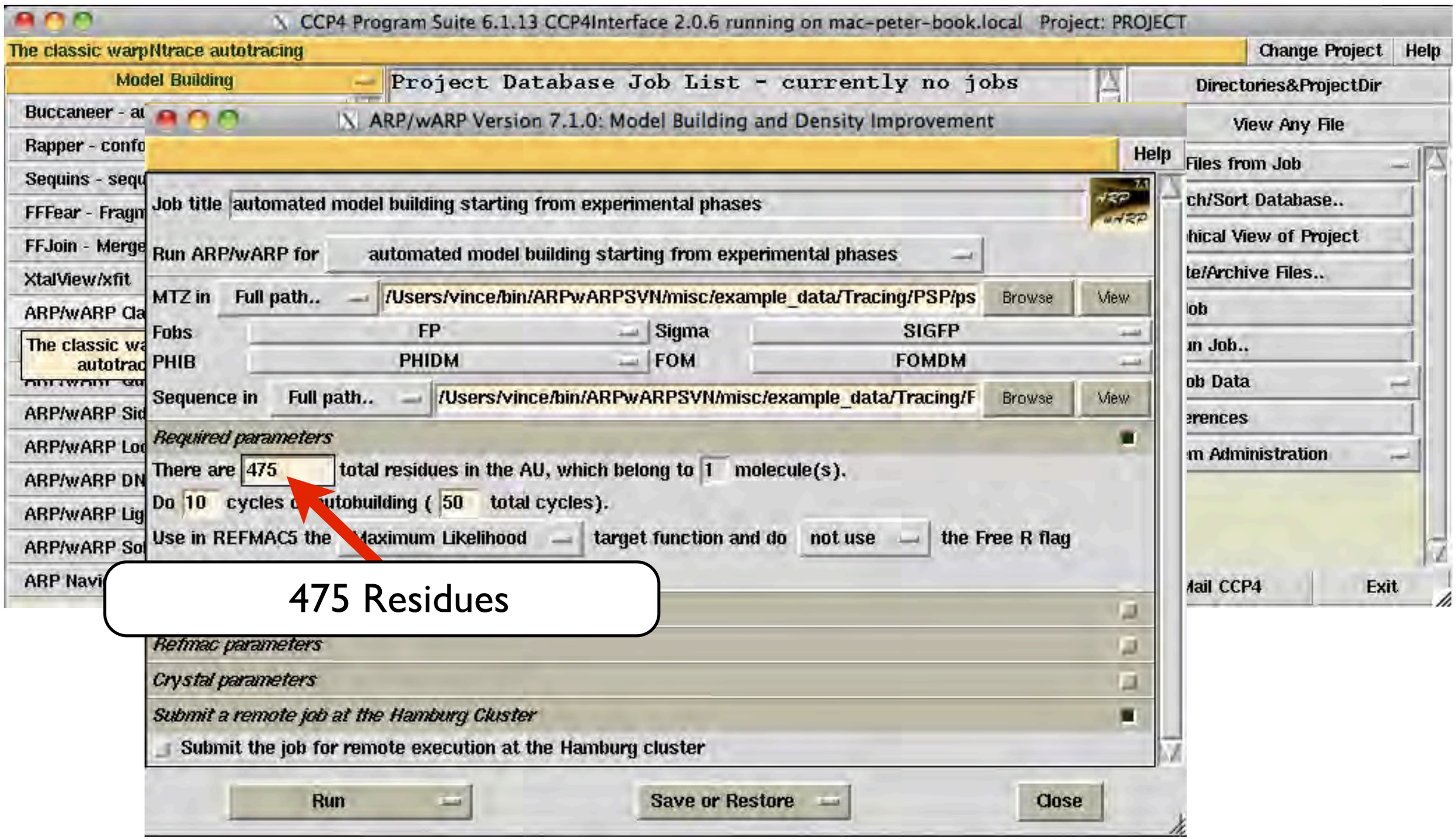

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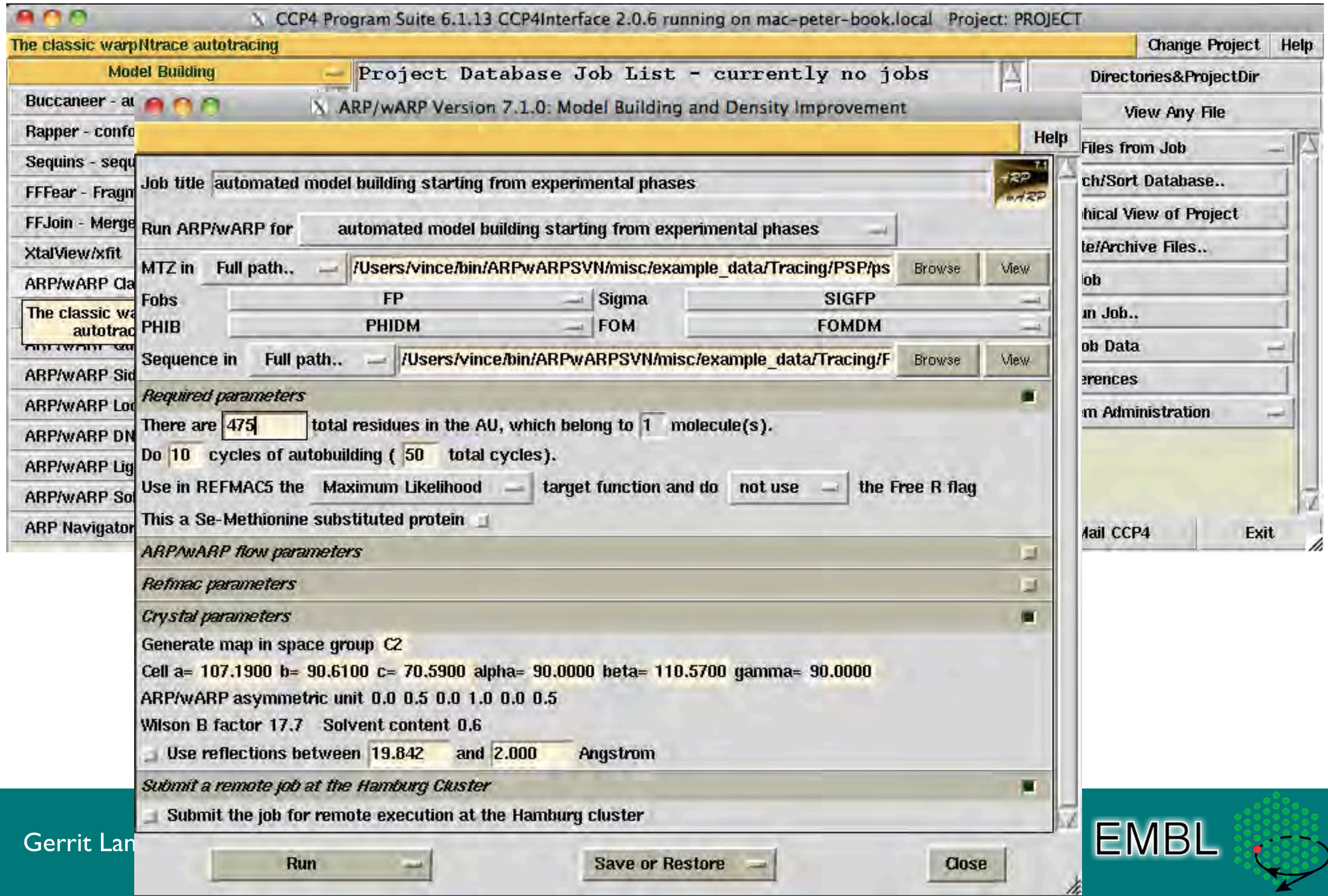

EMBL

ARP/wARP: Tracing (warp_tracing)

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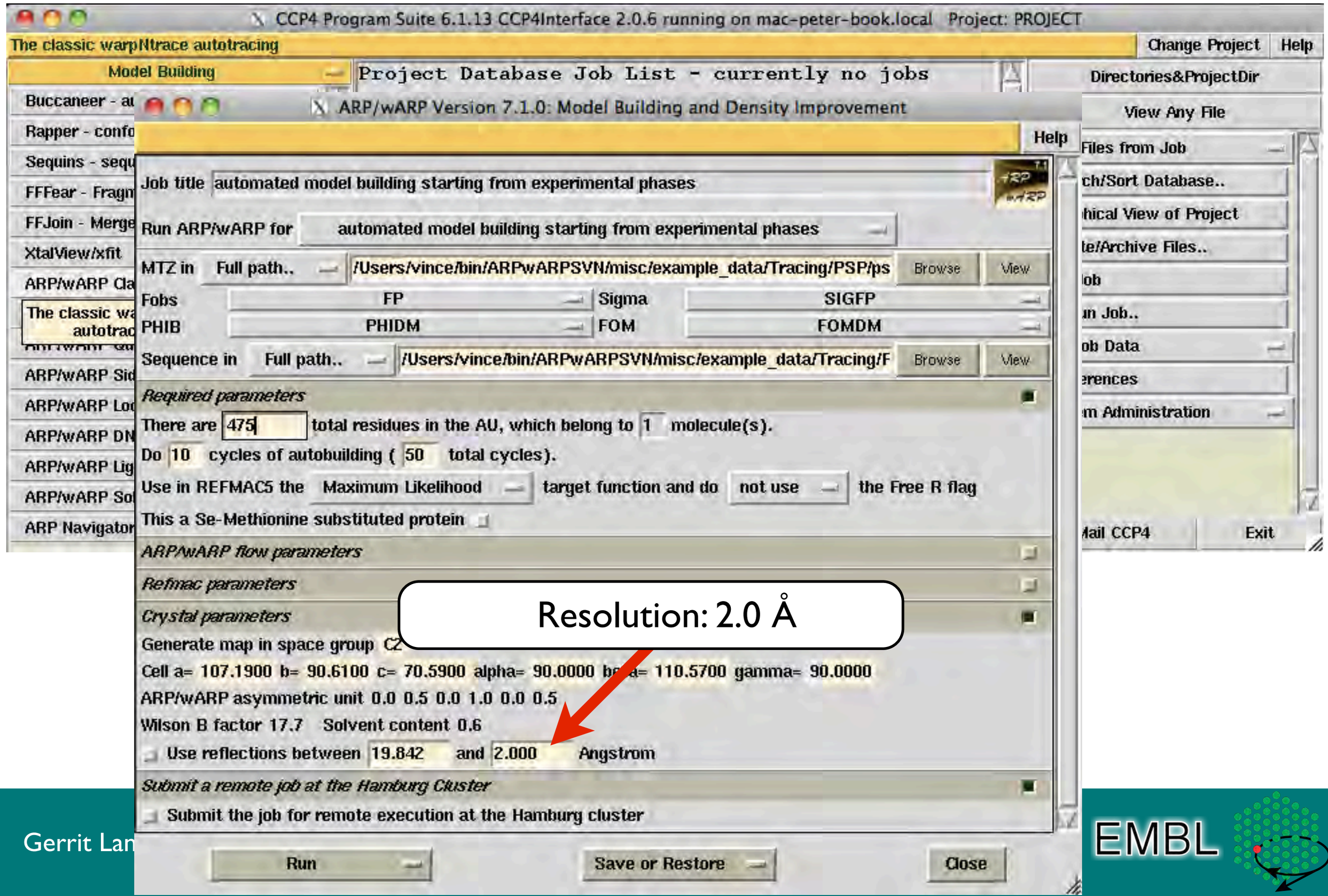

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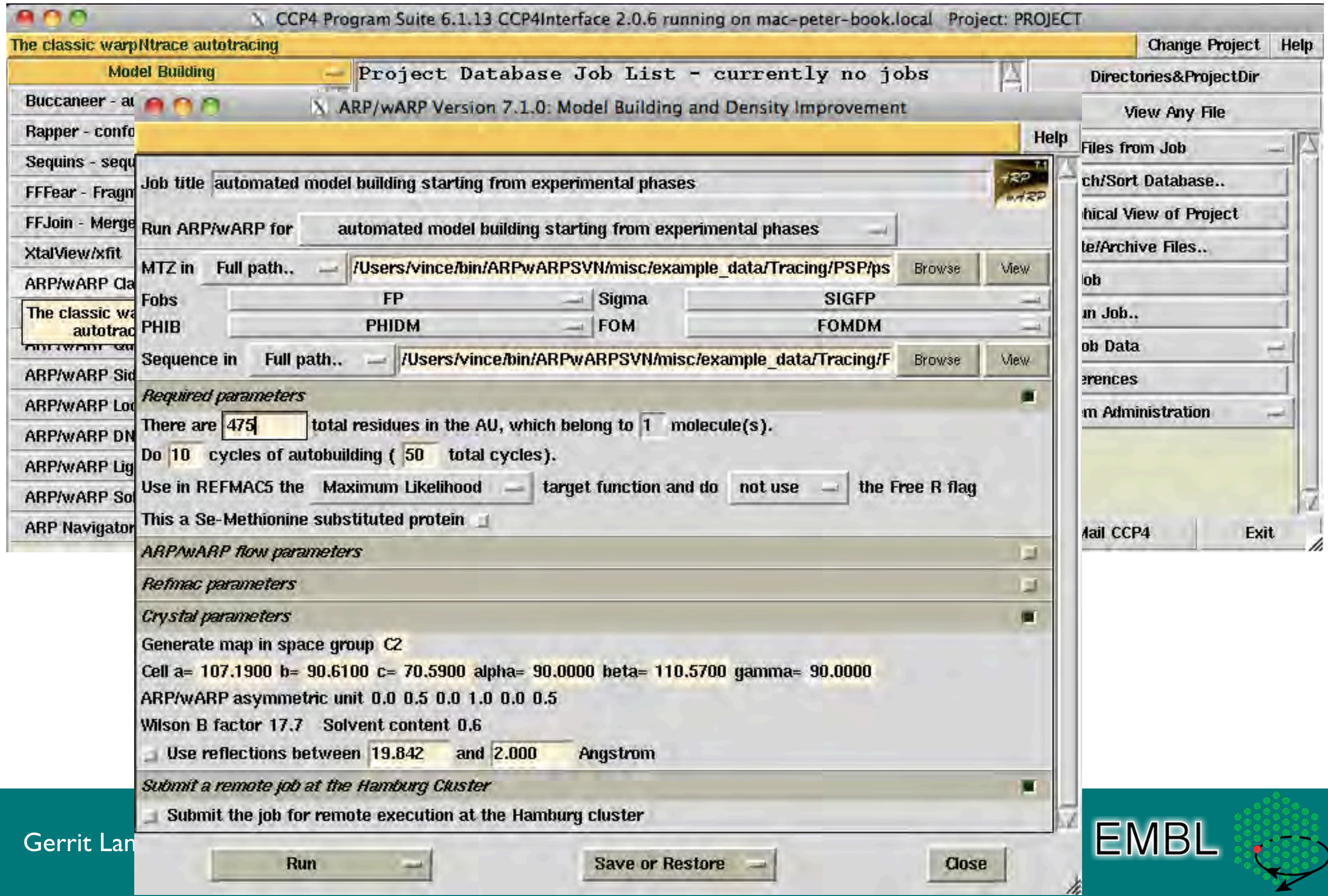

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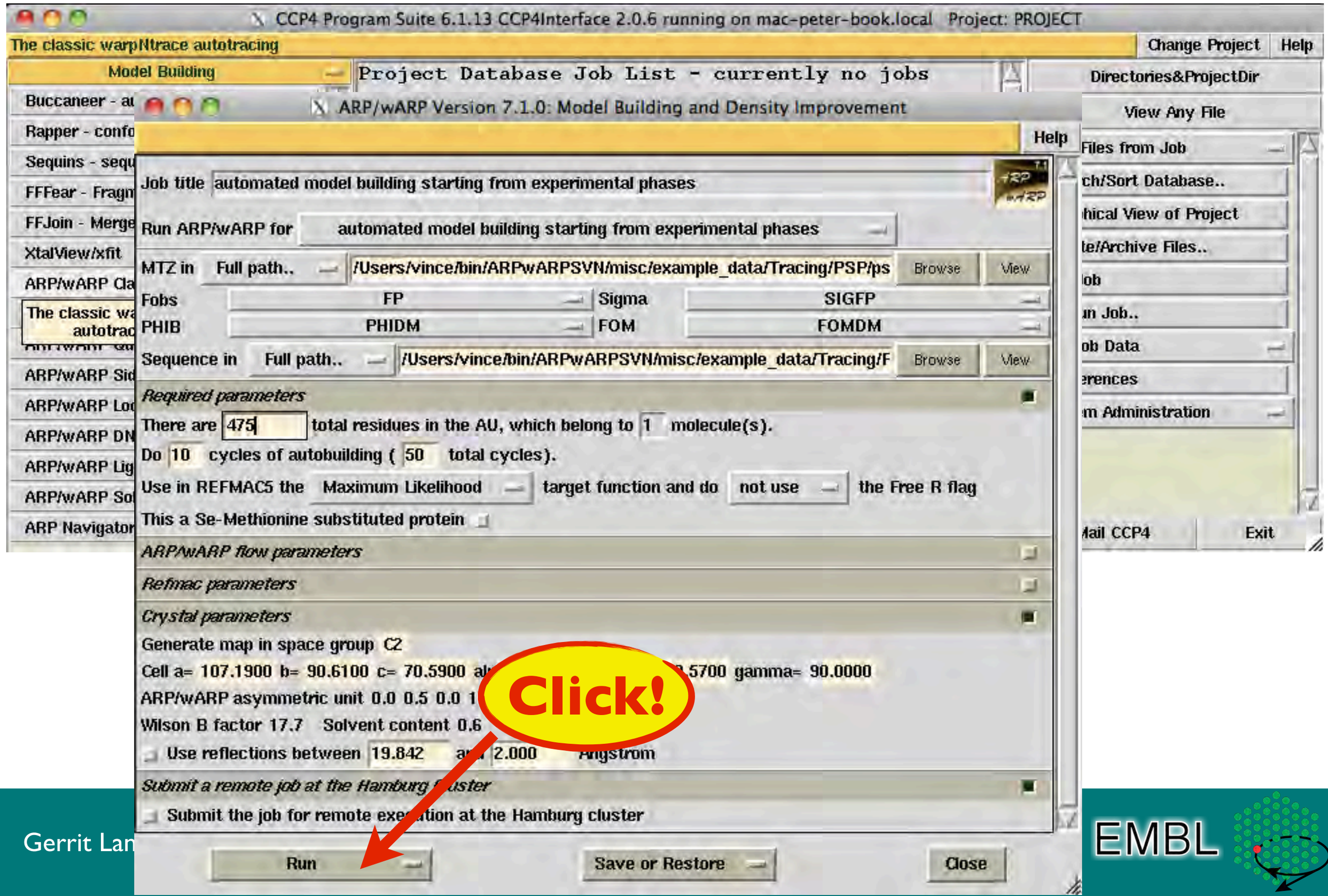
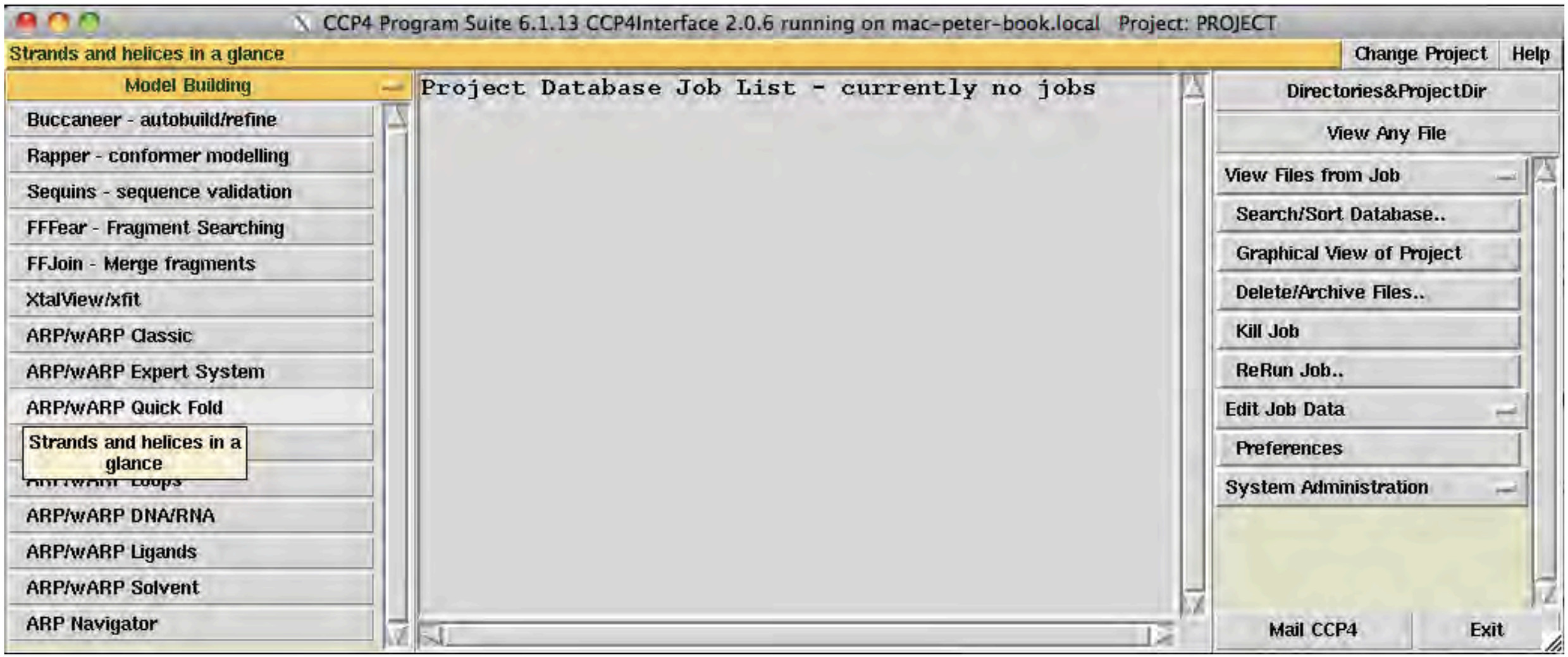


EMBL

ARP/wARP: Secondary Structure (albe)



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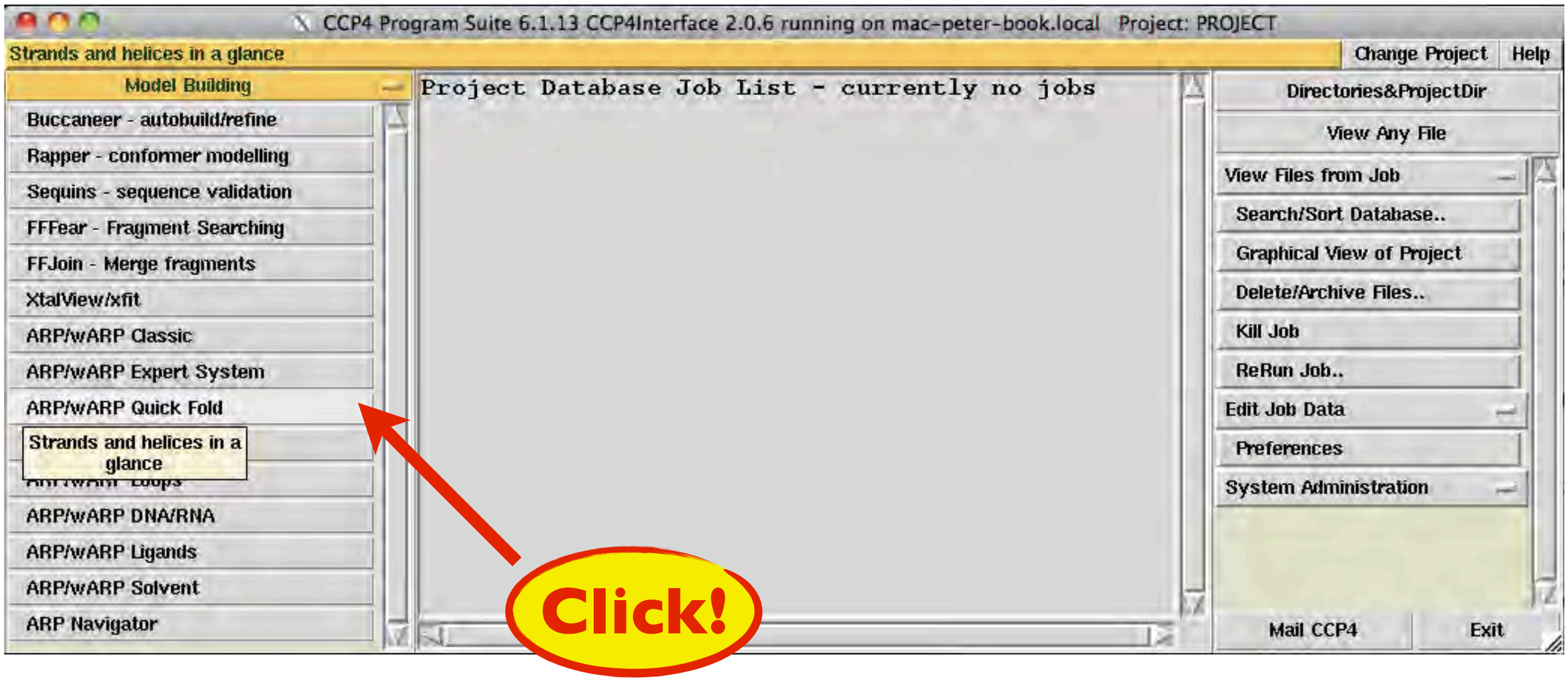

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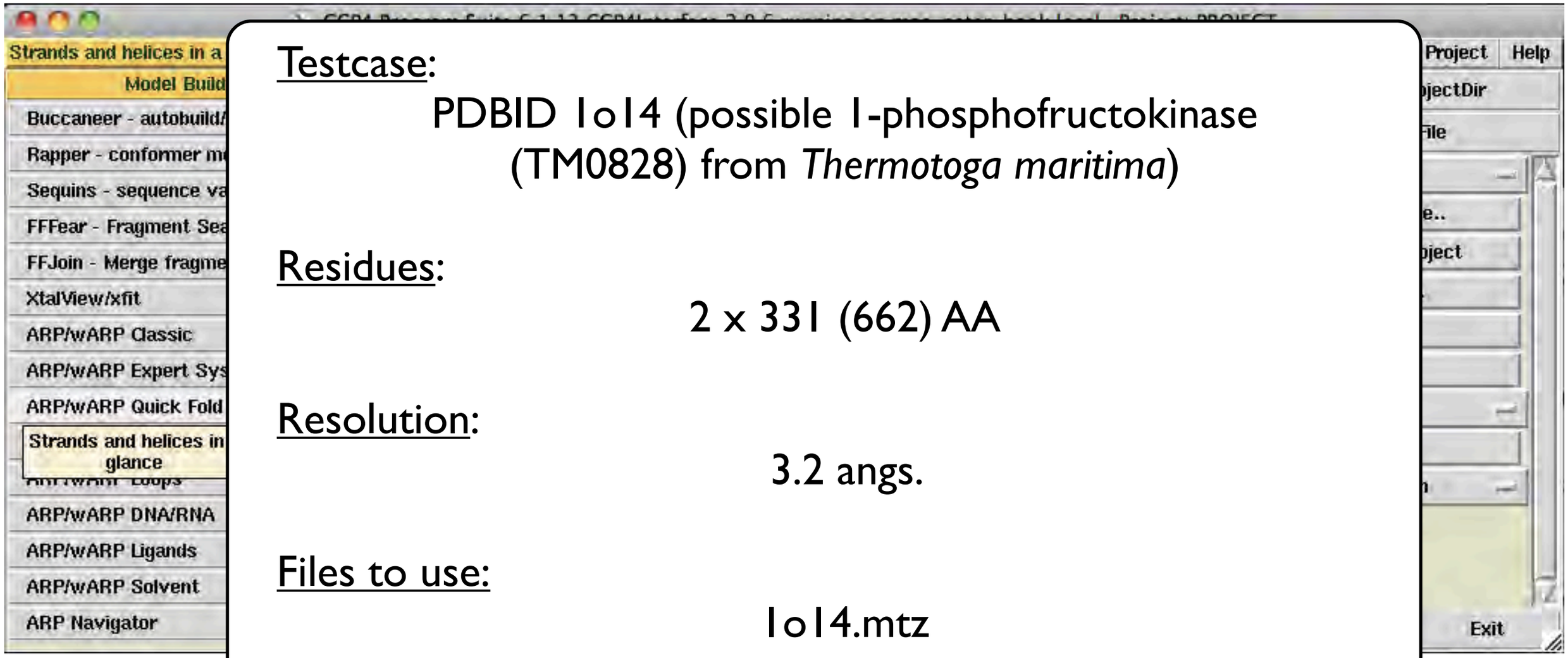


Testcase:

PDBID 1o14 (possible 1-phosphofructokinase (TM0828) from *Thermotoga maritima*)

Residues:

2 x 331 (662) AA

Resolution:

3.2 angs.

