Distribution: EFDA-TF-ITM-IMP3

ETS: European Transport Solver

Current Status.

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1 Background

The European Transport Solver (ETS) is a new 1d core transport codes being developed by members of Integrated Modelling Project 3 ("Transport Code and Discharge Evolution") of the EFDA Task Force on Integrated Tokamak Modelling (ITM). The approach taken by the ITM is to couple codes so that the only exchange is via well specified data structures (CPOs, Consistent Physical Objects), with the aim of having the workflow managed by Kepler, a Scientific Workflow engine.

Thus the work of the ETS group is both to prepare the core 1d transport solver, and, in conjunction with other parts of the ITM, to prepare workflows using the ETS.

The ITM has defined the CPO definitions for the physics inputs and outputs for a number of physics areas. Those relevant for the ETS include: (a) equilibrium, (b) core sources, (c) core transport, (d) core profile, (e) neoclassical transport, and (f) core impurities.

The current version of the core ETS code expects to receive as input: (a) equilibrium CPOs representing the equilibrium at the previous time-step, and at the present iteration (b) core source and transport CPOs representing the sources of current, particles, momentum and electron and ion energies, as well as the transport coefficients of these quantities represented as diffusion coefficients and convective velocities at the present iteration, (c) the plasma state as represented by the core profile at the previous time step and the previous iteration. It then returns an updated plasma state in a new core profile.

In addition to the core ETS routine, the ETS group within IMP3 has also prepared a number of workflows represented by code wrappers (these will ultimately be converted to Kepler workflows).

The first of these encompasses an analytical test case where the method of manufactured solutions is used to prepare an analytical solution to the test problem which can then be compared to the numerical solution. The test case incorporates a time varying problem with coupled poloidal flux, ion density, toroidal velocity and electron and ion temperature equations.

The second workflow takes sources and transport coefficients from a previously saved case in the ITM data-base, and then solves for the poloidal flux, density, velocity and temperatures including self-consistent calculations of the equilibrium (or with a "cylindrical" equilibrium). For these cases, the results are compares with the results from the ASTRA 1d core transport code (or with analytical results).

One of the features of the ETS is that internally there is a separation of the physics and the numerics. All of the equations are cast in the same form characterized by a number of vectors of coefficients, and these are then passed to one of the implemented solvers.

2 Analytical comparisons

Two versions of the work-flow calling the ETS are used.

The first, solver_test, uses the method of manufactures solutions to provide analytical results against which the numerical solutions can be compared.

The second, eq_ets_test, obtains sorces and transport coefficients by reading from a specified shot/run. The equilibrium is either cylindrixaol read the same way, or obtained from an equilibrium solver (EMEQ).

A number of solvers are implemented in the ETS:

solver 1 "standard" RITM

solver 2 "integral" RITM

solver 3 "PROGONKA" (block Thomas)

solver 6 Huysmans' solver

solver 7 RITM differential solver ???

solver 10 COS solver

2.1 Behaviour as a function of δx for solver_test

2.1.1 Solver 1

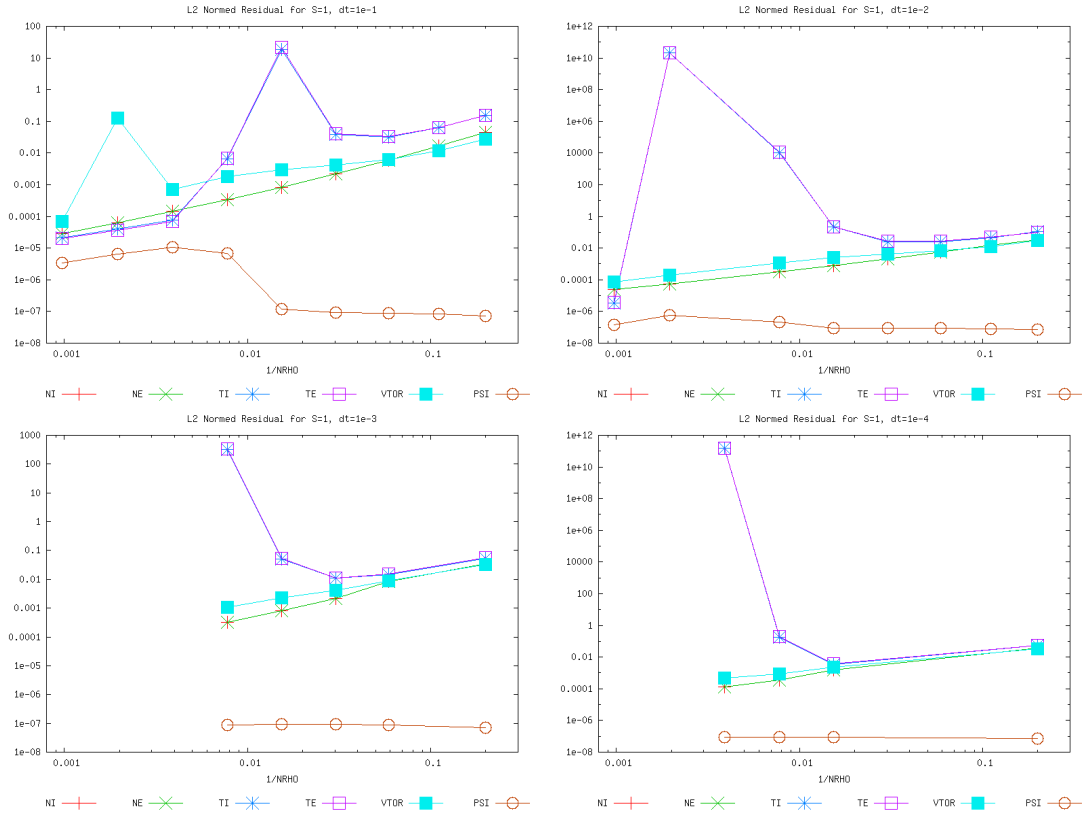

Figure 1: L2 norm for solver 1 as function of δx.

2.1.2 Solver 2

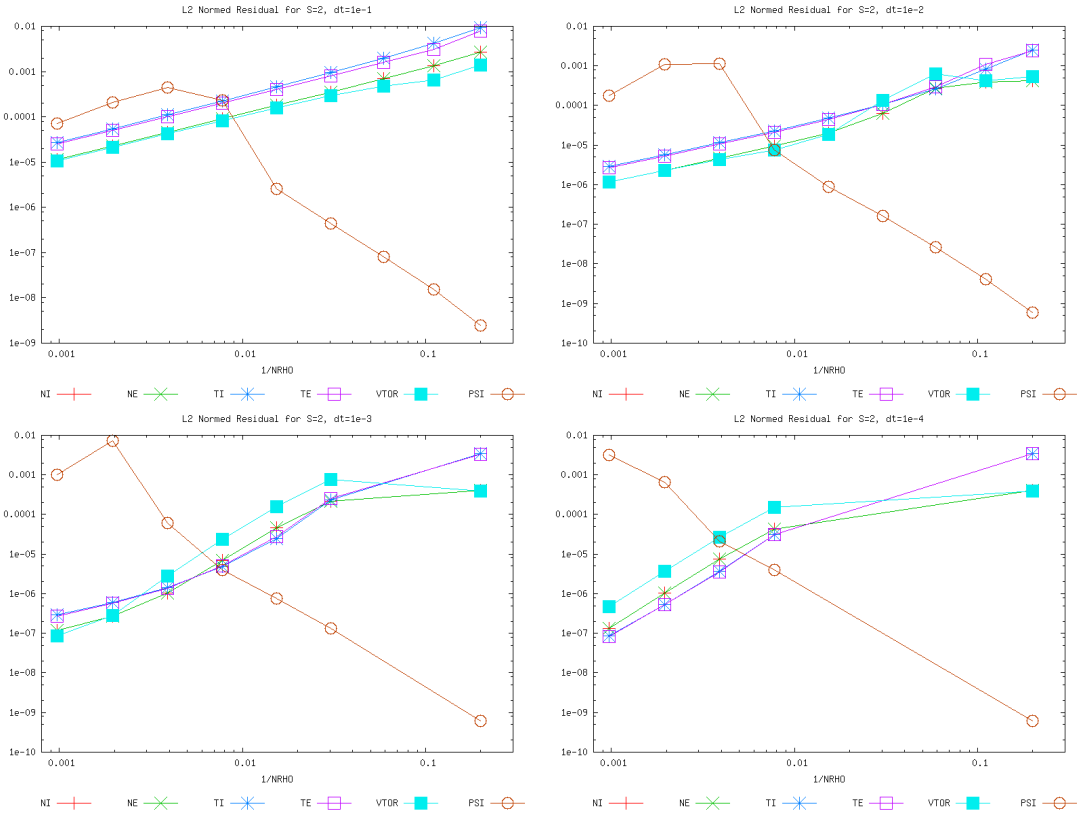

Figure 2: L2 norm for solver 2 as function of δx.

2.1.3 Solver 3

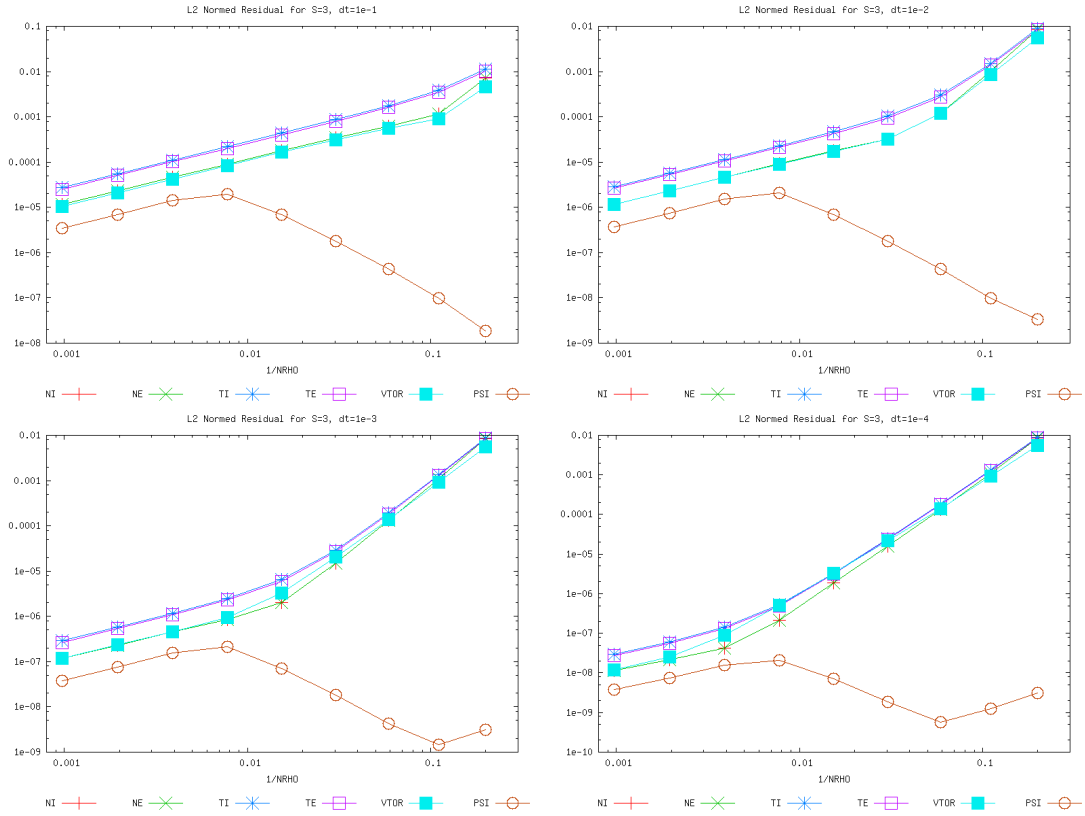

Figure 3: L2 norm for solver 3 as function of δx.

2.1.4 Solver 6

Figure 4: L2 norm for solver 6 as function of δx.

2.1.5 Solver 7

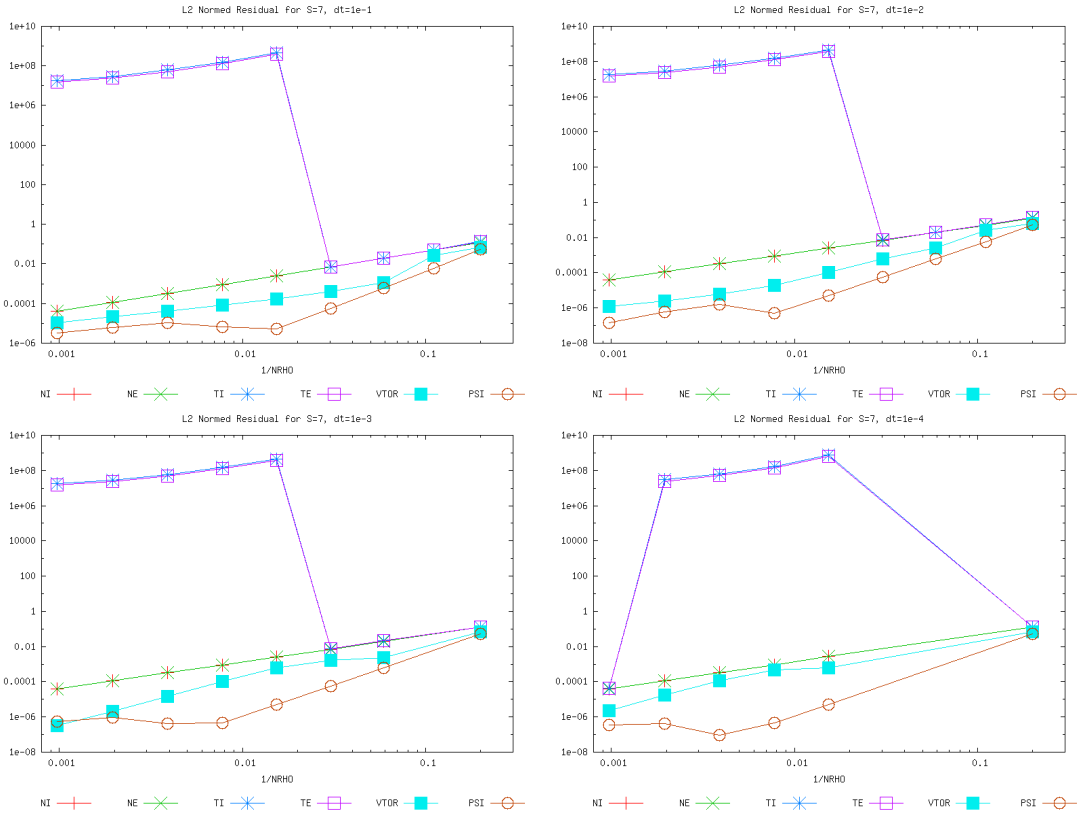

Figure 5: L2 norm for solver 7 as function of δx.

2.1.6 Solver 10

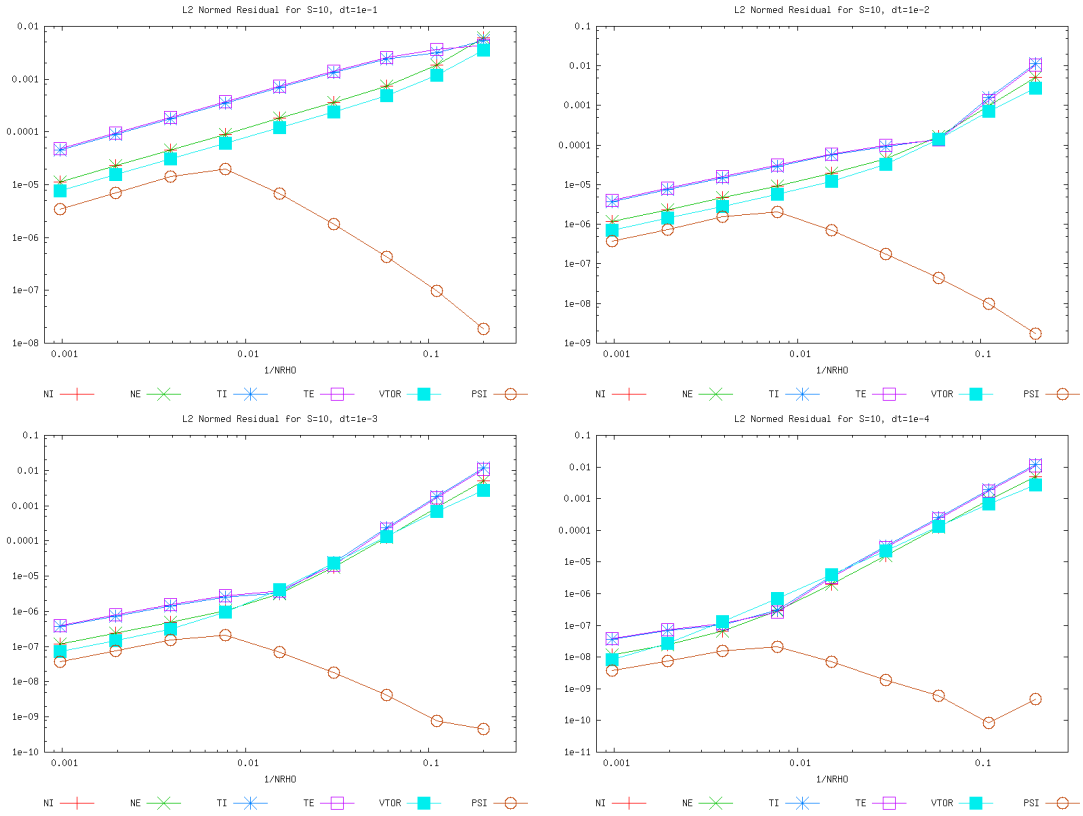

Figure 6: L2 norm for solver 10 as function of δx.

2.2 Behaviour as a function of δt for solver_test

2.2.1 Solver 1

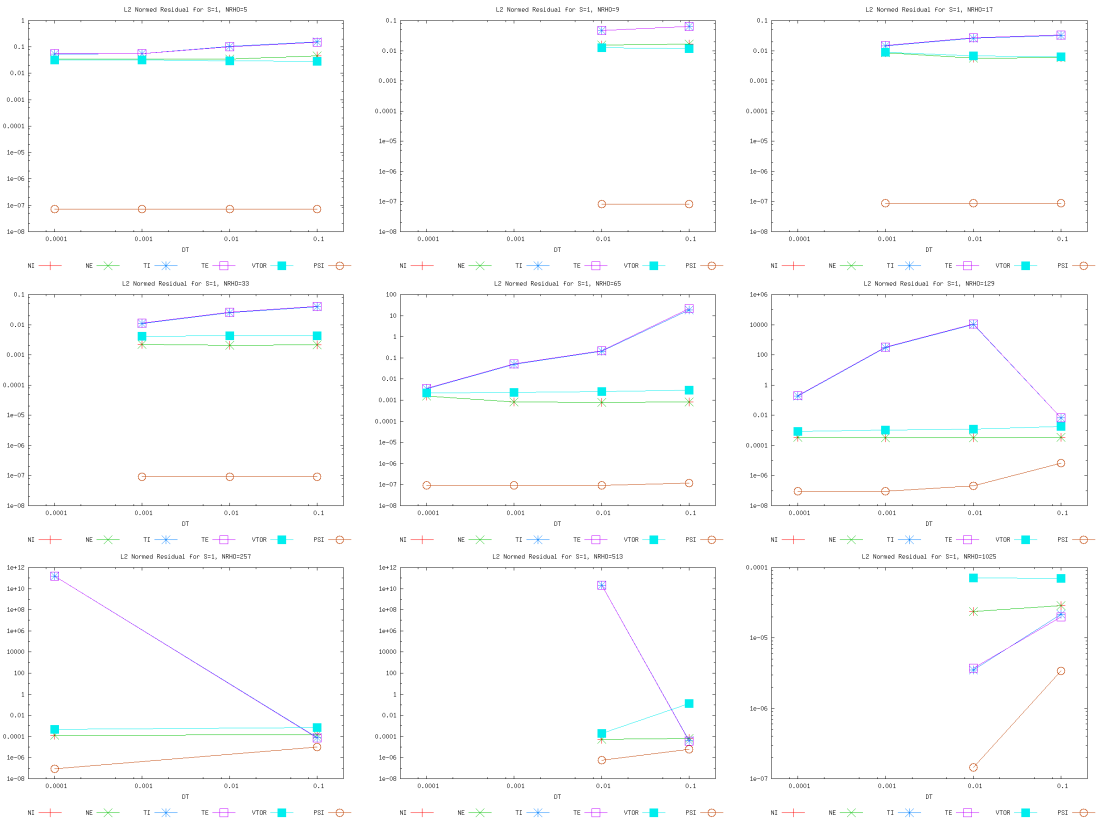

Figure 7: L2 norm for solver 1 as function of δt.

2.2.2 Solver 2

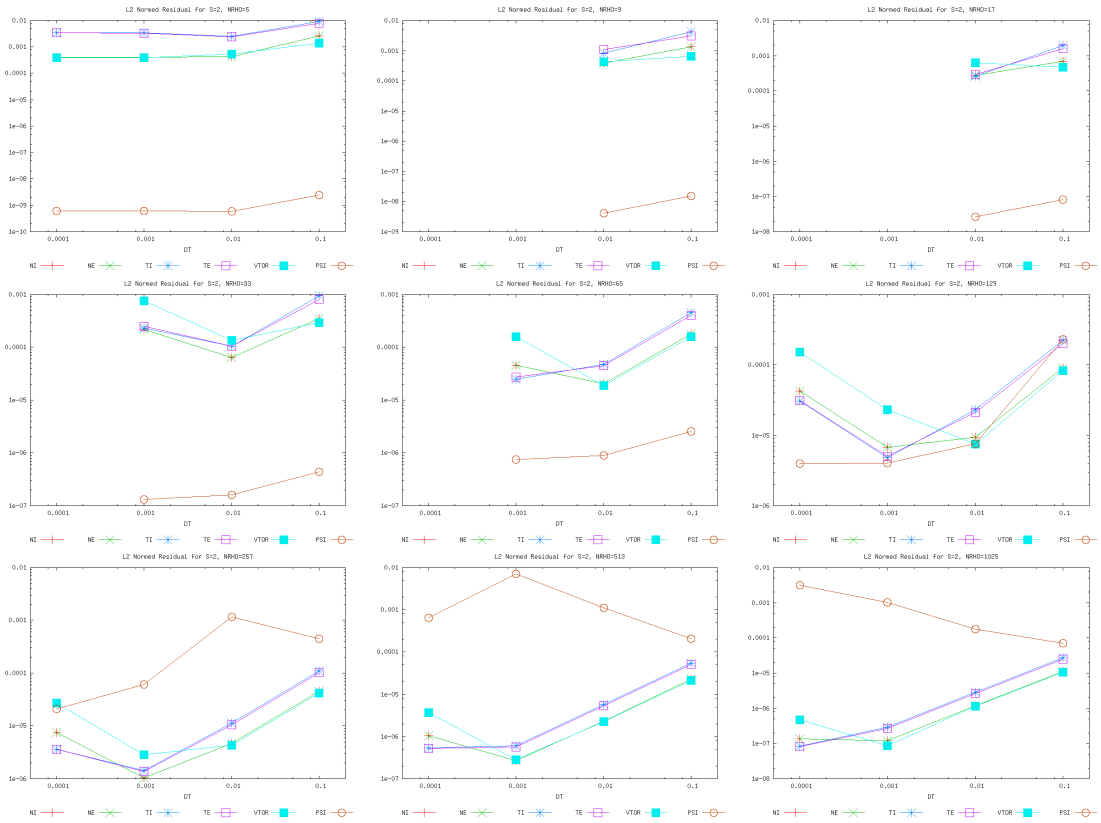

Figure 8: L2 norm for solver 2 as function of δt.

2.2.3 Solver 3

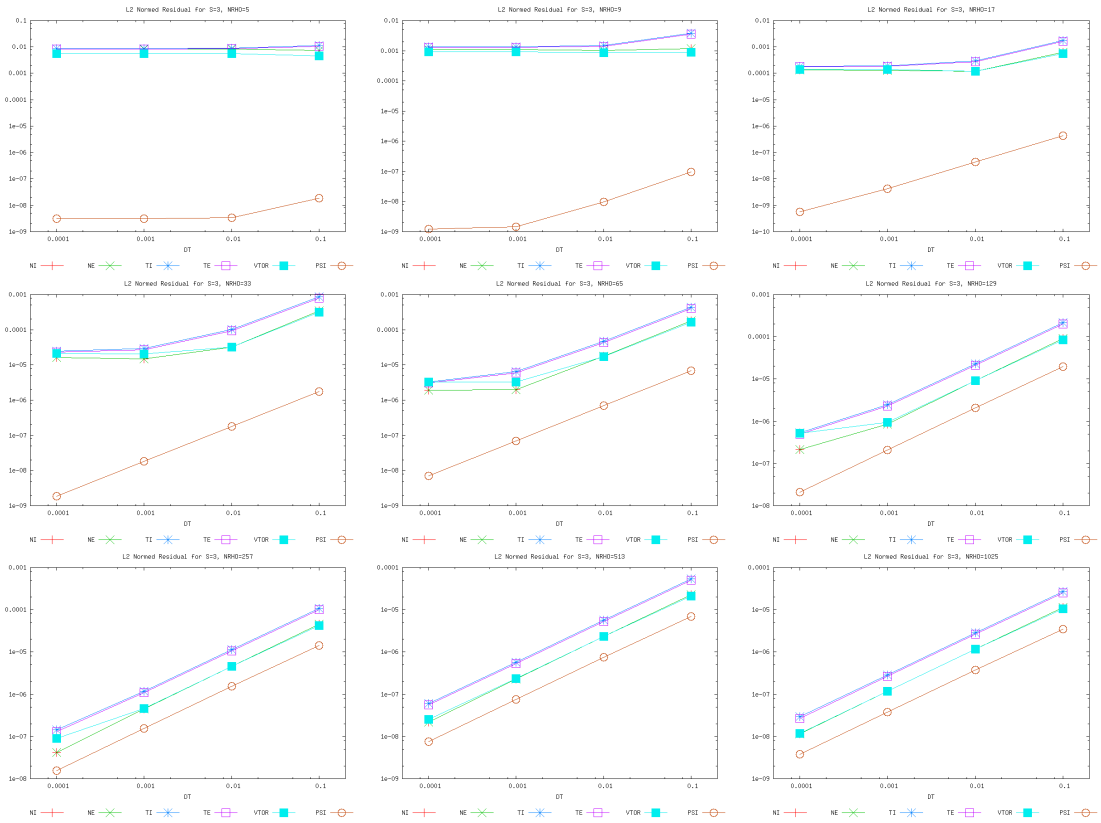

Figure 9: L2 norm for solver 3 as function of δt.

2.2.4 Solver 6

Figure 10: L2 norm for solver 6 as function of δt.

2.2.5 Solver 7

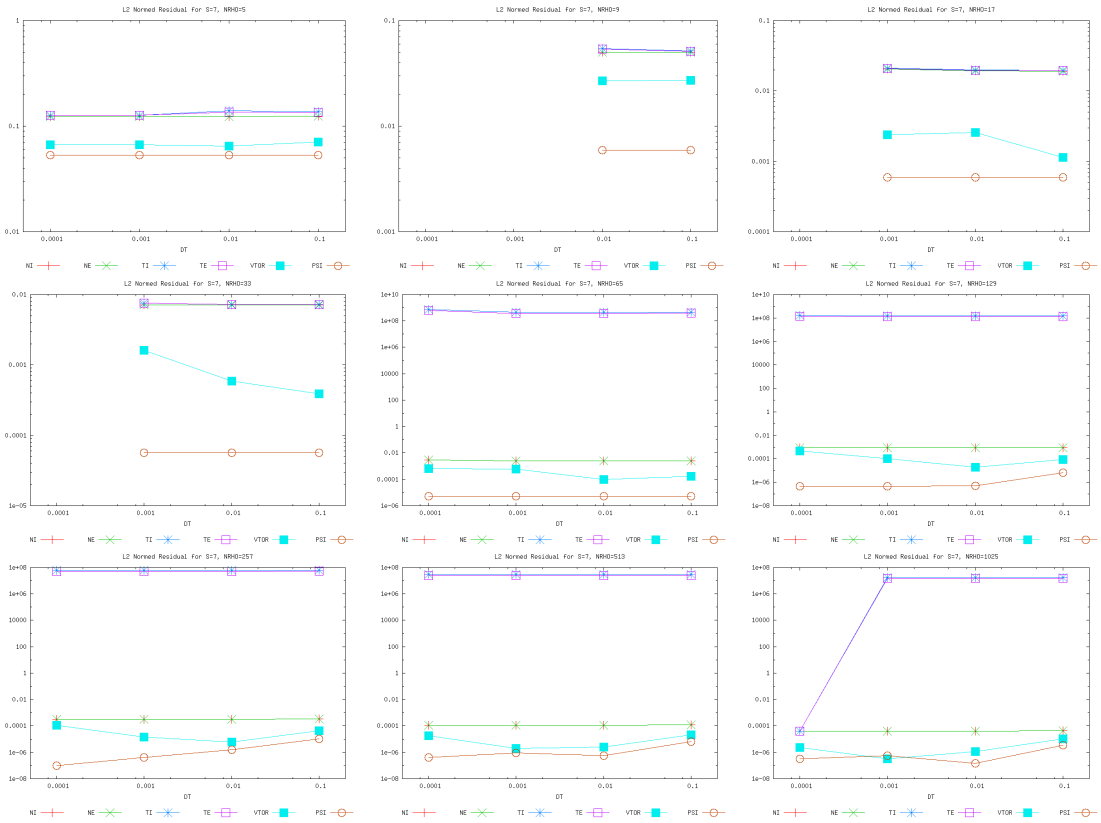

Figure 11: L2 norm for solver 7 as function of δt.

