Ab initio modelling: Guided tutorial

Clement Blanchet, EMBL Hamburg

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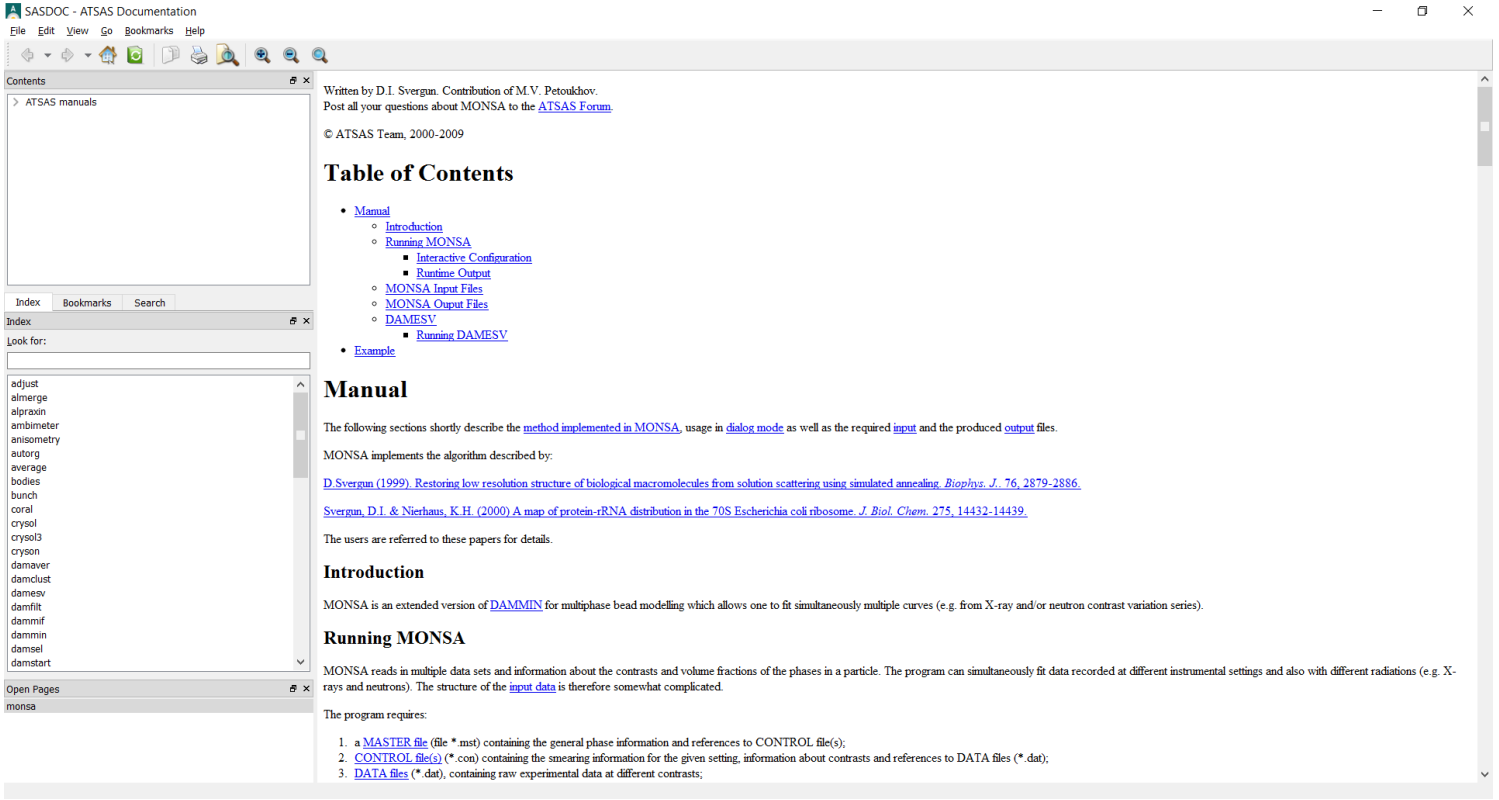
Ressources: Atsas help - Sasdoc