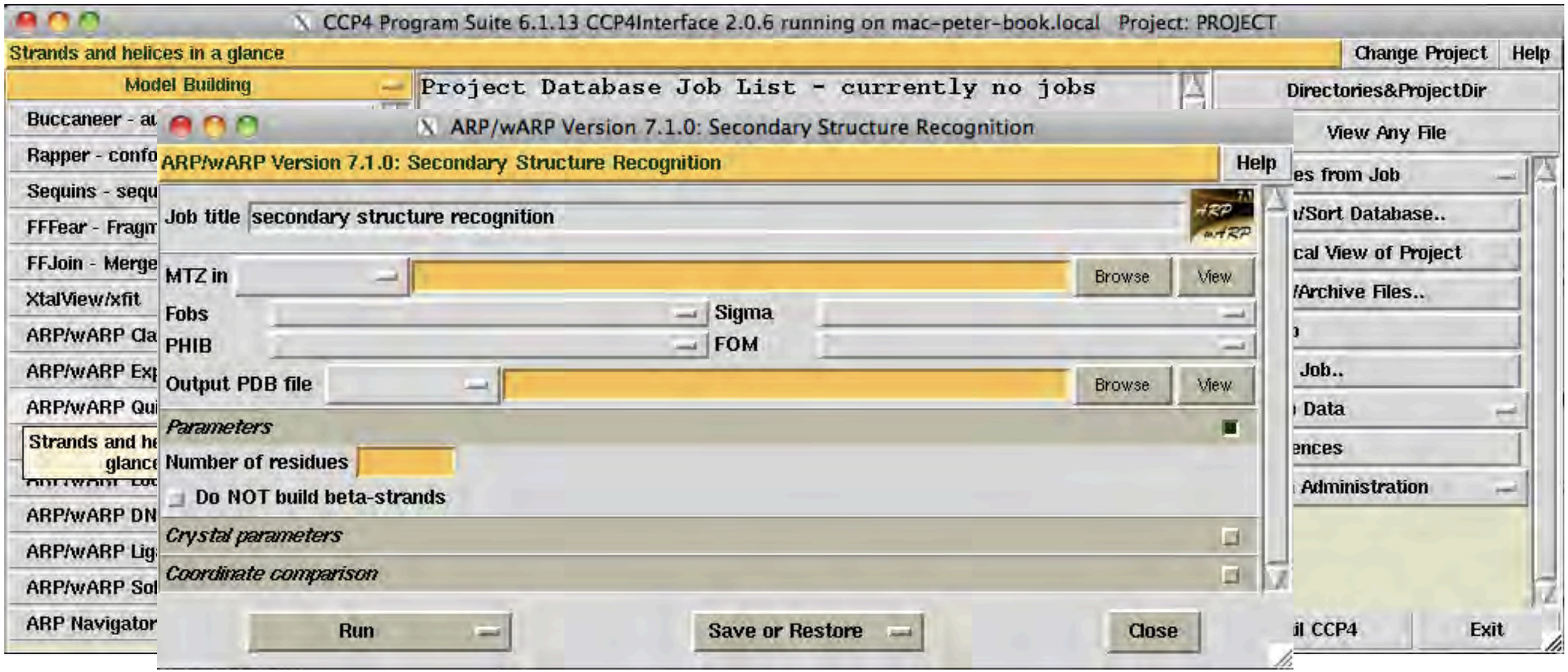
Files to use:

1o14.mtz

MTS labels to use:

F, PHIC, FOM

ARP/wARP: Secondary Structure (albe)



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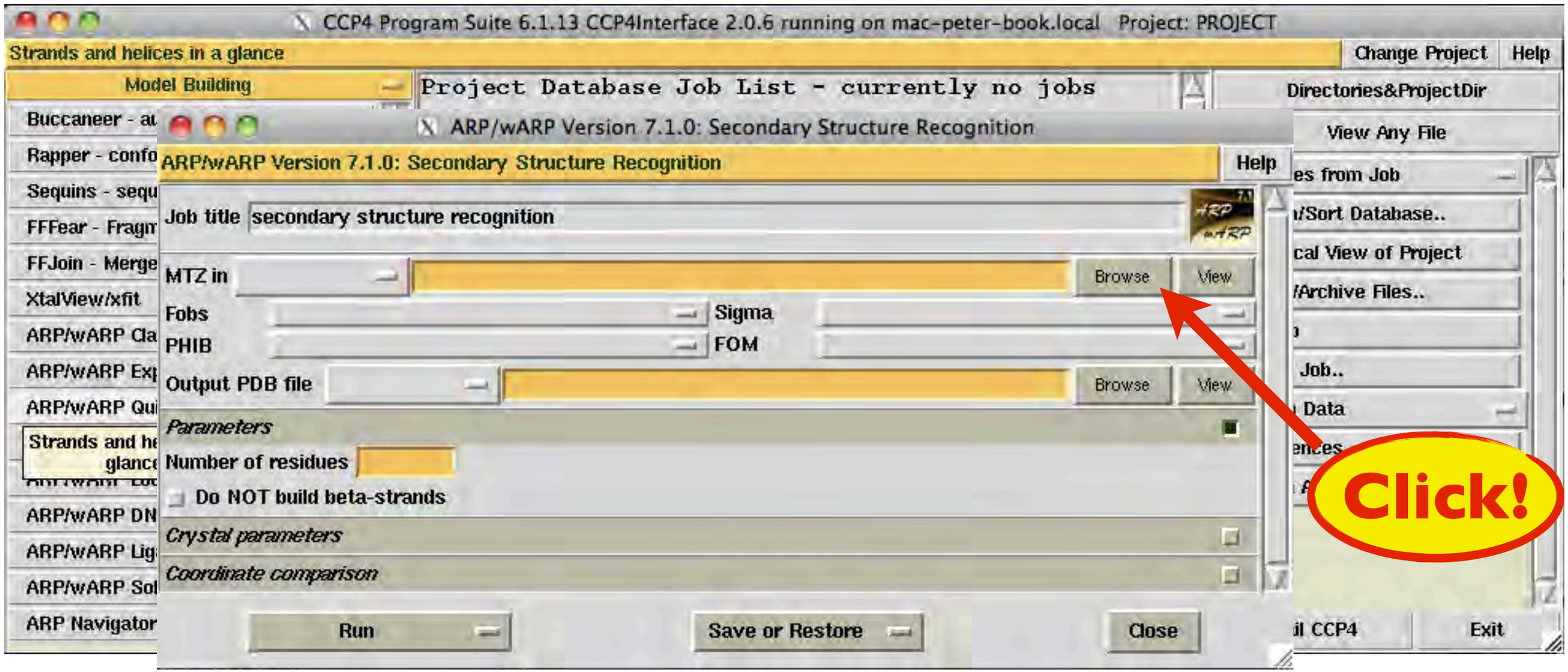

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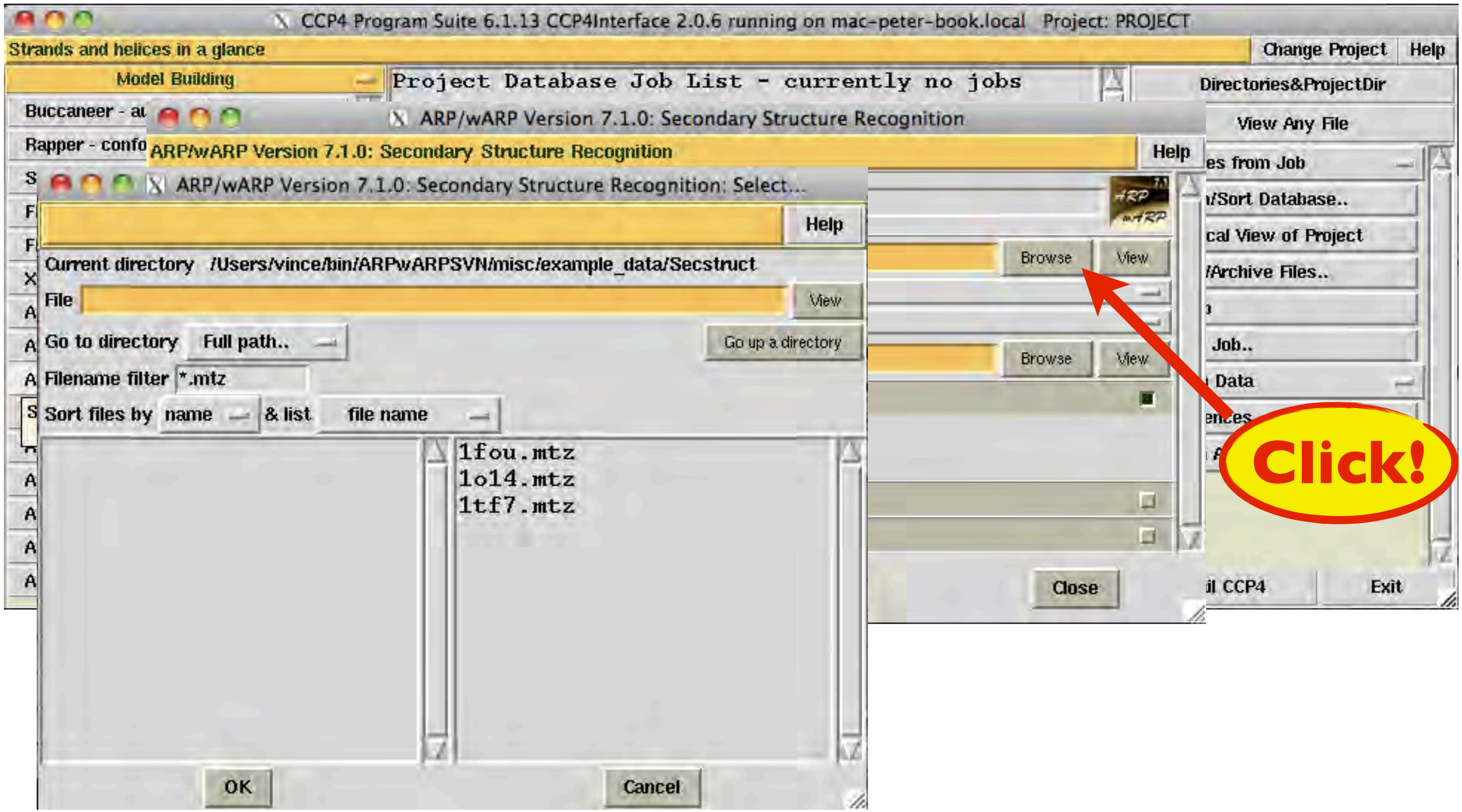

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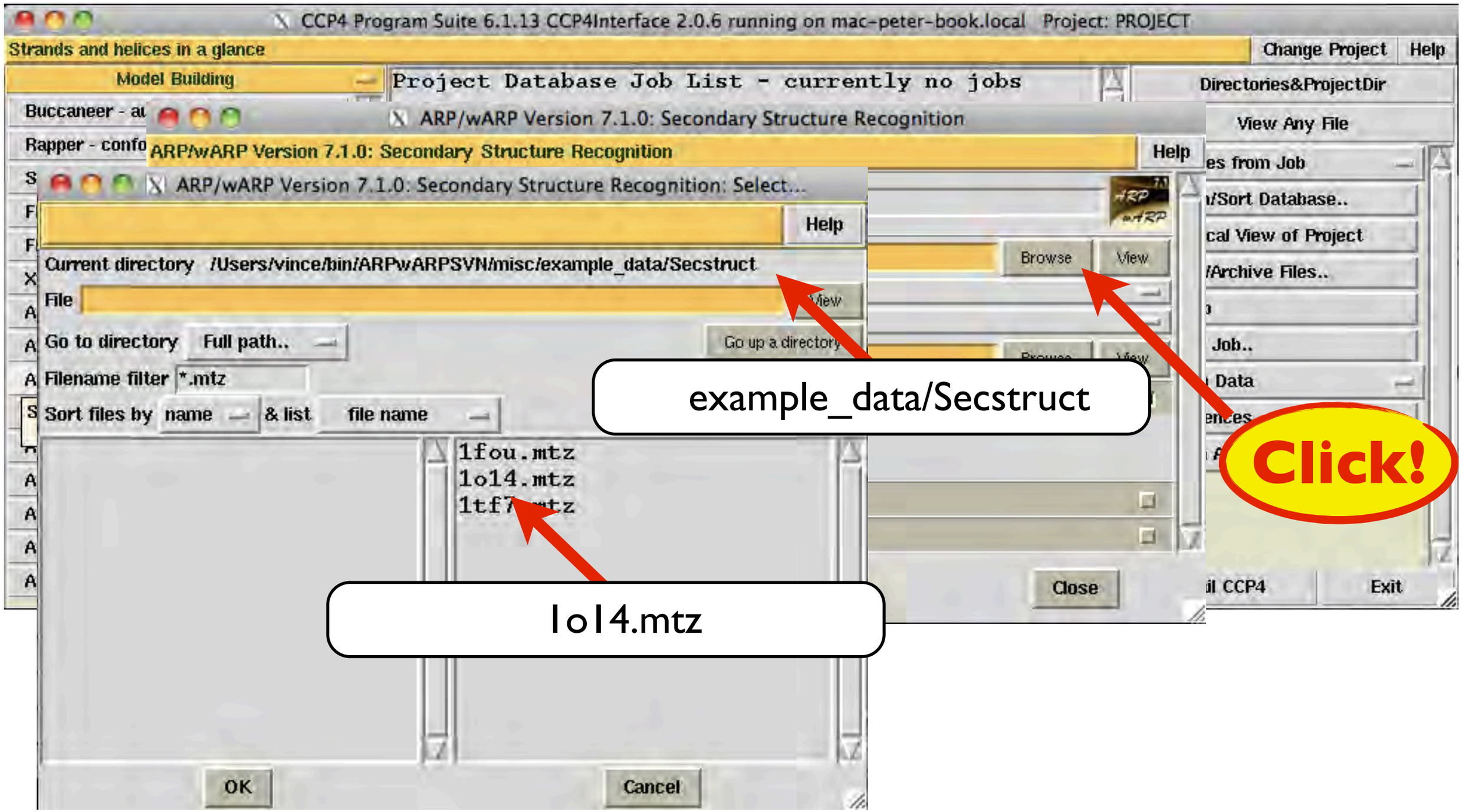

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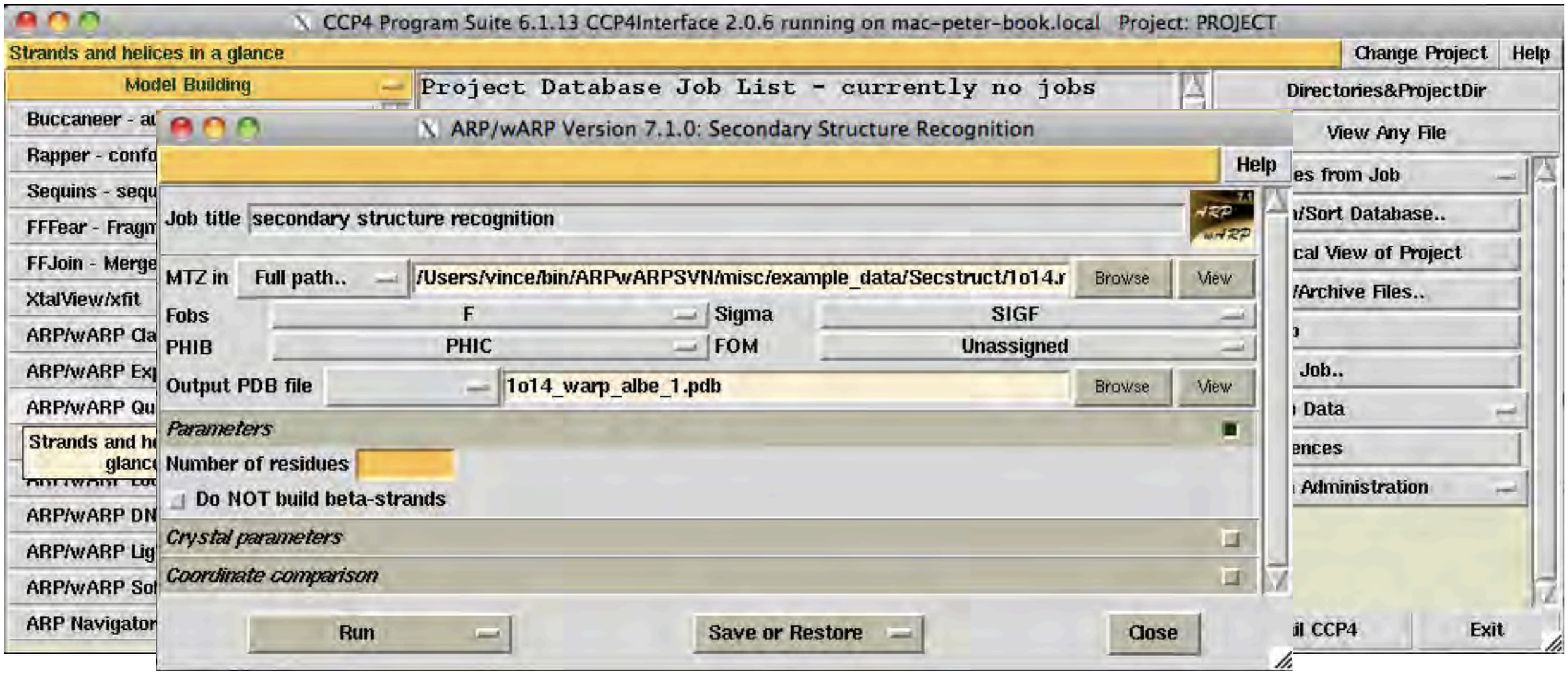

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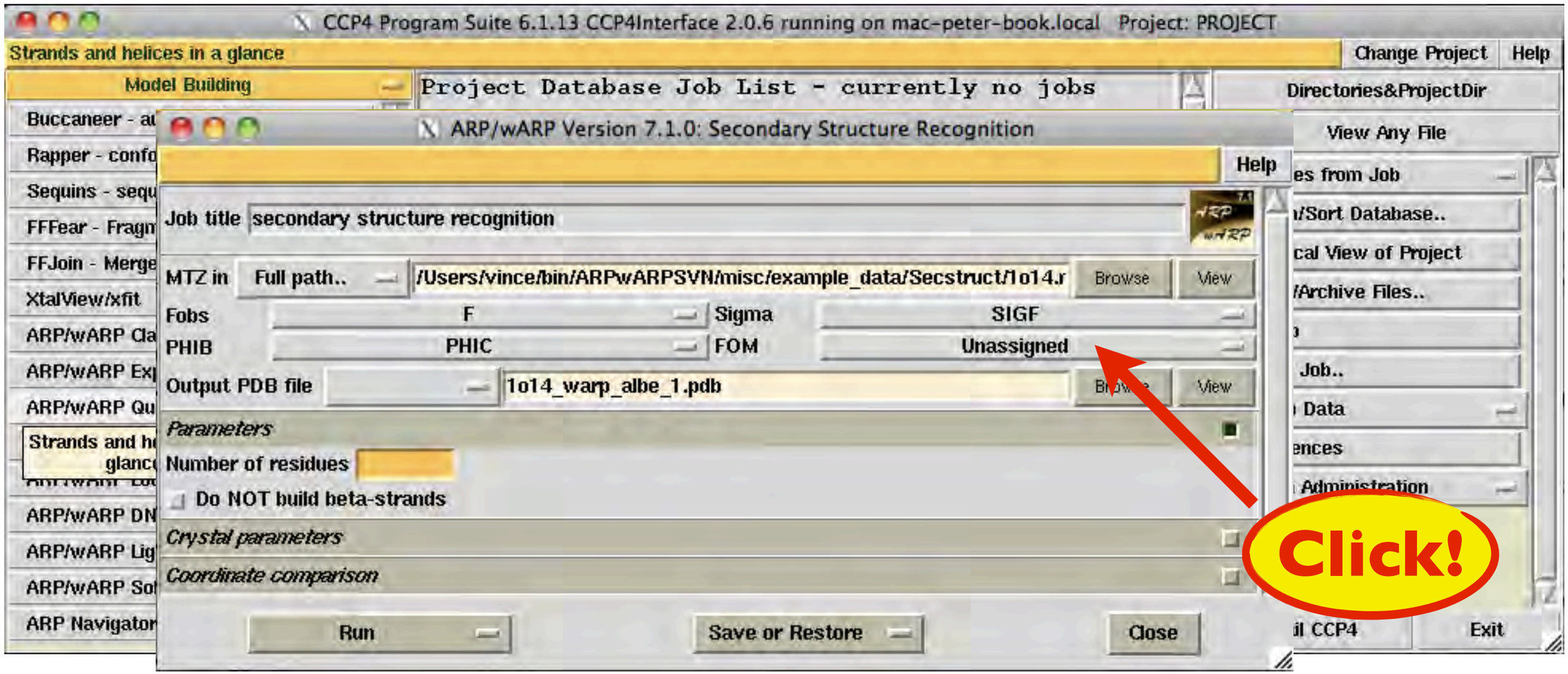

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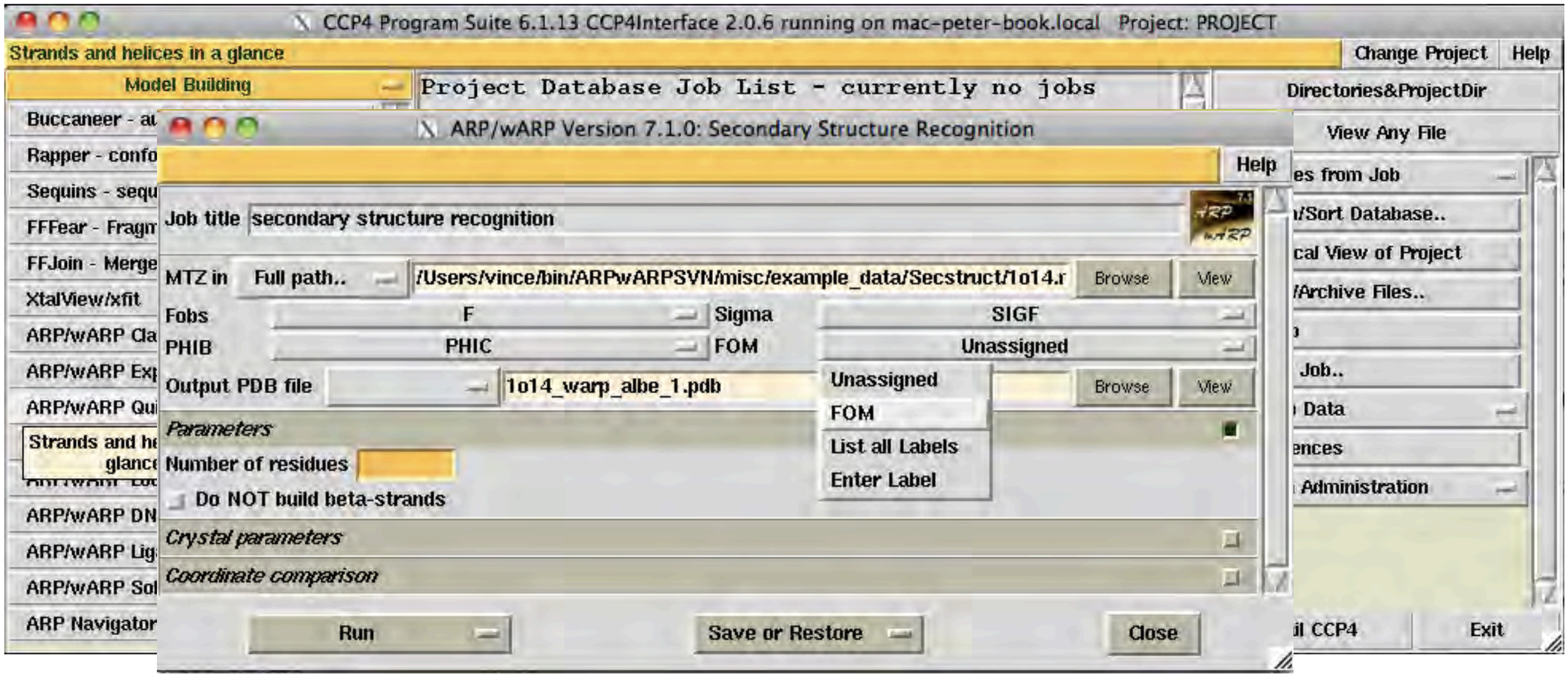

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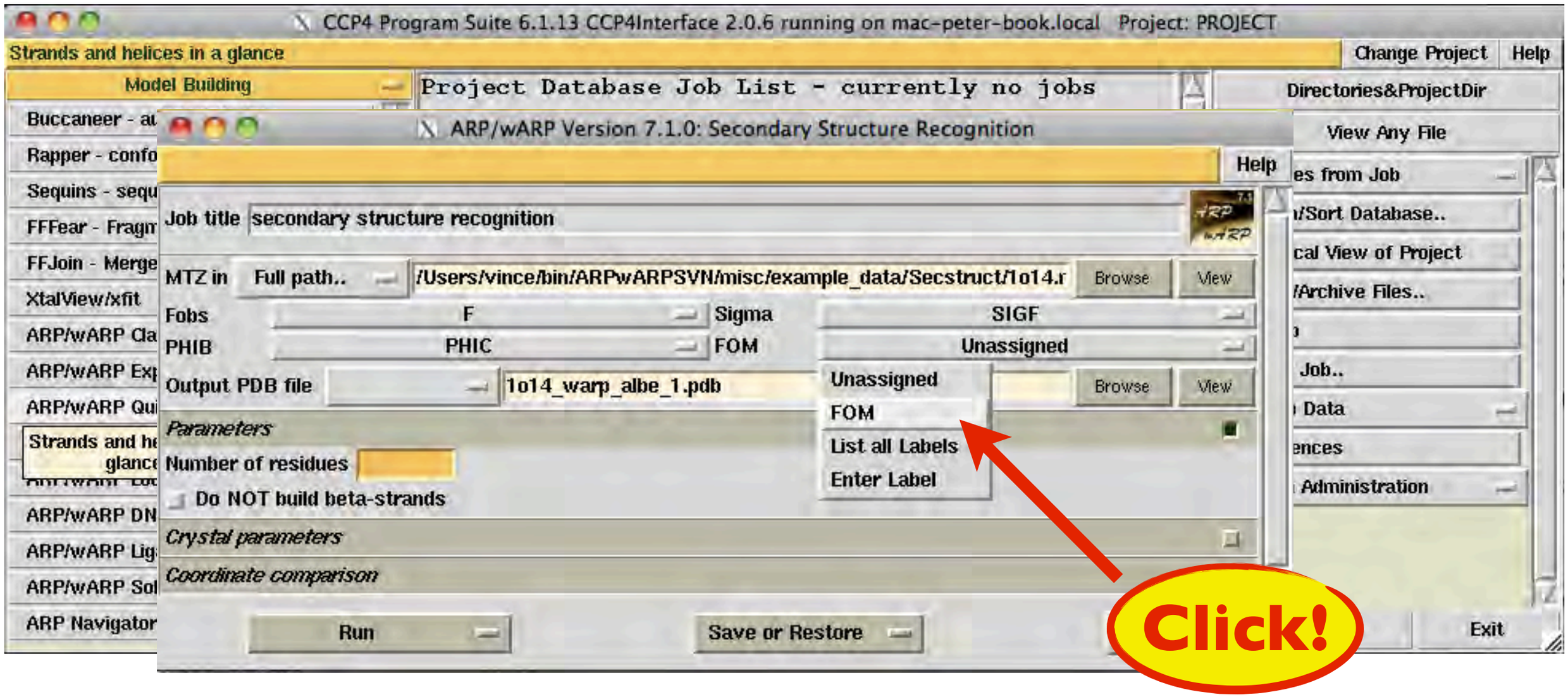

