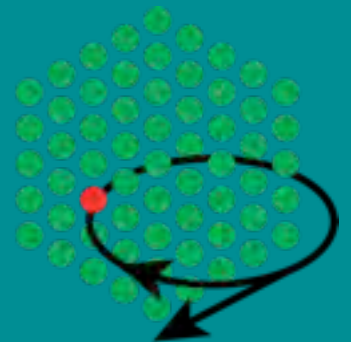


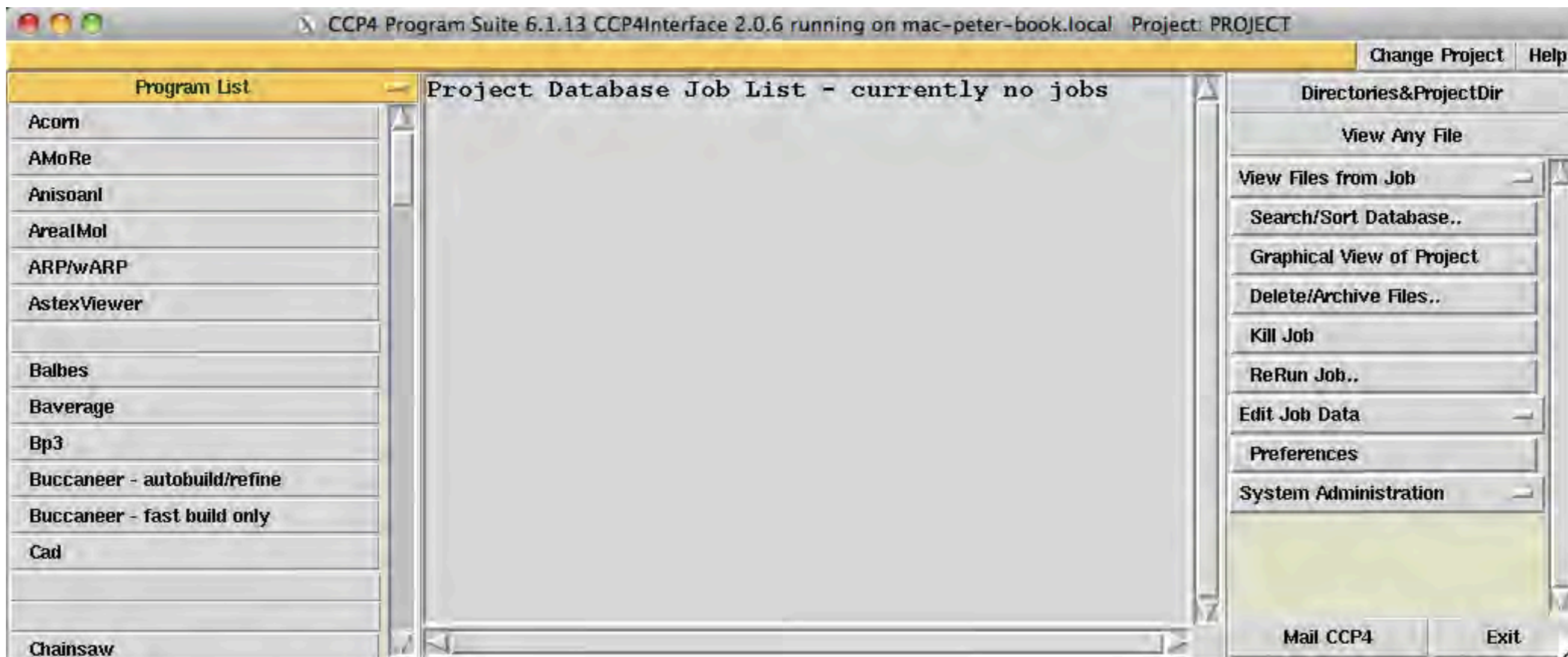
ARP/wARP Tutorial

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

EMBL



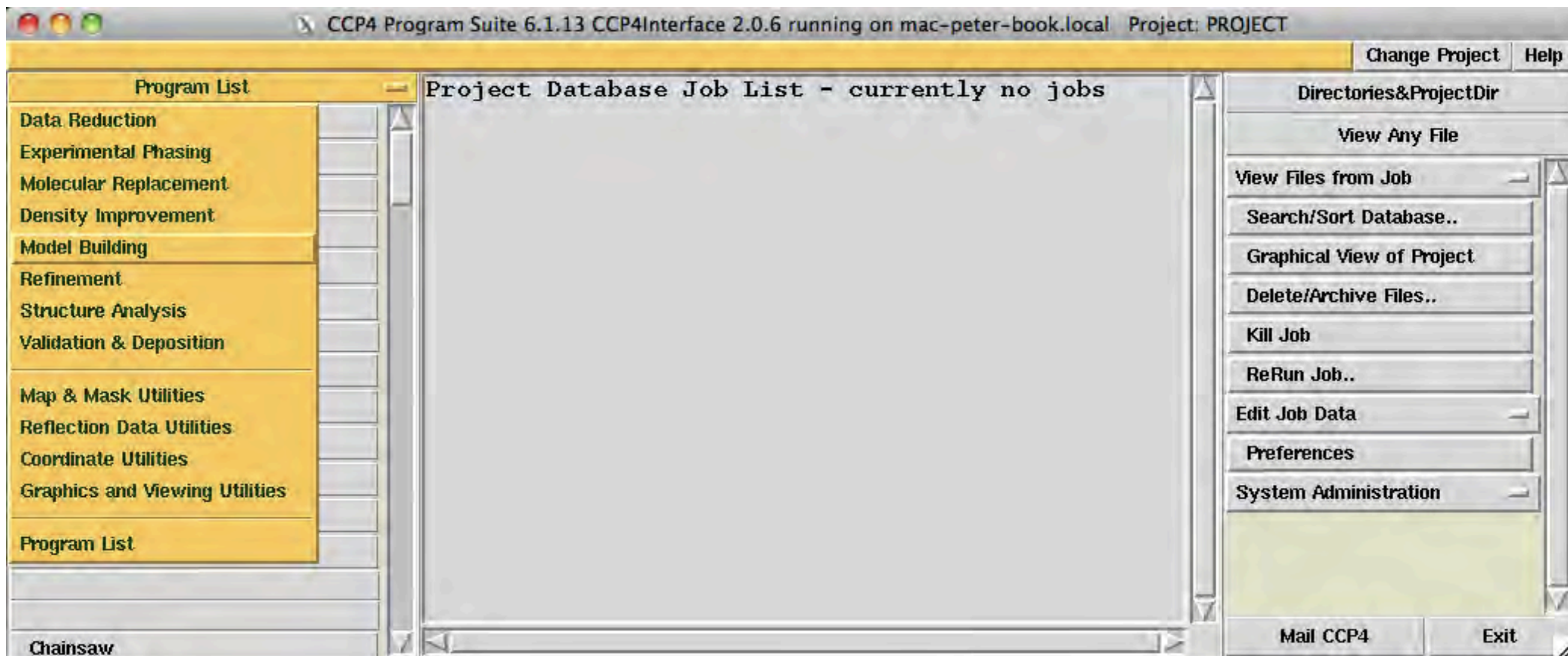
Where to go...



Where to go...



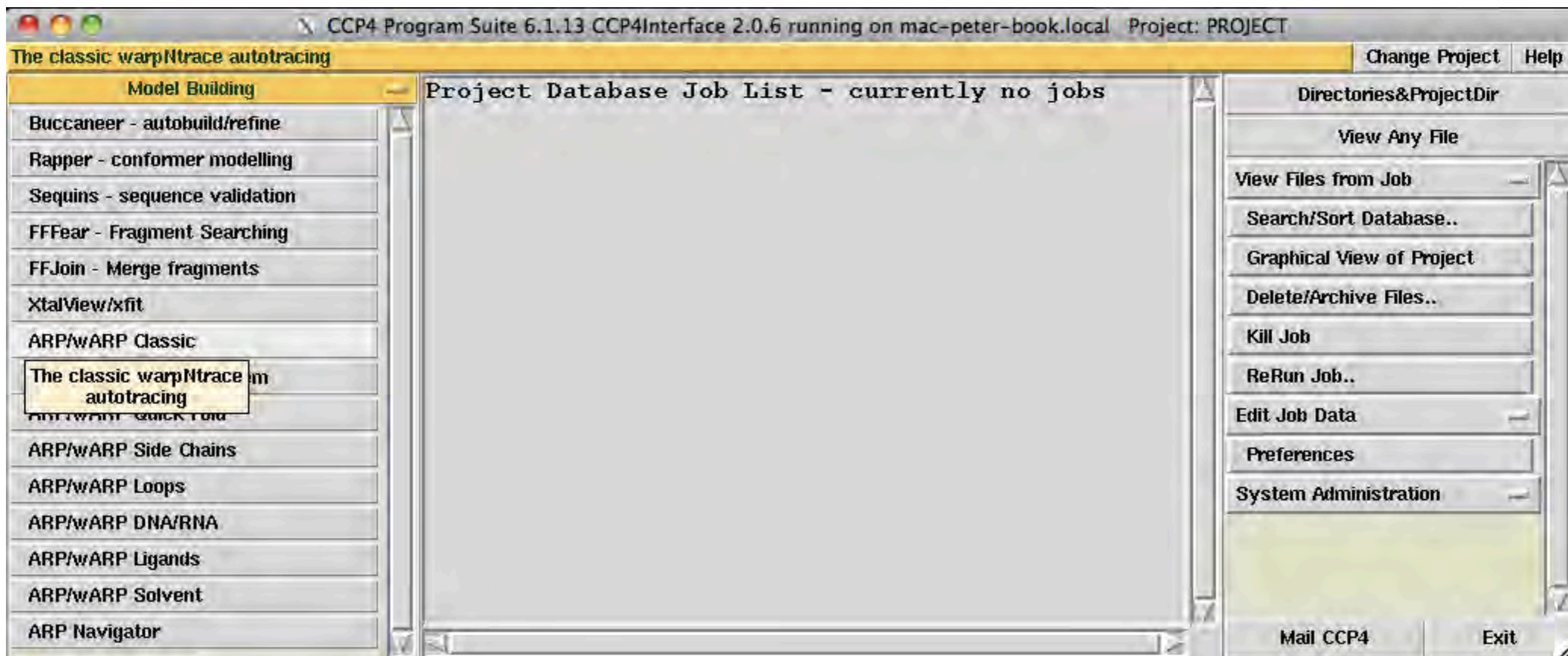
Where to go...



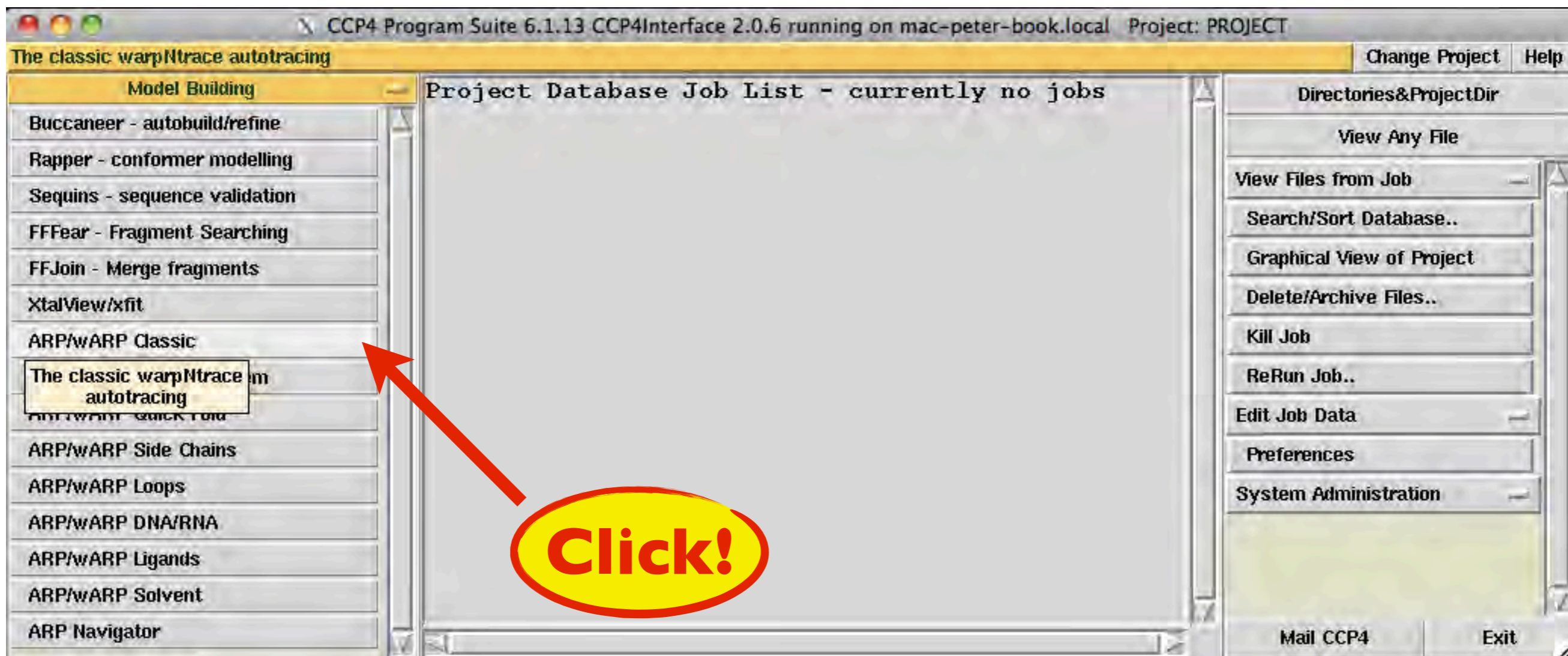
Where to go...



ARP/wARP: Tracing (warp_tracing)



ARP/wARP: Tracing (warp_tracing)



Testcase:

PSP / PDBID 1lml (Leishmanolysin)

Residues:

1 x 475 AA

Resolution:

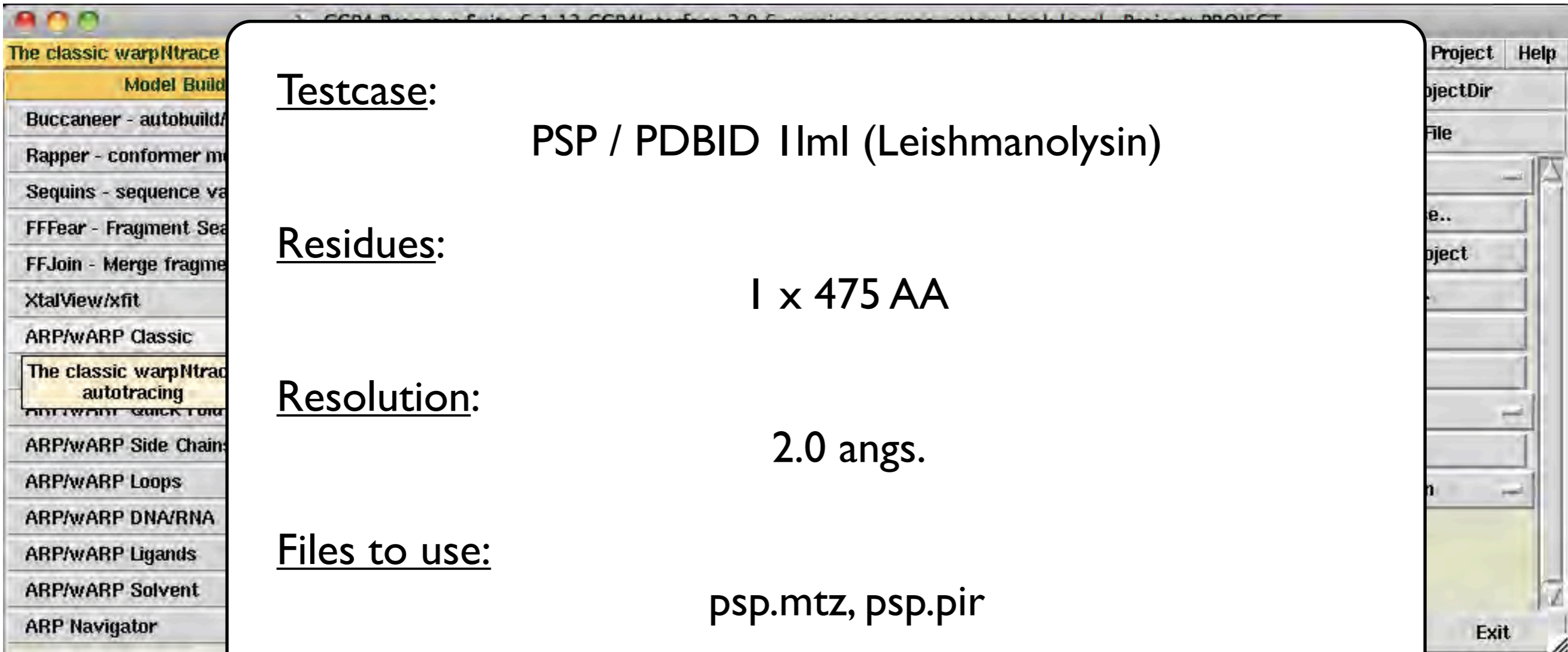
2.0 ang.

Files to use:

psp.mtz, psp.pir

MTS labels to use:

FP, SIGFP, PHIDM, FOMDM



ARP/wARP: Tracing (warp_tracing)

PSP

The screenshot displays the ARP/wARP Version 7.1.0: Model Building and Density Improvement window. The interface includes a menu bar with 'Change Project' and 'Help'. Below the menu bar, there are several tabs: 'Model Building', 'Project Database Job List - currently no jobs', and 'Directories&ProjectDir'. The main window contains the following fields and options:

- Job title:** automated model building starting from experimental phases
- Run ARP/wARP for:** automated model building starting from experimental phases
- MTZ in:** [Yellowed out] Browse View
- Fobs:** [Yellowed out] Sigma [Yellowed out]
- PHIB:** [Yellowed out] FOM [Yellowed out]
- Sequence in:** [Yellowed out] Browse View
- Required parameters:** There are [Yellowed out] total residues in the AU, which belong to [1] molecule(s). Do [10] cycles of autobuilding ([50] total cycles). Use in REFMAC5 the [Maximum Likelihood] target function and do [not use] the Free R flag. This a Se-Methionine substituted protein
- ARP/wARP flow parameters:**
- Refmac parameters:**
- Crystal parameters:**
- Submit a remote job at the Hamburg Cluster:** Submit the job for remote execution at the Hamburg cluster

Buttons at the bottom include 'Run', 'Save or Restore', and 'Close'. A sidebar on the right contains a 'View Any File' section and a list of files from the job.

ARP/wARP: Tracing (warp_tracing)

PSP

The screenshot shows the ARP/wARP Version 7.1.0: Model Building and Density Improvement window. The window title is "The classic warpNtrace autotracing". The main area contains the following fields and options:

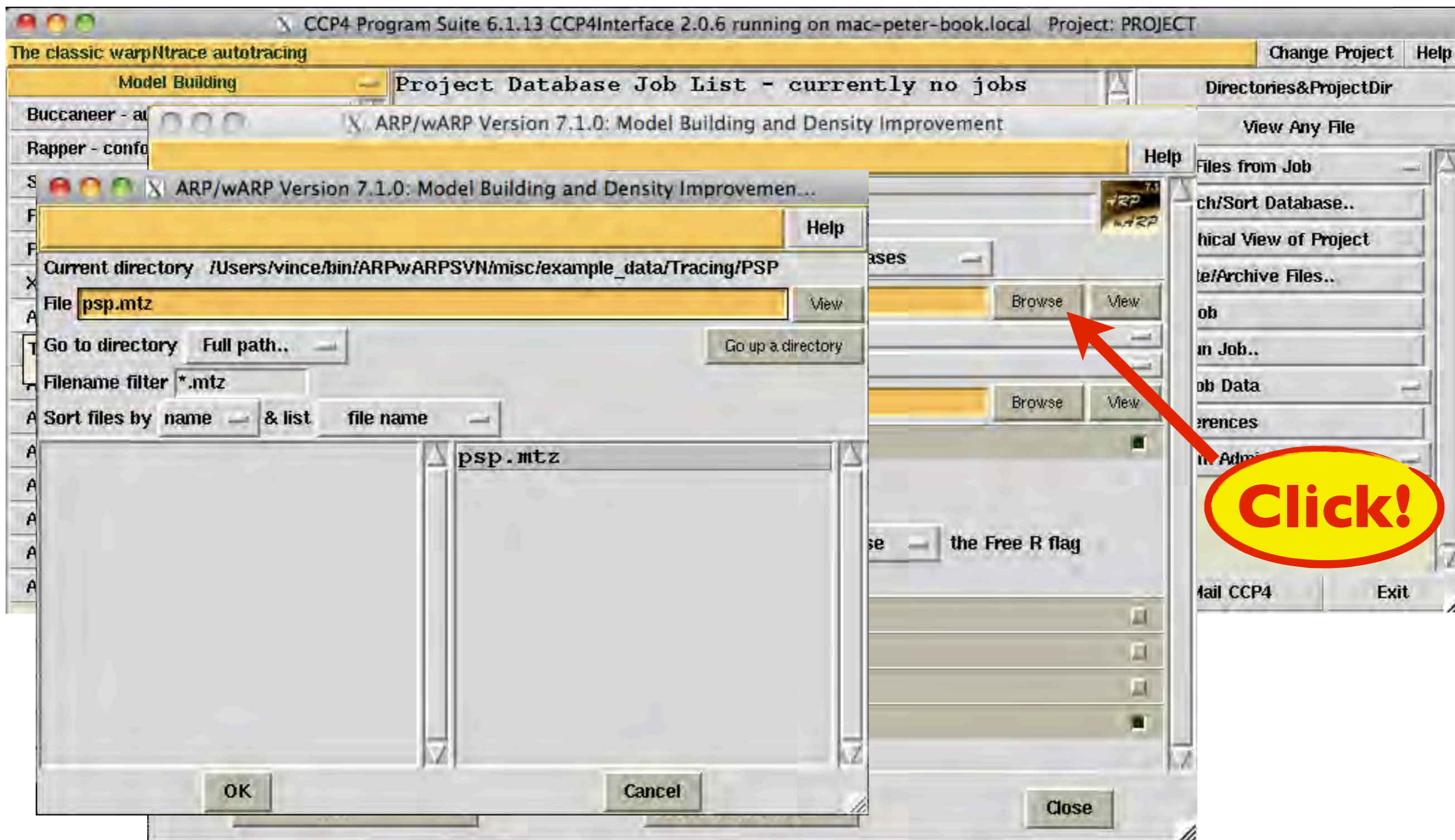
- Job title: automated model building starting from experimental phases
- Run ARP/wARP for: automated model building starting from experimental phases
- MTZ in: [empty field] Browse View
- Fobs: [empty field] Sigma: [empty field]
- PHIB: [empty field] FOM: [empty field]
- Sequence in: [empty field] Browse View
- Required parameters: There are [empty field] total residues in the AU, which belong to [1] molecule(s).
- Do [10] cycles of autobuilding ([50] total cycles).
- Use in REFMAC5 the [Maximum Likelihood] target function and do [not use] the Free R flag
- This a Se-Methionine substituted protein
- ARP/wARP flow parameters:
- Refmac parameters:
- Crystal parameters:
- Submit a remote job at the Hamburg Cluster:
- Submit the job for remote execution at the Hamburg cluster:

Buttons at the bottom: Run, Save or Restore, Close.

A red arrow points to the "Browse" button next to the "MTZ in" field. A yellow oval with the text "Click!" is overlaid on the right side of the window.

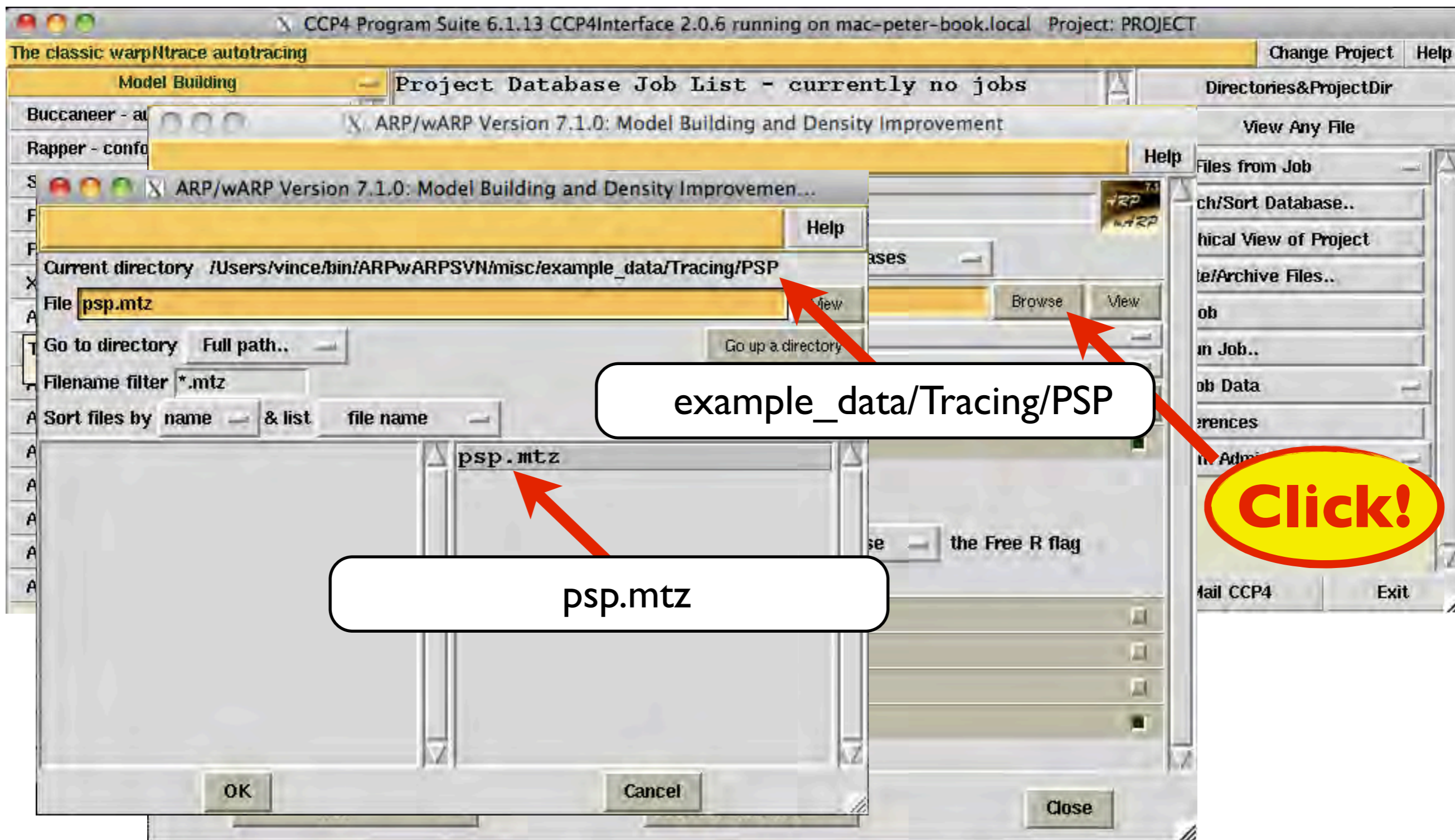
ARP/wARP: Tracing (warp_tracing)