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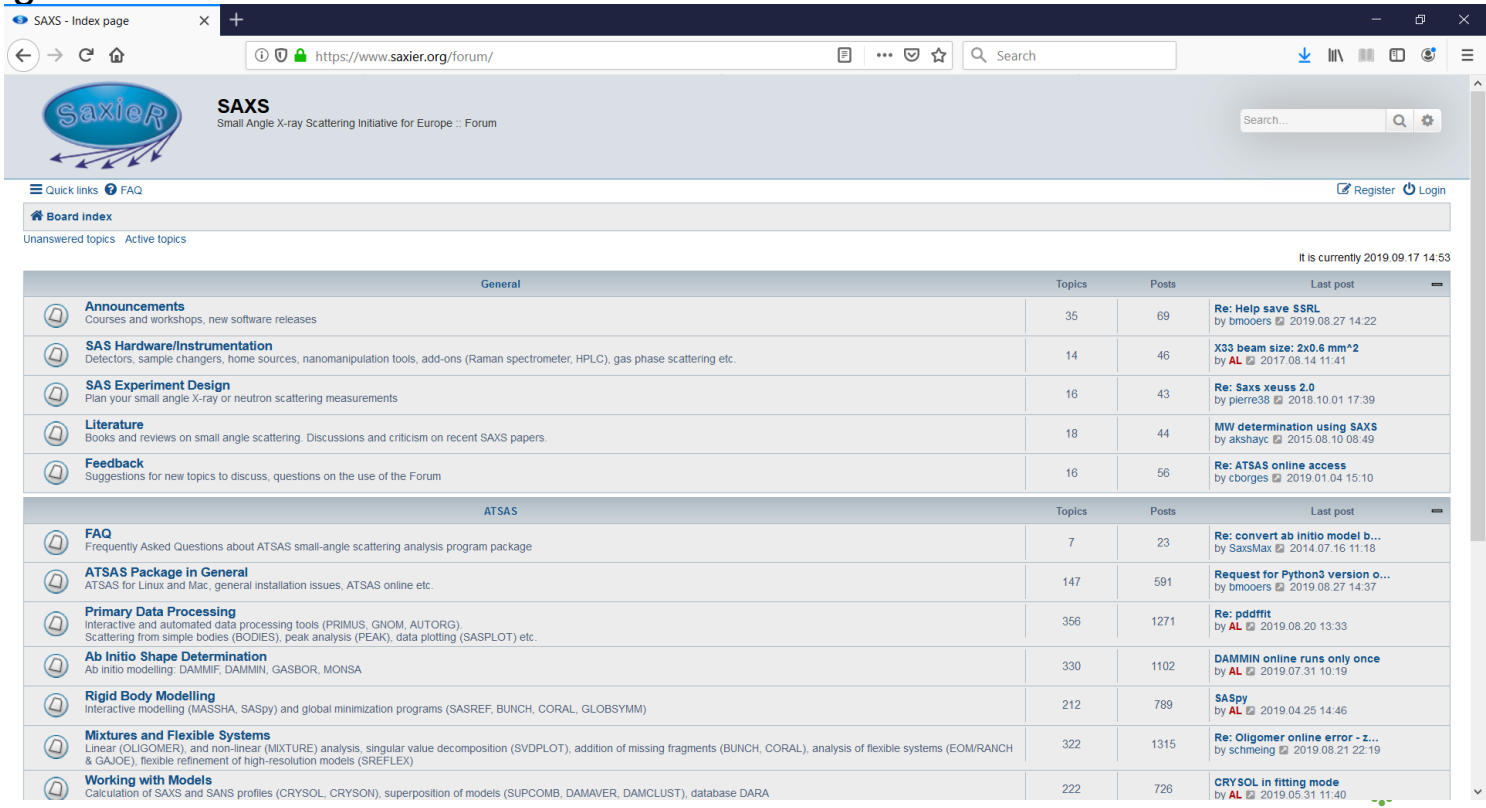
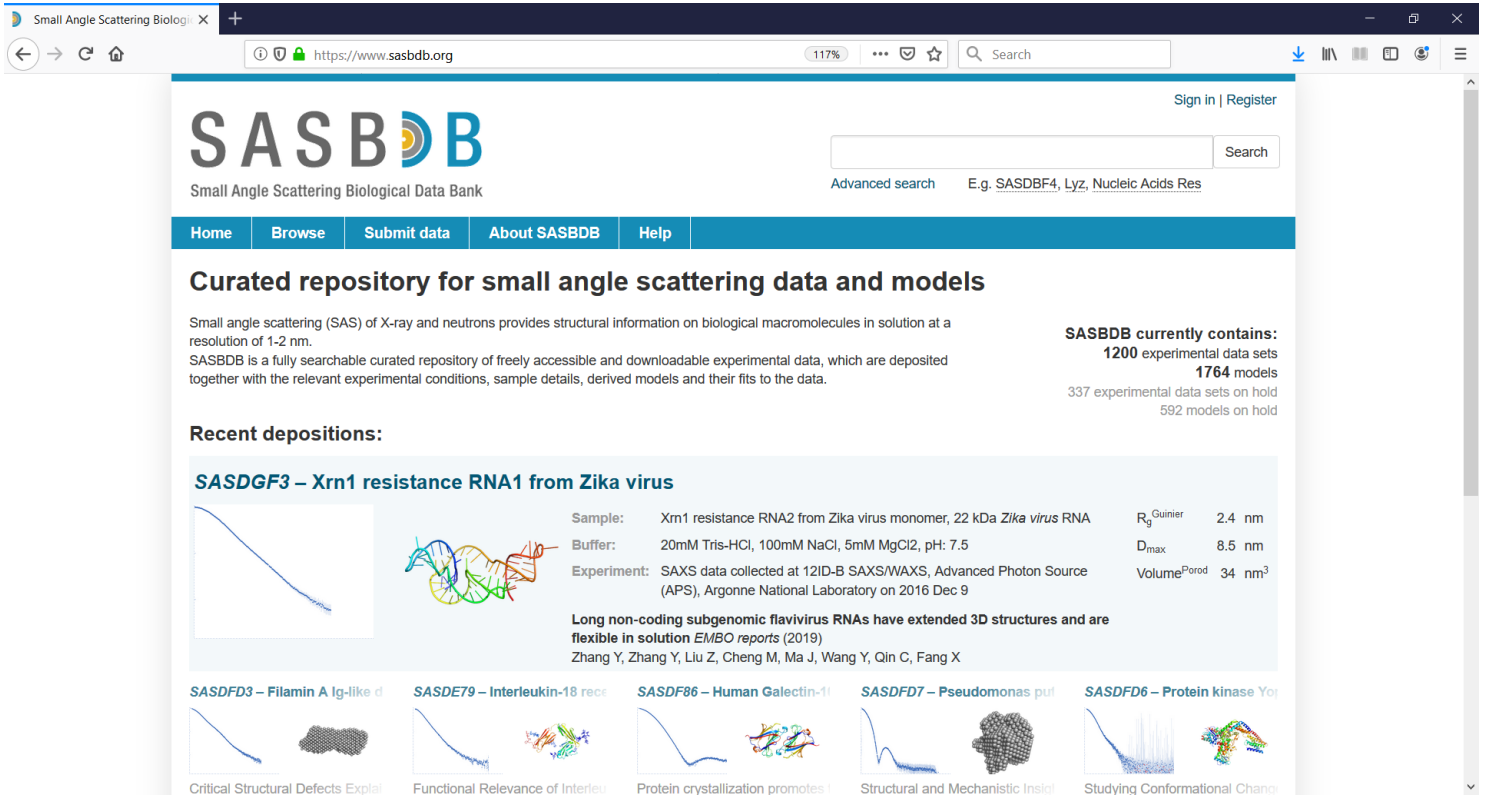
Ressources: Saxier forum

- www.saxier.org/forum/



Ressources: SASBDB – www.sasbdb.org



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Running atsas program - DAMMIN