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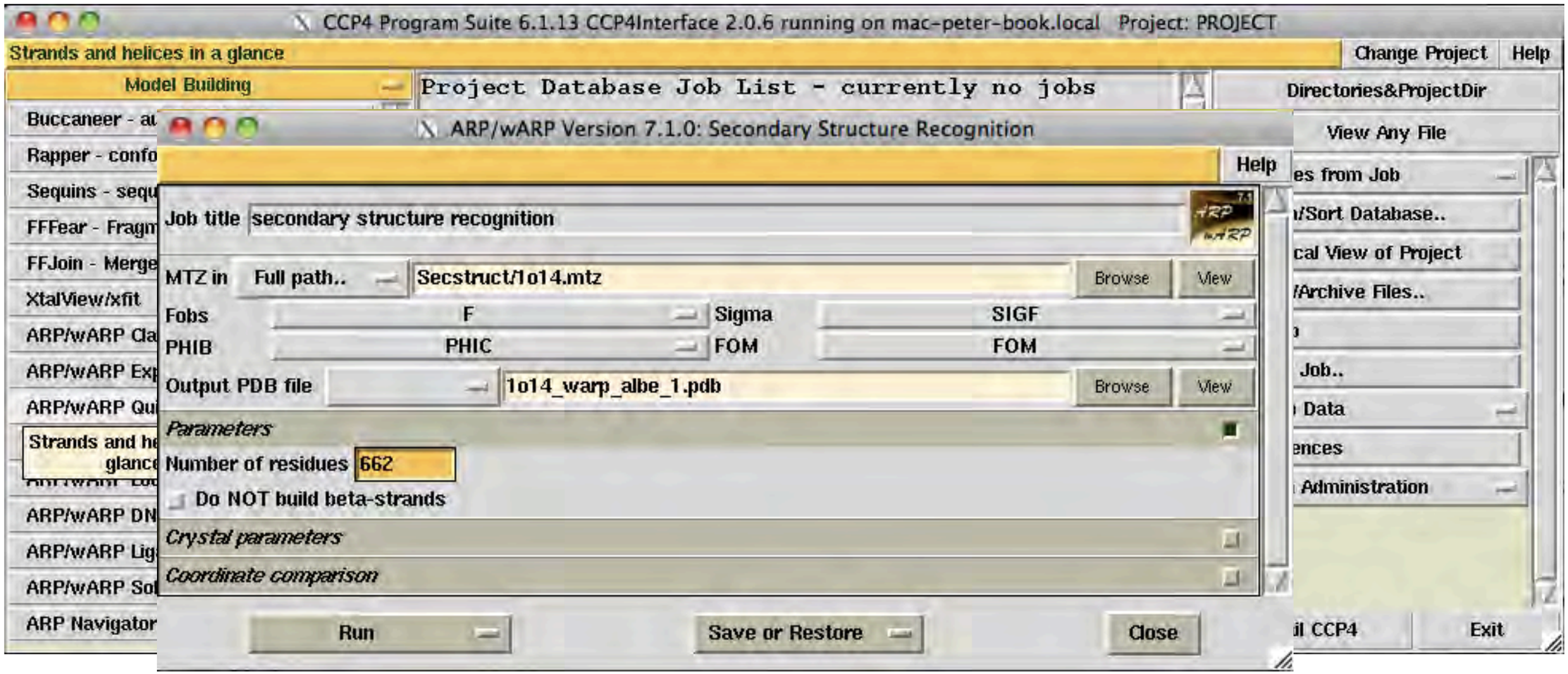

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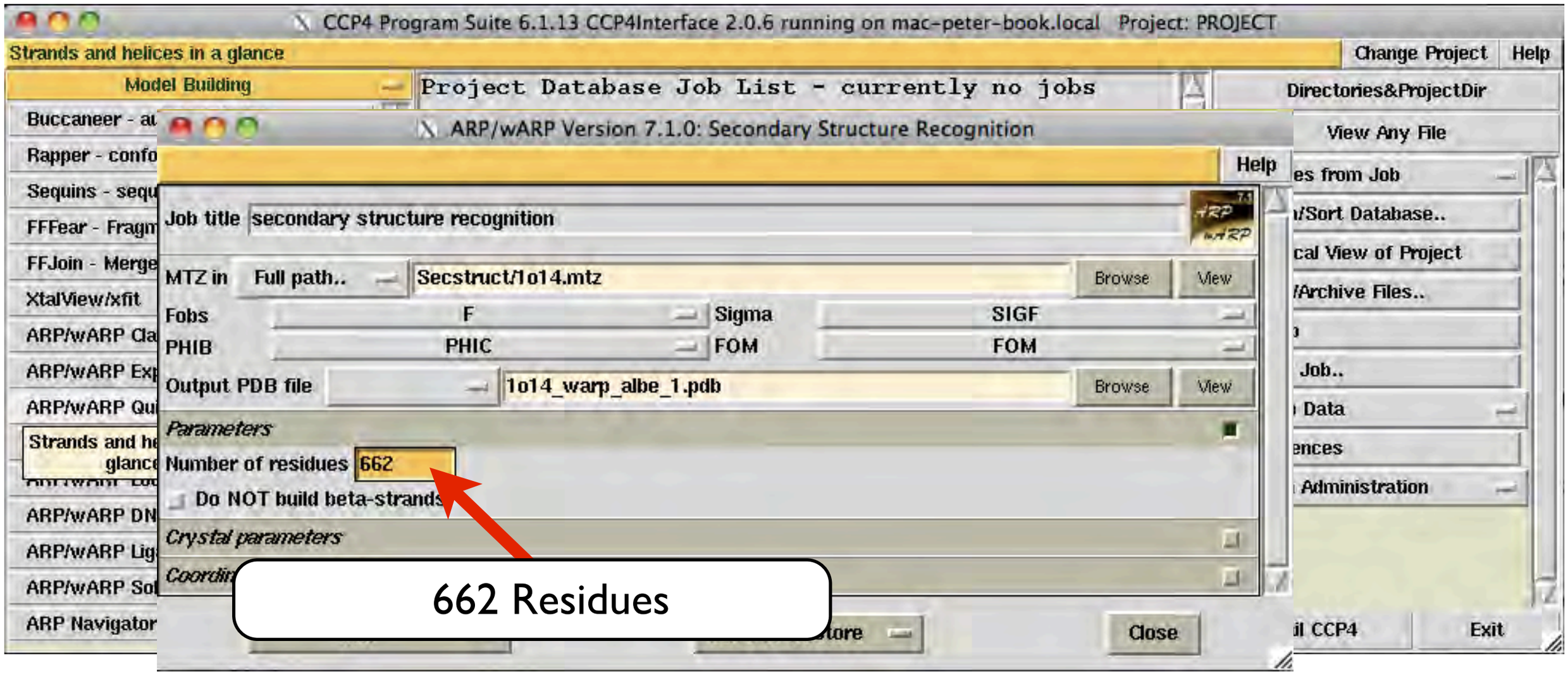

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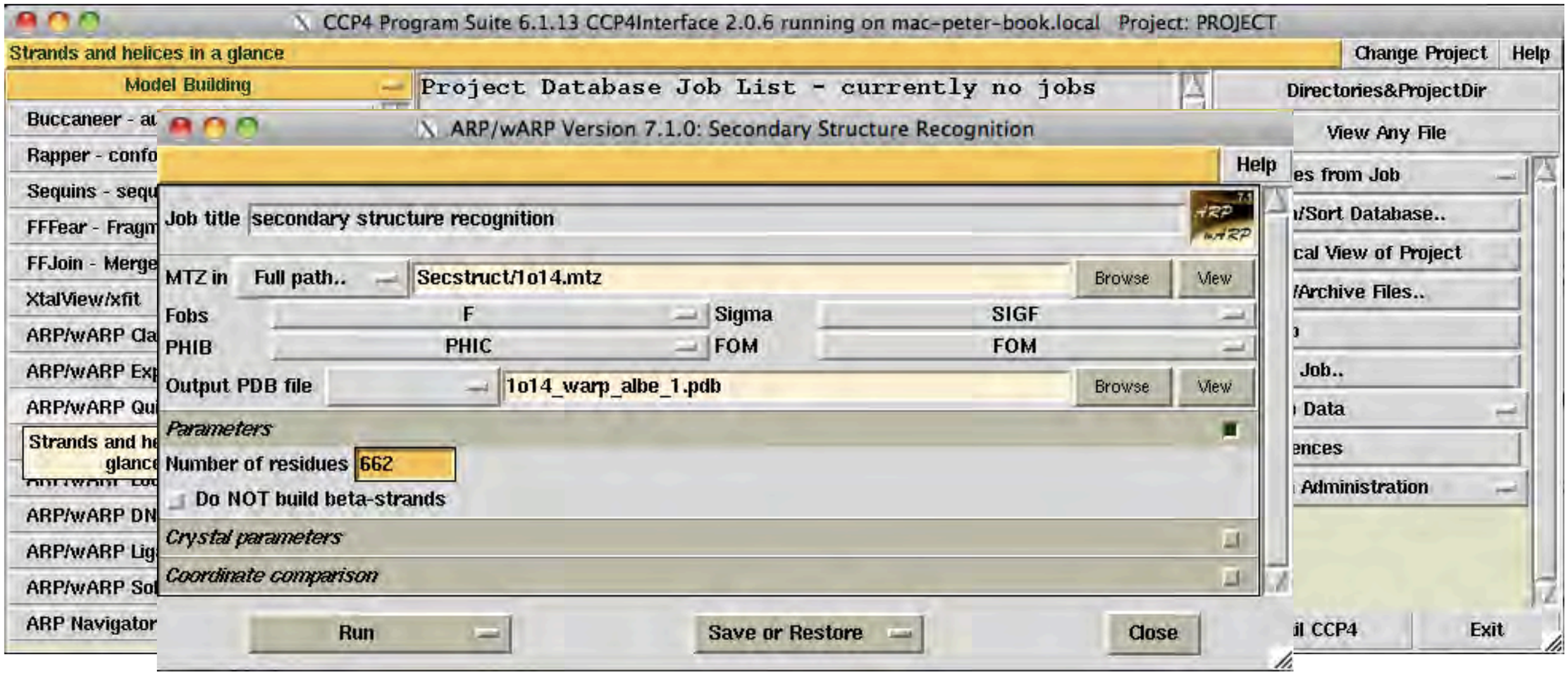

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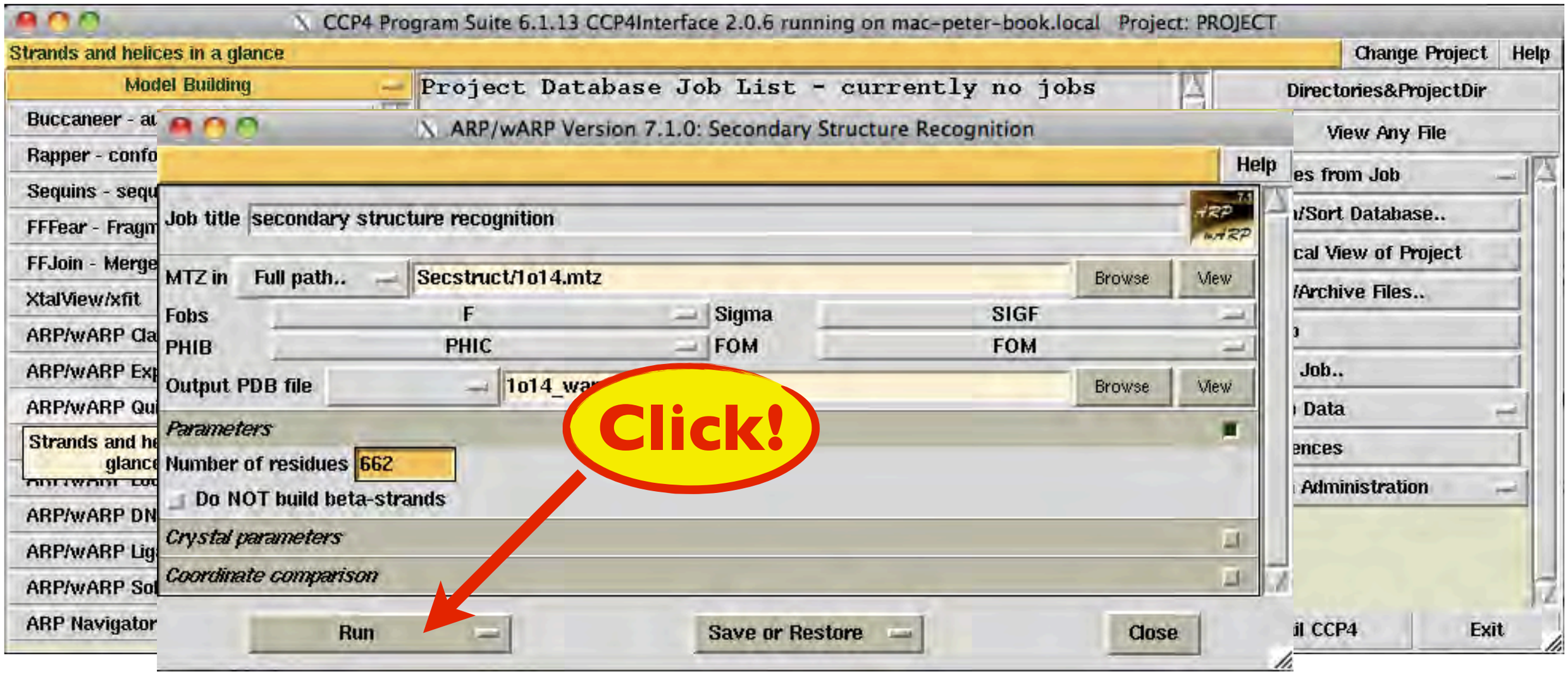
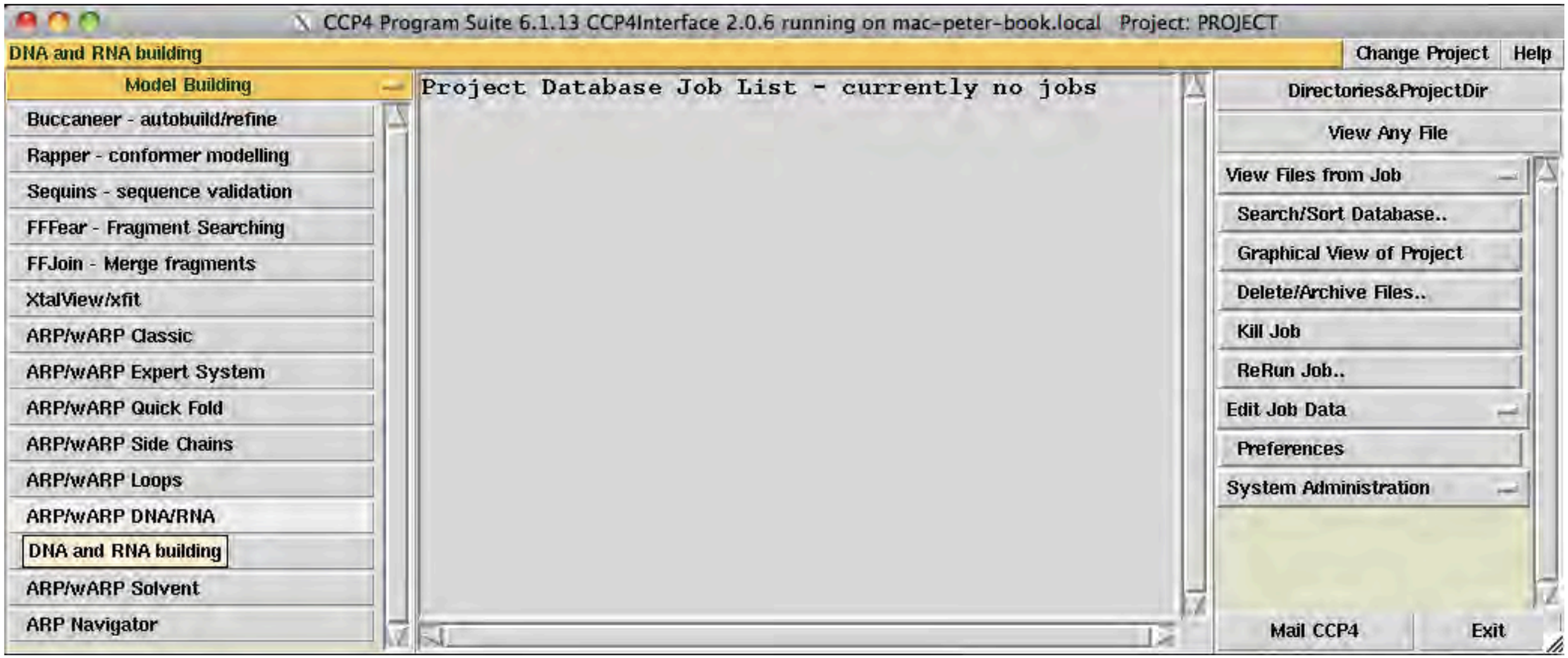


ARP/wARP: Nucleotide Building (nuce)

1e3m



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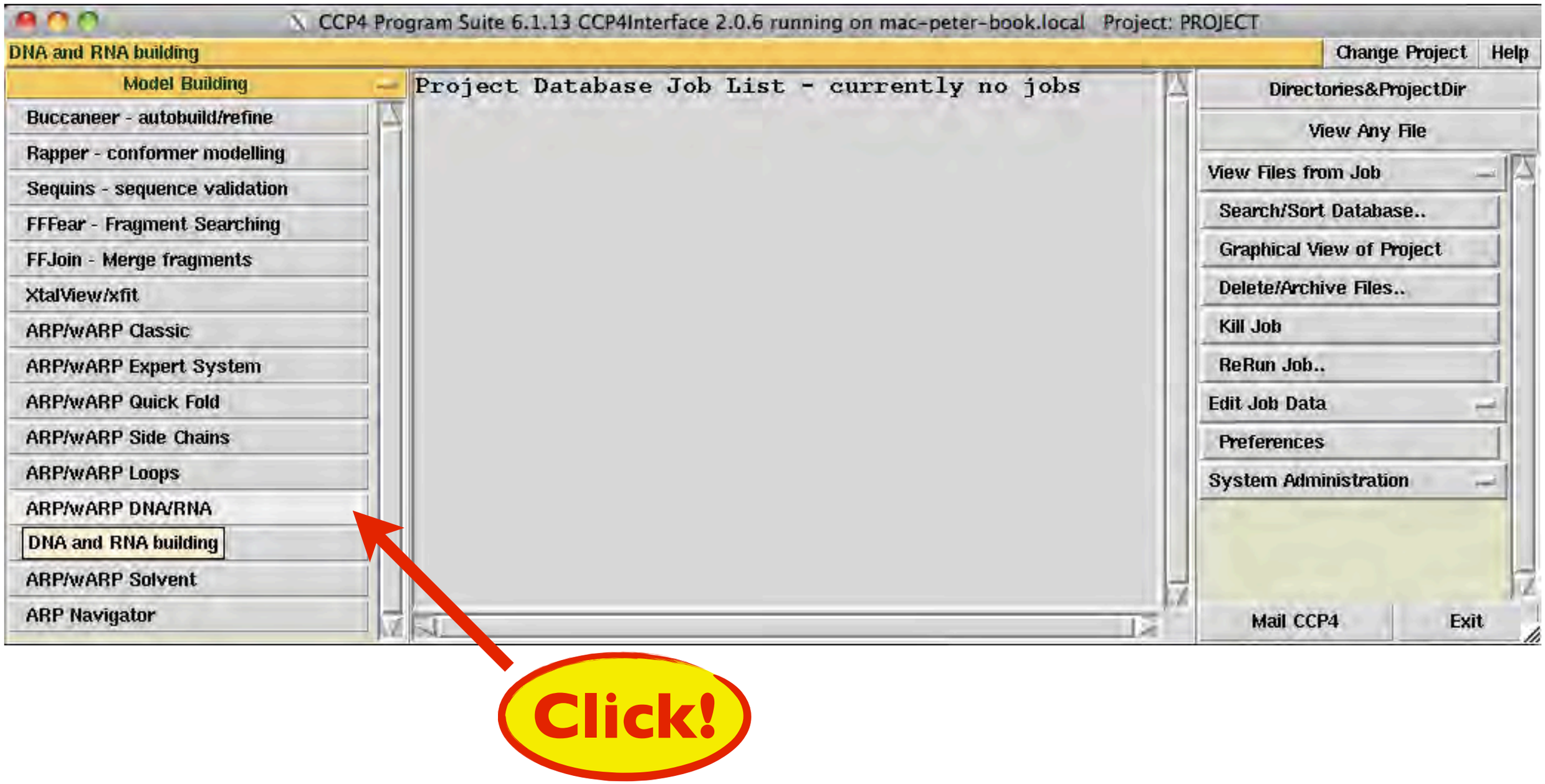

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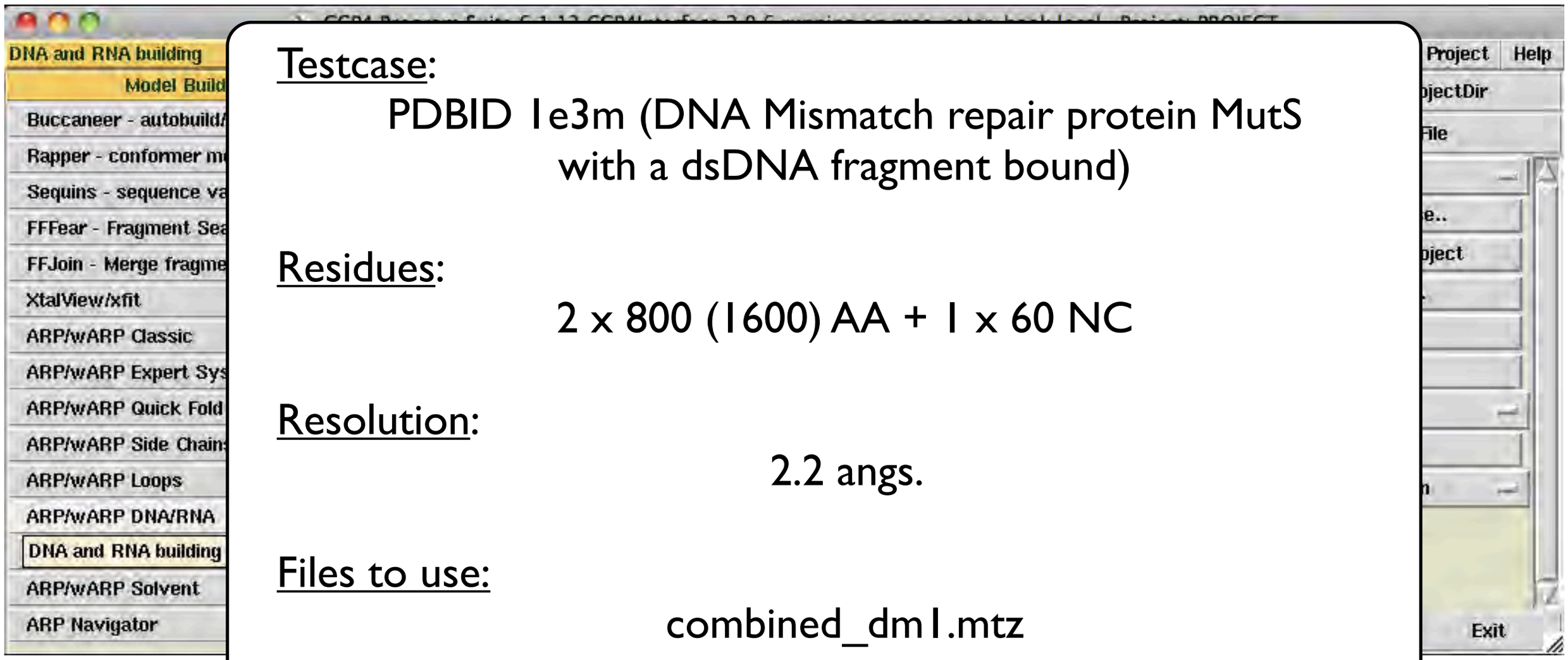


Testcase:

PDBID 1e3m (DNA Mismatch repair protein MutS with a dsDNA fragment bound)

Residues:

2 x 800 (1600) AA + 1 x 60 NC

Resolution:

2.2 angs.

Files to use:

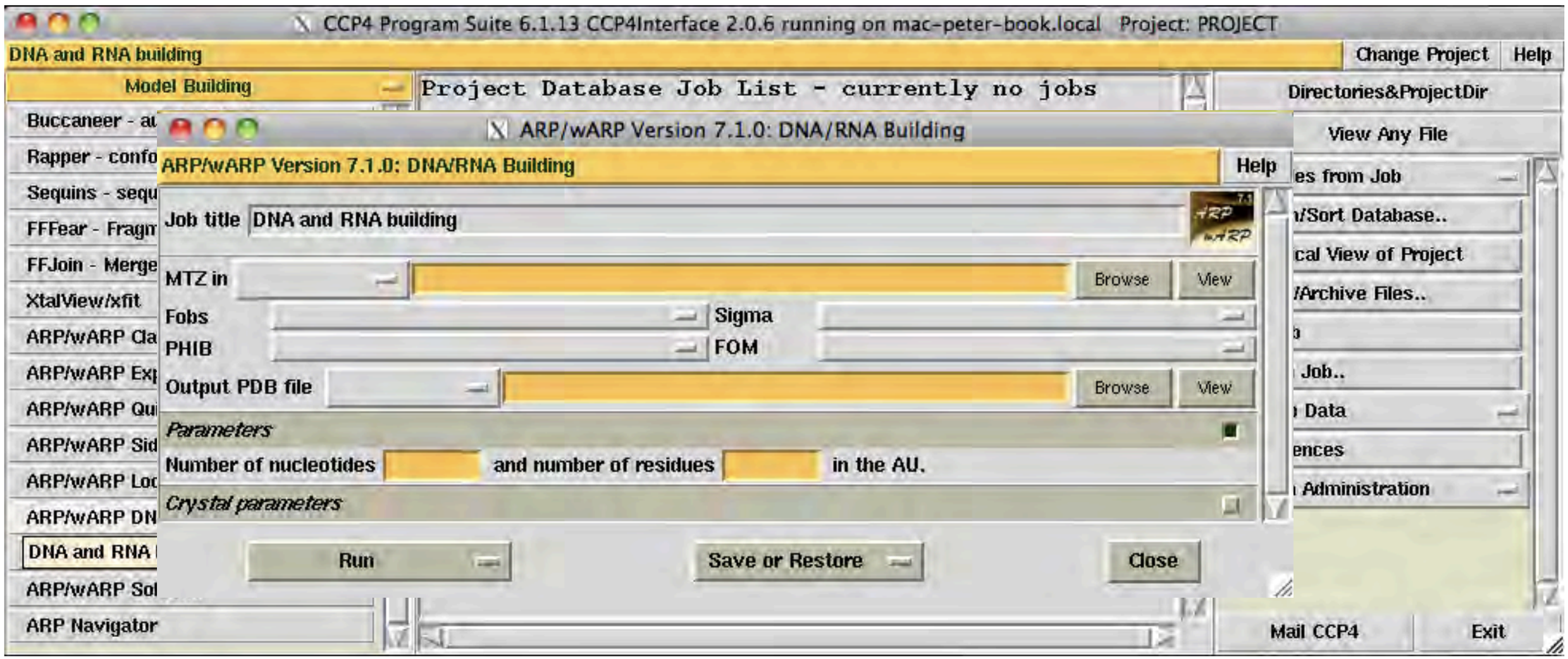
combined_dm1.mtz

MTS labels to use:

F_eh2nm, SIGF_eh2nm, PHIDM, FOMDM

ARP/wARP: Nucleotide Building (nuce)

1e3m



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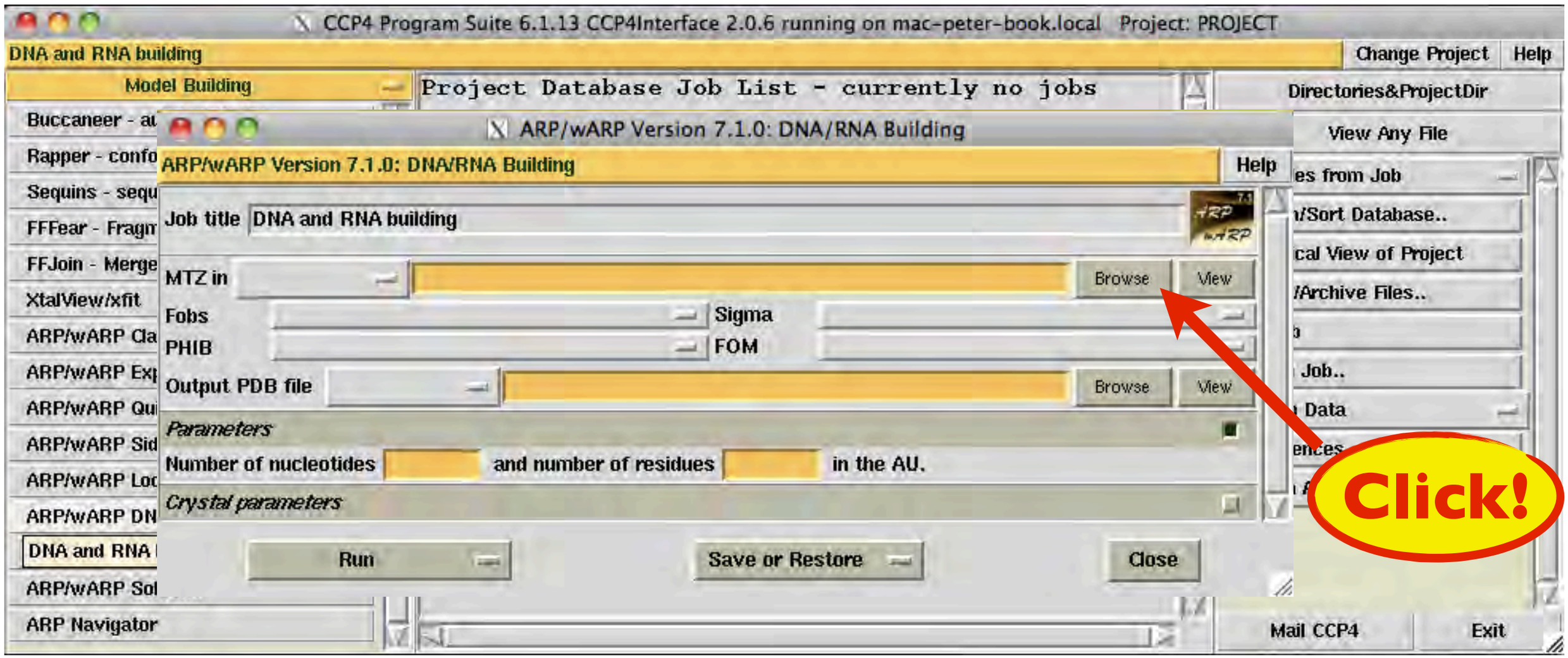