PSP



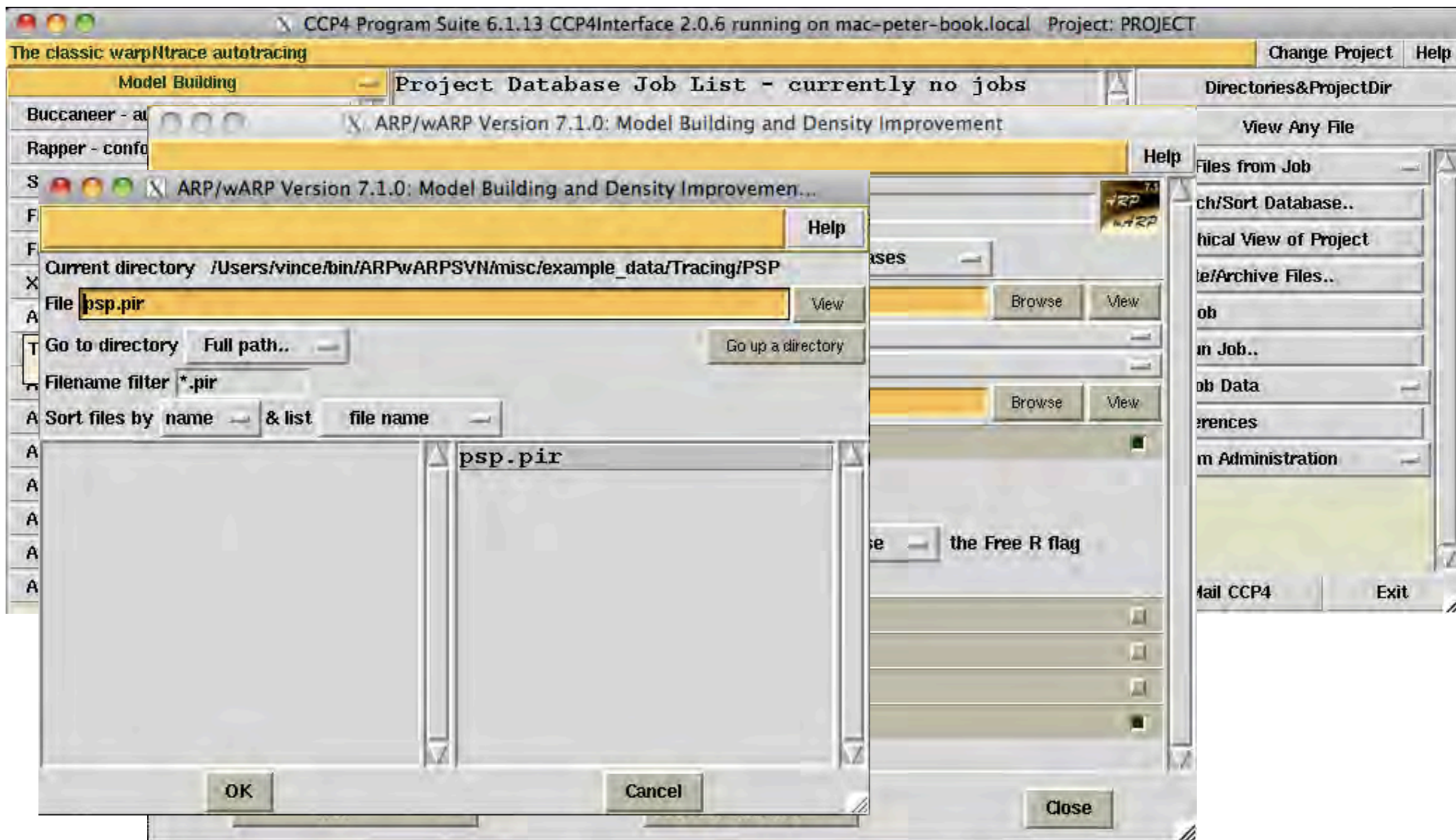
ARP/wARP: Tracing (warp_tracing)

PSP



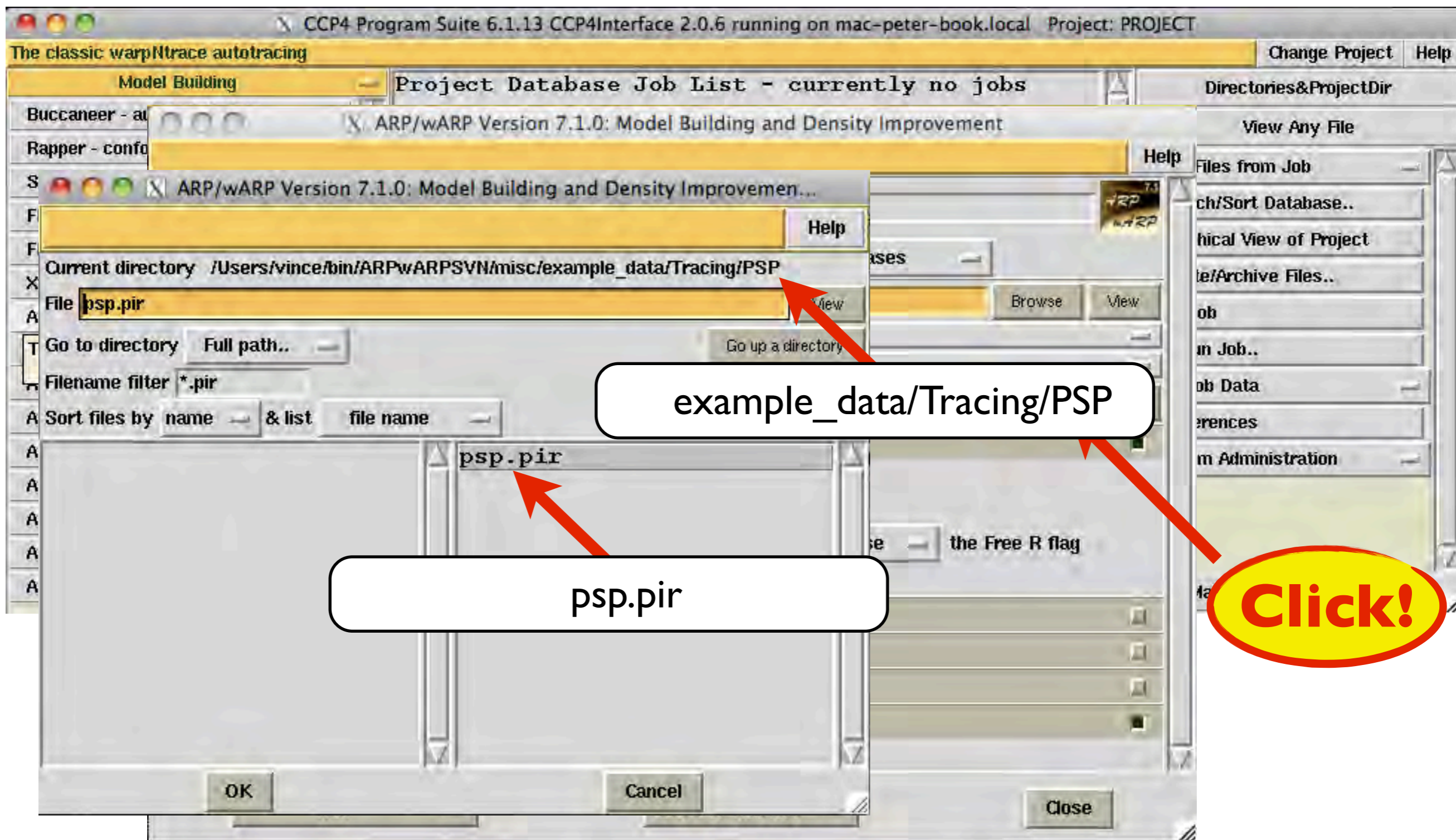
ARP/wARP: Tracing (warp_tracing)

PSP



ARP/wARP: Tracing (warp_tracing)

PSP



ARP/wARP: Tracing (warp_tracing)

PSP

The screenshot displays the ARP/wARP Version 7.1.0 interface. The main window is titled 'The classic warp/trace autotracing' and shows a 'Project Database Job List - currently no jobs'. The 'Job title' is 'automated model building starting from experimental phases'. The 'Run ARP/wARP for' field is also set to 'automated model building starting from experimental phases'. The 'MTZ in' field is set to '/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/PSP/ps'. The 'Sequence in' field is set to '/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/F'. The 'Required parameters' section shows '475' total residues in the AU, belonging to '1' molecule(s), with '10' cycles of autobuilding (50 total cycles). The 'Use in REFMAC5' target function is set to 'Maximum Likelihood' and the 'Free R flag' is set to 'not use'. The 'Submit a remote job at the Hamburg Cluster' checkbox is checked. The interface includes buttons for 'Run', 'Save or Restore', and 'Close'. A sidebar on the right contains various file management options like 'View Any File', 'Files from Job', and 'Mail CCP4'.

ARP/wARP: Tracing (warp_tracing)

PSP

The screenshot displays the ARP/wARP Version 7.1.0 interface. The main window is titled "The classic warp/trace autotracing" and shows a "Project Database Job List - currently no jobs". The "Job title" is "automated model building starting from experimental phases". The "Run ARP/wARP for" field is also "automated model building starting from experimental phases". The "MTZ in" field is "/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/PSP/ps". The "Sequence in" field is "/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/F". The "Required parameters" section shows "There are 475 total residues in the AU, which belong to 1 molecule(s)." and "Do 10 cycles of autobuilding (50 total cycles)". The "Use in REFMAC5 the" field is "Maximum Likelihood" and "do" is "not use". The "Free R flag" is "not use". The "475" value is highlighted in a white callout box with the text "475 Residues".

ARP/wARP: Tracing (warp_tracing)

PSP

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

The classic warp/trace autotracing

Model Building Project Database Job List - currently no jobs

ARP/wARP Version 7.1.0: Model Building and Density Improvement

Job title automated model building starting from experimental phases

Run ARP/wARP for automated model building starting from experimental phases

MTZ in Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/PSP/ps Browse View

Fobs FP Sigma SIGFP

PHIB PHIDM FOM FOMDM

Sequence in Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/F Browse View

Required parameters

There are 475 total residues in the AU, which belong to 1 molecule(s).

Do 10 cycles of autobuilding (50 total cycles).

Use in REFMAC5 the Maximum Likelihood target function and do not use the Free R flag

This a Se-Methionine substituted protein

ARP/wARP flow parameters

Refmac parameters

Crystal parameters

Generate map in space group C2

Cell a= 107.1900 b= 90.6100 c= 70.5900 alpha= 90.0000 beta= 110.5700 gamma= 90.0000

ARP/wARP asymmetric unit 0.0 0.5 0.0 1.0 0.0 0.5

Wilson B factor 17.7 Solvent content 0.6

Use reflections between 19.842 and 2.000 Angstrom

Submit a remote job at the Hamburg Cluster

Submit the job for remote execution at the Hamburg cluster

Run Save or Restore Close

Directories&ProjectDir

View Any File

Files from Job

ch/Sort Database..

hical View of Project

te/Archive Files..

ob

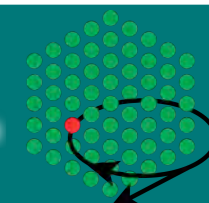
in Job..

ob Data

erences

m Administration

Mail CCP4 Exit



ARP/wARP: Tracing (warp_tracing)

PSP

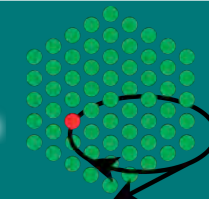
The screenshot displays the ARP/wARP Version 7.1.0: Model Building and Density Improvement interface. The main window is titled "The classic warp/trace autotracing" and shows a "Project Database Job List - currently no jobs". The "Job title" is "automated model building starting from experimental phases". The "Run ARP/wARP for" field is also "automated model building starting from experimental phases". The "MTZ in" field is set to "/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/PSP/ps". The "Fobs" field is "FP" and "Sigma" is "SIGFP". The "PHIB" field is "PHIDM" and "FOM" is "FOMDM". The "Sequence in" field is "/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/F".

Under "Required parameters", it states: "There are 475 total residues in the AU, which belong to 1 molecule(s). Do 10 cycles of autobuilding (50 total cycles). Use in REFMAC5 the Maximum Likelihood target function and do not use the Free R flag. This a Se-Methionine substituted protein".

Under "ARP/wARP flow parameters", "Refmac parameters", and "Crystal parameters", it shows: "Generate map in space group C2", "Cell a= 107.1900 b= 90.6100 c= 70.5900 alpha= 90.0000 beta= 110.5700 gamma= 90.0000", "ARP/wARP asymmetric unit 0.0 0.5 0.0 1.0 0.0 0.5", "Wilson B factor 17.7 Solvent content 0.6", and "Use reflections between 19.842 and 2.000 Angstrom".

A callout box with a red arrow points to the resolution value "2.000" in the "Use reflections between" field, with the text "Resolution: 2.0 Å".

At the bottom, there are buttons for "Run", "Save or Restore", and "Close".



ARP/wARP: Tracing (warp_tracing)

PSP

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

The classic warp/trace autotracing

Model Building Project Database Job List - currently no jobs

Directories&ProjectDir

View Any File

Files from Job

ch/Sort Database..

hical View of Project

te/Archive Files..

ob

in Job..

ob Data

erences

m Administration

Mail CCP4

Exit

ARP/wARP Version 7.1.0: Model Building and Density Improvement

Job title automated model building starting from experimental phases

Run ARP/wARP for automated model building starting from experimental phases

MTZ in Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/PSP/ps Browse View

Fobs FP Sigma SIGFP

PHIB PHIDM FOM FOMDM

Sequence in Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/F Browse View

Required parameters

There are 475 total residues in the AU, which belong to 1 molecule(s).

Do 10 cycles of autobuilding (50 total cycles).

Use in REFMAC5 the Maximum Likelihood target function and do not use the Free R flag

This a Se-Methionine substituted protein

ARP/wARP flow parameters

Refmac parameters

Crystal parameters

Generate map in space group C2

Cell a= 107.1900 b= 90.6100 c= 70.5900 alpha= 90.0000 beta= 110.5700 gamma= 90.0000

ARP/wARP asymmetric unit 0.0 0.5 0.0 1.0 0.0 0.5

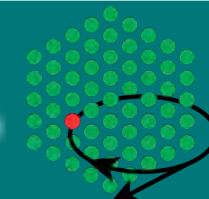
Wilson B factor 17.7 Solvent content 0.6

Use reflections between 19.842 and 2.000 Angstrom

Submit a remote job at the Hamburg Cluster

Submit the job for remote execution at the Hamburg cluster

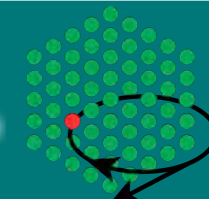
Run Save or Restore Close



ARP/wARP: Tracing (warp_tracing)

PSP

The screenshot displays the ARP/wARP Version 7.1.0: Model Building and Density Improvement interface. The window title is "CCP4 Program Suite 6.1.13 CCP4Interface 2.0.6 running on mac-peter-book.local Project: PROJECT". The main window is titled "The classic warp/trace autotracing" and contains a "Project Database Job List - currently no jobs" pane. The "Job title" is "automated model building starting from experimental phases". The "Run ARP/wARP for" field is also "automated model building starting from experimental phases". The "MTZ in" field is "/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/PSP/ps" with "Browse" and "View" buttons. The "Fobs" field is "FP" and "Sigma" is "SIGFP". The "PHIB" field is "PHIDM" and "FOM" is "FOMDM". The "Sequence in" field is "/Users/vince/bin/ARPwARPSVN/misc/example_data/Tracing/F" with "Browse" and "View" buttons. The "Required parameters" section shows "There are 475 total residues in the AU, which belong to 1 molecule(s)." and "Do 10 cycles of autobuilding (50 total cycles)." The "Use in REFMAC5 the Maximum Likelihood target function and do not use the Free R flag" is selected. The "This a Se-Methionine substituted protein" checkbox is unchecked. The "ARP/wARP flow parameters", "Refmac parameters", and "Crystal parameters" sections are also visible. The "Crystal parameters" section shows "Generate map in space group C2" and "Cell a= 107.1900 b= 90.6100 c= 70.5900 alpha= 90.0000 beta= 90.0000 gamma= 90.0000". The "Wilson B factor" is 17.7 and "Solvent content" is 0.6. The "Use reflections between 19.842 and 2.000 Angstrom" checkbox is checked. The "Submit a remote job at the Hamburg cluster" checkbox is also checked. A red arrow points to the "Run" button, which is highlighted with a yellow oval containing the text "Click!".



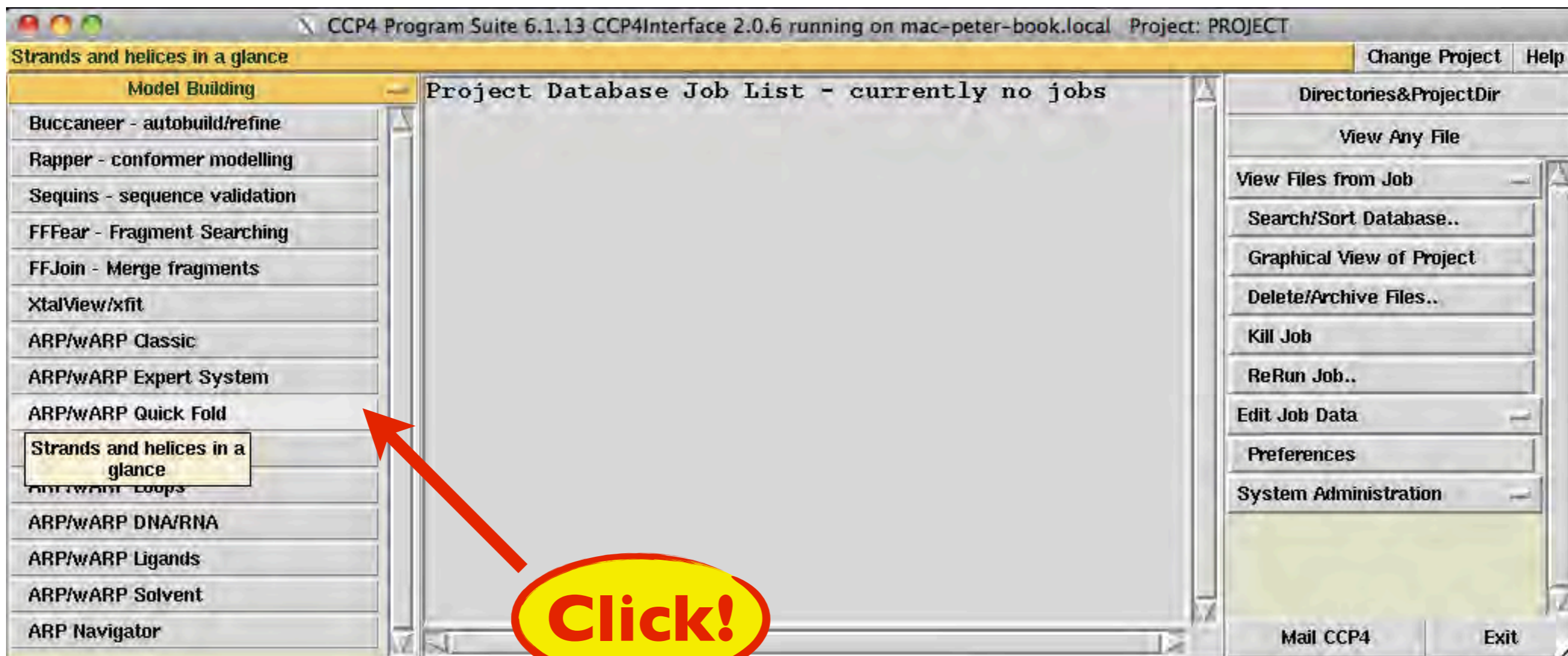
ARP/wARP: Secondary Structure (albe)

1014



ARP/wARP: Secondary Structure (albe)

1014



Testcase:

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

Residues:

2 x 331 (662) AA

Resolution:

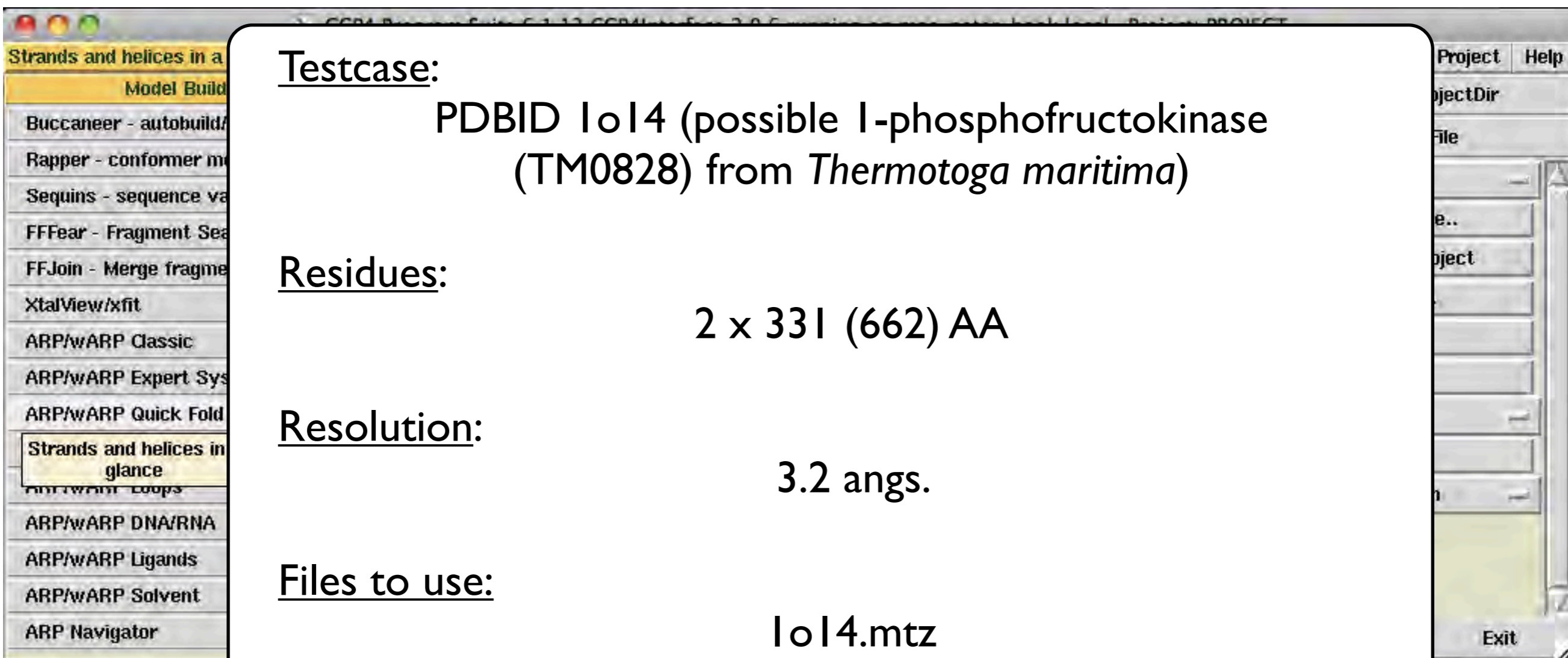
3.2 ang.

Files to use:

1o14.mtz

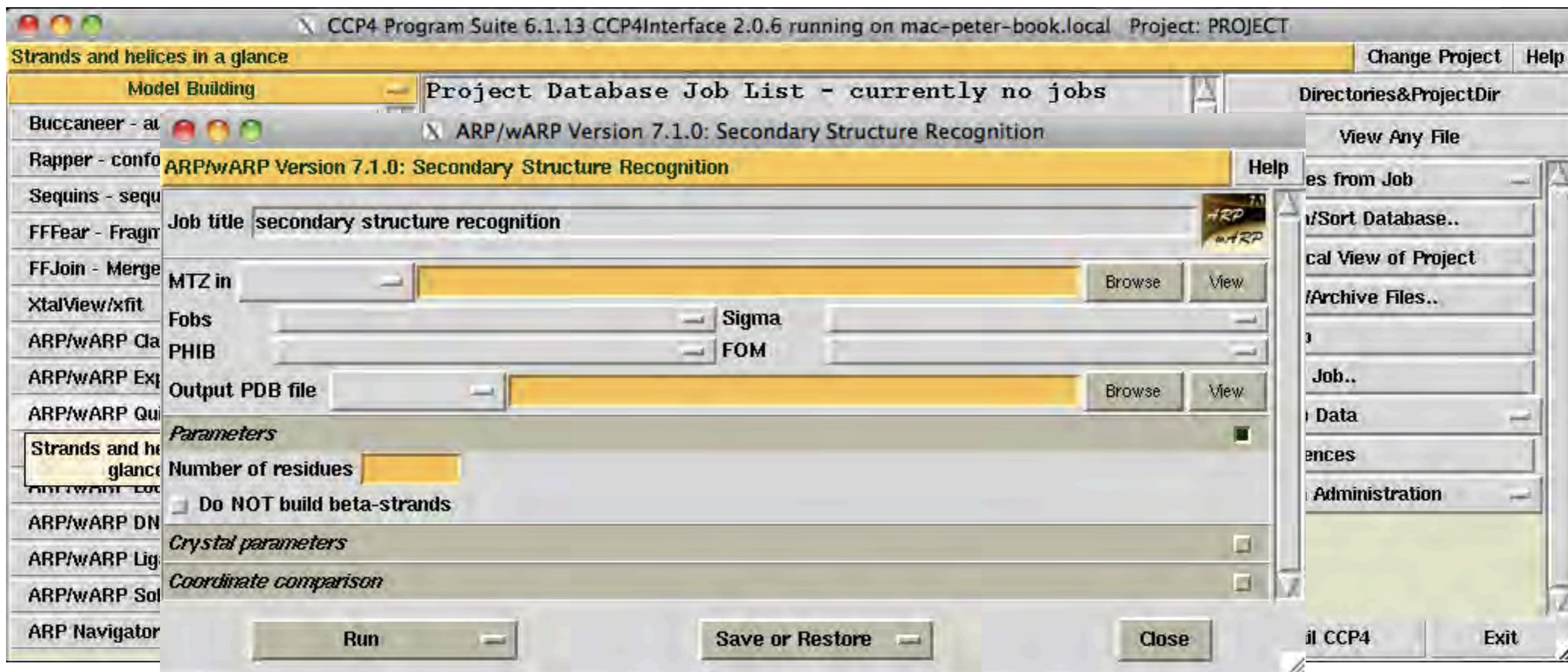
MTS labels to use:

F, PHIC, FOM



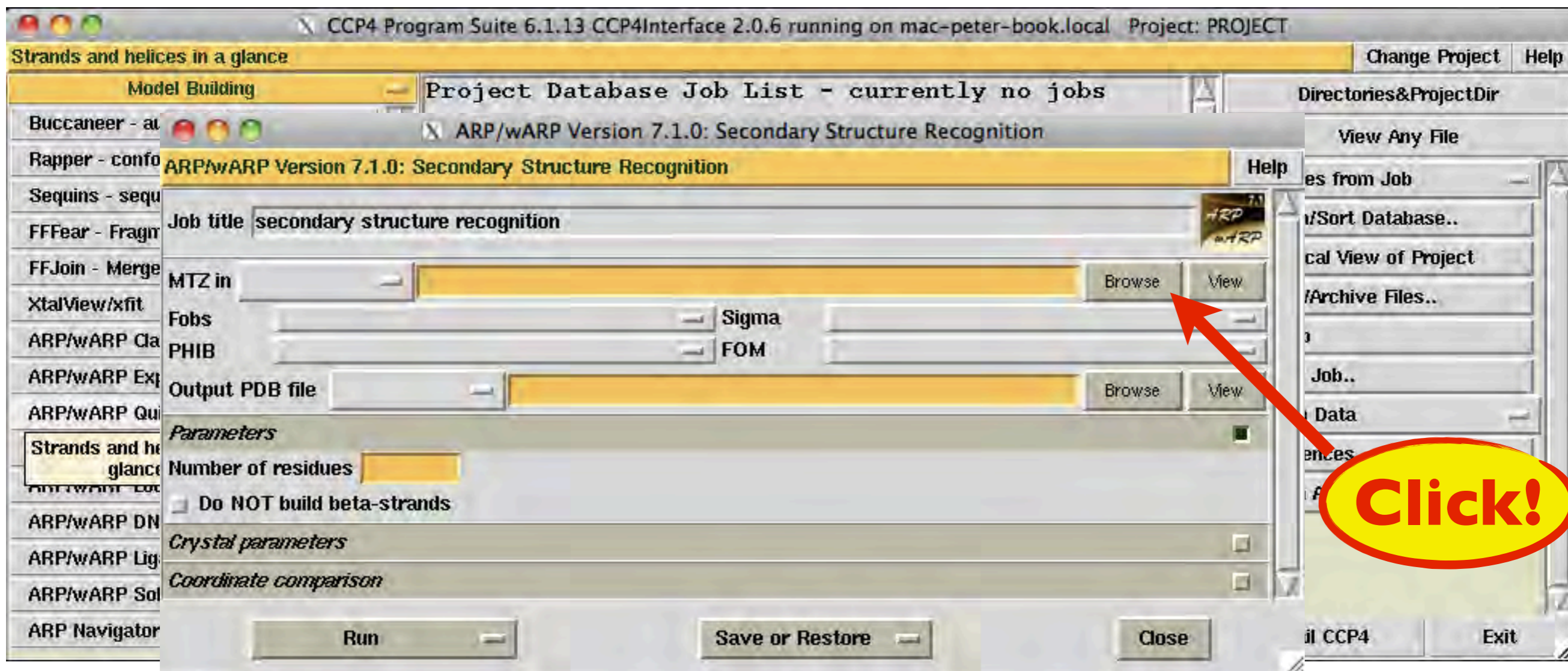
ARP/wARP: Secondary Structure (albe)