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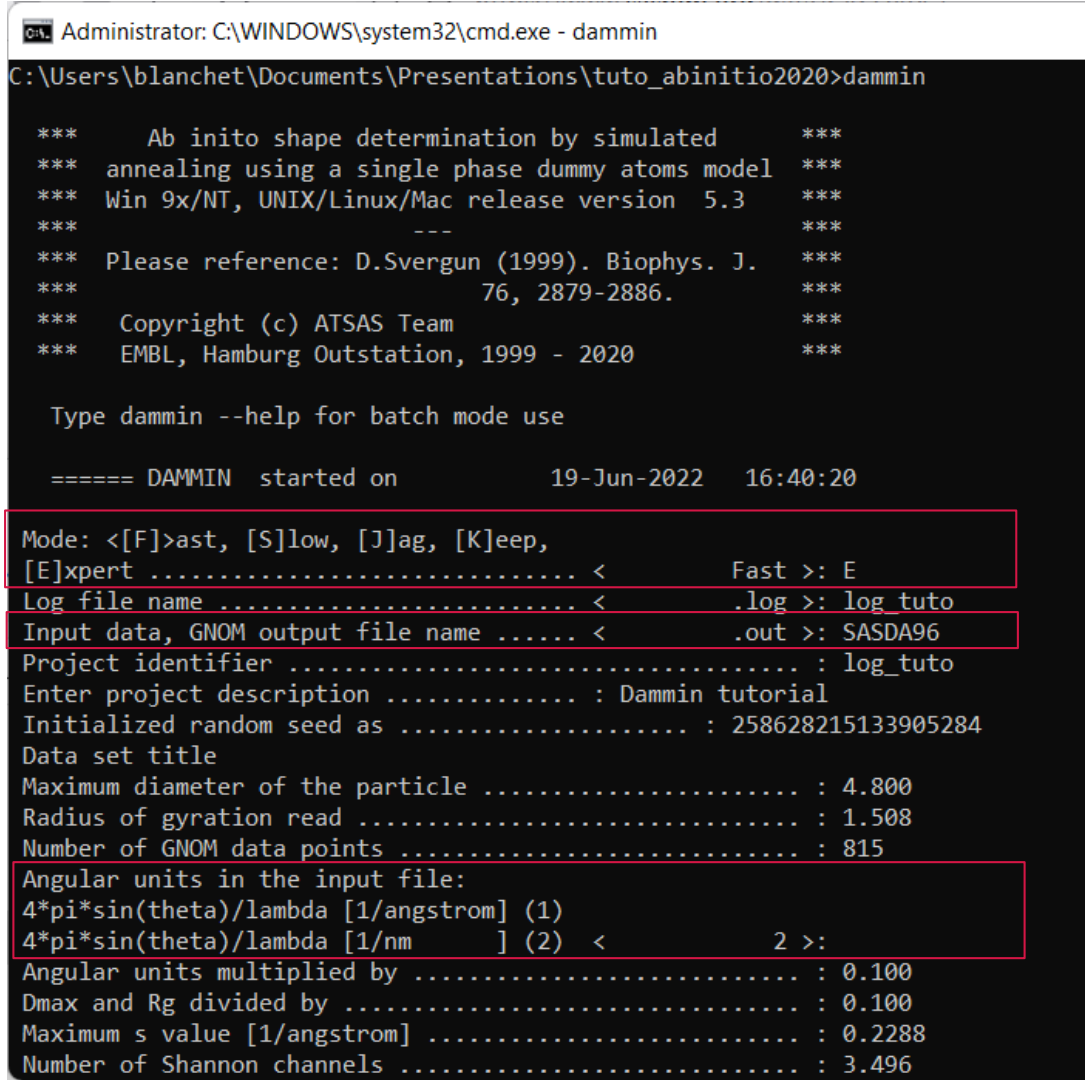

Mode: how much do you want to tune the
Fast (large beam, fast cool-down)
Slow (smaller beads and slower cool-dow

Name of the gnom output file

Angular unit of the input file

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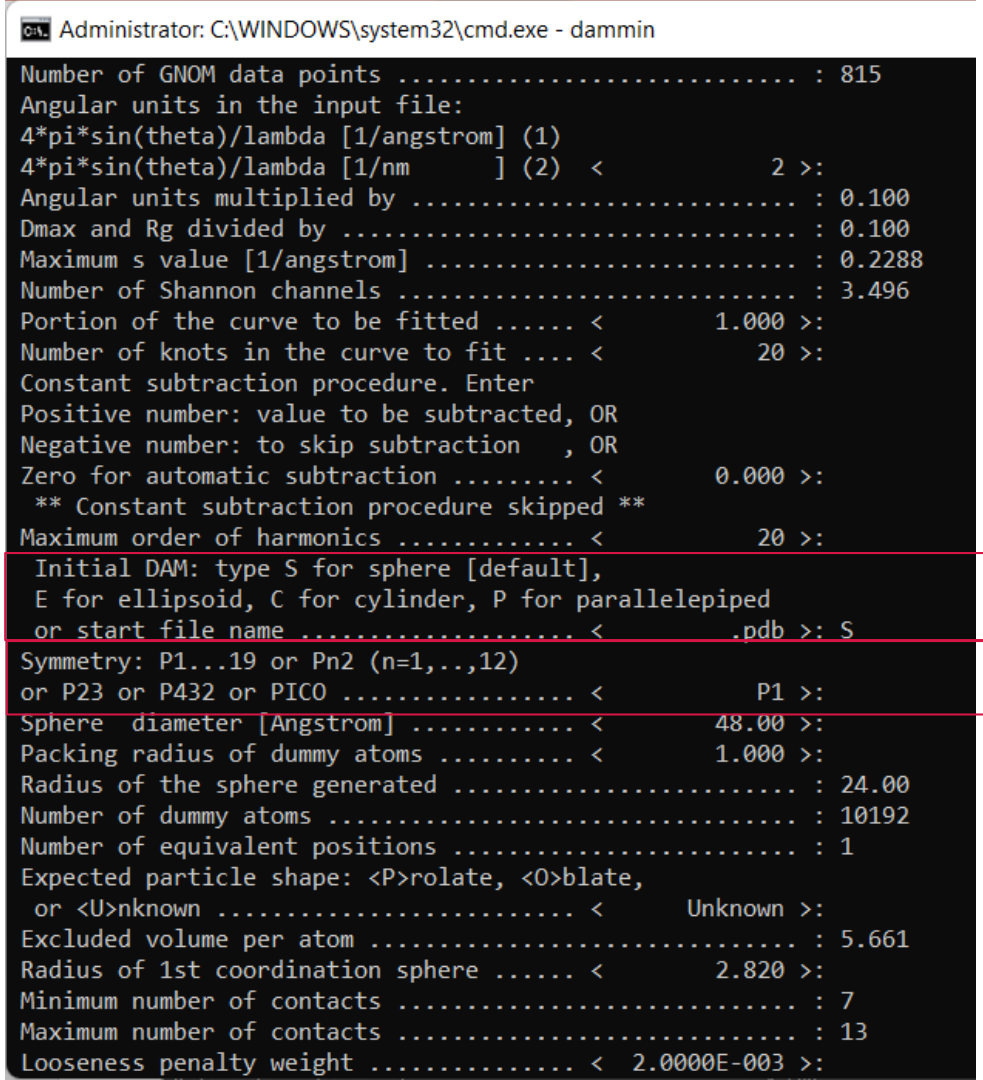