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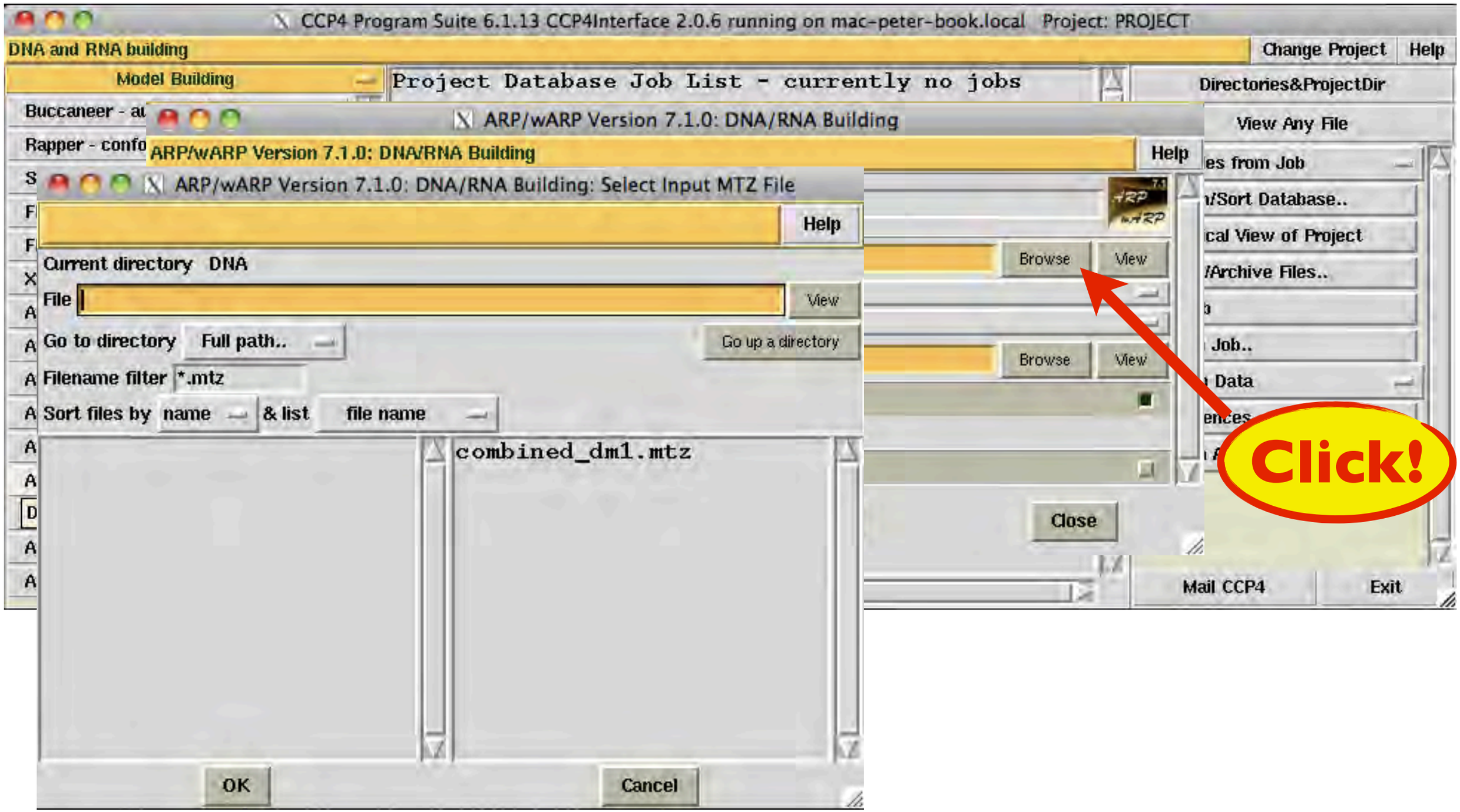

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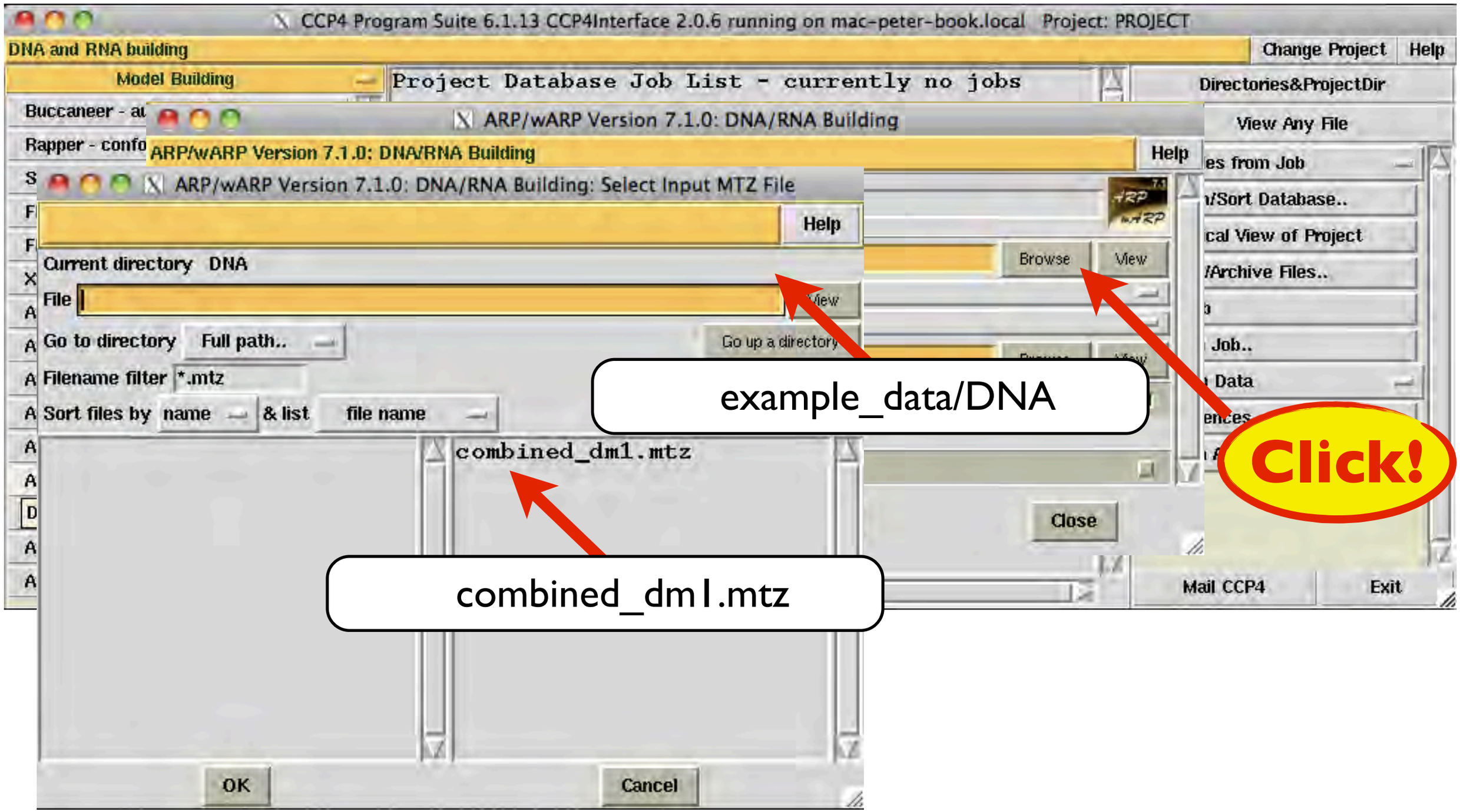

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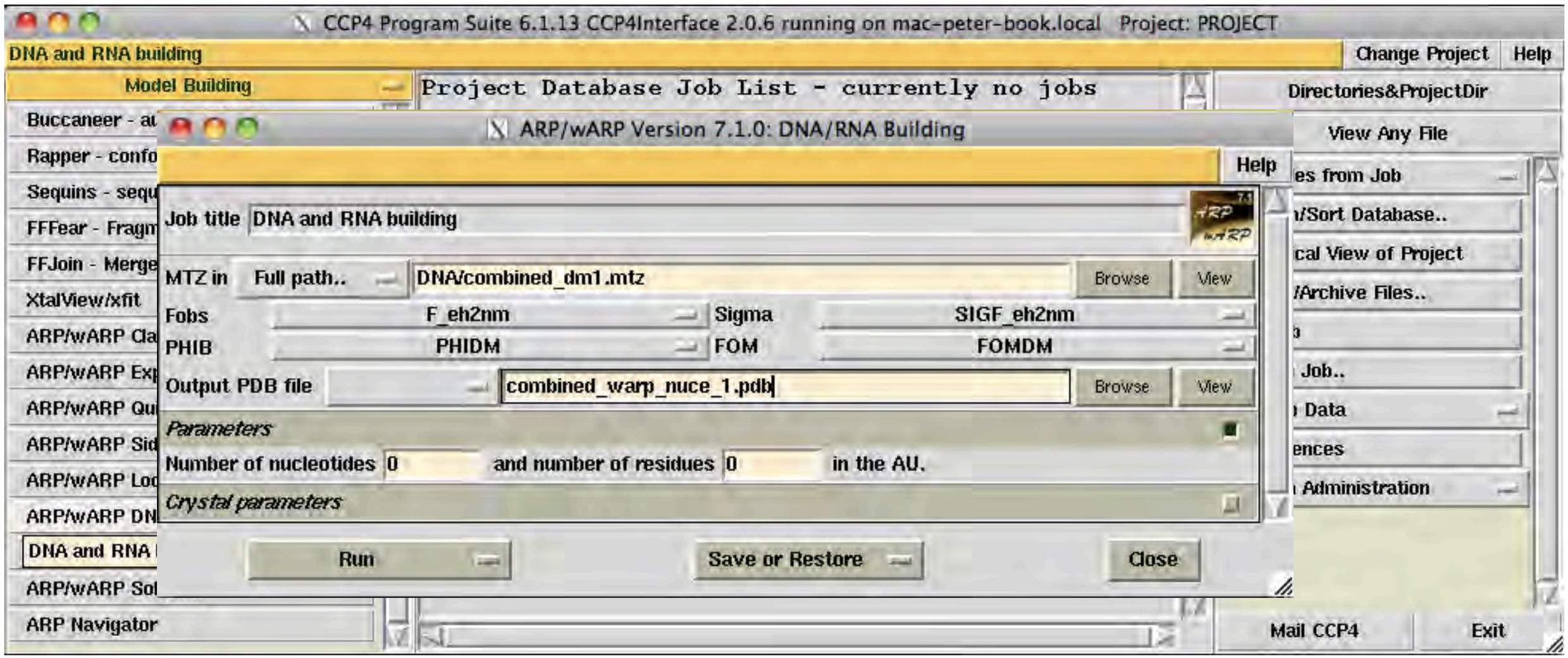

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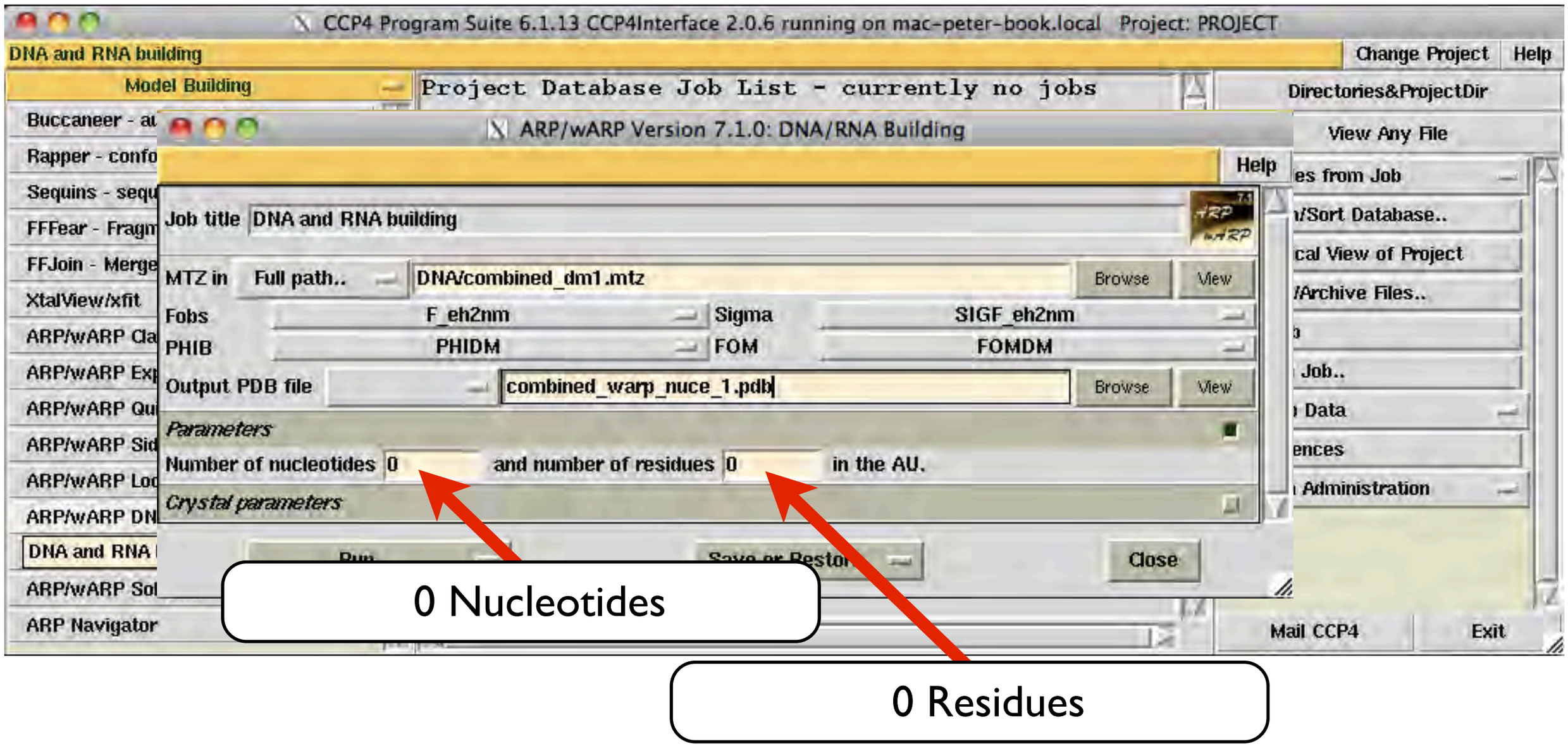

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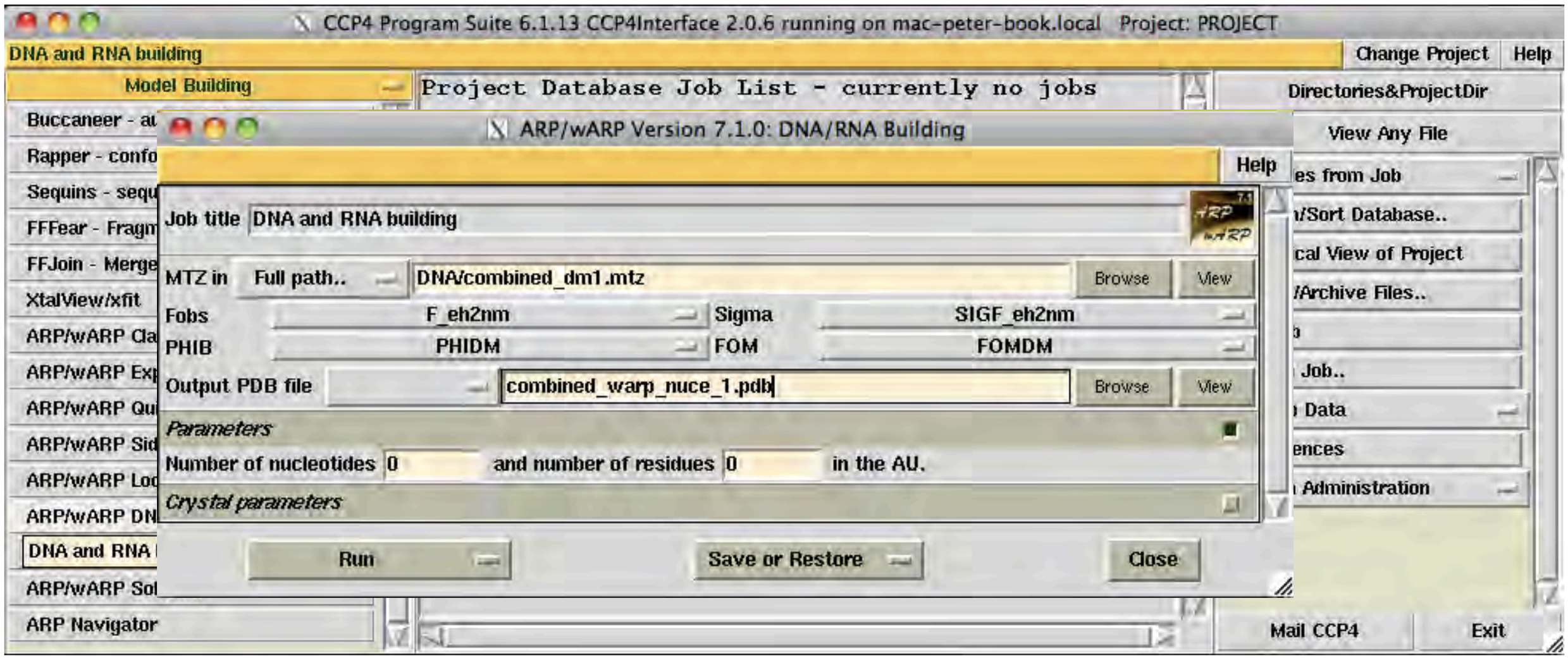

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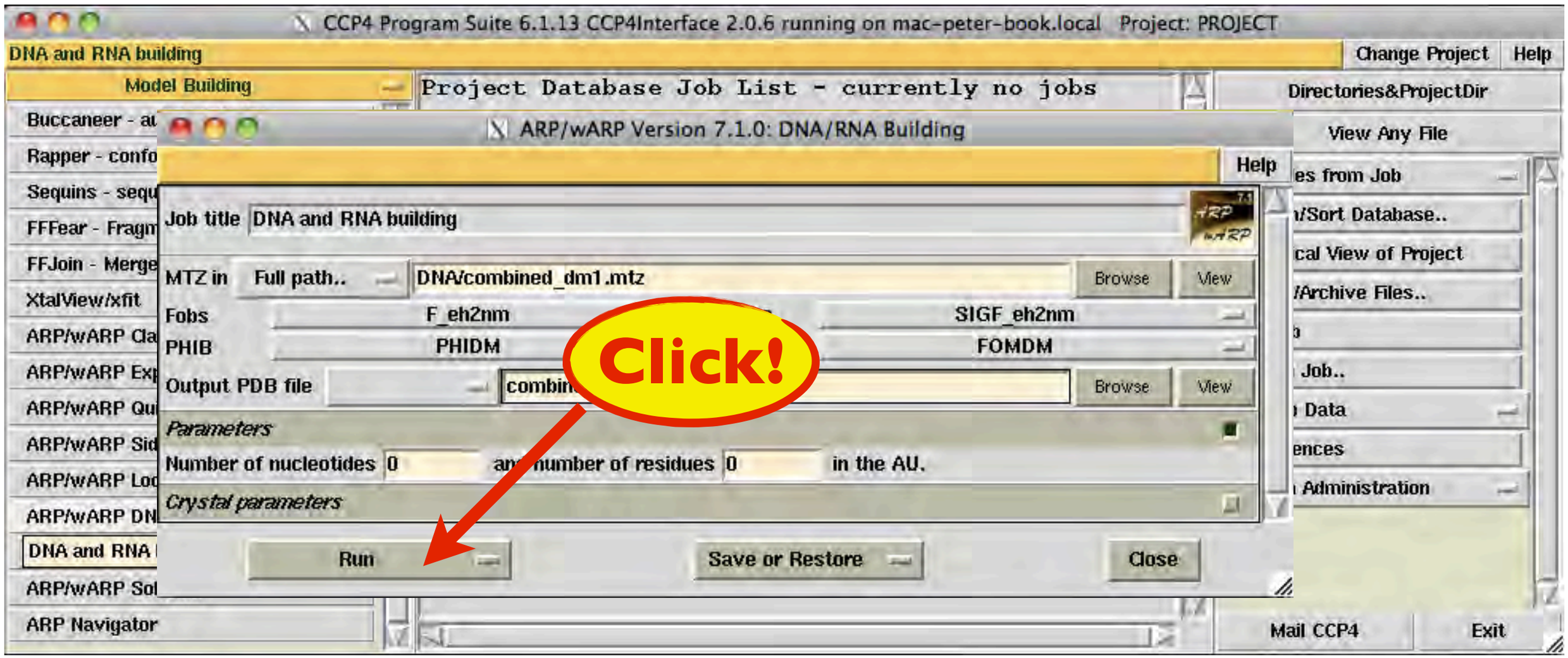

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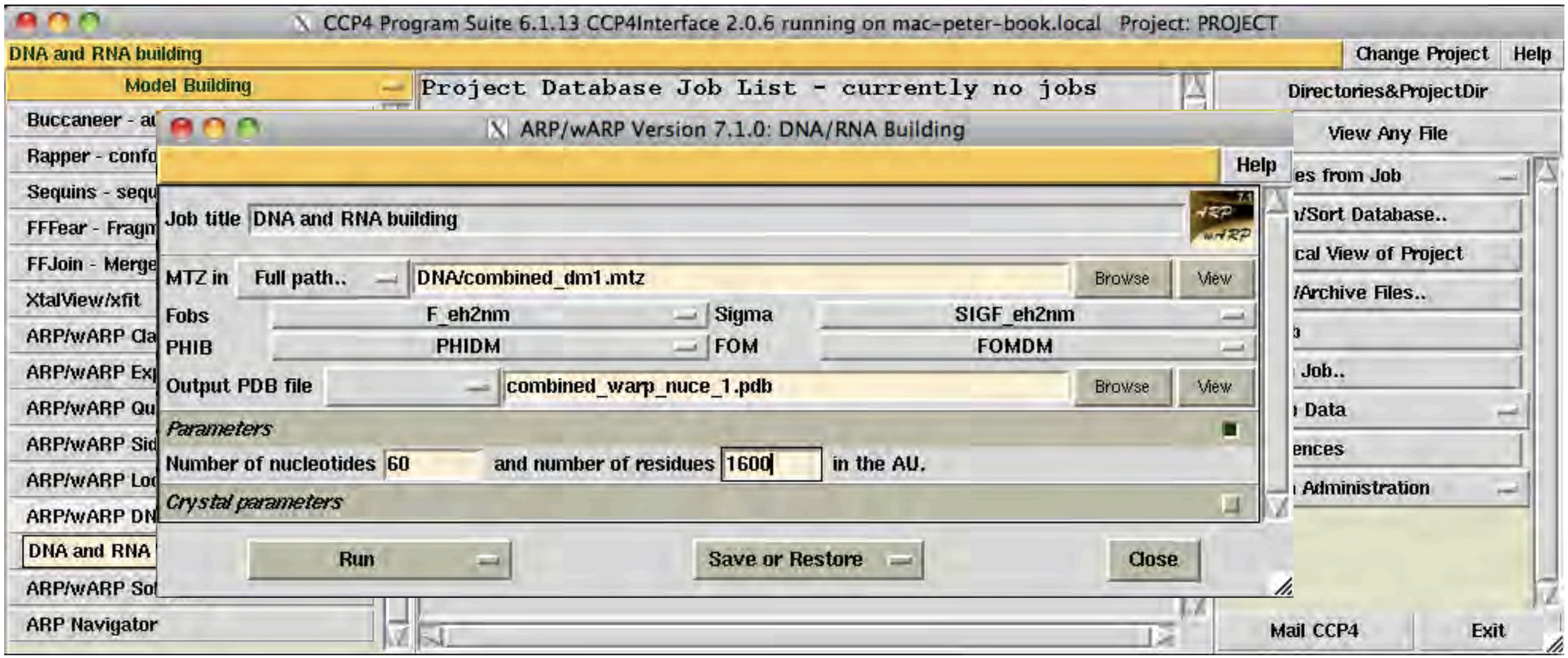

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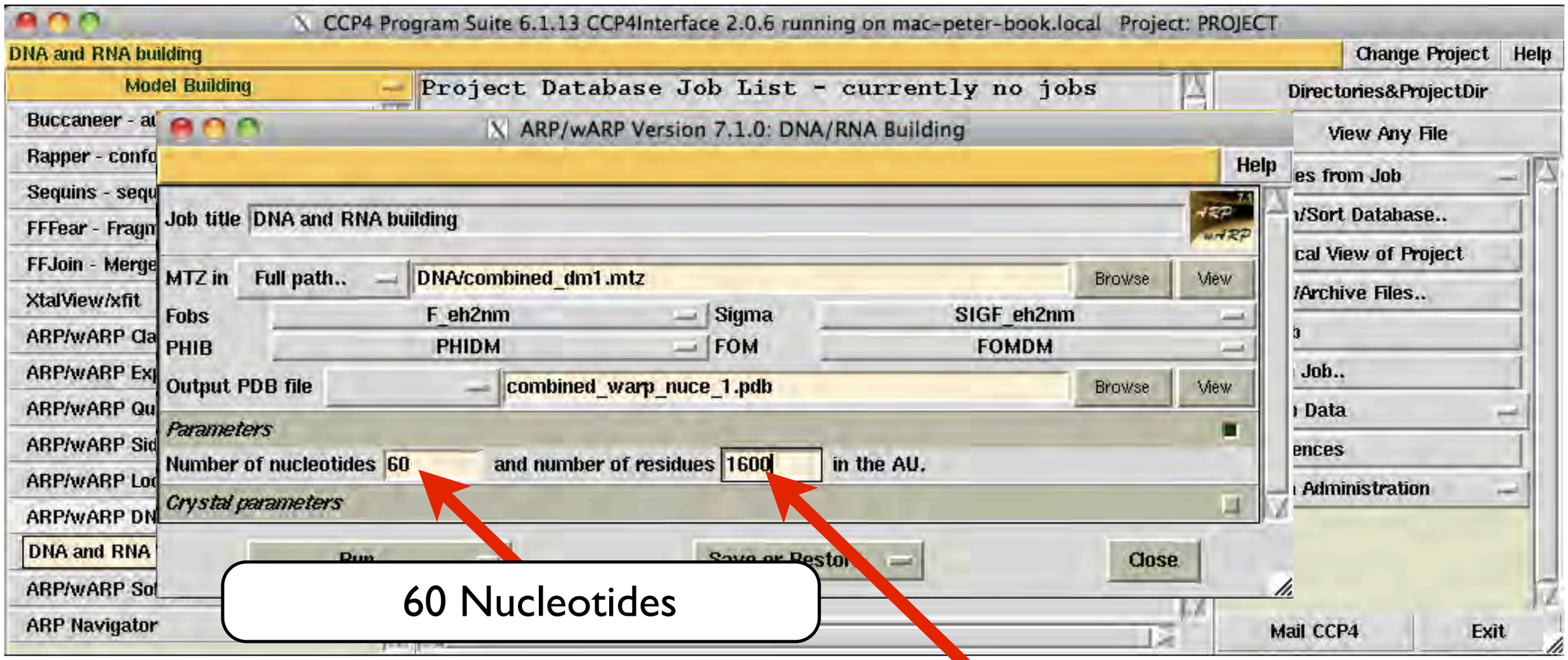
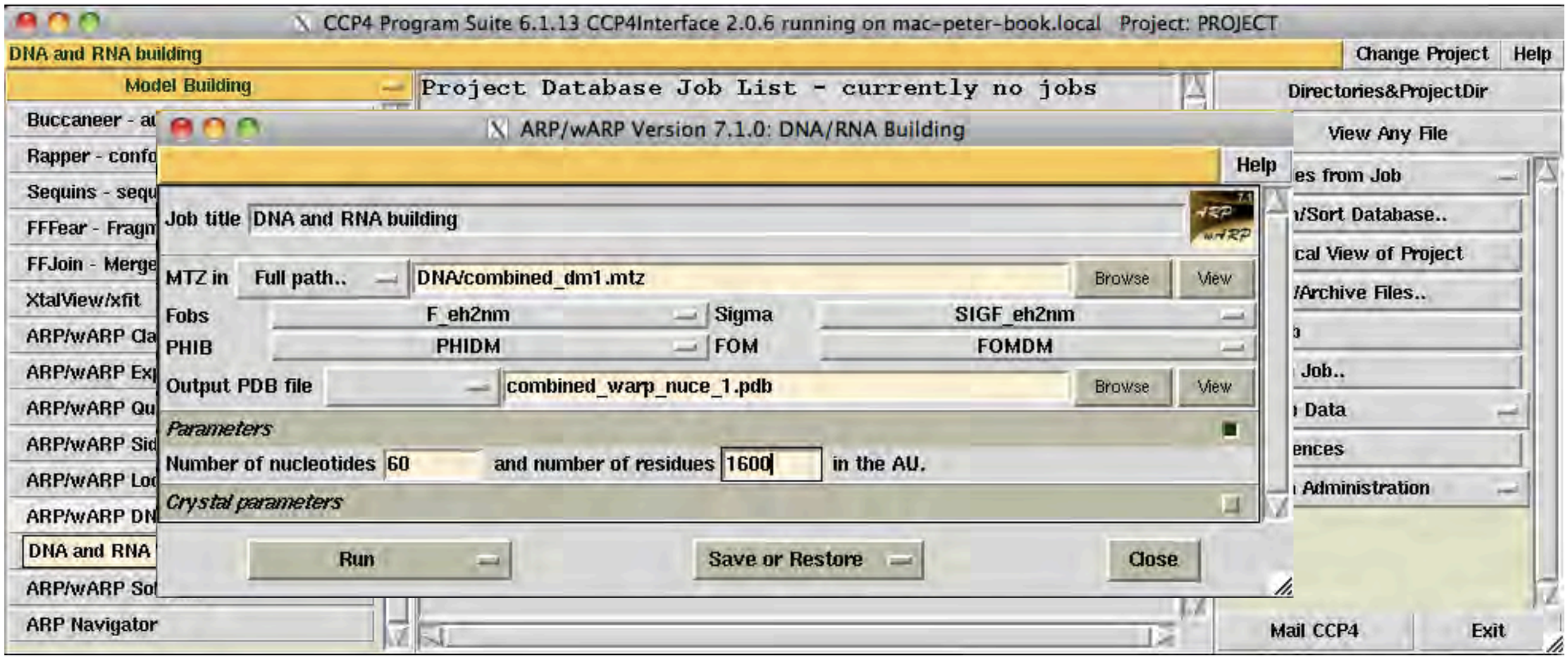