1014



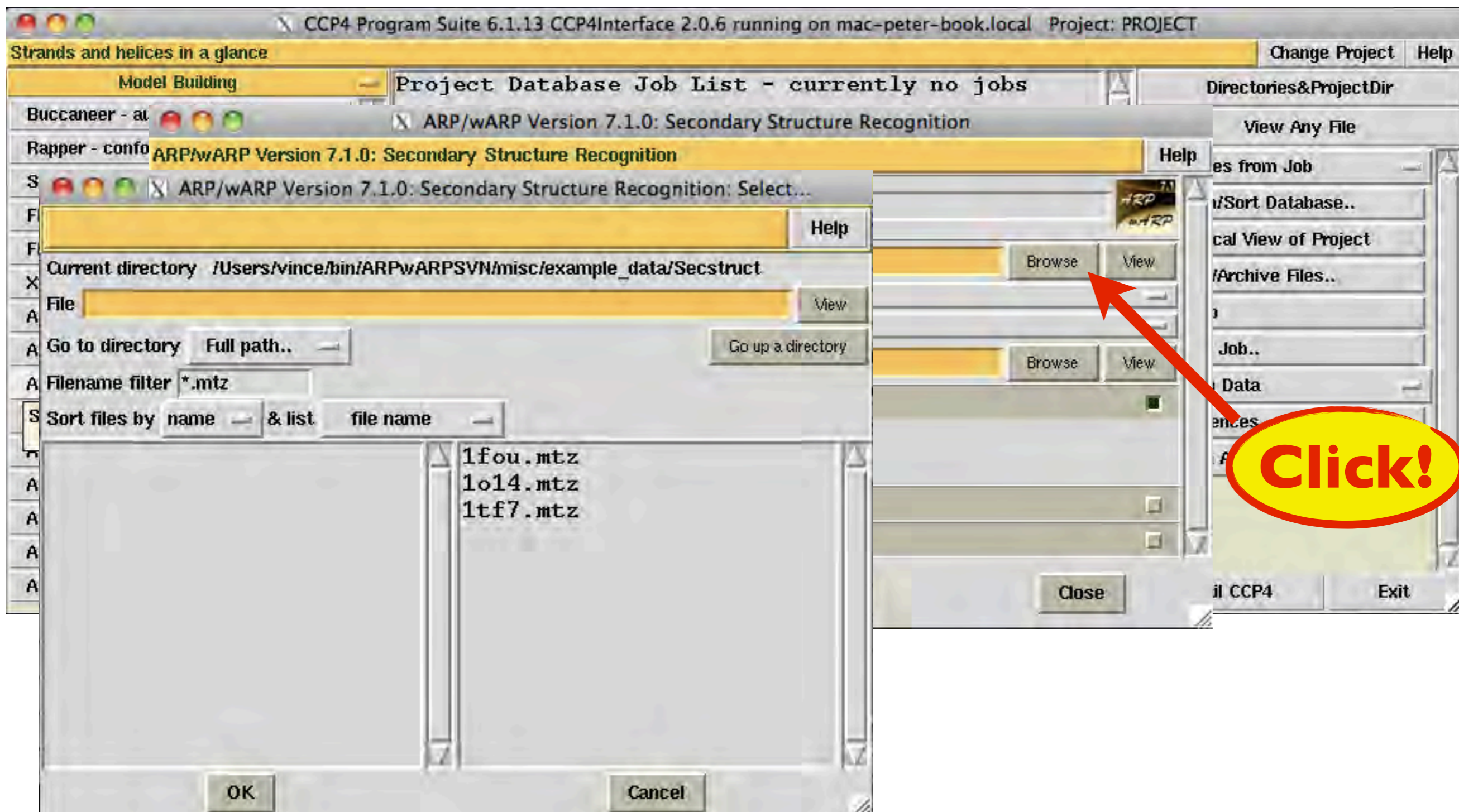
ARP/wARP: Secondary Structure (albe)

1014



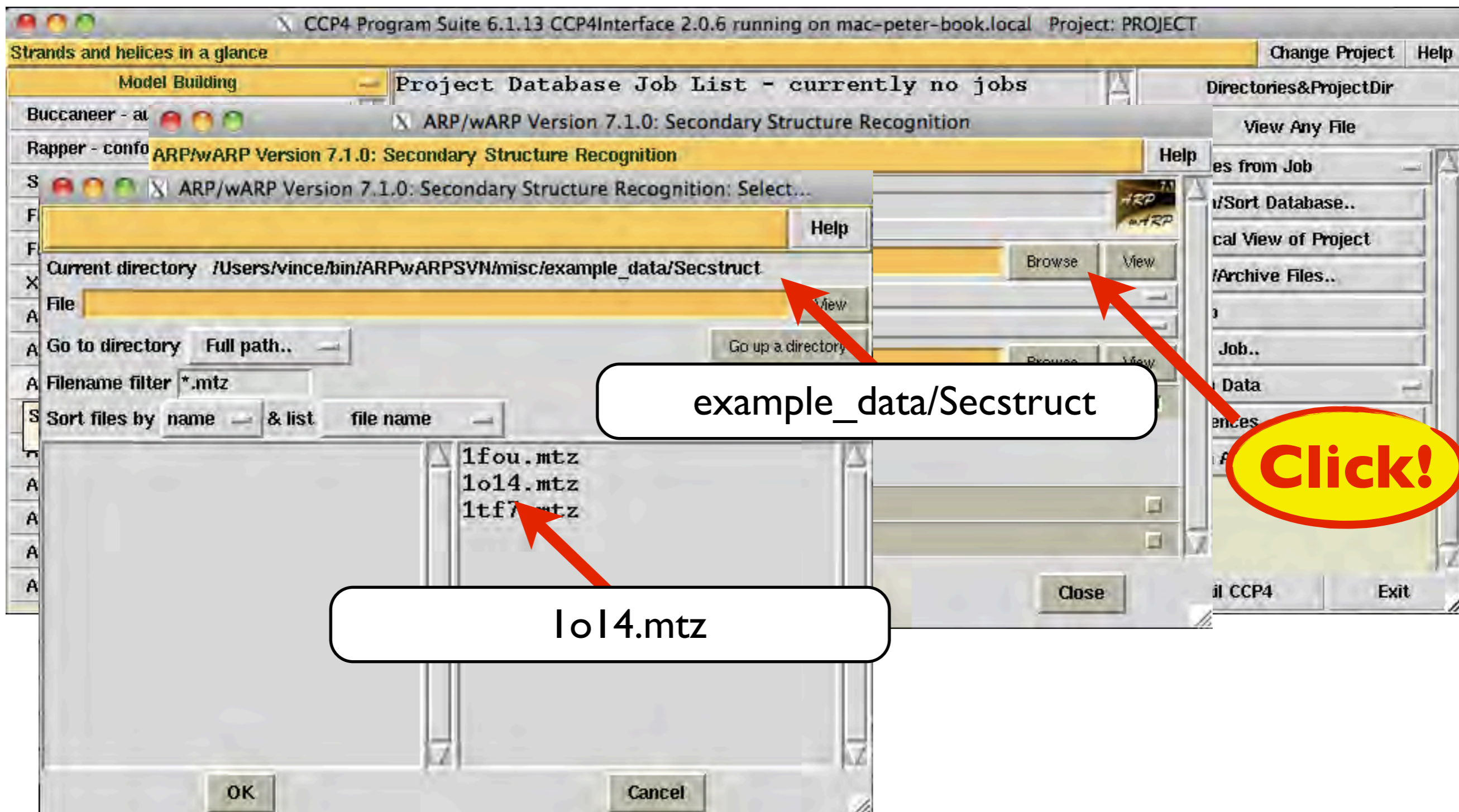
ARP/wARP: Secondary Structure (albe)

1o14



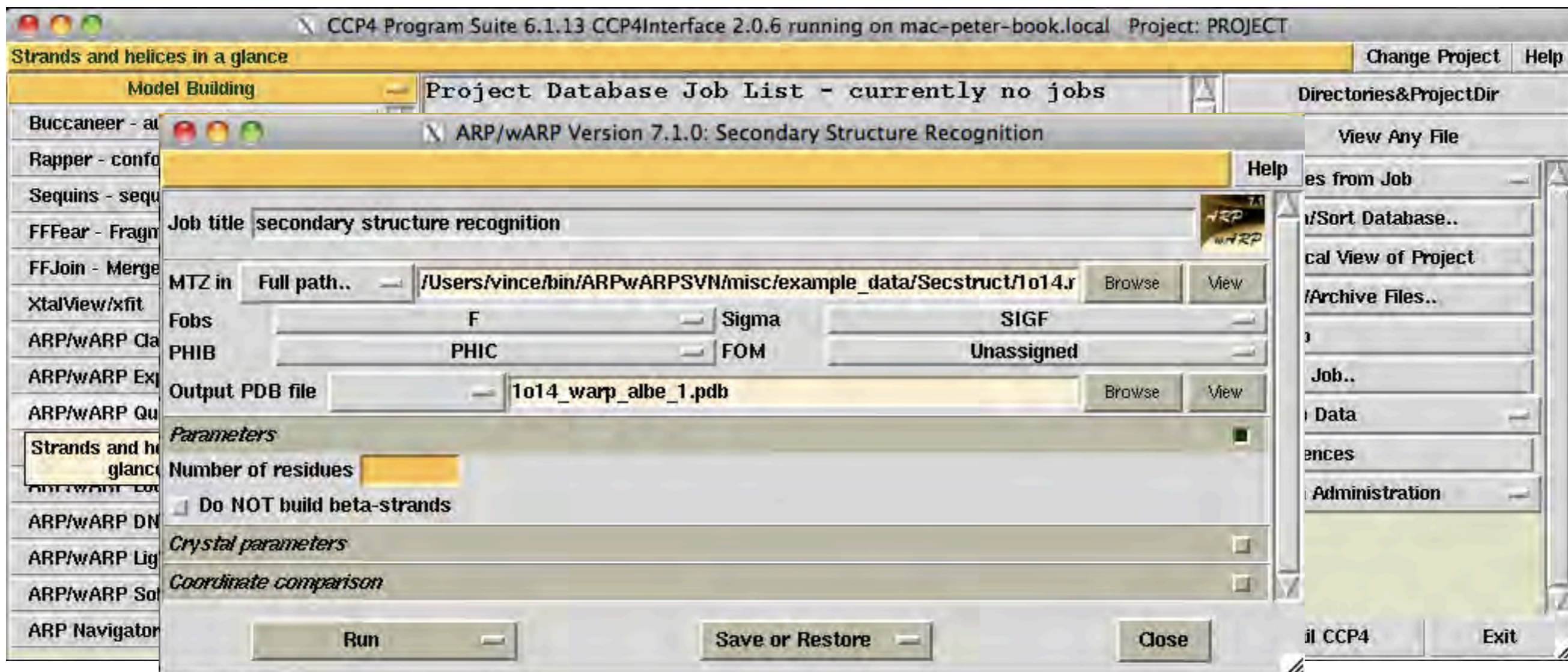
ARP/wARP: Secondary Structure (albe)

lo14



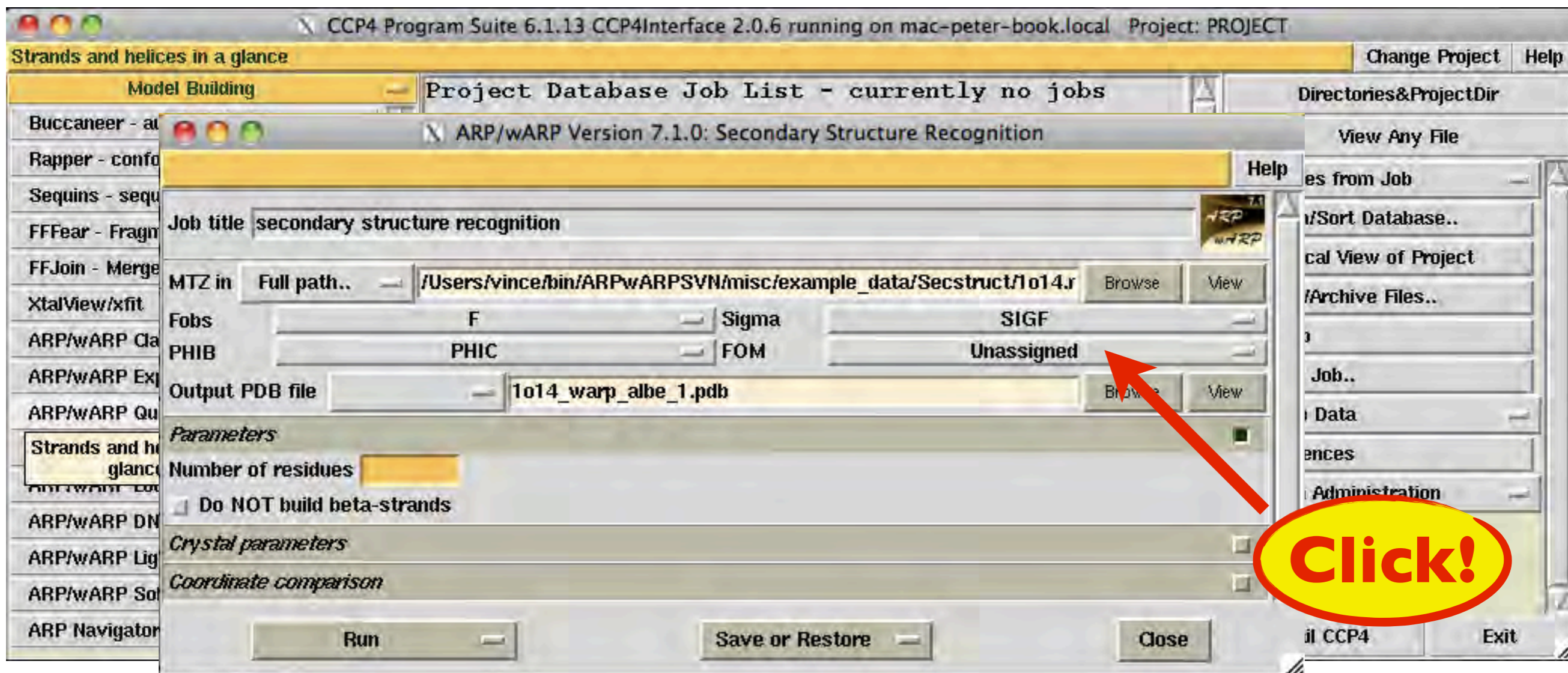
ARP/wARP: Secondary Structure (albe)

1o14



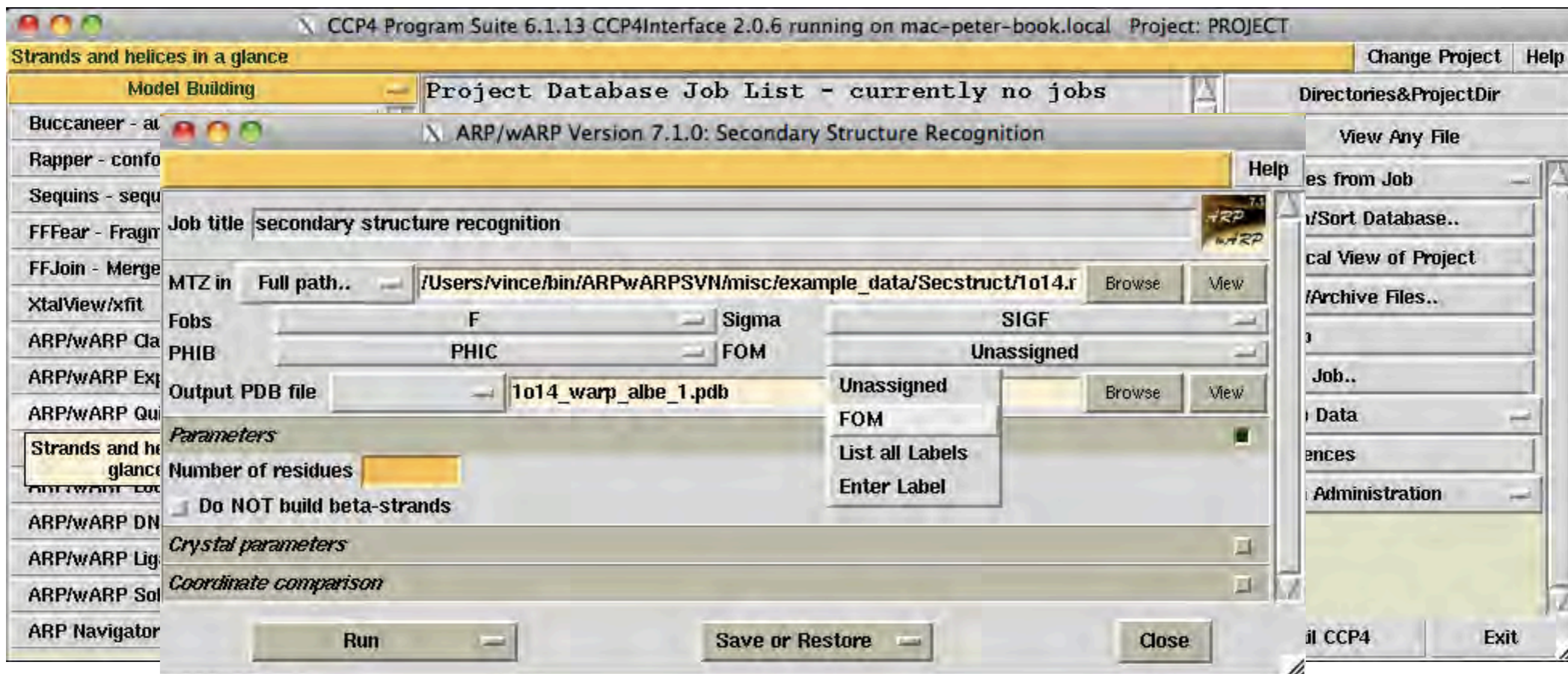
ARP/wARP: Secondary Structure (albe)

1o14



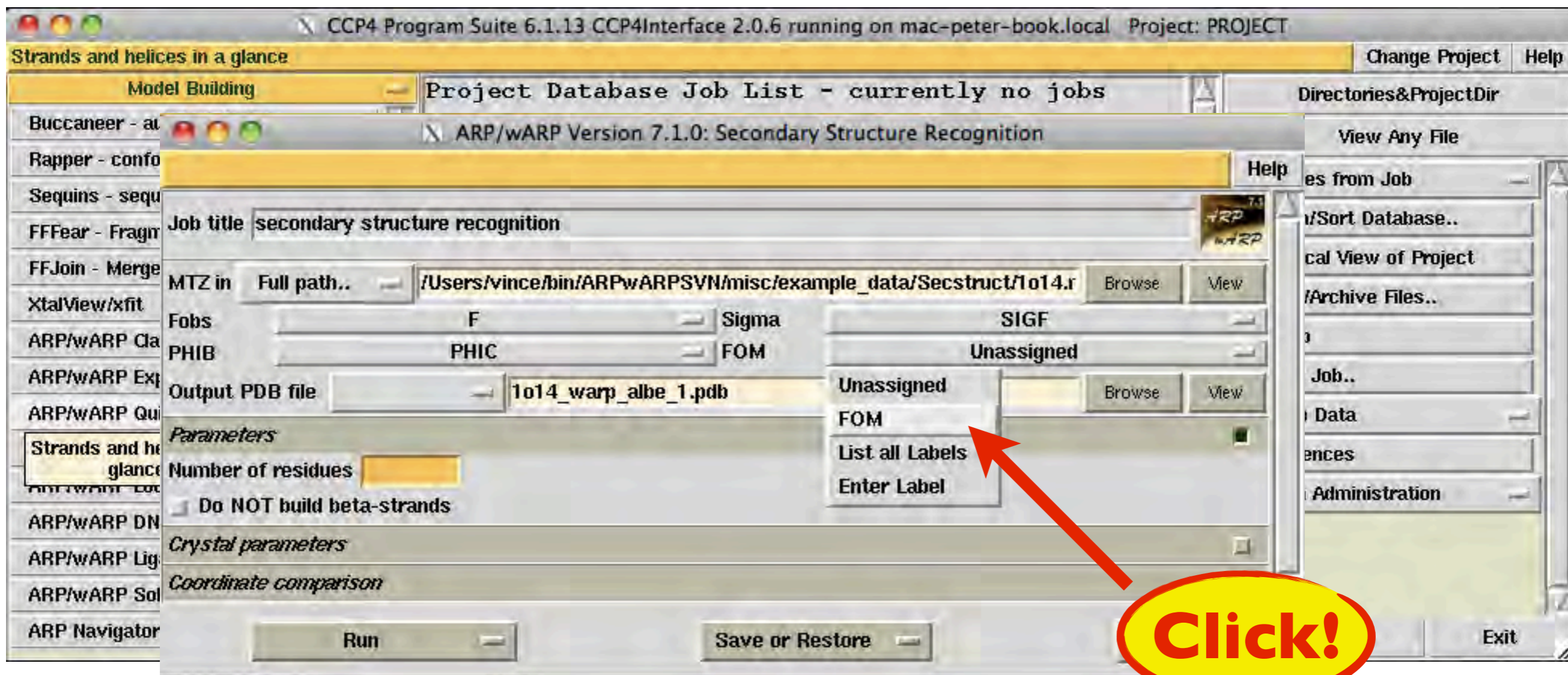
ARP/wARP: Secondary Structure (albe)

1o14



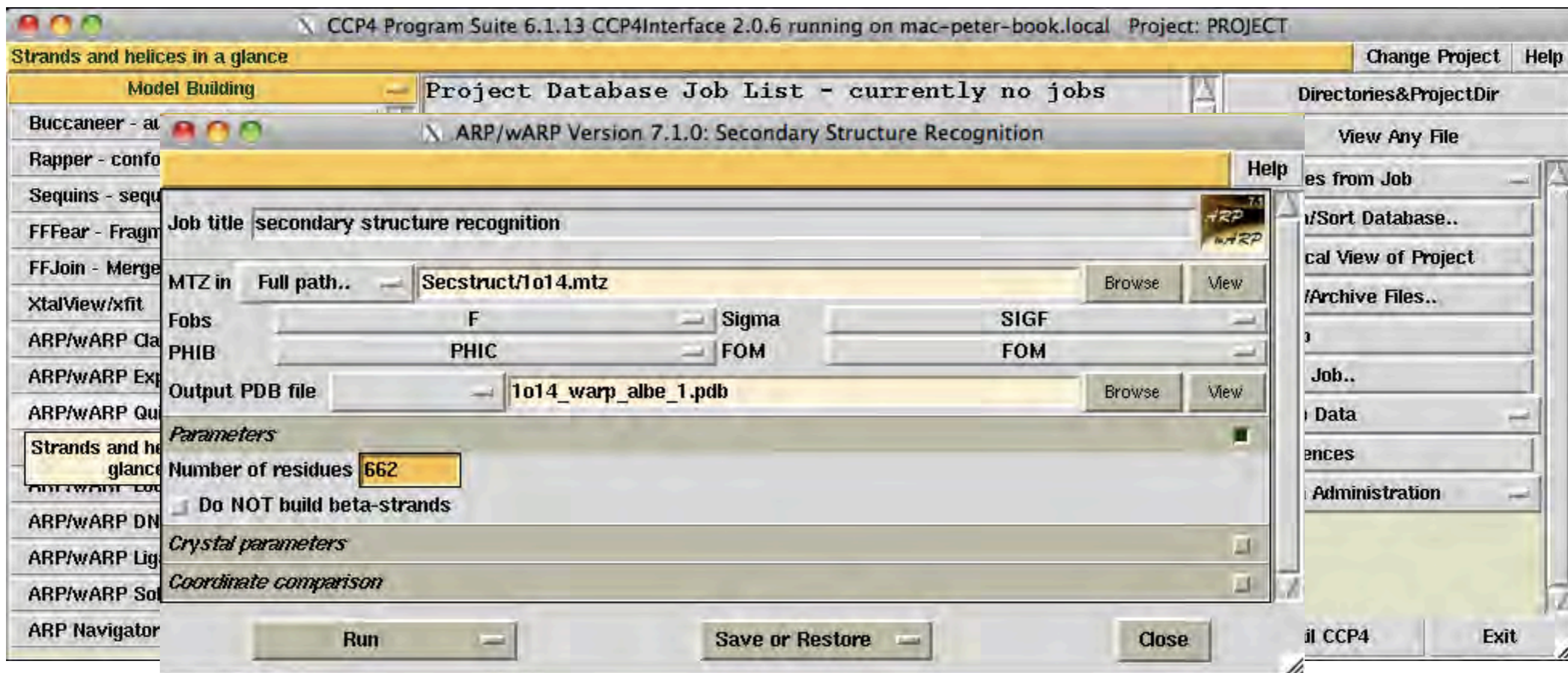
ARP/wARP: Secondary Structure (albe)

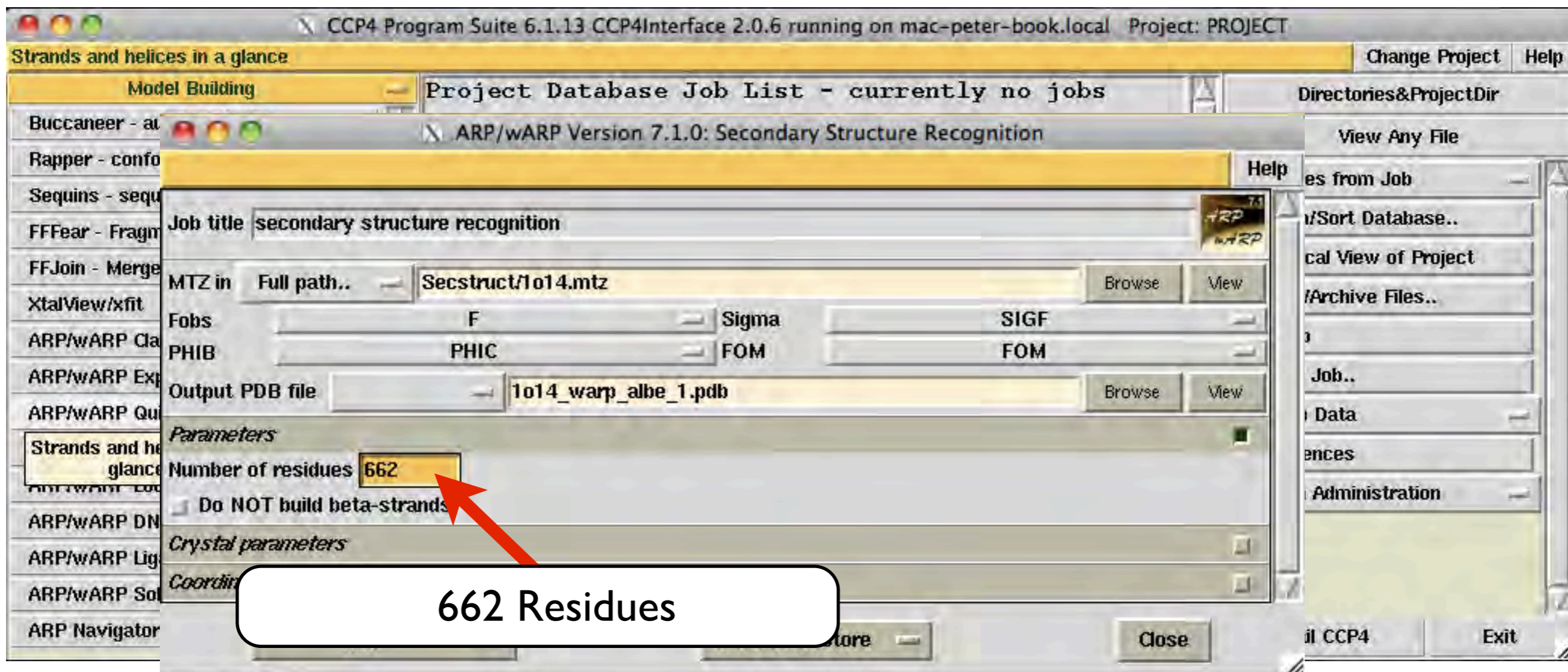
1o14



ARP/wARP: Secondary Structure (albe)