Input curve (unit, portion to be fitted, etc…)

Model (search volume, symmetry, bead size

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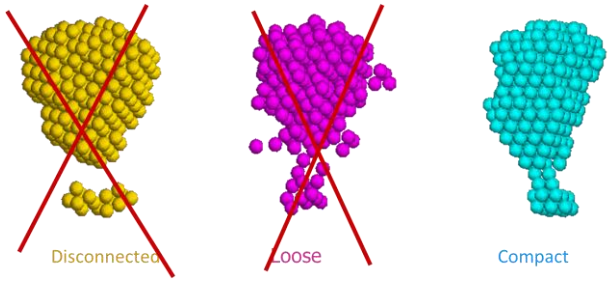
```
Administrator: C:\WINDOWS\system32\cmd.exe - dammin
Sphere  diameter [Angstrom] ..... <        48.00 >:
Packing radius of dummy atoms ..... <        1.000 >:
Radius of the sphere generated ..................... : 24.00
Number of dummy atoms .............................. : 10192
Number of equivalent positions ..................... : 1
Expected particle shape: <P>rolate, <O>blate,
 or <U>nknown ..................... <      Unknown >:
Excluded volume per atom ........................... : 5.661
Radius of 1st coordination sphere ..... <        2.820 >:
Minimum number of contacts ......................... : 7
Maximum number of contacts ......................... : 13
Looseness penalty weight ............ <  2.0000E-003 >:
No of non-solvent atoms ............................ : 10192
Initial DAM looseness .............................. : 1.342E-03
Disconnectivity penalty weight ..... <  2.0000E-003 >:
Initial DAM # of graphs ............................ : 1
Discontiguity   value .............................. : 0.0
Center of the initial DAM:    0.0000   0.0000  -0.0000
Peripheral penalty weight ........... <       0.3000 >:
Peripheral penalty value ........................... : 0.6046
Fixing thresholds Los and Rf <  5.0000E-002, 2.0000E-002 >:
Randomize the structure [ Y / N ] ..... <          Yes >:
No of non-solvent atoms ............................ : 5116
Randomized DAM looseness ........................... : 5.350E-02
Randomized DAM # of graphs ......................... : 12
Discontiguity   value .............................. : 2.152E-03
Randomized peripheral penalty value ................ : 0.6026
Initial DAM shape anisometry ....................... : 7.217E-03
Initial DAM non-prolateness ........................ : 5.555E-03
Initial DAM non-oblateness ......................... : 0.0
Weight: 0=s^2, 1=Emphas.s->0, 2=Log .... <           1 >:
*** Porod weight with emphasis at low s ***
Initial scale factor ................ <  1.3056E-006 >:
```



Penalty terms

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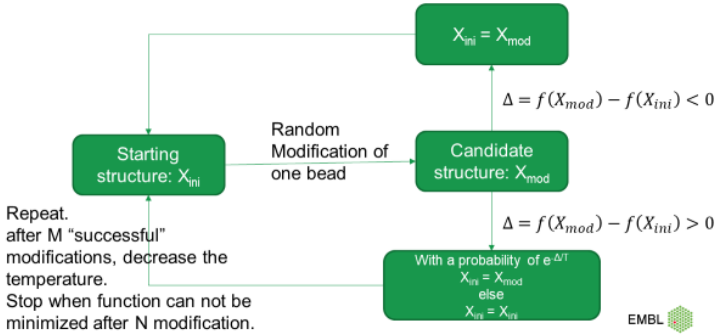
Administrator: C:\WINDOWS\system32\cmd.exe - dammin

```
Initial DAM non-oblateness ..............................  : 0.0
Weight: 0=s^2, 1=Emphas.s->0, 2=Log .... <           1 >:
*** Porod weight with emphasis at low s ***
Initial scale factor ..................  <  1.3056E-006 >:
Fix the scale factor [ Y / N ] .........  <          No >:
Initial R^2 factor ....................................  : 0.2315
Initial R   factor ....................................  : 0.4811
Initial penalty .......................................  : 0.1809
Initial fVal ..........................................  : 0.4124
 Tuning the annealing parameters. Please wait...
Variation of the target function ......................  : 7.469E-05
CPU per function call, seconds ........................  : 1.094E-03
Initial annealing temperature ..........  <  1.0000E-003 >:
Annealing schedule factor ..............  <       0.9500 >:
# of independent atoms to modify .......  <            1 >:
Max # of iterations at each T ..........  <       713440 >:
Max # of successes at each T ...........  <        71344 >:
Min # of successes to continue .........  <          237 >:
Max # of annealing steps ...............  <          200 >:
 ====  Simulated annealing procedure started  ====
j:   1 T: 0.100E-02 Suc: 71344 Eva:    73689 CPU:  0.817E+02 SqF: 0.6273
 Rf: 0.46553 Los:0.0519 Dis:0.0024 Per:  0.5891 Sca: 0.129E-05
j:   2 T: 0.950E-03 Suc: 71344 Eva:   147449 CPU:  0.163E+03 SqF: 0.6212
 Rf: 0.46657 Los:0.0522 Dis:0.0035 Per:  0.5898 Sca: 0.127E-05
j:   3 T: 0.903E-03 Suc: 71344 Eva:   221346 CPU:  0.244E+03 SqF: 0.6096
 Rf: 0.46121 Los:0.0545 Dis:0.0035 Per:  0.5866 Sca: 0.130E-05
j:   4 T: 0.857E-03 Suc: 71344 Eva:   295383 CPU:  0.326E+03 SqF: 0.6034
 Rf: 0.46144 Los:0.0570 Dis:0.0020 Per:  0.5873 Sca: 0.135E-05
j:   5 T: 0.815E-03 Suc: 71344 Eva:   369539 CPU:  0.407E+03 SqF: 0.5980
 Rf: 0.46265 Los:0.0562 Dis:0.0028 Per:  0.5868 Sca: 0.133E-05
j:   6 T: 0.774E-03 Suc: 71344 Eva:   443803 CPU:  0.488E+03 SqF: 0.5901
 Rf: 0.46053 Los:0.0551 Dis:0.0020 Per:  0.5859 Sca: 0.132E-05
```