2.2.6 Solver 10

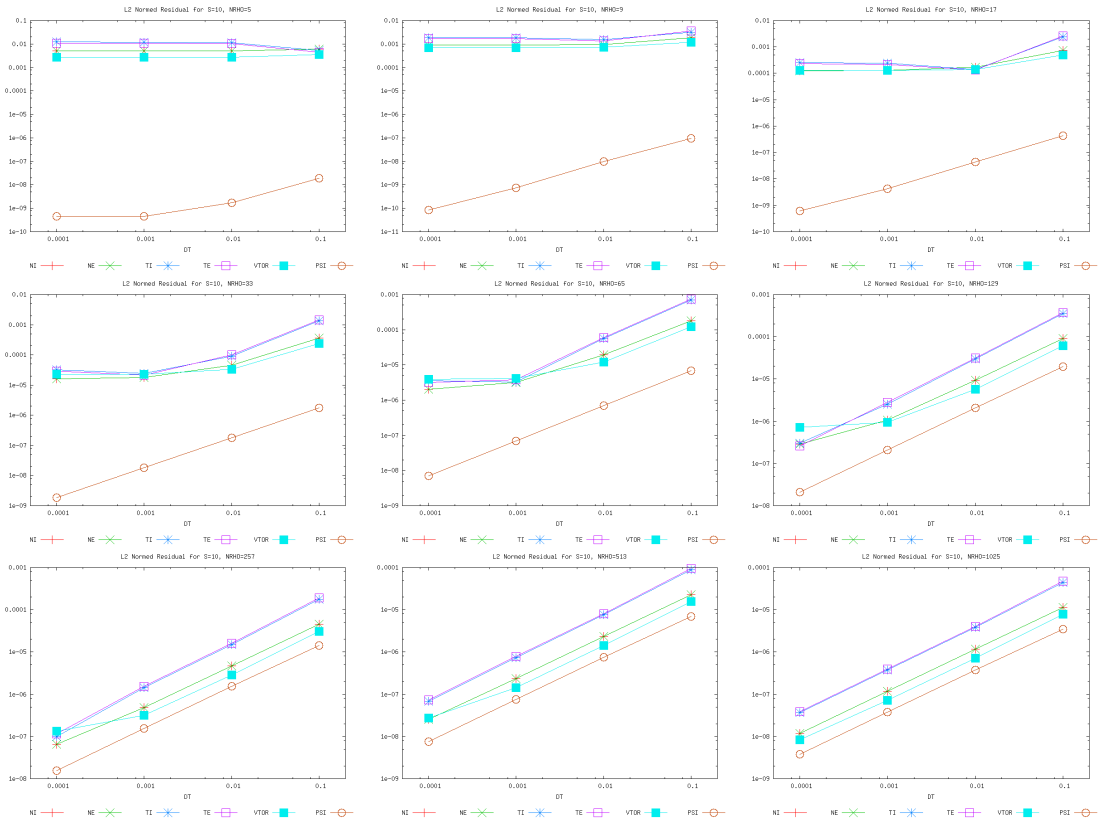

Figure 12: L2 norm for solver 10 as function of δt.

2.3 Analytical cases with eq_ets_test

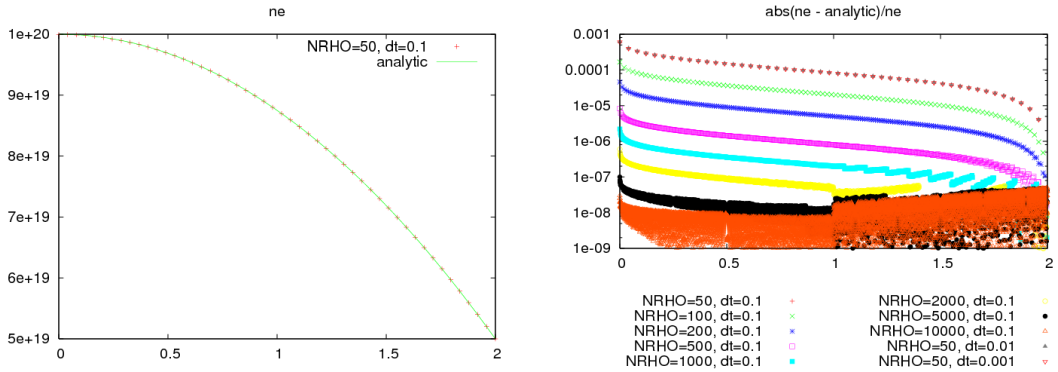

Figure 13: Cylindrical case, density profiles.

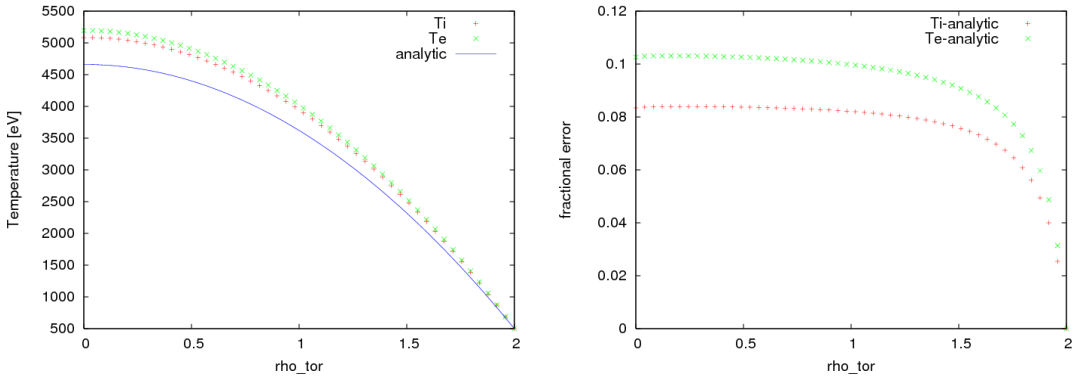

Figure 14: Cylindrical case, temperature profiles.

3 Further convergence studies with eq_ets_test

3.1 Convergence as a function of NRHO

3.1.1 $\delta t = 10^{-1} s$

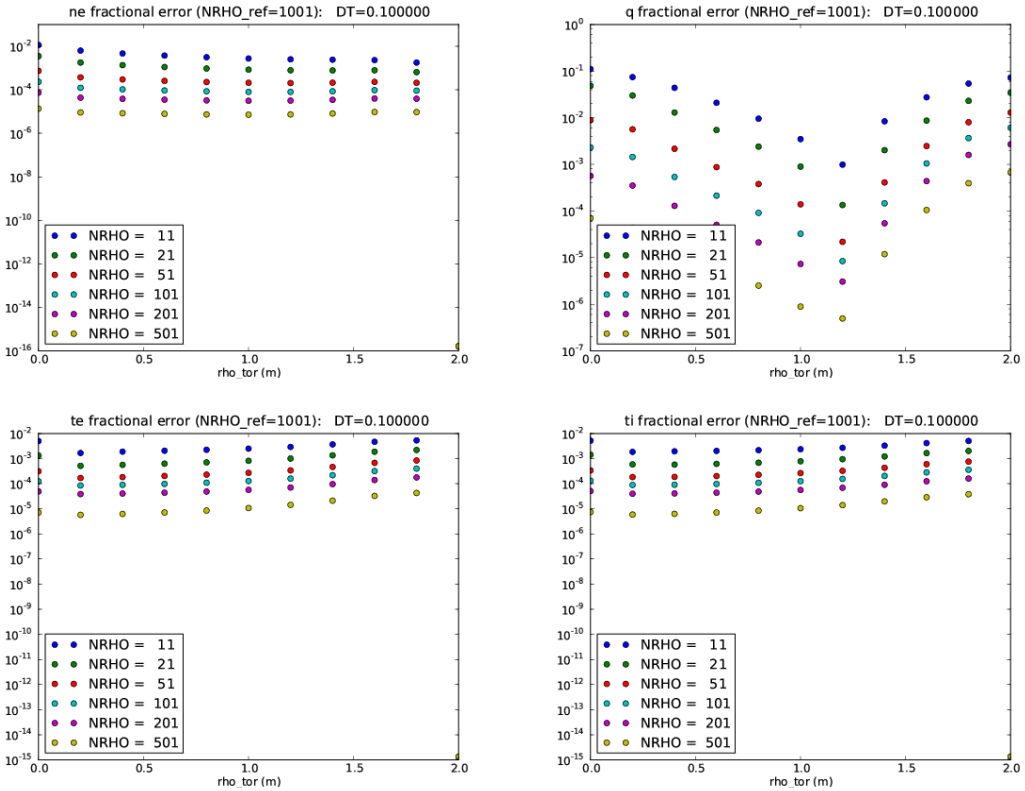

Figure 15: Fractional deviation for density, q and temperature profiles for a toroidal case with dt=1e-1.

3.1.2 $\delta t = 10^{-2} s$

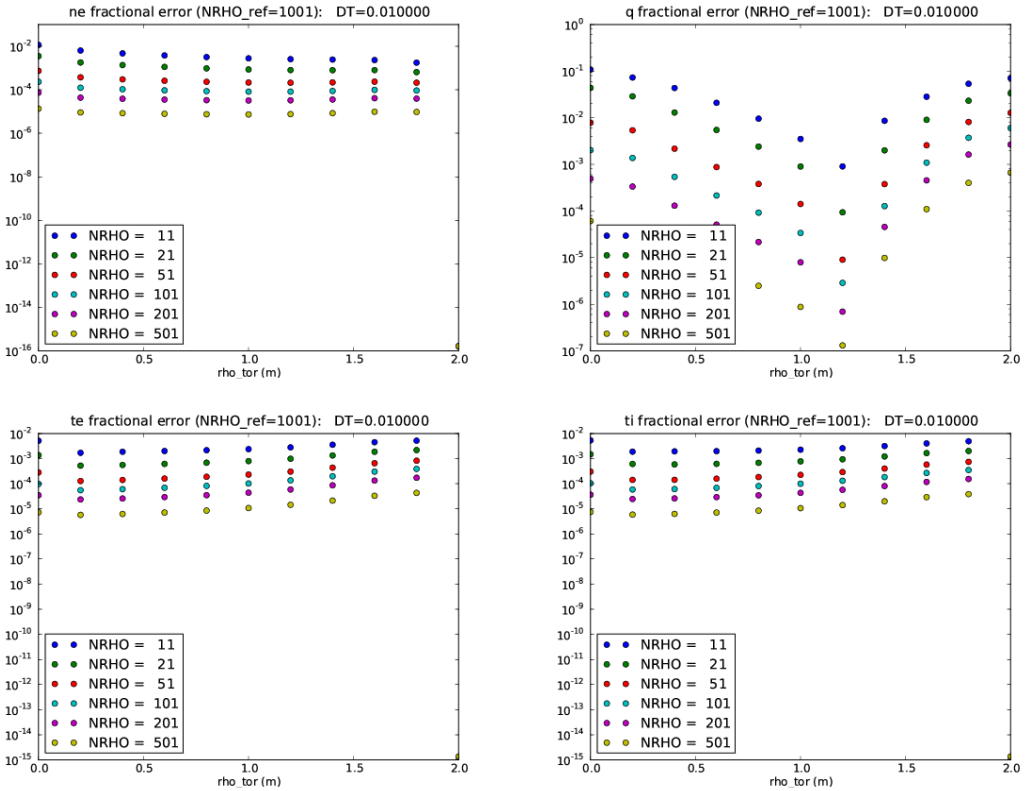

Figure 16: Fractional deviation for density, q and temperature profiles for a toroidal case with dt=1e-2.

3.1.3 $\delta t = 10^{-3} s$

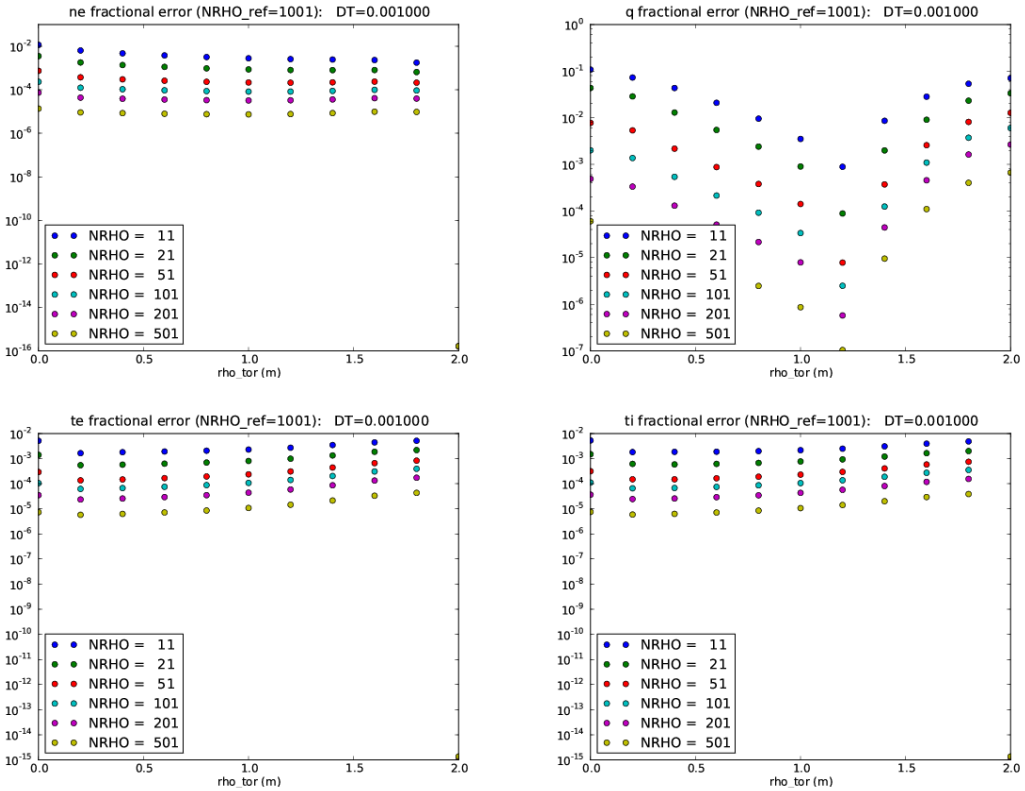

Figure 17: Fractional deviation for density, q and temperature profiles for a toroidal case with dt=1e-3.

3.1.4 $\delta t = 10^{-4} s$

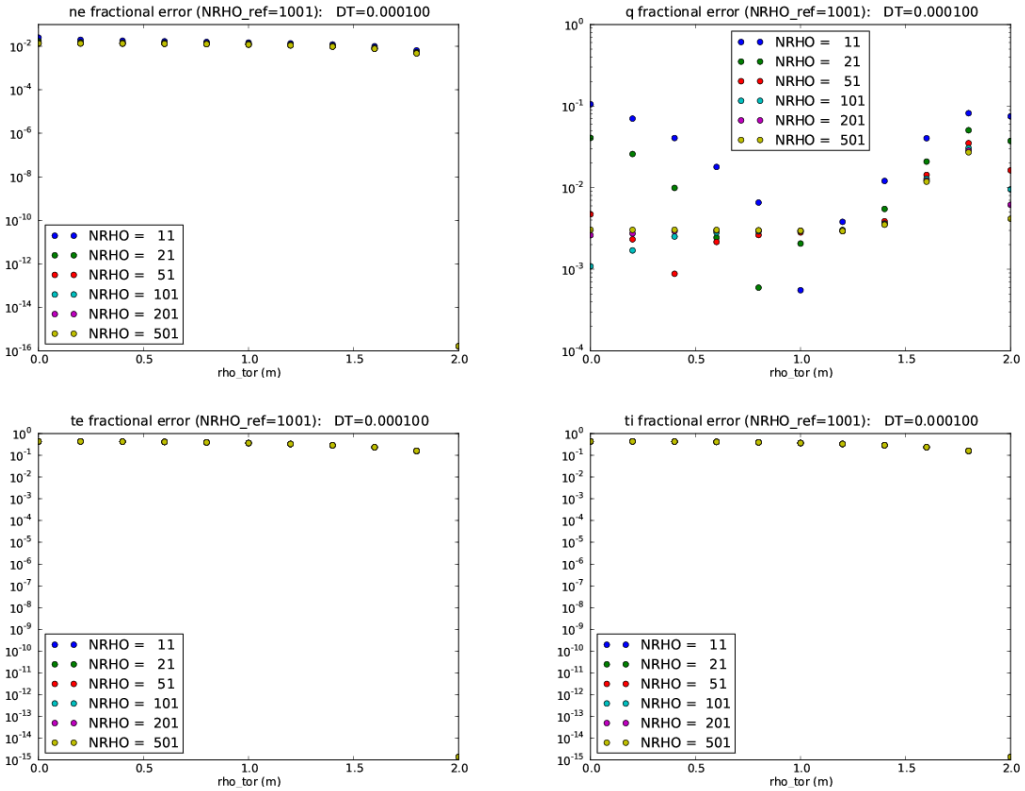

Figure 18: Fractional deviation for density, q and temperature profiles for a toroidal case with dt=1e-4.

3.2 Convergence as a function of time-step

3.2.1 NRHO=11

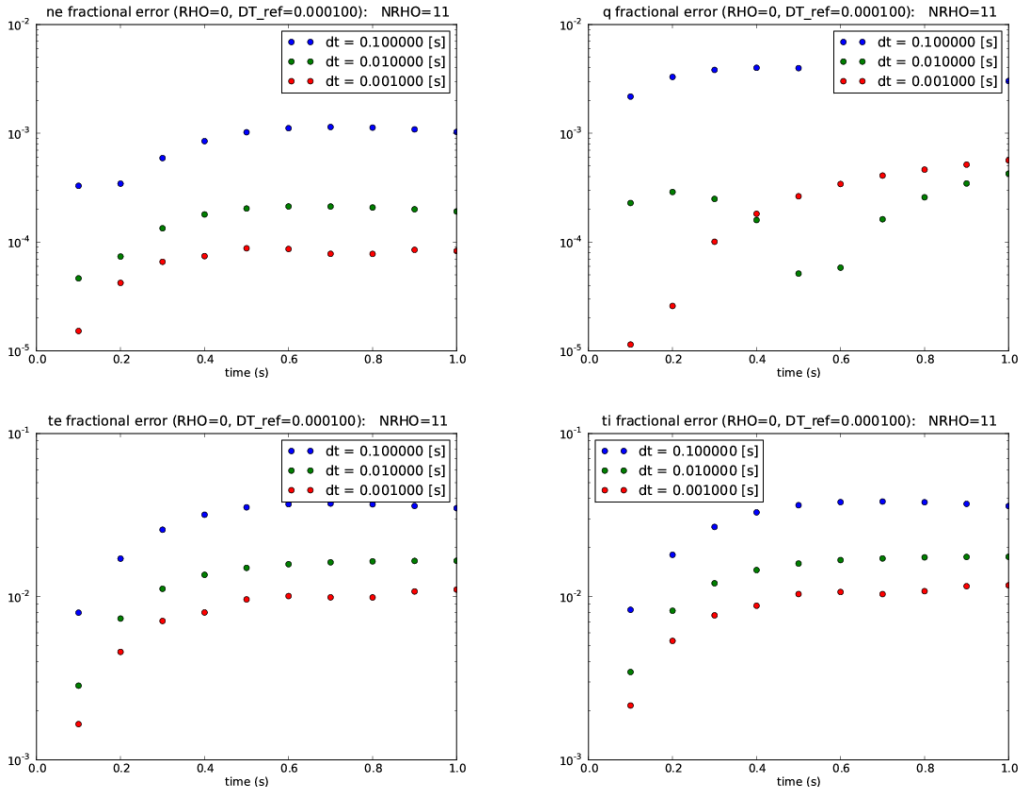

Figure 19: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=11, taken at $\rho = 0$.

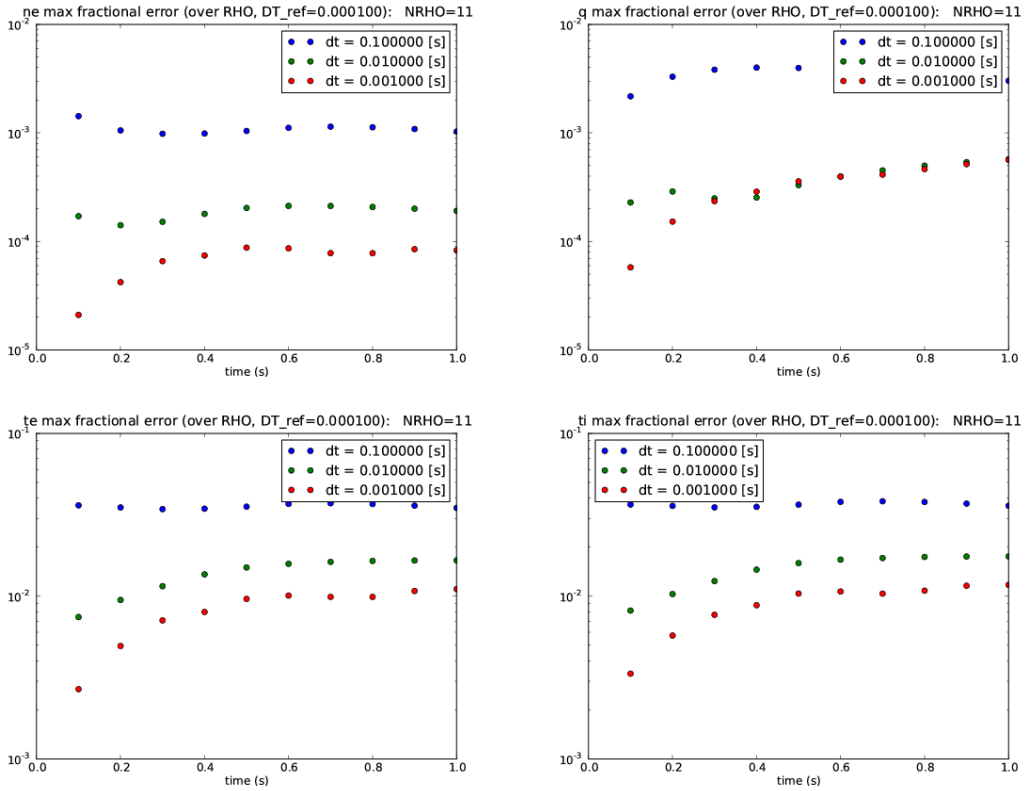

Figure 20: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=11, taken over ρ.

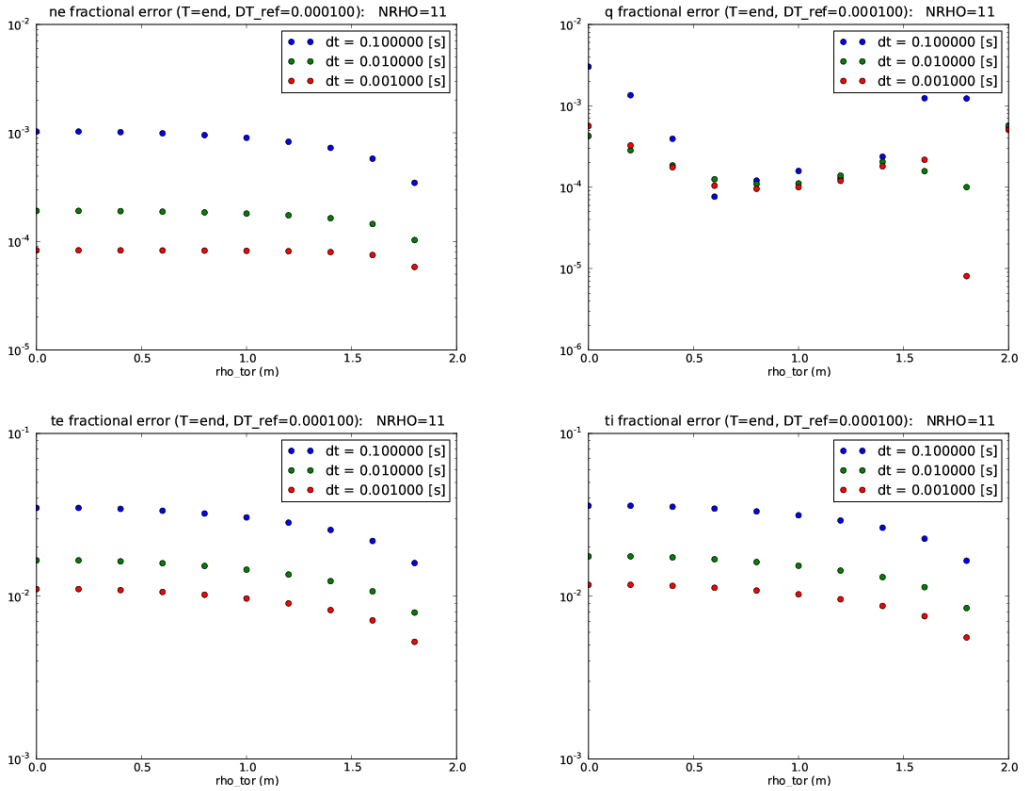

Figure 21: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=11, taken at the end time.

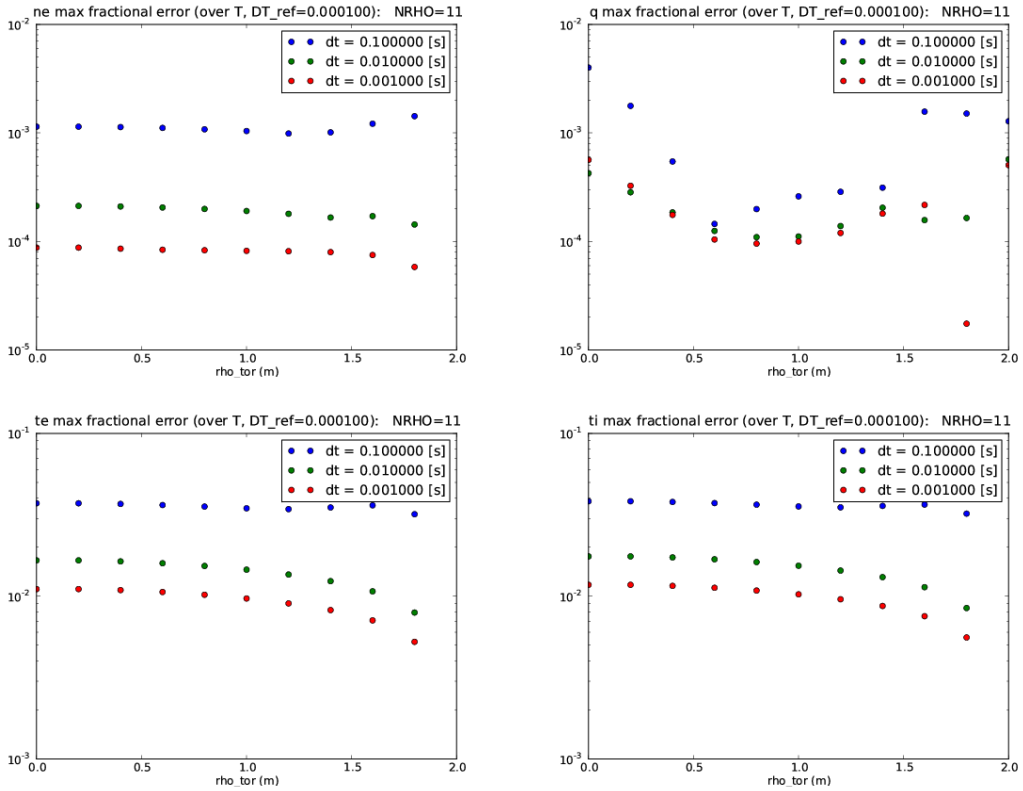

Figure 22: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=11, taken over time.

3.2.2 NRHO=21

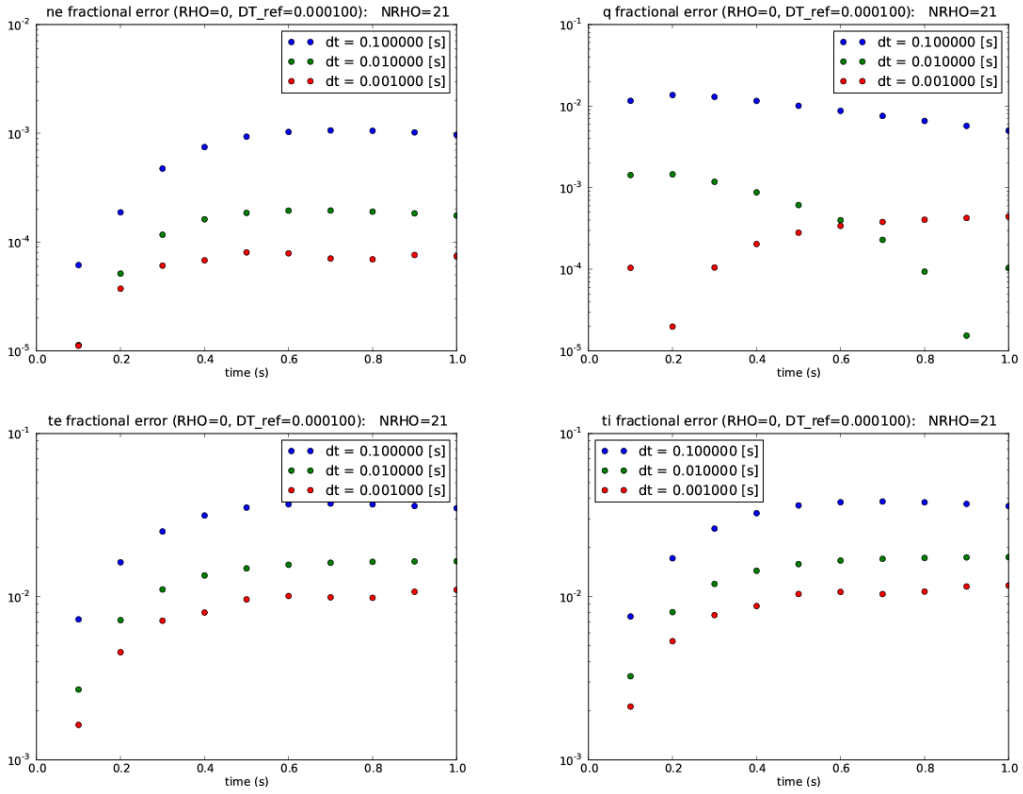

Figure 23: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=21, taken at $\rho = 0$.