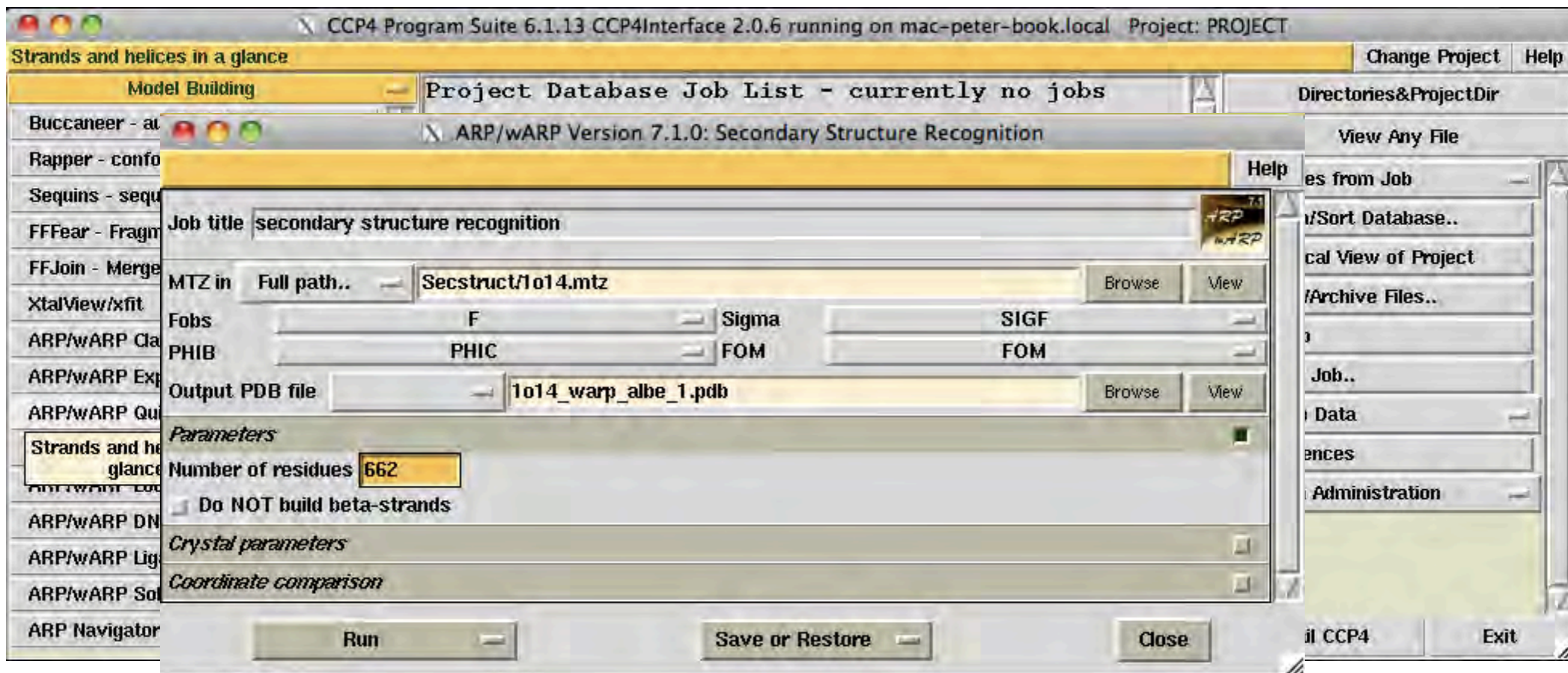
1o14





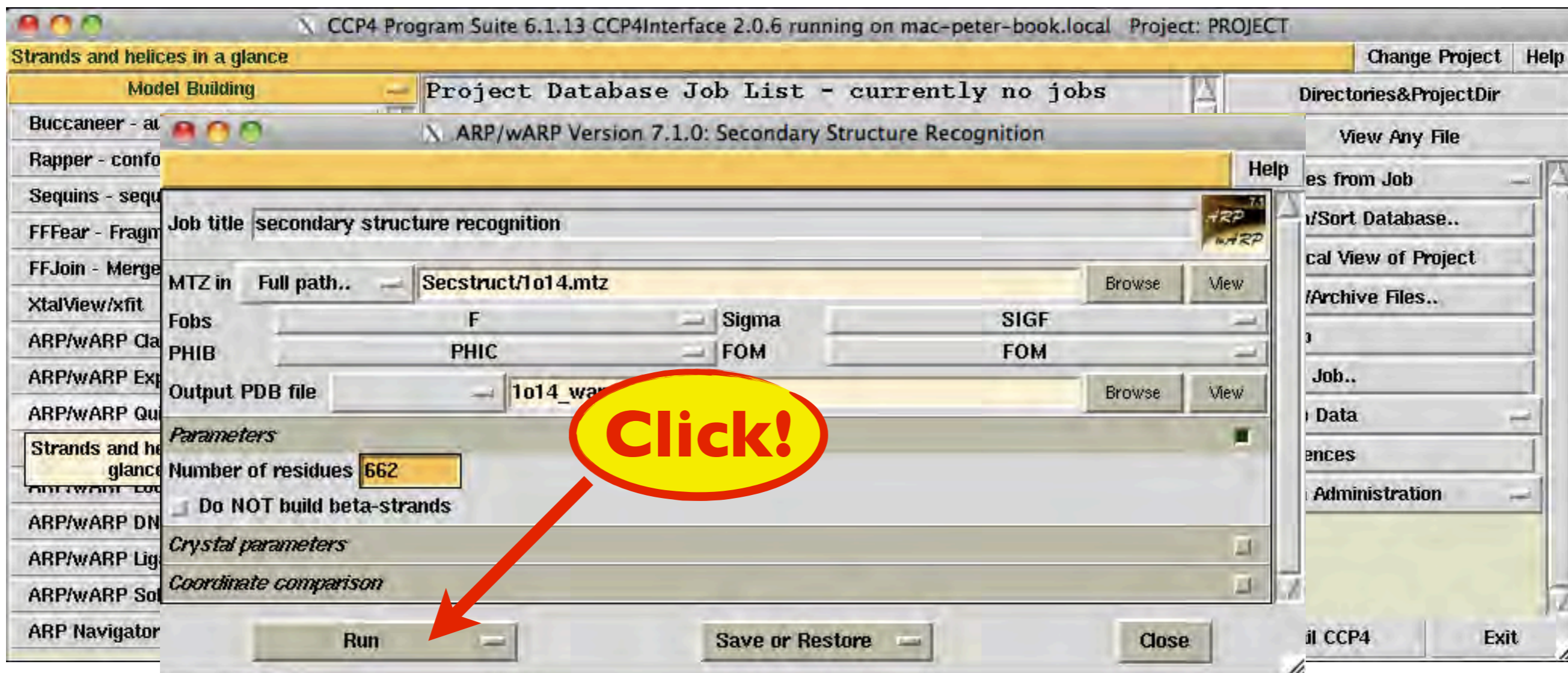
ARP/wARP: Secondary Structure (albe)

1o14



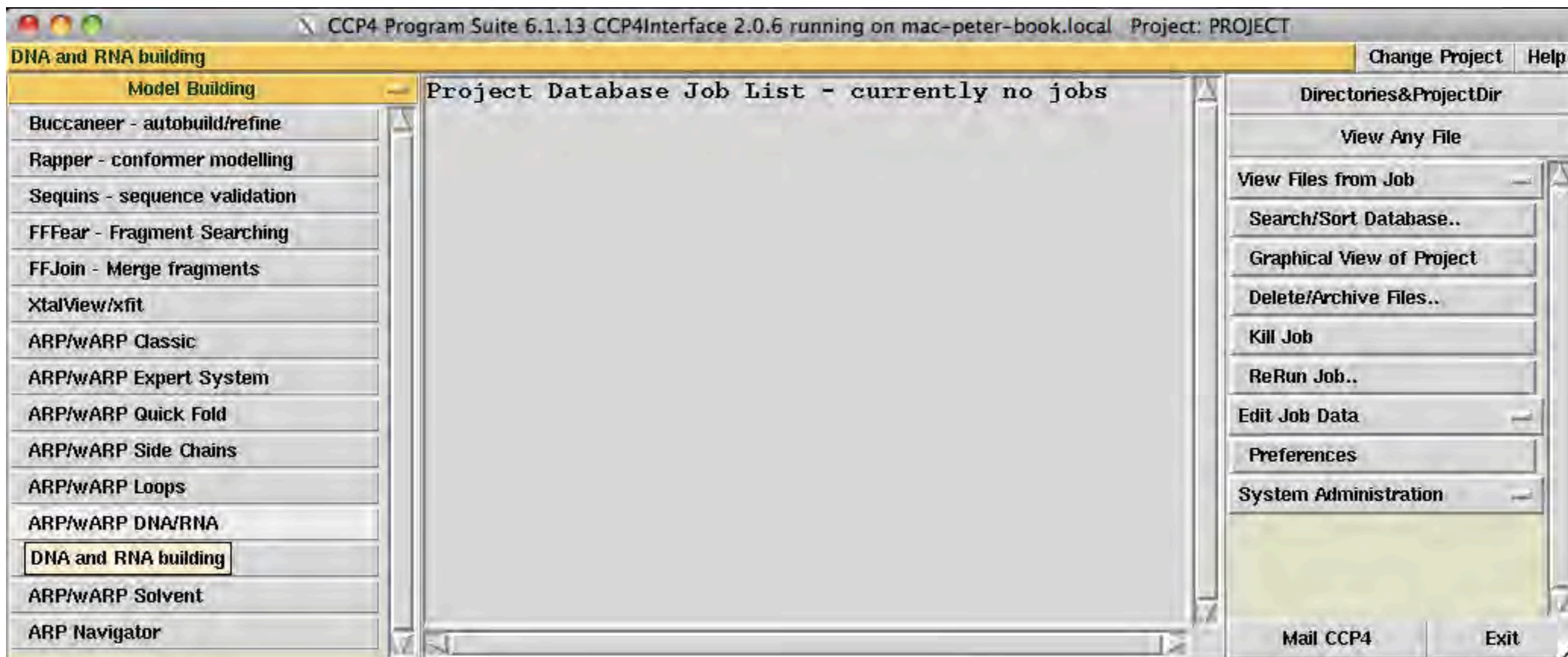
ARP/wARP: Secondary Structure (albe)

1o14



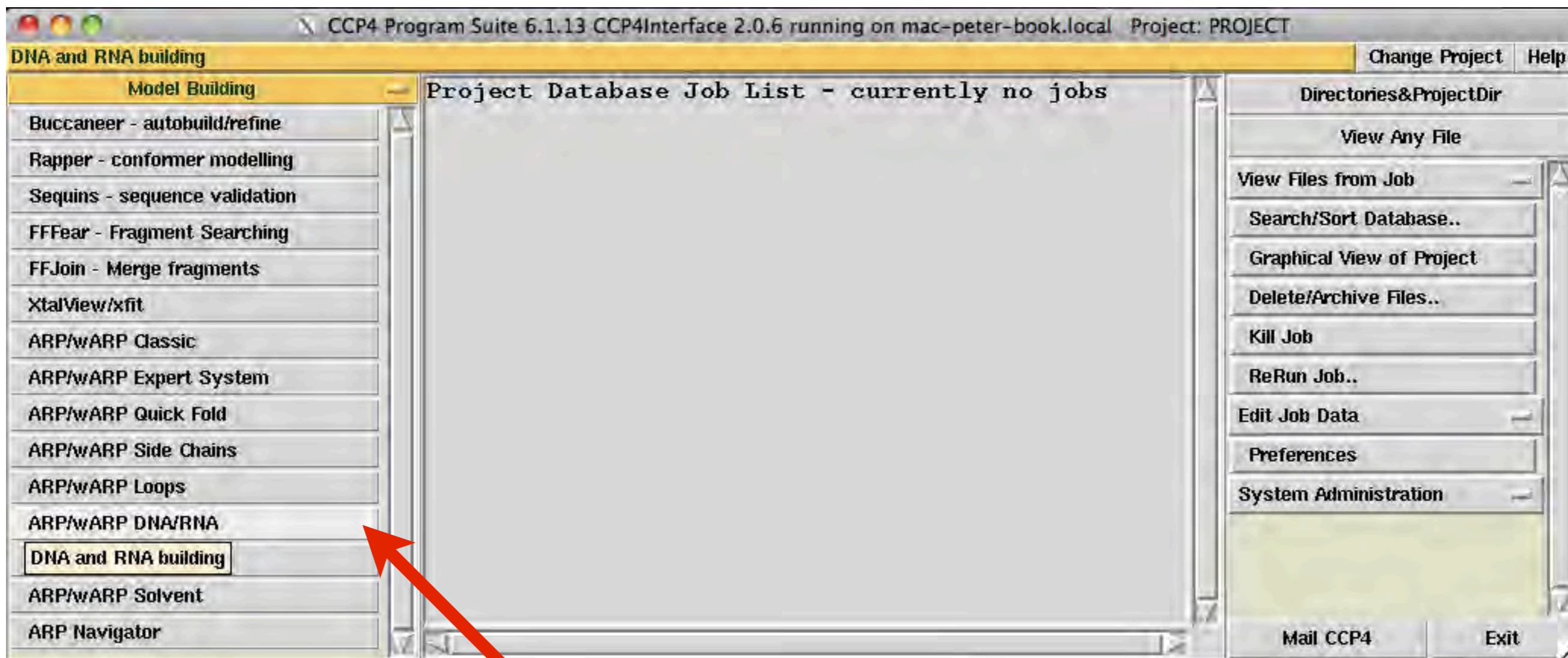
ARP/wARP: Nucleotide Building (nuce)

le3m



ARP/wARP: Nucleotide Building (nuce)

le3m



Click!

Testcase:

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

Residues:

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

Resolution:

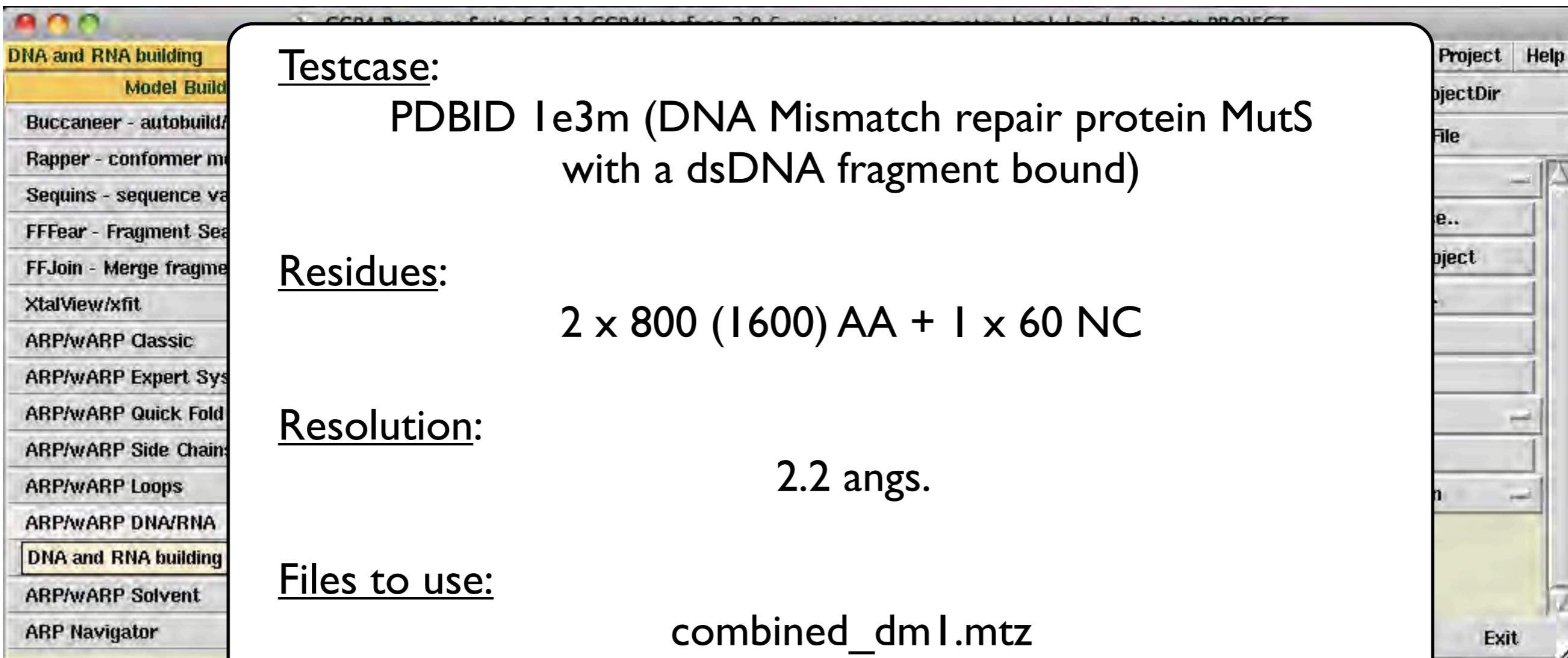
2.2 ang.

Files to use:

combined_dm1.mtz

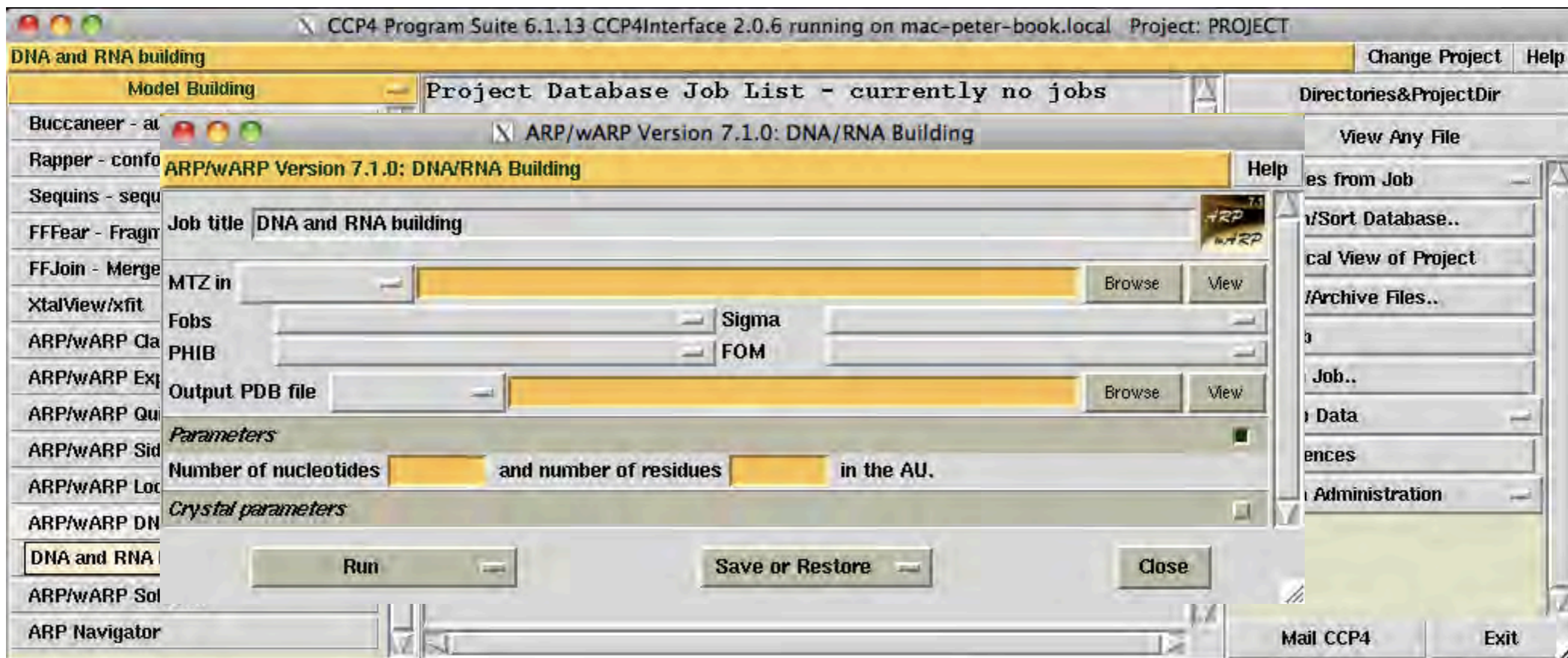
MTS labels to use:

F_eh2nm, SIGF_eh2nm, PHIDM, FOMDM



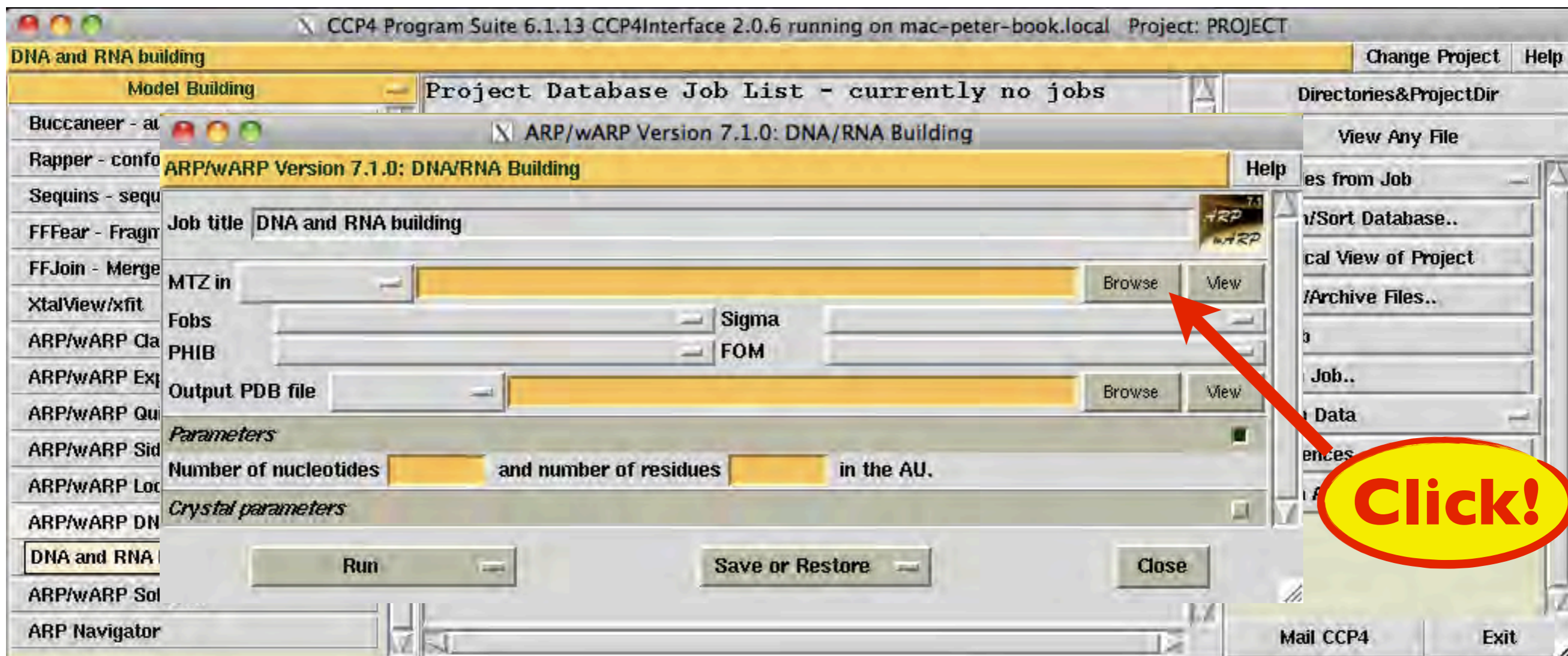
ARP/wARP: Nucleotide Building (nuce)

le3m



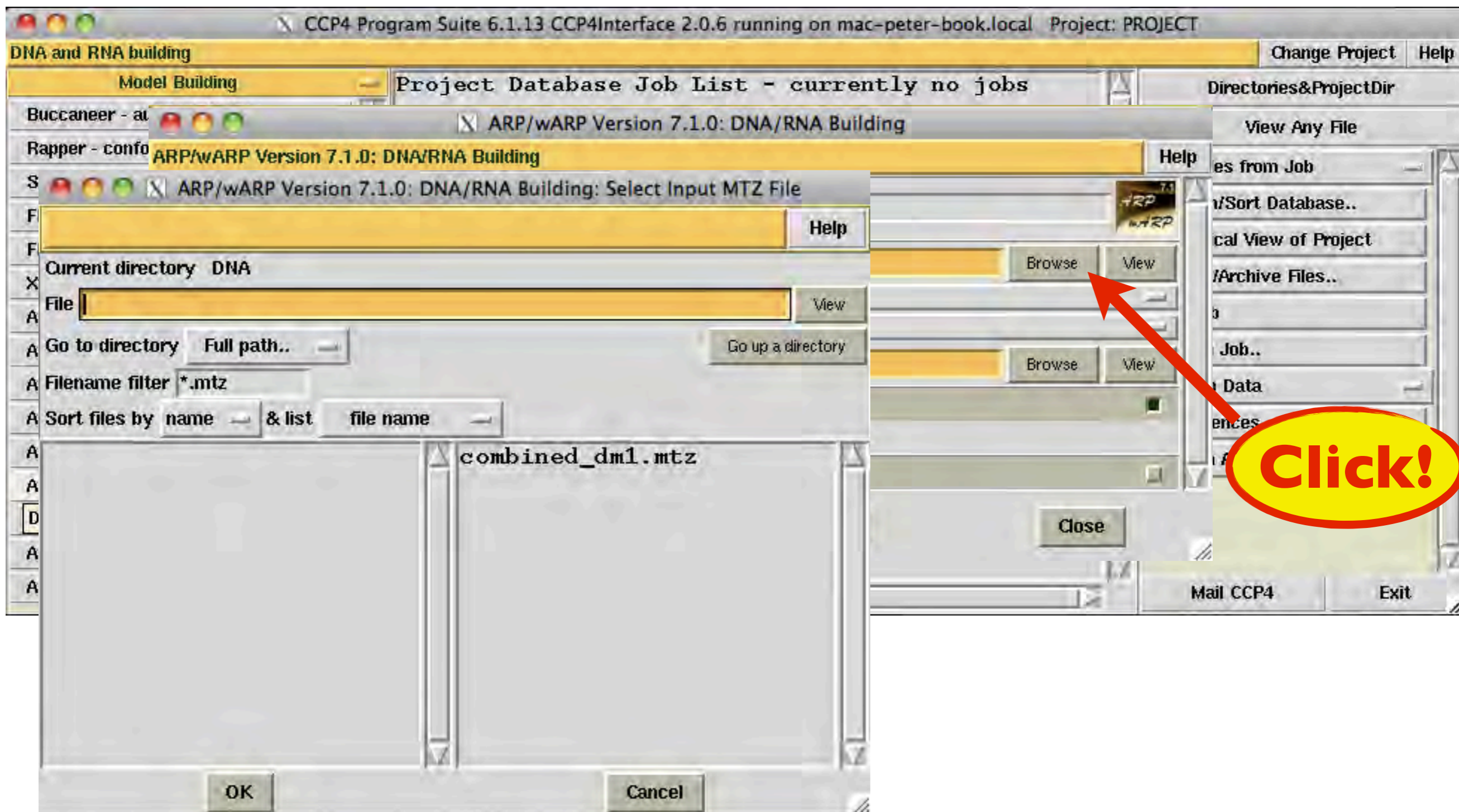
ARP/wARP: Nucleotide Building (nuce)

le3m



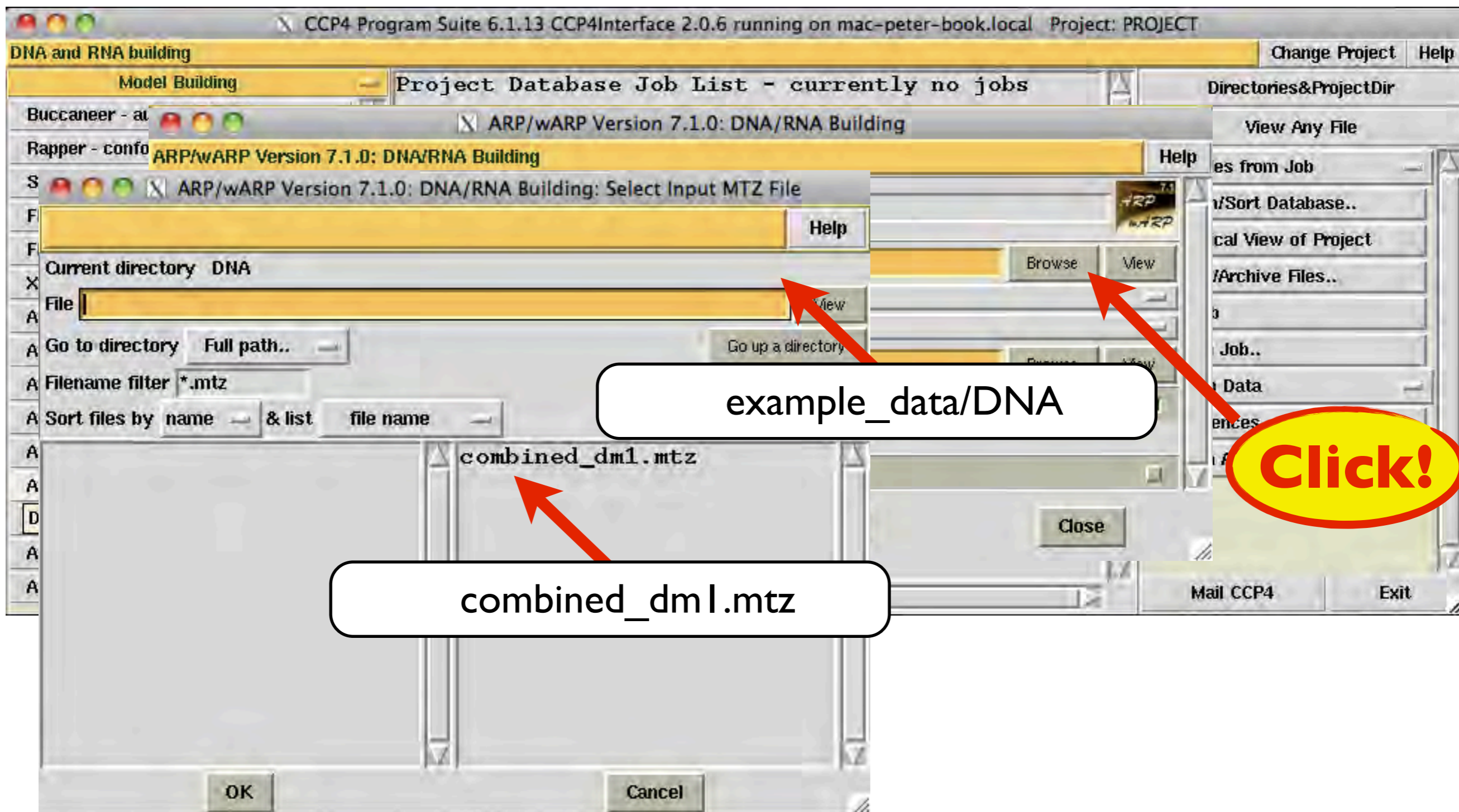
ARP/wARP: Nucleotide Building (nuce)