Simulated annealing



Simulated annealing parameters

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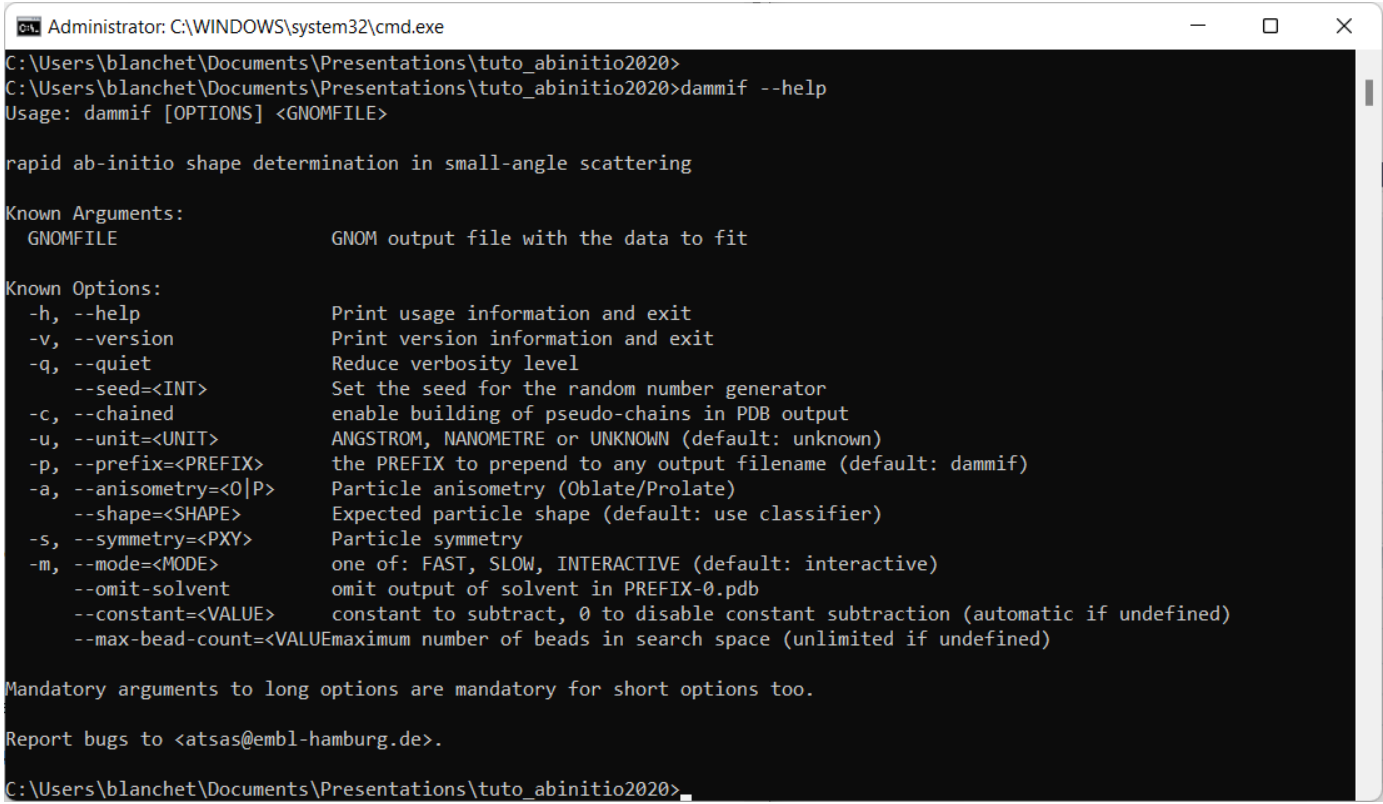
DAMMIF command line

- For all atsas program: Use `--help` in command line to see available options




```
dammif lys.out --mode=slow --prefix lys1
```

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windows

```
dammif lys.out --mode=slow --prefix lys1
dammif lys.out --mode=slow --prefix lys2
dammif lys.out --mode=slow --prefix lys3
dammif lys.out --mode=slow --prefix lys4
dammif lys.out --mode=slow --prefix lys5
dammif lys.out --mode=slow --prefix lys6
dammif lys.out --mode=slow --prefix lys7
dammif lys.out --mode=slow --prefix lys8
dammif lys.out --mode=slow --prefix lys9
dammif lys.out --mode=slow --prefix lys10
```

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On linux/macOS

```
for i in ‘seq1 10‘ ; do
dammif --prefix=lys-$i --mode=slow lys.out;
done
```

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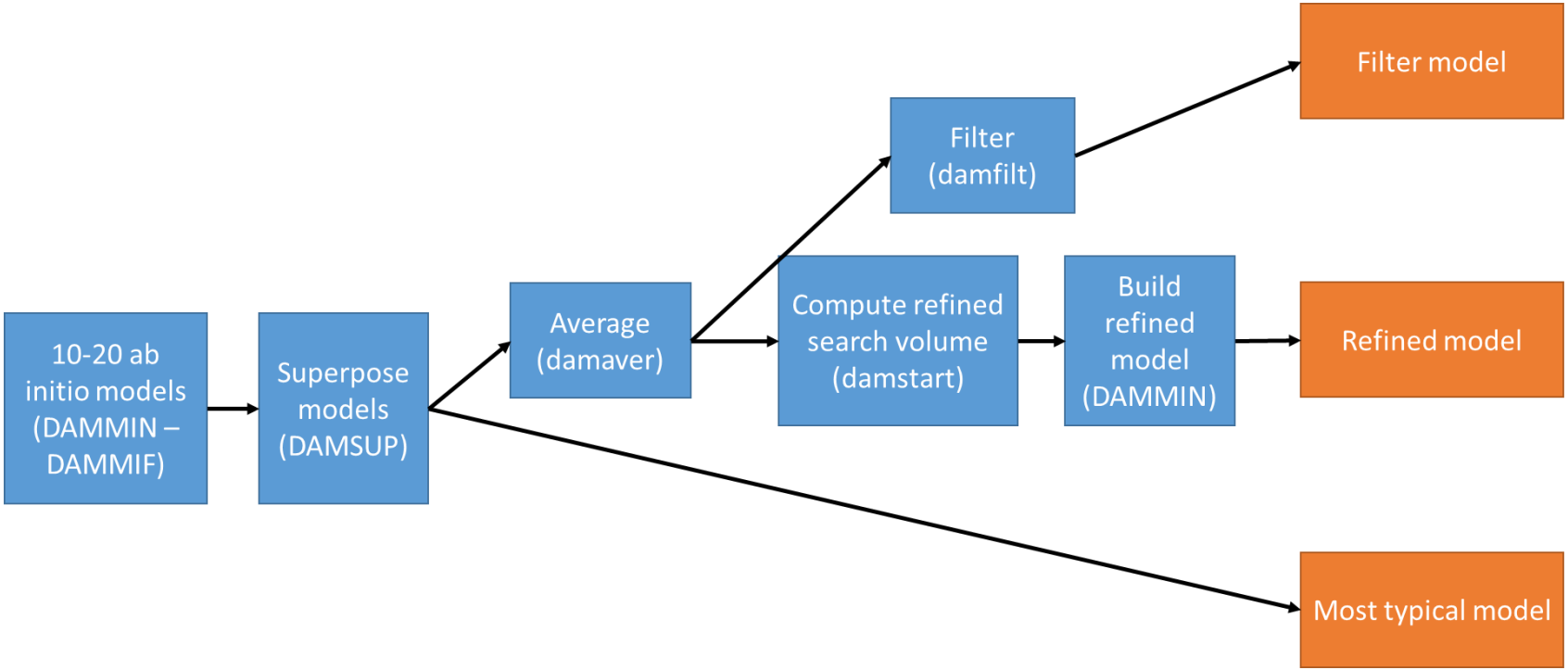
10-20 ab initio models (DAMMIN – DAMMIF)
Superpose models (DAMSUP)
Average (damaver)
Filter (damfilt)
Filter model
Compute refined search volume (damstart)
Build refined model (DAMMIN)
Refined model
Most typical model