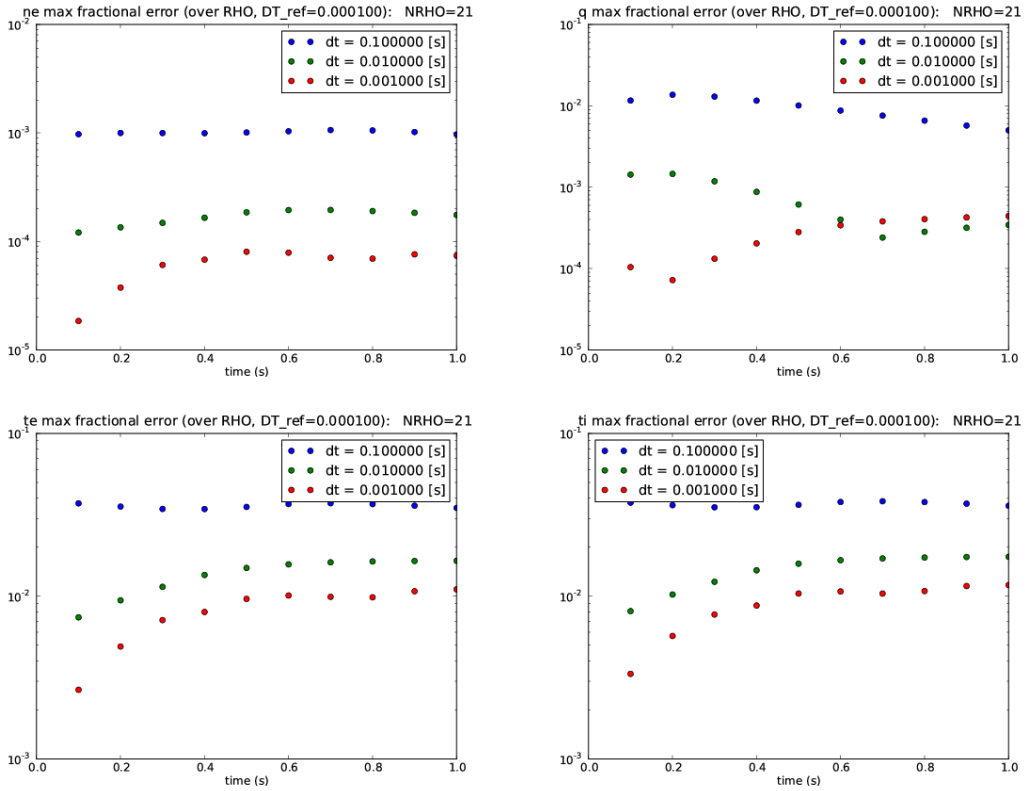

Figure 24: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=21, taken over ρ.

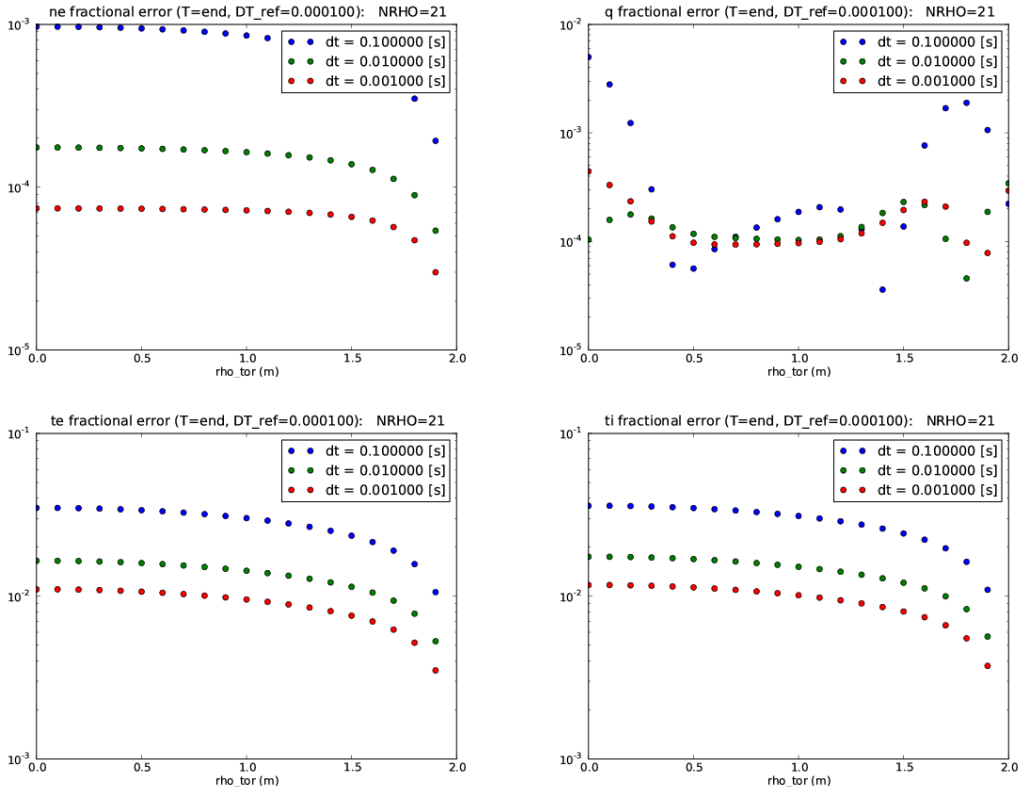

Figure 25: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=21, taken at the end time.

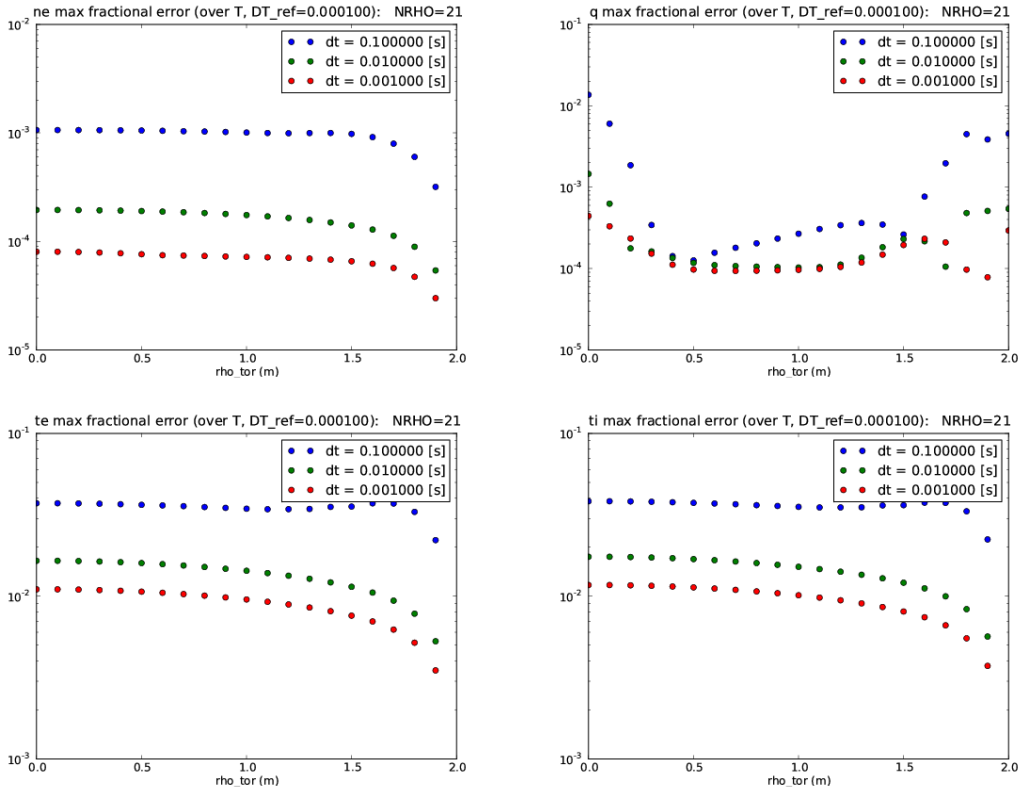

Figure 26: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=21, taken over time.

3.2.3 NRHO=51

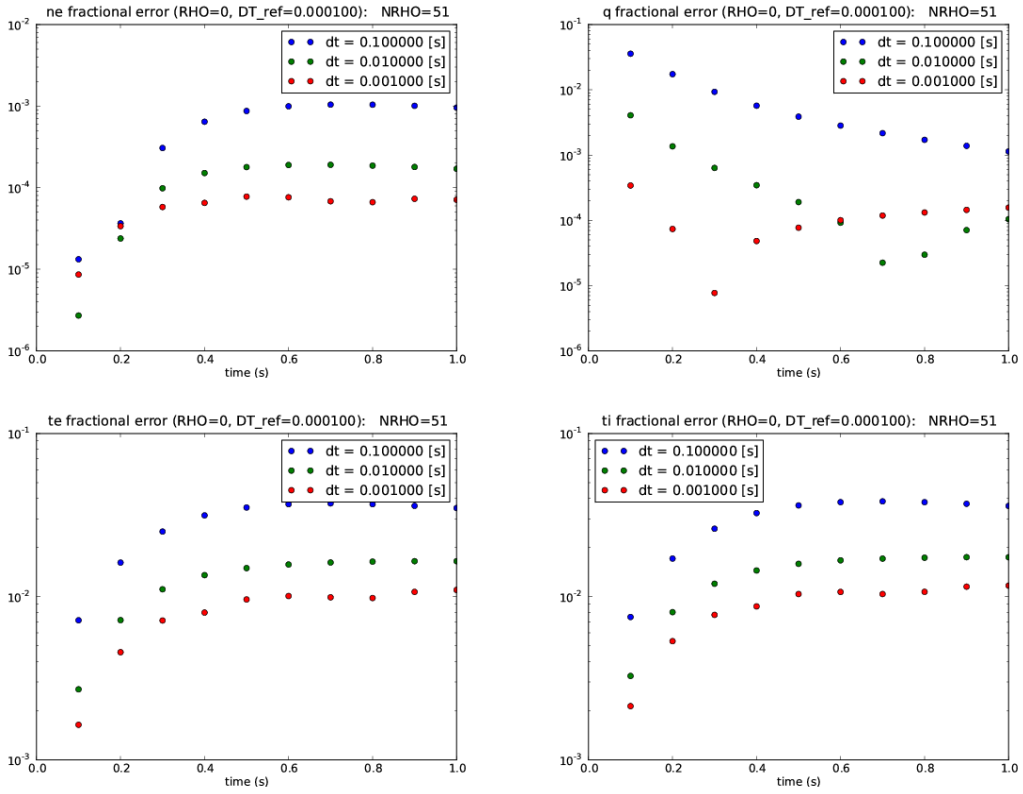

Figure 27: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=51, taken at $\rho = 0$.

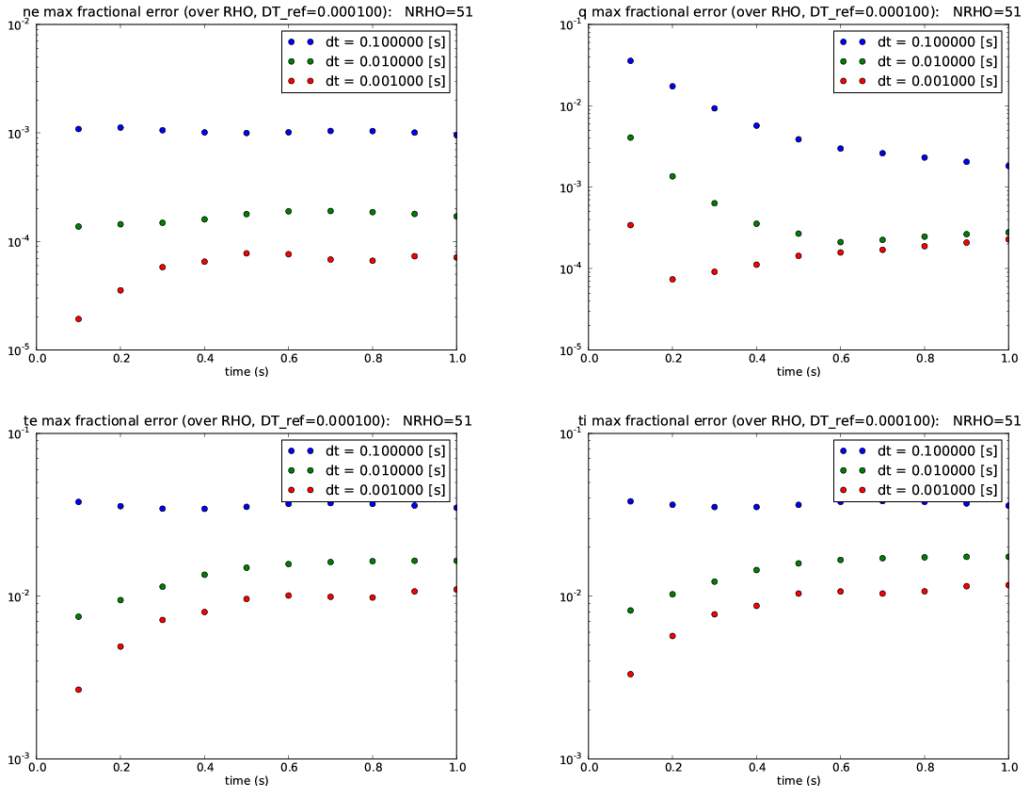

Figure 28: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=51, taken over ρ.

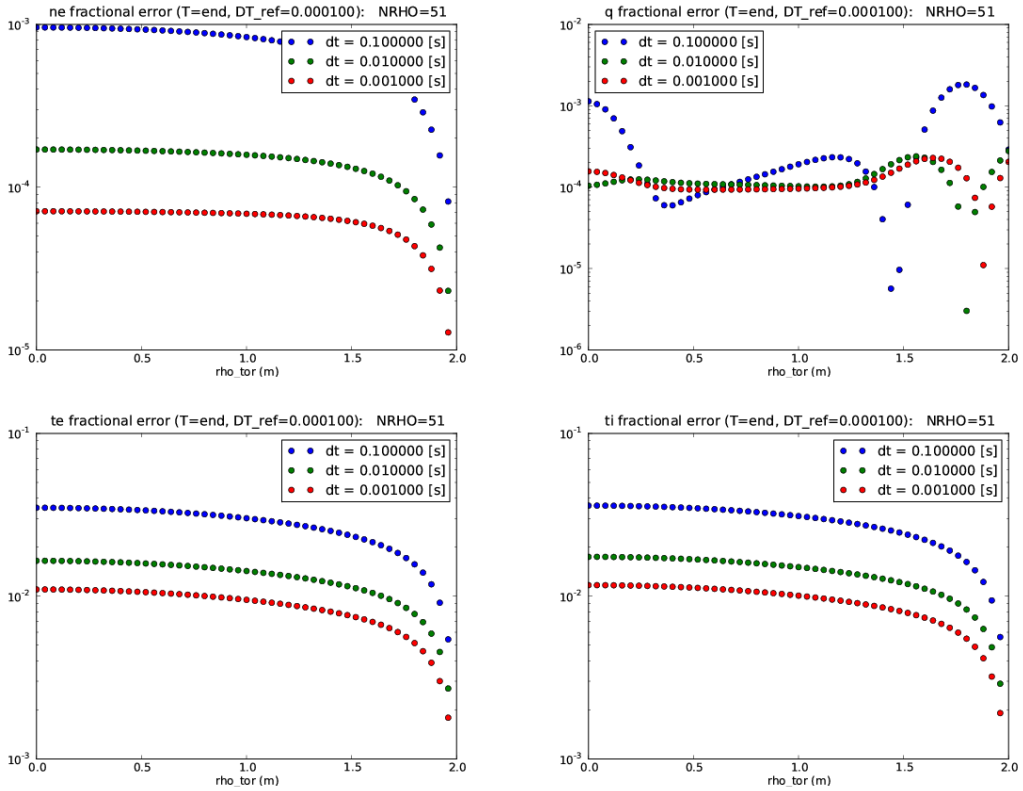

Figure 29: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=51, taken at the end time.

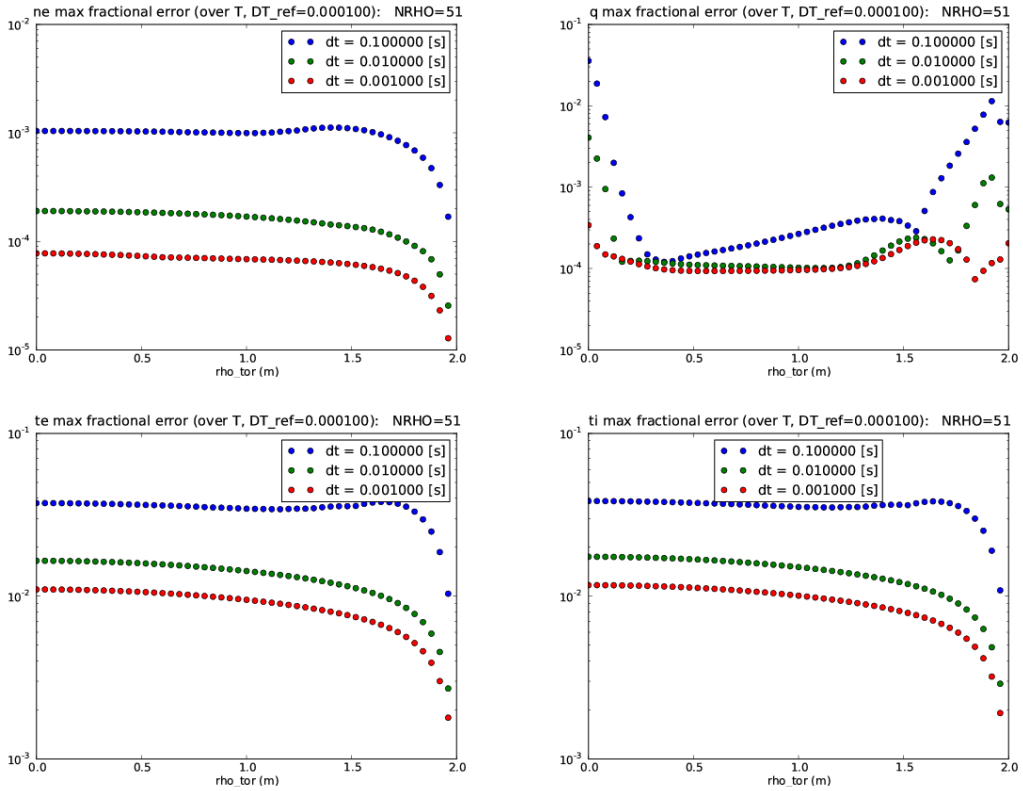

Figure 30: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=51, taken over time.

3.2.4 NRHO=101

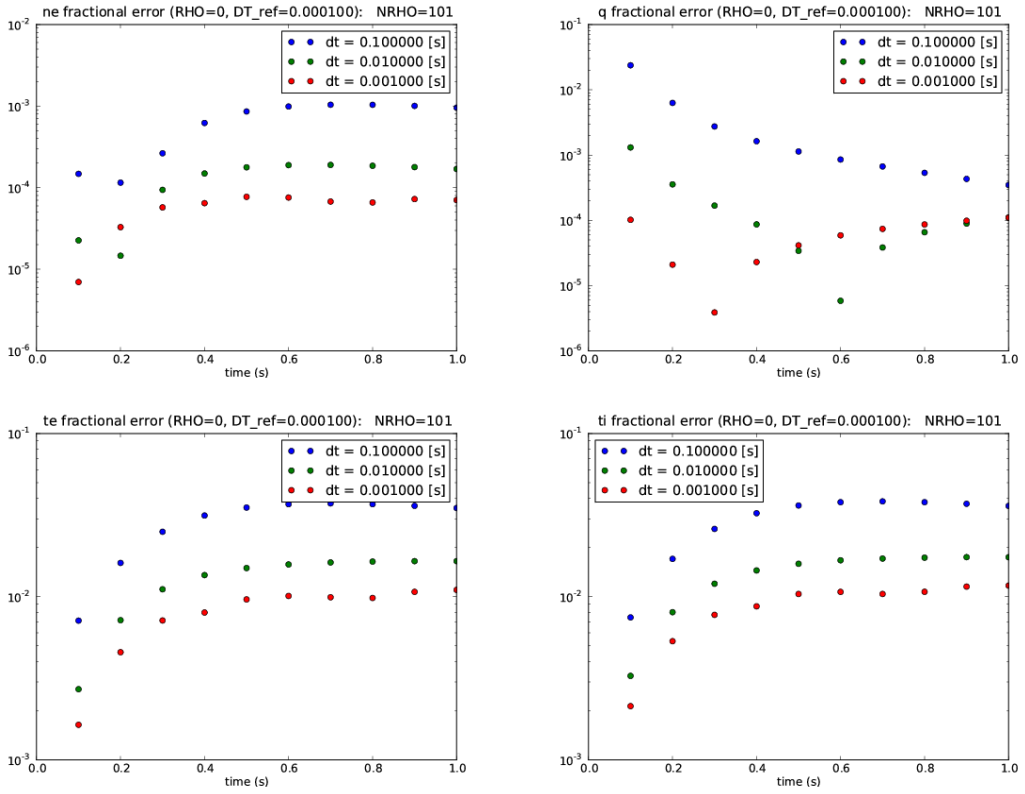

Figure 31: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=101, taken at $\rho = 0$.

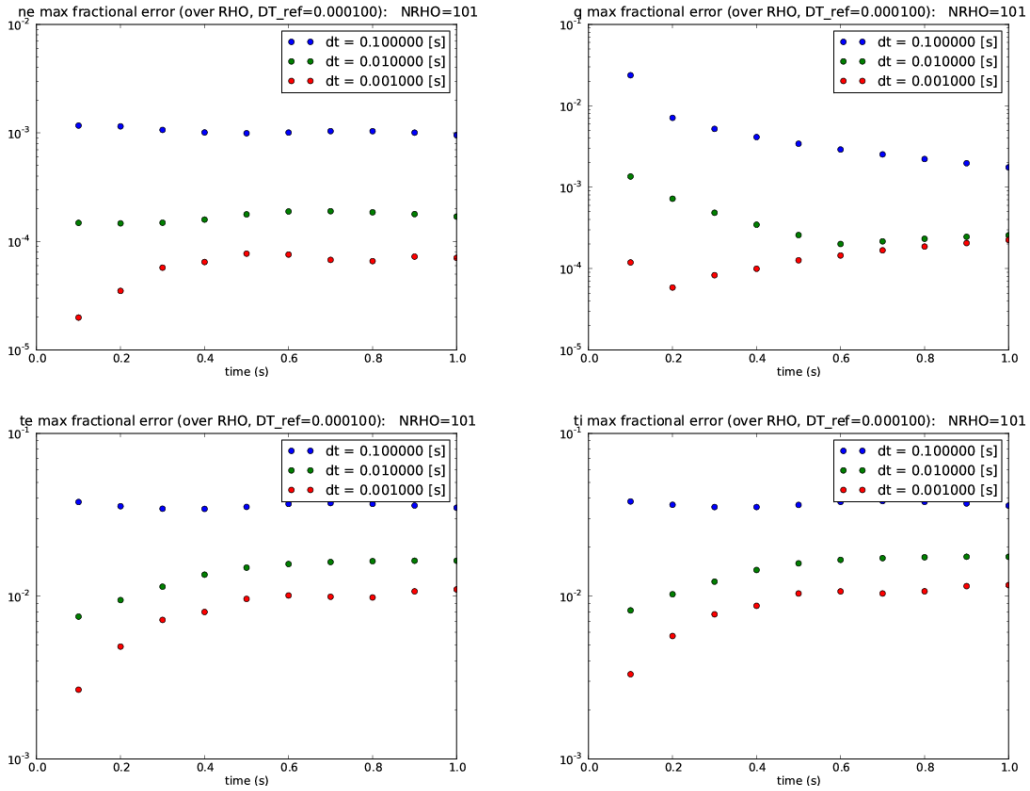

Figure 32: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=101, taken over ρ.

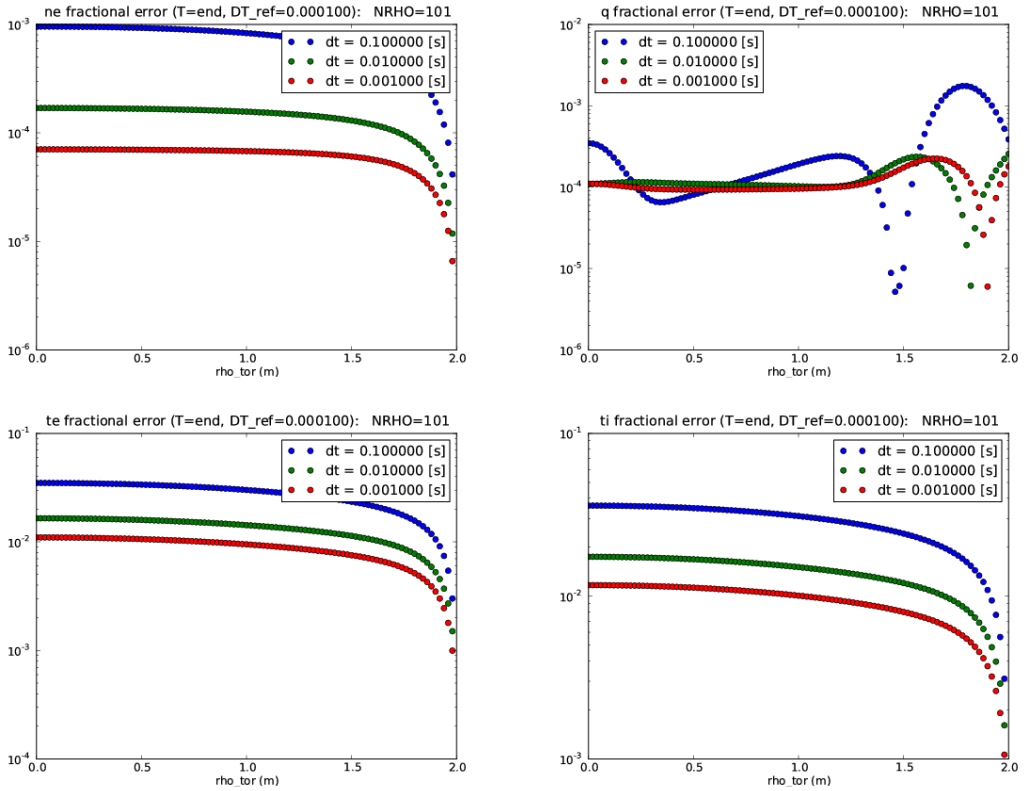

Figure 33: Fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=101, taken at the end time.

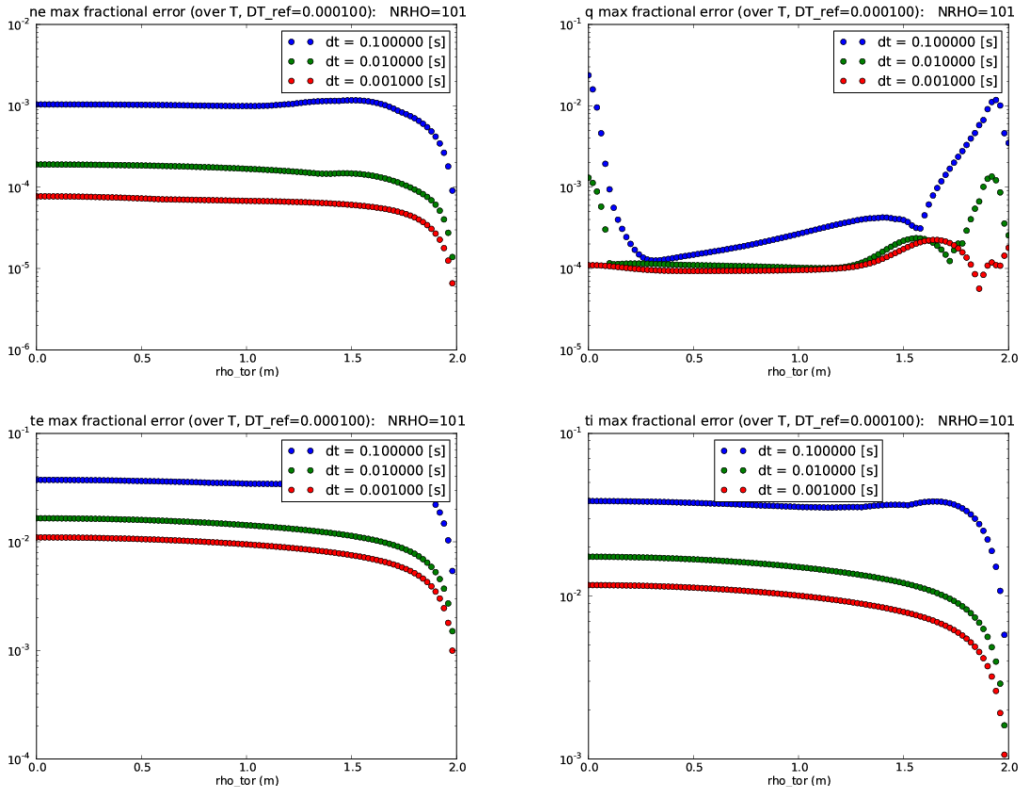

Figure 34: Max fractional deviation for density, q and temperature profiles for a toroidal case with NRHO=101, taken over time.

4 Comparisons with ASTRA

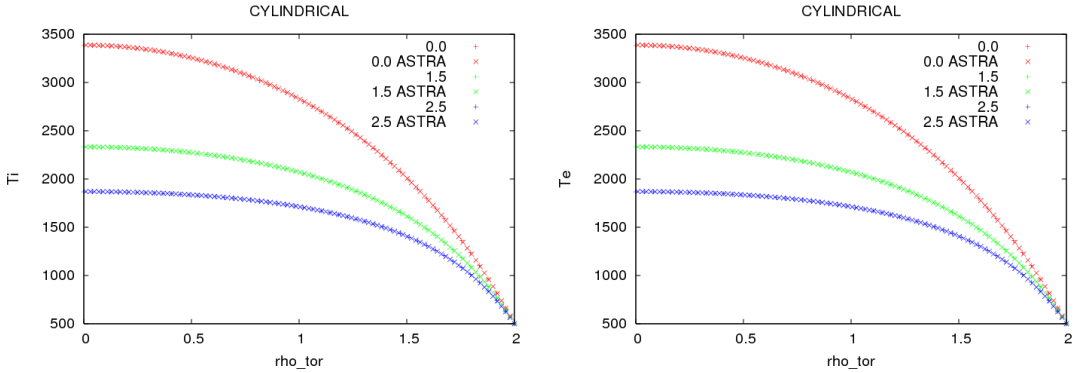

Figure 35: Comparison of temperatures for convective heat multipliers of 0.0, 1.5 and 2.5.