le3m



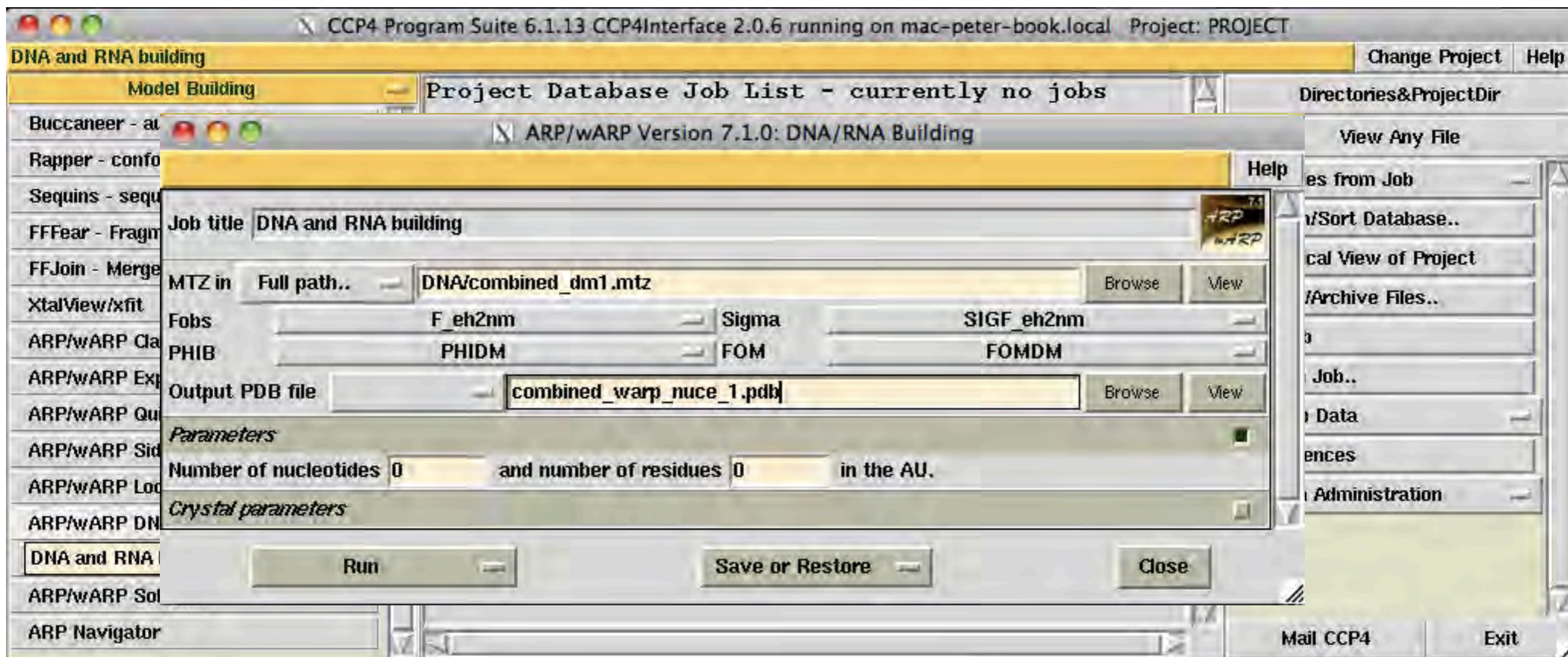
ARP/wARP: Nucleotide Building (nuce)

le3m



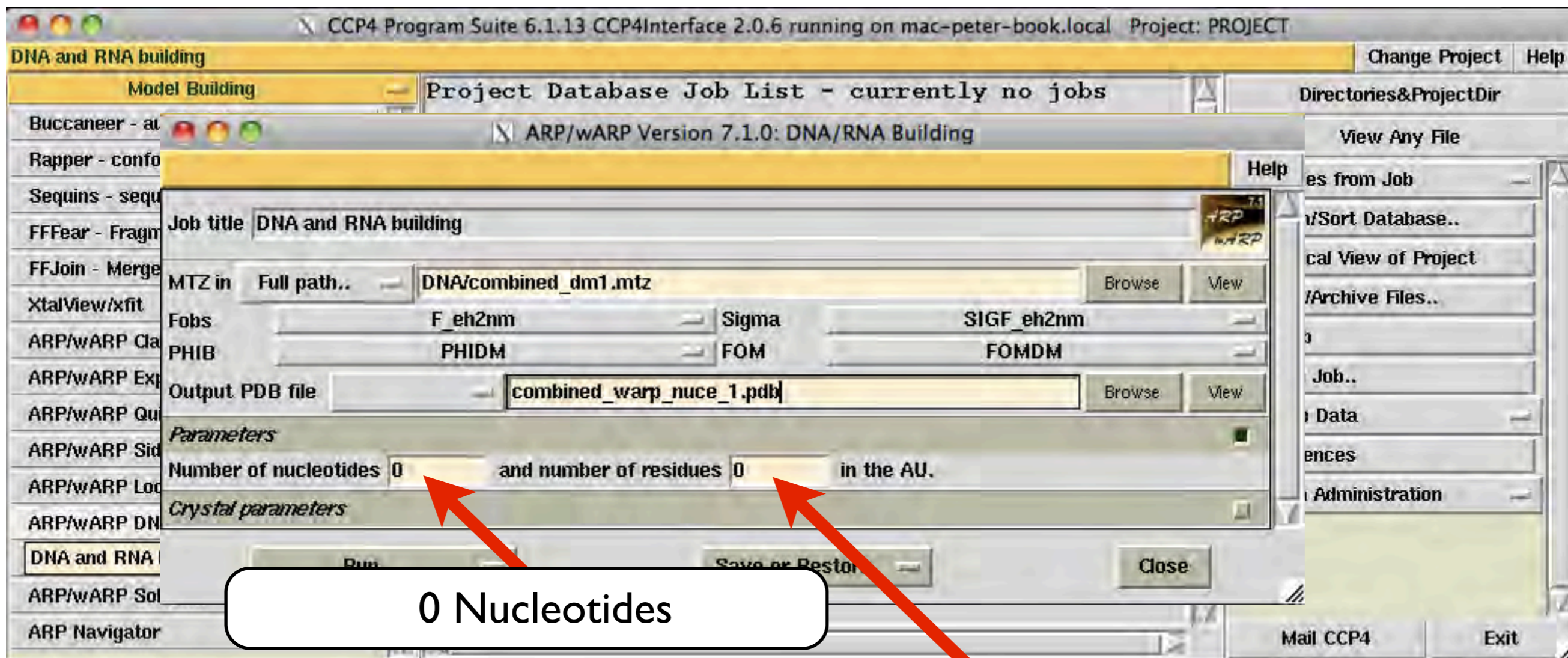
ARP/wARP: Nucleotide Building (nuce)

le3m



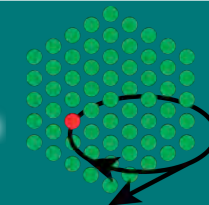
ARP/wARP: Nucleotide Building (nuce)

le3m



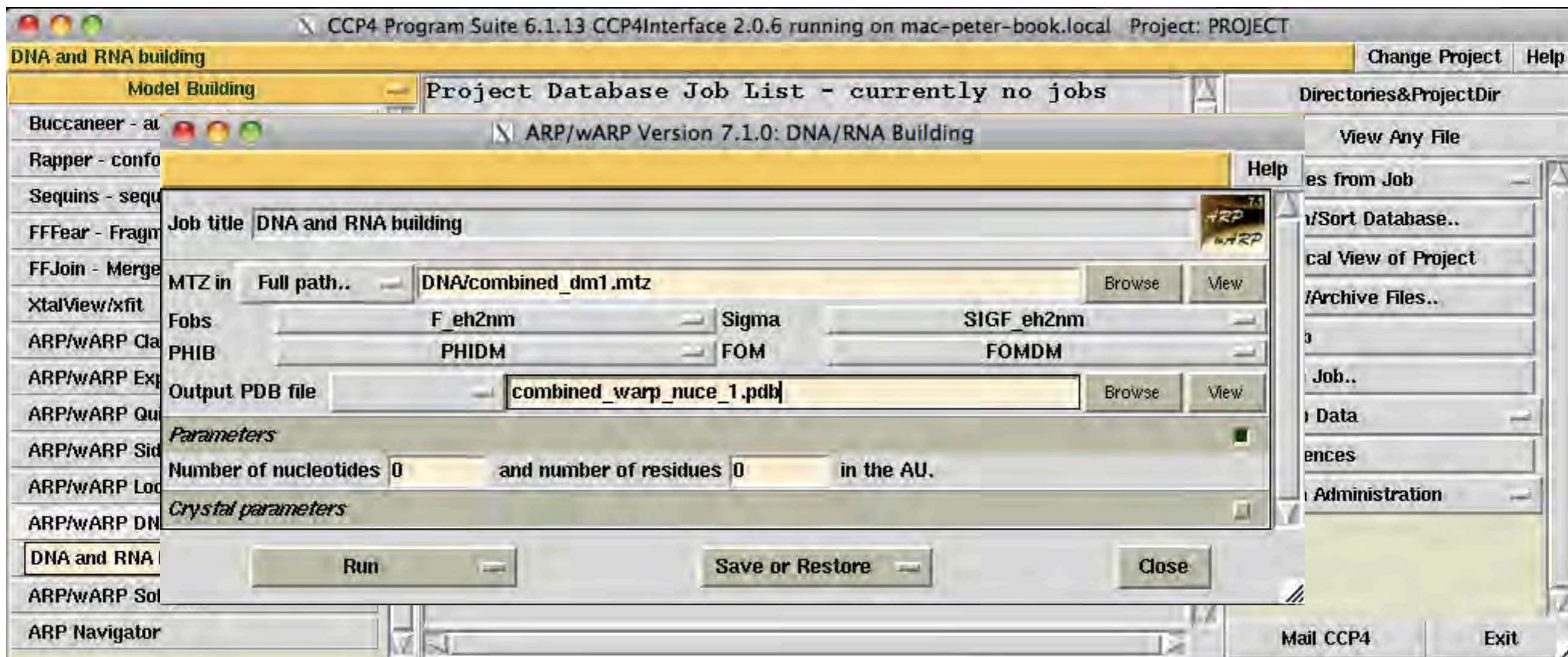
0 Nucleotides

0 Residues



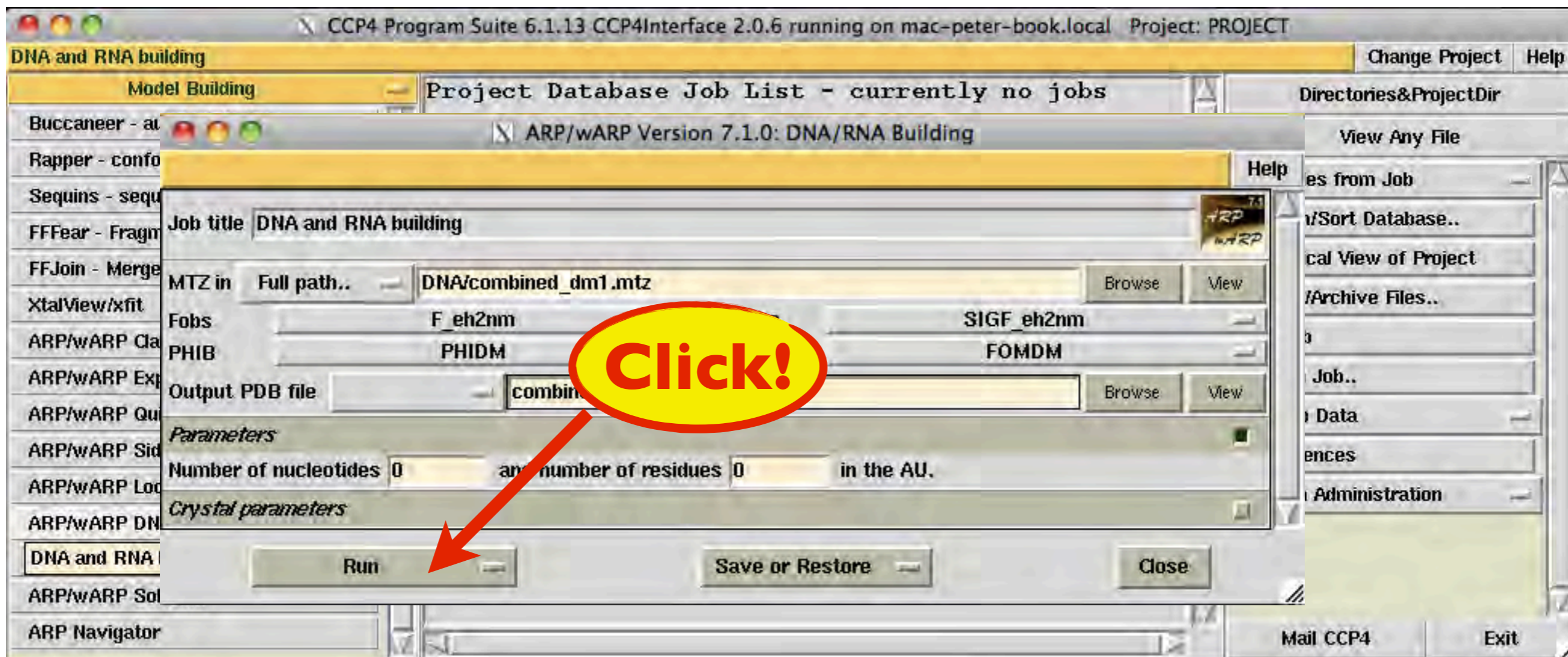
ARP/wARP: Nucleotide Building (nuce)

le3m



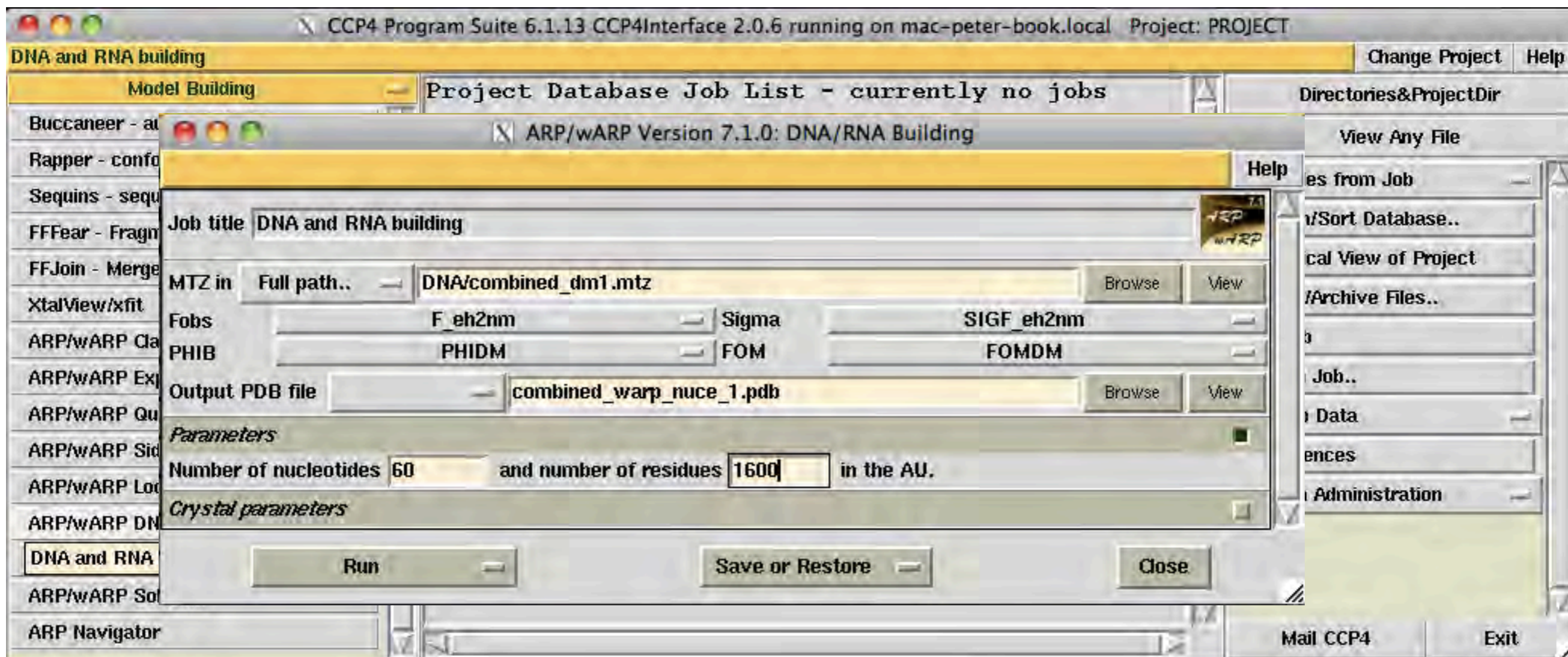
ARP/wARP: Nucleotide Building (nuce)

le3m



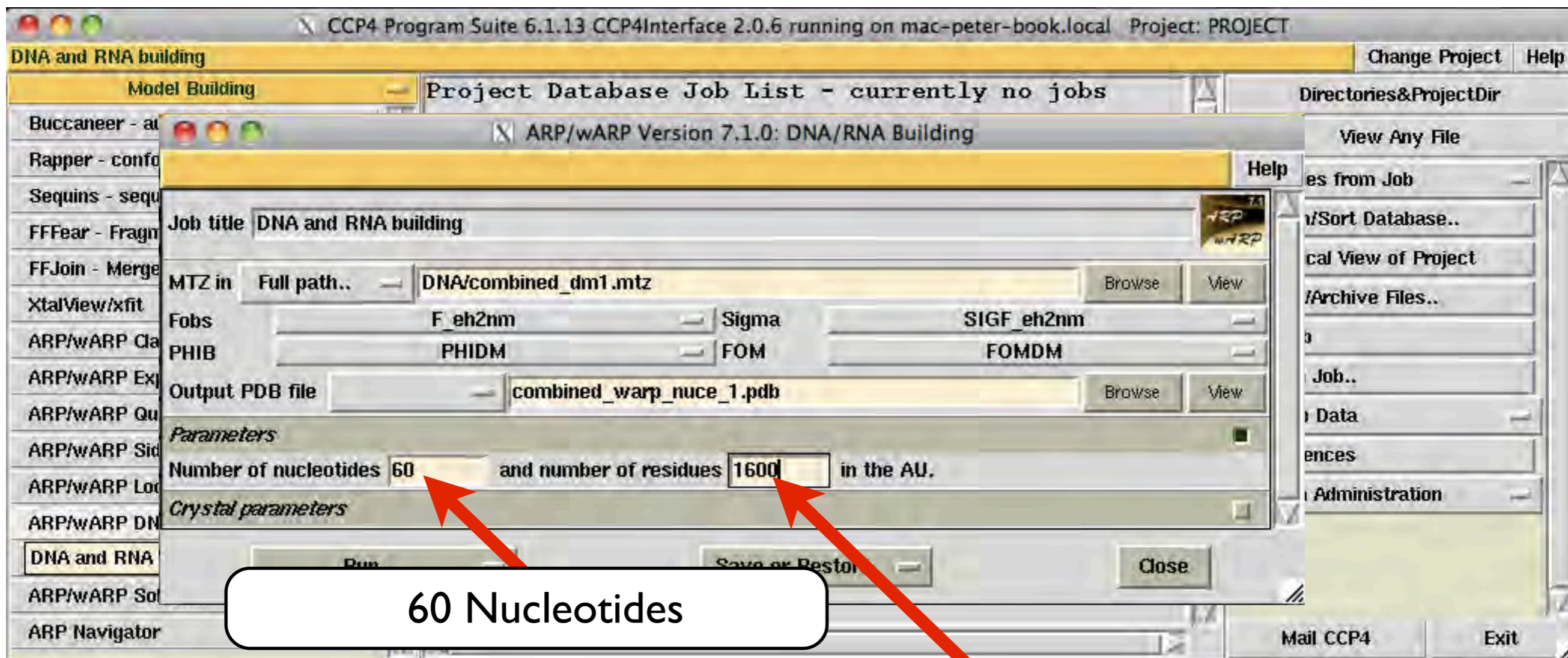
ARP/wARP: Nucleotide Building (nuce)

le3m



ARP/wARP: Nucleotide Building (nuce)

le3m

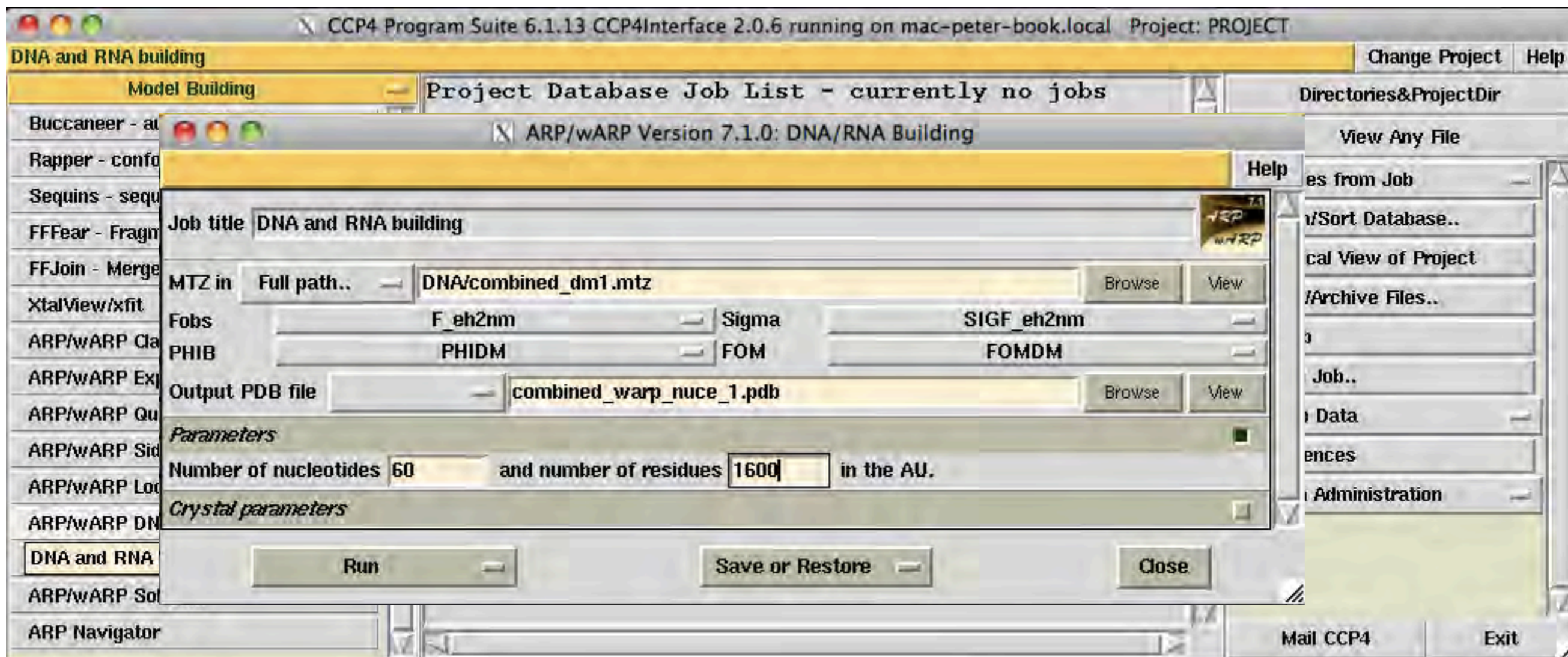


60 Nucleotides

1600 Residues

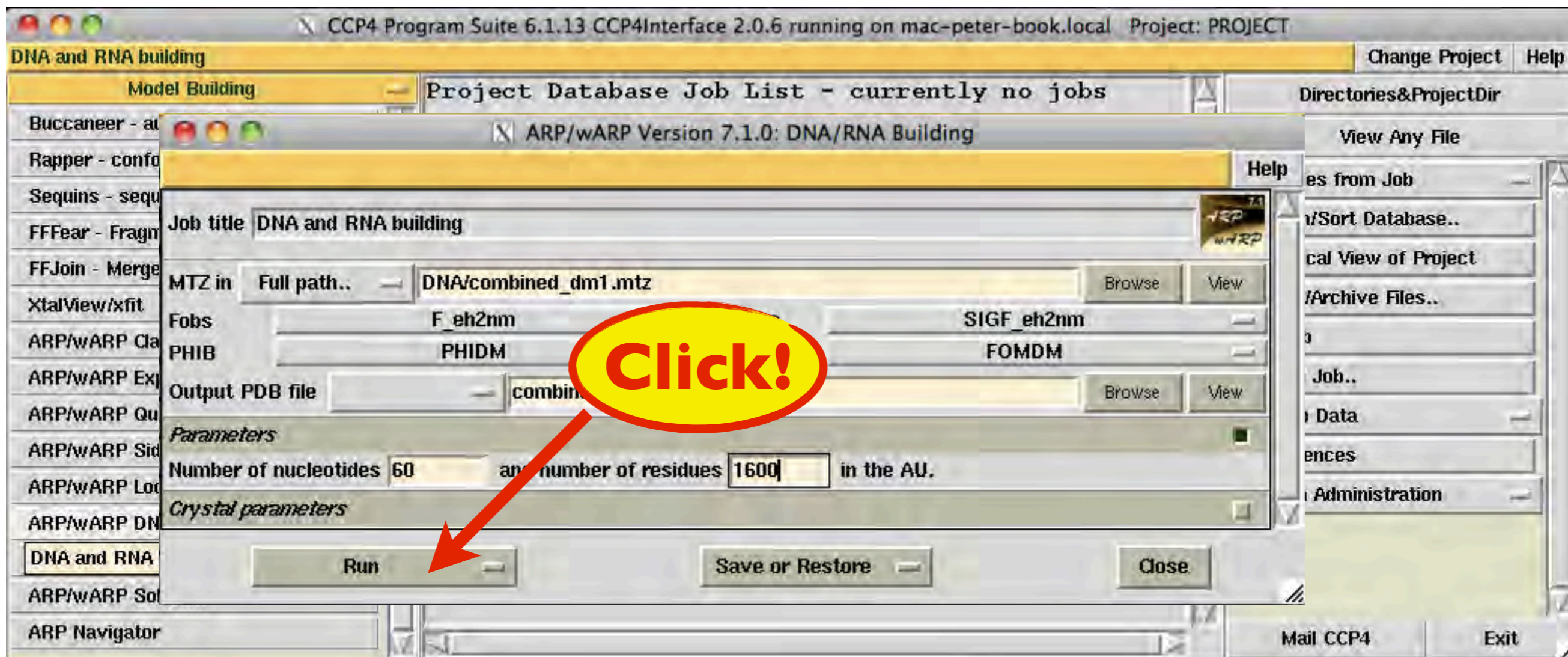
ARP/wARP: Nucleotide Building (nuce)

le3m



ARP/wARP: Nucleotide Building (nuce)

le3m



ARP/wARP: Solvent (warp_solvent)

PSP

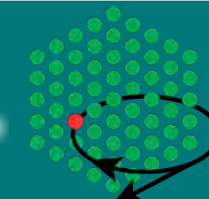


ARP/wARP: Solvent (warp_solvent)

PSP



Click!



Testcase:

PSP / PDBID 1lml (Leishmanolysin)

Residues:

1 x 475 AA

Resolution:

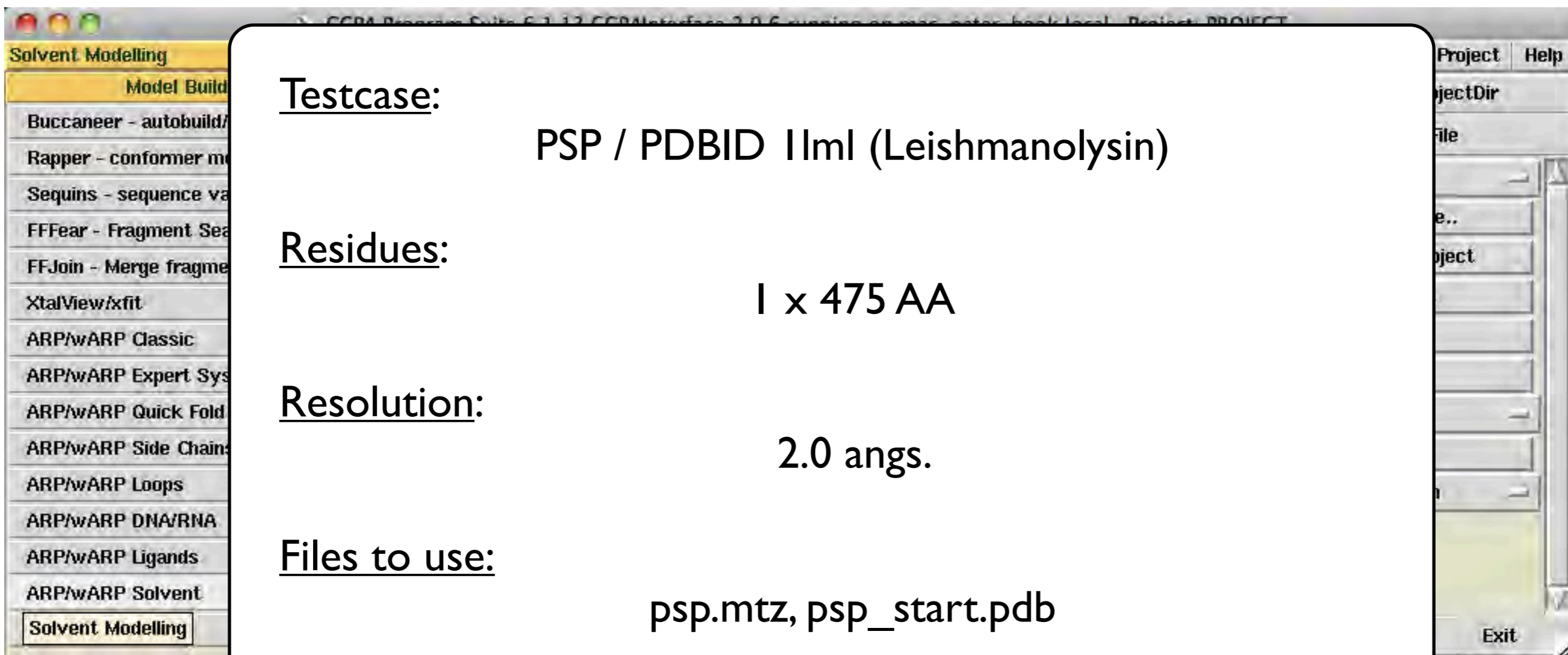
2.0 ang.