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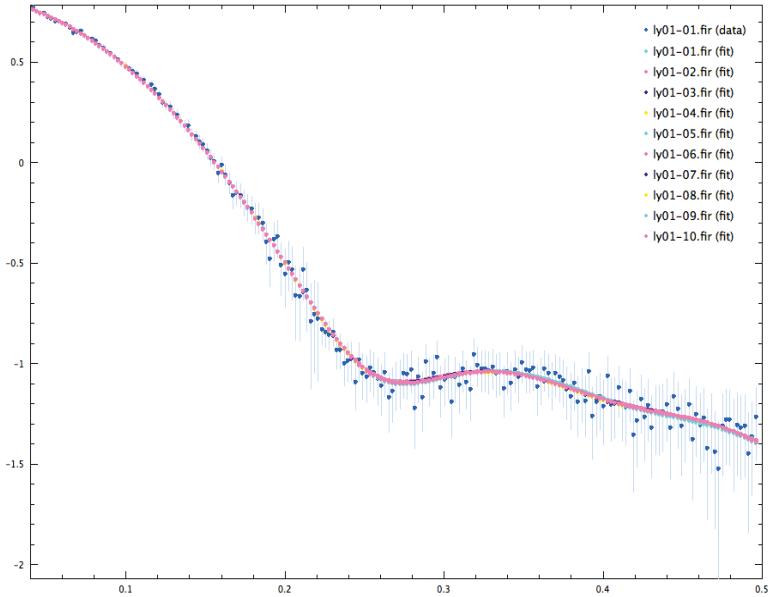
DAMMIF fits



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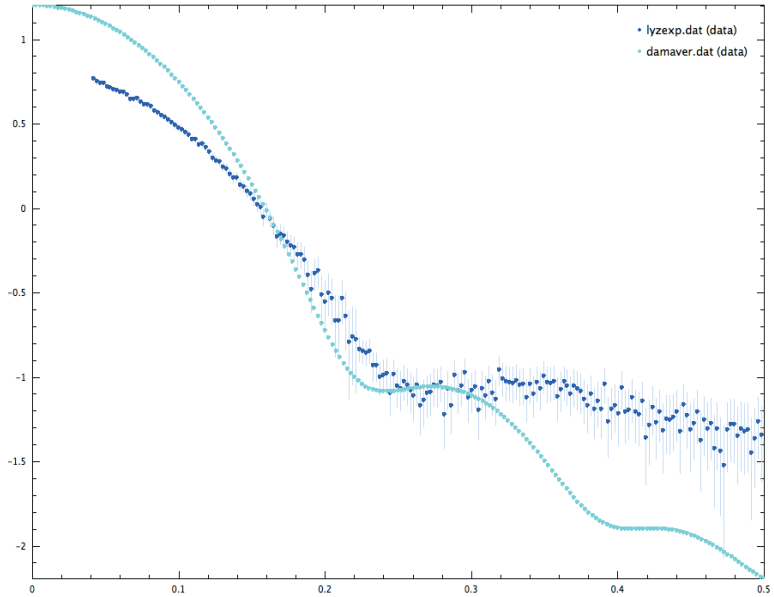
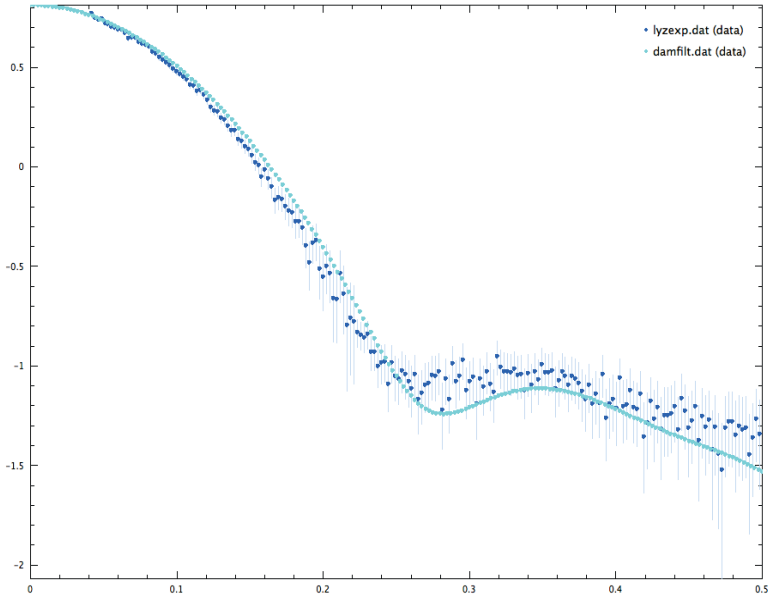
DAMAVER fit