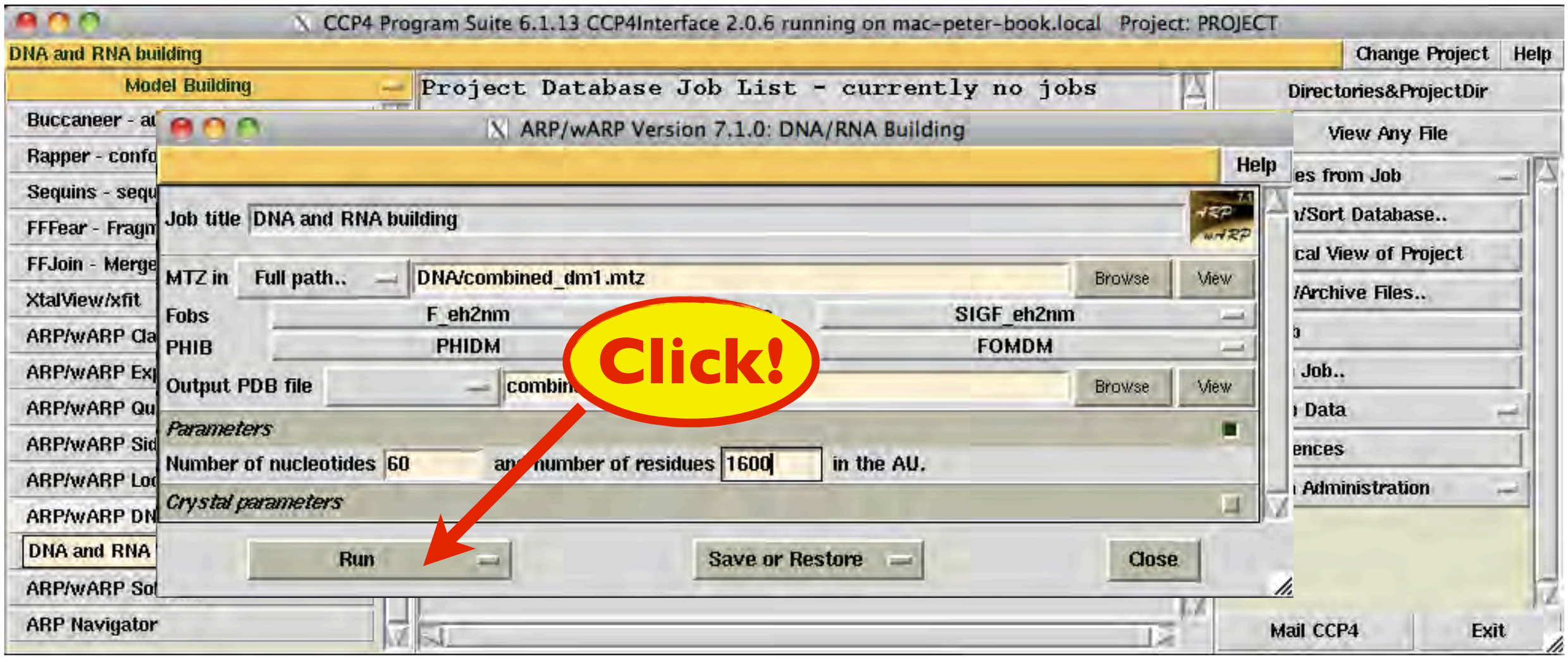
ARP/wARP: Nucleotide Building (nuce)

1e3m



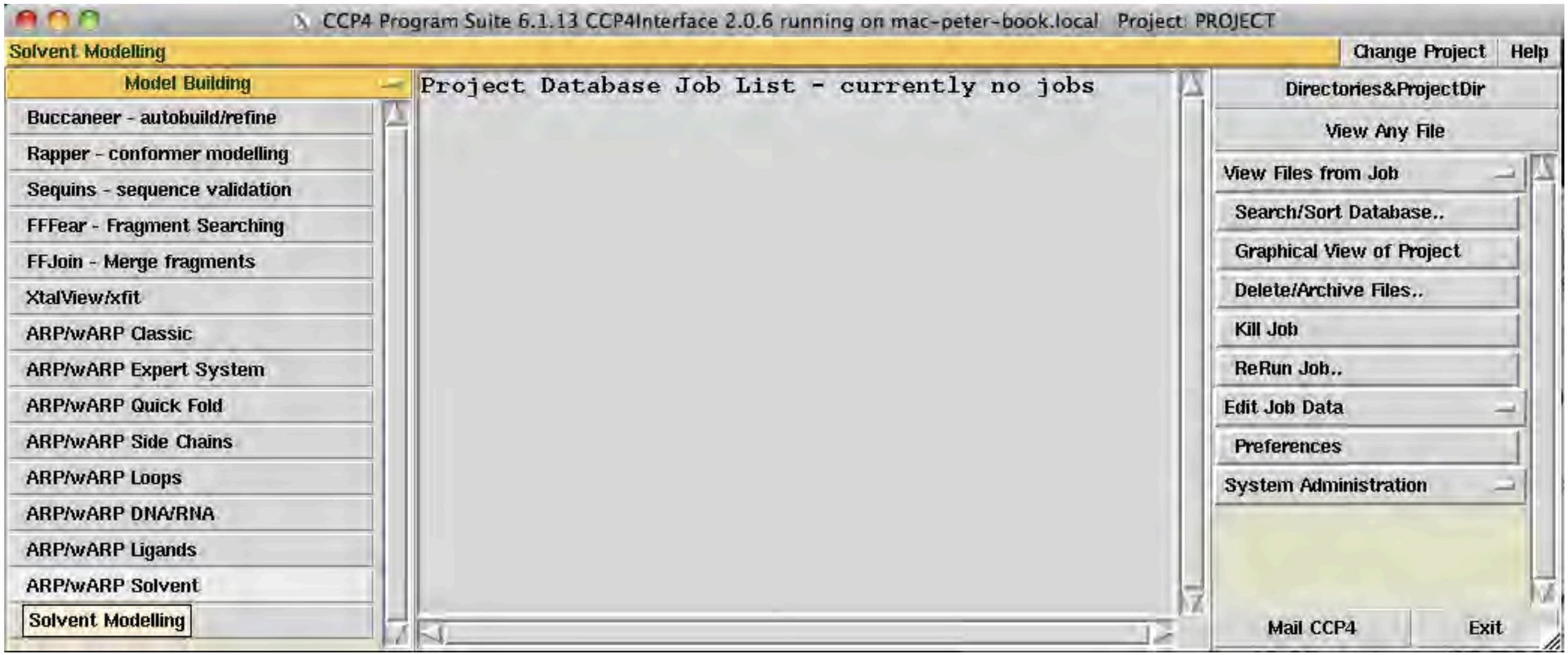
ARP/wARP: Nucleotide Building (nuce)

1e3m



ARP/wARP: Solvent (warp_solvent)

PSP



ARP/wARP: Solvent (warp_solvent)

PSP

CCP4 Program Suite 6.1.13 CCP4Interface 2.0.6 running on mac-peter-book.local Project: PROJECT

Solvent Modelling | Change Project | Help

Model Building
- Buccaneer - autobuild/refine
- Rapper - conformer modelling
- Sequins - sequence validation
- FFFear - Fragment Searching
- FFJoin - Merge fragments
- XtalView/xfit
- ARP/wARP Classic
- ARP/wARP Expert System
- ARP/wARP Quick Fold
- ARP/wARP Side Chains
- ARP/wARP Loops
- ARP/wARP DNA/RNA
- ARP/wARP Ligands
- ARP/wARP Solvent
- Solvent Modelling

Project Database Job List - currently no jobs

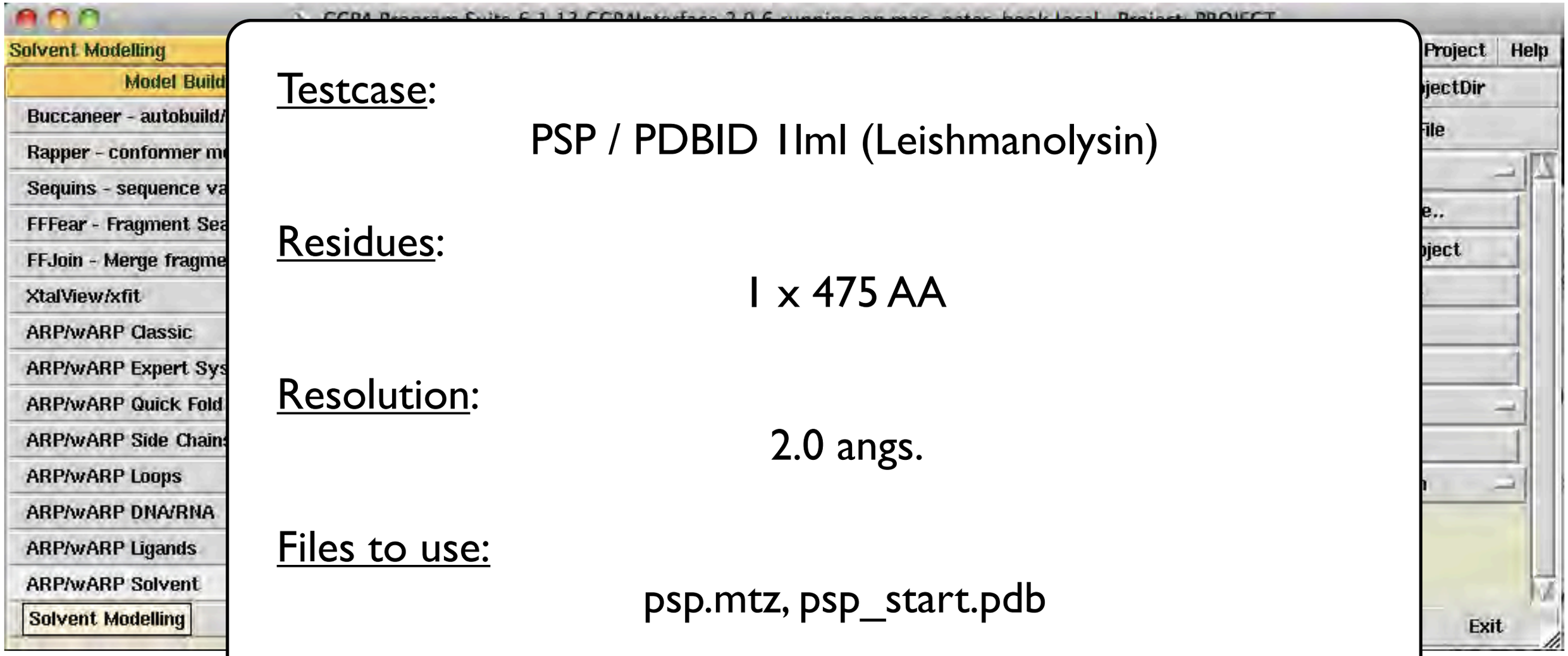
Directories&ProjectDir
View Any File
View Files from Job
Search/Sort Database..
Graphical View of Project
Delete/Archive Files..
Kill Job
ReRun Job..
Edit Job Data
Preferences
System Administration

Mail CCP4 | Exit

Click!

ARP/wARP: Solvent (warp_solvent)

PSP



Testcase:

PSP / PDBID 1lml (Leishmanolysin)

Residues:

1 x 475 AA

Resolution:

2.0 angs.

Files to use:

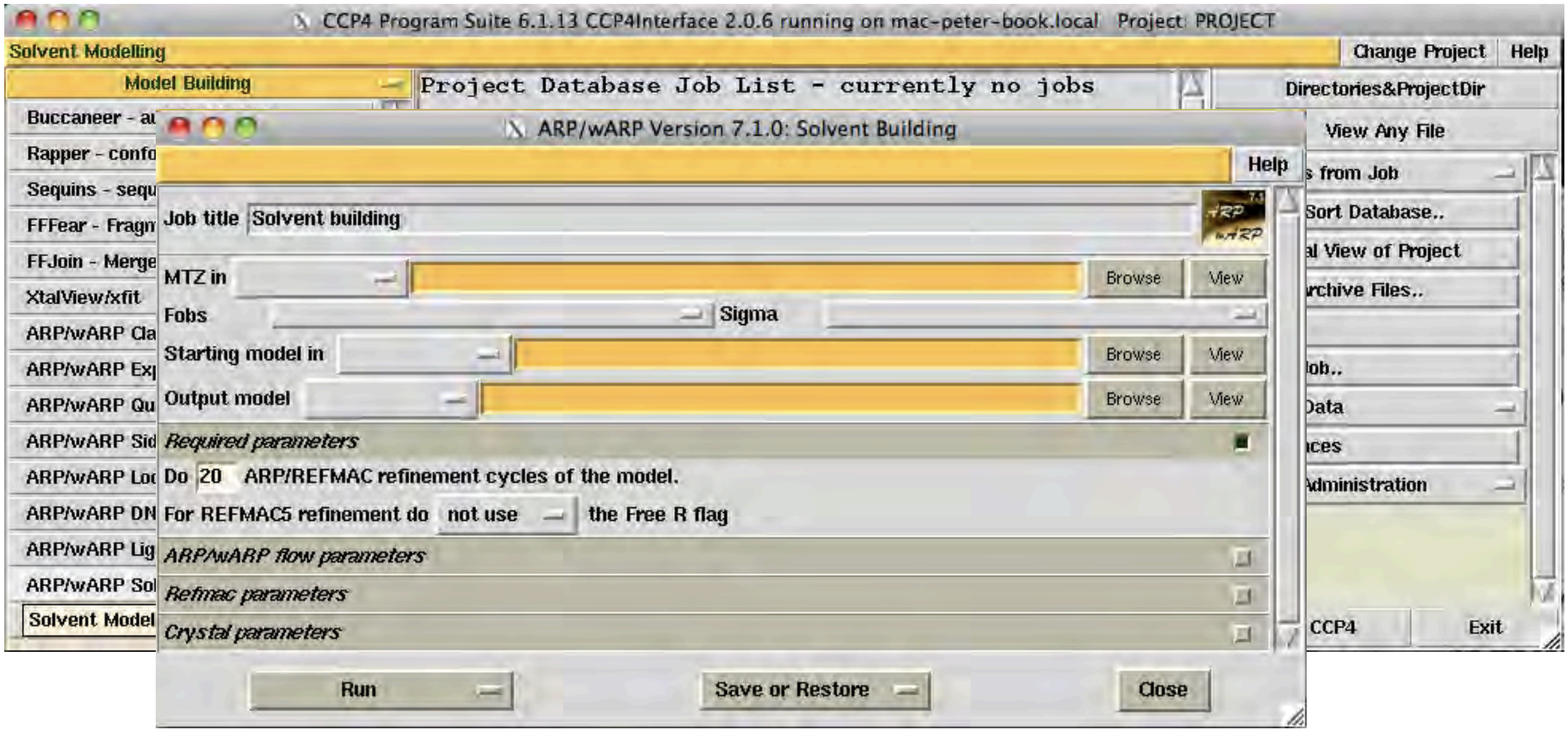
psp.mtz, psp_start.pdb

MTS labels to use:

FP, SIGFP

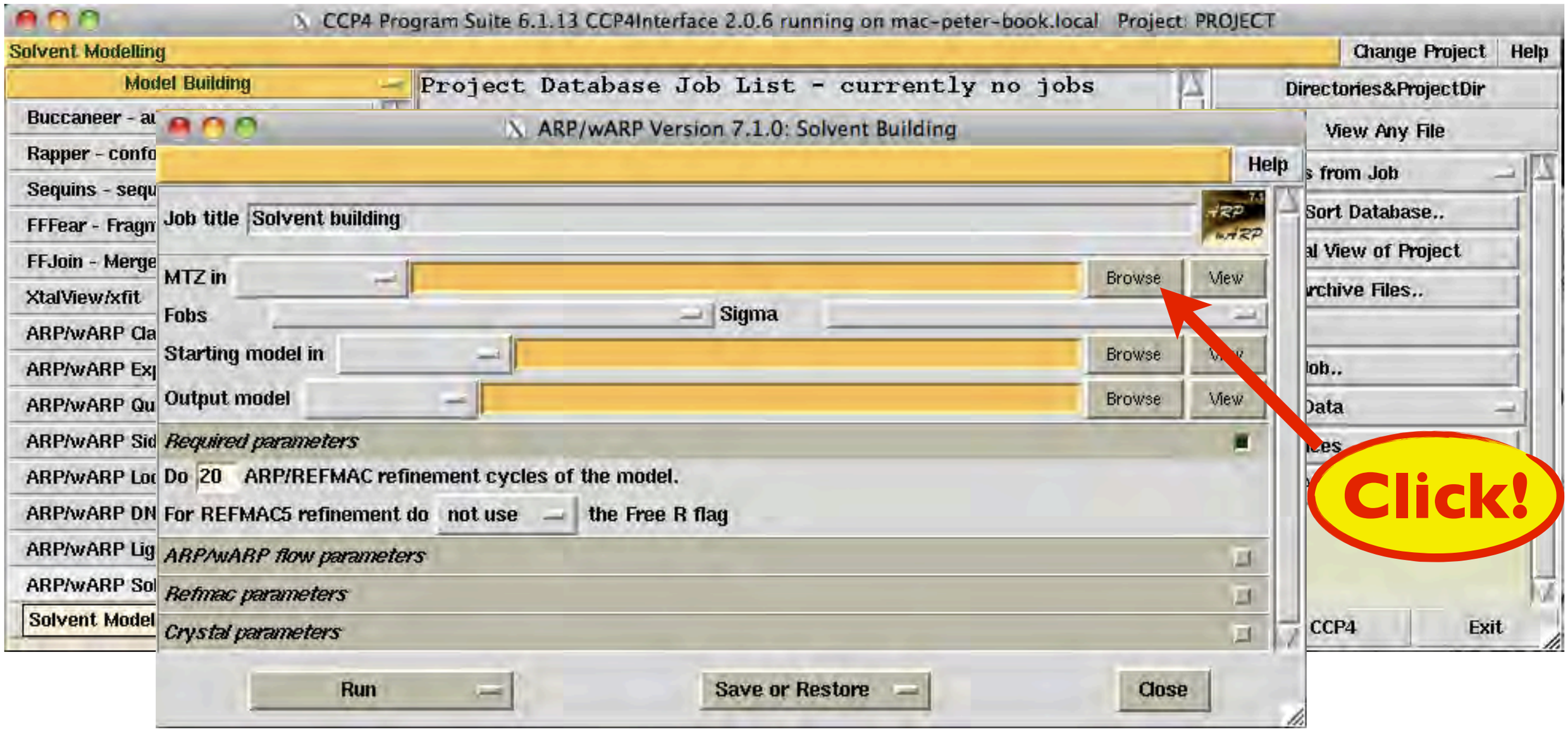
ARP/wARP: Solvent (warp_solvent)

PSP



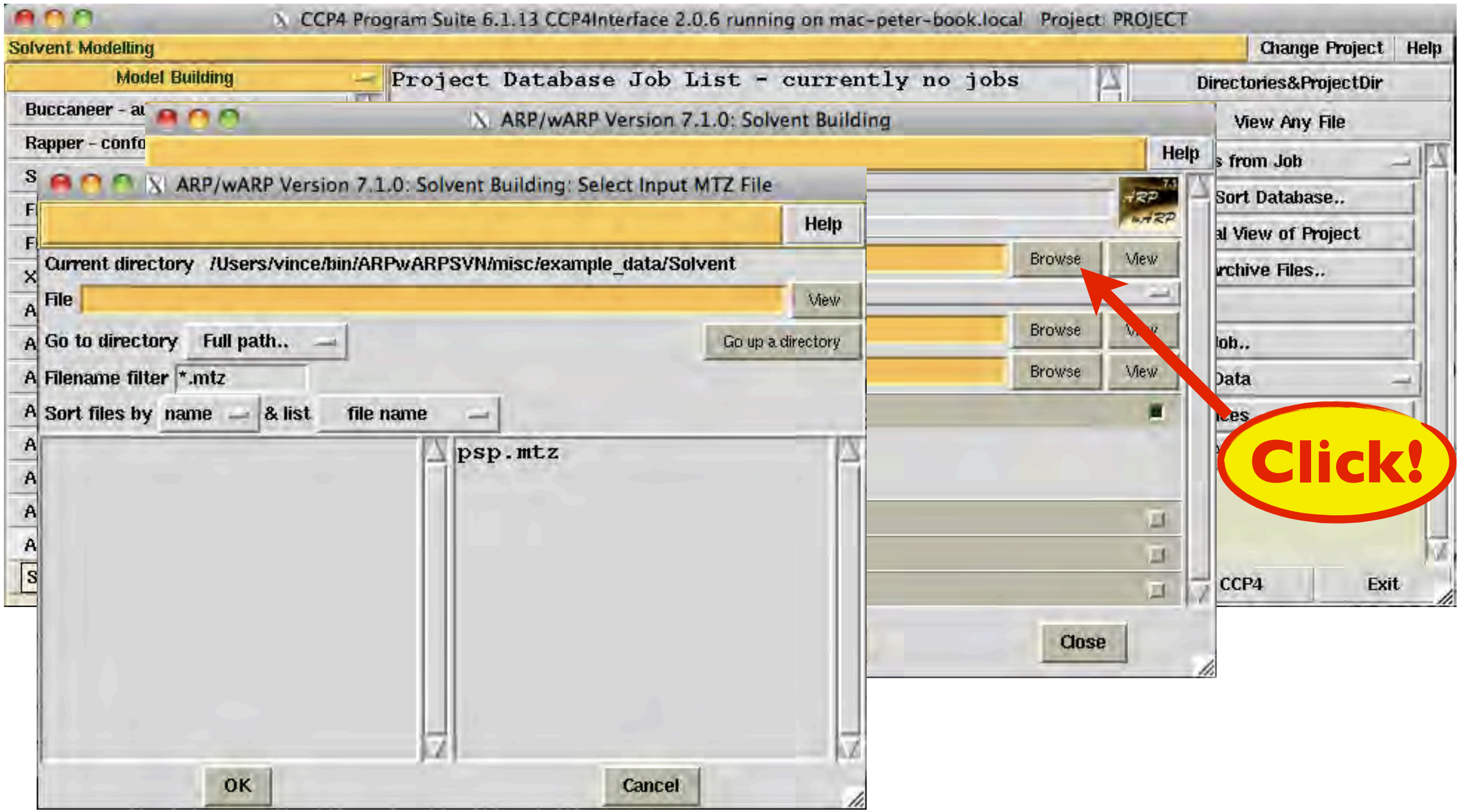
ARP/wARP: Solvent (warp_solvent)

PSP



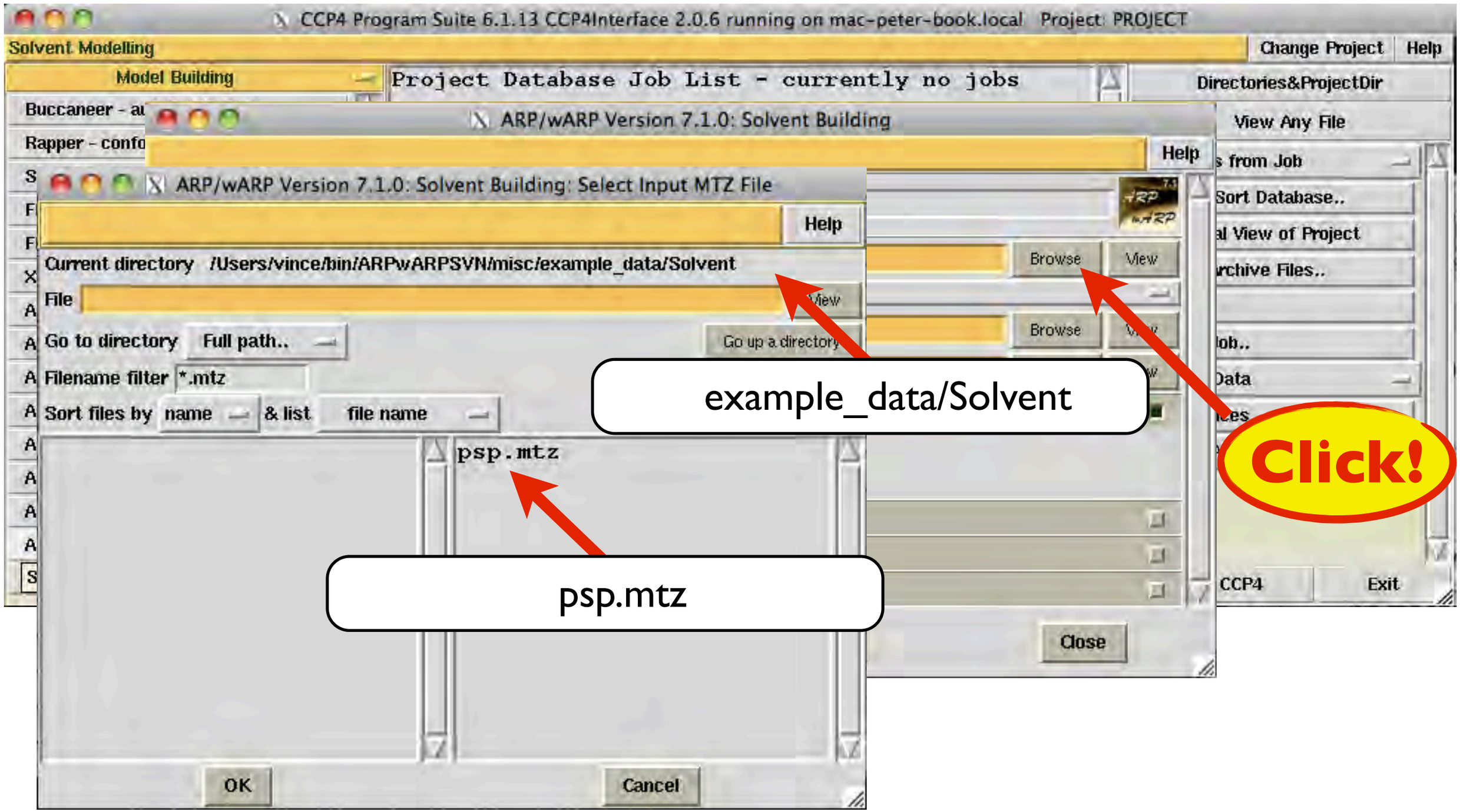
ARP/wARP: Solvent (warp_solvent)