Files to use:

psp.mtz, psp_start.pdb

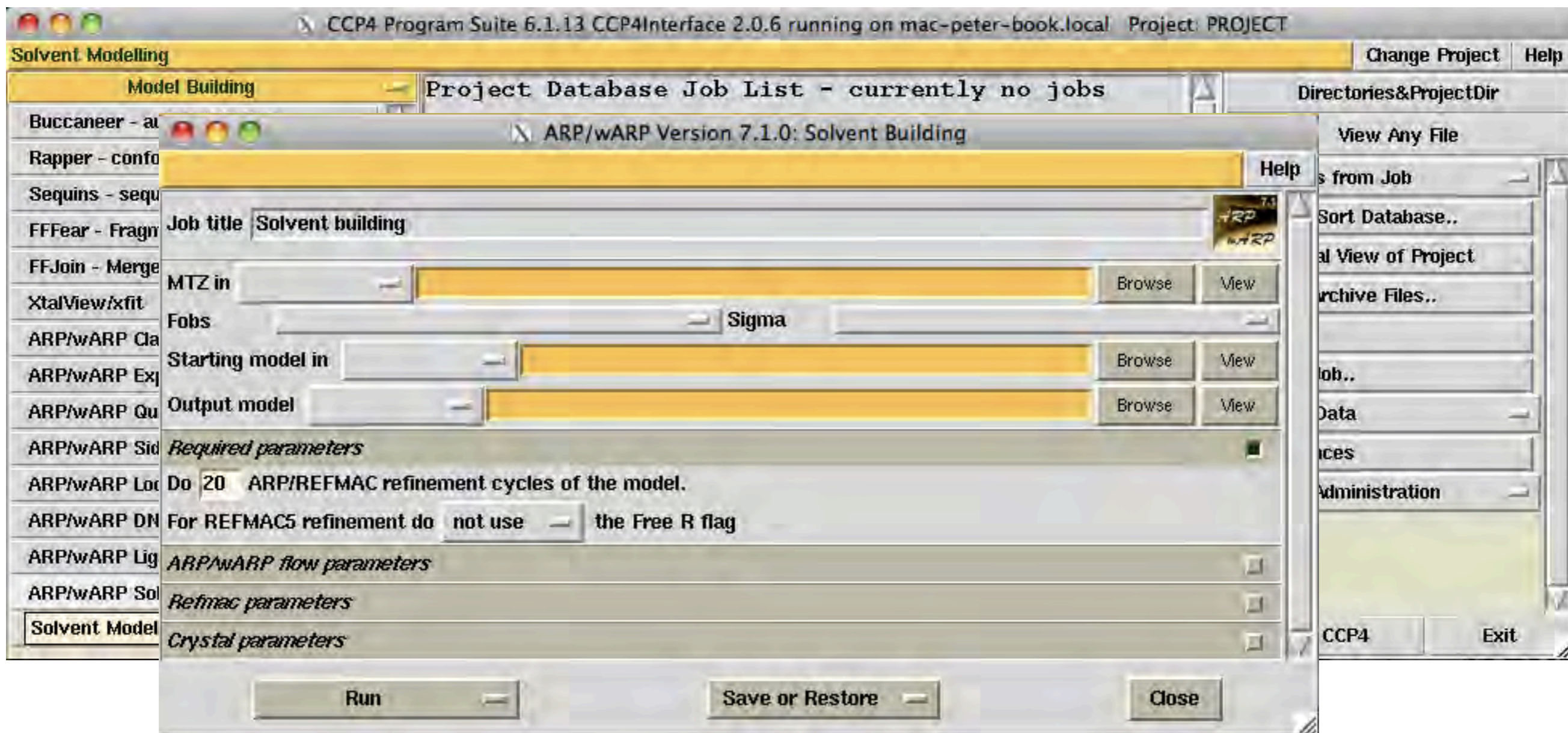
MTS labels to use:

FP, SIGFP



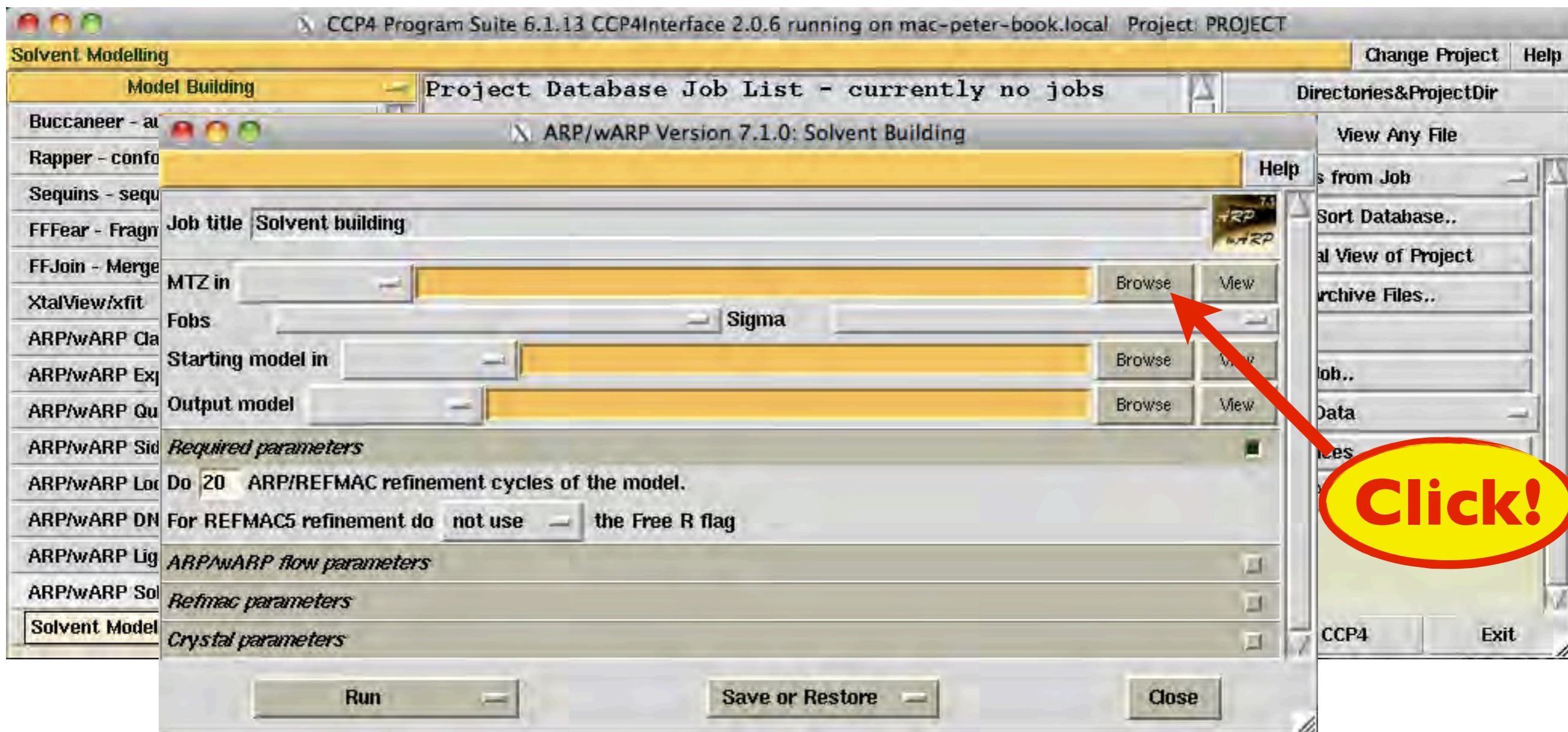
ARP/wARP: Solvent (warp_solvent)

PSP



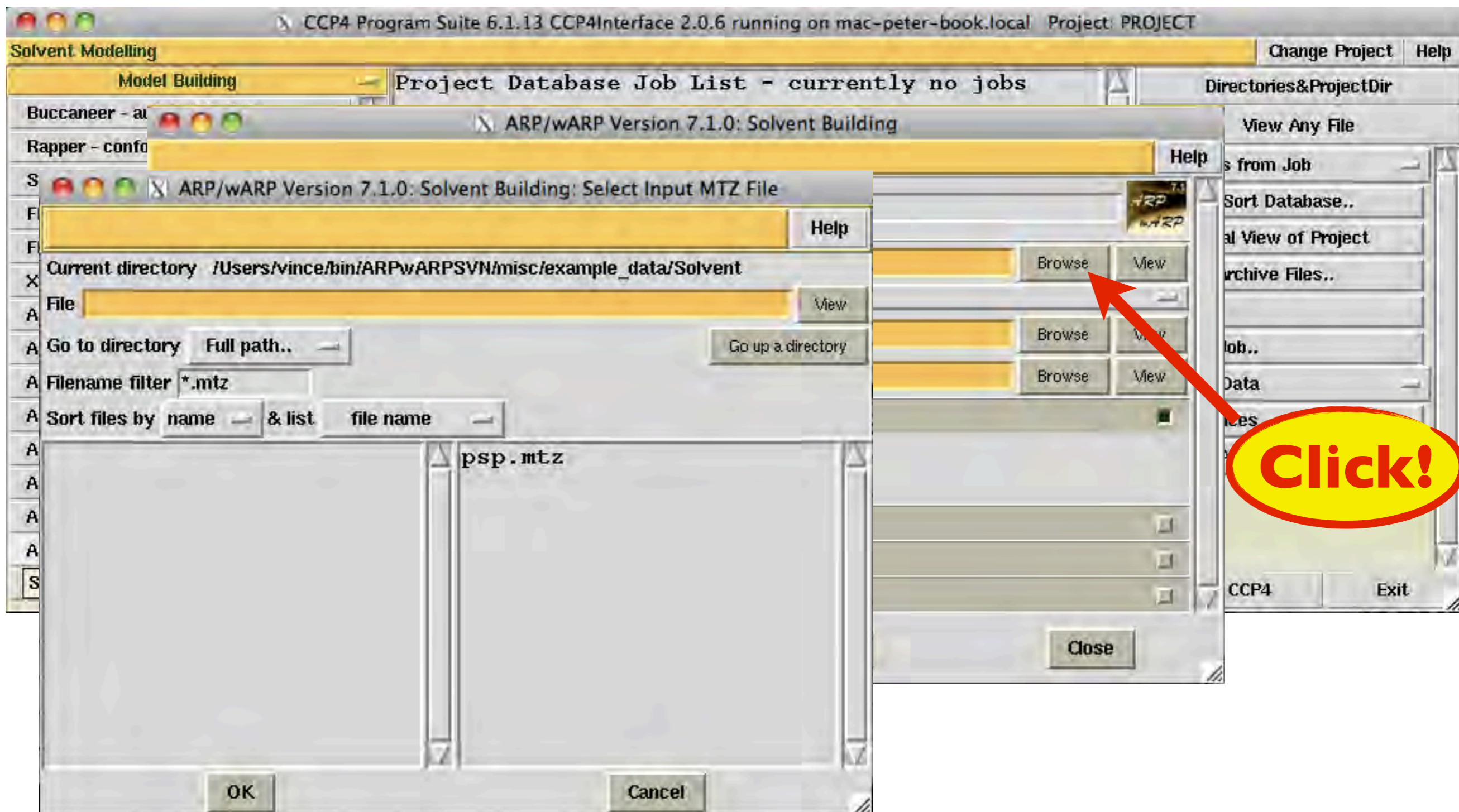
ARP/wARP: Solvent (warp_solvent)

PSP



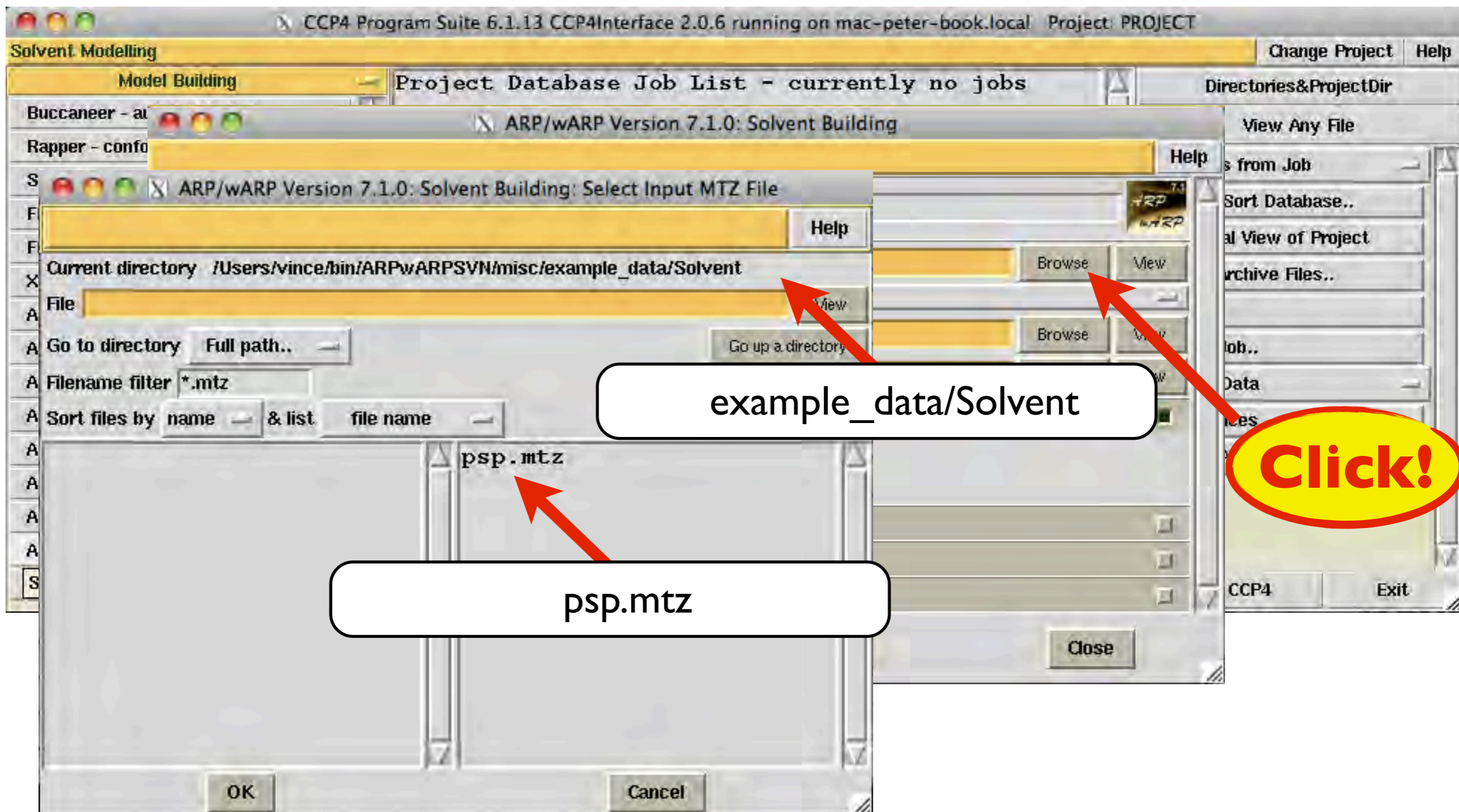
ARP/wARP: Solvent (warp_solvent)

PSP



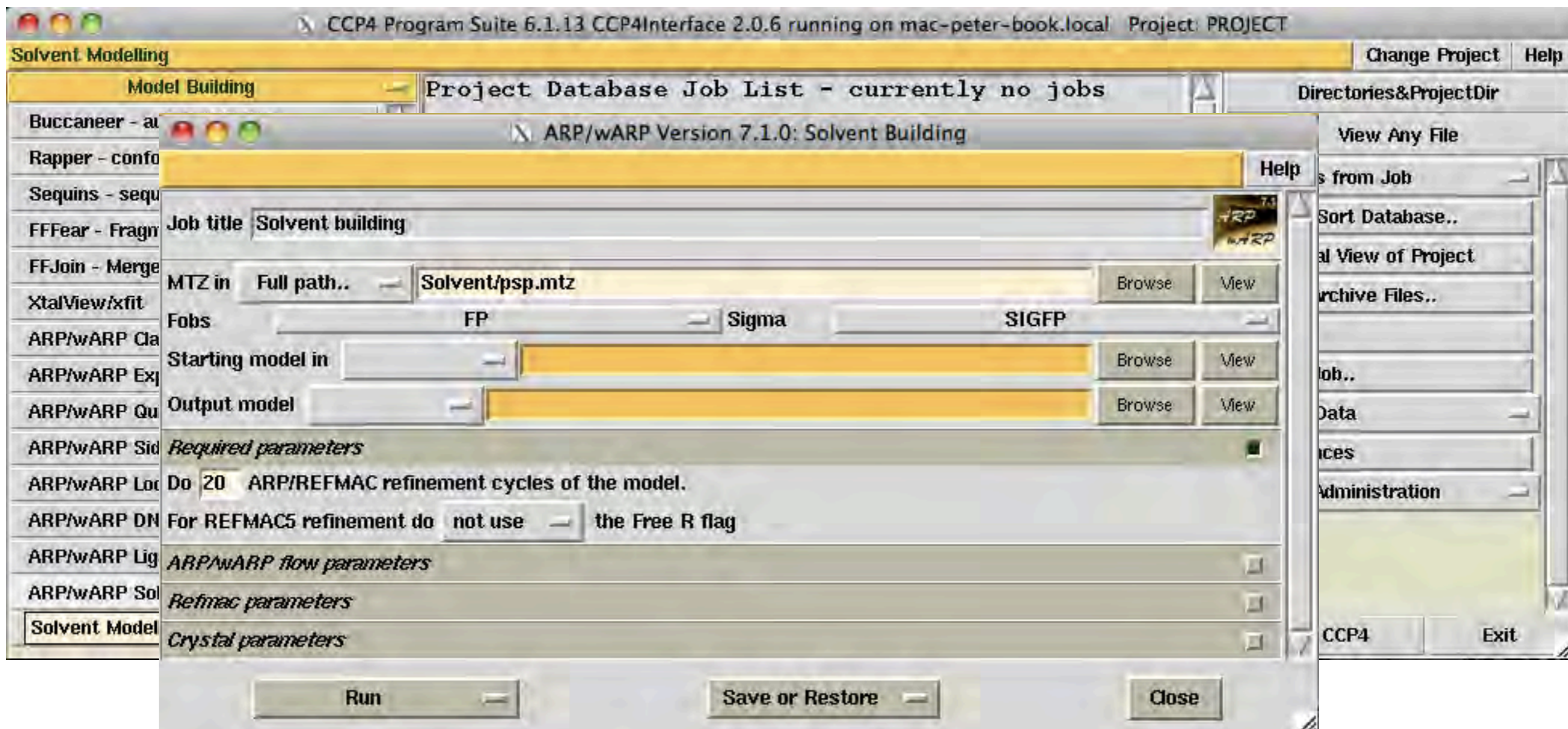
ARP/wARP: Solvent (warp_solvent)

PSP



ARP/wARP: Solvent (warp_solvent)

PSP



ARP/wARP: Solvent (warp_solvent)

PSP

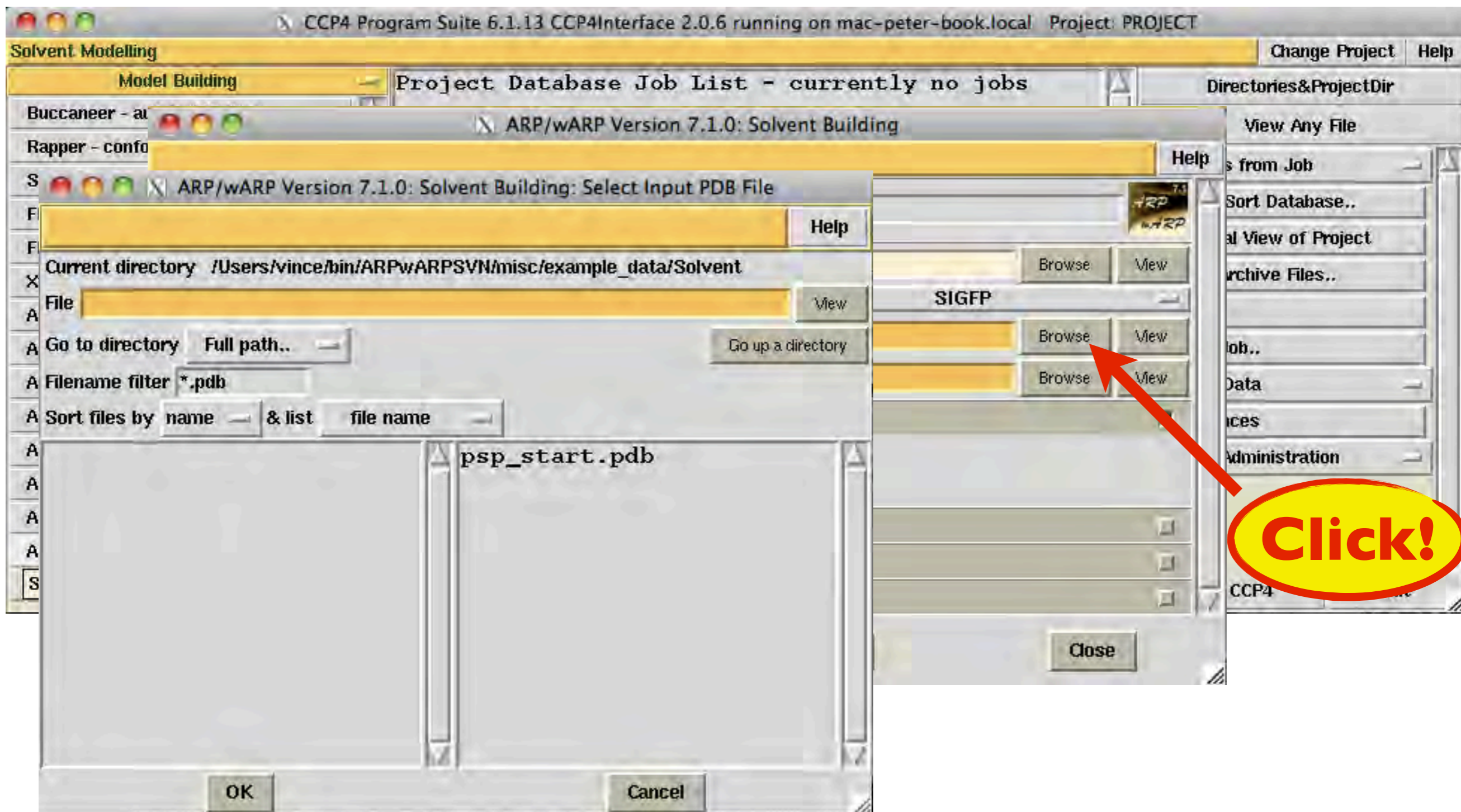
The screenshot shows the CCP4 Program Suite interface. The main window is titled 'Solvent Modelling' and contains a 'Model Building' tab. A secondary window, 'ARP/wARP Version 7.1.0: Solvent Building', is open in the foreground. This dialog box has the following fields and controls:

- Job title:** Solvent building
- MTZ in:** Full path.. Solvent/psp.mtz (with 'Browse' and 'View' buttons)
- Fobs:** FP (with 'Sigma' and 'SIGFP' options)
- Starting model in:** [Empty field] (with 'Browse' and 'View' buttons)
- Output model:** [Empty field] (with 'Browse' and 'View' buttons)
- Required parameters:** Do 20 ARP/REFMAC refinement cycles of the model.
- For REFMAC5 refinement do:** not use the Free R flag
- ARP/wARP flow parameters:** [Checkbox]
- Refmac parameters:** [Checkbox]
- Crystal parameters:** [Checkbox]

At the bottom of the dialog are 'Run', 'Save or Restore', and 'Close' buttons. A red arrow points to the 'Browse' button next to the 'Starting model in' field, with a yellow oval containing the text 'Click!' next to it.

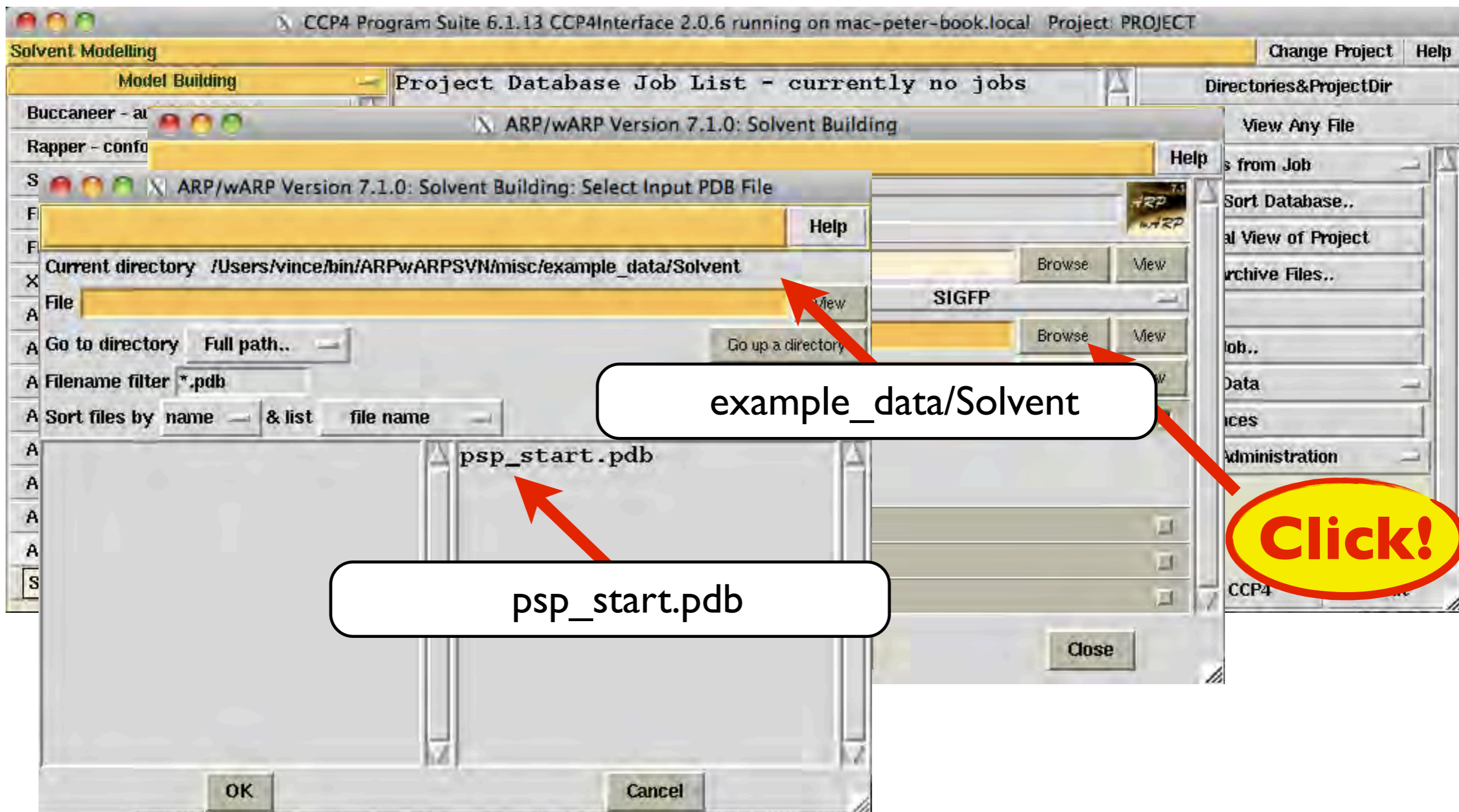
ARP/wARP: Solvent (warp_solvent)

