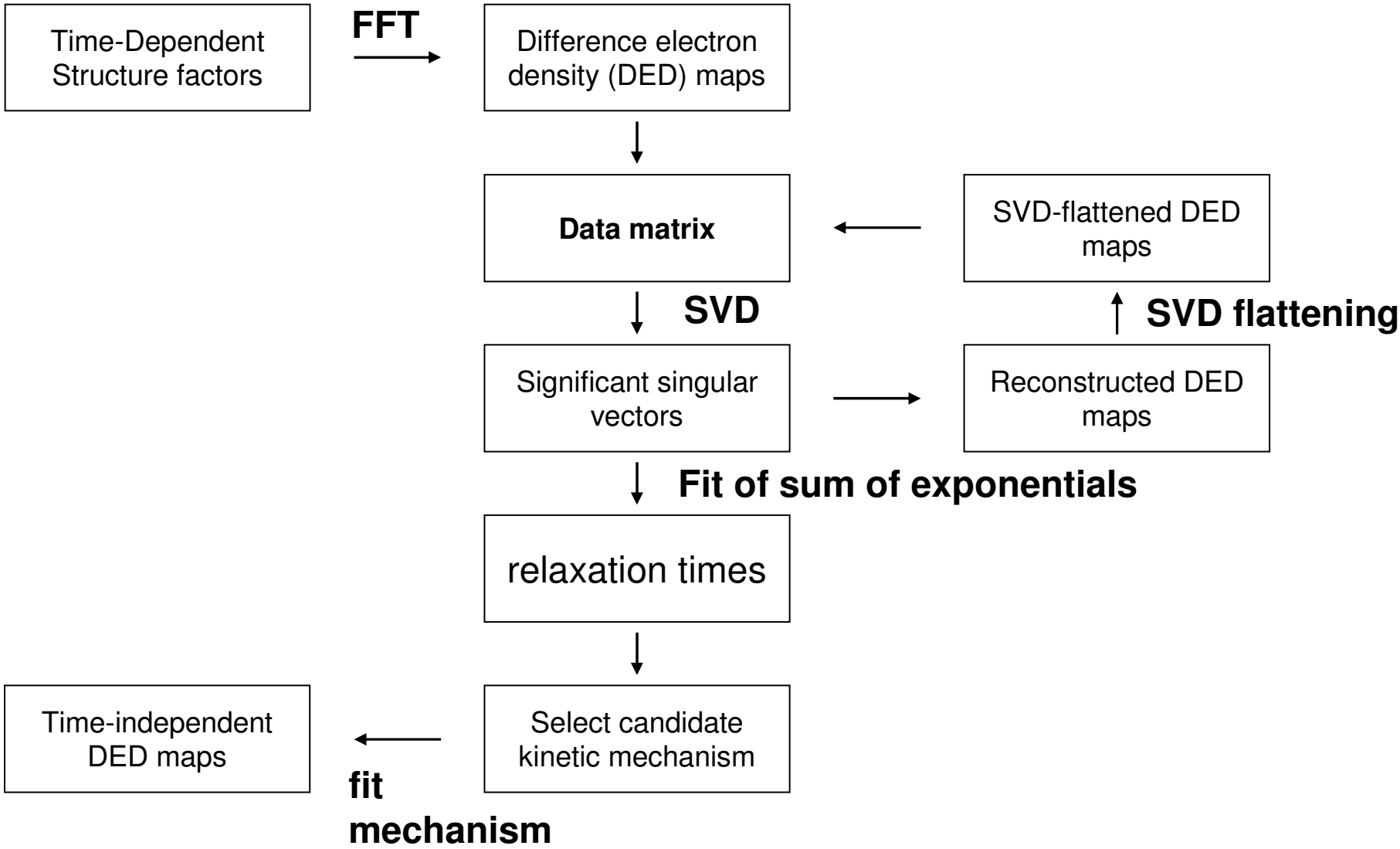
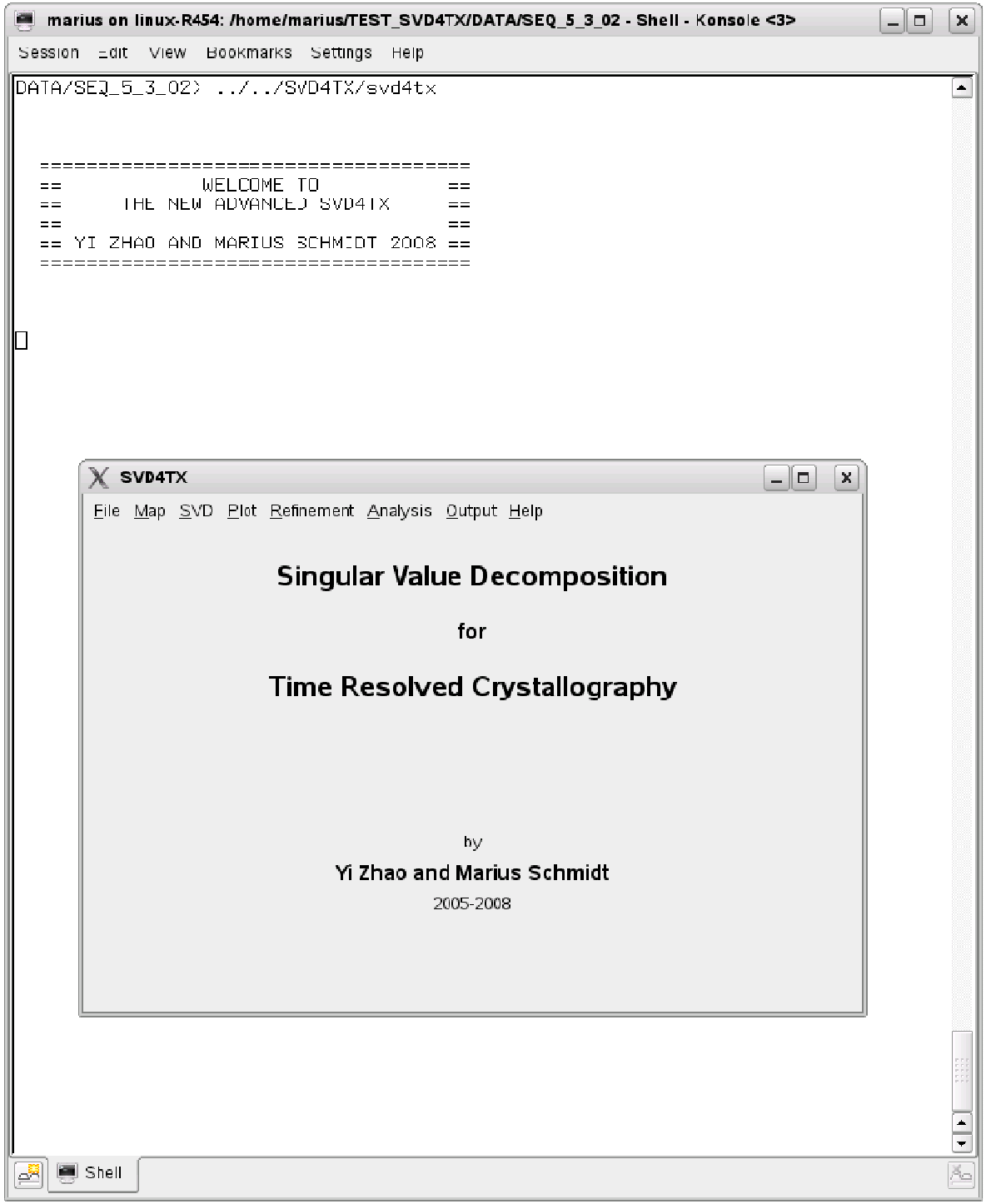
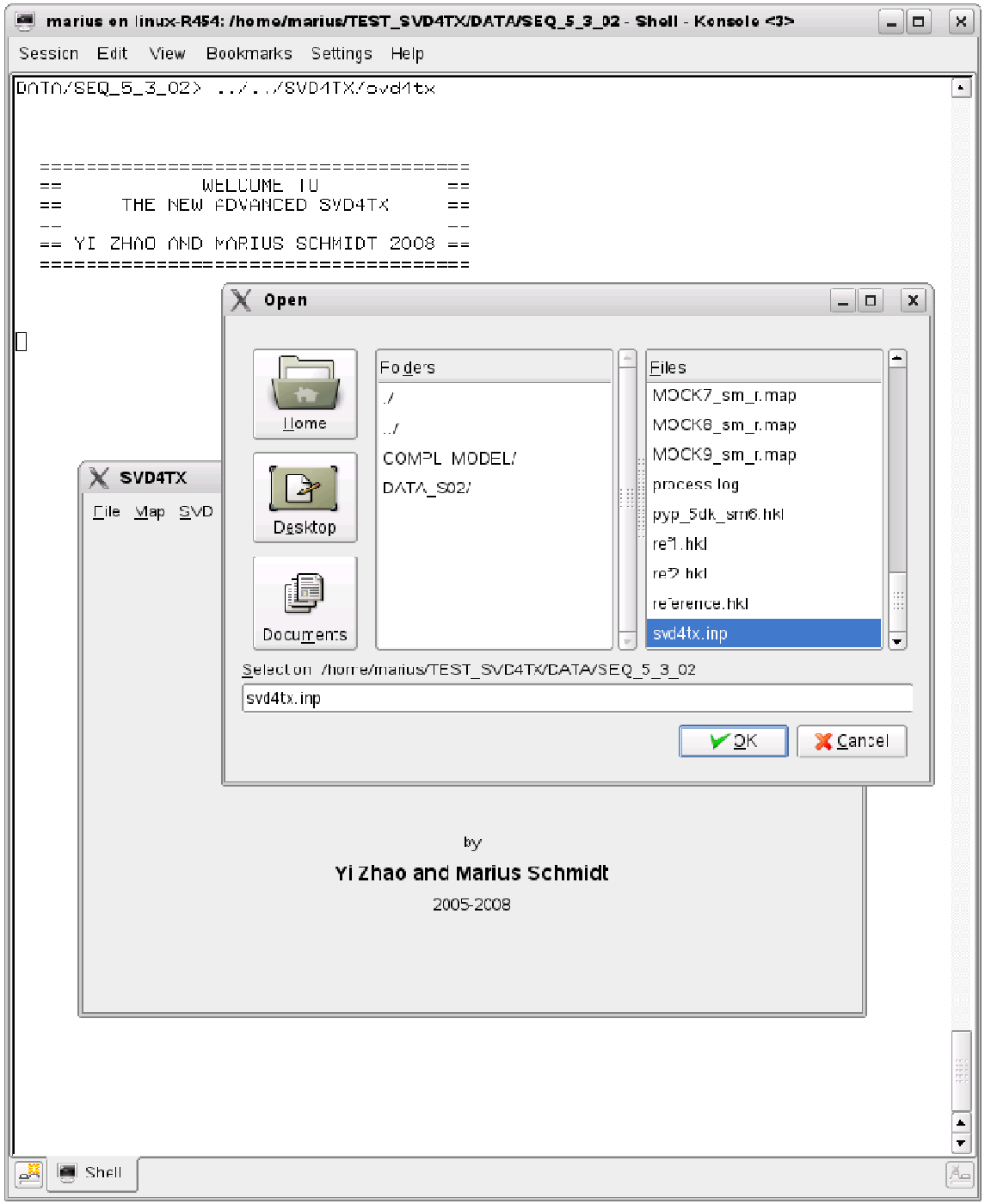
General Outline for Data Analysis with SVD4TX

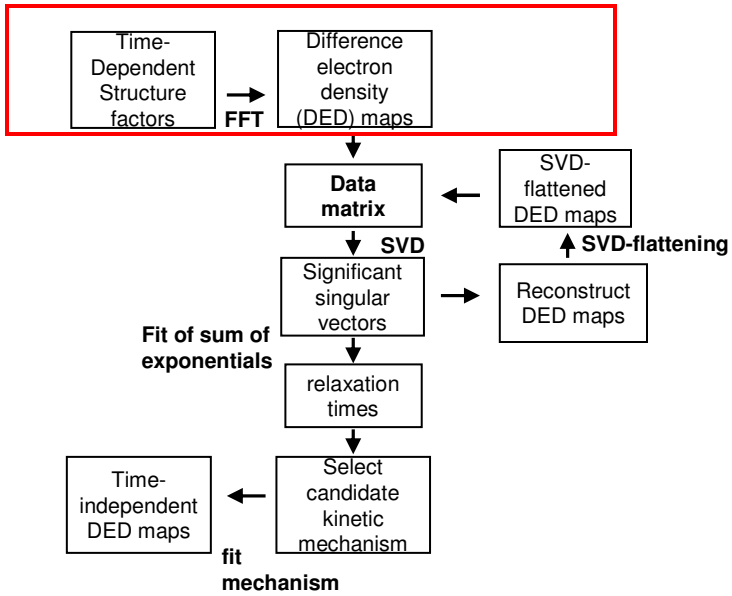




This is the new SVD4TX GUI

Programmed in GTK+ and C


marius on linux-R454: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02 - Shell - Konsole <3>
Session Edit View Bookmarks Settings Help
DATA/SEQ_5_3_02> ../../SVD4TX/svd4tx
WELCOME TO
THE NEW ADVANCED SVD4TX
YI ZHAO AND MARIUS SCHMIDT 2008
Open
Home
Desktop
Documents
Folders
./
../
COMPL_MODEL/
DATA_S02/
Files
MOCK7_sm_r.map
MOCK8_sm_r.map
MOCK9_sm_r.map
process.log
pyp_5dk_sm6.hkl
ref1.hkl
ref2.hkl
reference.hkl
svd4tx.inp
Selection: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02
svd4tx.inp
OK
Cancel
SVD4TX
File Map SVD
by
Yi Zhao and Marius Schmidt
2005-2008
Shell

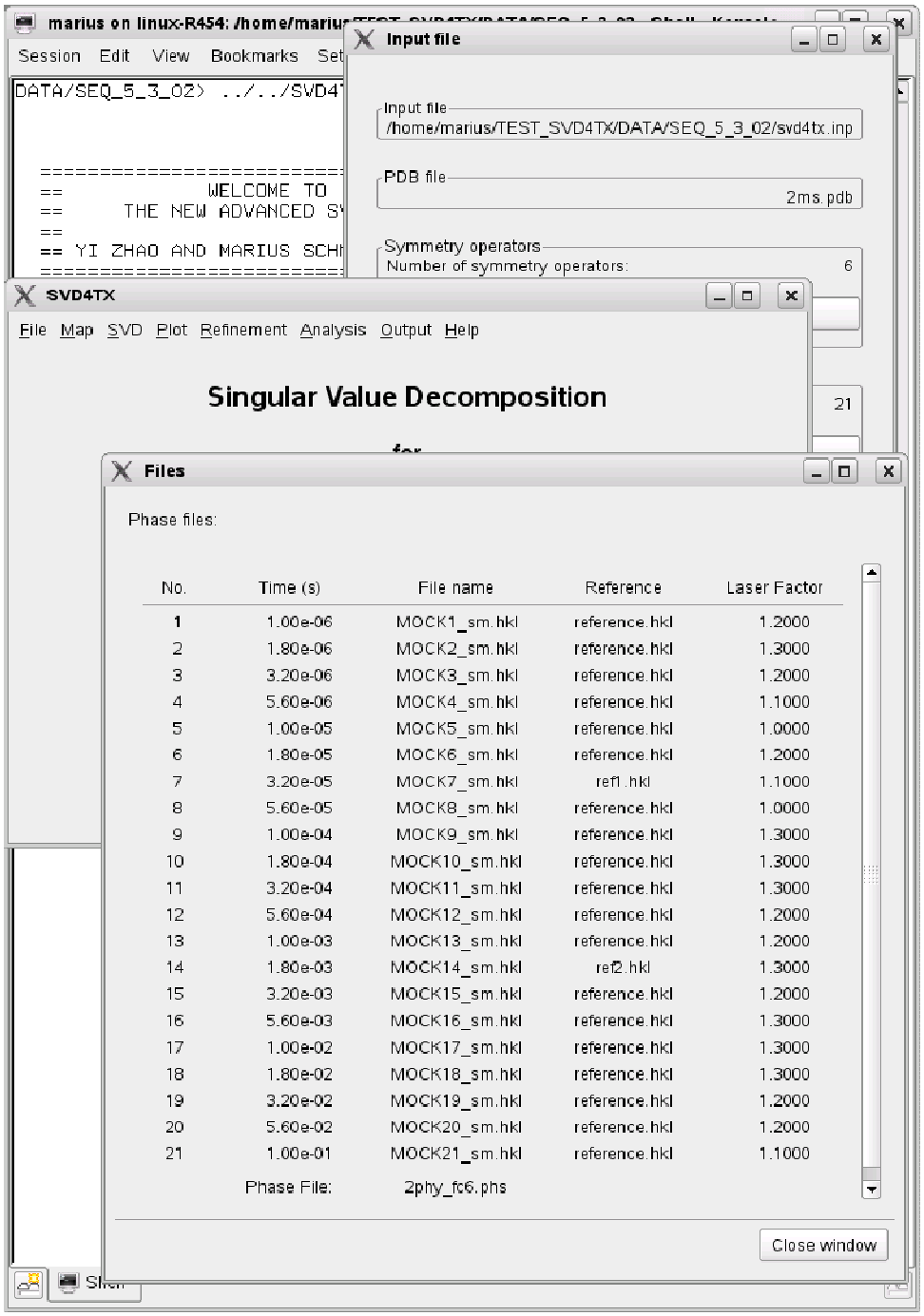

Time-Dependent Structure factors
FFT
Difference electron density (DED) maps
Data matrix
SVD-flattened DED maps
SVD-flattening
SVD
Significant singular vectors
Reconstruct DED maps
Fit of sum of exponentials
relaxation times
Select candidate kinetic mechanism
Time-independent DED maps
fit mechanism