PSP



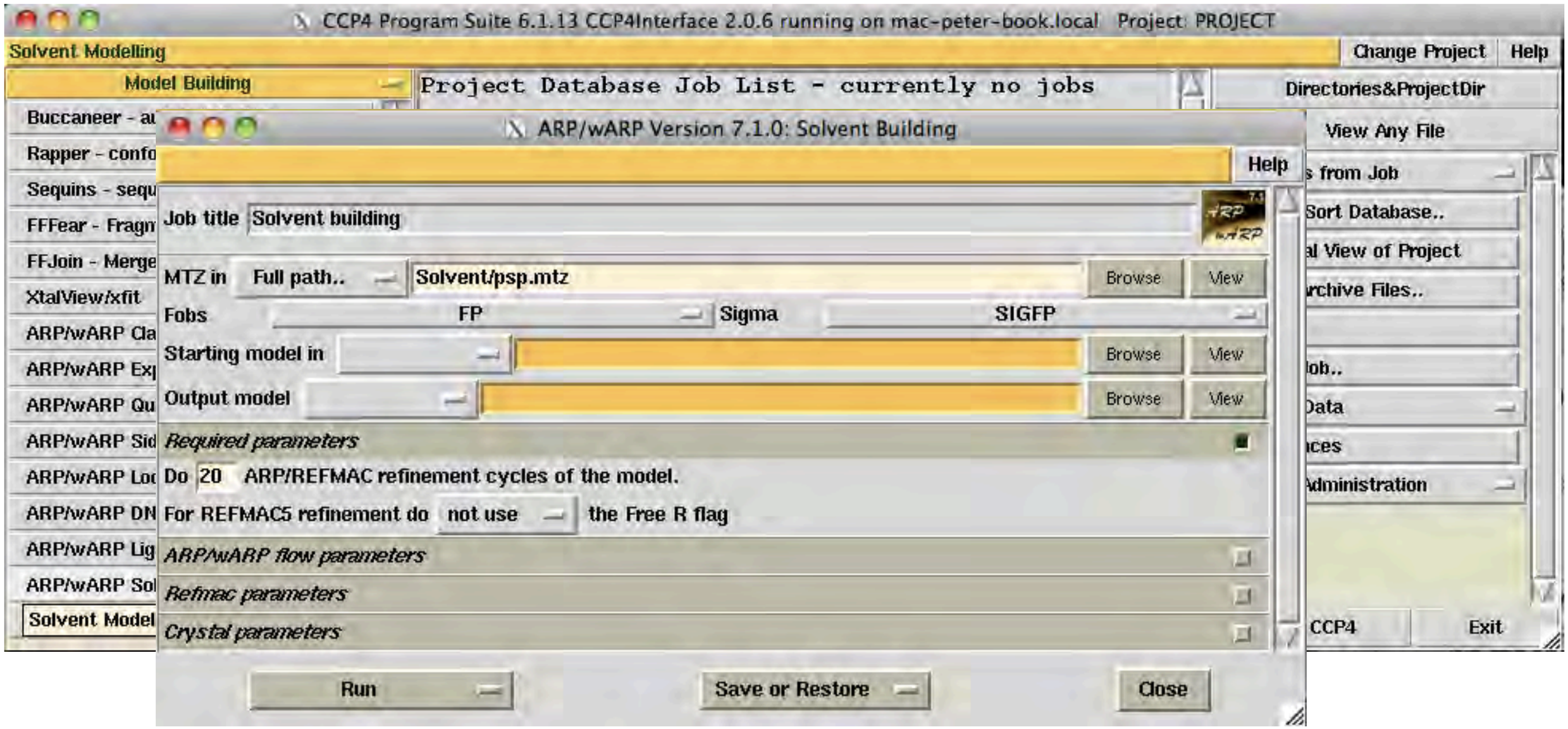
ARP/wARP: Solvent (warp_solvent)

PSP



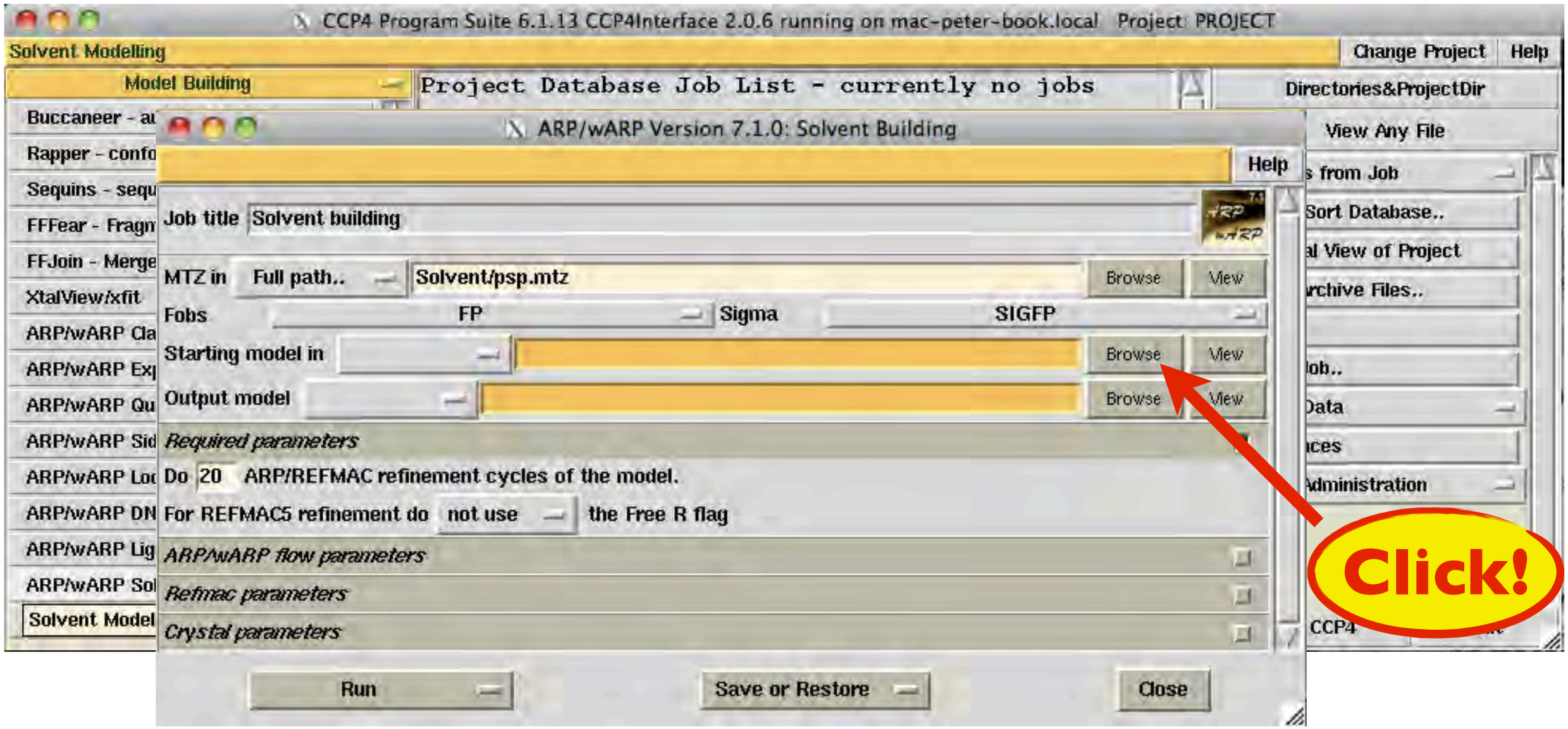
ARP/wARP: Solvent (warp_solvent)

PSP



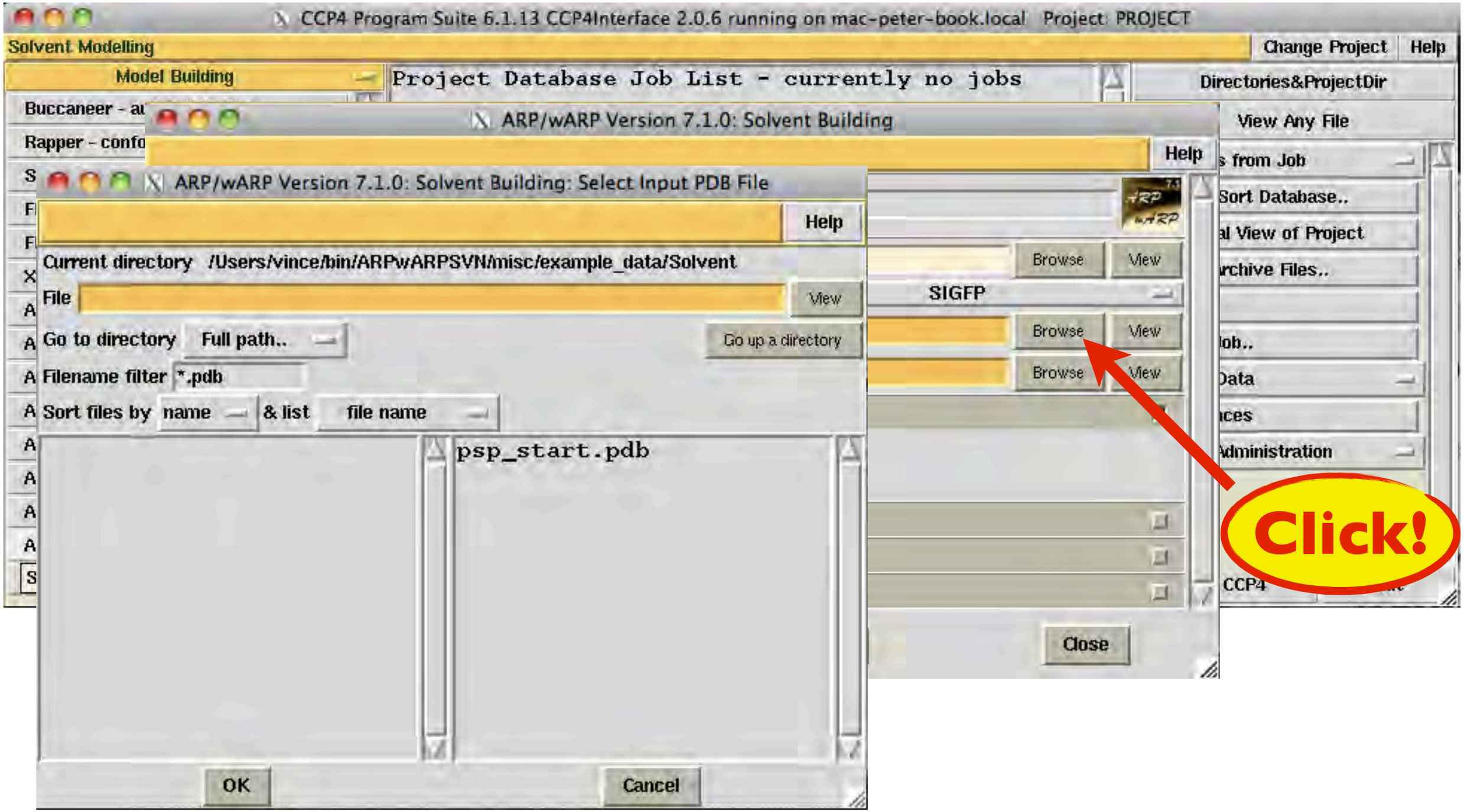
ARP/wARP: Solvent (warp_solvent)

PSP



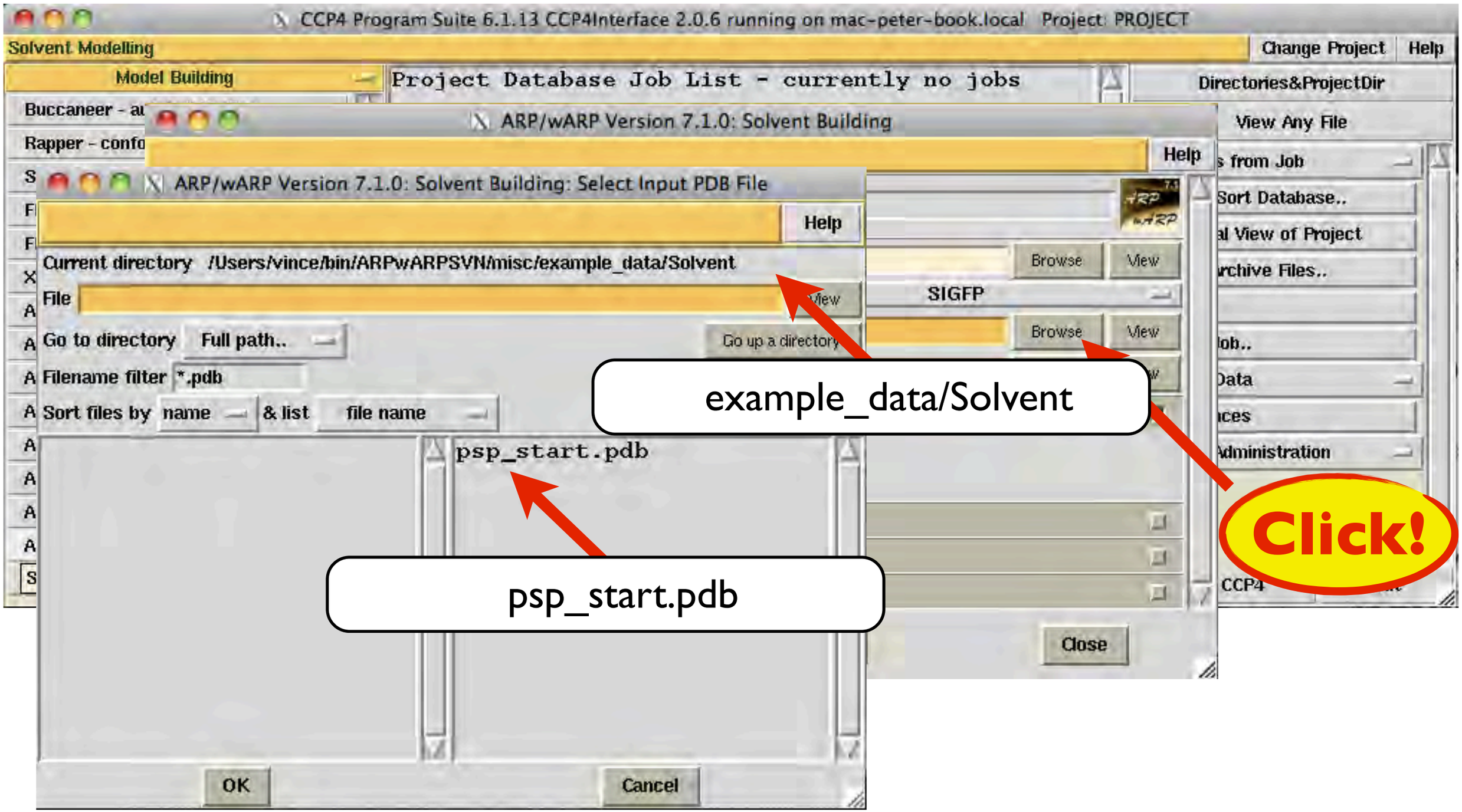
ARP/wARP: Solvent (warp_solvent)

PSP



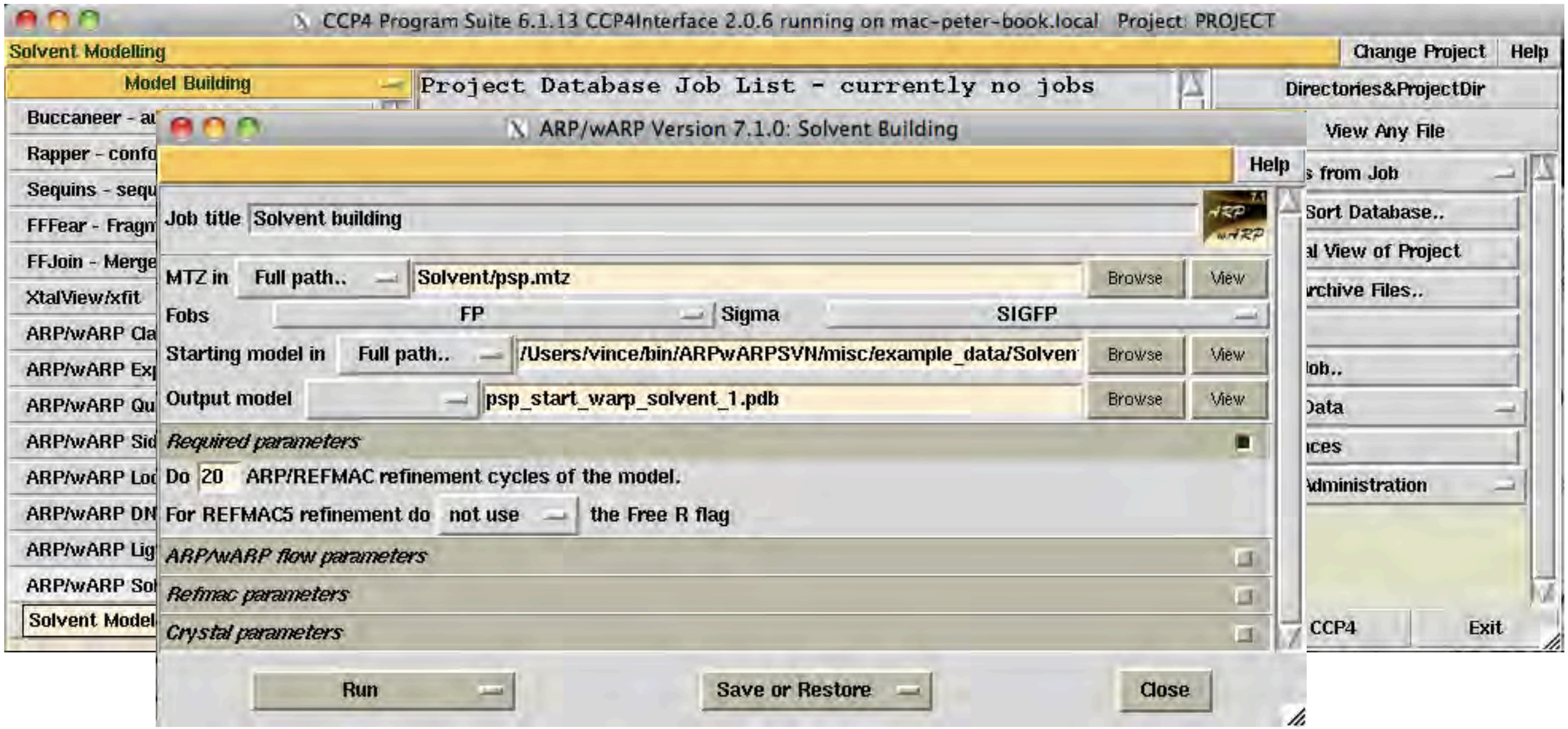
ARP/wARP: Solvent (warp_solvent)

PSP



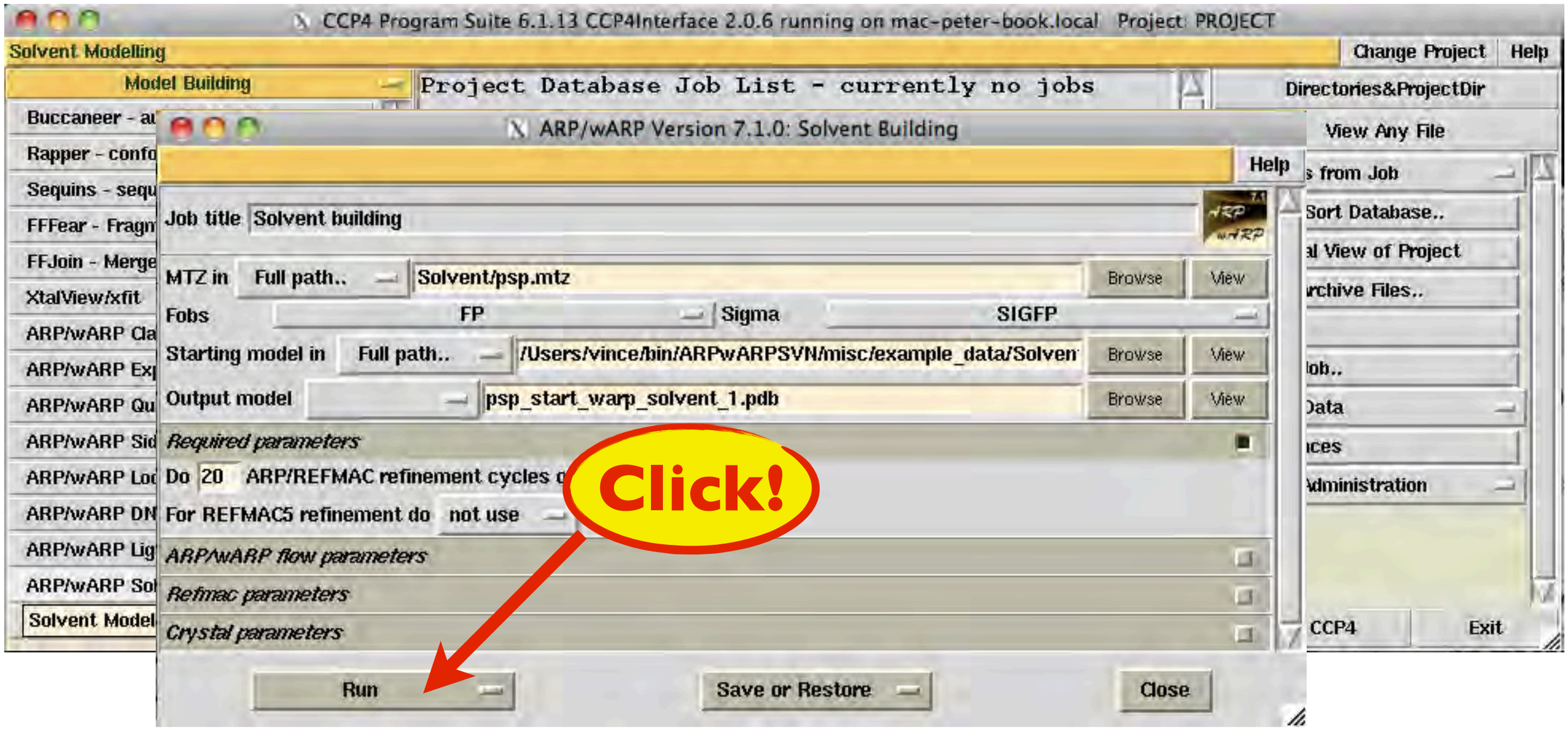
ARP/wARP: Solvent (warp_solvent)

PSP



ARP/wARP: Solvent (warp_solvent)

PSP

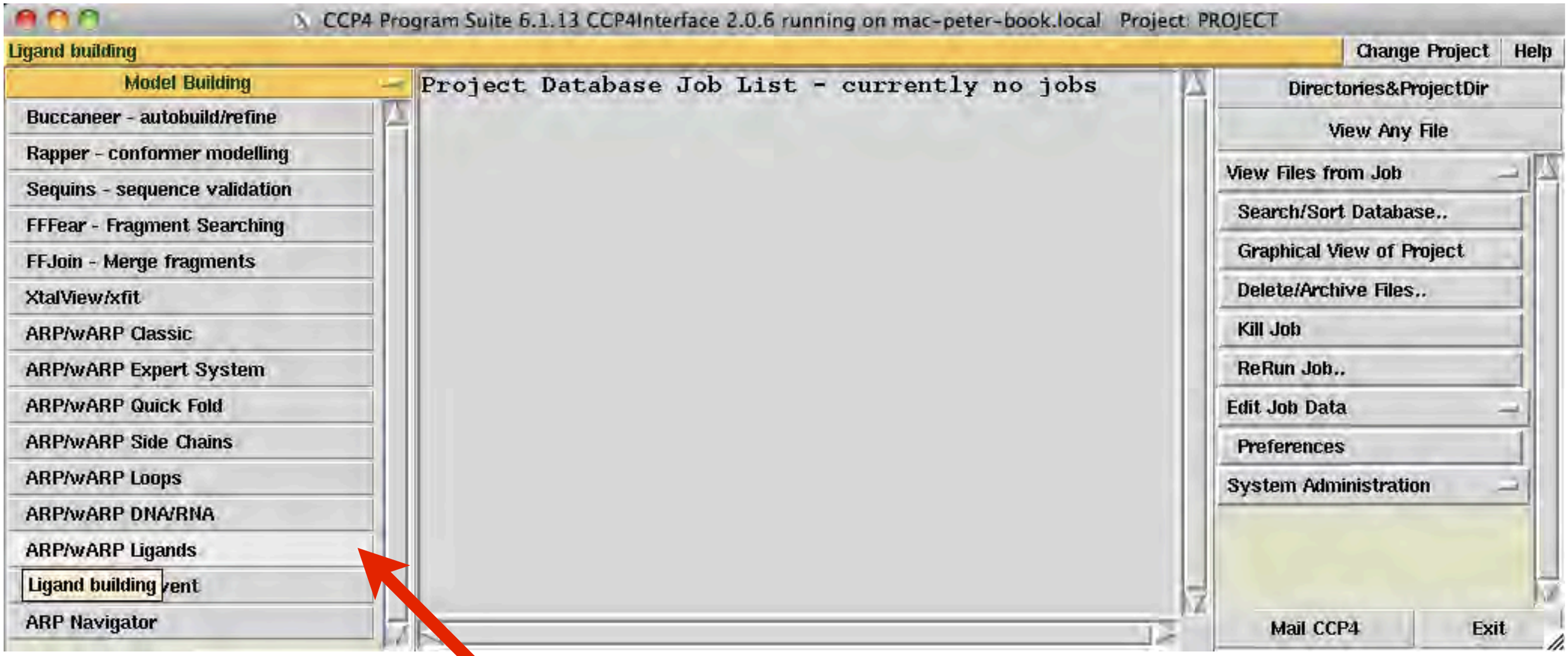


ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA

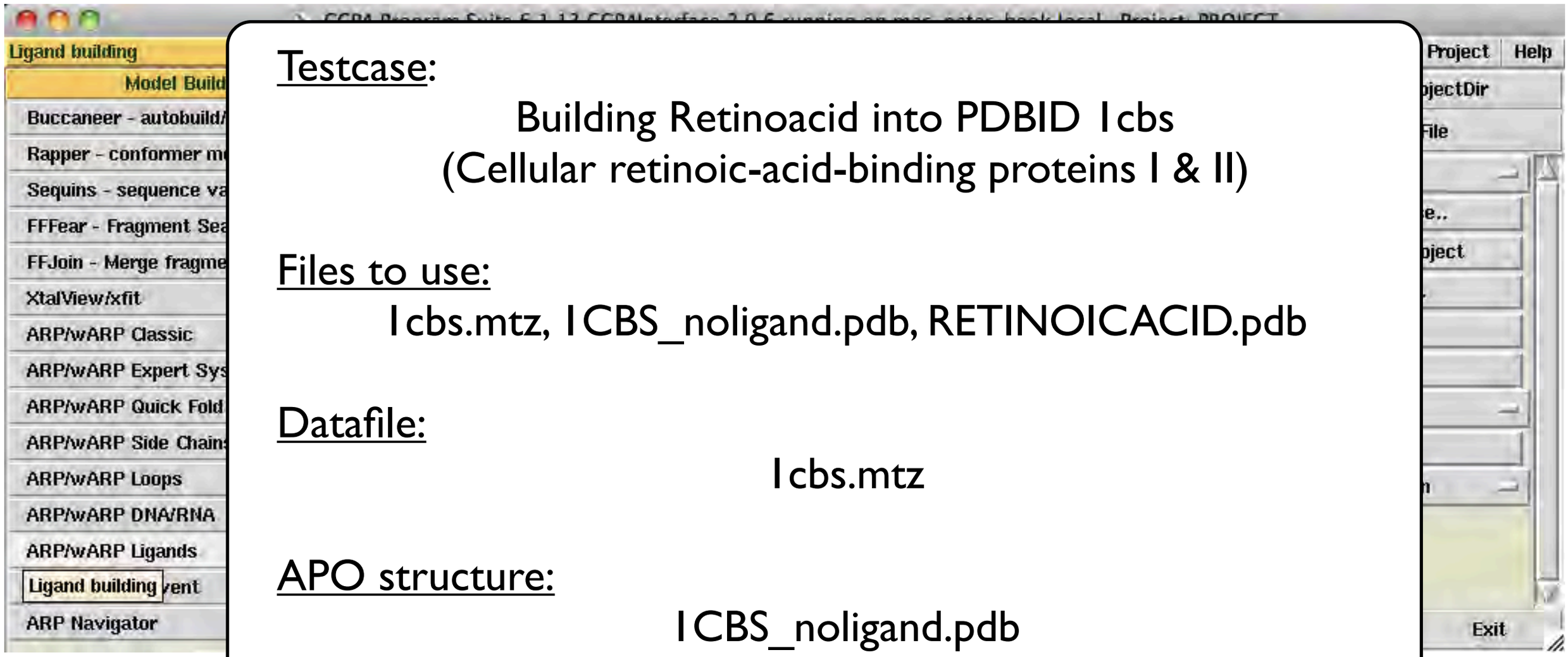
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