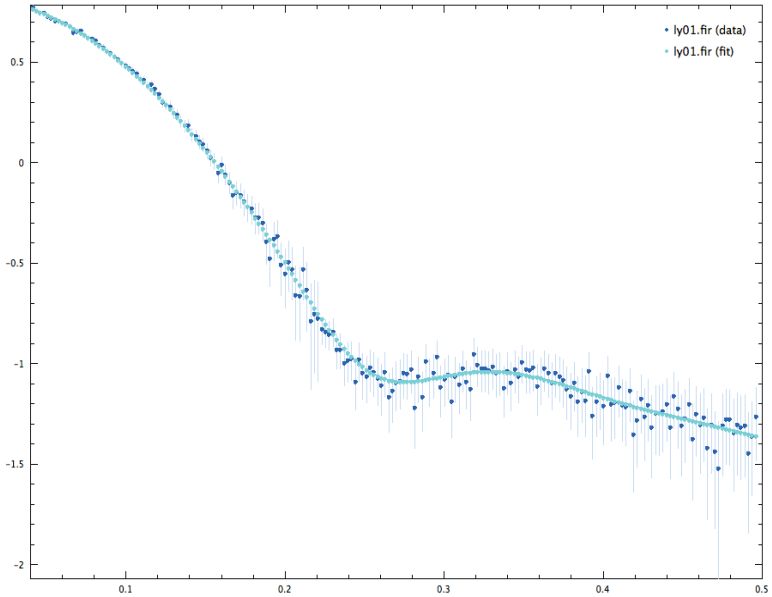
EMBL

DAMFILT fit



EMBL

DAMMIN fit



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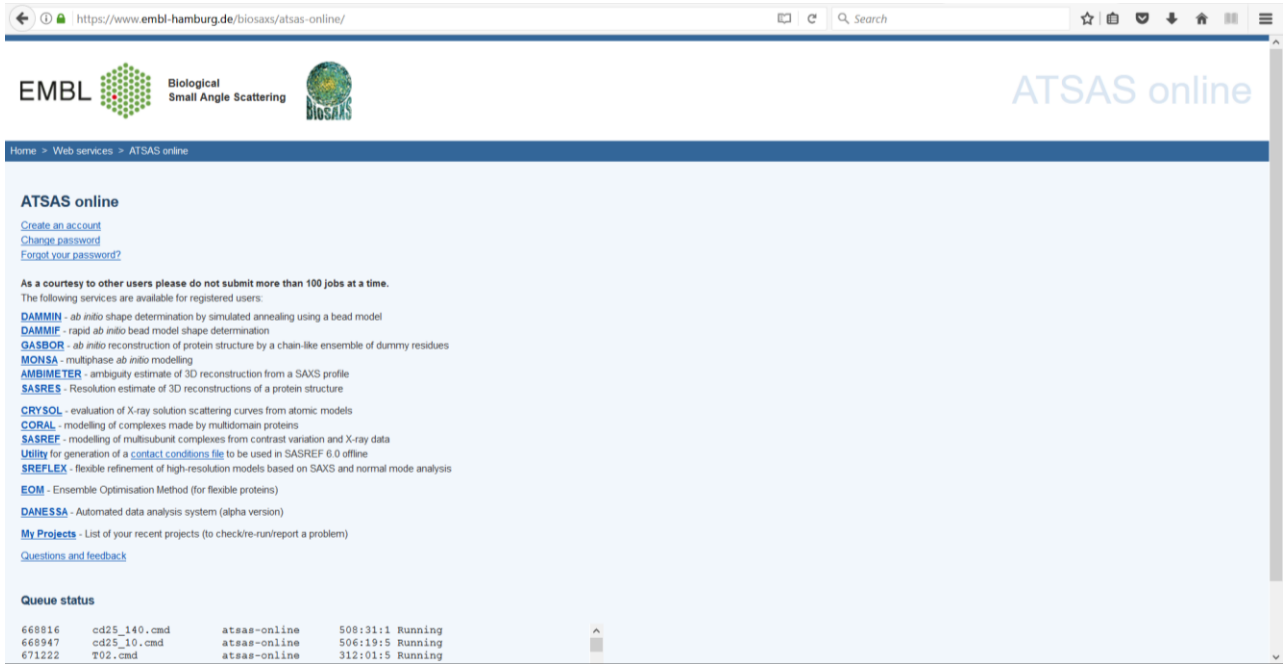
Using Primus

Atsas online



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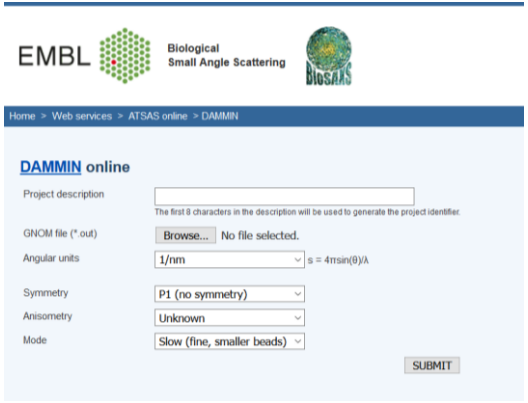
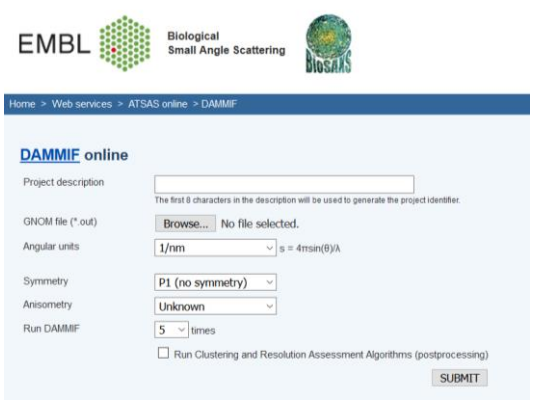
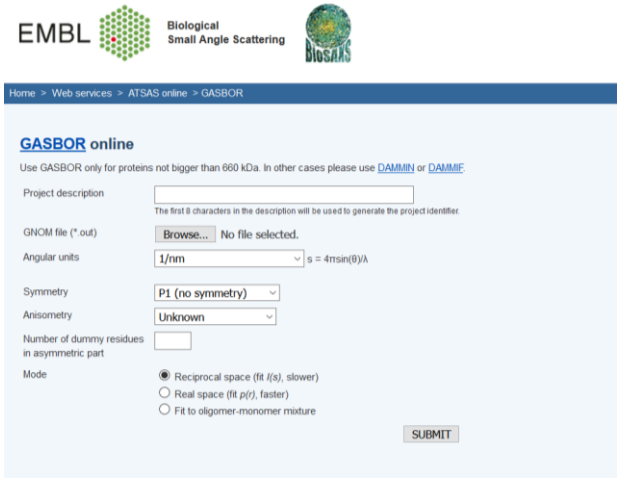
DAMMIN