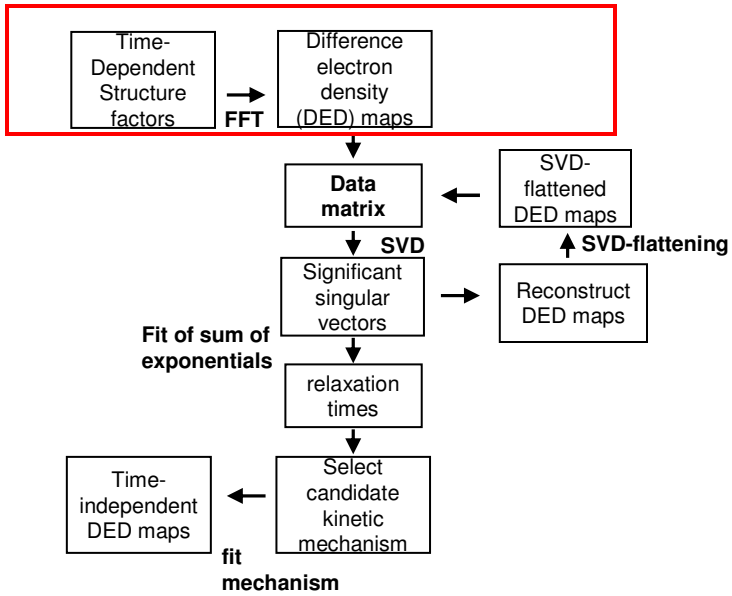
marius on linux-R454: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02 - Shell - Konsole

Session Edt View Bookmarks Settings Help

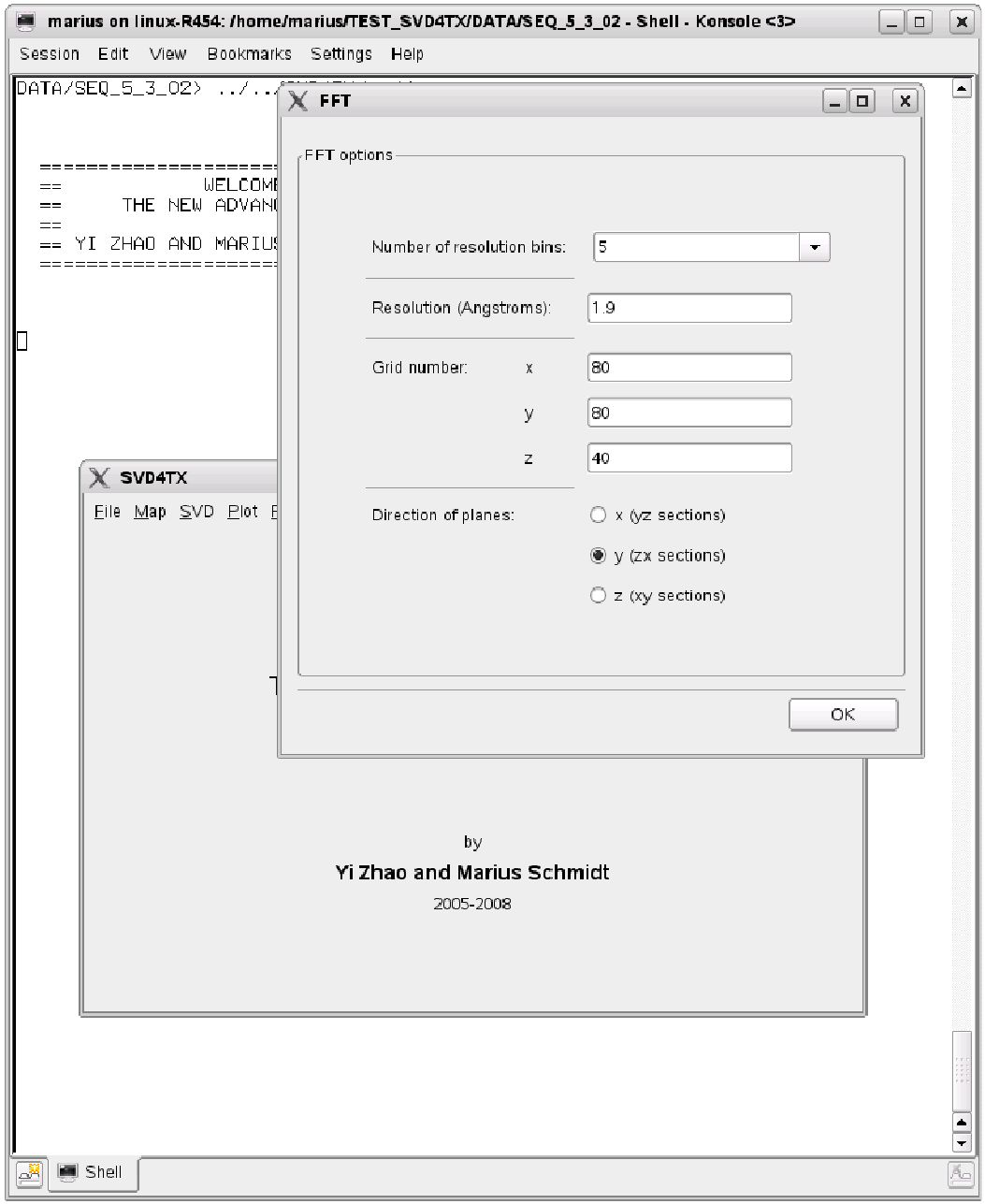
```
PDBFILE  2ms.pdb
SYMMETRY OPERATORS 6
X,Y,Z
-Y,X-Y,Z
Y-X,-X,Z
-X,-Y,1/2+Z
Y,Y-X,1/2+Z
X-Y,X,1/2+Z
PHASE FILES FSFOUR 21
1.0E-6    DATA_SO2/MOCK1_sm.hkl reference.hkl   1.2
1.8E-6    DATA_SO2/MOCK2_sm.hkl reference.hkl   1.3
3.2E-6    DATA_SO2/MOCK3_sm.hkl reference.hkl   1.2
5.6E-6    DATA_SO2/MOCK4_sm.hkl reference.hkl   1.1
10.0E-6   DATA_SO2/MOCK5_sm.hkl reference.hkl   1.0
18.0E-6   DATA_SO2/MOCK6_sm.hkl reference.hkl   1.2
32.0E-6   DATA_SO2/MOCK7_sm.hkl ref1.hkl        1.1
56.0E-6   DATA_SO2/MOCK8_sm.hkl reference.hkl   1.0
100.0E-6  DATA_SO2/MOCK9_sm.hkl reference.hkl   1.3
180.0E-6  DATA_SO2/MOCK10_sm.hkl reference.hkl  1.3
320.0E-6  DATA_SO2/MOCK11_sm.hkl reference.hkl  1.3
560.0E-6  DATA_SO2/MOCK12_sm.hkl reference.hkl  1.2
1.0E 3    DATA_SO2/MOCK13_sm.hkl reference.hkl  1.2
1.8E-3    DATA_SO2/MOCK14_sm.hkl ref2.hkl       1.3
3.2E-3    DATA_SO2/MOCK15_sm.hkl reference.hkl  1.2
5.6E-3    DATA_SO2/MOCK16_sm.hkl reference.hkl  1.3
10.0E-3   DATA_SO2/MOCK17_sm.hkl reference.hkl  1.3
18.0E-3   DATA_SO2/MOCK18_sm.hkl reference.hkl  1.3
32.0E-3   DATA_SO2/MOCK19_sm.hkl reference.hkl  1.2
56.0E-3   DATA_SO2/MOCK20_sm.hkl reference.hkl  1.2
100.0E-3  DATA_SO2/MOCK21_sm.hkl reference.hkl  1.1
DARK_CALC 2phy_fc6.phs
~
~
~
~
"svd4tx.inp" 31L, 1236C                          11,1          All
```

Shel





pairs of reference/time dependent Laue
-preferentially scaled to Fc
-All files 6 column: h k l Fobs sigma " 0 "
h k l " 0 " Fcalc ϕ