4.1 Cylindrical geometry

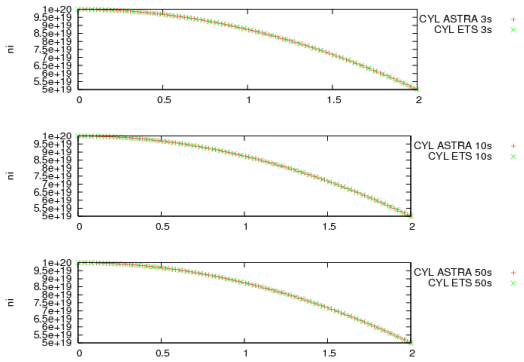

Figure 36: Comparison of ion densities at 3, 10 and 50s.

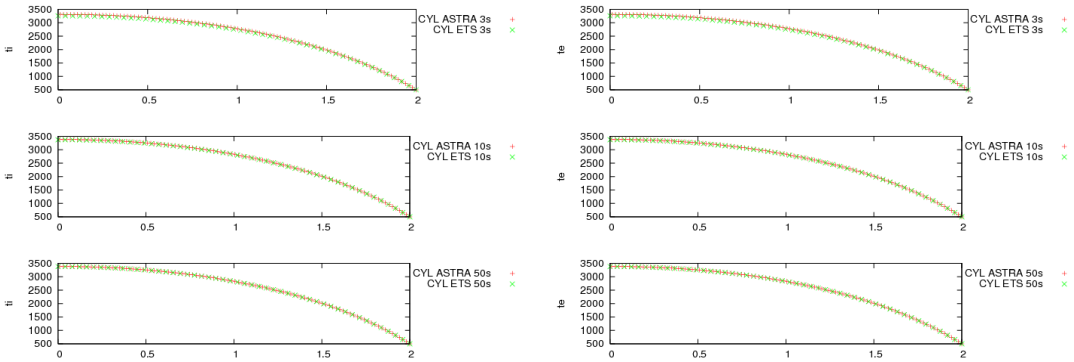

Figure 37: Comparison of ion and electron temperatures at 3, 10 and 50s.

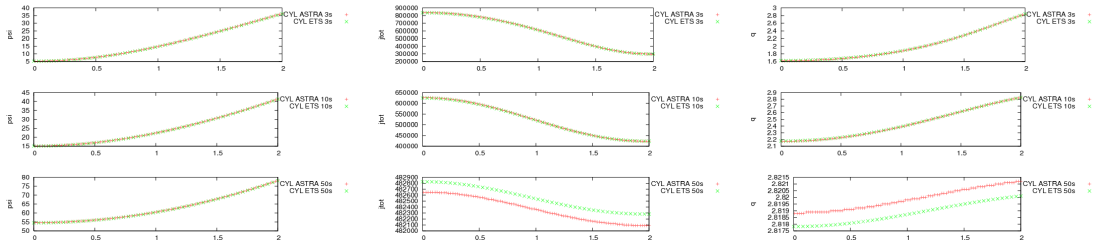

Figure 38: Comparison of ψ, total current and q at 3, 10 and 50s.

4.2 Toroidal geometry

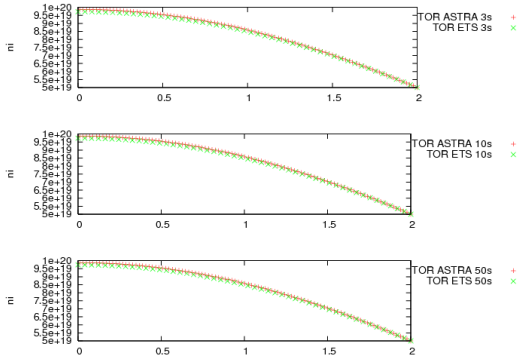

Figure 39: Comparison of ion densities at 3, 10 and 50s.

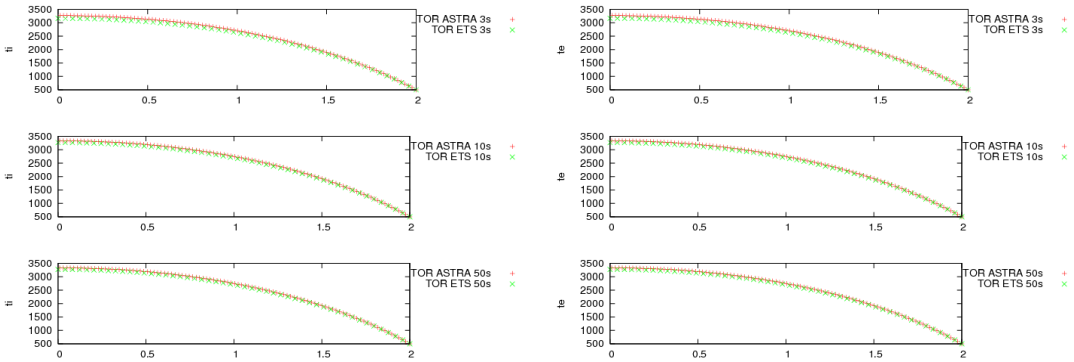

Figure 40: Comparison of ion and electron temperatures at 3, 10 and 50s.

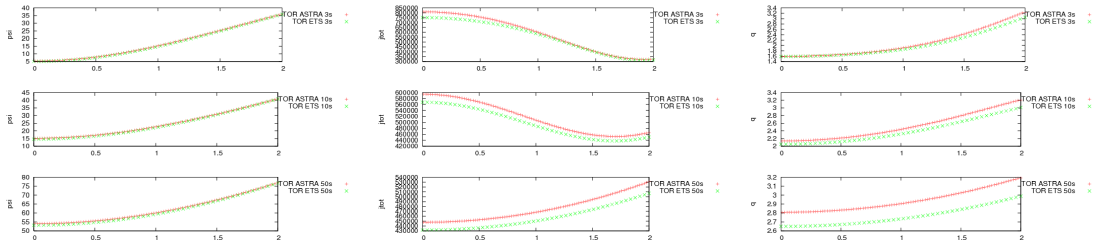

Figure 41: Comparison of ψ, total current and q at 3, 10 and 50s.

5 Equilibrium code comparisons

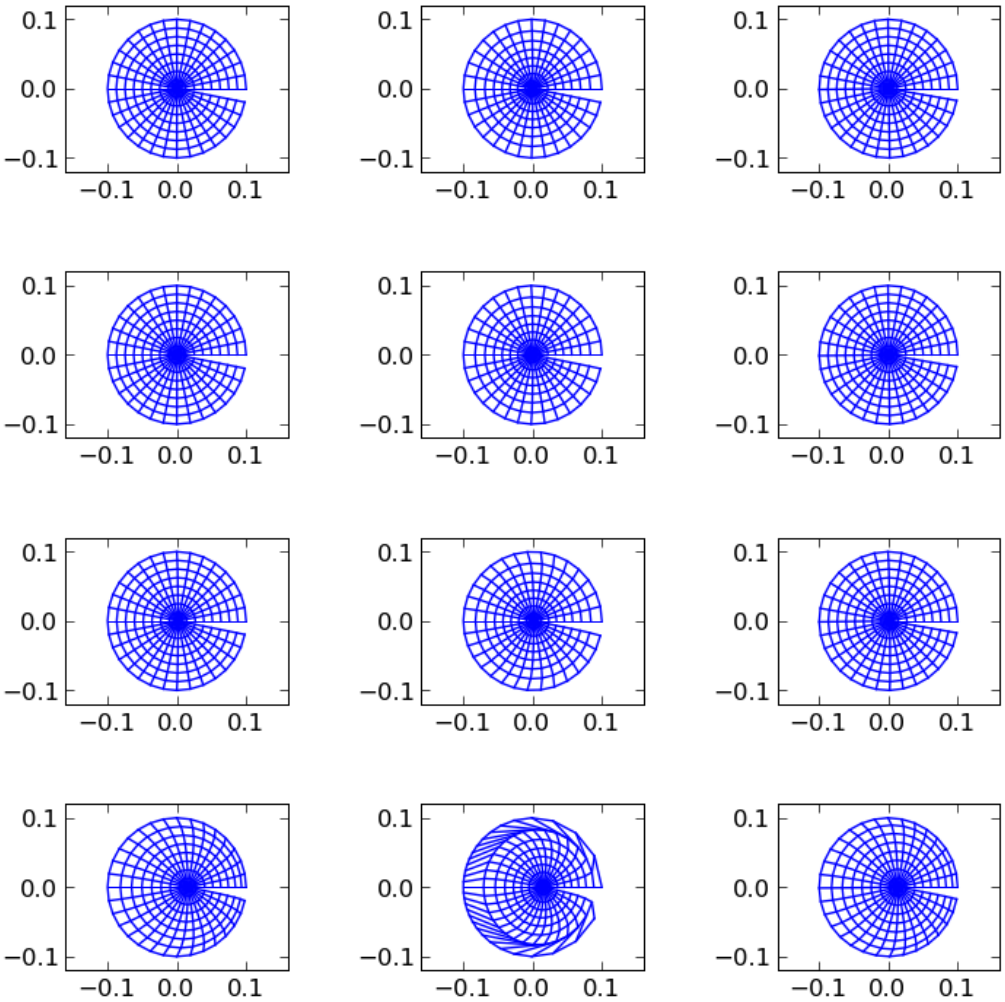

Figure 42: From left to right, BDSEQ, HELENA, EMEQ. From top to bottom, central pressures of 5, 50, 500 and 5000.

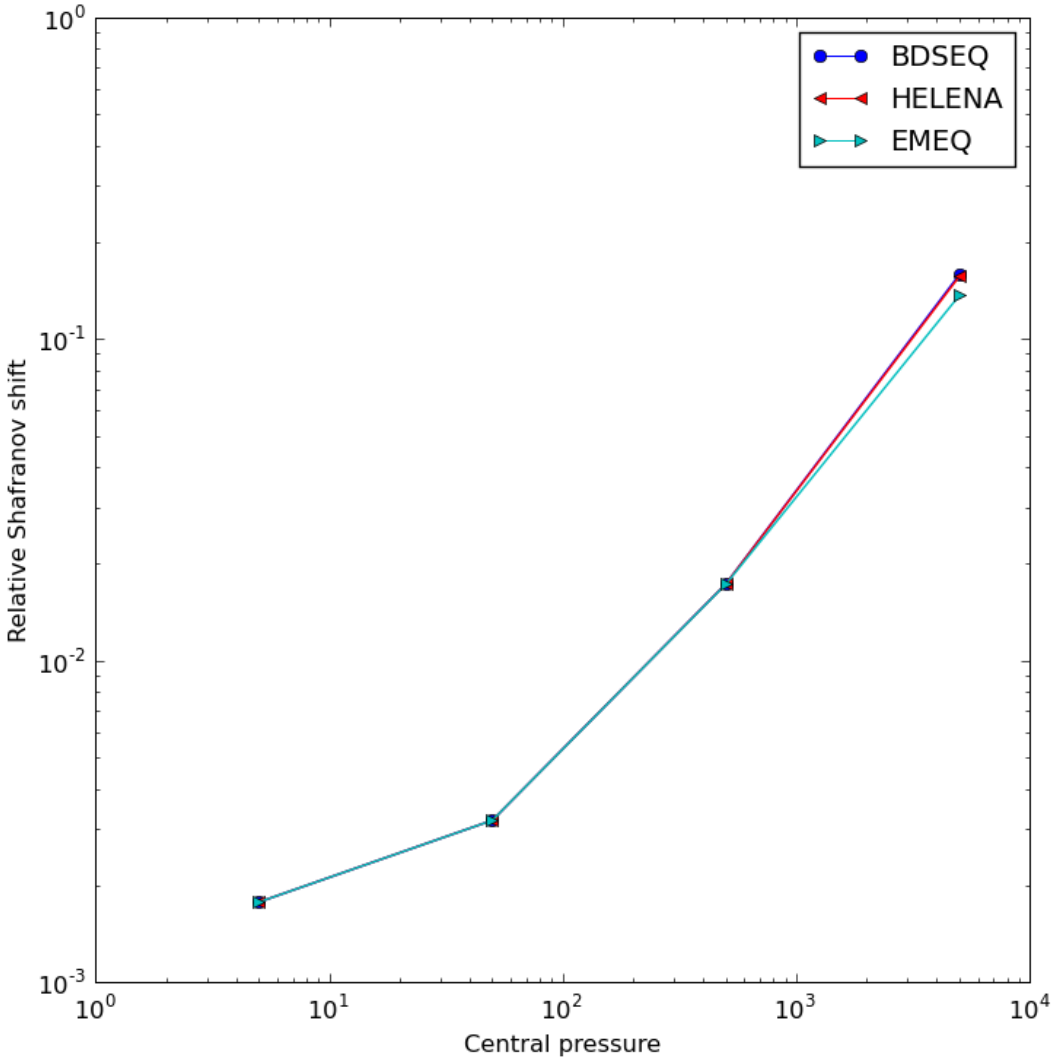

Figure 43: Relative Shafranov shifts.

6 Convergence studies with HELENA

6.1 Standalone HELENA

These studies were done with the end state of a calculation of the ETS coupled to HELENA. The number of radial point (NR) and poloidal points (NP) in helena were varied and the results compared.

The results for key quantities are shown in figures 44, 45, 46, 47 and 48.

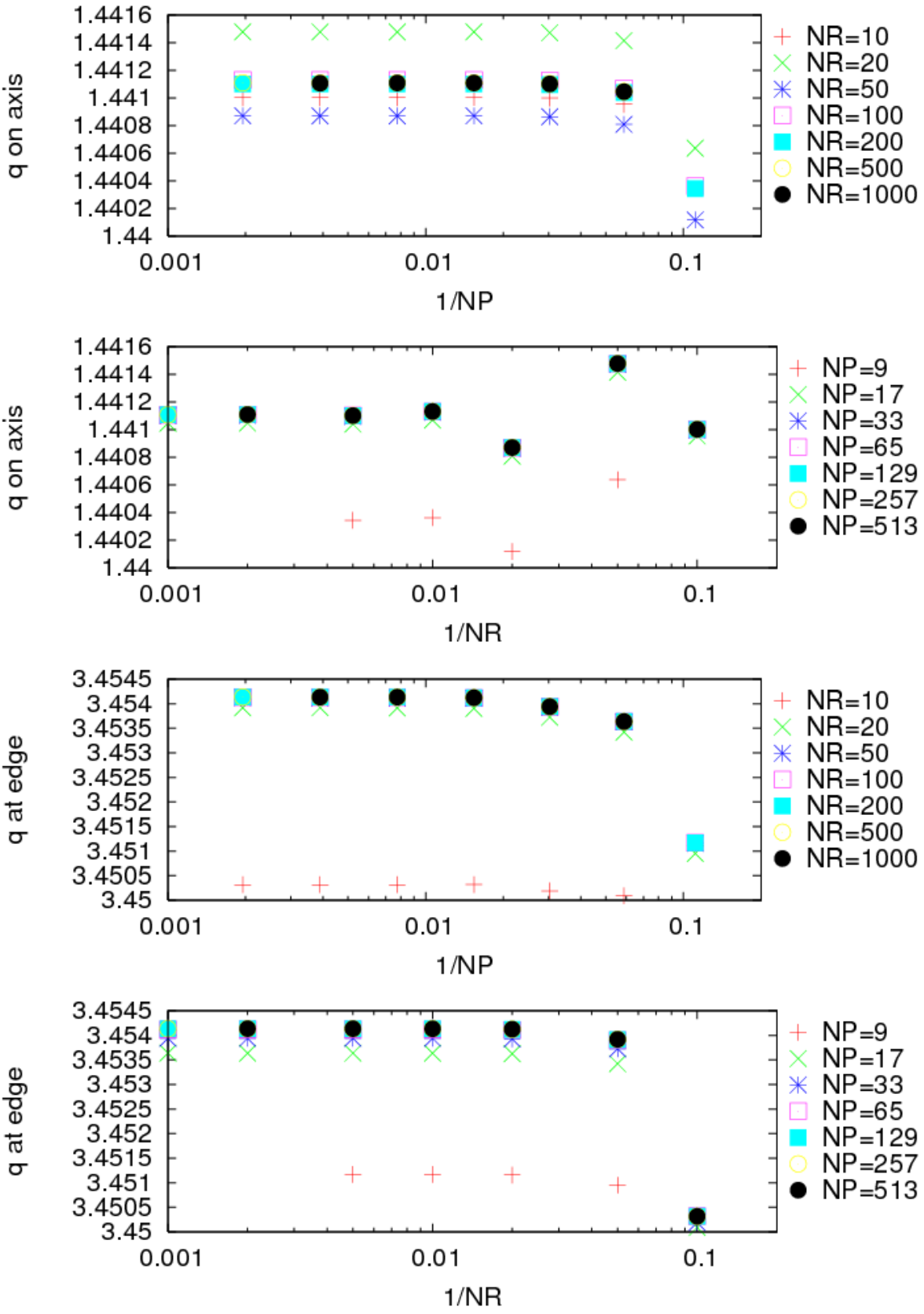

Figure 44: Convergence of q.

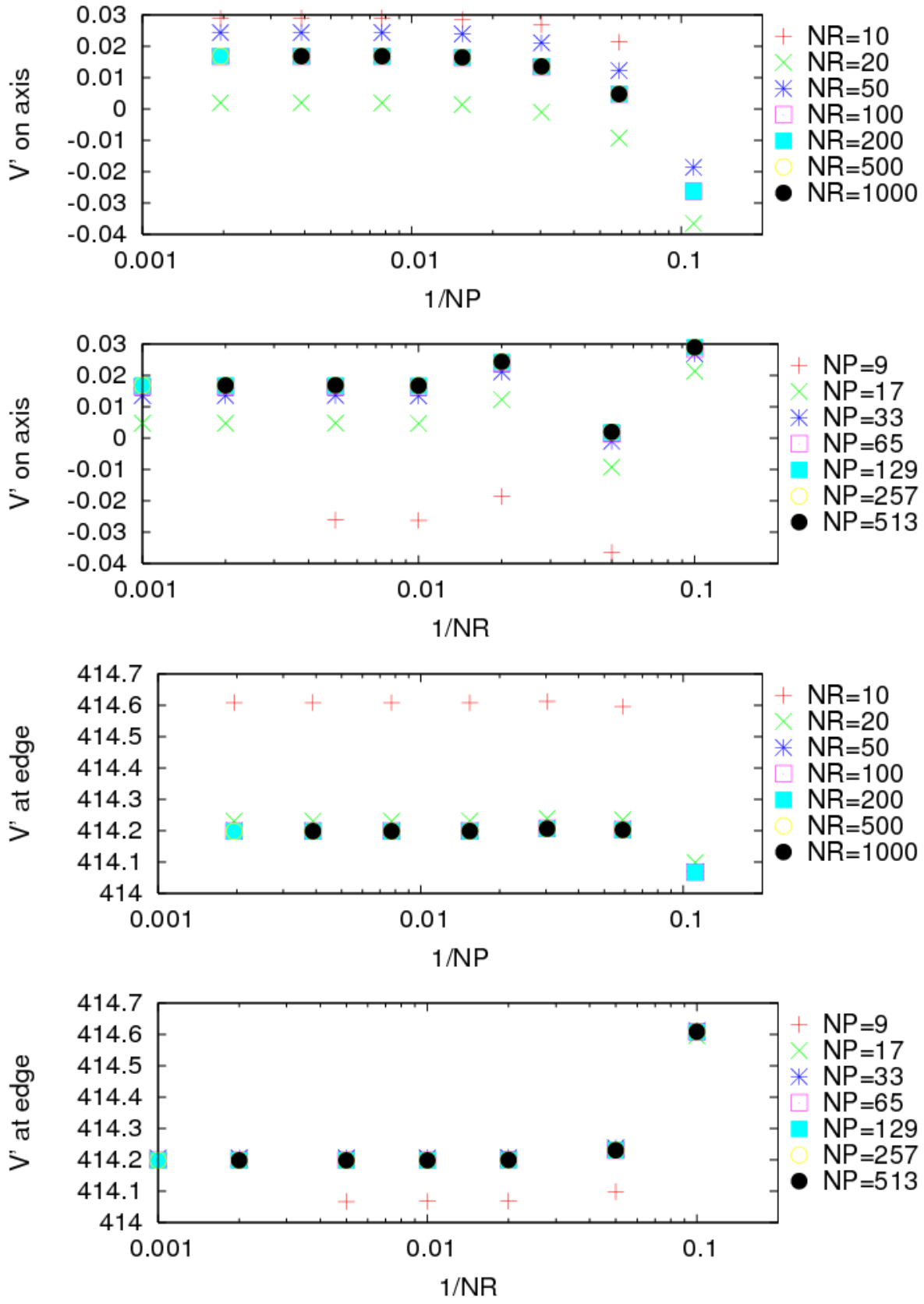

Figure 45: Convergence of V'

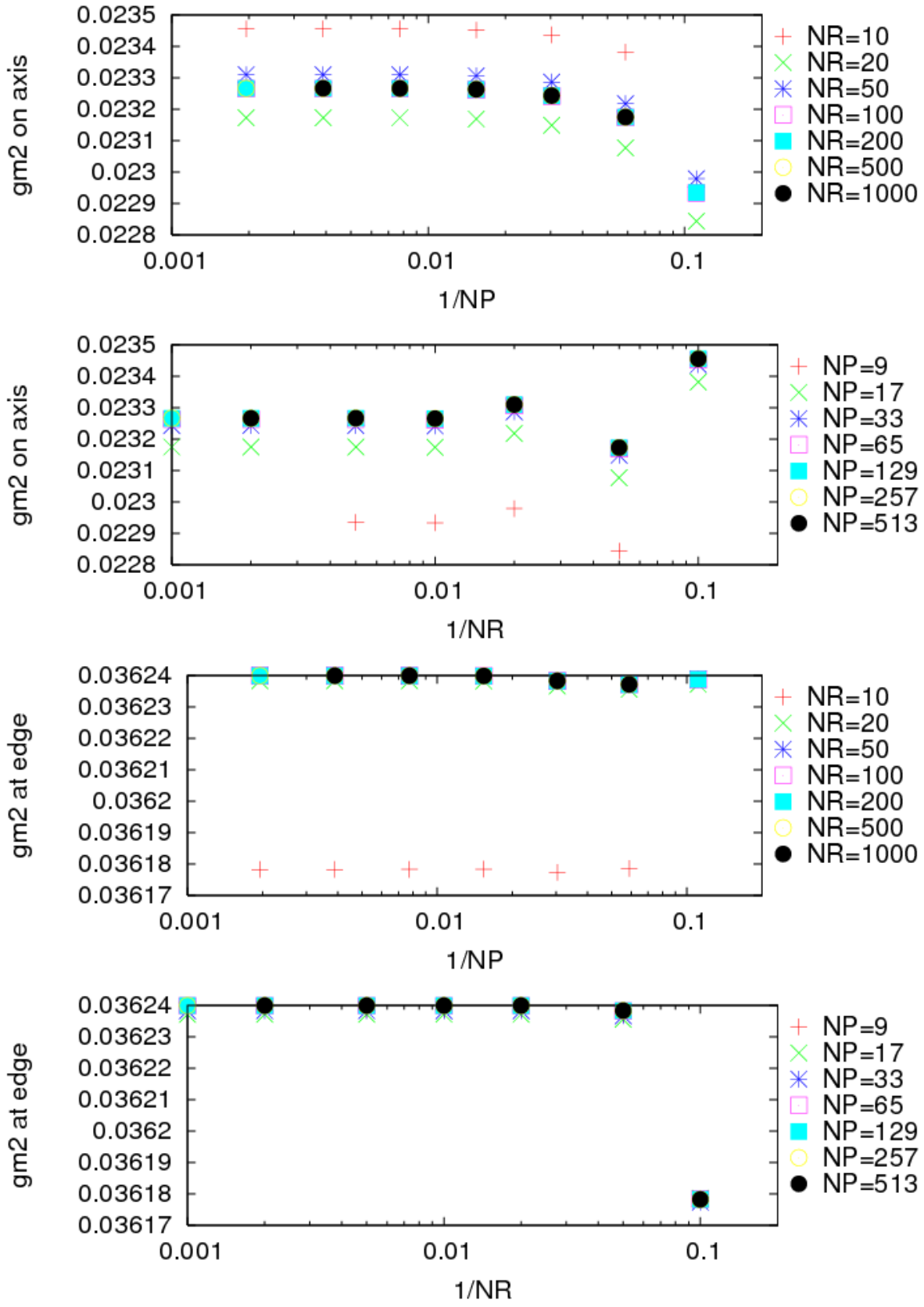

Figure 46: Convergence of gm2

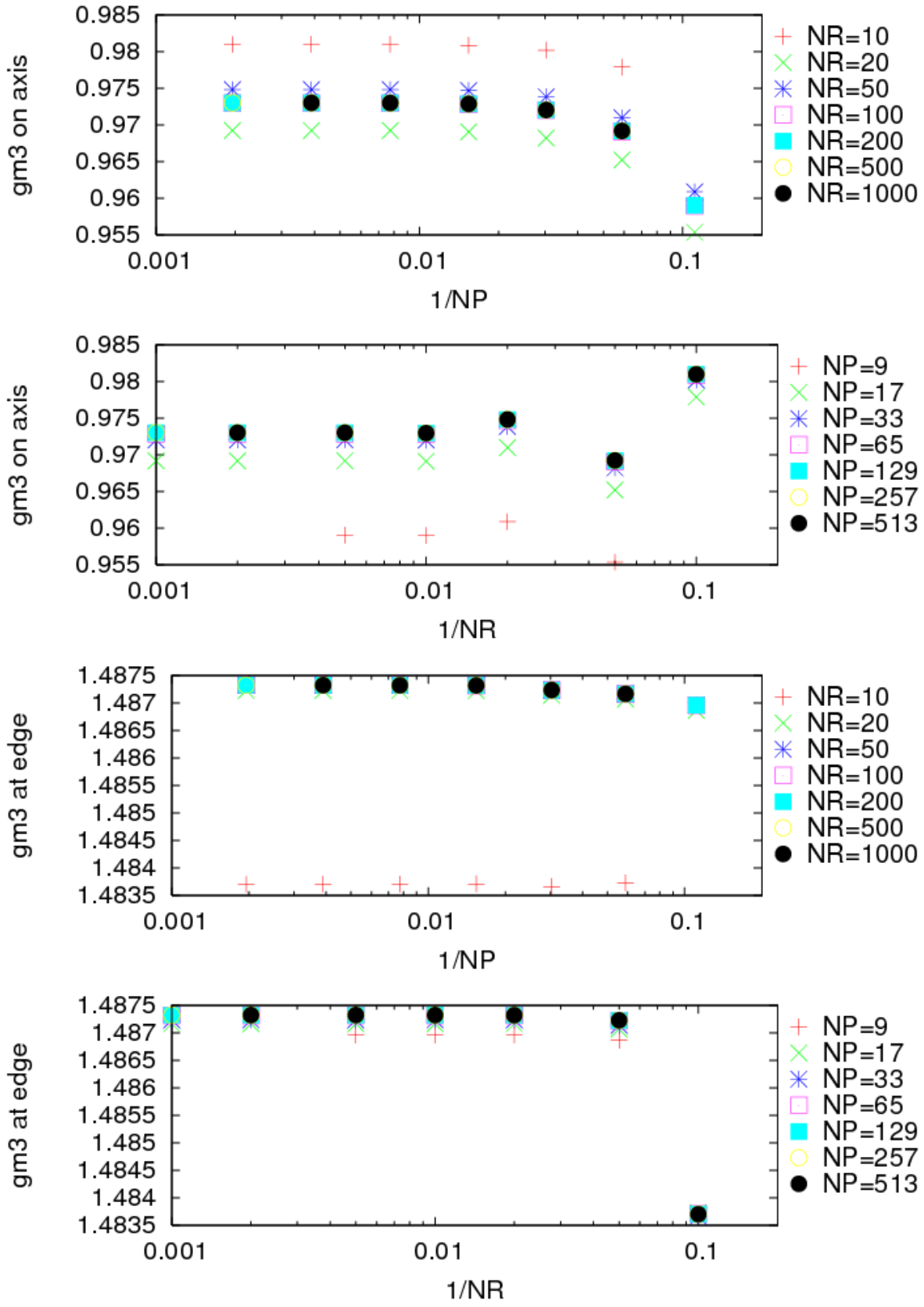

Figure 47: Convergence of gm3

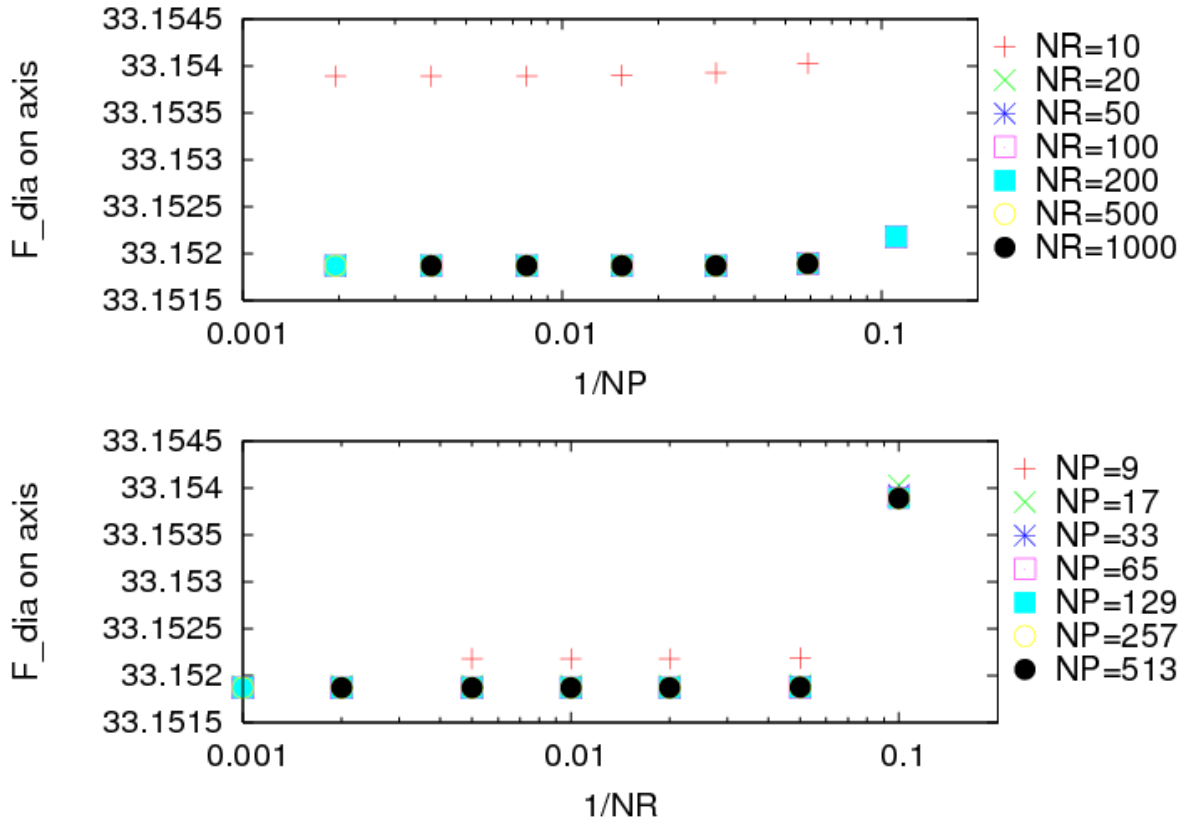

Figure 48: convergence of F_{dia}

6.2 Coupled ETS/HELENA runs

These comparisons involved running the ETS with HELENA with varying NR and NP to 10s. The results are shown in figures 49, 50, 51, 52, 53, 54, 55 and 56.