Testcase:

Building Retinoacid into PDBID 1cbs
(Cellular retinoic-acid-binding proteins I & II)

Files to use:

1cbs.mtz, 1CBS_noligand.pdb, RETINOICACID.pdb

Datafile:

1cbs.mtz

APO structure:

1CBS_noligand.pdb

Ligand template:

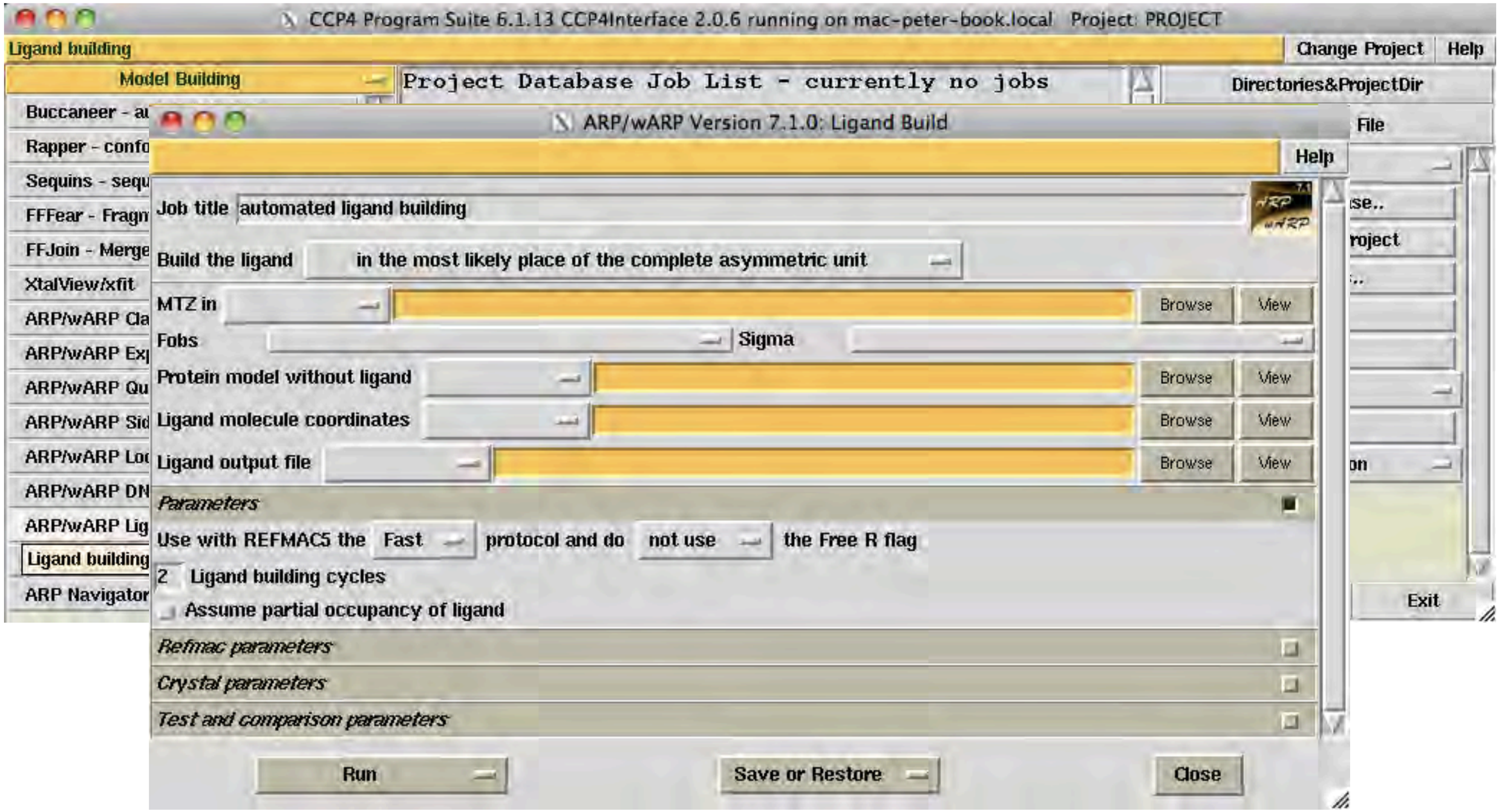
RETINOICACID.pdb

MTS labels to use:

FP, SIGFP

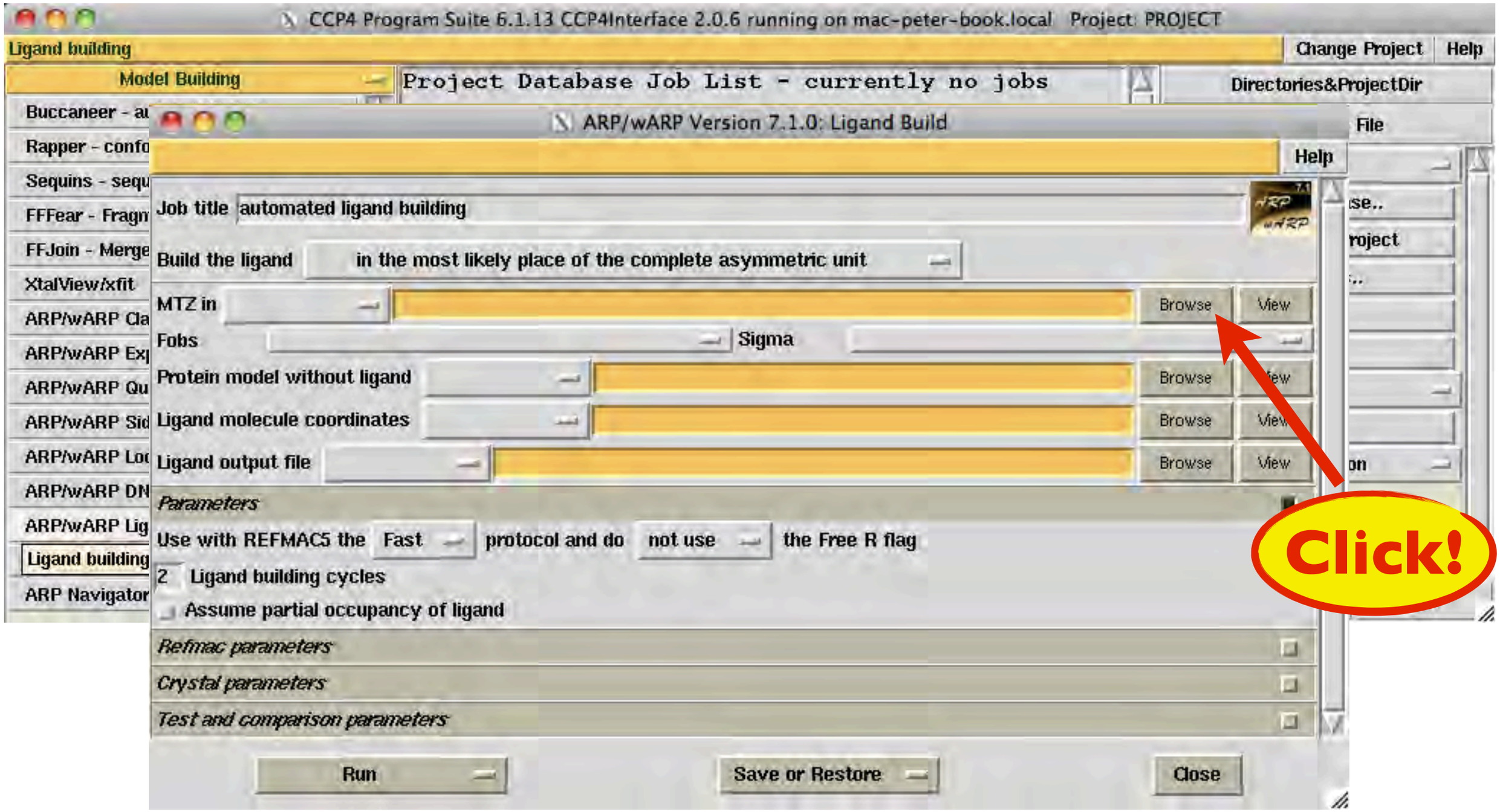
ARP/wARP: Ligands (warp_ligand)

Icbs, Lig: RA



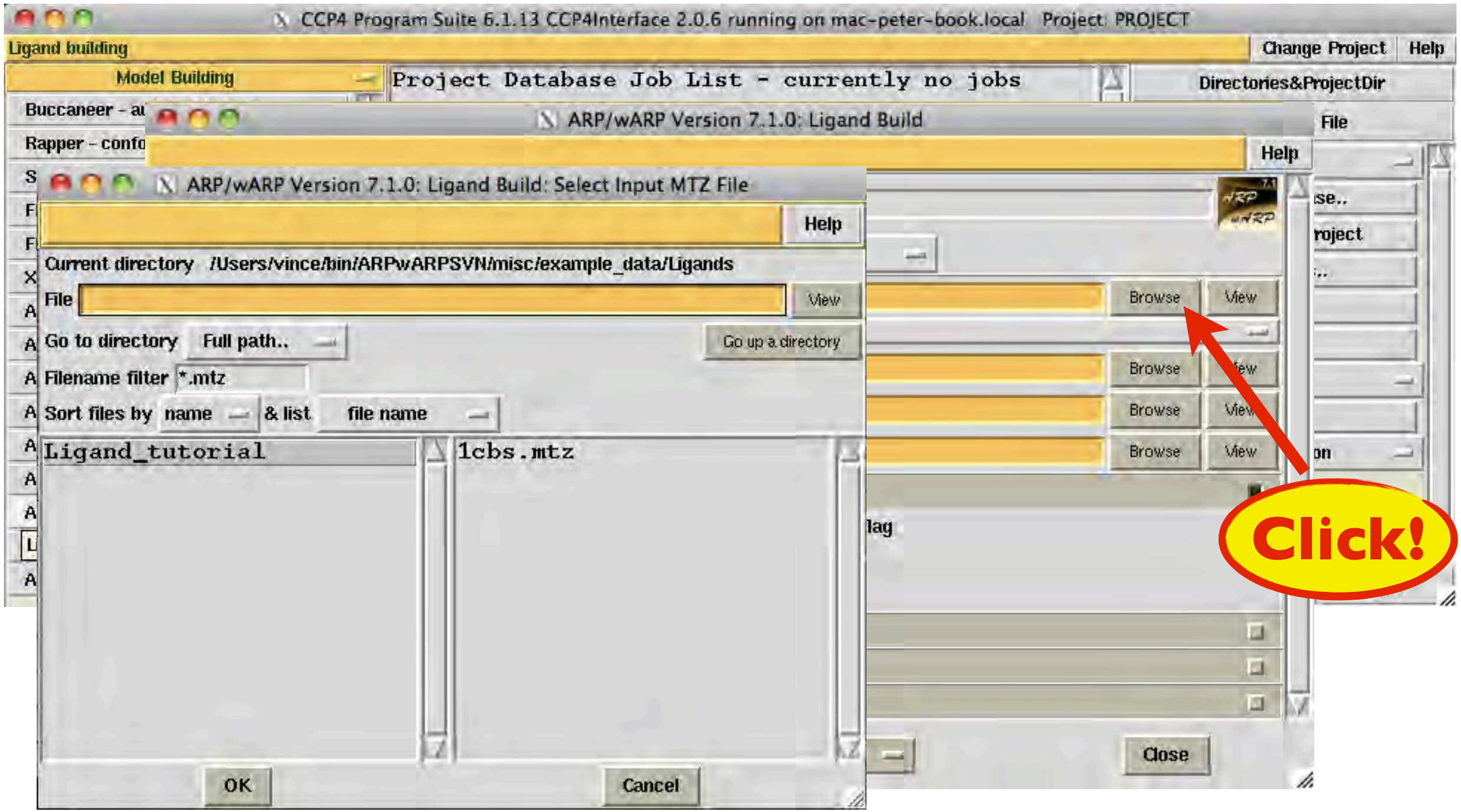
ARP/wARP: Ligands (warp_ligand)

Icbs, Lig: RA



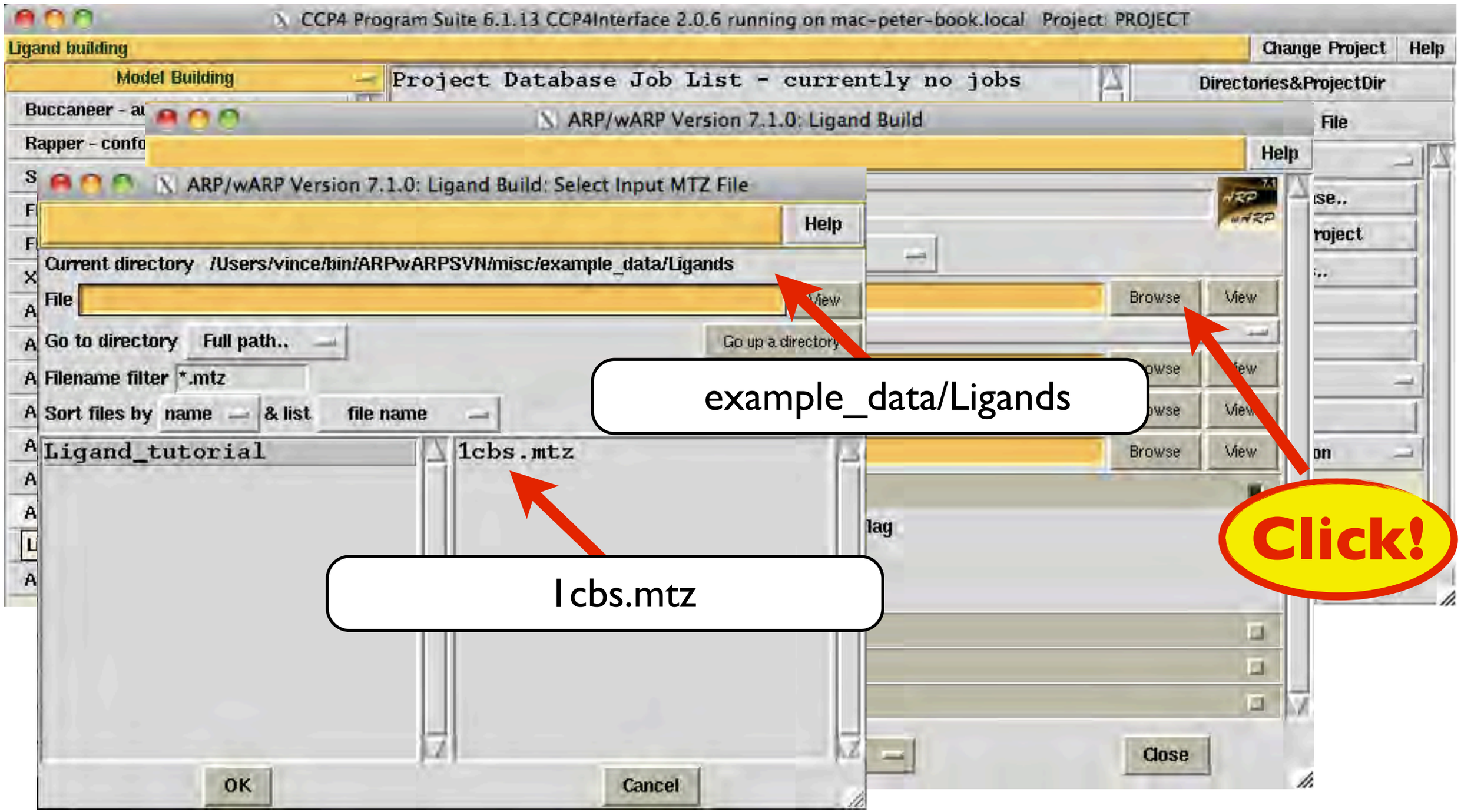
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



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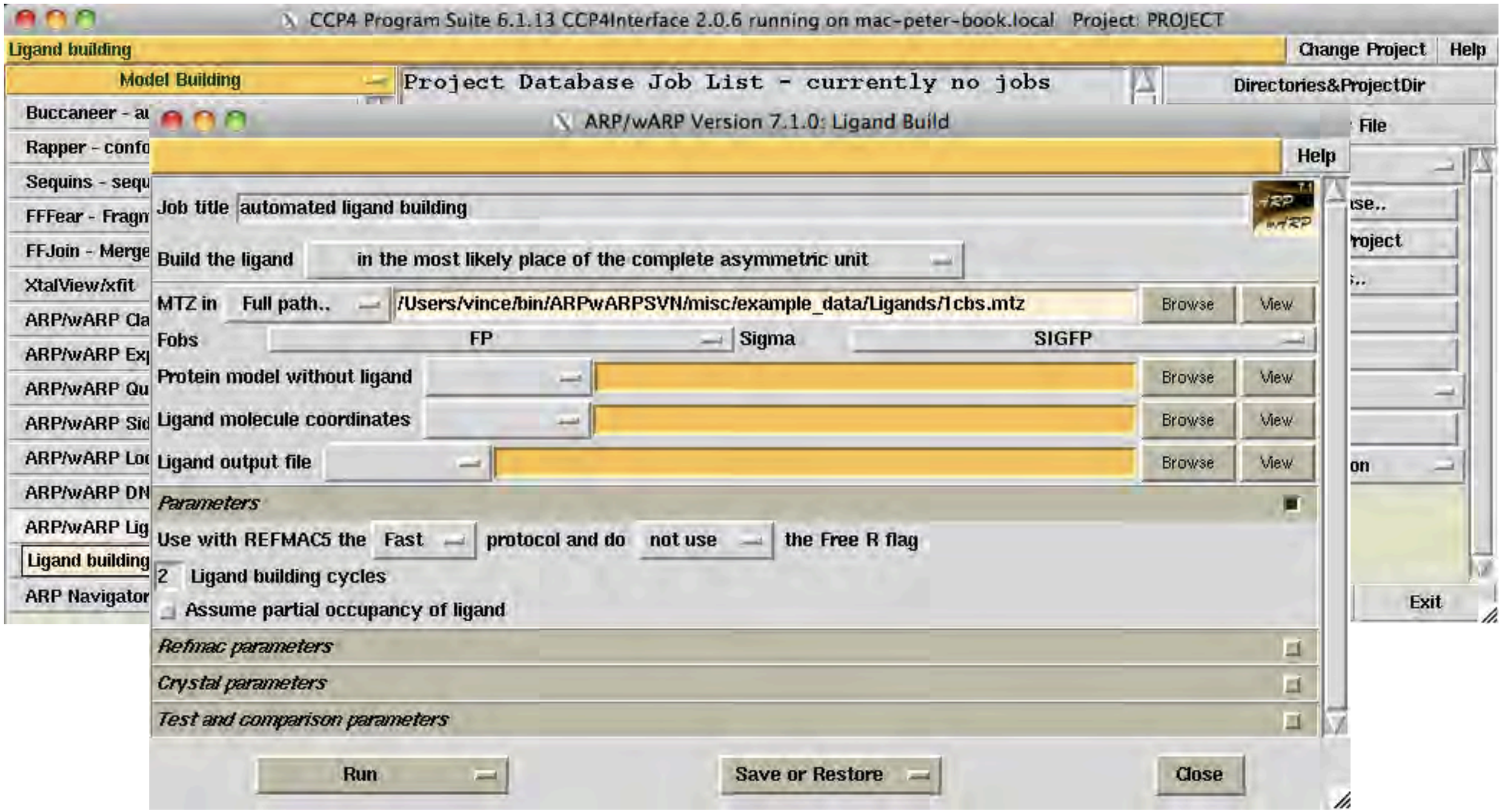
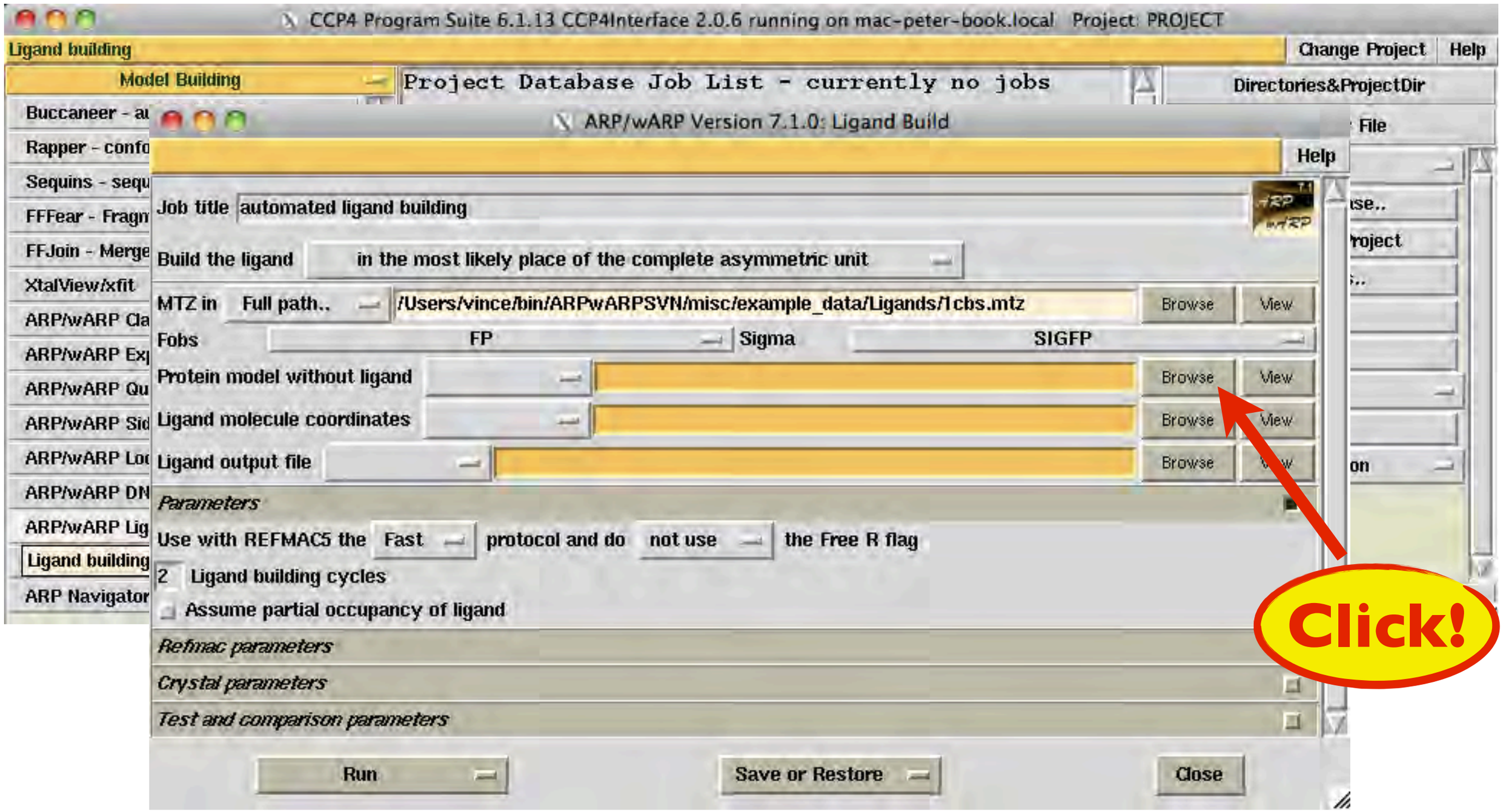
1cbs, Lig: RA



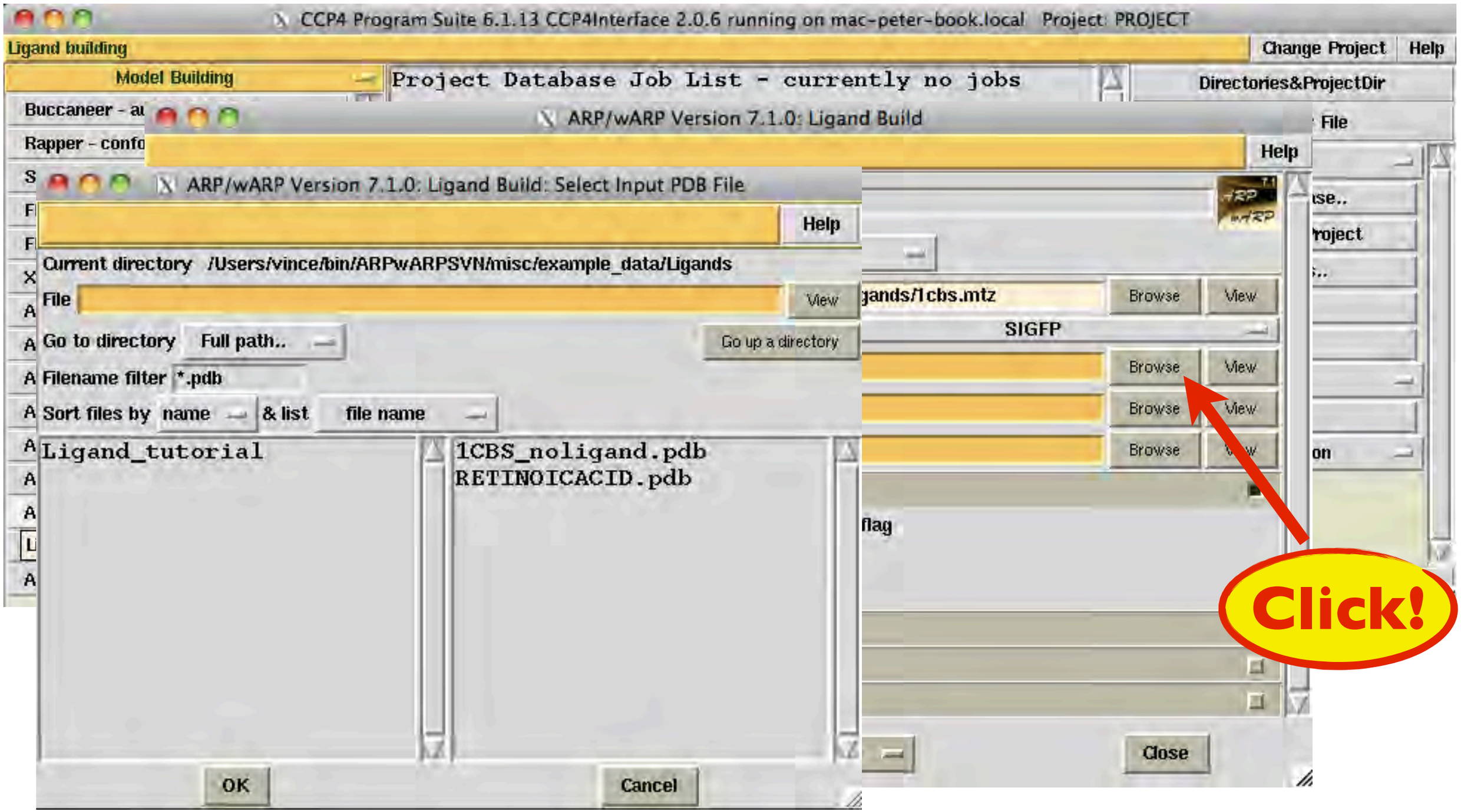
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