marius on linux-R454: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02 - Shell - Konsole <3>
Session Edit View Bookmarks Settings Help
FFT
FFT options
Number of resolution bins: 5
Resolution (Angstroms): 1.9
Grid number: x 80
y 80
z 40
Direction of planes:
x (yz sections)
y (zx sections)
z (xy sections)
OK
SVD4TX
File Map SVD Plot
by
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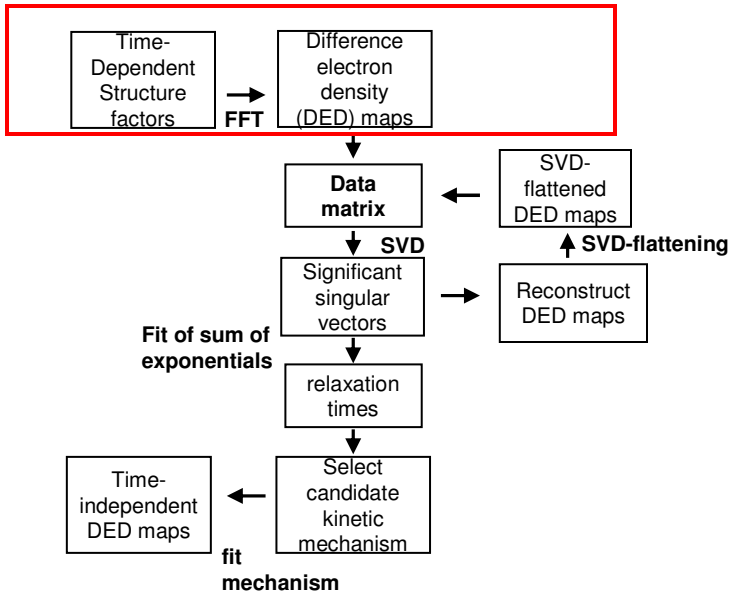
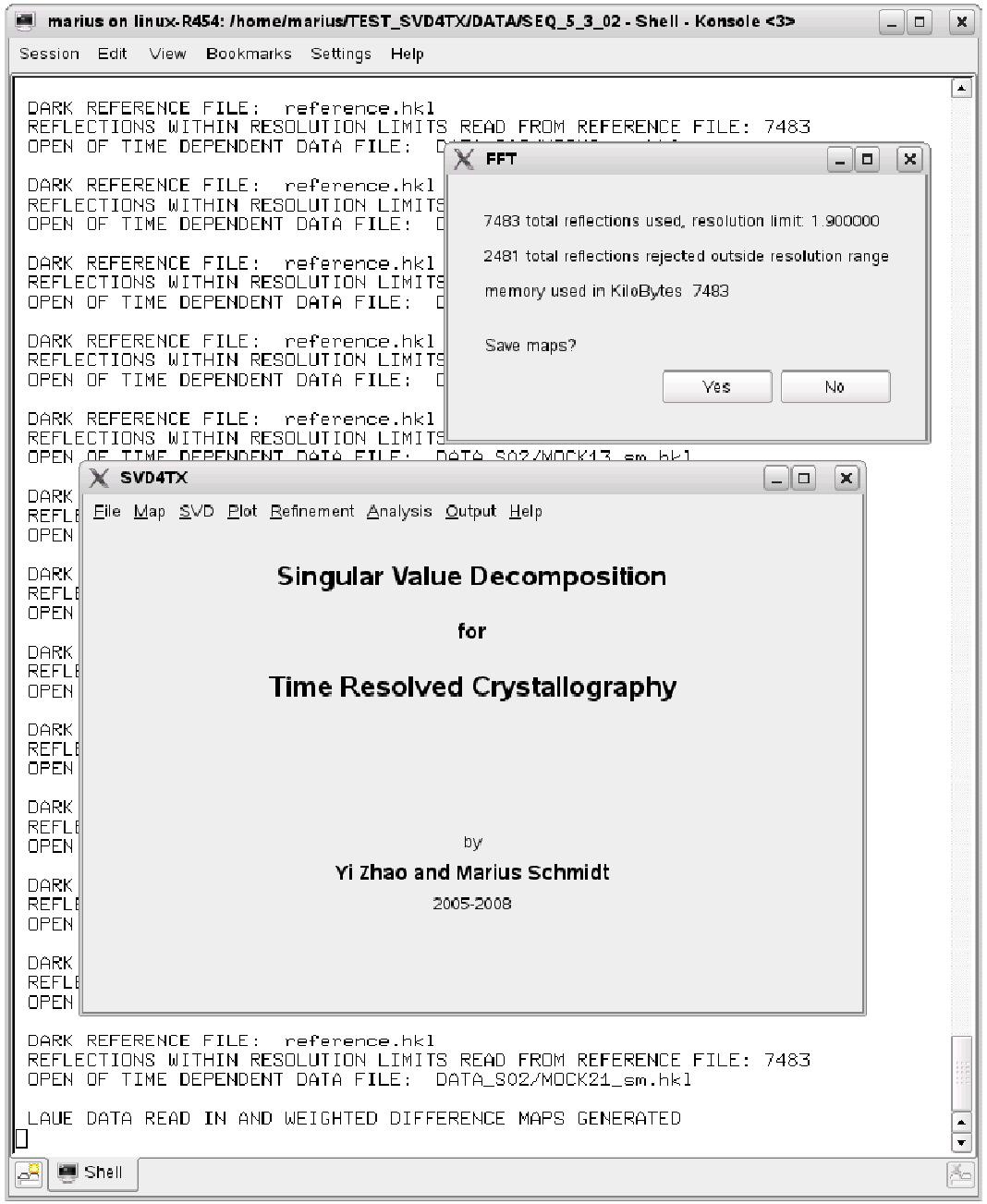
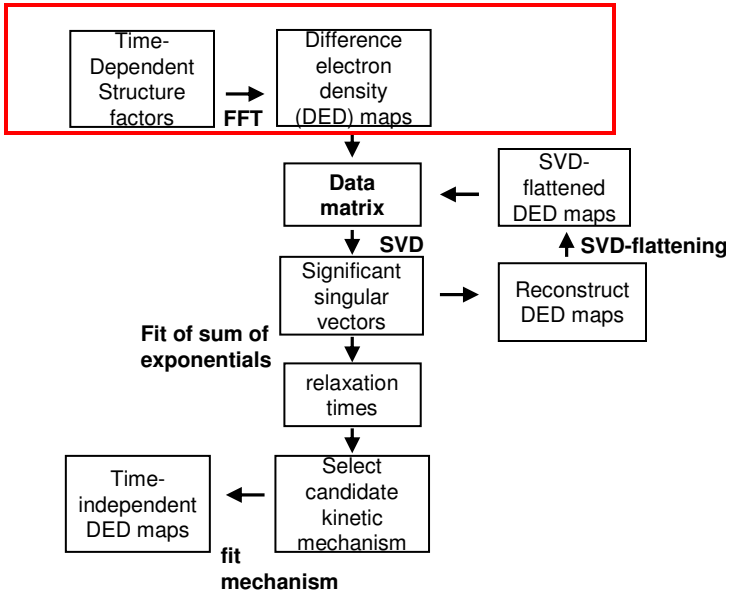
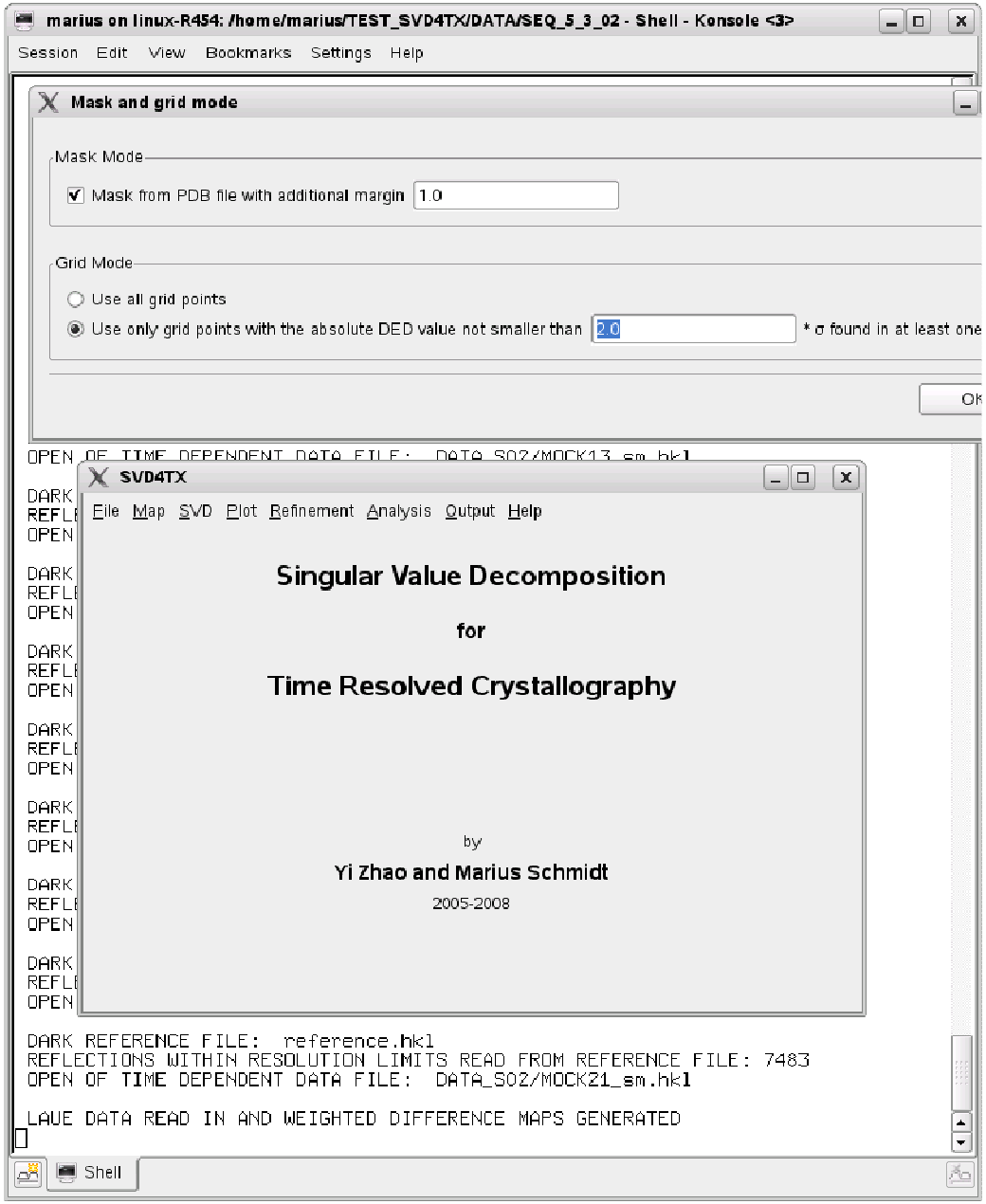
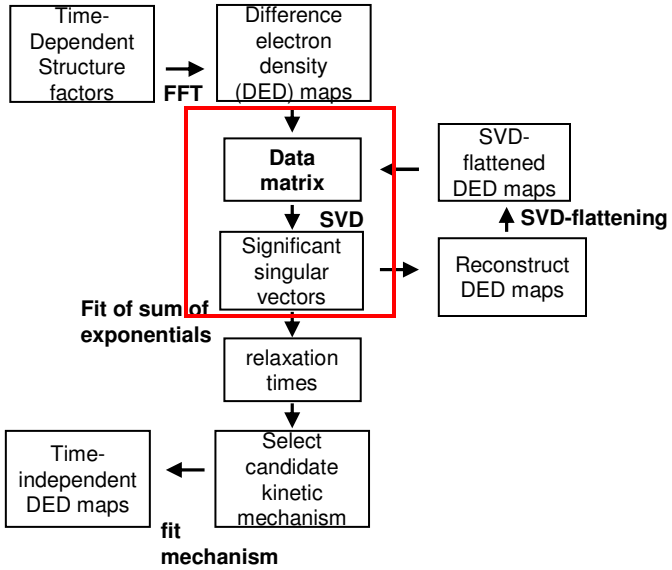

Time-Dependent Structure factors
FFT
Difference electron density (DED) maps
Data matrix
SVD-flattened DED maps
SVD-flattening
SVD
Significant singular vectors
Reconstruct DED maps
Fit of sum of exponentials
relaxation times
Select candidate kinetic mechanism
Time-independent DED maps
fit mechanism



Data imported into Program




marius on linux-R454: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02 - Shell - Konsole <3>
Session Edit View Bookmarks Settings Help
Mask and grid mode
Mask Mode
Mask from PDB file with additional margin 1.0
Grid Mode
Use all grid points
Use only grid points with the absolute DED value not smaller than 2.0 * σ found in at least one
OK
SVD4TX
File Map SVD Plot Refinement Analysis Output Help
Singular Value Decomposition
for
Time Resolved Crystallography
by
Yi Zhao and Marius Schmidt
2005-2008
DARK REFERENCE FILE: reference.hkl
REFLECTIONS WITHIN RESOLUTION LIMITS READ FROM REFERENCE FILE: 7483
OPEN OF TIME DEPENDENT DATA FILE: DATA_SOZ/MOCK21_sm.hkl
LAUE DATA READ IN AND WEIGHTED DIFFERENCE MAPS GENERATED
Shell


Time-Dependent Structure factors
FFT
Difference electron density (DED) maps
Data matrix
SVD
Significant singular vectors
SVD-flattened DED maps
SVD-flattening
Reconstruct DED maps
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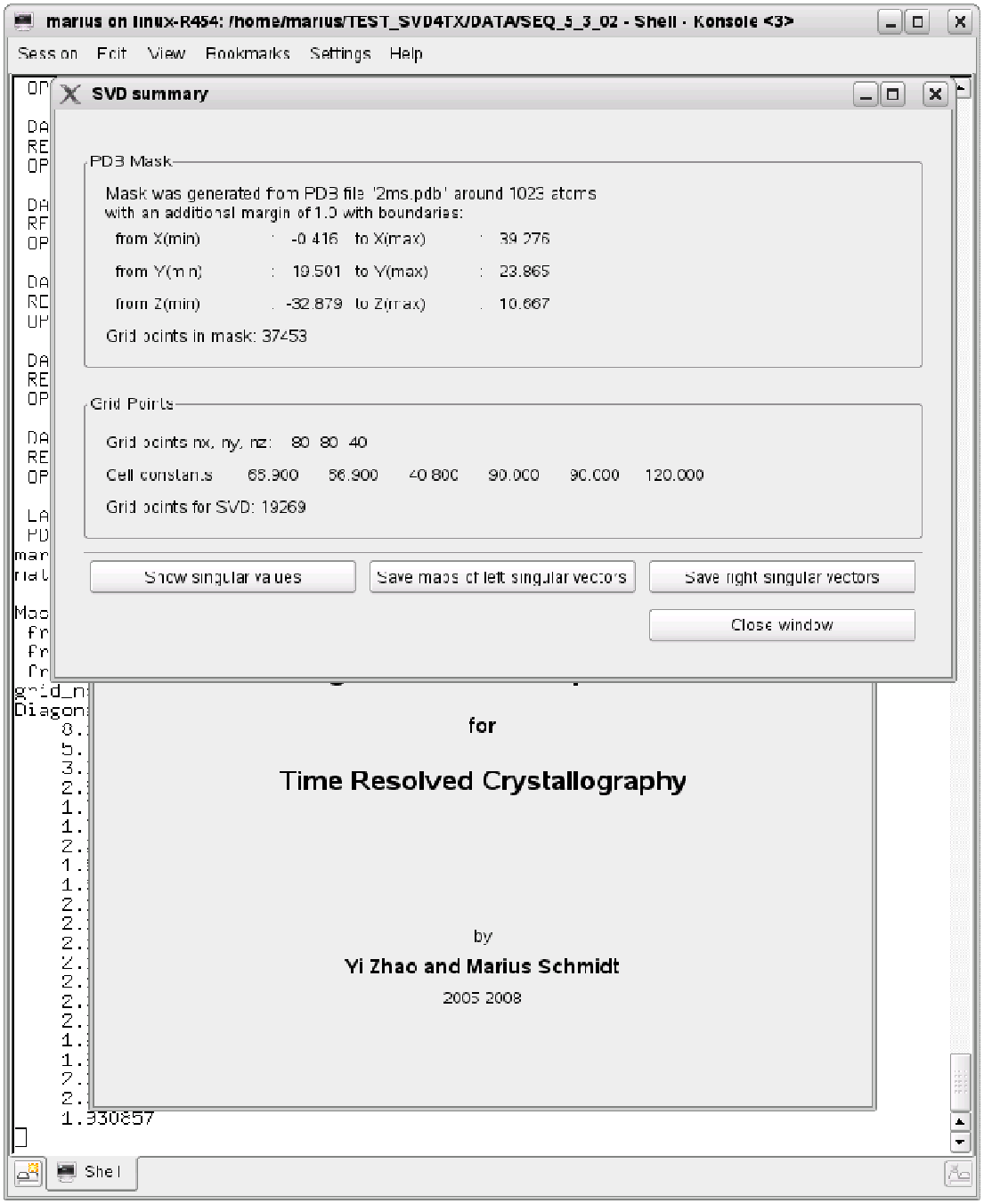
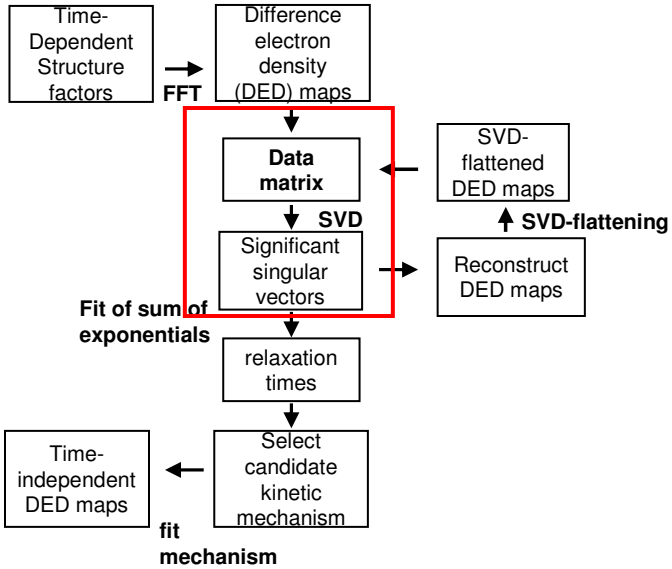
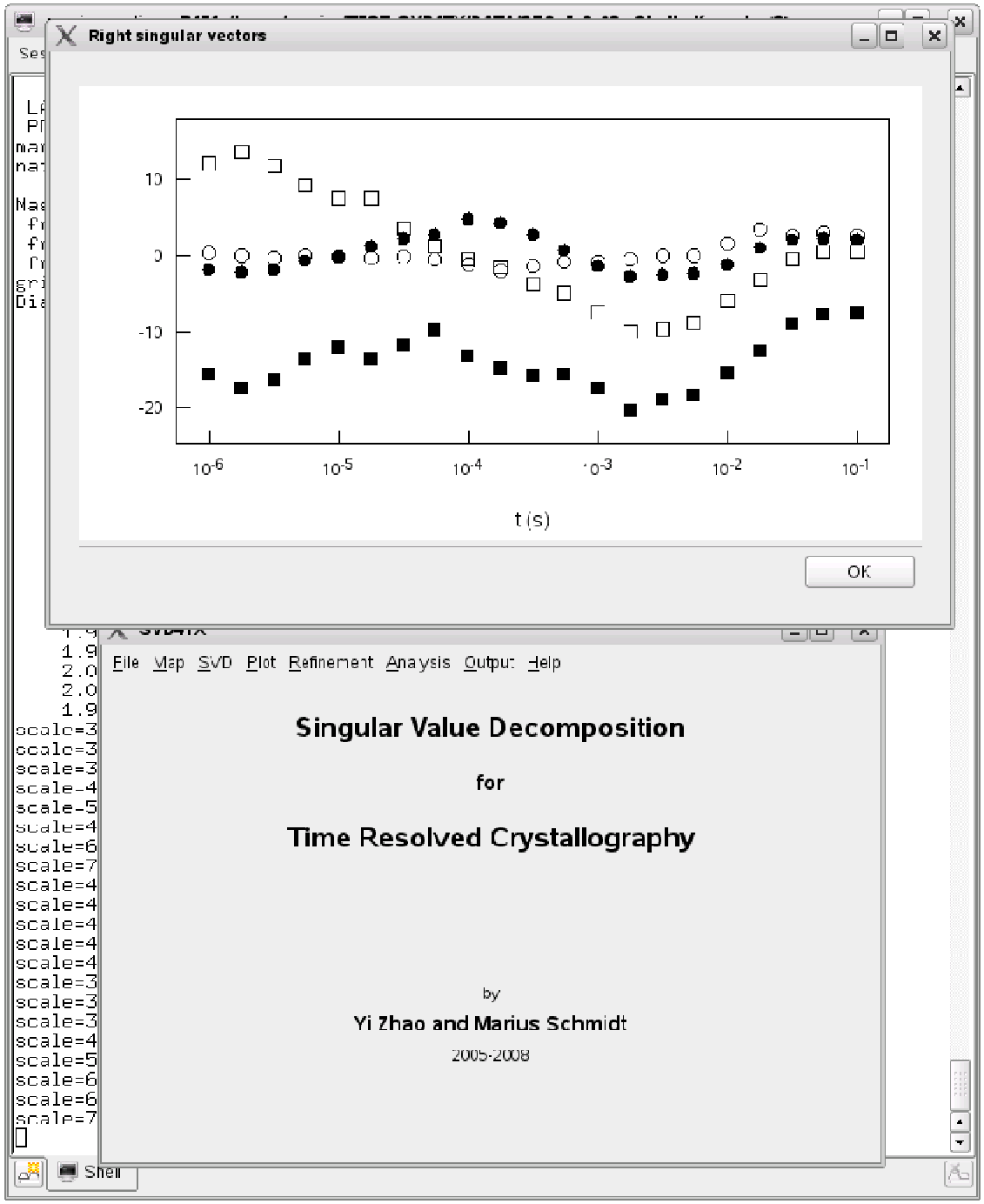
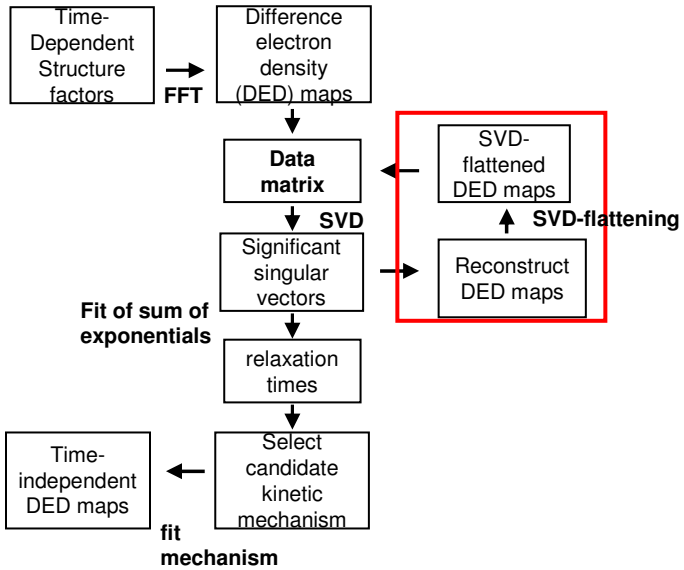
relaxation times
Select candidate kinetic mechanism
Time-independent DED maps
fit mechanism