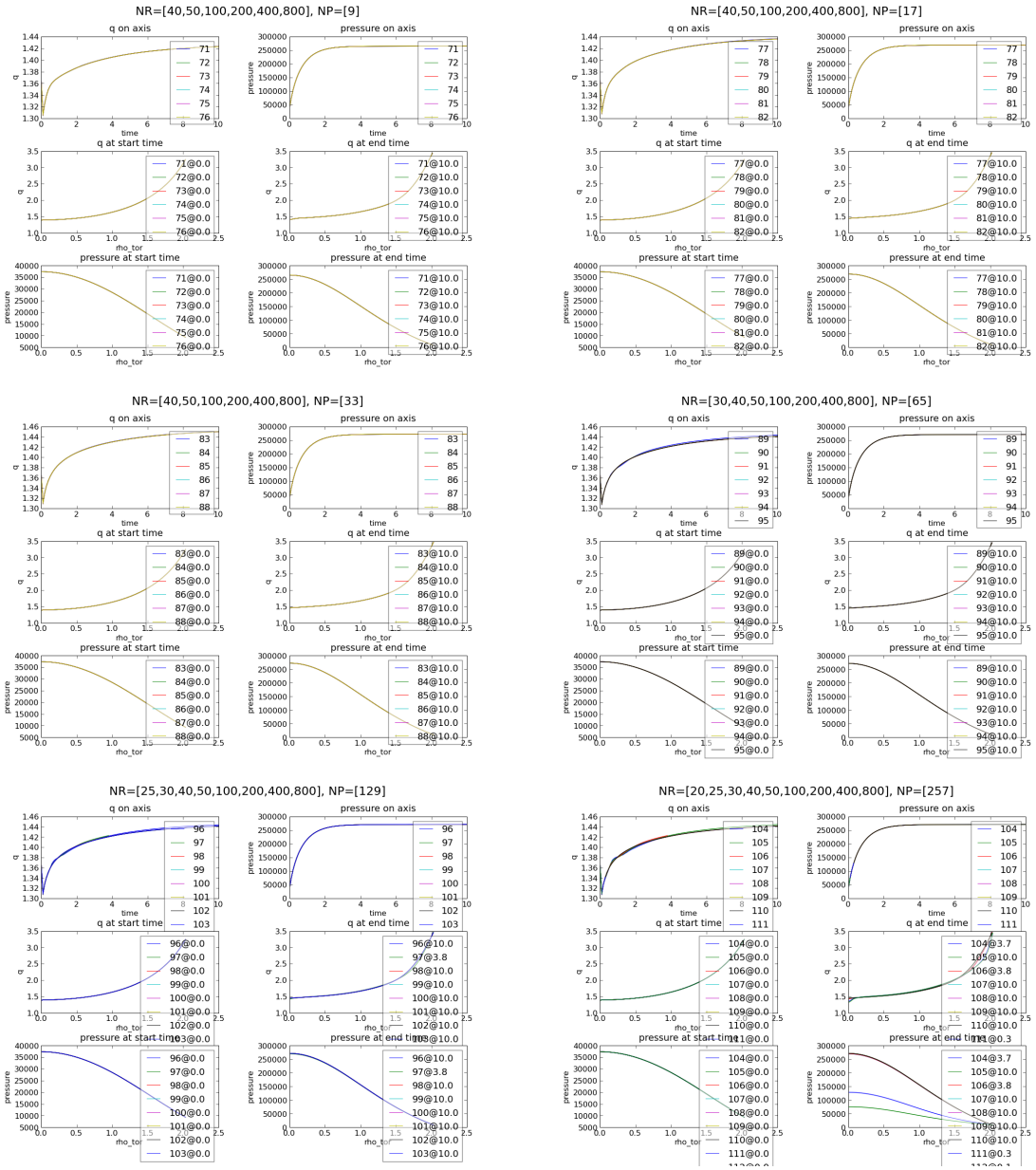

Figure 49: Convergence of equilibrium quantities for fixed NPs

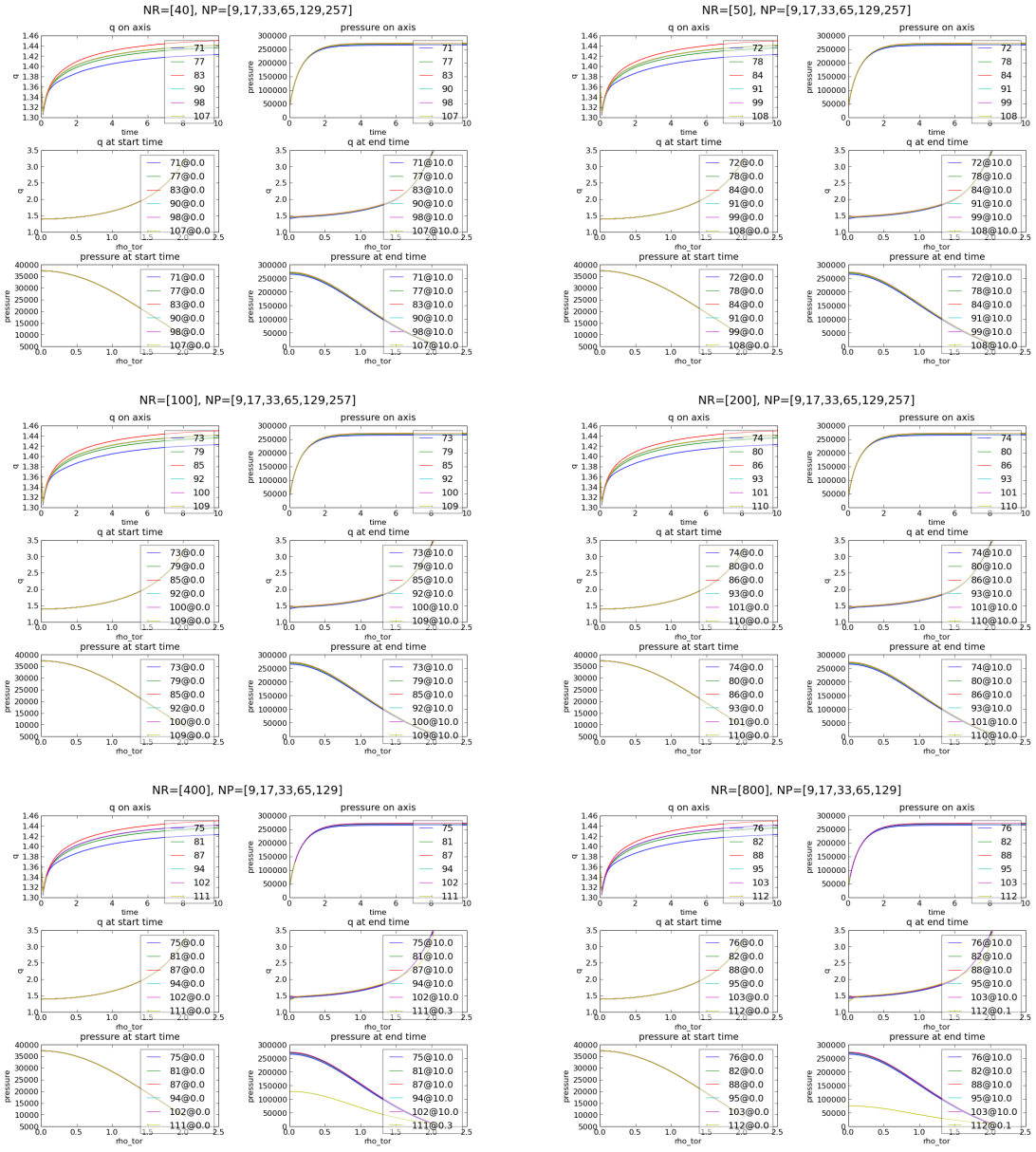

Figure 50: Convergence of equilibrium quantities for fixed NRs

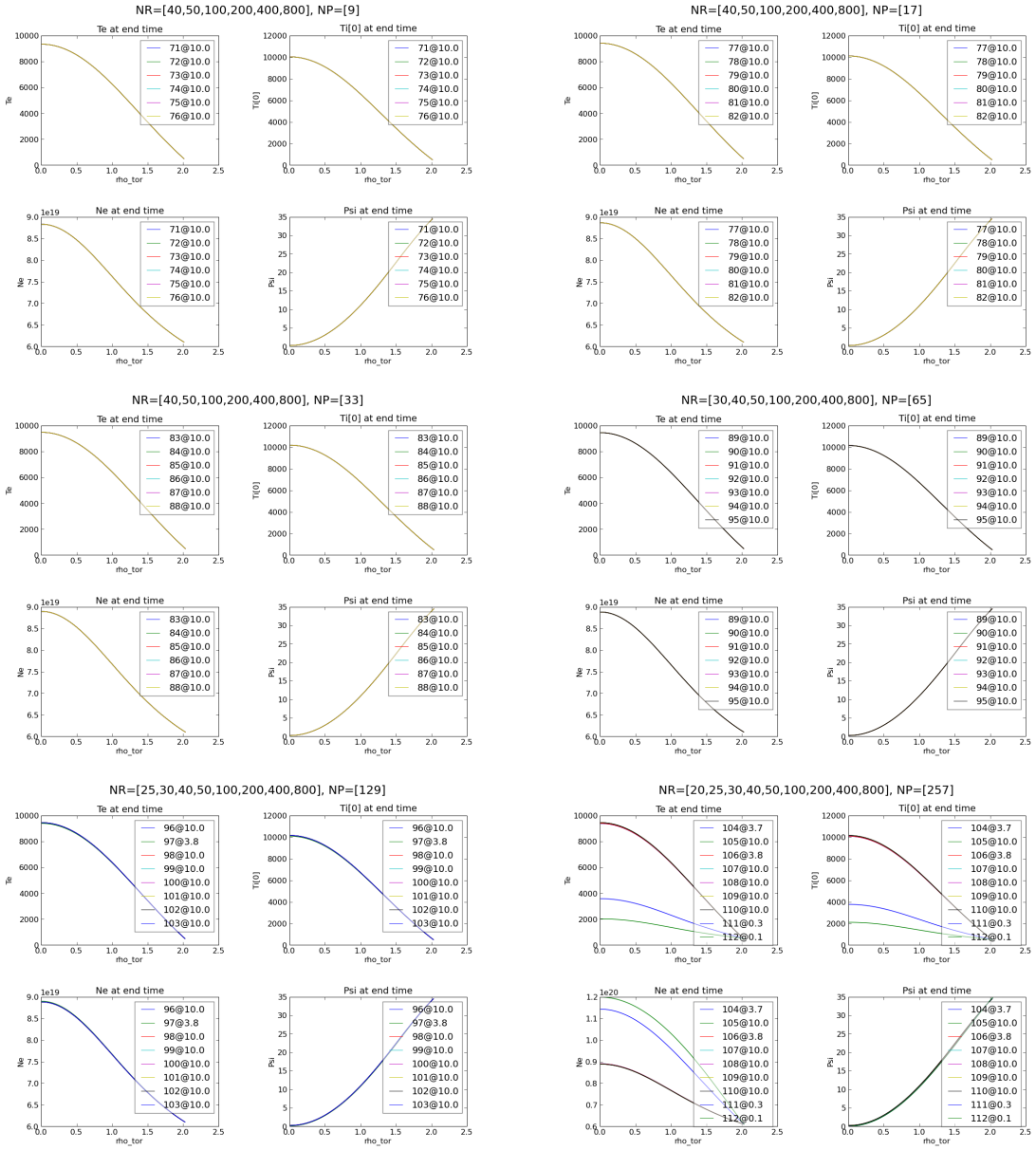

Figure 51: Convergence of coreprof quantities for fixed NPs

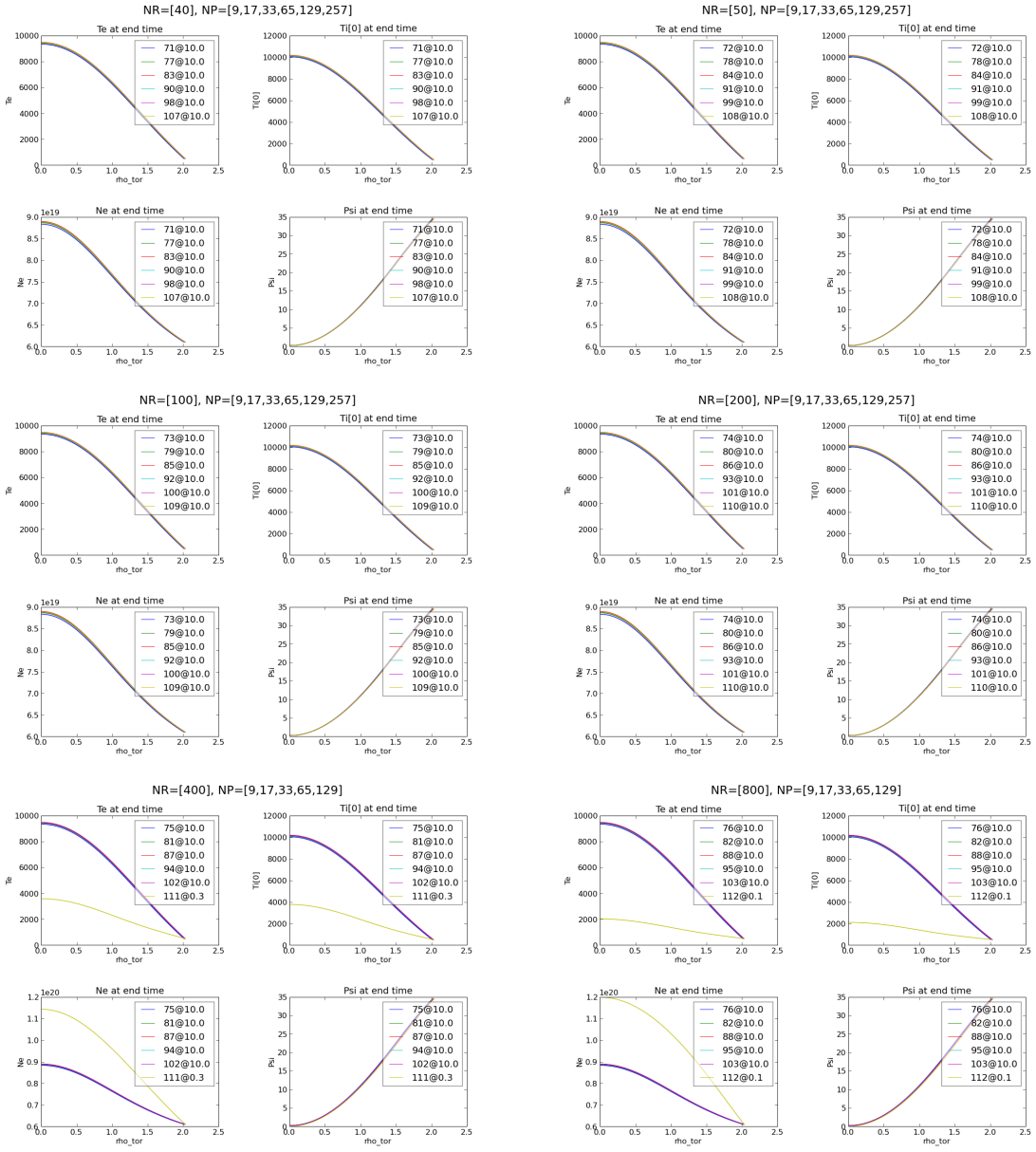

Figure 52: Convergence of coreprof quantities for fixed NRs

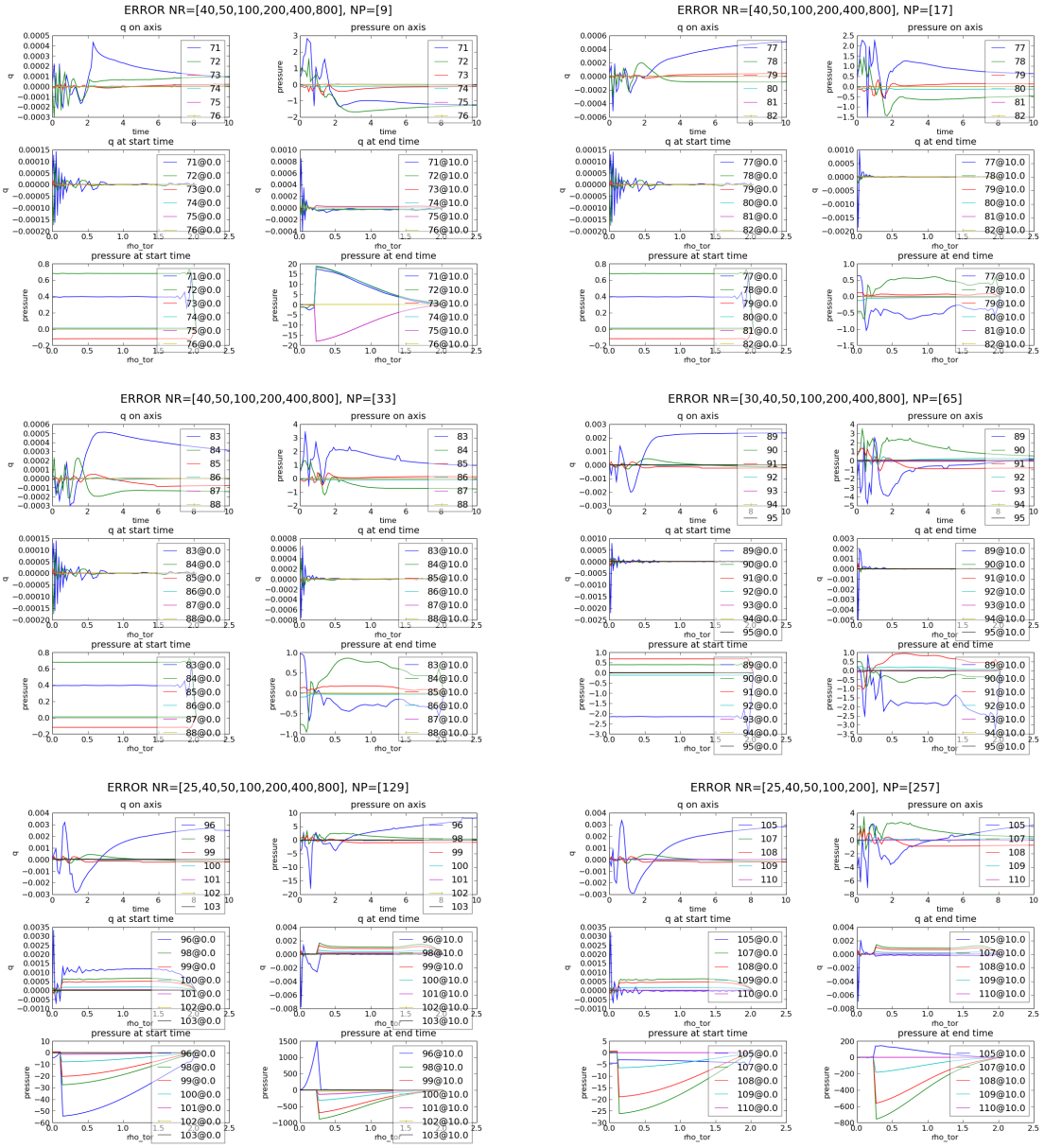

Figure 53: Convergence of equilibrium quantities for fixed NPs

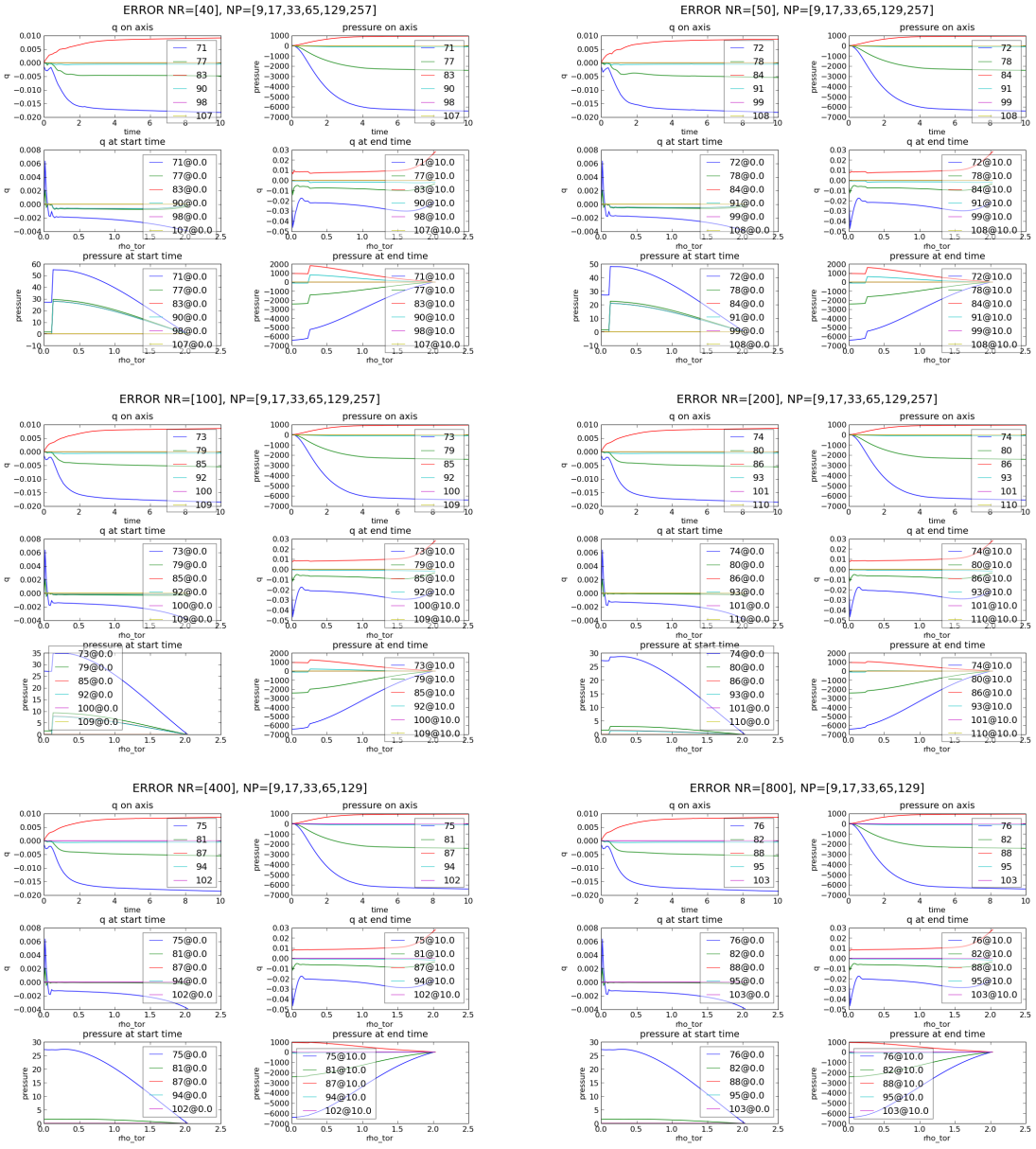

Figure 54: Convergence of equilibrium quantities for fixed NRs

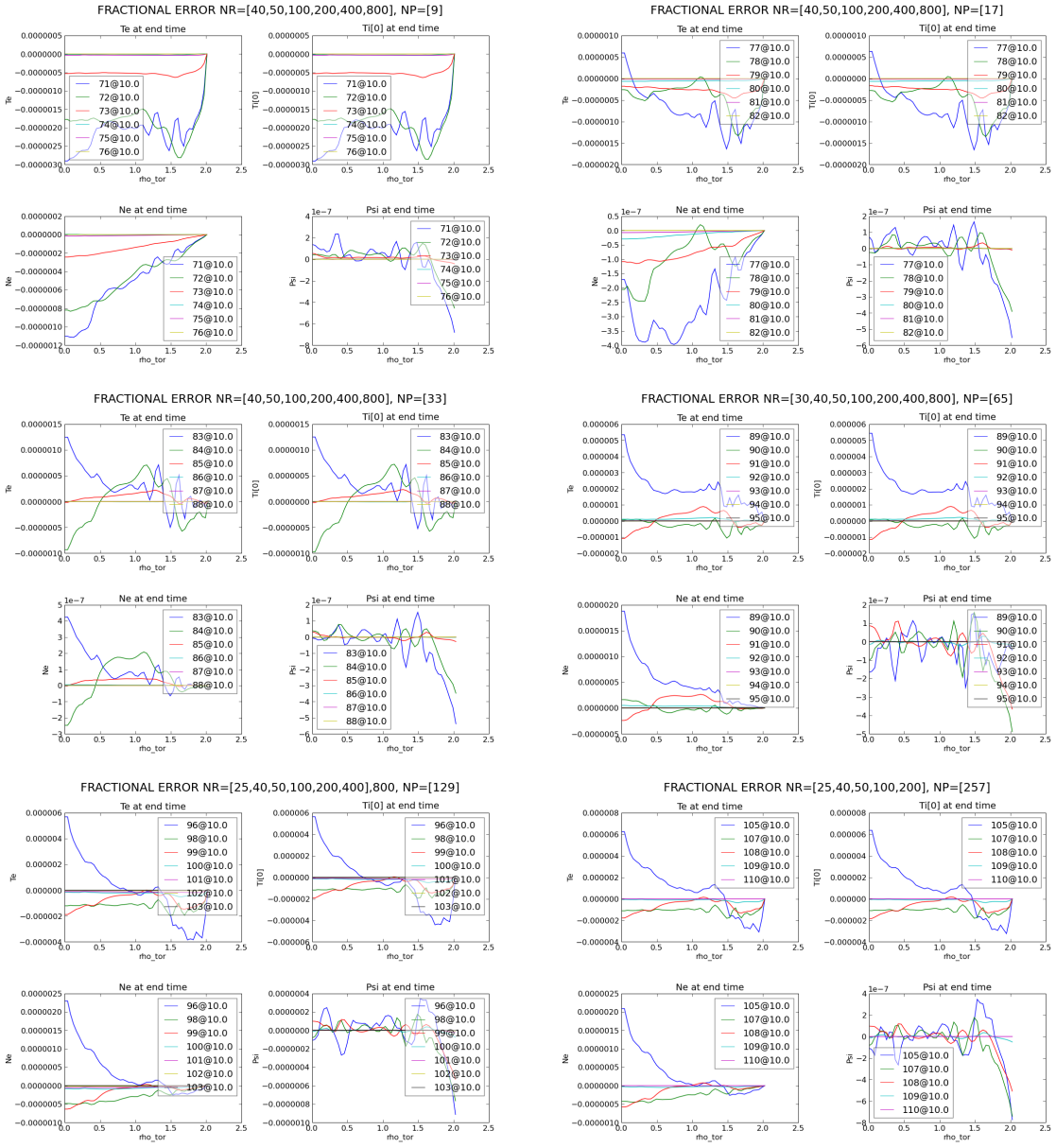

Figure 55: Convergence of coreprof quantities for fixed NPs

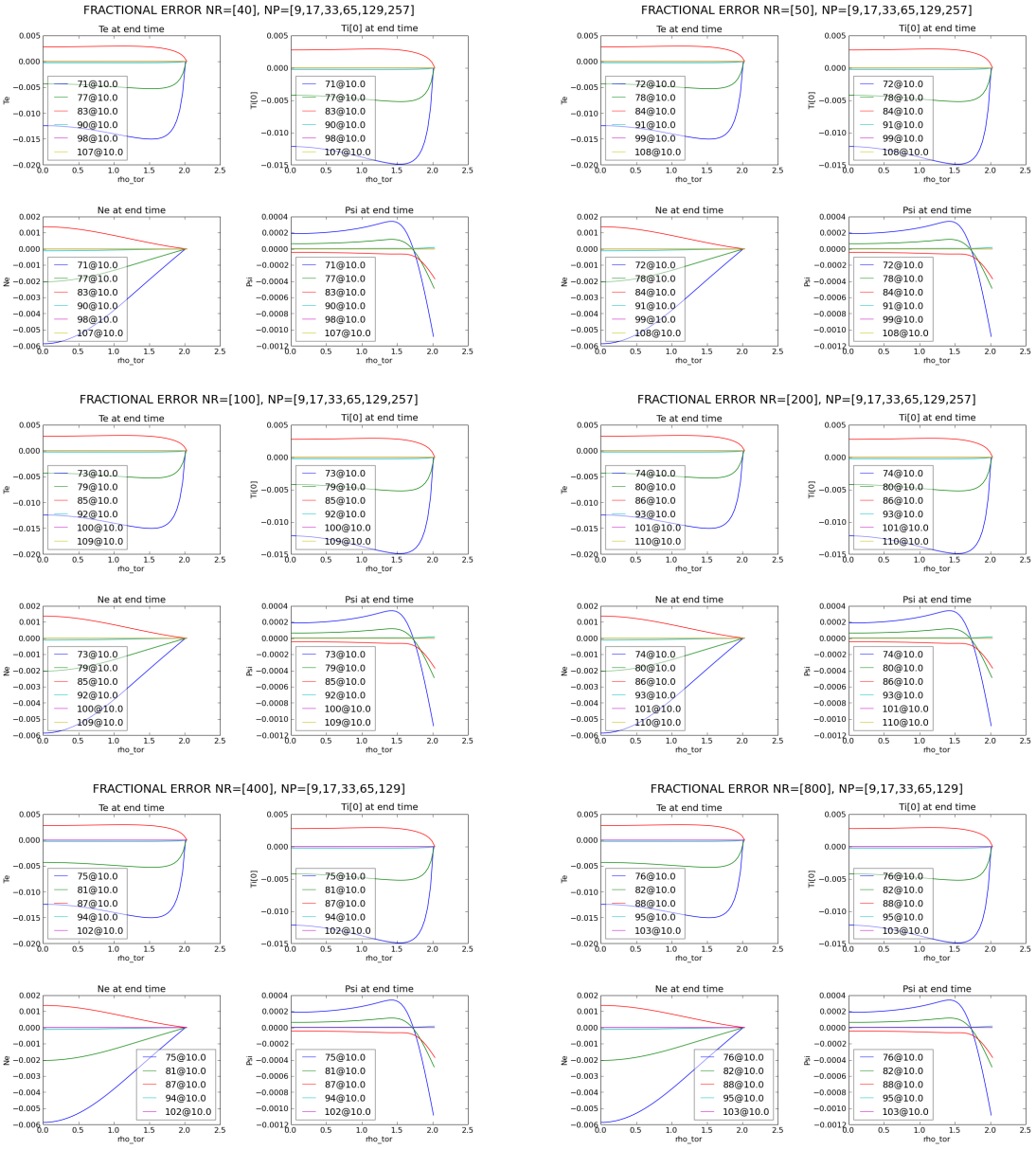

Figure 56: Convergence of coreprof quantities for fixed NRs

7 Comparison of cases with BDSEQ, EMEQ and HELENA

Results are shown in figures 57, 58, 59, 60 and 61.