PSP



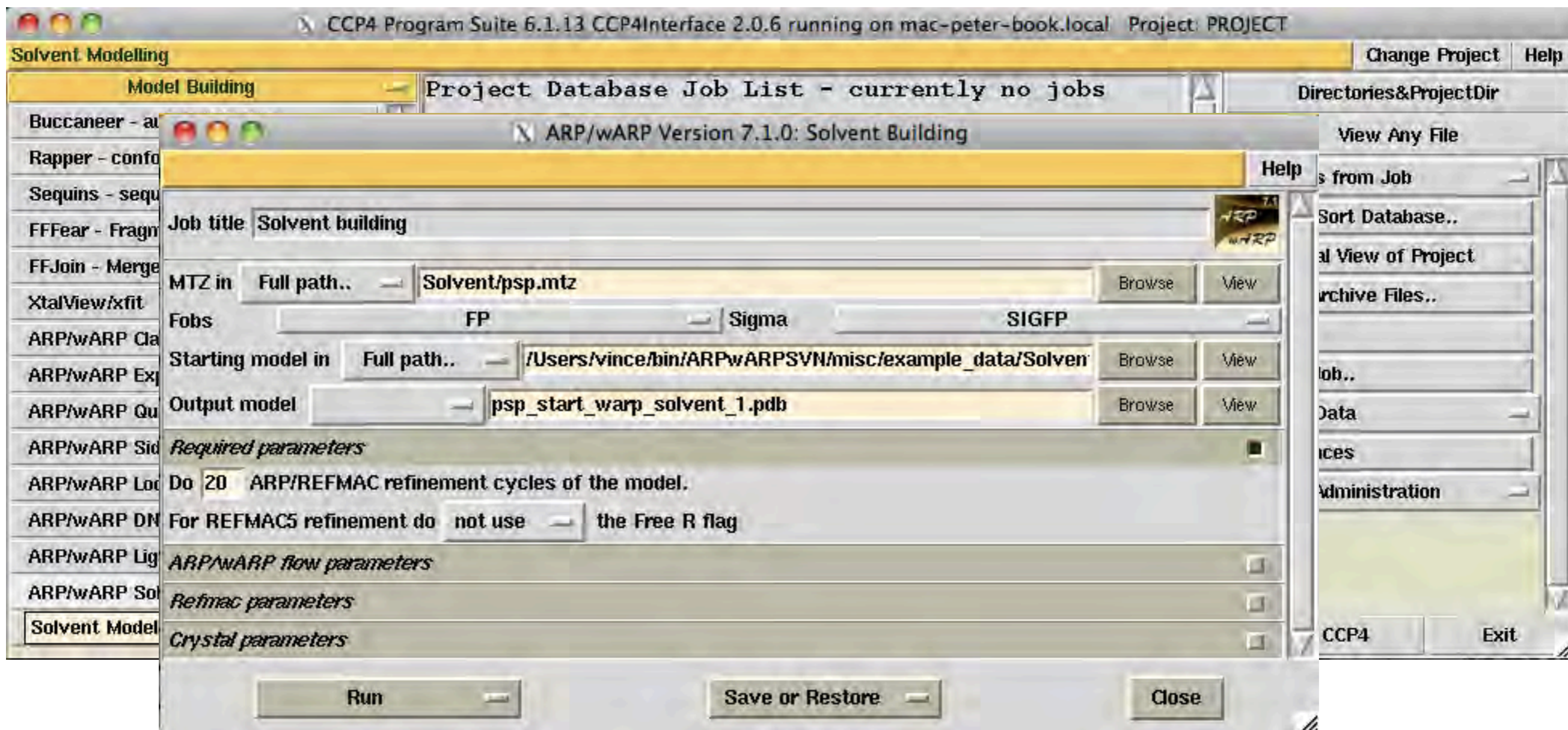
ARP/wARP: Solvent (warp_solvent)

PSP



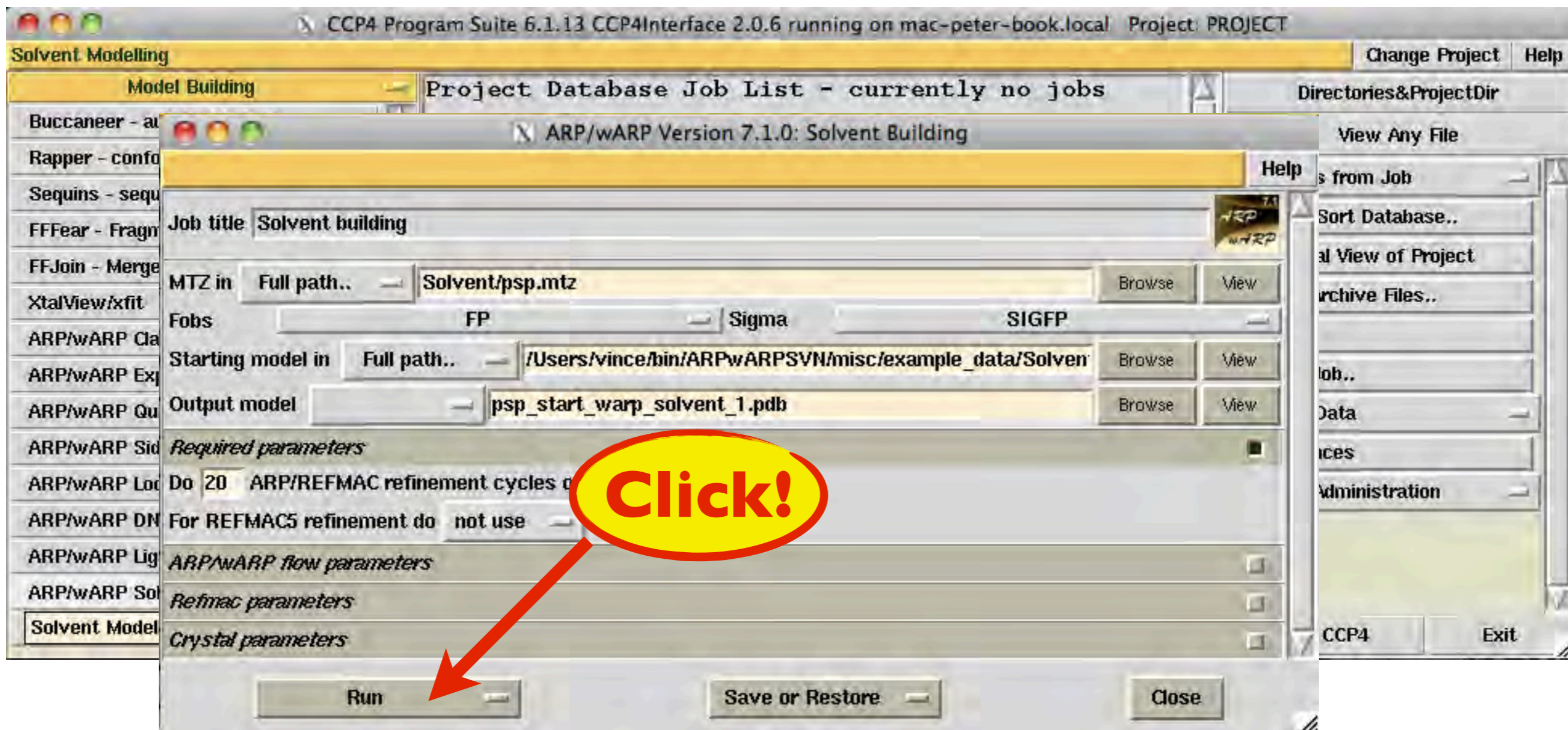
ARP/wARP: Solvent (warp_solvent)

PSP



ARP/wARP: Solvent (warp_solvent)

PSP



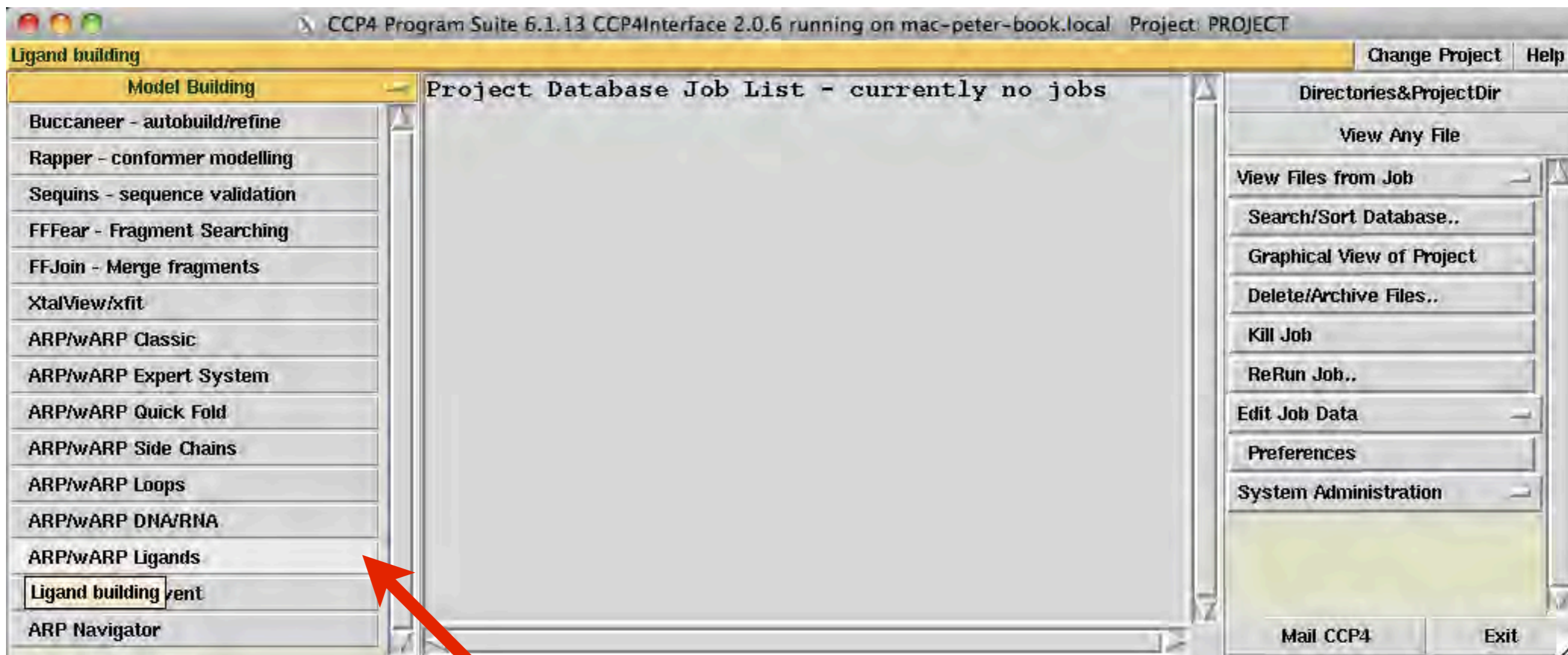
ARP/wARP: Ligands (warp_ligand)

I cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

I cbs, Lig: RA



Click!

Testcase:

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

Files to use:

I cbs.mtz, ICBS_noligand.pdb, RETINOICACID.pdb

Datafile:

I cbs.mtz

APO structure:

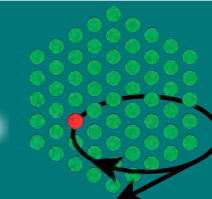
ICBS_noligand.pdb

Ligand template:

RETINOICACID.pdb

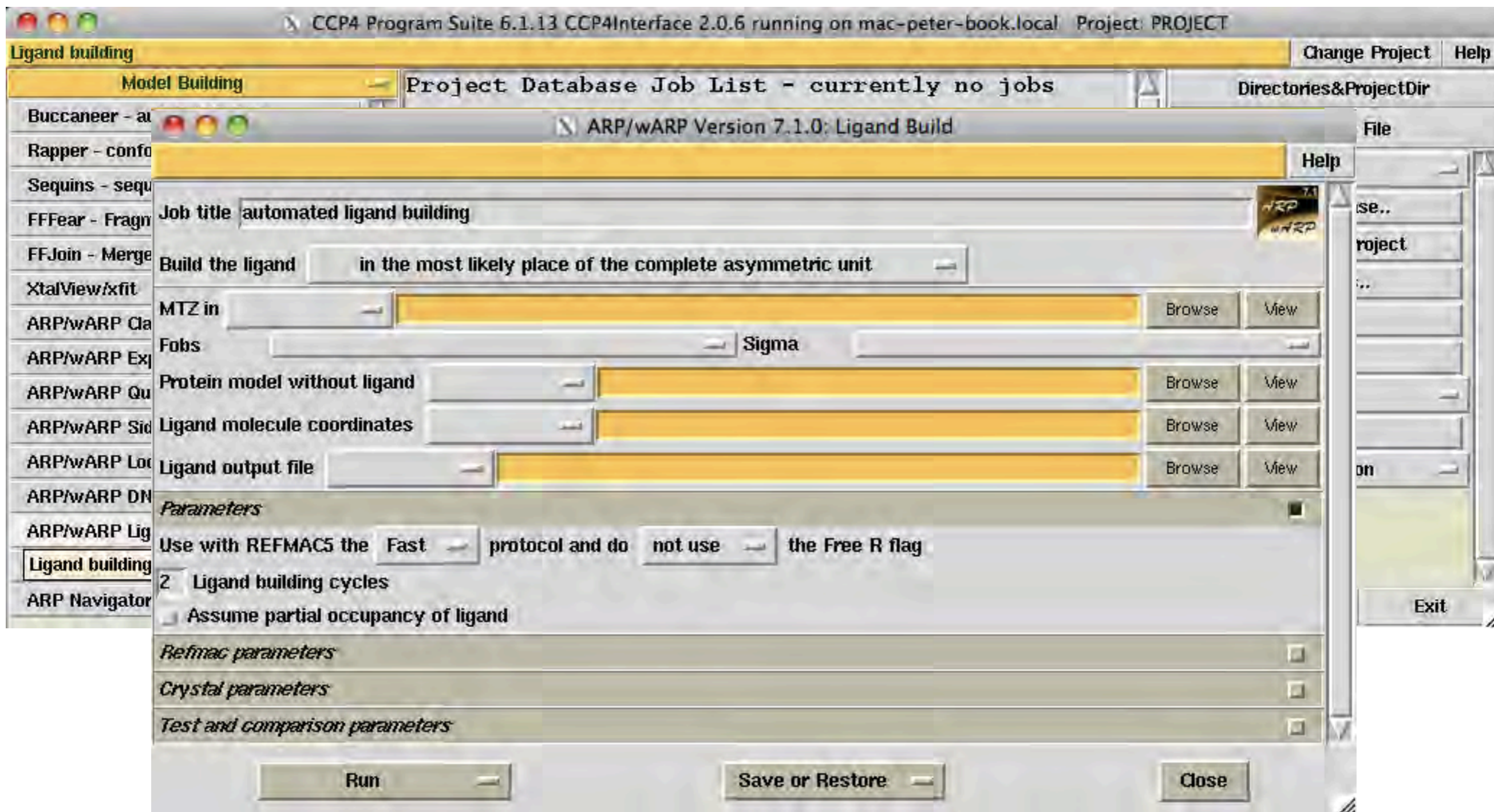
MTS labels to use:

FP, SIGFP



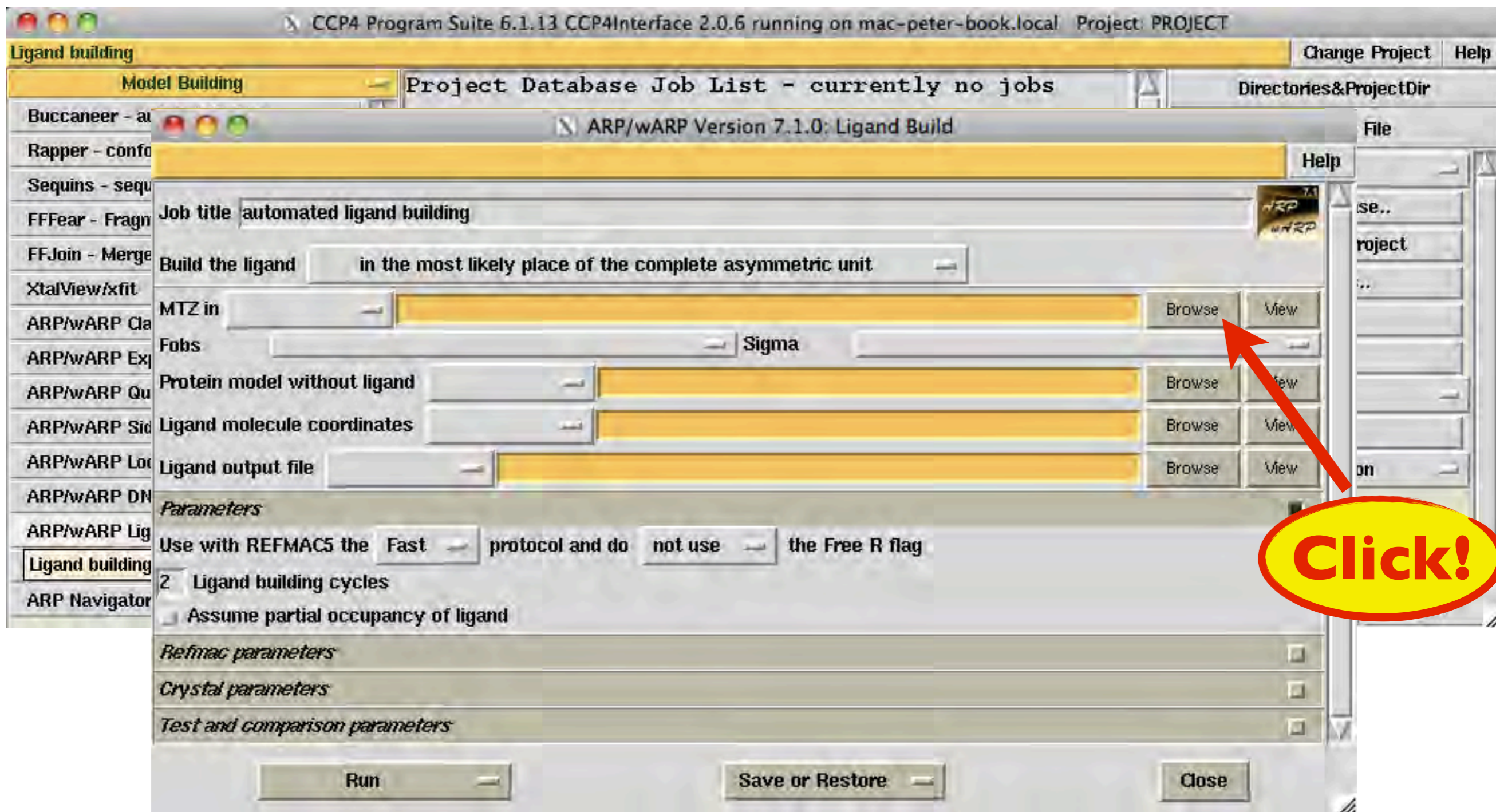
ARP/wARP: Ligands (warp_ligand)

I cbs, Lig: RA



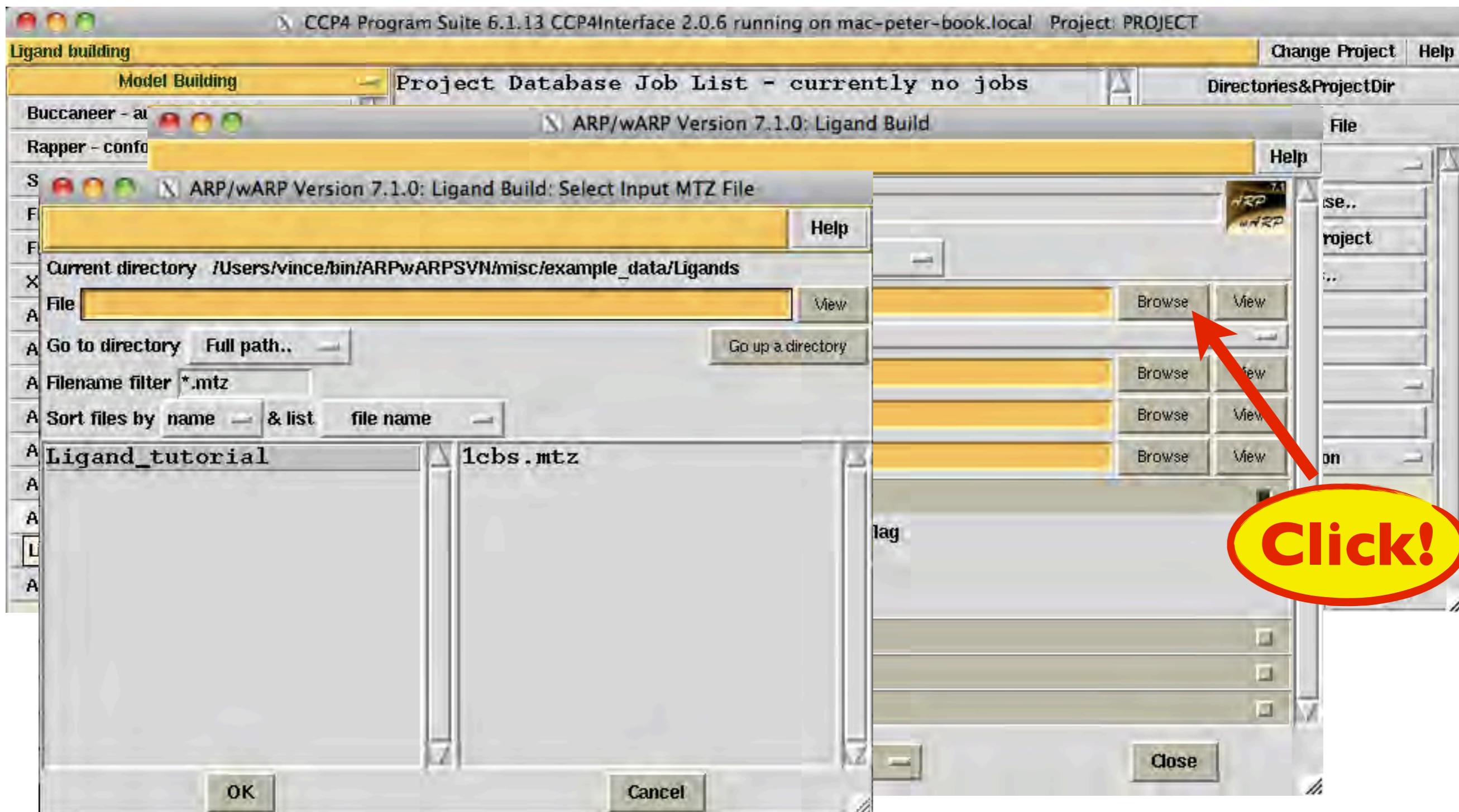
ARP/wARP: Ligands (warp_ligand)

I cbs, Lig: RA



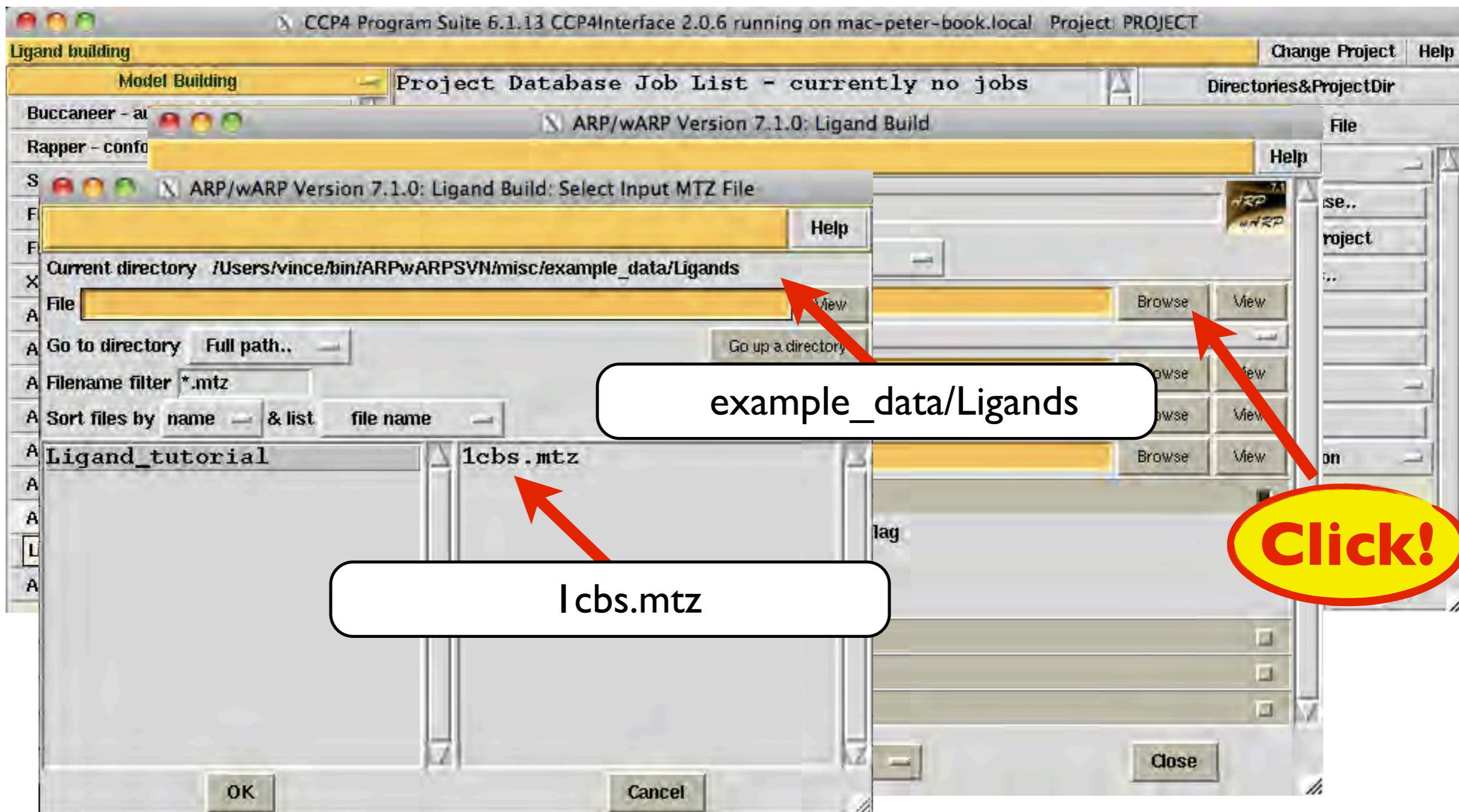
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



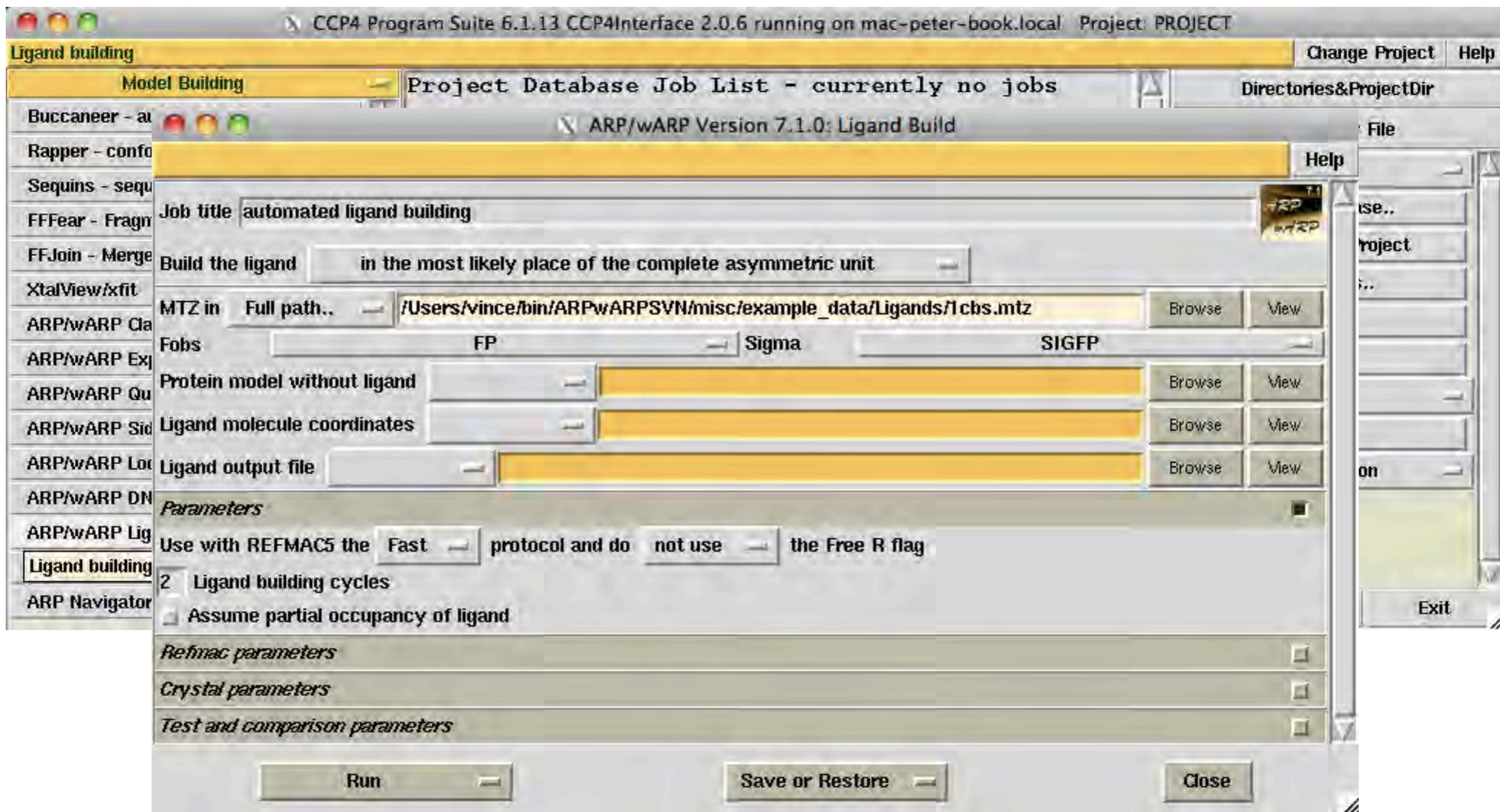
ARP/wARP: Ligands (warp_ligand)