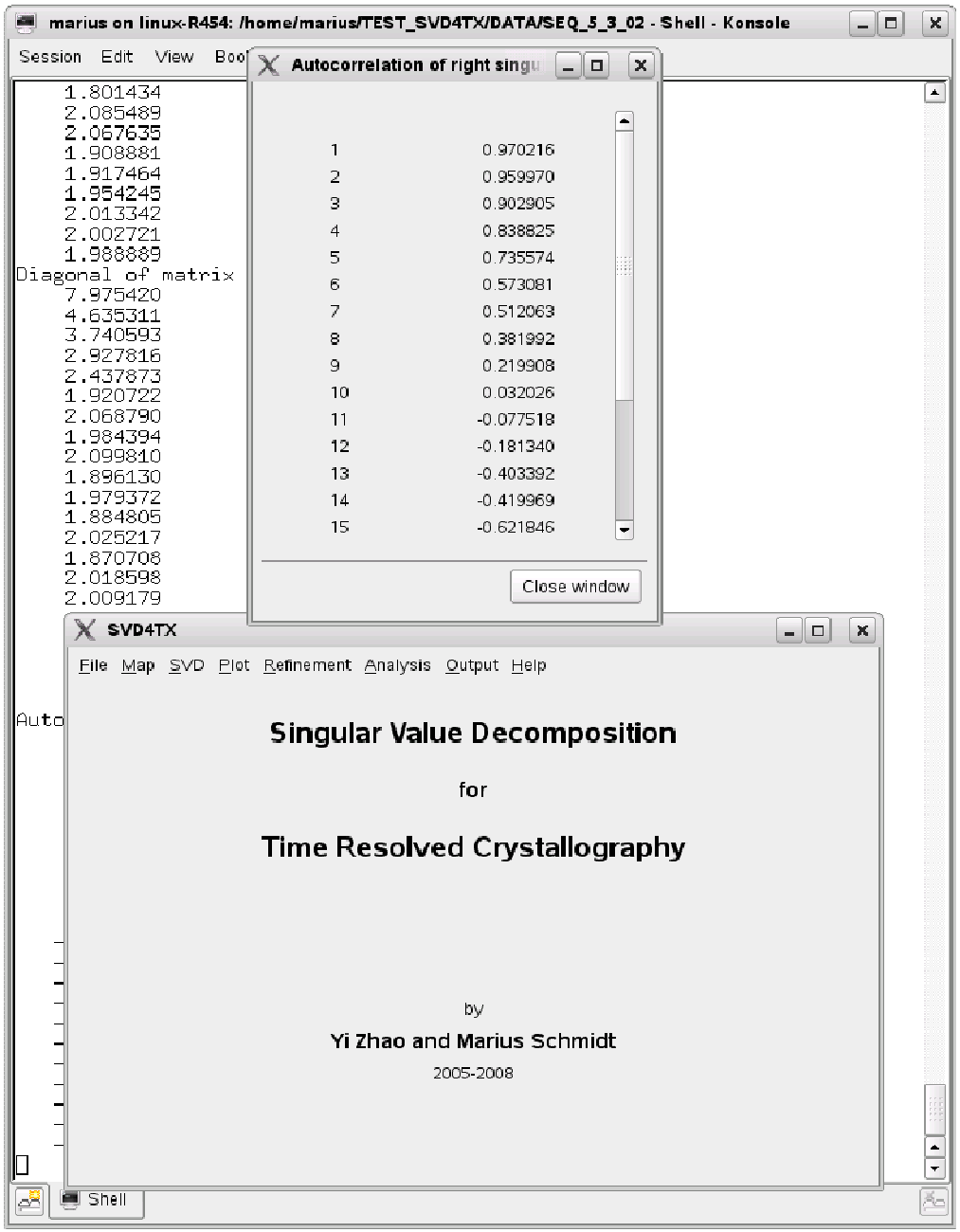
-Prepare Mask
-Select significant voxels
-Perform SVD





Select significant singular vectors
-Singular values
-Autocorrelation of right singular vectors
-Automatic Quality Factors

Rajagopal et al., 2004


marius on linux-R454: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02 - Shell - Konsole
Session Edit View Boo
1.801434
2.085489
2.067635
1.908881
1.917464
1.954245
2.013342
2.002721
1.988889
Diagonal of matrix
7.975420
4.635311
3.740593
2.927816
2.437873
1.920722
2.068790
1.984394
2.099810
1.896130
1.979372
1.884805
2.025217
1.870708
2.018598
2.009179
Auto
Autocorrelation of right singu
1 0.970216
2 0.959970
3 0.902905
4 0.838825
5 0.735574
6 0.573081
7 0.512063
8 0.381992
9 0.219908
10 0.032026
11 -0.077518
12 -0.181340
13 -0.403392
14 -0.419969
15 -0.621846
Close window
SVD4TX
File Map SVD Plot Refinement Analysis Output Help
Singular Value Decomposition
for
Time Resolved Crystallography
by
Yi Zhao and Marius Schmidt
2005-2008
Shell

marius on linux-R454: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02 - Shell - Konsole <2>

Session Edit View Bookmarks Settings Help

```
    3.360358
    3.19208
    3.52431
    3.19285
    2.93714
    3.25030
    3.45569
    3.30460
    3.37072
    3.12730
    3.36478
    3.29298
    3.24459
    3.17081
    3.19837
Autocorrela
    0.96979
    0.94762
    0.89613
    0.82839
    0.66201
    0.50334
    0.37258
    0.27999
    0.03435
   -0.05493
   -0.34281
   -0.45647
   -0.59313
   -0.647902
   -0.816063
   -0.9149
   -0.9529
   -0.0108
   -0.1769
   -0.3061
   -0.2209
i=1      2
i=2      2
i=3      1
i=4      1
i=5      1
i=6      0
i=7      0
i=8      1
i=9      1
i=10     1
i=11     0
i=12     1
i=13     1
i=14     0
i=15     0
i=16     1
i=17     0
i=18     0
i=19     1
i=20     0
i=21     0
```

Quality Factors

Quality factors:

1	2.4563 (1)	2.3080 (1)
2	2.1020 (2)	1.2749 (4)
3	1.7527 (3)	1.1618 (3)
4	1.6072 (5)	0.8805 (7)
5	1.3955 (4)	0.8743 (10)
6	1.3383 (16)	0.8676 (21)
7	1.2502 (9)	0.8559 (18)
8	1.2028 (12)	0.8406 (16)
9	1.1477 (19)	0.8329 (8)
10	1.1267 (10)	0.8168 (14)
11	1.1079 (13)	0.8059 (2)
12	1.0285 (8)	0.7929 (6)