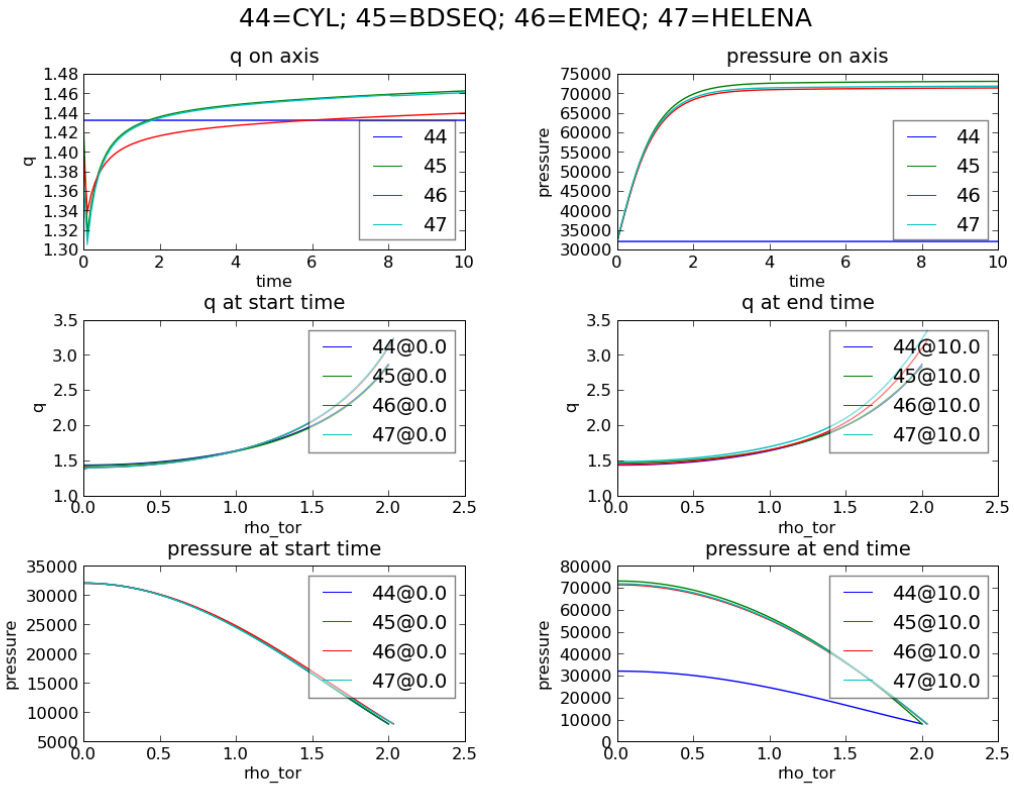

Figure 57: Cylindrical and toroidal cases.

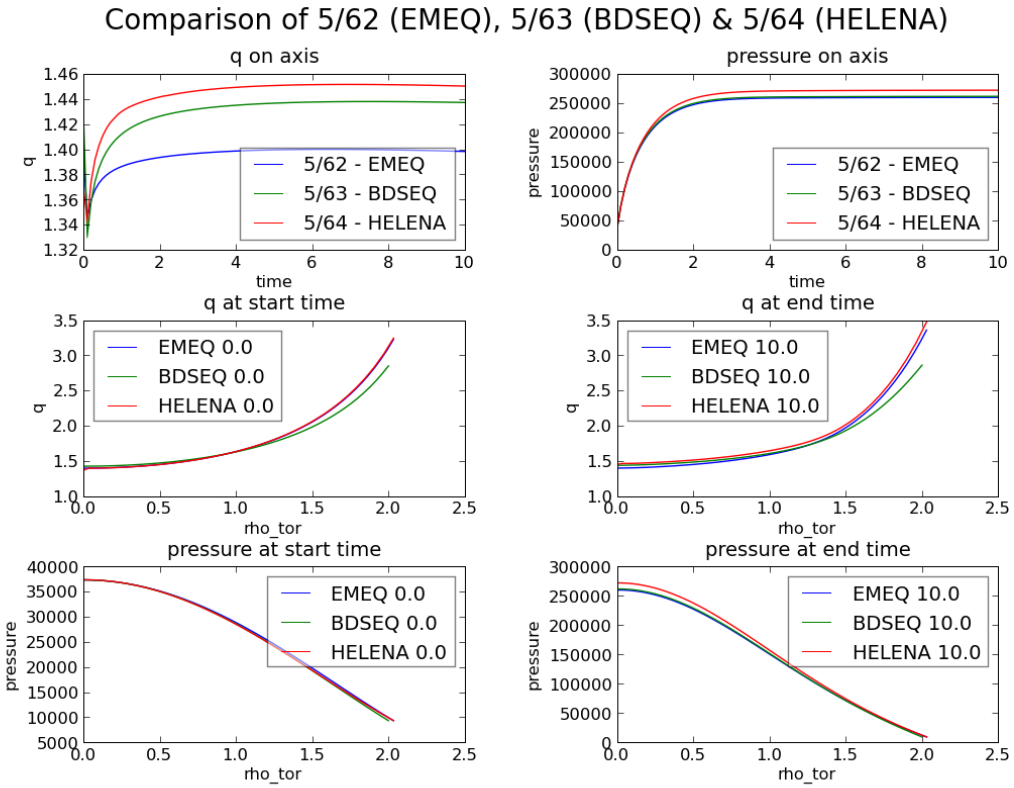

Figure 58: Comparisons of ETS cases with EMEQ, BDSEQ and HELENA (without equilibrium augmentation).

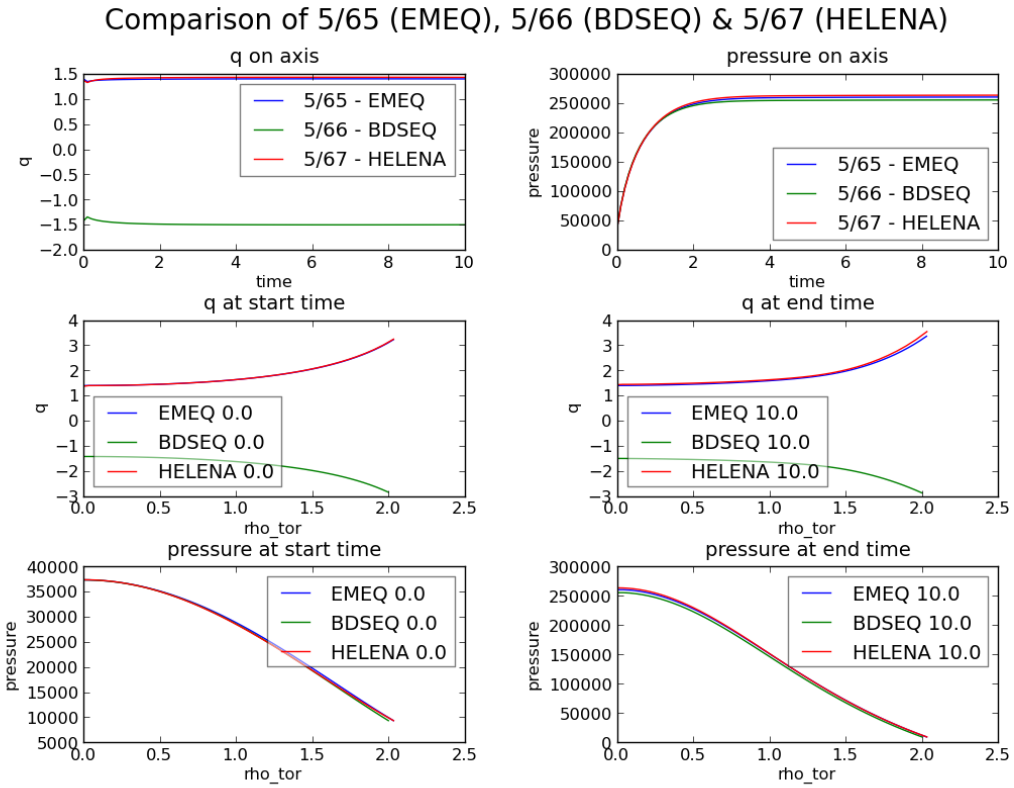

Figure 59: Comparisons of ETS cases with EMEQ, BDSEQ and HELENA (with equilibrium augmentation).

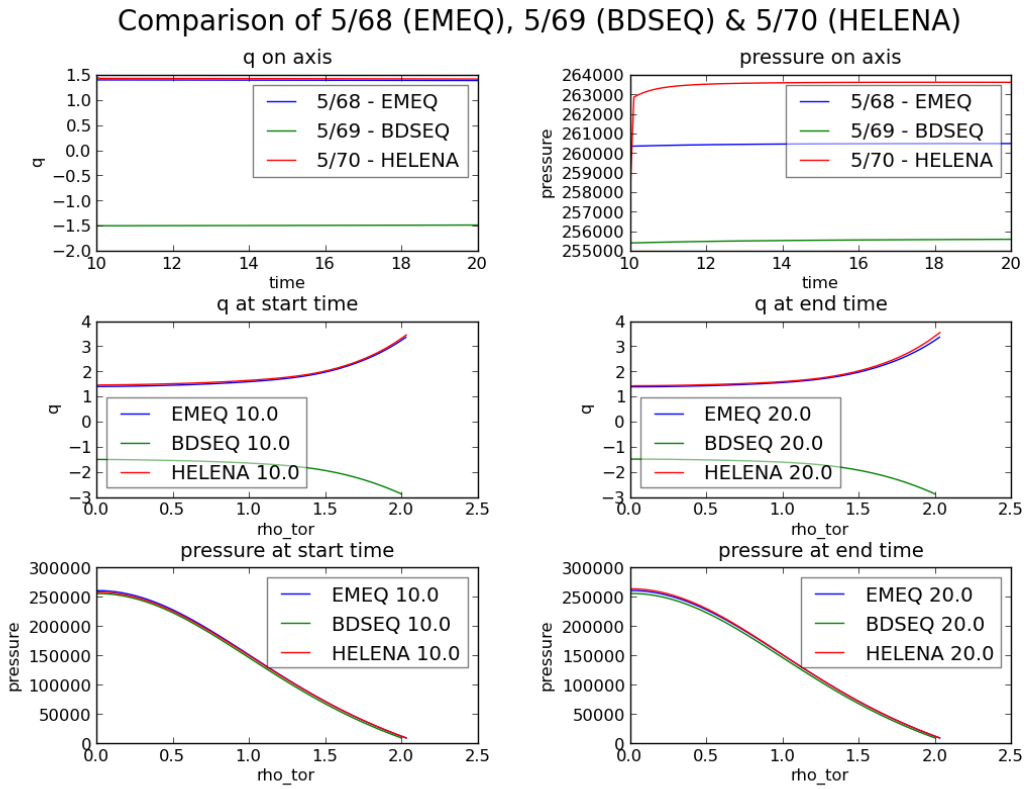

Figure 60: Comparisons of ETS cases with EMEQ, BDSEQ and HELENA. Continued from 65–67.

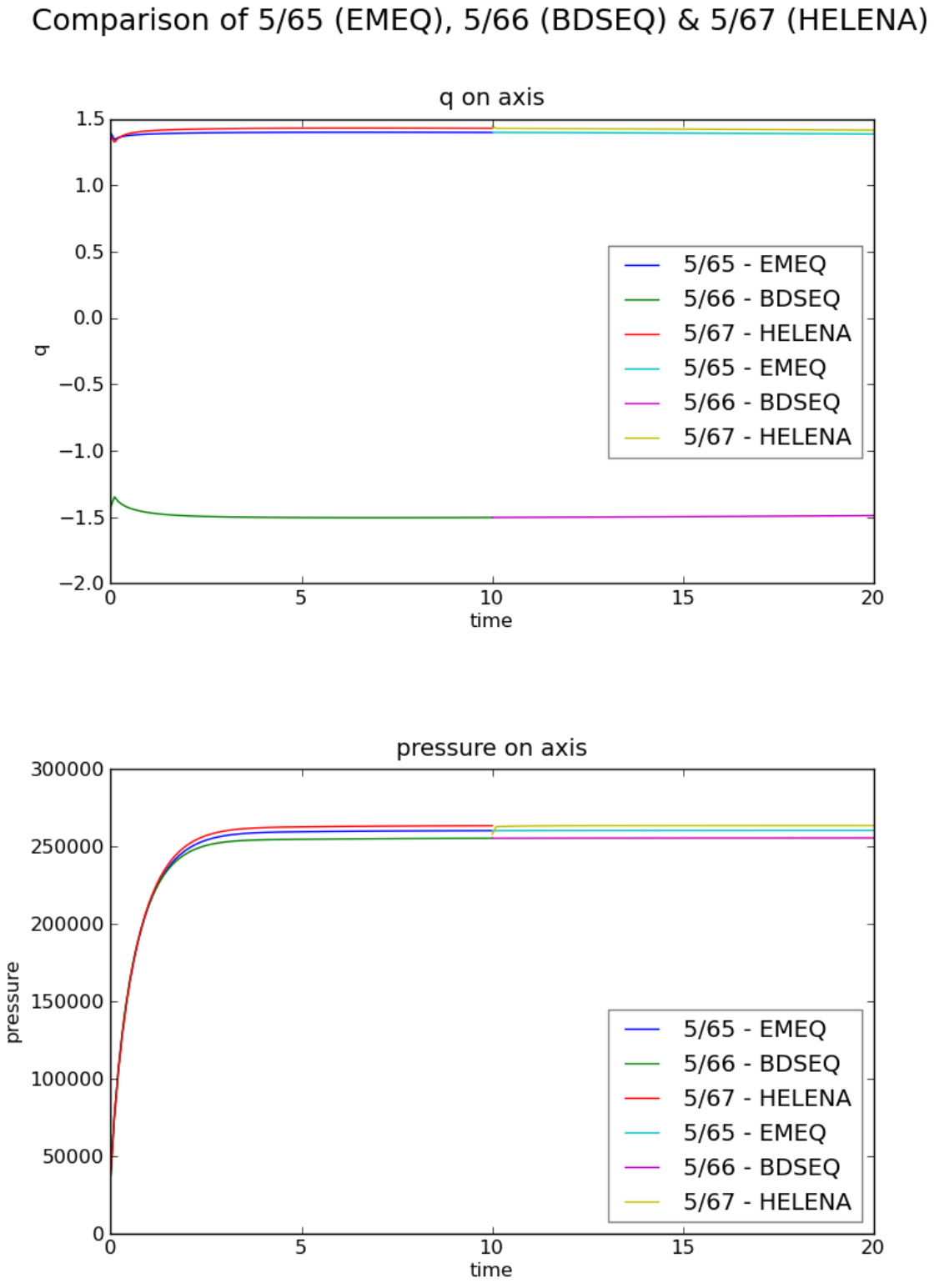

Figure 61: Comparisons of ETS cases with EMEQ, BDSEQ and HELENA. Showing the combined runs.

8 Comparison of ITM neoclassical modules

The results of comparing "NEOWES" from IMP4 and "NEO" (an implementation of NCLASS done as part of thye COS branch of the ETS) are presented.

8.1 Circular plasma; D only

The results for `test/5/64` at 10s with D are shown in figure 62. In the cases shown, the neoclassical coefficients presented were not used in the calculations.

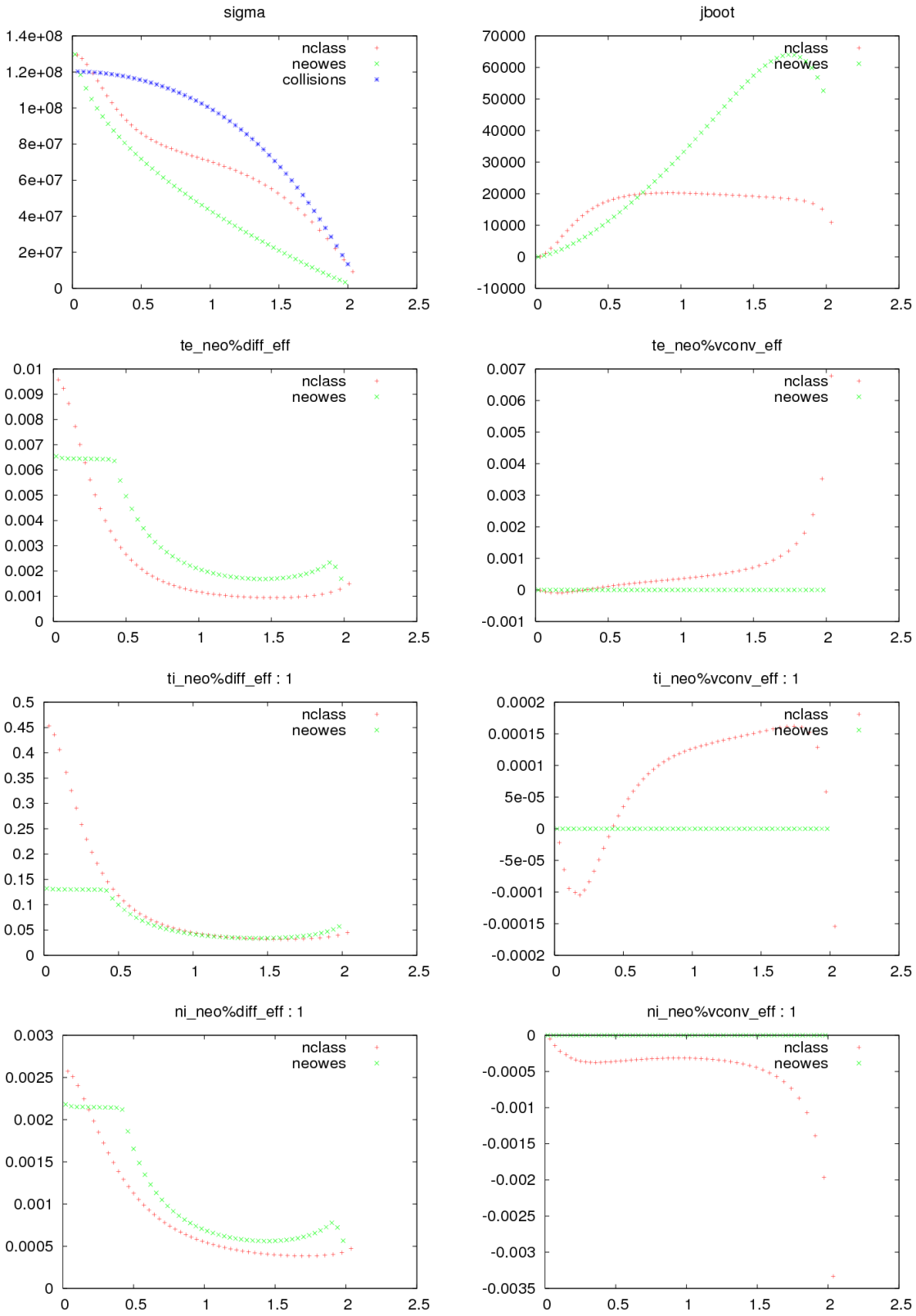

Figure 62: Neoclassical comparison between "NEO" (= NCLASS) and "NEOWES" for a pure D case.

8.2 Circular plasma; D, T and two isotopes of He

The results for `test/5/64` at 10s with D, T, ^3He and ^4He are shown in figure 63.

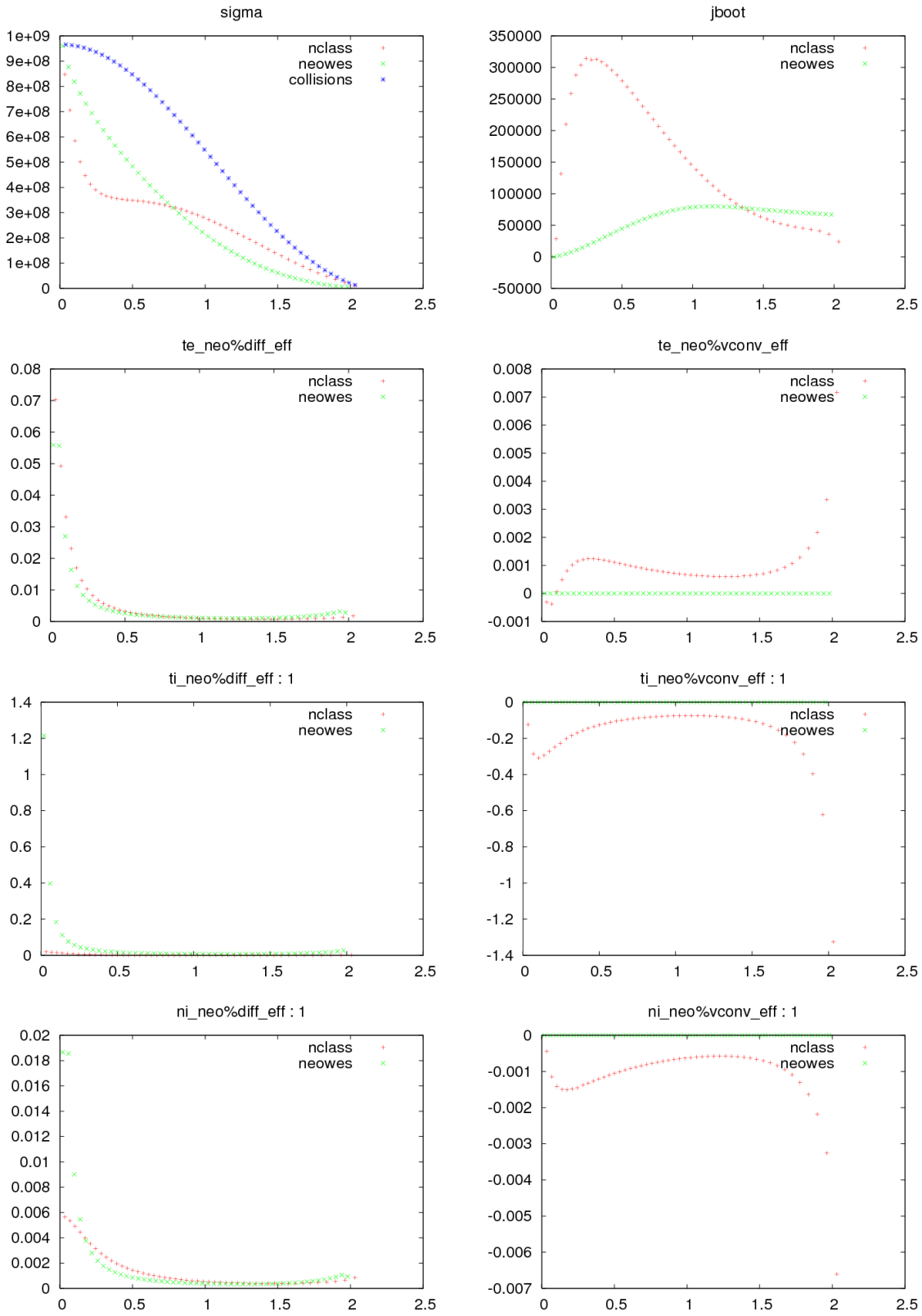

Figure 63: Neoclassical comparison between "NEO" (= NCLASS) and "NEOWES" for a multi-species case.

9 Impurities

9.1 Cases 5/113 – 5/116: 2 impurities

These cases are run with 2 impurity species for a cylindrical case, and then with BDSEQ, EMEQ and HELENA. The resultant charge state density profiles are shown in figure 64. These cases use atomic physics data from Roman Zagorski.

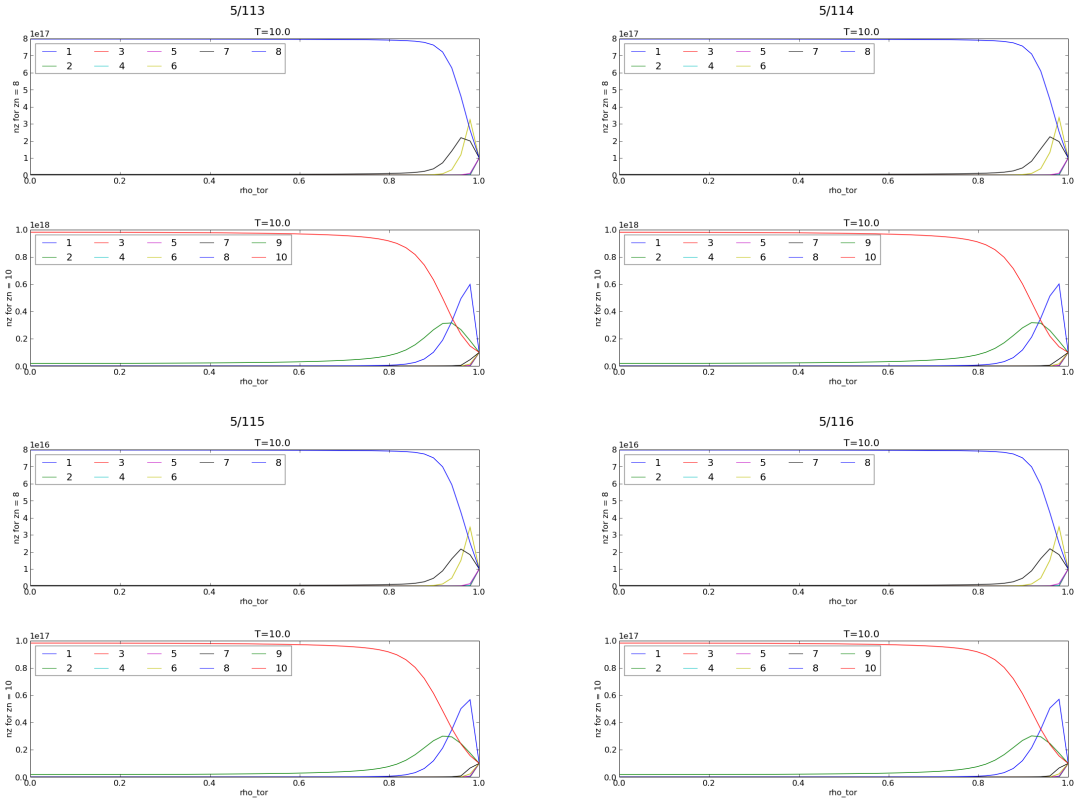

Figure 64: Runs with 2 species of impurities with a cylindrical equilibrium, BDSEQ, EMEQ and HELENA.

9.2 W

Profiles of the charge states of W are shown in figure 65. This case uses atomic physics data from Roman Zagorski.

9.3 Atomic physics

Figure 66 shows a comparison beween the ETS using atomic physics data from Roman Zagorksi and the ITM AMNSPROTO package.