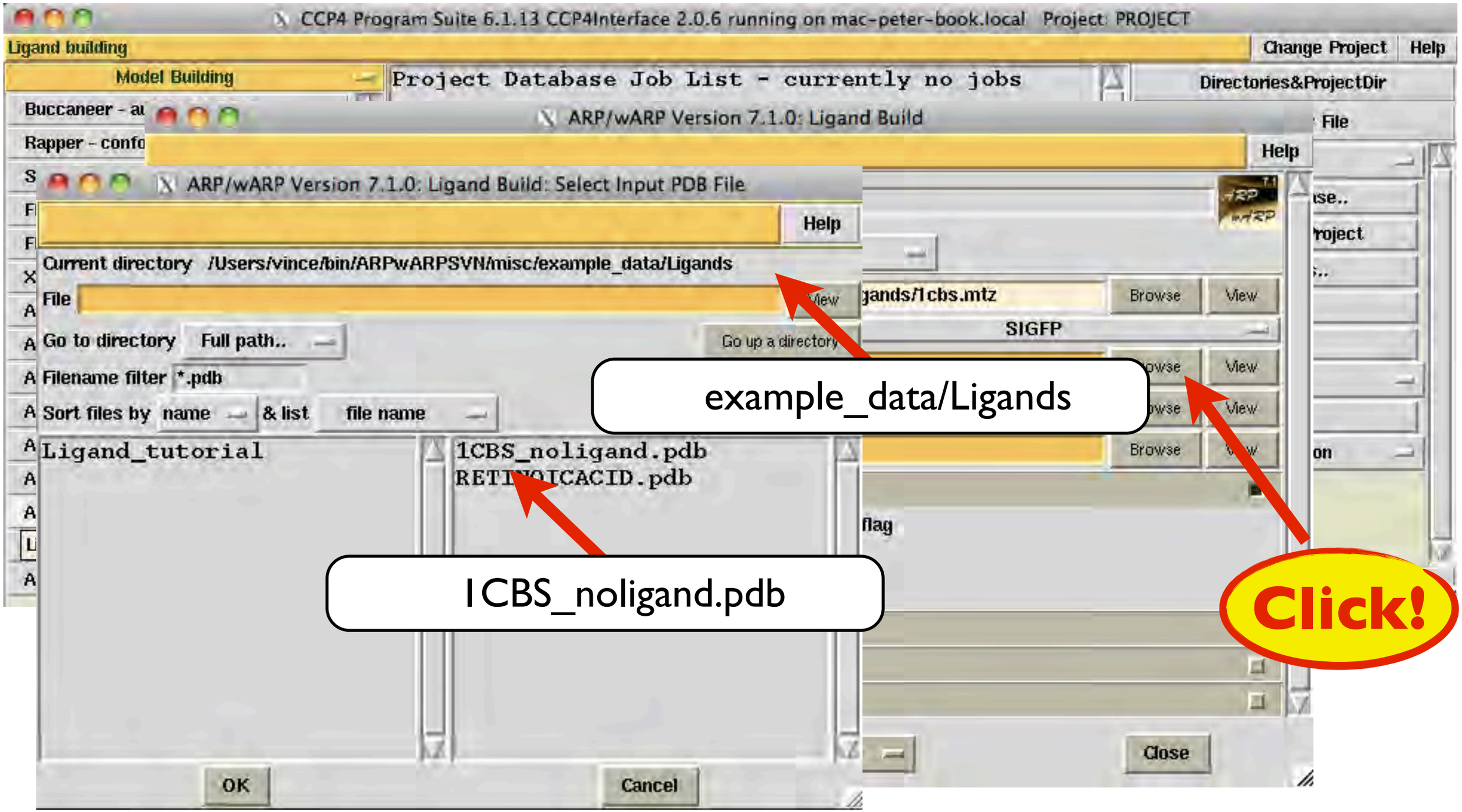
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



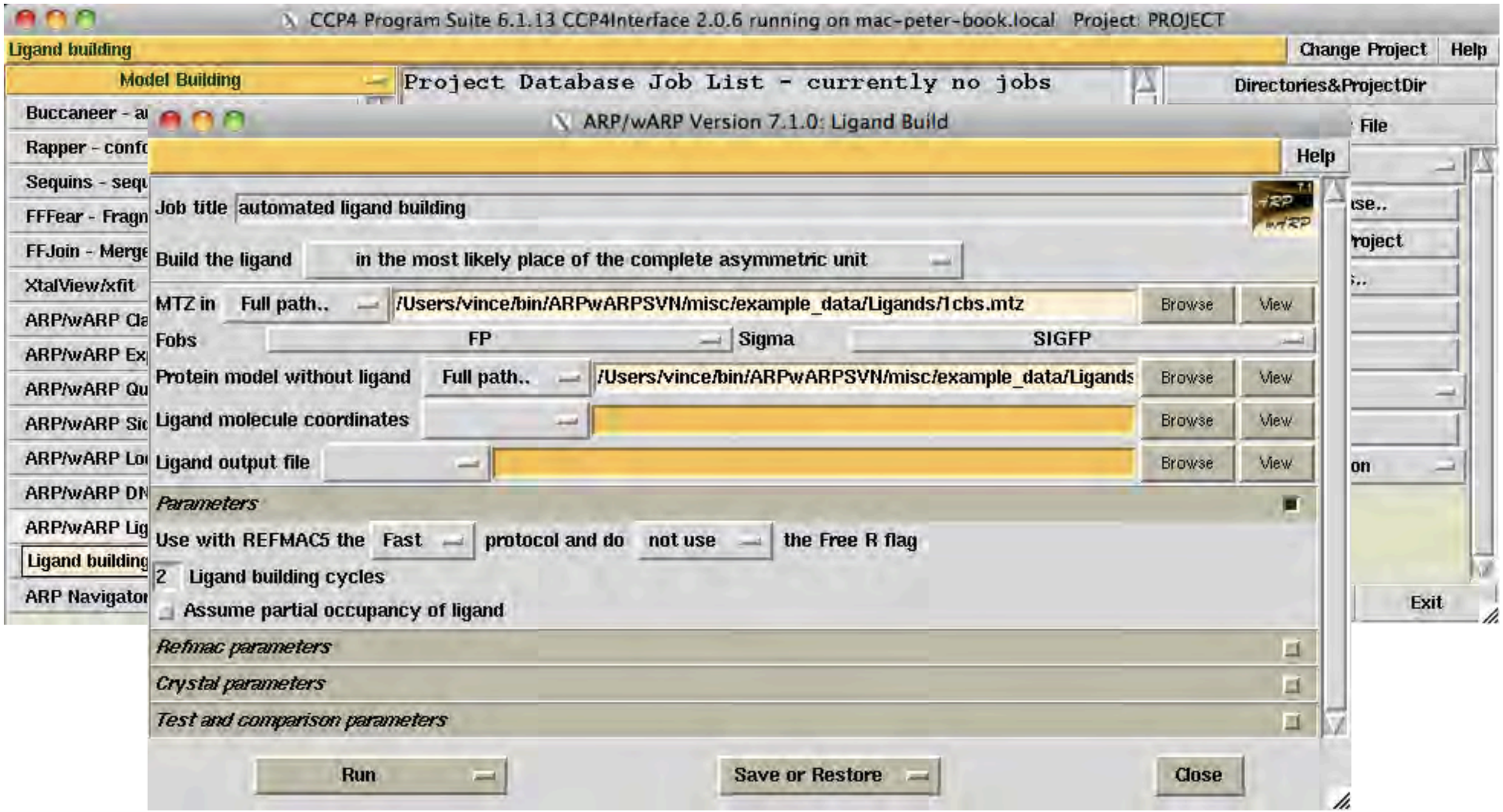
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



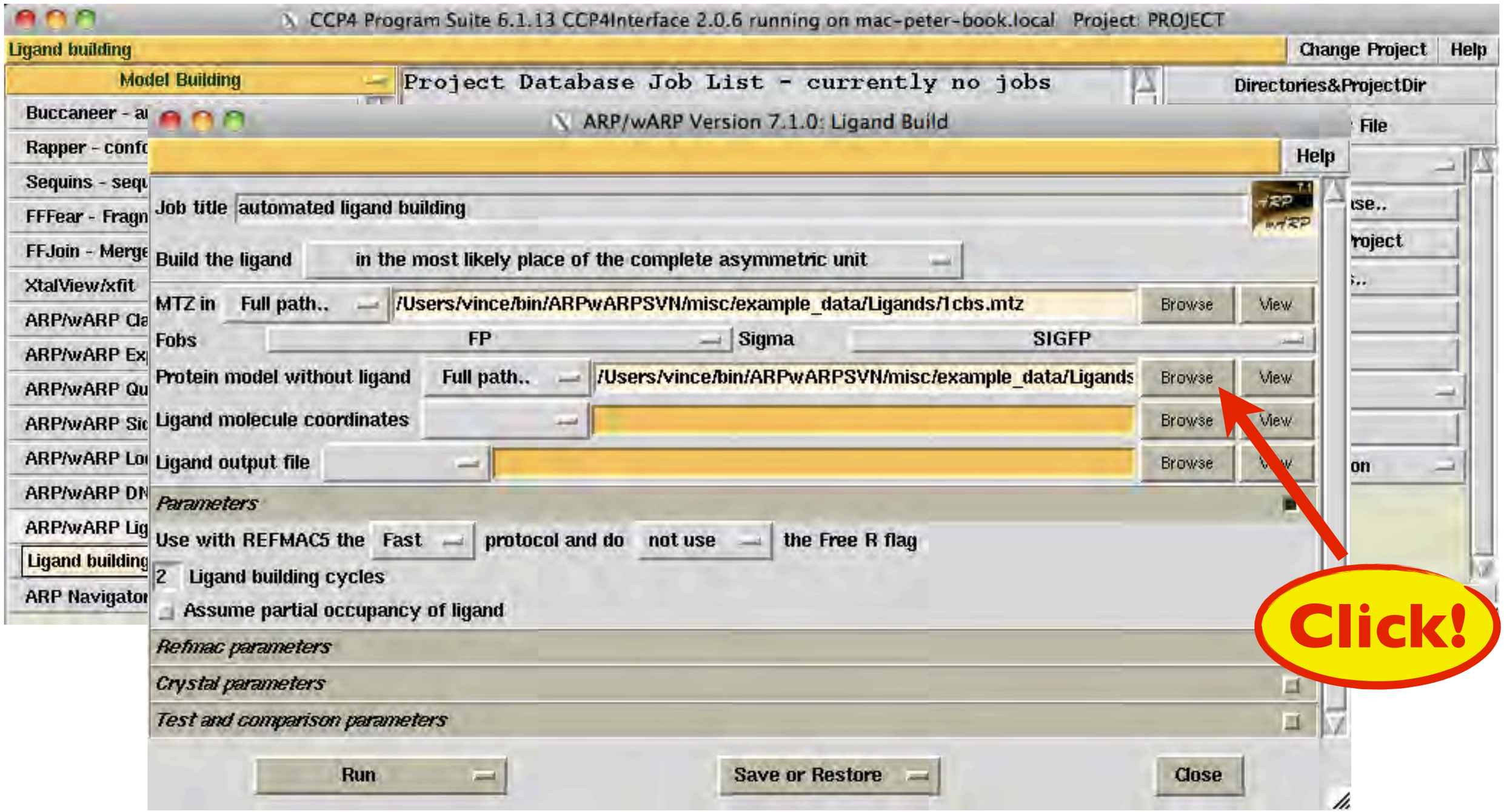
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

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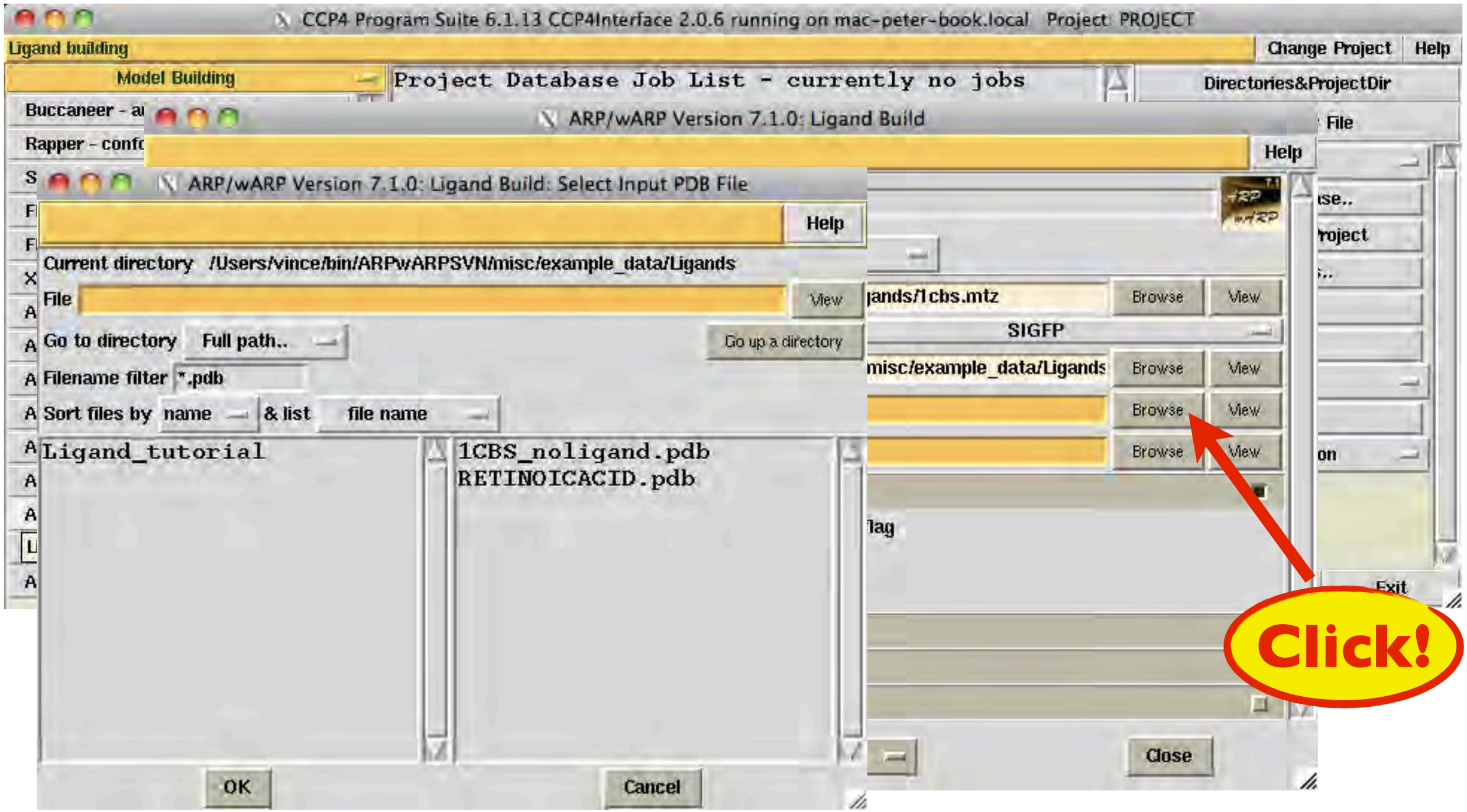

ARP/wARP: Ligands (warp_ligand)

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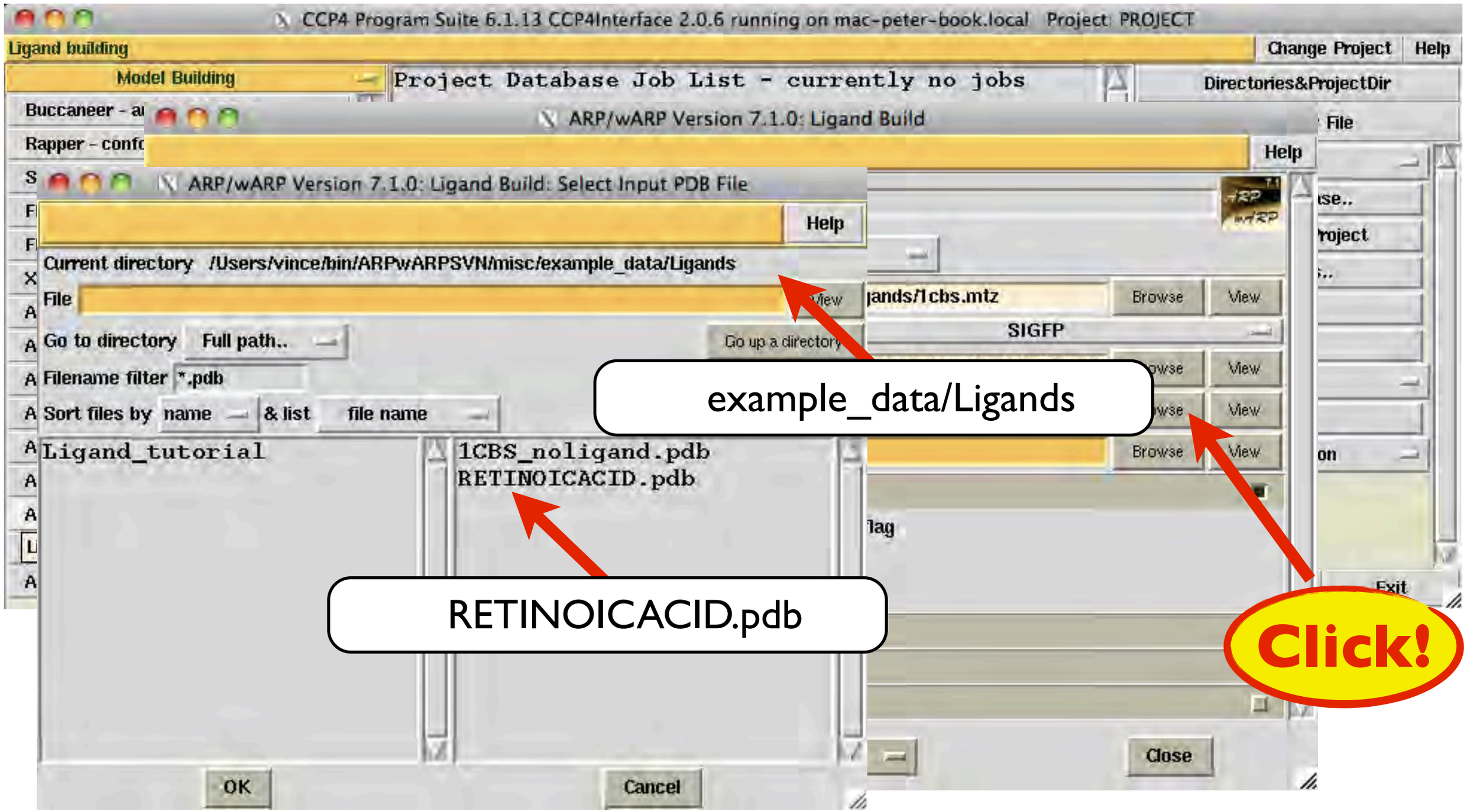
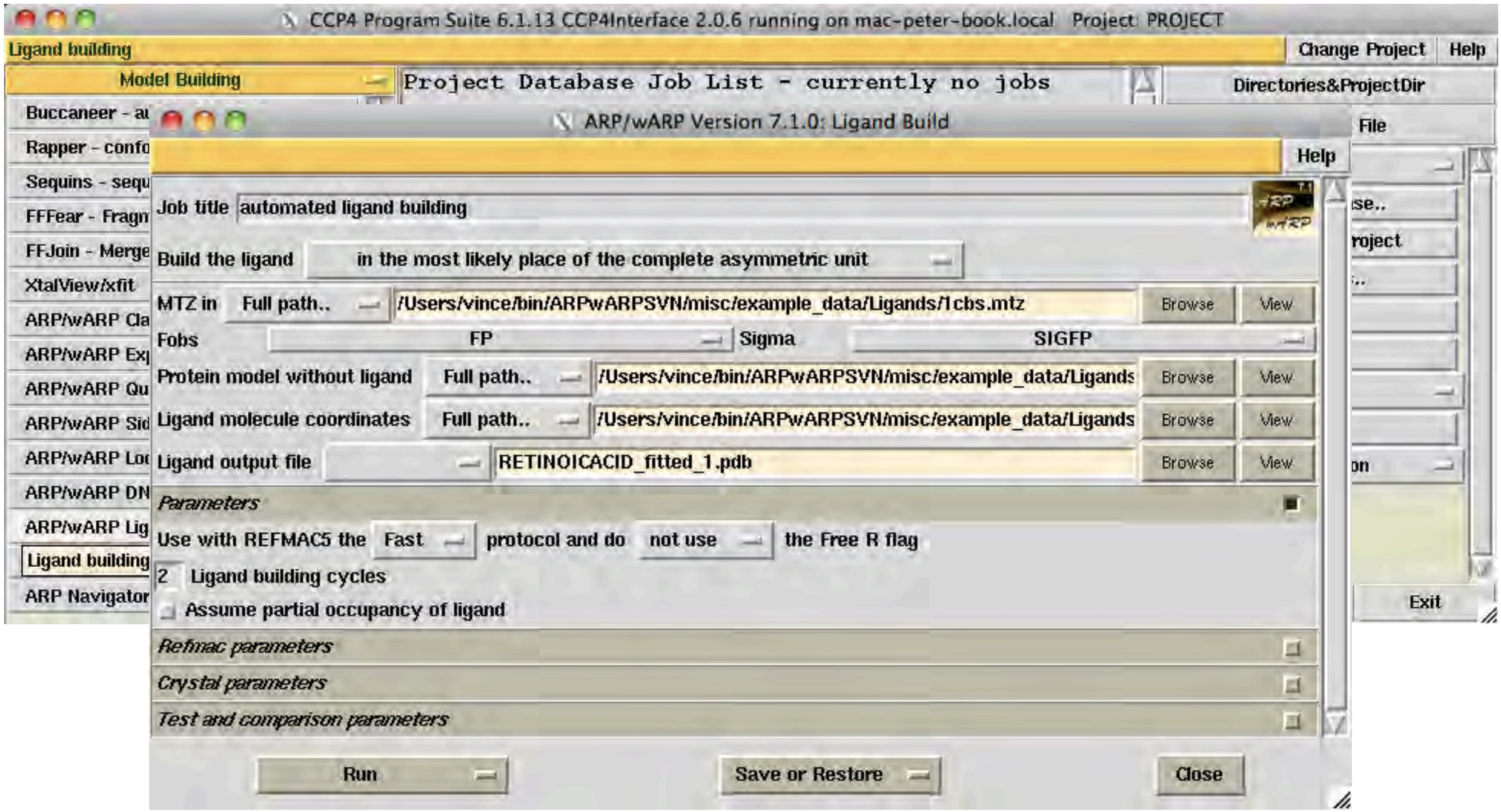


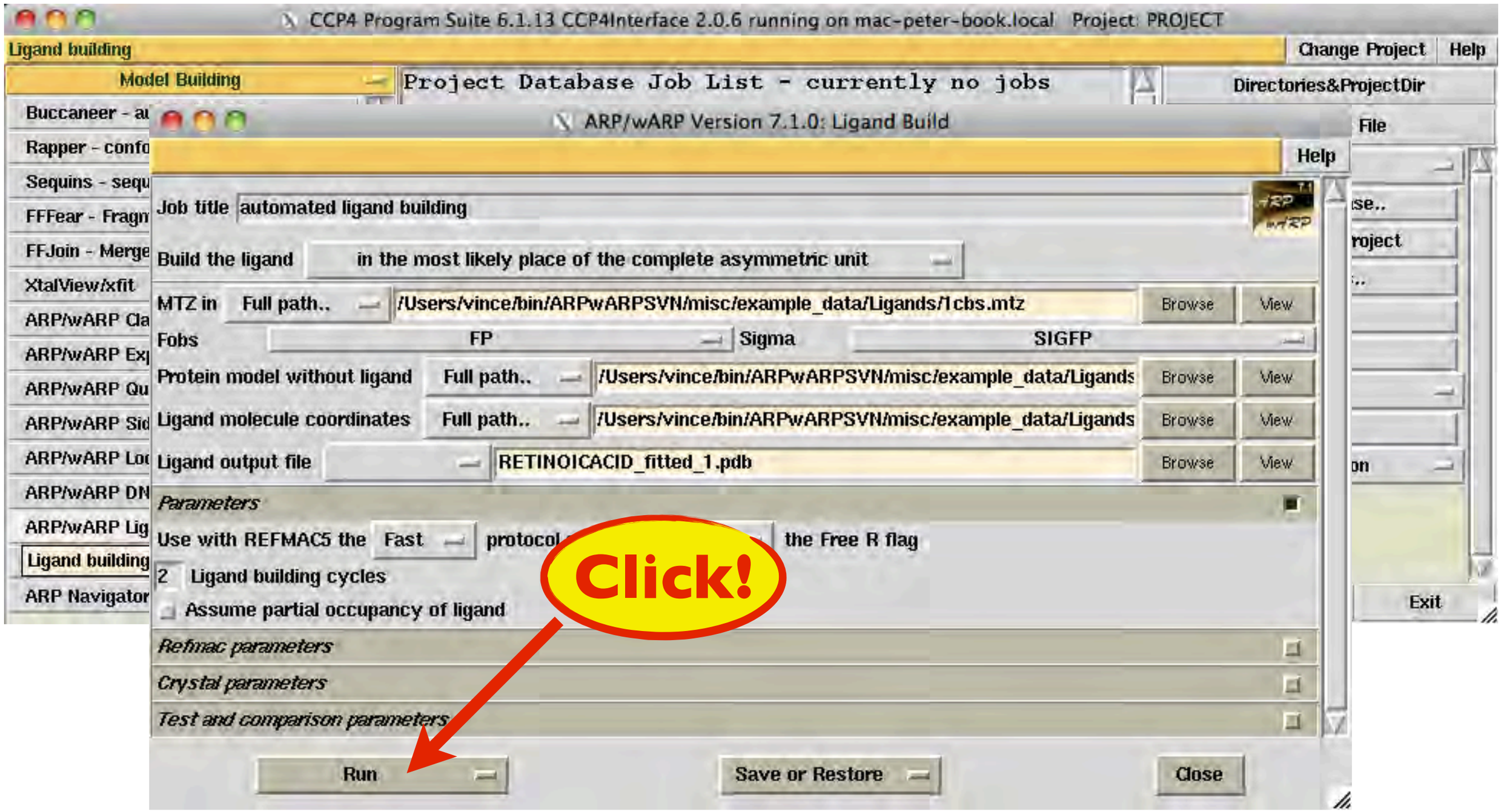
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA

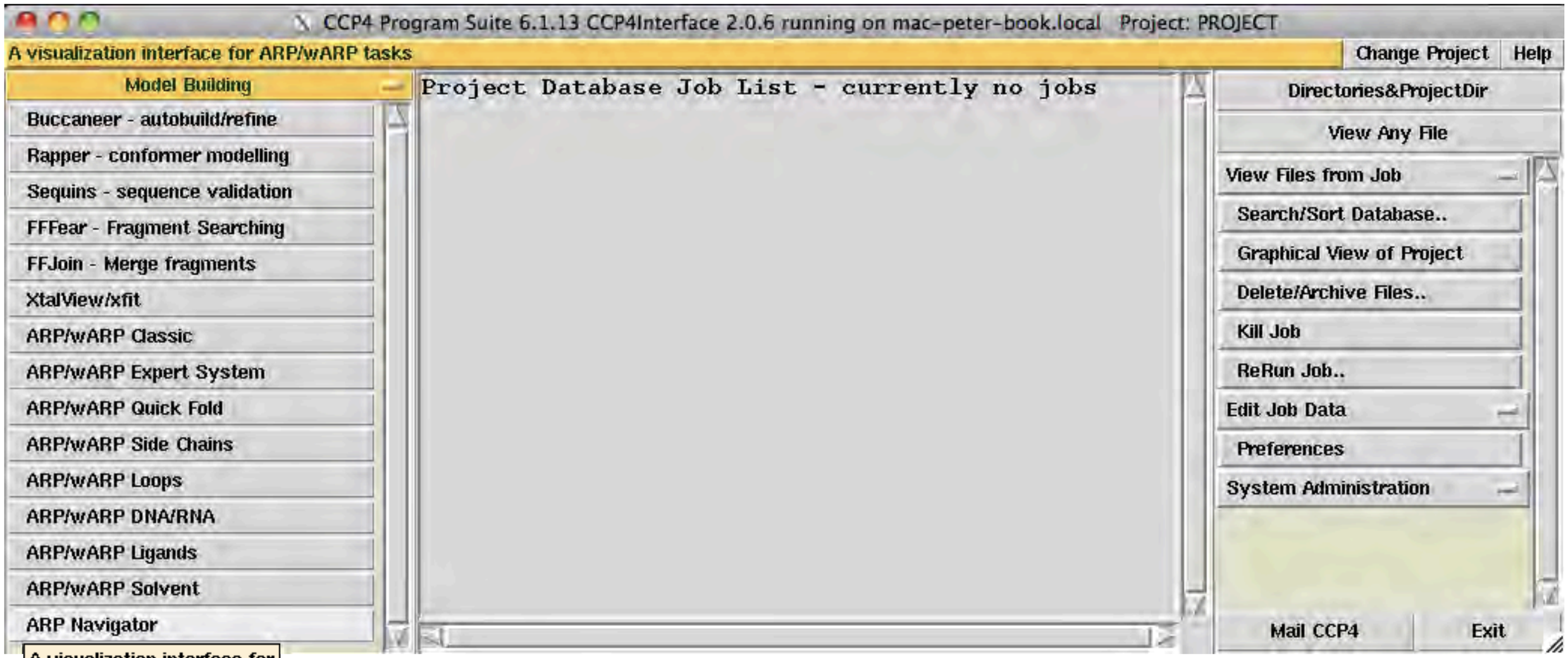


ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



ARP/wARP: ARPNavigator



ARP/wARP: ARPNavigator