Select significant singular vectors Close window

SVD4TX

File Map SVD Plot Refinement Analysis Output Help

Singular Value Decomposition

for

Time Resolved Crystallography

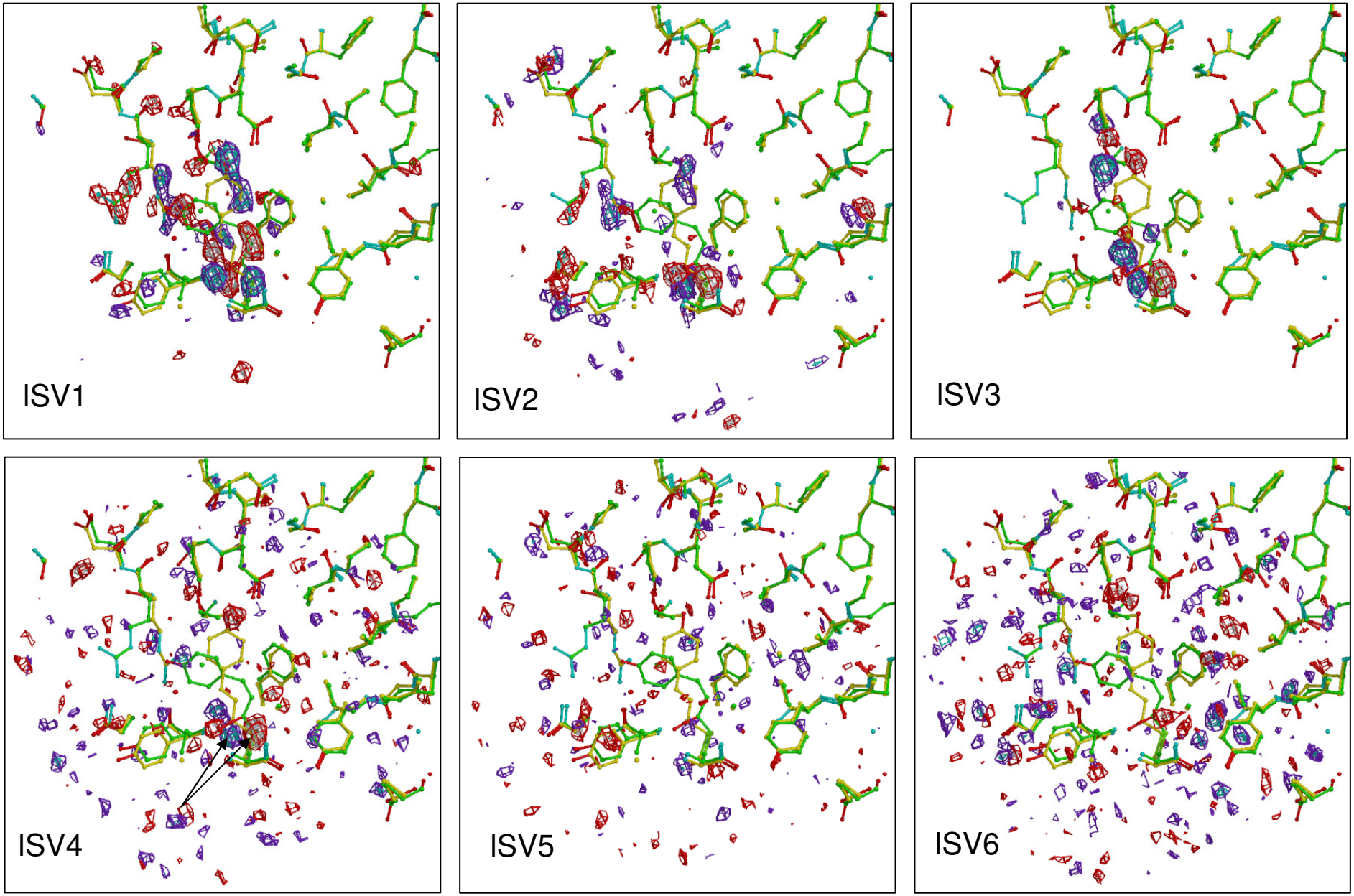
by

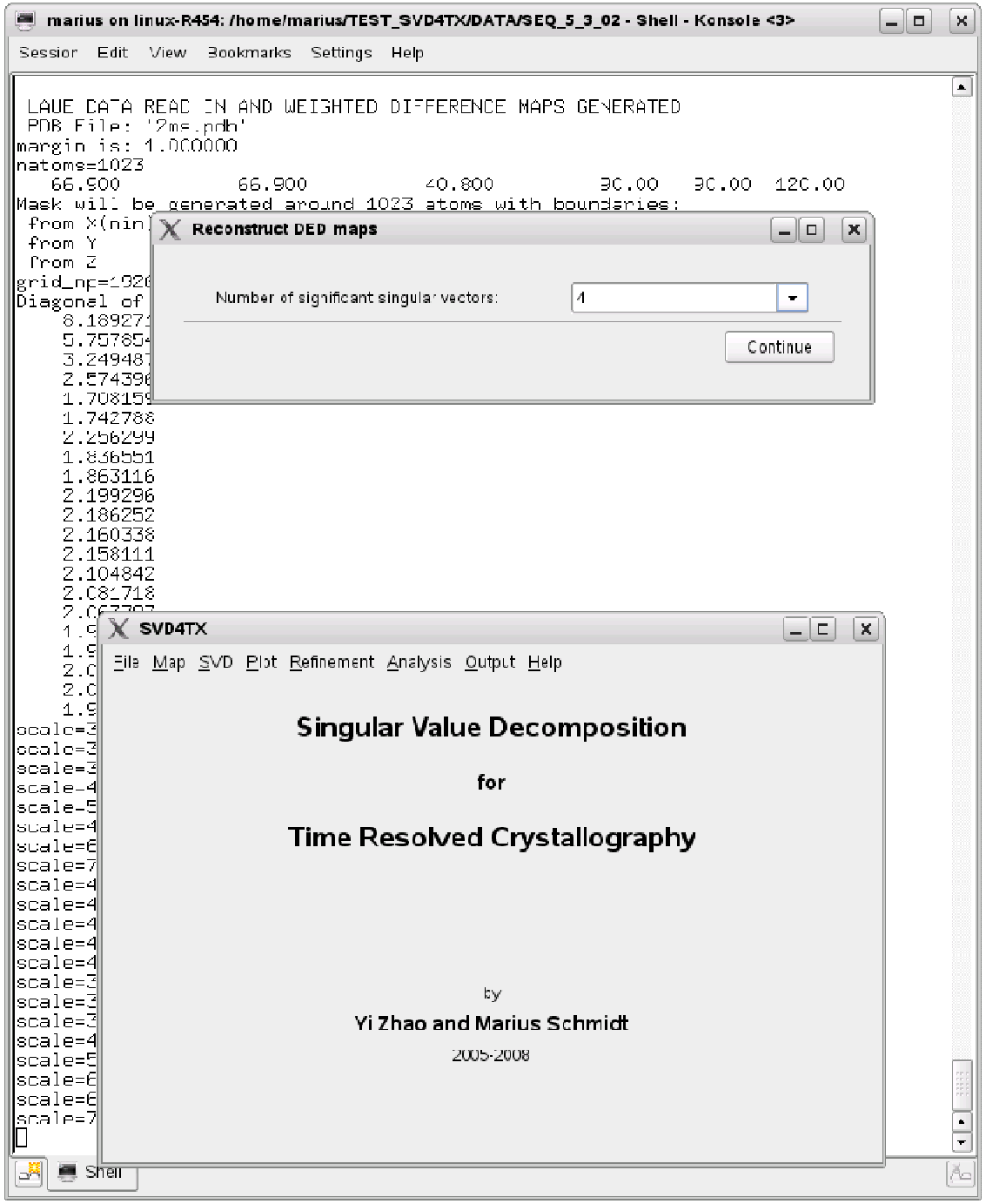
Yi Zhao and Marius Schmidt

2005-2008

Shell

The left singular vectors = difference maps

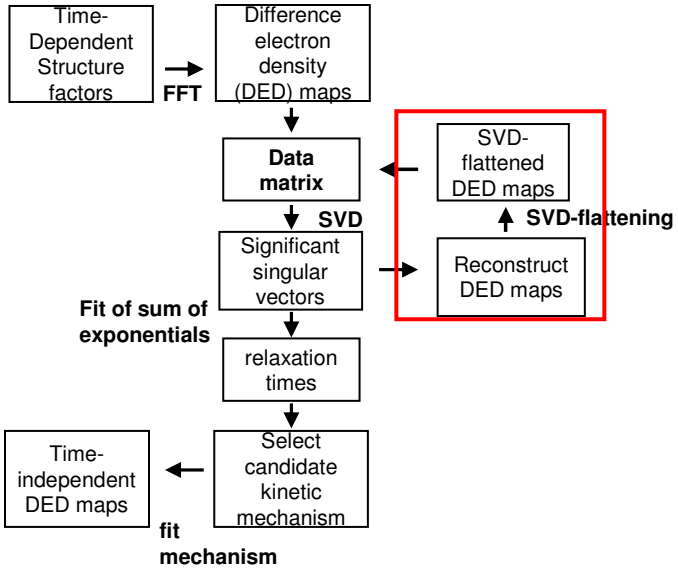


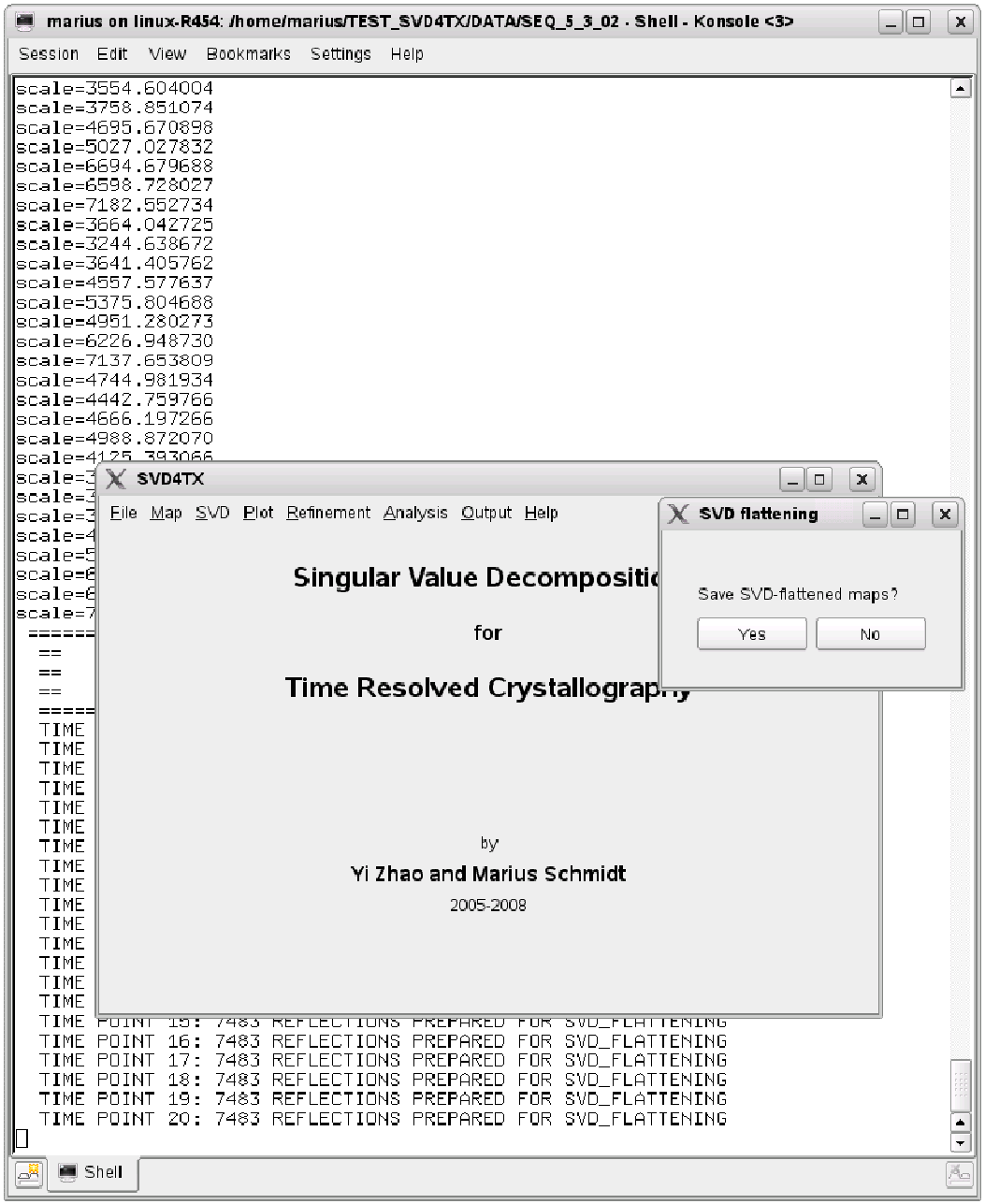


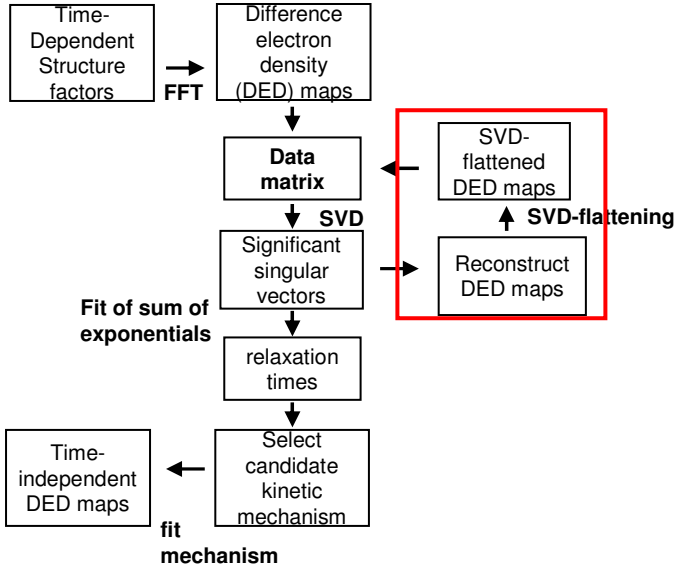
4 significant SV selected for reconstruction

$$U_s\, S_s\, V_S^T = A'$$

noise reduced




marius on linux-R454: /home/marius/TEST_SVD4TX/DATA/SEQ_5_3_02 - Shell - Konsole <3>
Session Edit View Bookmarks Settings Help
scale=3554.604004
scale=3758.851074
scale=4695.670898
scale=5027.027832
scale=6694.679688
scale=6598.728027
scale=7182.552734
scale=3664.042725
scale=3244.638672
scale=3641.405762
scale=4557.577637
scale=5375.804688
scale=4951.280273
scale=6226.948730
scale=7137.653809
scale=4744.981934
scale=4442.759766
scale=4666.197266
scale=4988.872070
SVD4TX
File Map SVD Plot Refinement Analysis Output Help
Singular Value Decomposition
for
Time Resolved Crystallography
by
Yi Zhao and Marius Schmidt
2005-2008
SVD flattening
Save SVD-flattened maps?
Yes
No
TIME POINT 16: 7483 REFLECTIONS PREPARED FOR SVD_FLATTENING
TIME POINT 17: 7483 REFLECTIONS PREPARED FOR SVD_FLATTENING
TIME POINT 18: 7483 REFLECTIONS PREPARED FOR SVD_FLATTENING
TIME POINT 19: 7483 REFLECTIONS PREPARED FOR SVD_FLATTENING
TIME POINT 20: 7483 REFLECTIONS PREPARED FOR SVD_FLATTENING
Shell


Time-Dependent Structure factors
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Difference electron density (DED) maps
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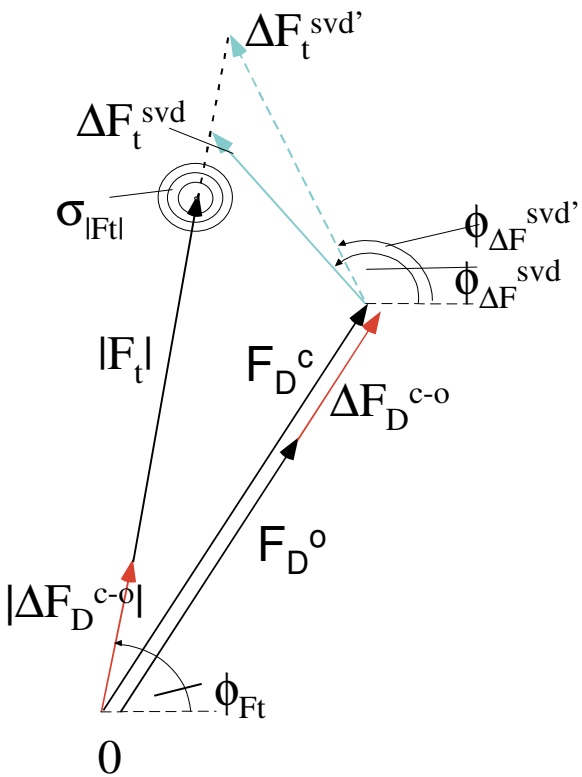
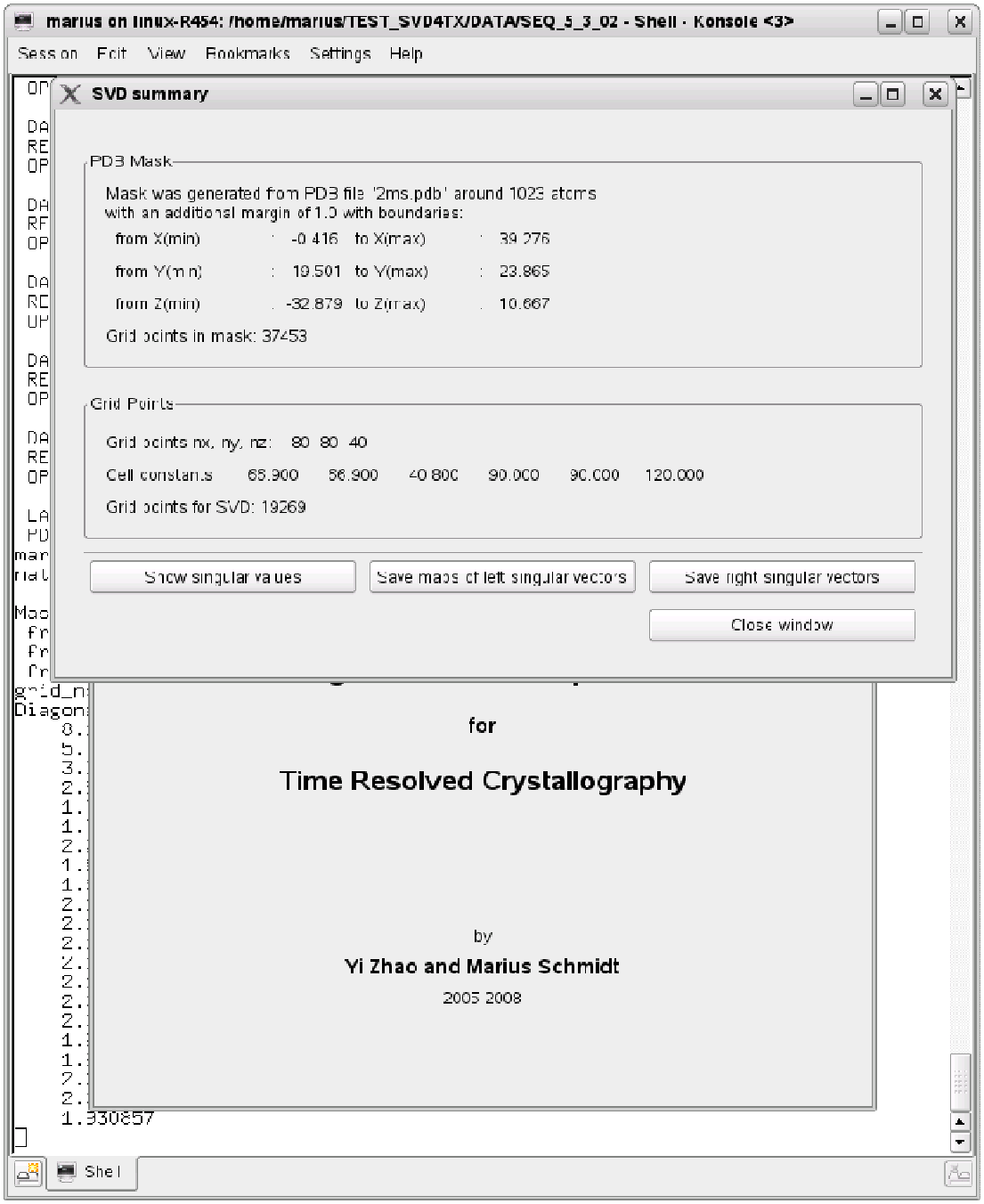
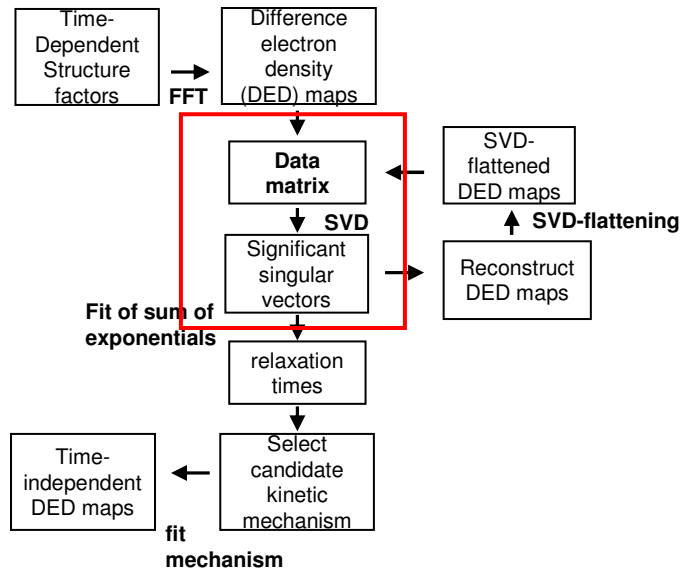
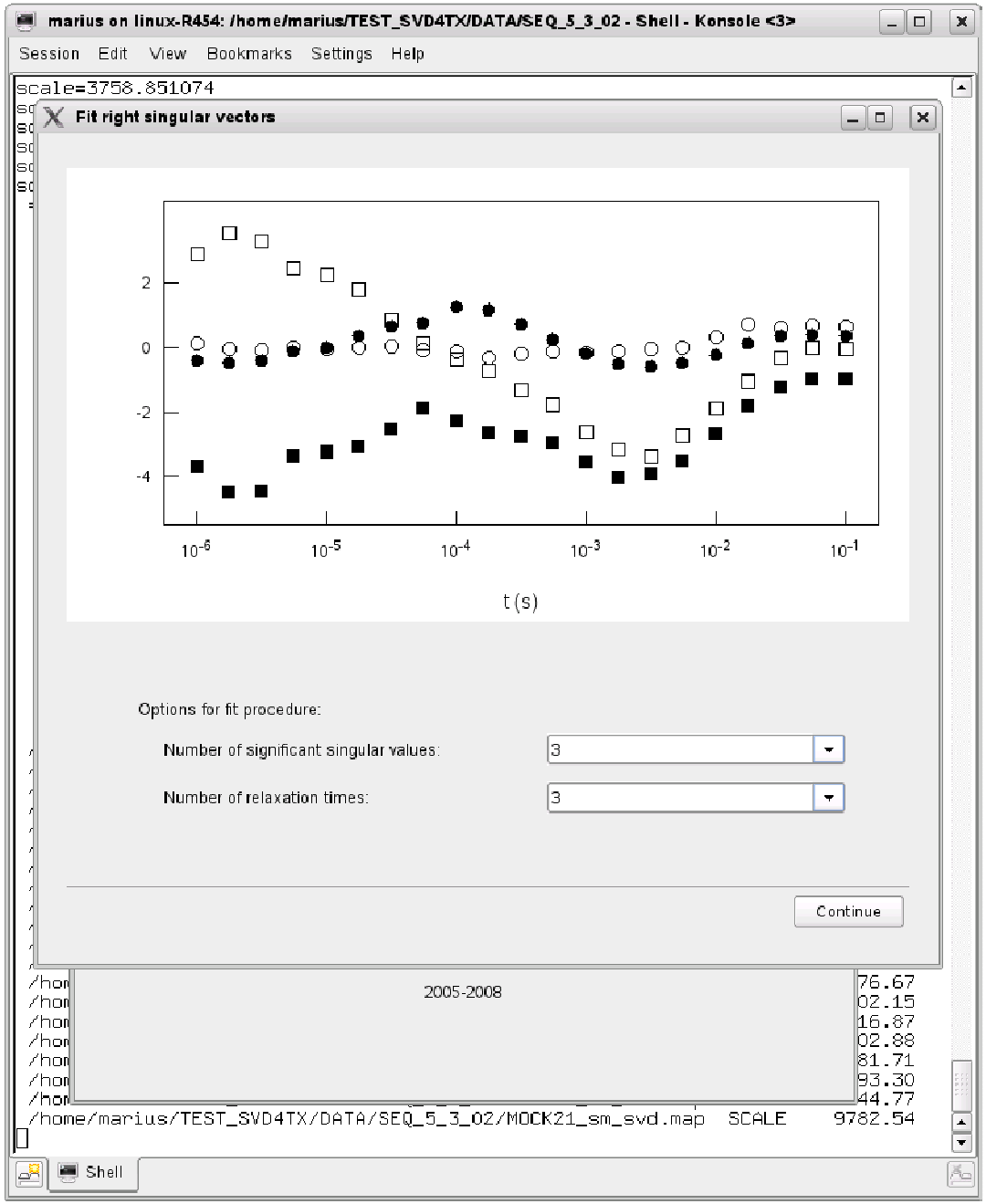
Reconstruct DED maps