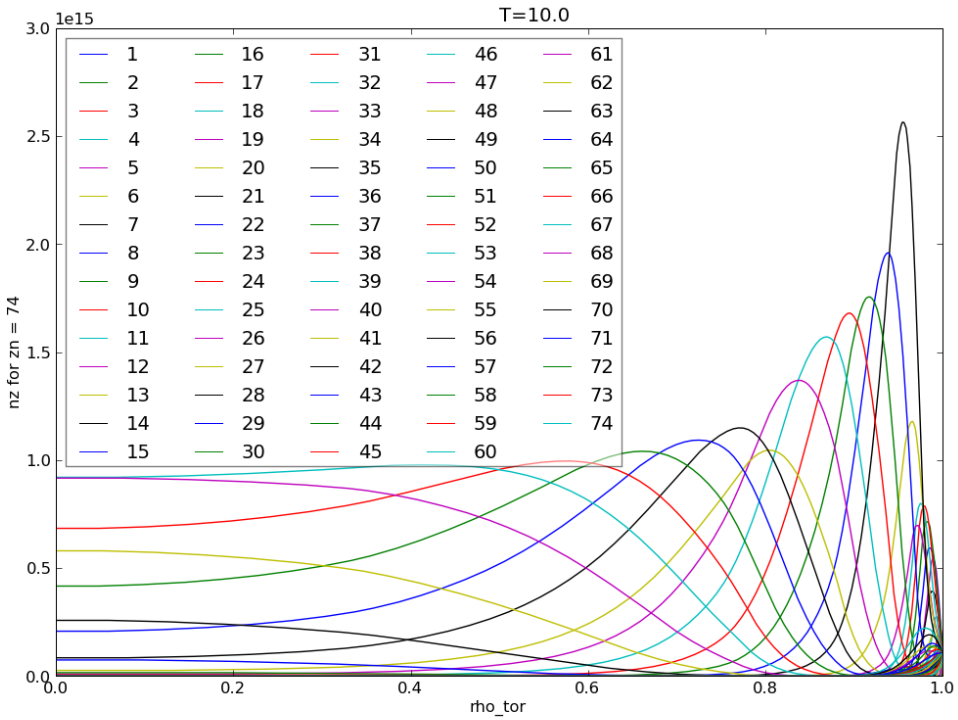

Figure 65: Runs with W.

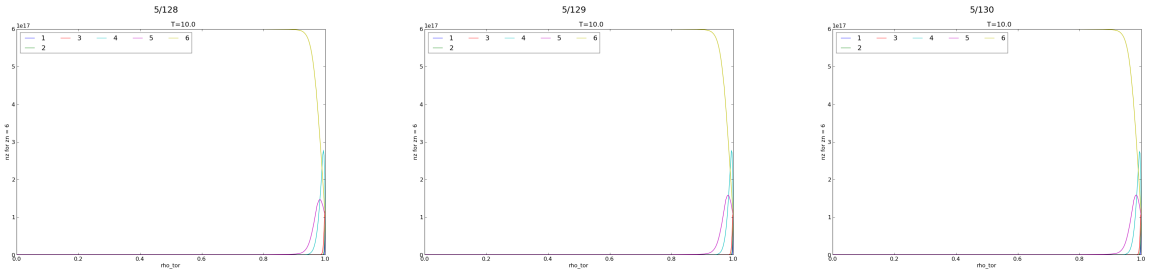

Figure 66: Runs with C: on the left a case with atomic physics from Zagorski, in the middle using the AMNSPROTO version of the ITM AMNS concept, and on the right using the UAL version of AMNSPROTO.

9.3.1 Use of the ITM AMNS routines

This is still using a development version!

To initialize the rates:

```
write(*,*) 'ITM AMNSPROTO data used (via UAL)'
allocate(amns_ei(0:max_nzimp, nimp), amns_rc(0:max_nzimp, nimp), species(0:max_nzimp, nimp))
call ITM_AMNS_SETUP(amns)
call ITM_AMNS_QUERY(amns,query,answer)
write(*,*) 'AMNS data base version = ',trim(answer%string)
ei_rx%string='EI'
```

```
rc_rx%string='RC'
do iimp=1, nimp
! the following should be done behind the user's back!
  shot= COREIMPUR_OLD(1)%DESC_IMPUR%zn(IIMP)
  run = 1
  treename = 'euitm'
  call getenv('USER', USER)
  call euitm_open_env(treename,shot,run,idx,trim(USER),'amns','4.08a')
  call euitm_get(idx,'amns',amns_cpo)
  call euitm_close(idx)
!
   do izimp=0, COREIMPUR_OLD(1)%DESC_IMPUR%zn(IIMP)
      allocate(species(izimp,iimp)%components(1))
      species(izimp,iimp)%components(1)%ZN=COREIMPUR_OLD(1)%DESC_IMPUR%zn(IIMP)
      species(izimp,iimp)%components(1)%ZA=izimp
      species(izimp,iimp)%components(1)%MI=COREIMPUR_OLD(1)%DESC_IMPUR%amn(IIMP)
   enddo
   do izimp=0, COREIMPUR_OLD(1)%DESC_IMPUR%zn(IIMP)-1
      call ITM_AMNS_SETUP_TABLE(amns, ei_rx, species(izimp, iimp), &
        amns_ei(izimp, iimp), amns_cpo)
   enddo
   do izimp=1, COREIMPUR_OLD(1)%DESC_IMPUR%zn(IIMP)
      call ITM_AMNS_SETUP_TABLE(amns, rc_rx, species(izimp, iimp), &
        amns_rc(izimp, iimp), amns_cpo)
   enddo
enddo
```

(note that the explicit call to "euitm_open_env" and "euitm_get" will in the future be done behind the user's back!)

Then to use the data

```
do izimp=1, nzimp+1
   if(izimp .ne. nzimp+1) then
      write(*,*) 'EI: ', izimp
      write(*,*) 'amns_ei%filled: ', izimp, shape(amns_ei(izimp)%grid%f2d)
      call ITM_AMNS_RX(amns_ei(izimp),alfa(:,izimp),te,ne)
   endif
   if(izimp .ne. 1) then
      write(*,*) 'RC: ', izimp
      write(*,*) 'amns_rc%filled: ', izimp, shape(amns_rc(izimp)%grid%f2d)
      call ITM_AMNS_RX(amns_rc(izimp),beta(:,izimp),te,ne)
   endif
enddo
```

10 JET Cases

10.1 JET 71827/21

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./ets.xsl" charset="ISO-8859-1"?>

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  <dimensions>
    <nrho>      100      </nrho>
    <nion>        1      </nion>
    <nimp>        0      </nimp>
    <max_nzimp>   0      </max_nzimp>
    <ntheta>    101      </ntheta>
  </dimensions>

  <output>
    <shot>    71827      </shot>
    <run>        11      </run>
  </output>

  <global>
    <time>     52.0      </time>
    <R0>        2.95     </R0>
    <B0>        2.56     </B0>
    <A0>        0.99     </A0>
    <Ip>        2.558e6  </Ip>
    <Rgeo>      2.87     </Rgeo>
  </global>

  <equilibrium>
    <equilibrium_ext>  </equilibrium_ext>
    <el>        1.65     </el>
    <tr_u>      0.2      </tr_u>
    <tr_l>      0.2      </tr_l>
  </equilibrium>

  <coreprof>
    <coreprof_ext> coster/jet/4.08a/71827/11 </coreprof_ext>
    <zn>        1.0      </zn>
    <amn>       2.0      </amn>
    <zion>      1.0      </zion>
    <ni>                 </ni>
    <ti>                 </ti>
    <te>                 </te>
    <vtor>               </vtor>
    <jpar>               </jpar>
```

```
    <qsf>                 </qsf>
  </coreprof>

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    </sigma>
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    </ne_diff>
    <ne_conv>
0.0 0.0 0.0
    </ne_conv>
    <ni_diff>
0.0 1.0 0.0
    </ni_diff>
    <ni_conv>
0.0 0.0 0.0
    </ni_conv>
    <te_diff>
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    </te_diff>
    <te_conv>
0.0
    </te_conv>
    <ti_diff>
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    </ti_diff>
    <ti_conv>
0.0
    </ti_conv>
    <vtor_diff>
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    </vtor_diff>
    <vtor_conv>
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    </vtor_conv>
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    </j>
    <sigma_src>
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    </sigma_src>
    <qe_exp>
```

```
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    </qi_exp>
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    <si_exp>
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    <si_imp>
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    </si_imp>
    <ui_exp>
0.0
    </ui_exp>
    <ui_imp>
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    </ui_imp>
  </coresource>

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    <imp_amn>            </imp_amn>
    <nz>
    </nz>
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    </diff>
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    </conv>
  </coreimpur>

</parameters>
```

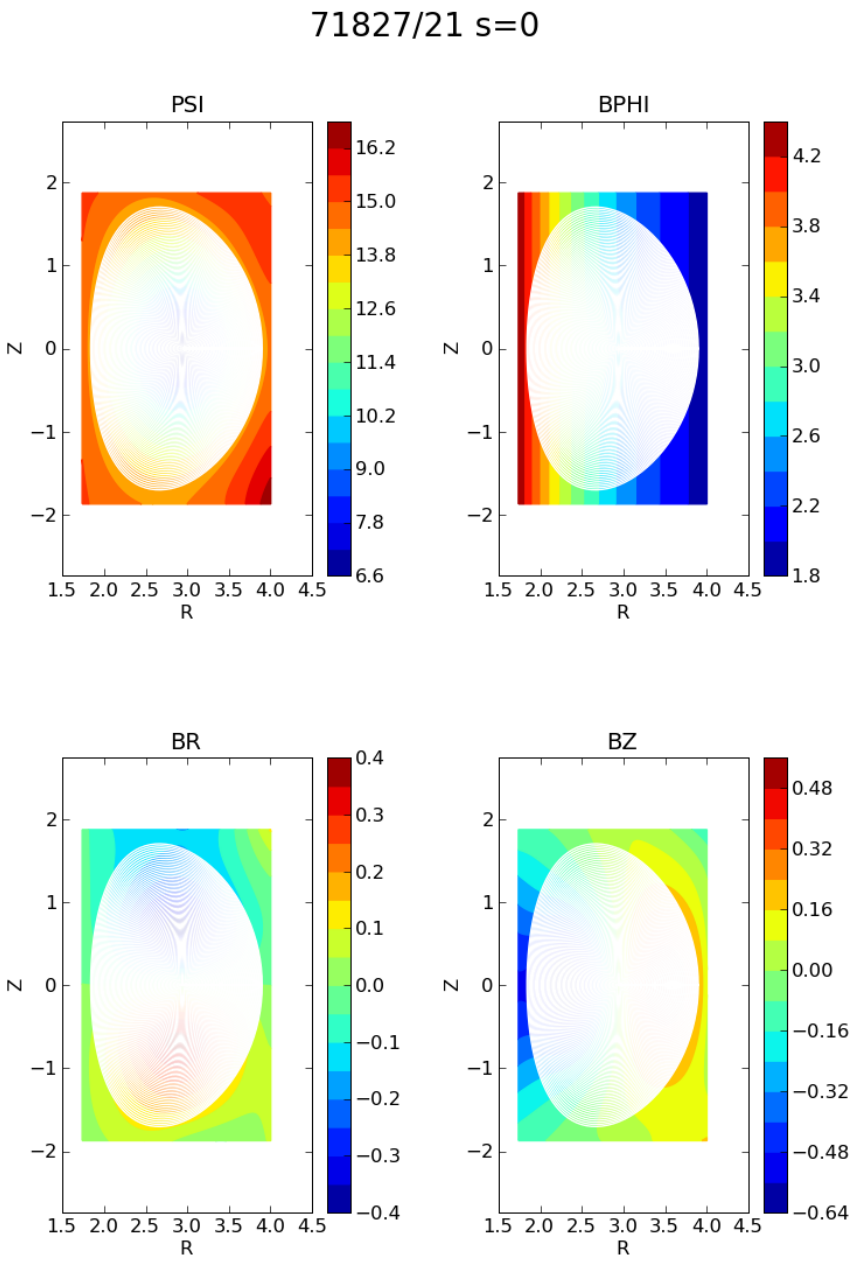

Figure 67: Plot reconstruction of $\psi(R, Z)$ as well as B_R, B_Z and B_ϕ.

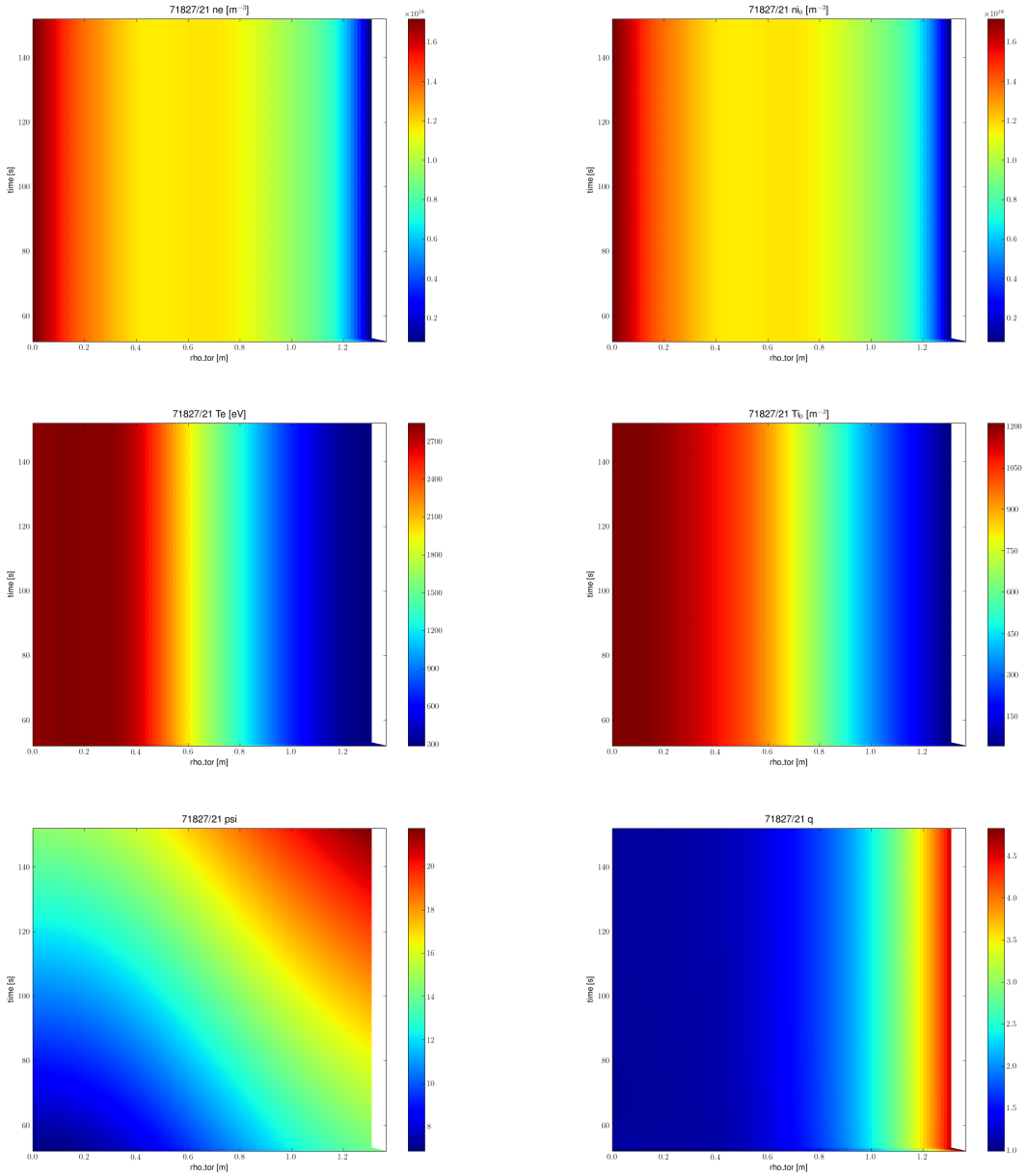

Figure 68: Results of a JET simulation for 71827 based on a start from data prepared by exp2itm. Current evolution only.

10.2 JET 71827/22

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./ets.xsl" charset="ISO-8859-1"?>

<parameters>

  <dimensions>
    <nrho>      100      </nrho>
    <nion>        1      </nion>
    <nimp>        0      </nimp>
    <max_nzimp>   0      </max_nzimp>
    <ntheta>    101      </ntheta>
  </dimensions>

  <output>
    <shot>    71827      </shot>
    <run>        12      </run>
  </output>

  <global>
    <time>     52.0      </time>
    <R0>        2.95     </R0>
    <B0>        2.56     </B0>
    <A0>        0.99     </A0>
    <Ip>        2.558e6  </Ip>
    <Rgeo>      2.87     </Rgeo>
  </global>

  <equilibrium>
    <equilibrium_ext>  </equilibrium_ext>
    <el>        1.65     </el>
    <tr_u>      0.2      </tr_u>
    <tr_l>      0.2      </tr_l>
  </equilibrium>

  <coreprof>
    <coreprof_ext> coster/jet/4.08a/71827/12 </coreprof_ext>
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    <ti>                 </ti>
    <te>                 </te>
    <vtor>               </vtor>
    <jpar>               </jpar>
    <qsf>                </qsf>
  </coreprof>
```

```
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    </sigma>
    <ne_diff>
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    </ne_diff>
    <ne_conv>
0.0 0.0 0.0
    </ne_conv>
    <ni_diff>
0.0 1.0 0.0
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0.0
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    </ti_conv>
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  <coresource>
    <coresource_ext>  </coresource_ext>
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    <sigma_src>
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5.0e4
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```

```
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5.0e4
    </qi_exp>
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  </coreimpur>

</parameters>
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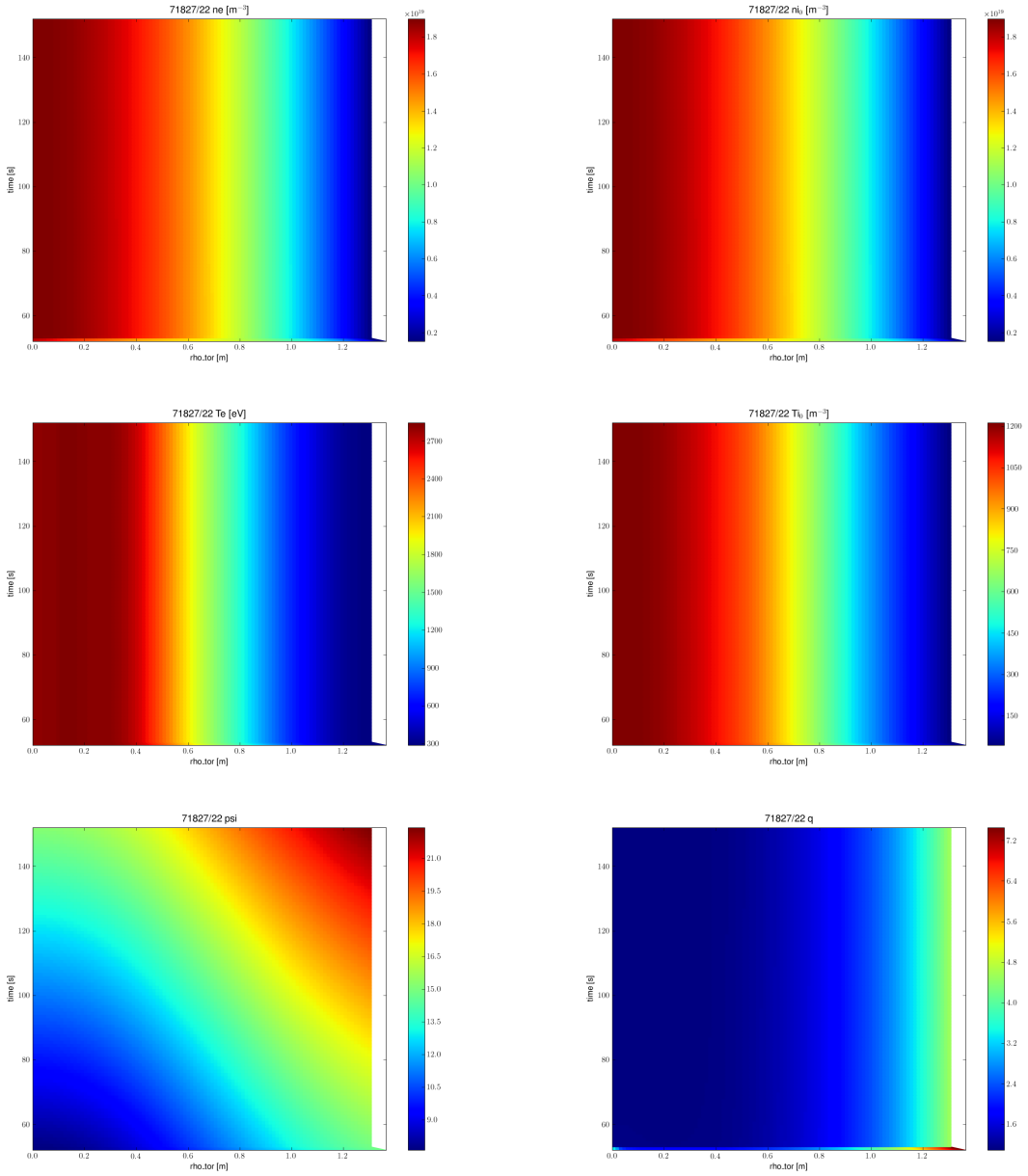

Figure 69: Results of a JET simulation for 71827 based on a start from data prepared by exp2itm. Current and density evolution only.

10.3 JET 71827/23

```
<?xml version="1.0"?>

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    <max_nzimp>   6      </max_nzimp>
    <ntheta>    101      </ntheta>
  </dimensions>

  <output>
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    <run>        13      </run>
  </output>

  <global>
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    <B0>        2.56     </B0>
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  </global>

  <equilibrium>
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    <tr_u>      0.2      </tr_u>
    <tr_l>      0.2      </tr_l>
  </equilibrium>

  <coreprof>
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```

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0.0
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    <vtor_conv>
0.0
    </vtor_conv>
  </coretransp>

  <coresource>
    <coresource_ext>  </coresource_ext>
    <j>
0.0
    </j>
    <sigma_src>
0.0
    </sigma_src>
    <qe_exp>
5.0e4
    </qe_exp>
```

```
    <qe_imp>
0.0
    </qe_imp>
    <qi_exp>
5.0e4
    </qi_exp>
    <qi_imp>
0.0
    </qi_imp>
    <si_exp>
5.0e19
    </si_exp>
    <si_imp>
0.0
    </si_imp>
    <ui_exp>
0.0
    </ui_exp>
    <ui_imp>
0.0
    </ui_imp>
  </coresource>

  <coreimpur>
    <coreimpur_ext>      </coreimpur_ext>
    <imp_zn>       6.0   </imp_zn>
    <imp_amn>     12.0   </imp_amn>
    <nz>
2.702E-13*(1.0E17) 1.489E-11*(1.0E17) 1.10E-7*(1.0E17) 0.18724*(1.0E17) 0.2065*(1.0E17) 0
    </nz>
    <diff>
1.0 1.0 1.0 1.0 1.0 1.0
    </diff>
    <conv>
0.0 0.0 0.0 0.0 0.0 0.0
    </conv>
  </coreimpur>

</parameters>
```

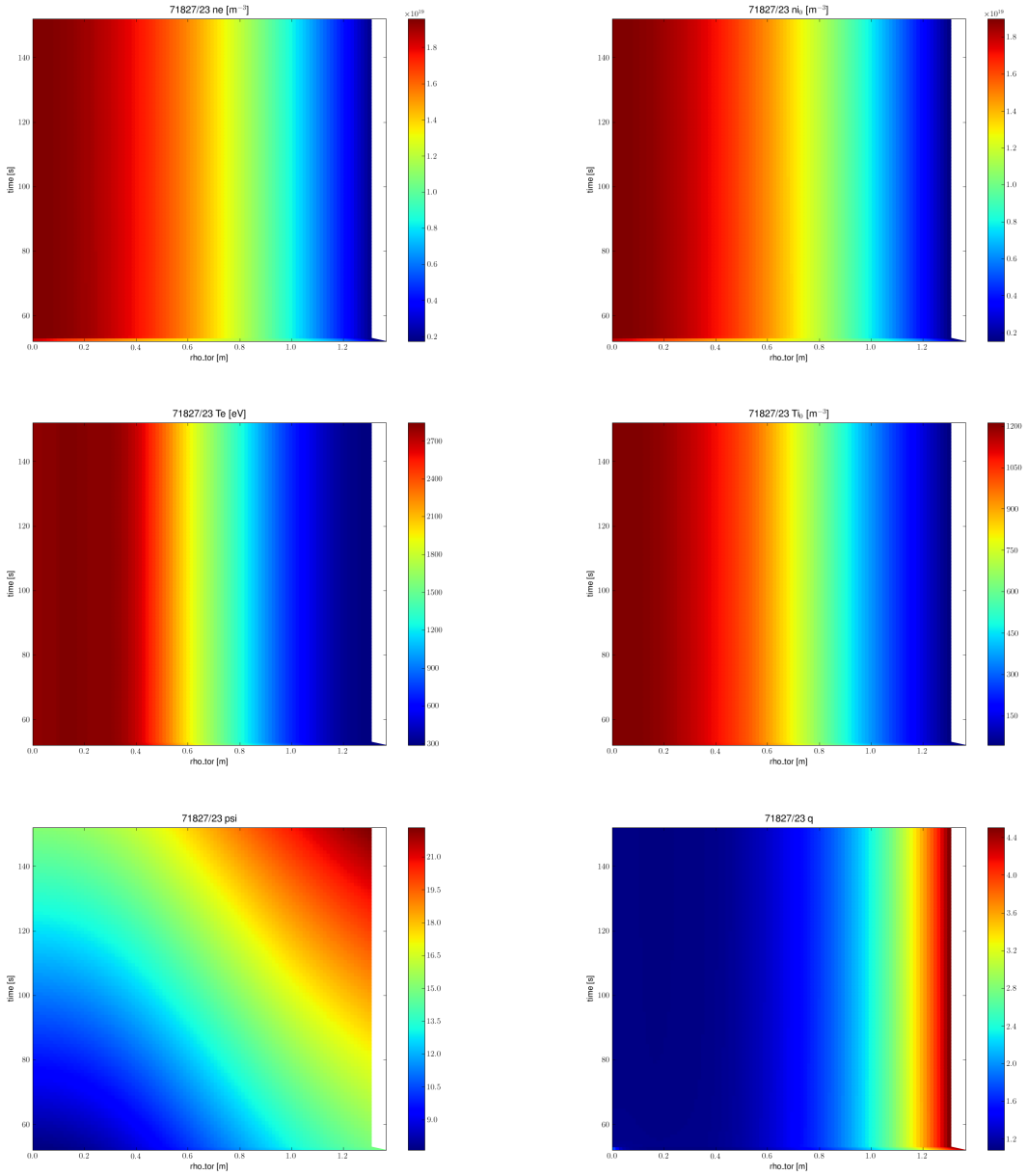

Figure 70: Results of a JET simulation for 71827 based on a start from data prepared by exp2itm. With impurities.

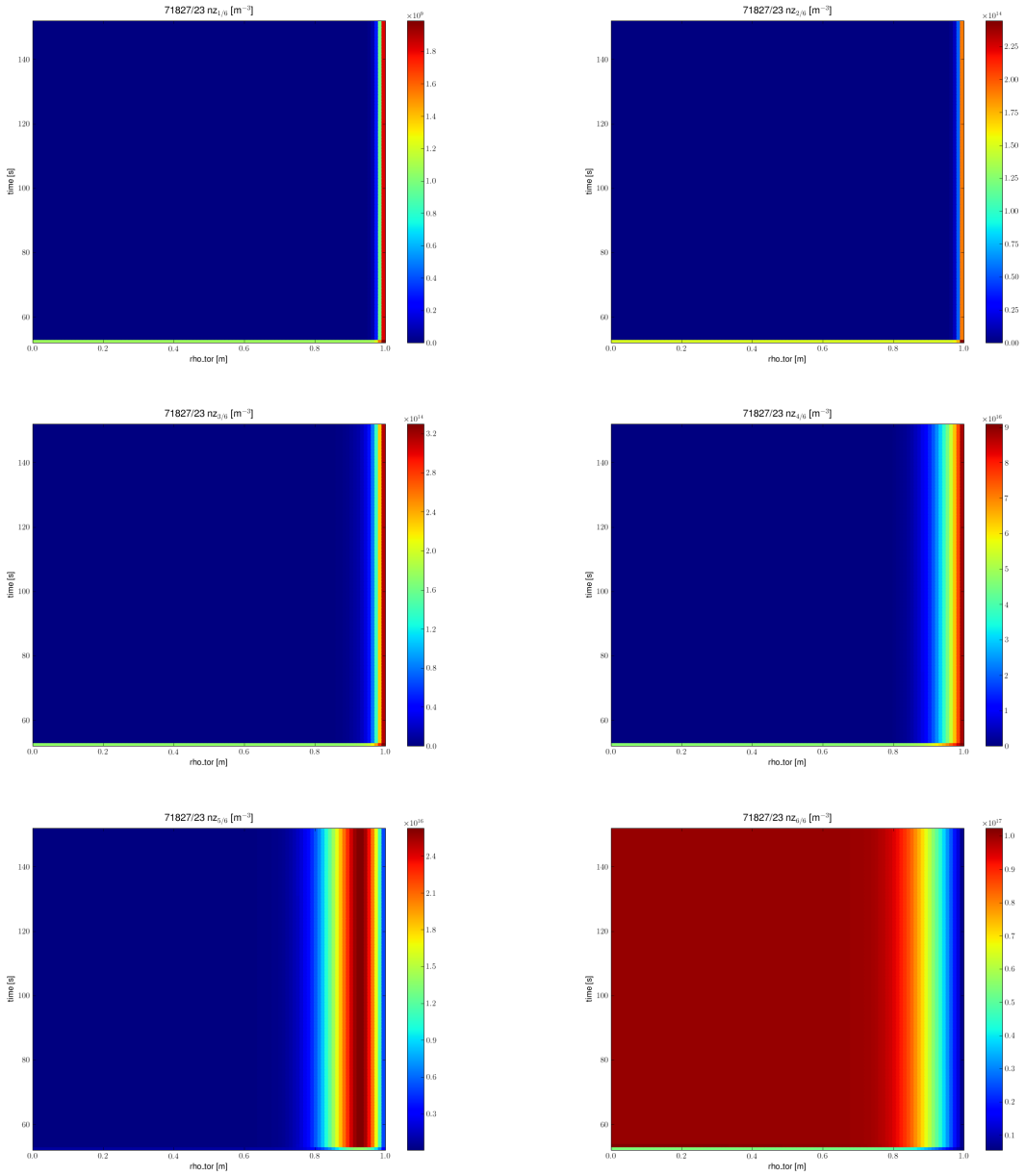

Figure 71: Results of a JET simulation for 71827 based on a start from data prepared by exp2itm. With impurities.