1 cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

l cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

l cbs, Lig: RA

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

Ligand building

Model Building Project Database Job List - currently no jobs Directories&ProjectDir

ARP/wARP Version 7.1.0: Ligand Build

Job title automated ligand building

Build the ligand in the most likely place of the complete asymmetric unit

MTZ in Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Ligands/l cbs.mtz Browse View

Fobs FP Sigma SIGFP

Protein model without ligand Browse View

Ligand molecule coordinates Browse View

Ligand output file Browse View

Parameters

Use with REFMAC5 the Fast protocol and do not use the Free R flag

2 Ligand building cycles

Assume partial occupancy of ligand

Refmac parameters

Crystal parameters

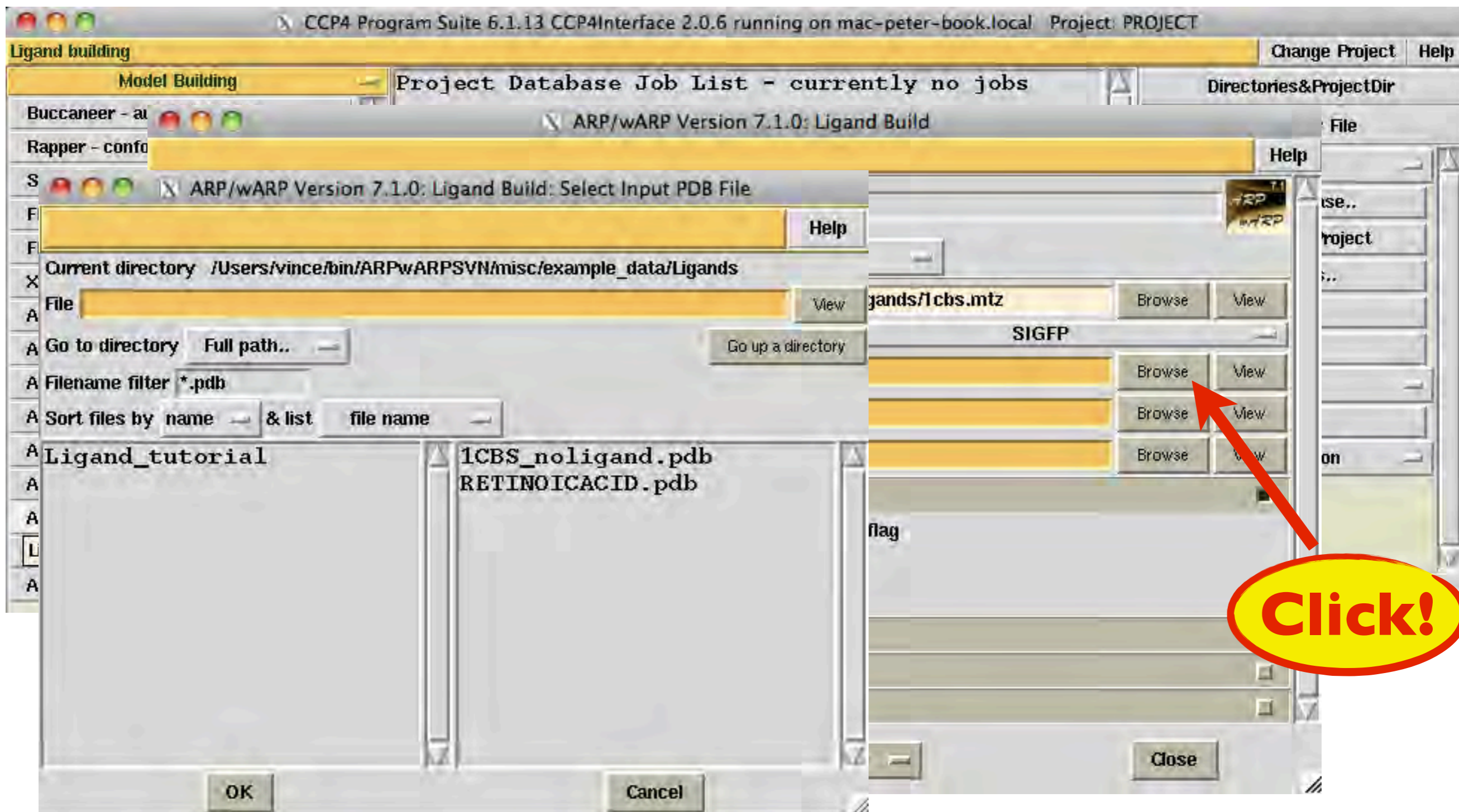
Test and comparison parameters

Run Save or Restore Close

Click!

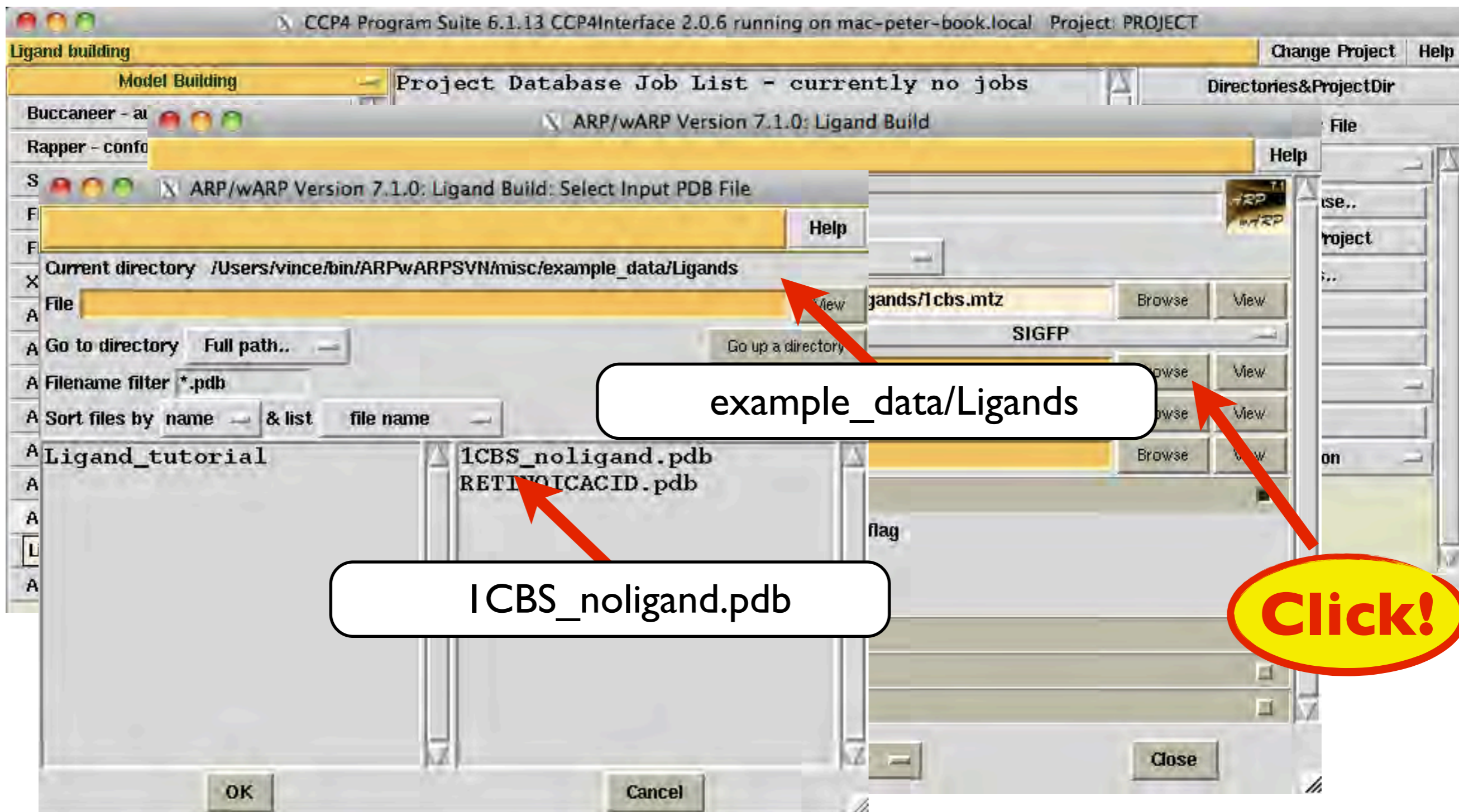
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



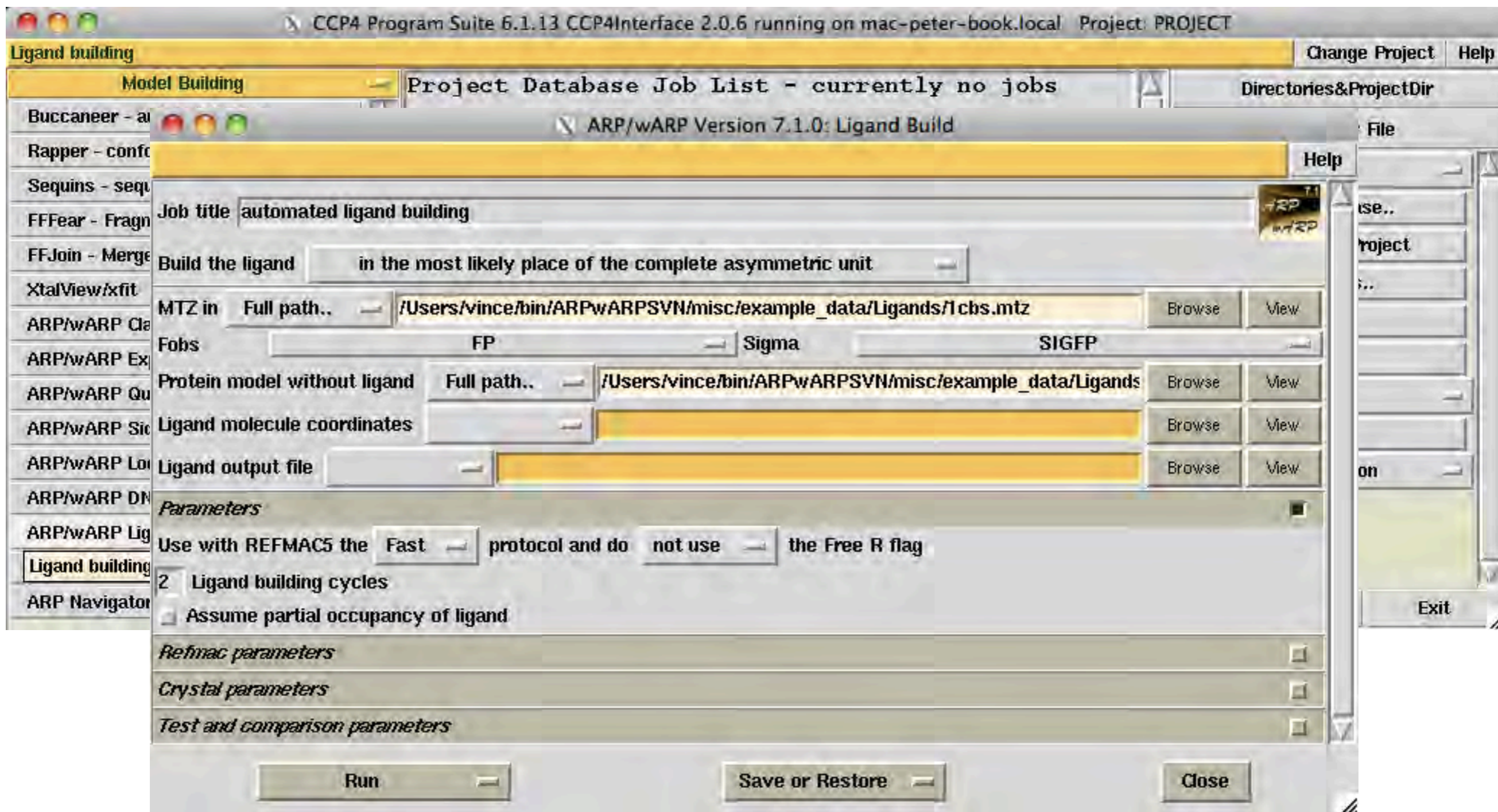
ARP/wARP: Ligands (warp_ligand)

l cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

I cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

l cbs, Lig: RA

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

Ligand building

Model Building Project Database Job List - currently no jobs Directories&ProjectDir

Buccaneer - a Rapper - conf Sequins - sequ FFFear - Fragn FFJoin - Merge XtalView/xfit ARP/wARP Cla ARP/wARP Ex ARP/wARP Qu ARP/wARP Sic ARP/wARP Lo ARP/wARP DN ARP/wARP Lig Ligand building ARP Navigator

ARP/wARP Version 7.1.0: Ligand Build

File Help

Job title automated ligand building

Build the ligand in the most likely place of the complete asymmetric unit

MTZ in Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Ligands/l cbs.mtz Browse View

Fobs FP Sigma SIGFP

Protein model without ligand Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Ligands Browse View

Ligand molecule coordinates Browse View

Ligand output file Browse View

Parameters

Use with REFMAC5 the Fast protocol and do not use the Free R flag

Ligand building cycles

Assume partial occupancy of ligand

Refmac parameters

Crystal parameters

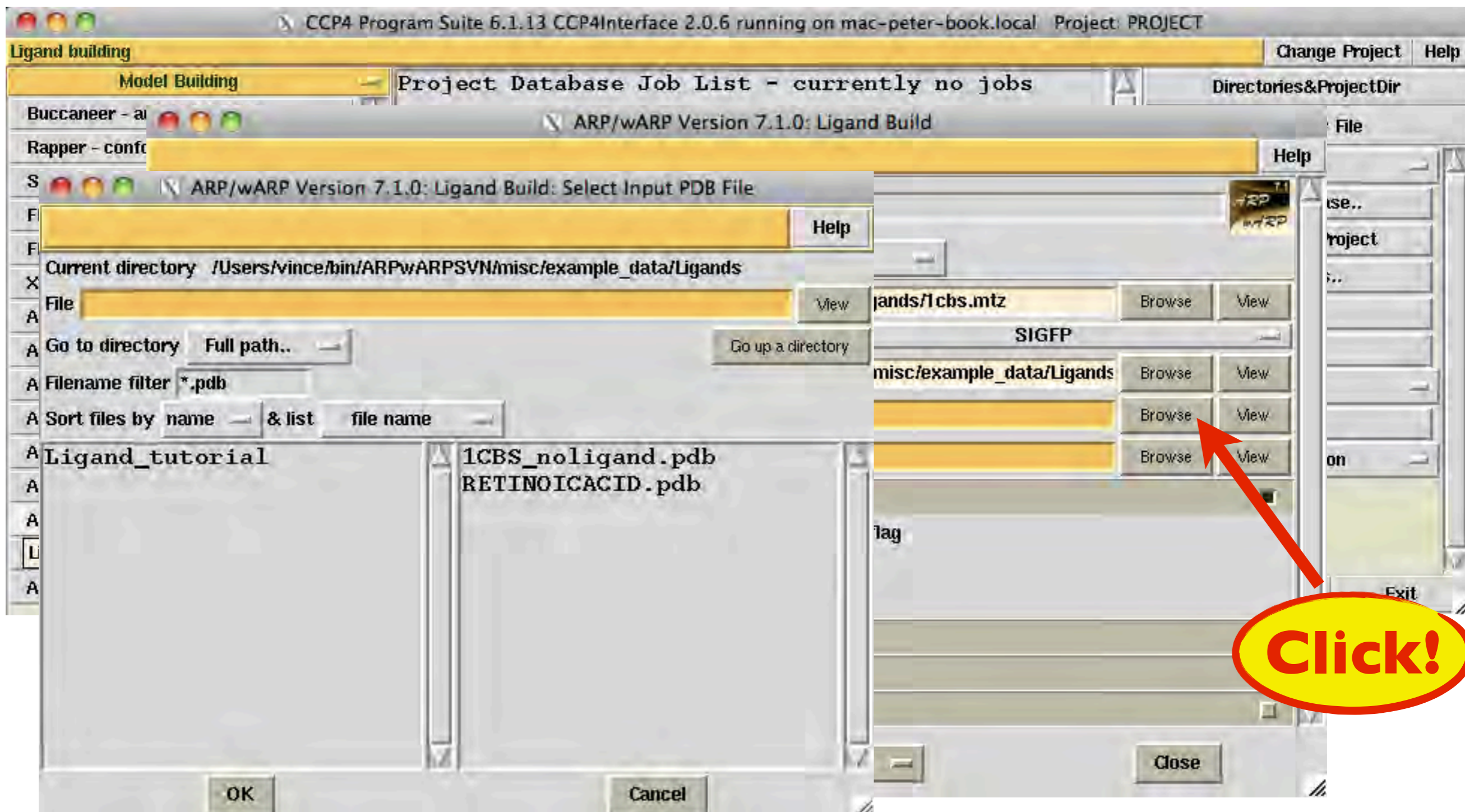
Test and comparison parameters

Run Save or Restore Close

Click!

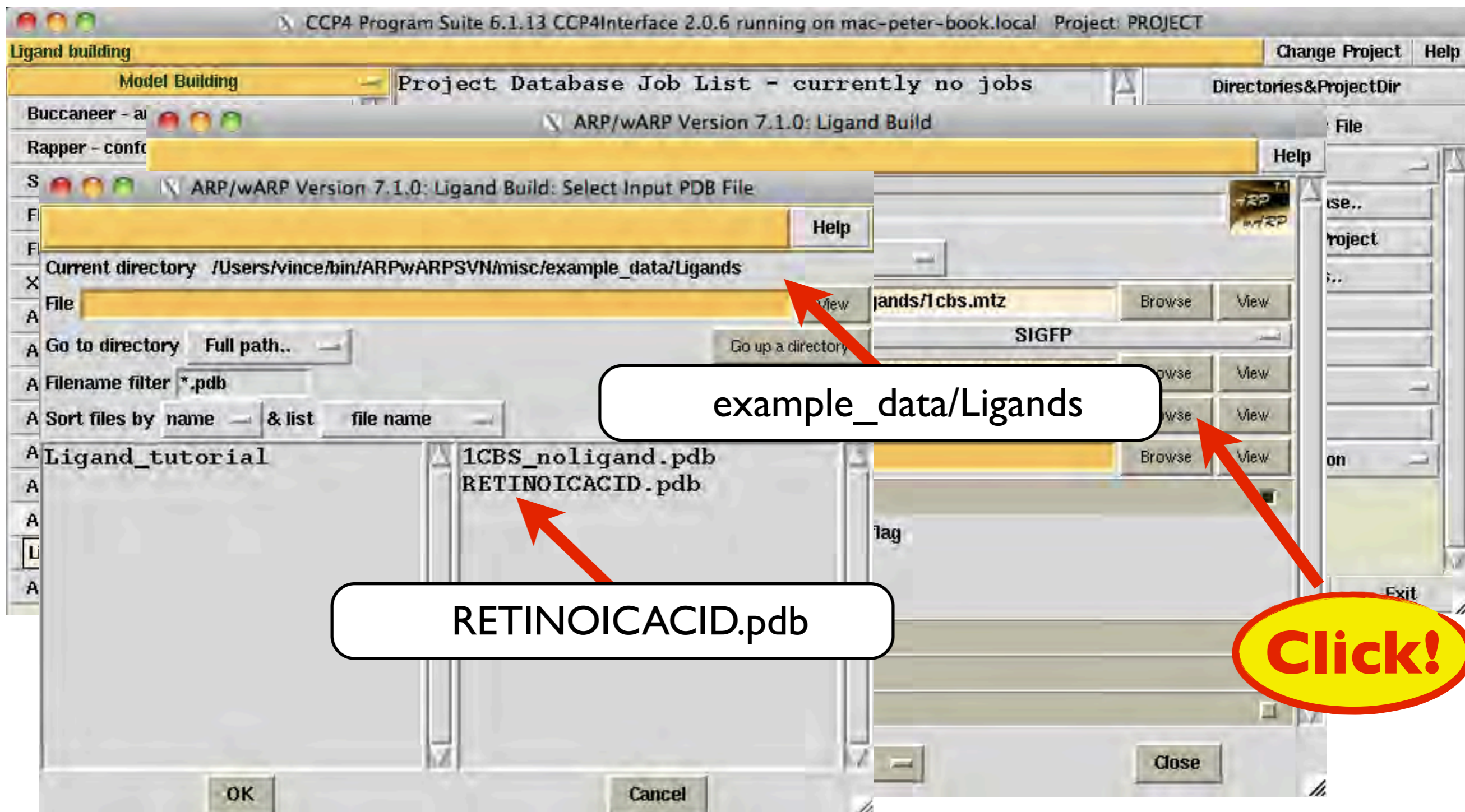
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



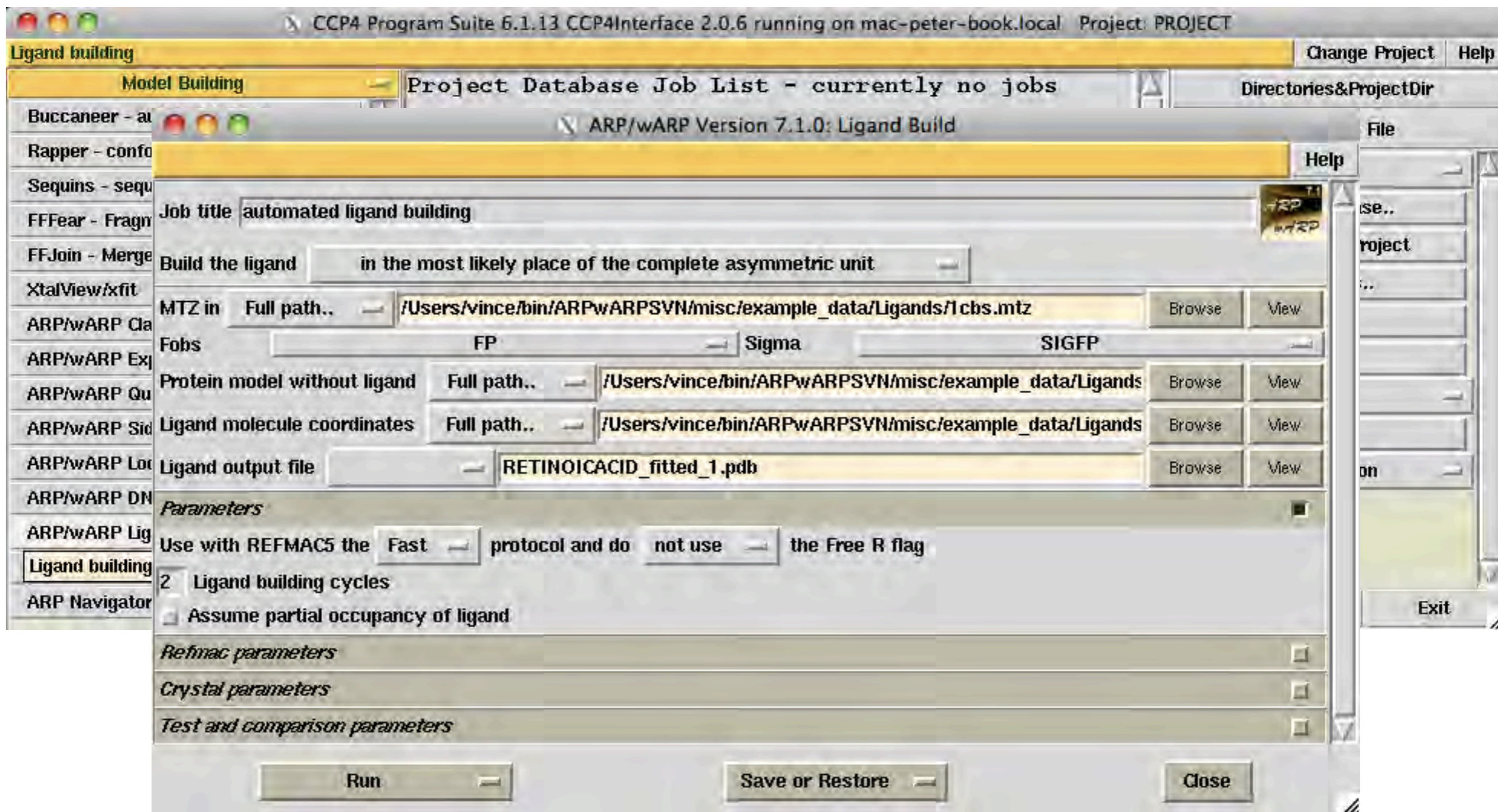
ARP/wARP: Ligands (warp_ligand)

1cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

l cbs, Lig: RA



ARP/wARP: Ligands (warp_ligand)

l cbs, Lig: RA

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

Ligand building

Model Building Project Database Job List - currently no jobs Directories&ProjectDir

ARP/wARP Version 7.1.0: Ligand Build

Job title automated ligand building

Build the ligand in the most likely place of the complete asymmetric unit

MTZ in Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Ligands/l cbs.mtz Browse View

Fobs FP Sigma SIGFP

Protein model without ligand Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Ligands Browse View

Ligand molecule coordinates Full path.. /Users/vince/bin/ARPwARPSVN/misc/example_data/Ligands Browse View

Ligand output file RETINOICACID_fitted_1.pdb Browse View

Parameters

Use with REFMAC5 the Fast protocol the Free R flag

2 Ligand building cycles

Assume partial occupancy of ligand

Refmac parameters

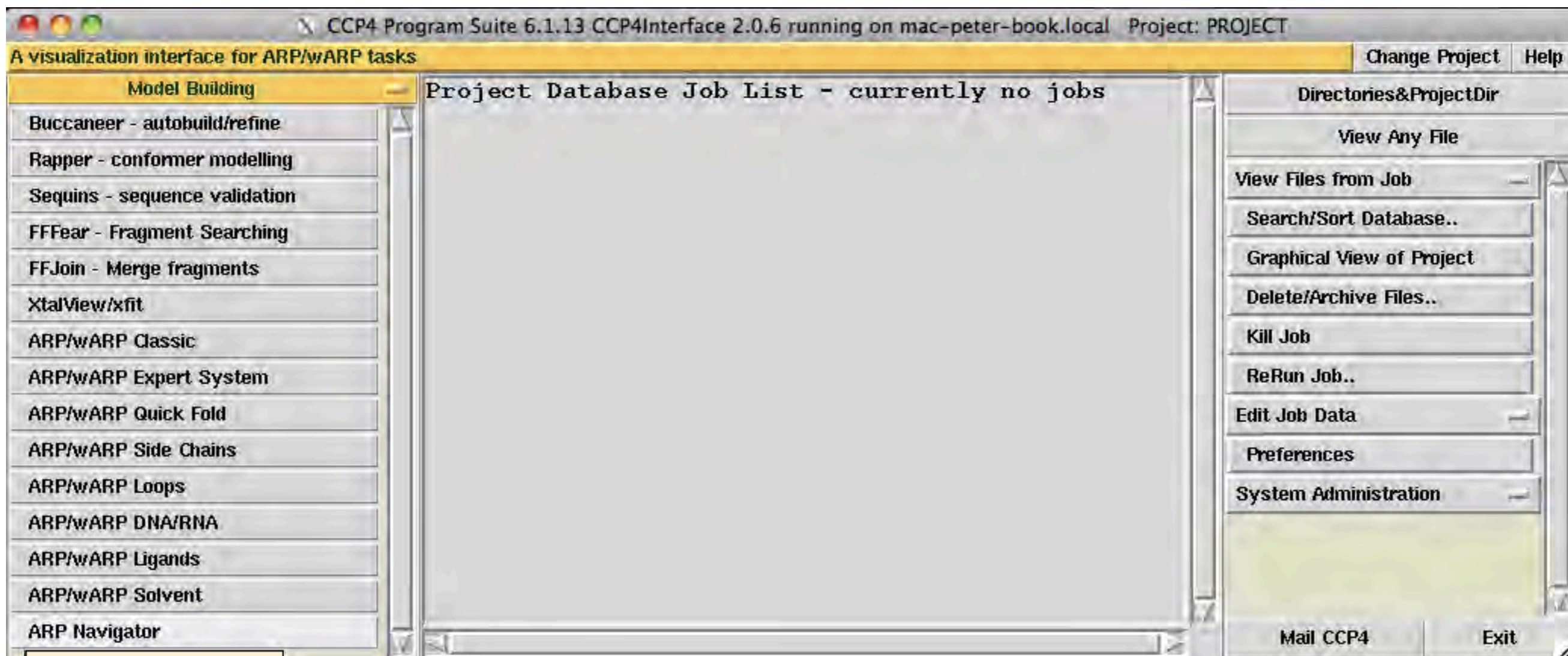
Crystal parameters

Test and comparison parameters

Run Save or Restore Close

Click!

ARP/wARP: ARPNavigator



A visualization interface for
ARP/wARP tasks

ARP/wARP: ARPNavigator



A visualization interface for ARP/wARP tasks

Click!