$\Delta F_t^{svd'}$
ΔF_t^{svd}
$\sigma_{|Ft|}$
$\phi_{\Delta F}^{svd'}$
$\phi_{\Delta F}^{svd}$
$|F_t|$
F_D^c
ΔF_D^{c-o}
F_D^o
$|\Delta F_D^{c-o}|$
ϕ_{Ft}
0



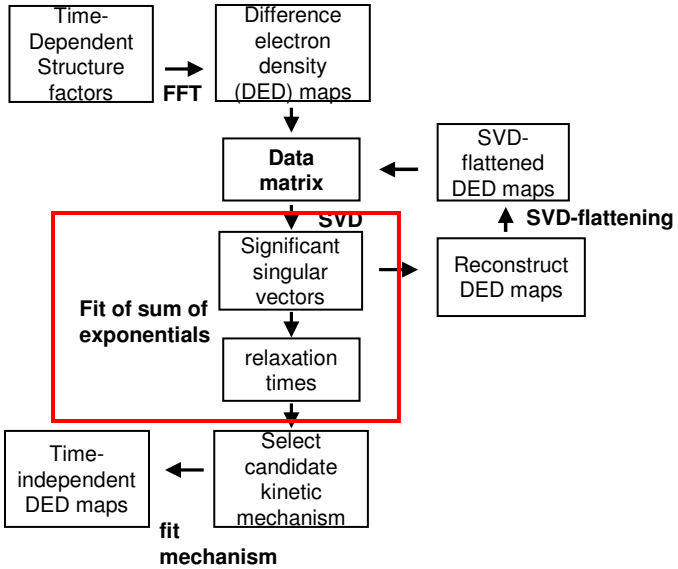
Re-SVD the SVD-flattened data

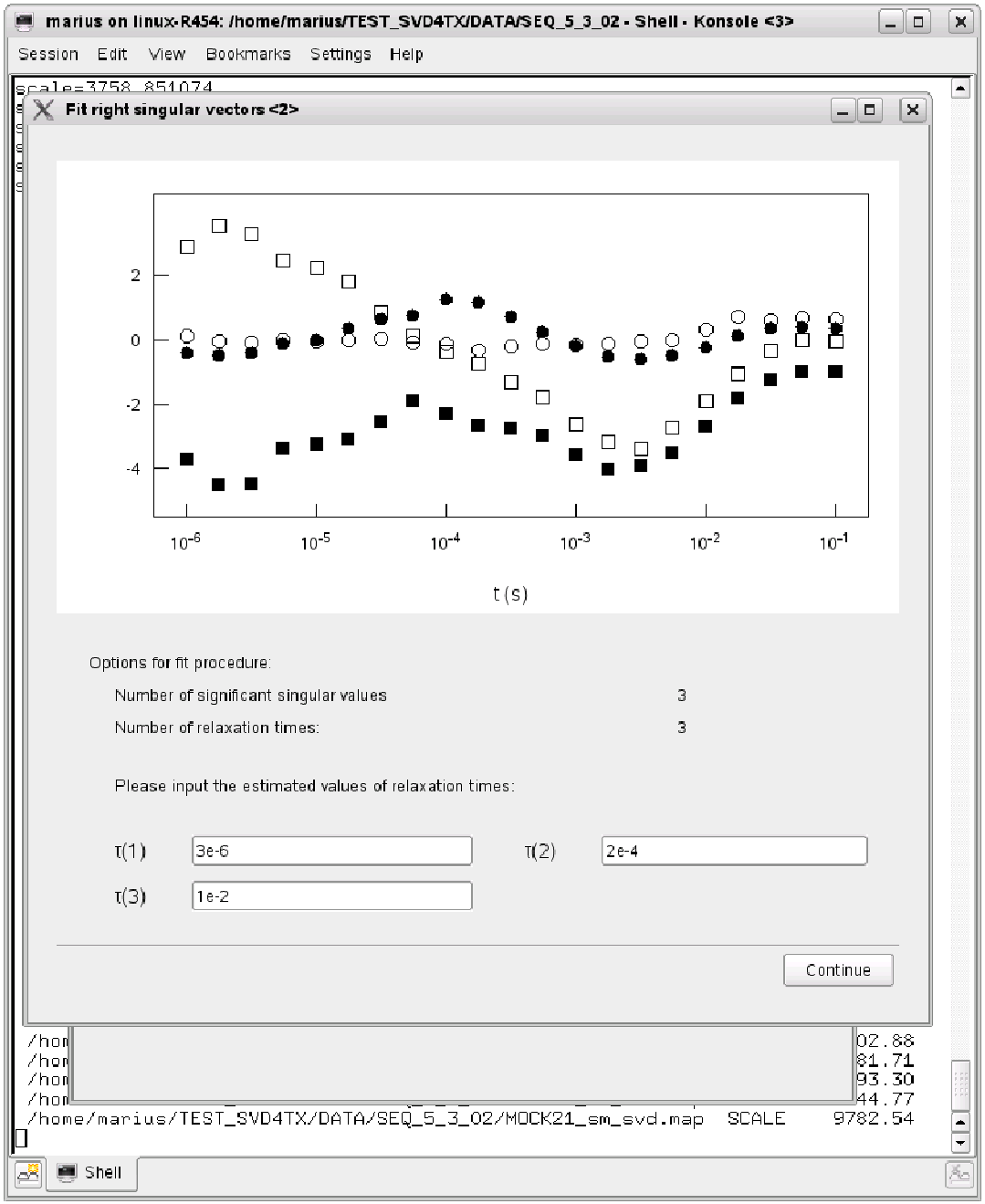




Determine relaxation times of the kinetics

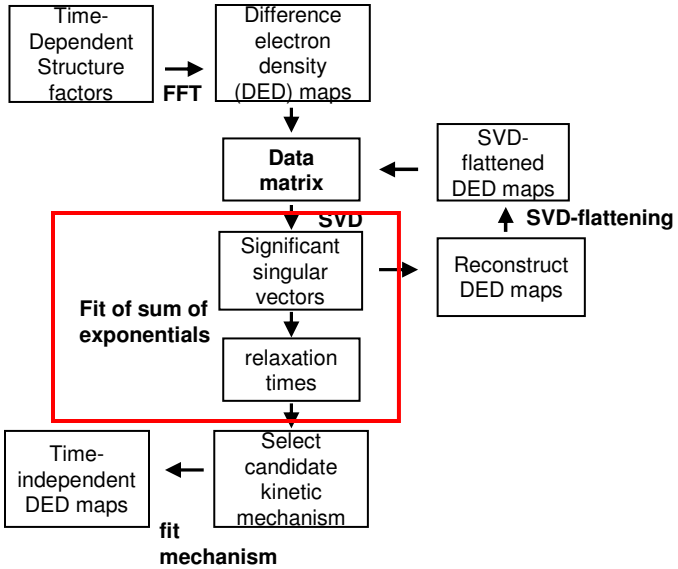
Step 1. Select significant rSV

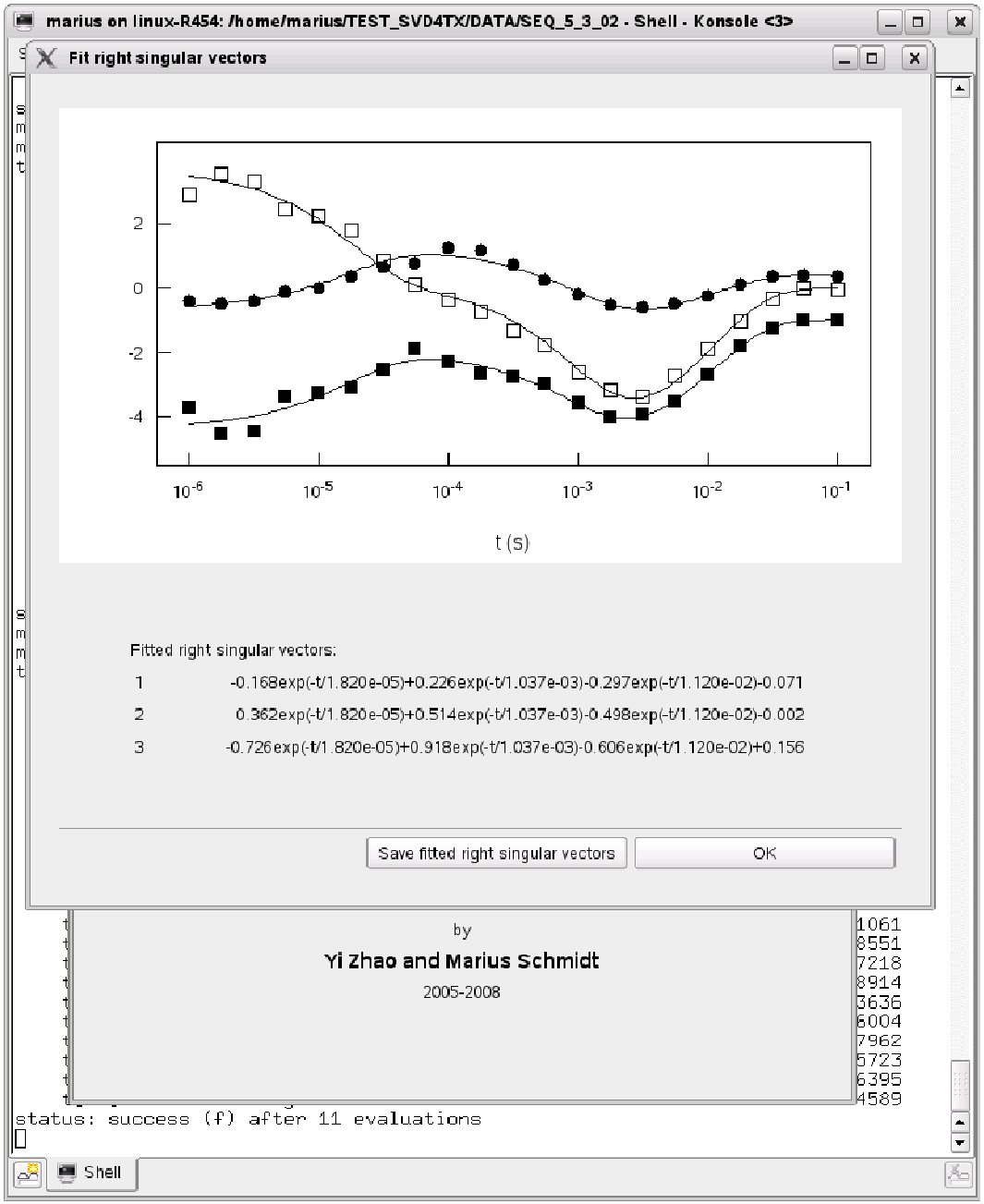




Determine relaxation times of the kinetics

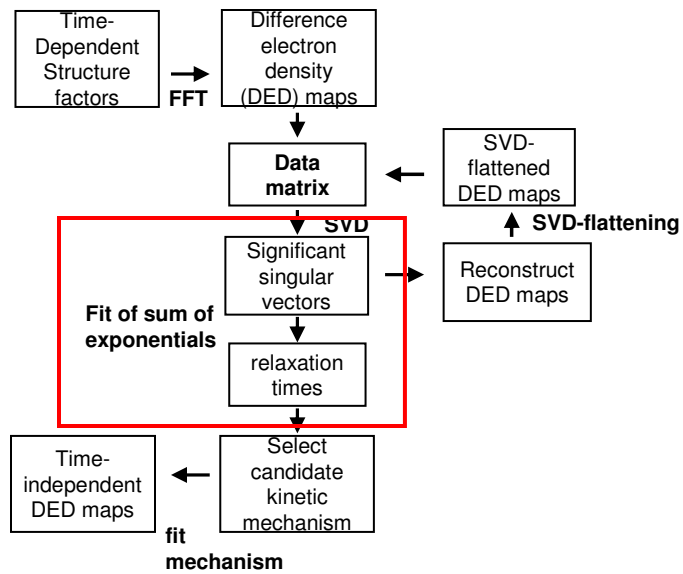
Step 2. initialize global fit





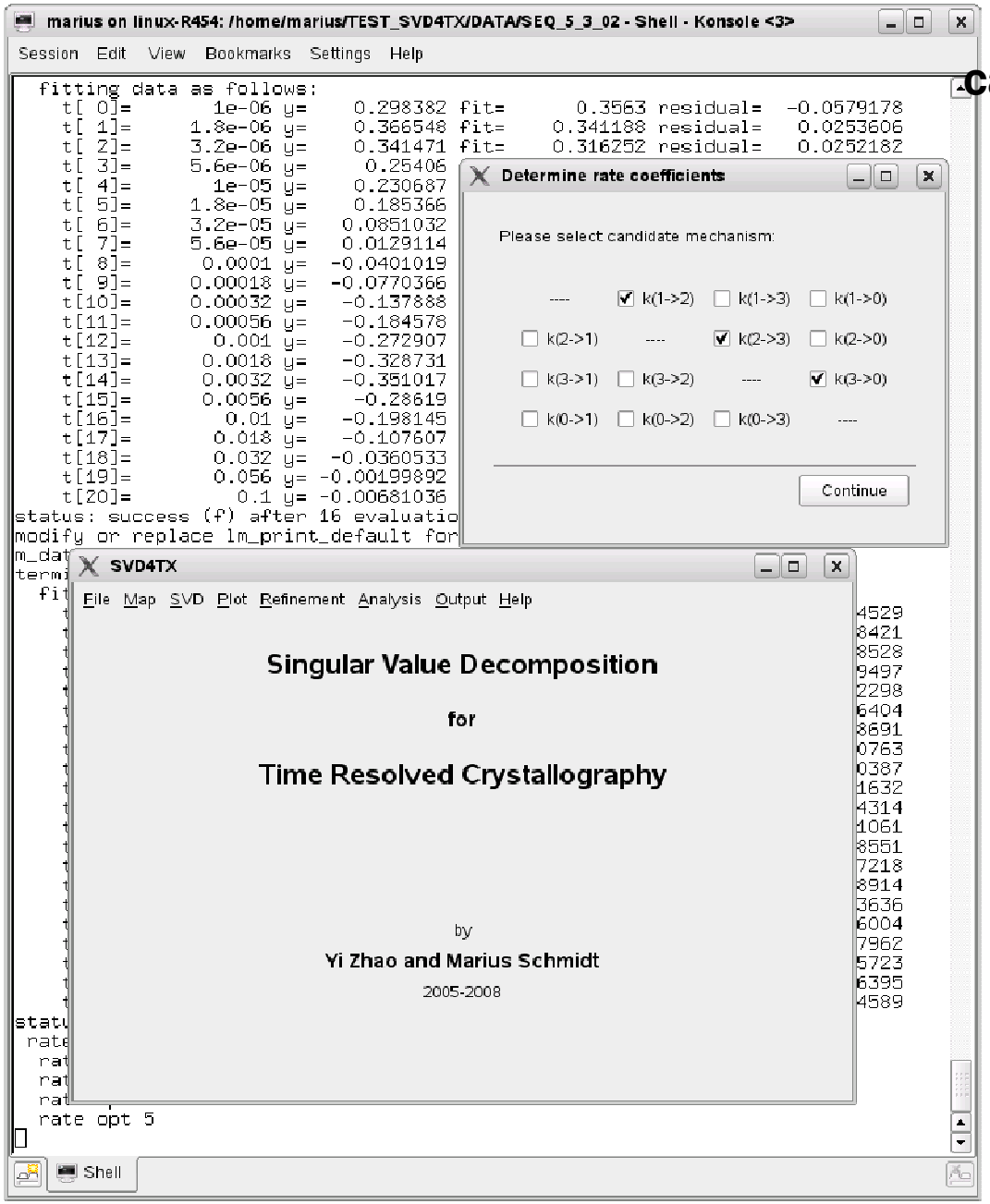
Determine relaxation times of the kinetics