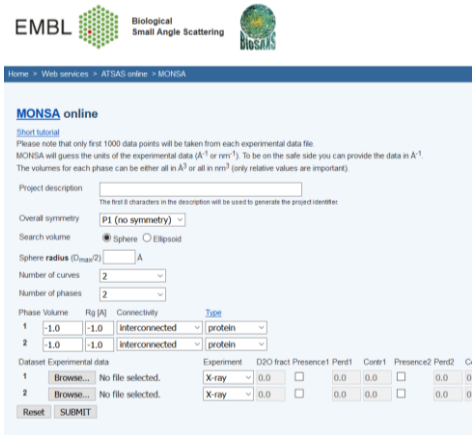
DAMMIF



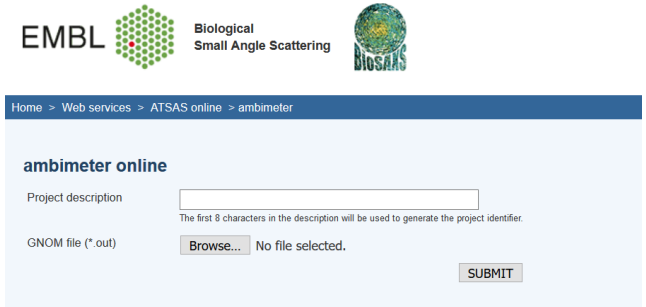
GASBOR



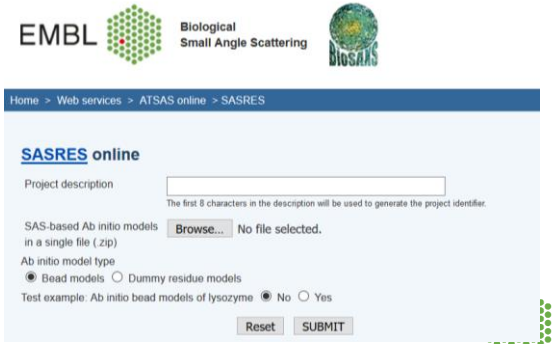
MONSA



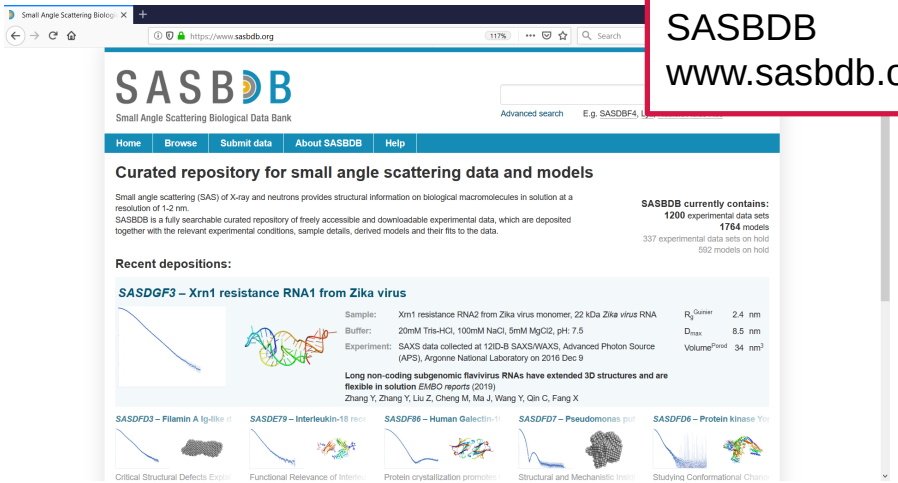
AMBIMETER



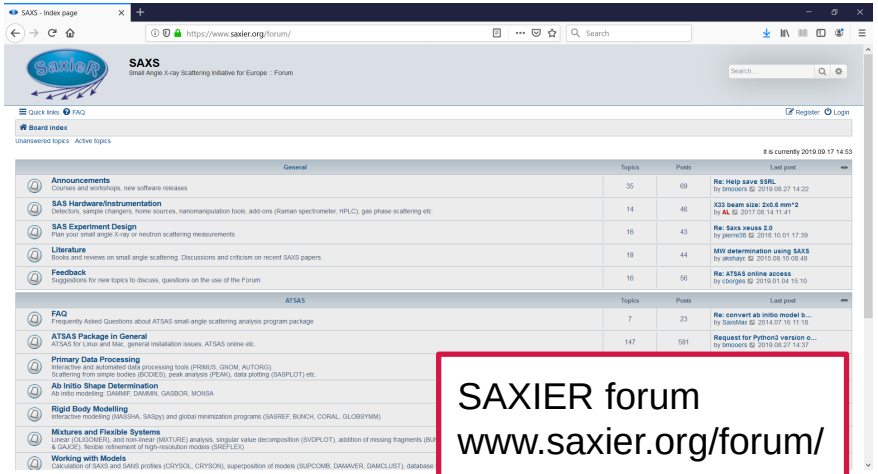
SASRES



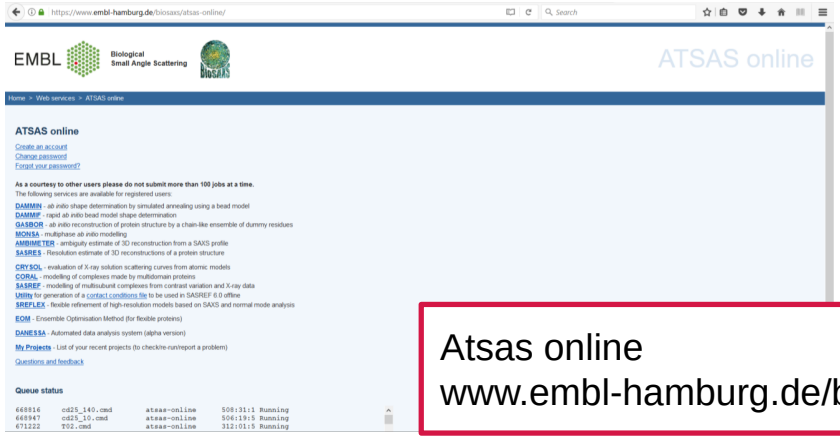
SASBDB
www.sasbdb.org



SAXIER forum
www.saxier.org/forum/



Atsas online
www.embl-hamburg.de/biosaxs/atsas-online/



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