Step 3. global fit

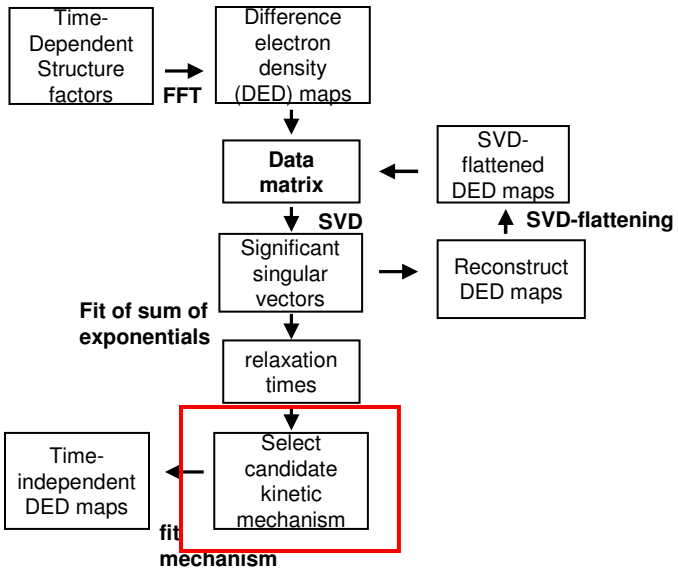


Fit and residuals are written out to standard output for easy cut and paste into favorite plot program (xmgrace recommended).

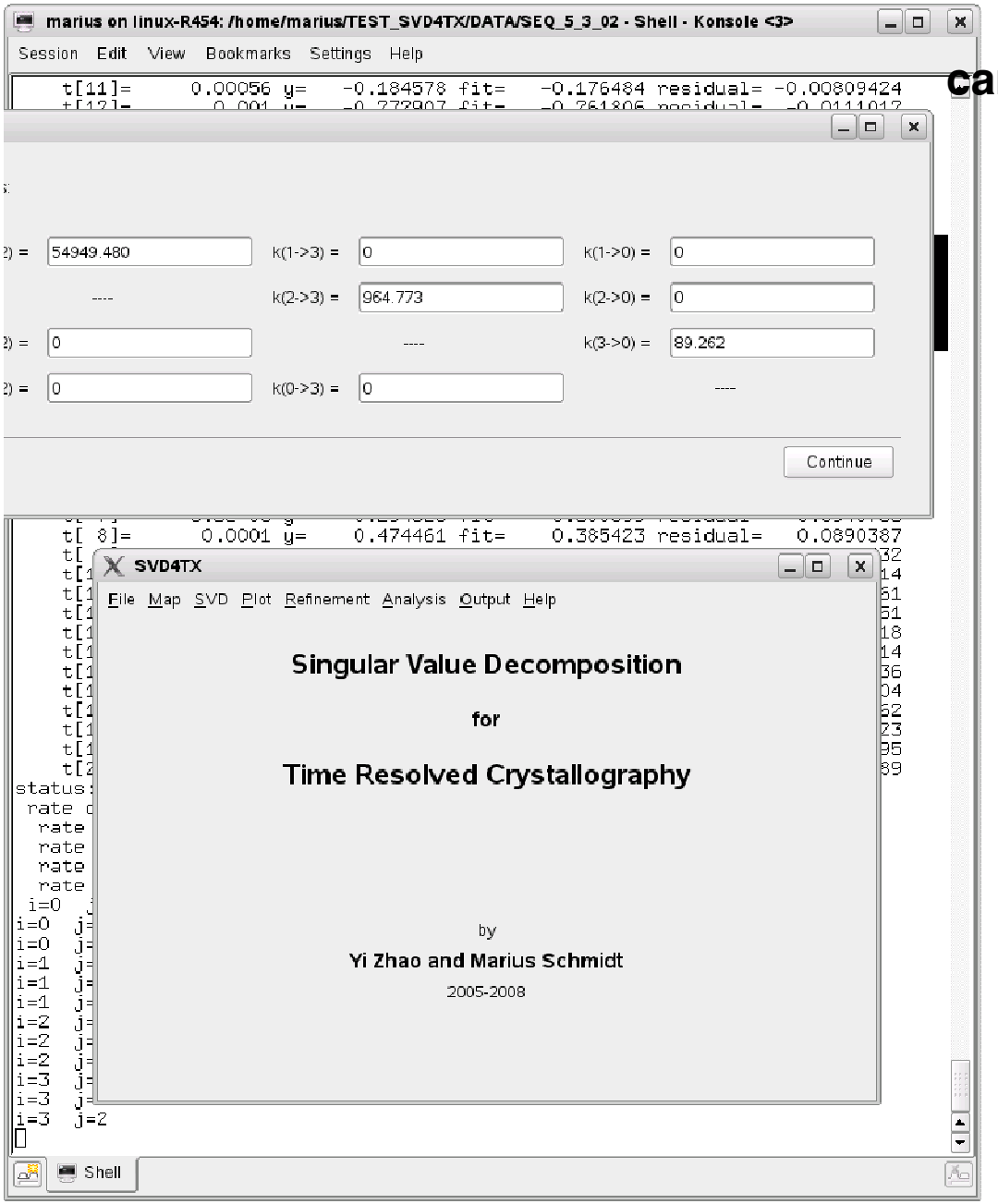
Determine rate constants for candidate chemical kinetic mechanism



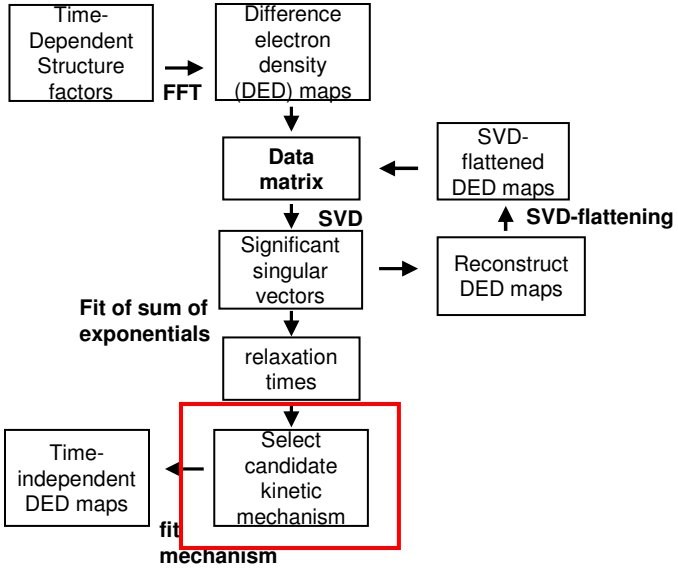
Step1. select candidate

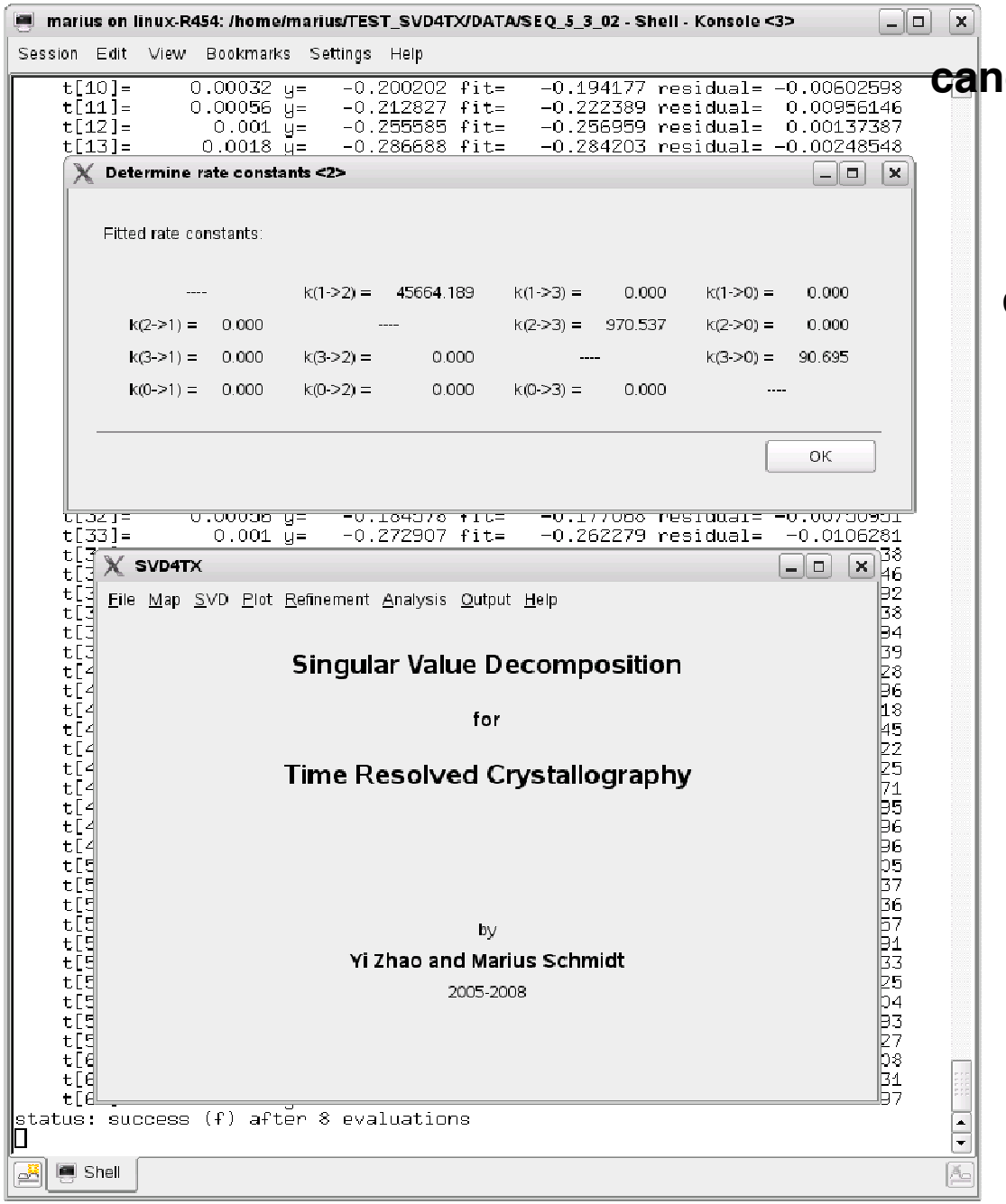


Determine rate constants for candidate chemical kinetic mechanism



Step2. initialize candidate
(automatic guess)





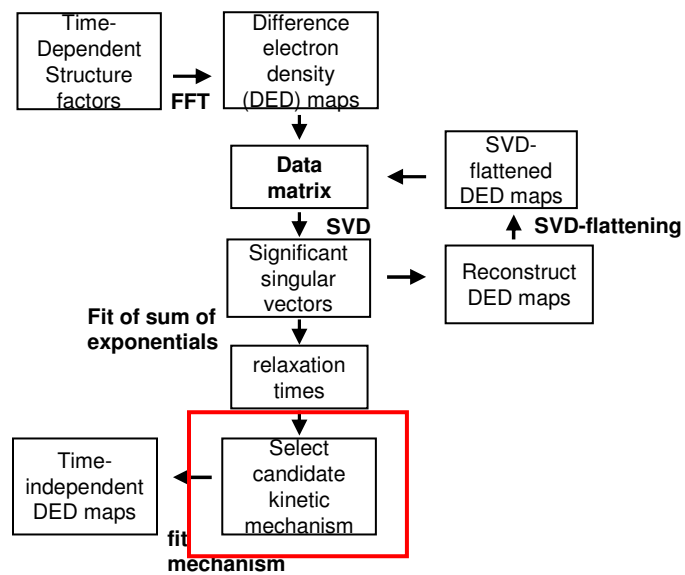
Determine rate constants for candidate chemical kinetic mechanism

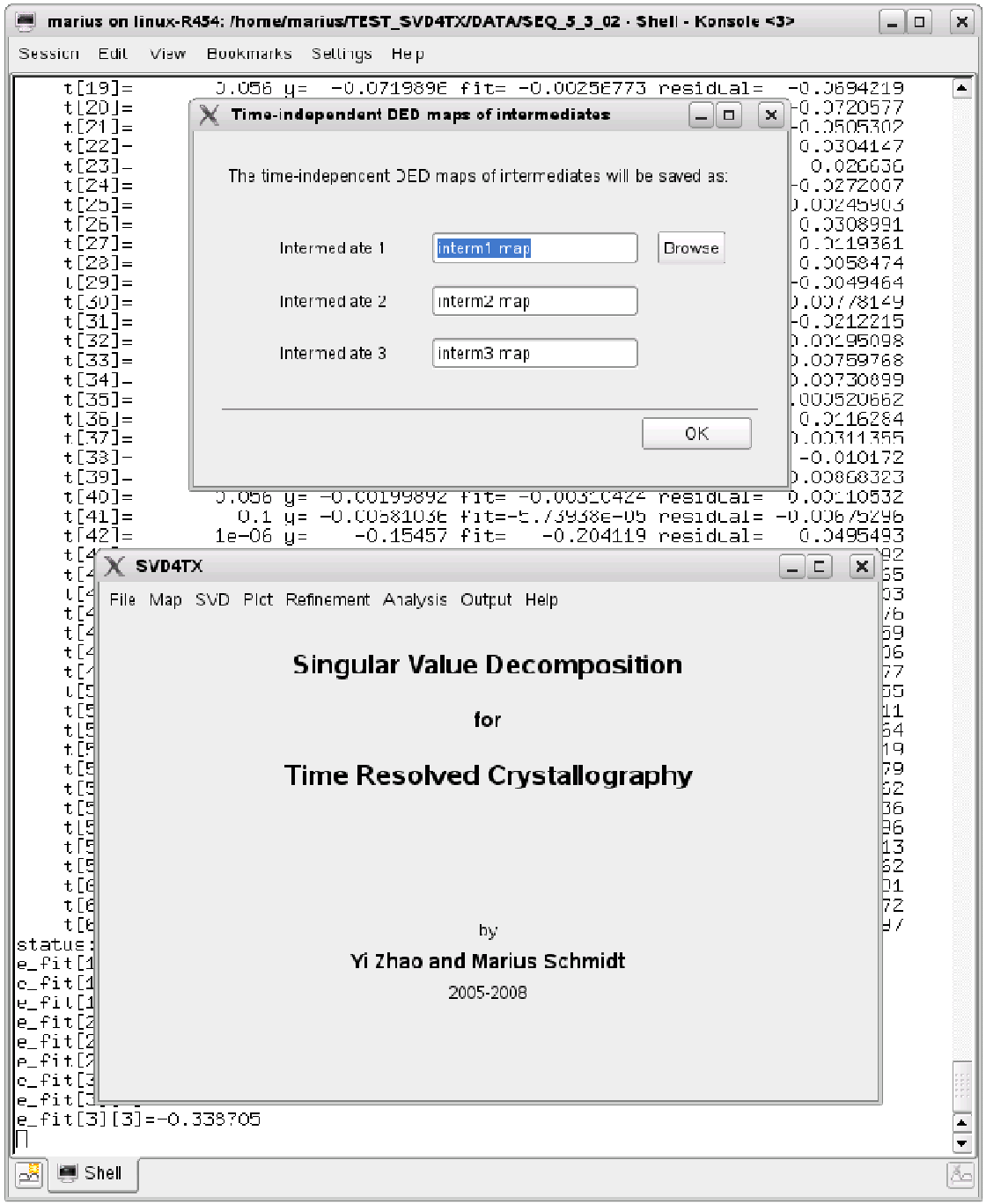
Step3. solve coupled differential eqn.
fit rate constants

diagonalize coefficient matrix

$$\begin{pmatrix} \frac{d[I_1]}{dt} \\ \frac{d[I_2]}{dt} \\ \frac{d[I_3]}{dt} \end{pmatrix} = \underbrace{\begin{pmatrix} -k_{+1} & \varepsilon & \varepsilon \\ \varepsilon & k_{+1}-k_{+2} & \varepsilon \\ \varepsilon & \varepsilon & k_{+2}-k_{+3} \end{pmatrix}}_{coefficient\ matrix\ K} \begin{pmatrix} [I_1] \\ [I_2] \\ [I_3] \end{pmatrix}$$

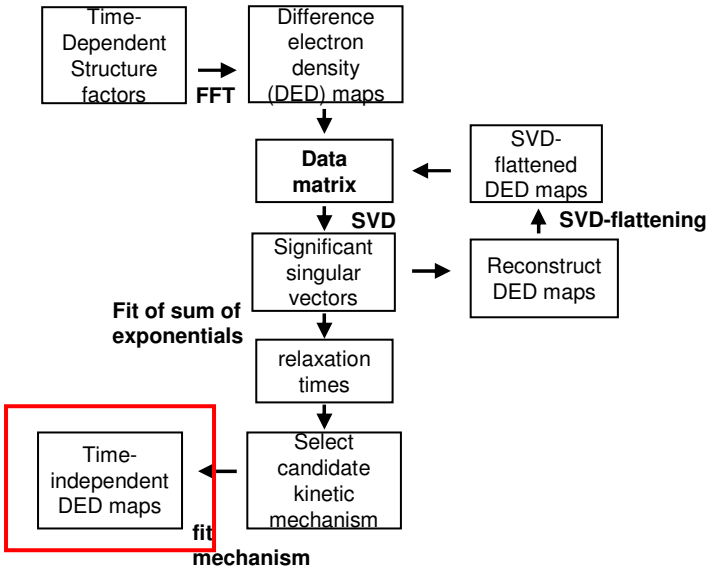
$$\varepsilon \sim 0$$

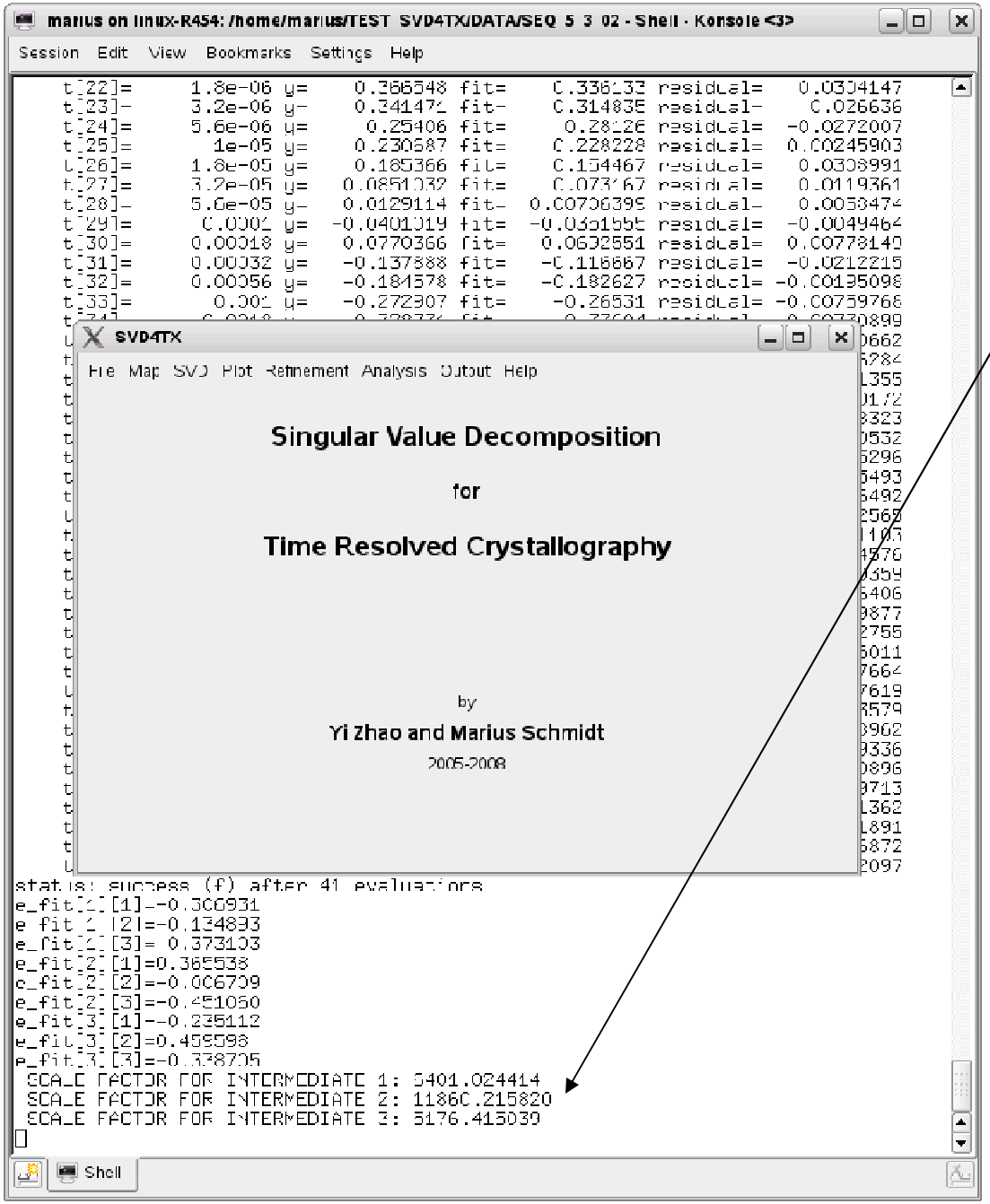




Determine time-independent DED of intermediates

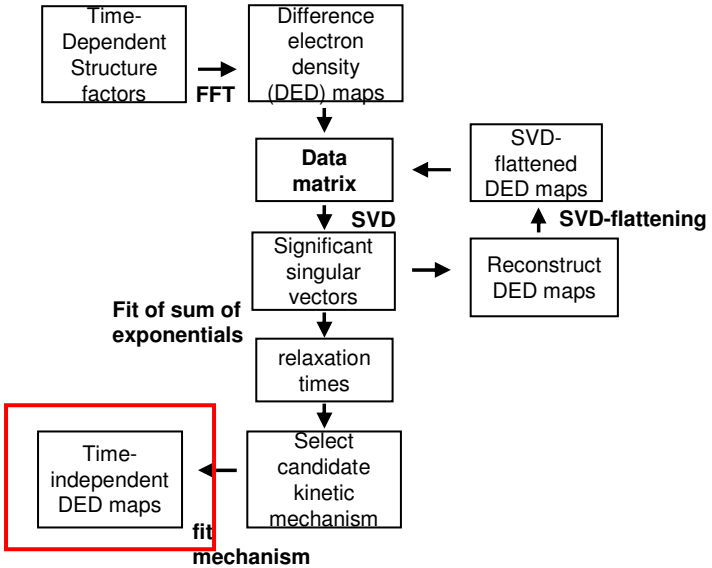
ask for filenames:





Write out maps

since maps are FSFOUR maps they must be scaled to 1σ=50



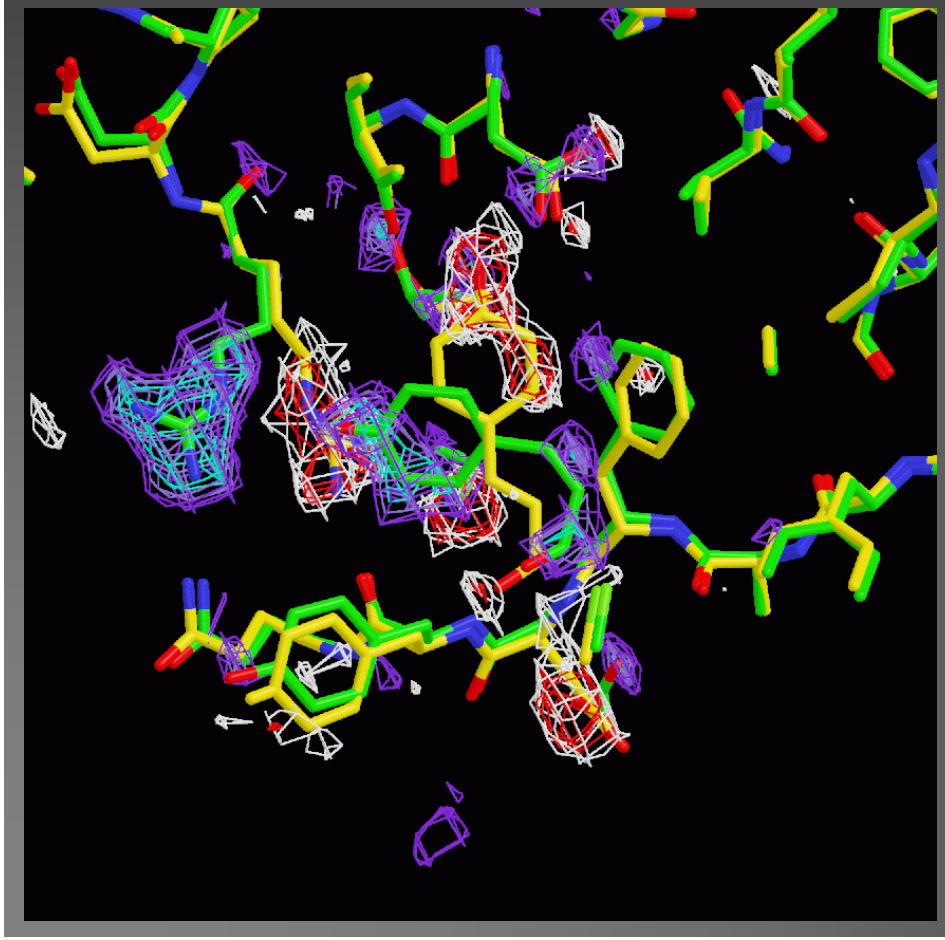
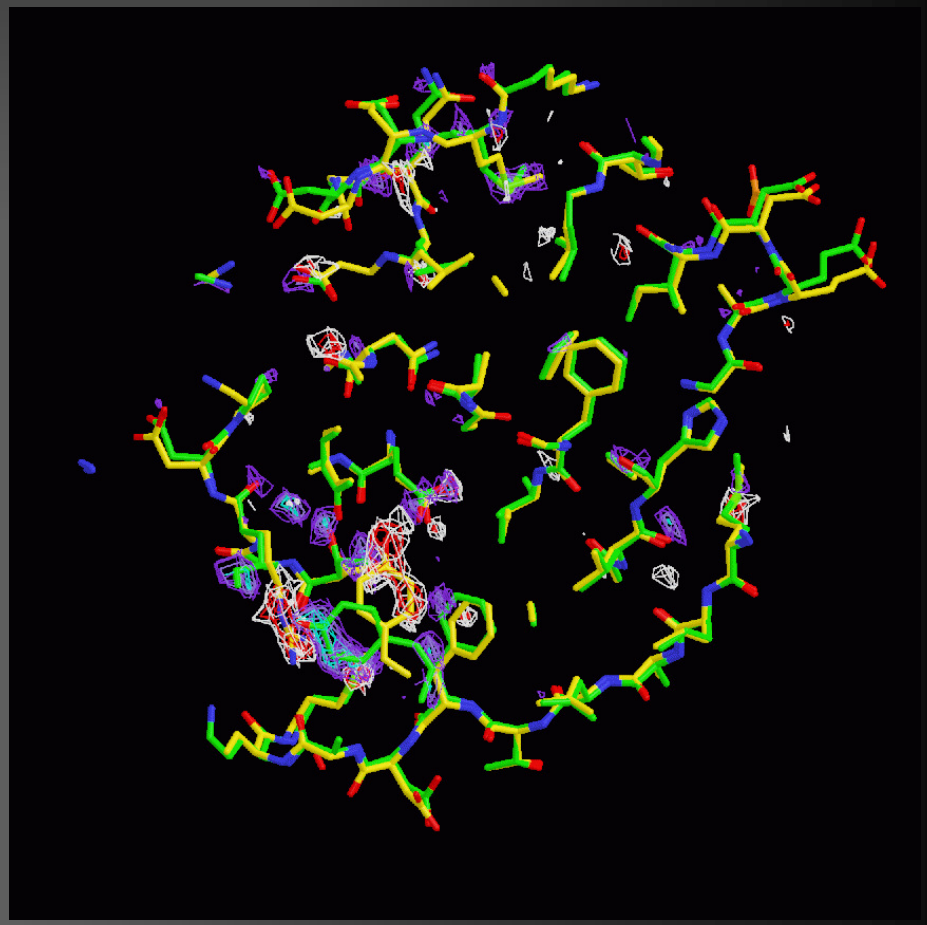
DONE !!!

Inspect difference electron density

Need to be implemented (but tools are already there)

- Back FFT of intermediate DED maps (back fft already implemented)

- Calculate extrapolated electron density (dark structure factors already in program)

structures of the intermediates

- POSTERIOR ANALYSIS (coefficient matrix solver already in place)