10.4 78092

This case starts from JET/78092/3 (originally from Konz) which was a HELENA run based on JET/78092/2, which in turn was an EQUAL reconstruction based on JET data in JET/78092/1.

The relevant input for preparing the initial CPO is

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./ets.xsl" charset="ISO-8859-1"?>

<parameters>

  <dimensions>
    <nrho>      100      </nrho>
    <nion>        1      </nion>
    <nimp>        0      </nimp>
    <max_nzimp>   0      </max_nzimp>
    <ntheta>    101      </ntheta>
  </dimensions>

  <output>
    <shot>    78092      </shot>
    <run>       103      </run>
  </output>

  <global>
    <time>      0.0      </time>
    <R0>        2.960000000000000     </R0>
    <B0>        2.245840415197474     </B0>
    <A0>        0.9359649590744112    </A0>
    <Ip>        1673037.784858907     </Ip>
    <Rgeo>      2.919332520294536     </Rgeo>
  </global>

  <equilibrium>
    <equilibrium_ext> coster/jet/4.08a/78092/3 </equilibrium_ext>
    <el>        1.65     </el>
    <tr_u>      0.2      </tr_u>
    <tr_l>      0.2      </tr_l>
  </equilibrium>

  <coreprof>
    <coreprof_ext>                                  </coreprof_ext>
    <zn>                     1.0                    </zn>
    <amn>                    2.0                    </amn>
    <zion>                   1.0                    </zion>
    <ni>        (1-x^2)*(1.0E20-5.0E19)+5.0E19      </ni>
```

```
    <ti>        (1-x^2)*(1.0E3-5.0E2)+5.0E2      </ti>
    <te>        (1-x^2)*(1.0E3-5.0E2)+5.0E2      </te>
    <vtor>                  0.0                  </vtor>
    <jpar>      (1-x^2)*(1.0E6-0.0E0)+0.0E0      </jpar>
    <qsf>       (1-x^2)*(1.0-3.0)+3.0            </qsf>
  </coreprof>

  <coretransp>
    <coretransp_ext>  </coretransp_ext>
    <sigma>
2.0e7
    </sigma>
    <ne_diff>
0.0 1.0 0.0
    </ne_diff>
    <ne_conv>
0.0 0.0 0.0
    </ne_conv>
    <ni_diff>
0.0 1.0 0.0
    </ni_diff>
    <ni_conv>
0.0 0.0 0.0
    </ni_conv>
    <te_diff>
1.5
    </te_diff>
    <te_conv>
0.0
    </te_conv>
    <ti_diff>
1.5
    </ti_diff>
    <ti_conv>
0.0
    </ti_conv>
    <vtor_diff>
1.0
    </vtor_diff>
    <vtor_conv>
0.0
    </vtor_conv>
  </coretransp>

  <coresource>
    <coresource_ext>  </coresource_ext>
    <j>
0.0
    </j>
```

```
    <sigma_src>
0.0
    </sigma_src>
    <qe_exp>
5.0e4
    </qe_exp>
    <qe_imp>
0.0
    </qe_imp>
    <qi_exp>
5.0e4
    </qi_exp>
    <qi_imp>
0.0
    </qi_imp>
    <si_exp>
5.0e19
    </si_exp>
    <si_imp>
0.0
    </si_imp>
    <ui_exp>
0.0
    </ui_exp>
    <ui_imp>
0.0
    </ui_imp>
  </coresource>

  <coreimpur>
    <coreimpur_ext>      </coreimpur_ext>
    <imp_zn>             </imp_zn>
    <imp_amn>            </imp_amn>
    <nz>
    </nz>
    <diff>
    </diff>
    <conv>
    </conv>
  </coreimpur>

</parameters>
```

The was then performed based on

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./ets.xsl" charset="ISO-8859-1"?>
```

```
<parameters>

  <input>
    <shot_in>          78092     </shot_in>          <!-- shot number -->
    <run_in>             103     </run_in>           <!-- run number -->
    <interpol>             1     </interpol>         <!-- interpolation index -->
    <time_dep_input>       0     </time_dep_input>   <!-- 1 implies time dependence in inp
  </input>

  <output>
    <shot_out>         78092     </shot_out>         <!-- shot number -->
    <run_out>            203     </run_out>          <!-- run number -->
    <tau_out>         1.0d-2     </tau_out>          <!-- output frequency -->
  </output>

  <dims>
    <nrho>               100     </nrho>             <!-- NRHO,  number of radial points -
    <neq>                 50     </neq>              <!-- NEQ,   number of equilibrium poi
    <nion>                 1     </nion>             <!-- NION,  number of ions -->
    <nimp>                 0     </nimp>             <!-- NIMP,  number of impurity types
    <max_nzimp>            0     </max_nzimp>        <!-- MAX_NZIMP, number of impurity io
  </dims>

  <solver>
   <solver_type>           3     </solver_type>      <!-- choice of numerical solver -->
   <sigma_source>          0     </sigma_source>     <!-- option for origin of Plasma elec
    <tau>             1.0d-2     </tau>              <!-- TAU, time step [s] -->
    <amix>            1.0d-0     </amix>             <!-- AMIX, mixing factor -->
    <convrec>         1.0d-4     </convrec>          <!-- PRECISION -->
    <ntime>             1000     </ntime>            <!-- NTIME, number of time points -->
    <time0>              0.0     </time0>            <!-- Start time [s] -->
    <nsol>                 2     </nsol>             <!-- Number of analytical example -->
    <ext_equil>            3     </ext_equil>        <!-- call external equilibrium: 0: no
    <augment_equil>        1     <augment_equil>        1     </augment_equil>    <!-- if
 </augment_equil>    <!-- if 1 add psi(R,Z), B(R,Z) using splines
    <ext_source>           0     </ext_source>       <!-- call external source routines: 1
    <ext_transport>        0     </ext_transport>    <!-- call external transport routines
  </solver>

  <boundary>
    <psi_bnd_type>         2     </psi_bnd_type>     <!-- Type of boundary conditions CURR
    <ni_bnd_type>          1     </ni_bnd_type>      <!-- Type of boundary conditions ION
    <ti_bnd_type>          1     </ti_bnd_type>      <!-- Type of boundary conditions ION
    <te_bnd_type>          1     </te_bnd_type>      <!-- Type of boundary conditions ELEC
    <vtor_bnd_type>        1     </vtor_bnd_type>    <!-- Type of boundary conditions ROTA
  </boundary>

  <experimental>
    <option>              -1     </option>           <!-- option #: 0: disabled -->
```

```
  </experimental>

</parameters>
```

producing output in JET/78092/203. The HELENA parameters used were

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./input_helena.xsl"
charset="ISO-8859-1"?>

<parameters>

<!-- profile parameters -->

 <profile_parameters>
   <hbt> .false. </hbt>
   <input_type> p and j_tor </input_type>
   <radial_coordinate> rho_vol </radial_coordinate>
 </profile_parameters>

<!-- shape parameters -->

 <shape_parameters>
   <ishape> 2 </ishape>
   <isol> 0 </isol>
   <ias> 1 </ias>
   <imesh> 2 </imesh>
   <equidistant> 0.5 </equidistant>
   <n_acc_points> 2 </n_acc_points>
   <s_acc> 0.0 1.0 </s_acc>
   <sig> 0.1 0.1 </sig>
   <weights> 0.1 0.1 </weights>
 </shape_parameters>

<!-- global parameters -->

 <global_parameters>
 </global_parameters>

<!-- numerical parameters -->

  <numerical_parameters>
    <nr> 100 </nr>
    <np> 17 </np>
    <nrmap> 100 </nrmap>
    <npmap> 64 </npmap>
    <nchi> 64 </nchi>
    <niter> 32 </niter>
```

```
    <nmesh> 20 </nmesh>
    <errcur> 1.000E-03 </errcur>
  </numerical_parameters>

<!-- diagnostics parameters -->

 <diagnostics_parameters>
   <verbosity> 0 </verbosity>
   <output> none </output>
   <diagnostics_on> .false. </diagnostics_on>
   <standard_output> .false. </standard_output>
   <xmgrace_output> .false. </xmgrace_output>
   <profiles_output> .false. </profiles_output>
 </diagnostics_parameters>

</parameters>
```

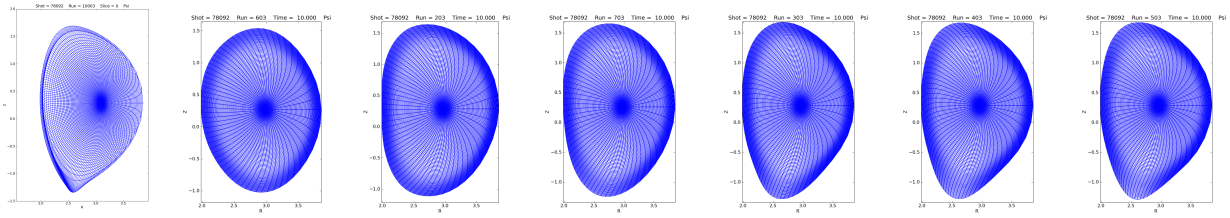

Figure 72: Original grid (high resolution) from Konz and the grid used in the computations for the resolution scan (NP = 9, 17, 33, 65, 129, 257).

The results are shown in figure 73, which was produced by

```
diagnostics/run_plot_eq_ets -t png 78092 603
diagnostics/run_plot_eq_ets -t png 78092 203
diagnostics/run_plot_eq_ets -t png 78092 703
diagnostics/run_plot_eq_ets -t png 78092 303
diagnostics/run_plot_eq_ets -t png 78092 403
diagnostics/run_plot_eq_ets -t png 78092 503
```

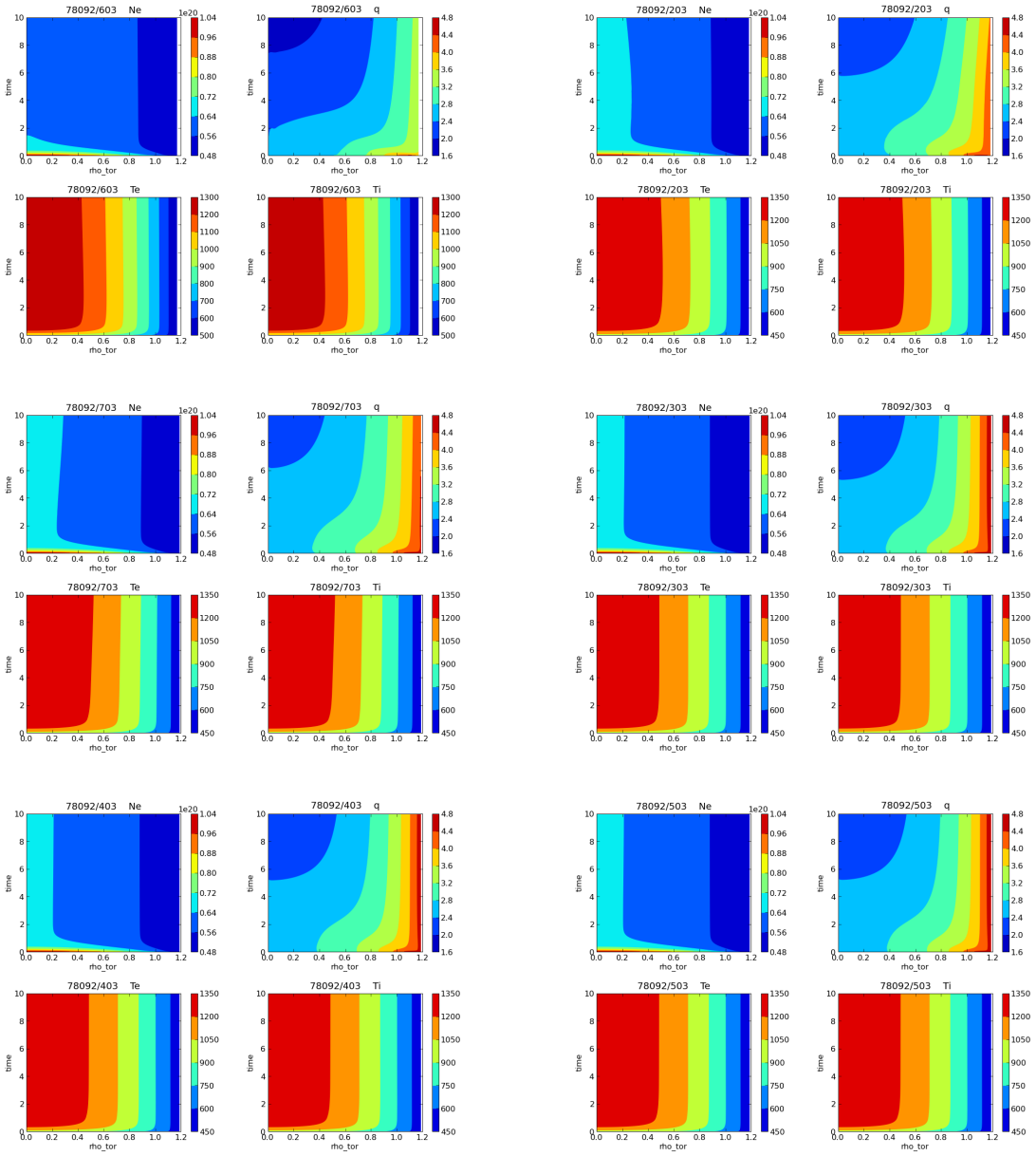

Figure 73: Results of JET simulations for 78092 (no physics other than the equilibrium!). Different poloidal resolutions in HELENA were used (NP = 9, 17, 33, 65, 129, 257).

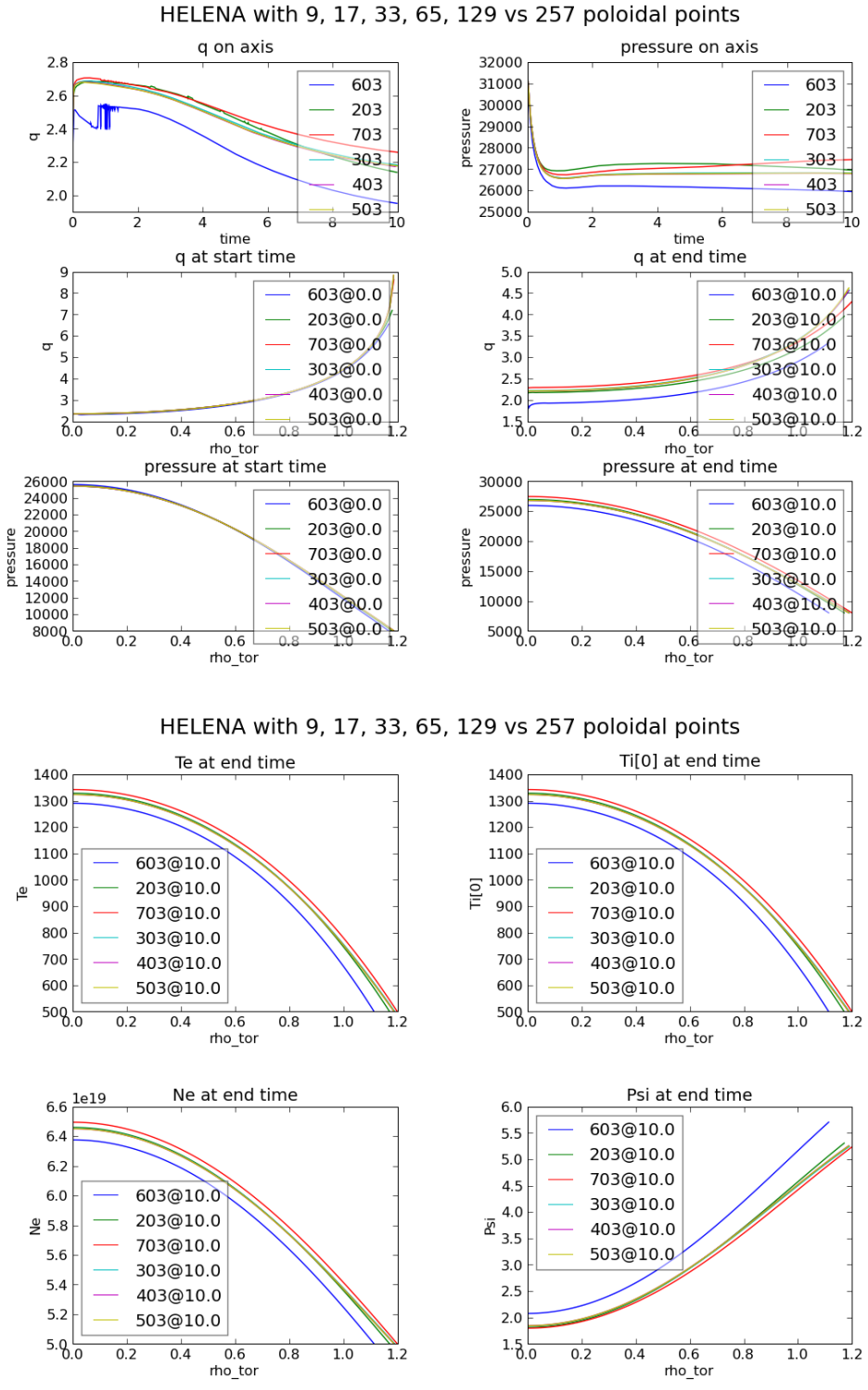

Figure 74: Comparison of the results of a JET simulation for 78092 for the NP resolution scan (no physics other than the equilibrium!).

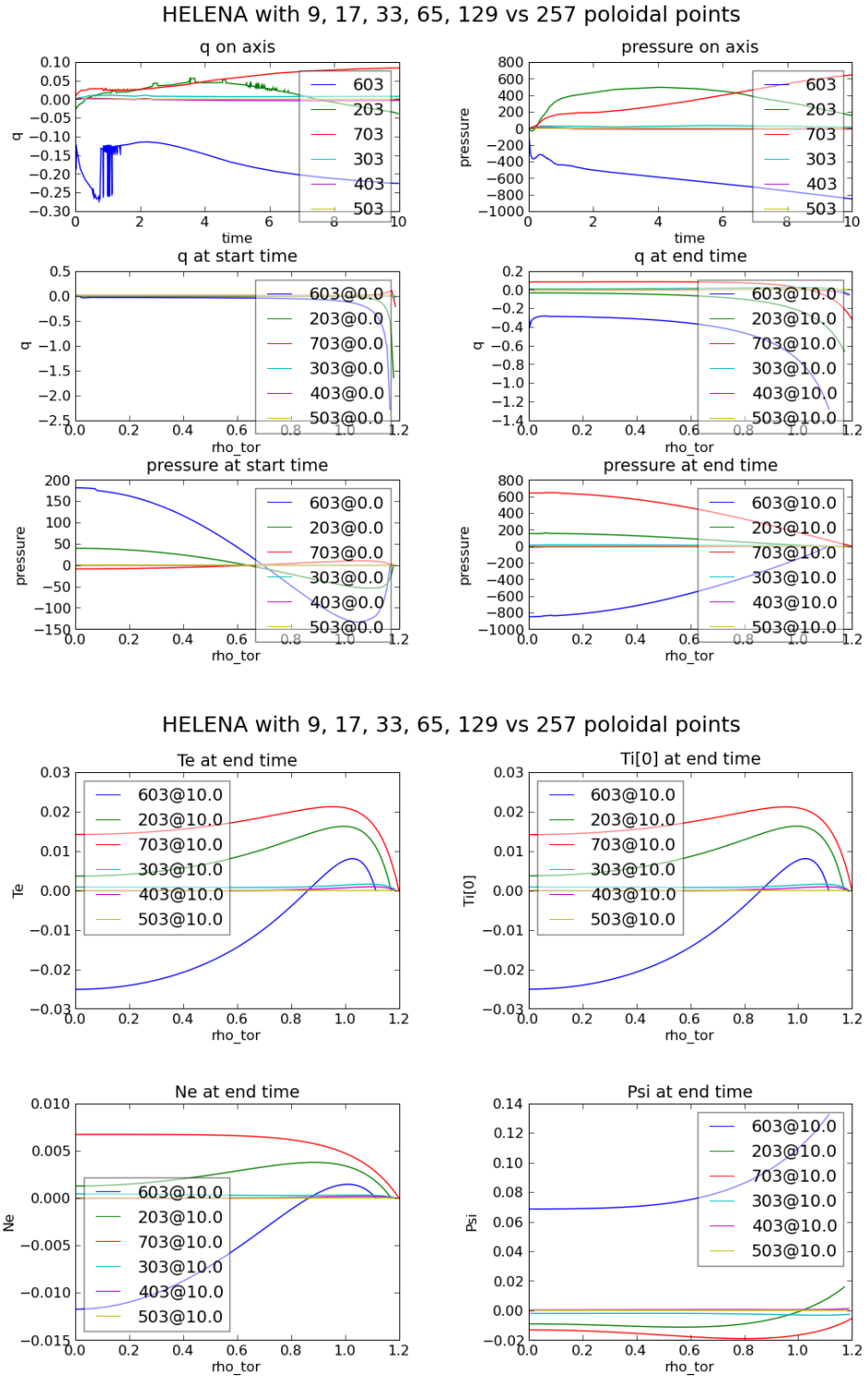

Figure 75: Comparison of the results of a JET simulation for 78092 for the NP resolution scan (no physics other than the equilibrium!).

11 AUG Cases

11.1 20116

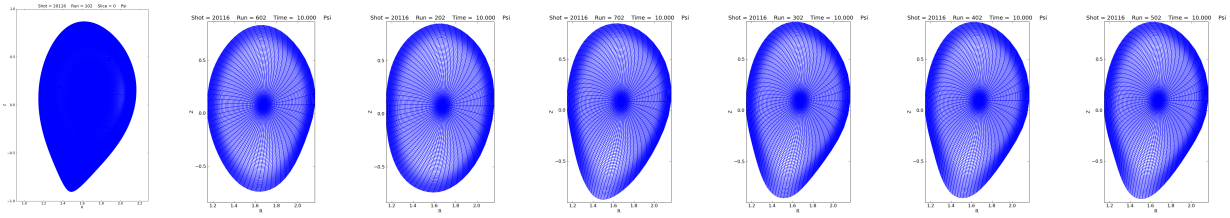

Figure 76: Original grid (high resolution) from Konz and the grid used in the computations for the resolution scan (NP = 9, 17, 33, 65, 129, 257).

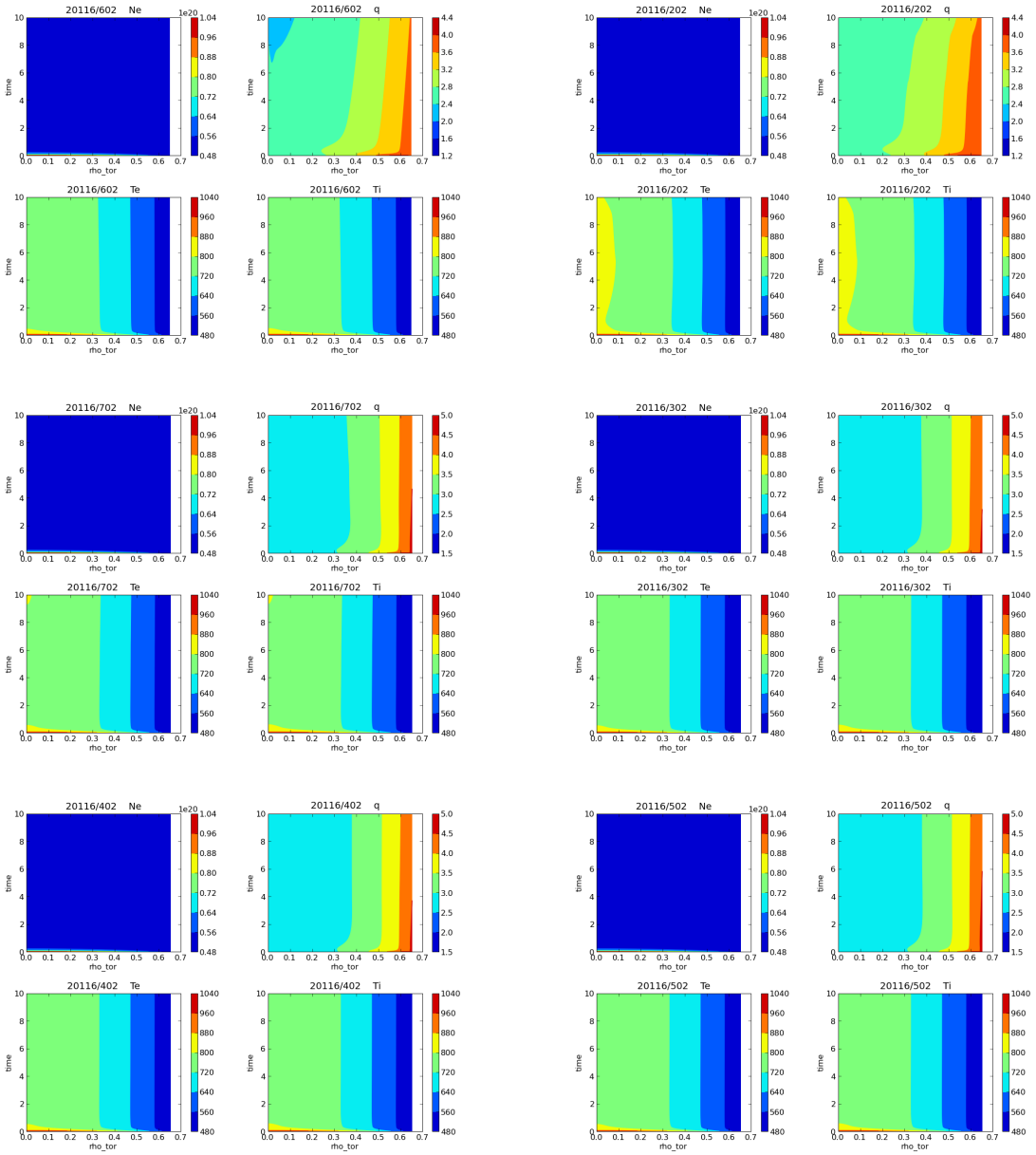

Figure 77: Results of AUG simulations for 20116 (no physics other than the equilibrium!). Different poloidal resolutions in HELENA were used (NP = 9, 17, 33, 65, 129, 257).

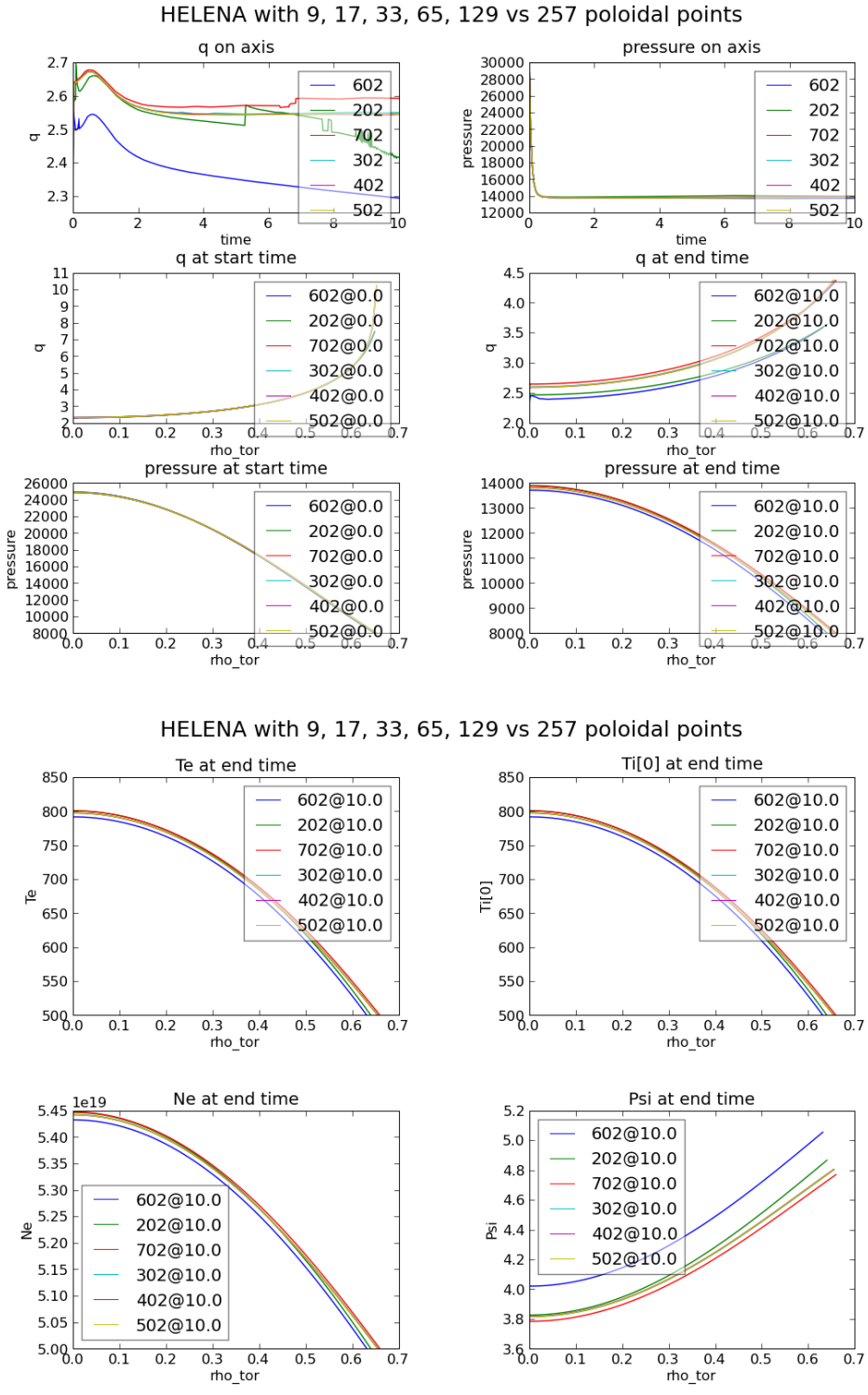

Figure 78: Comparison of the results of a JET simulation for 20116 for the NP resolution scan (no physics other than the equilibrium!).

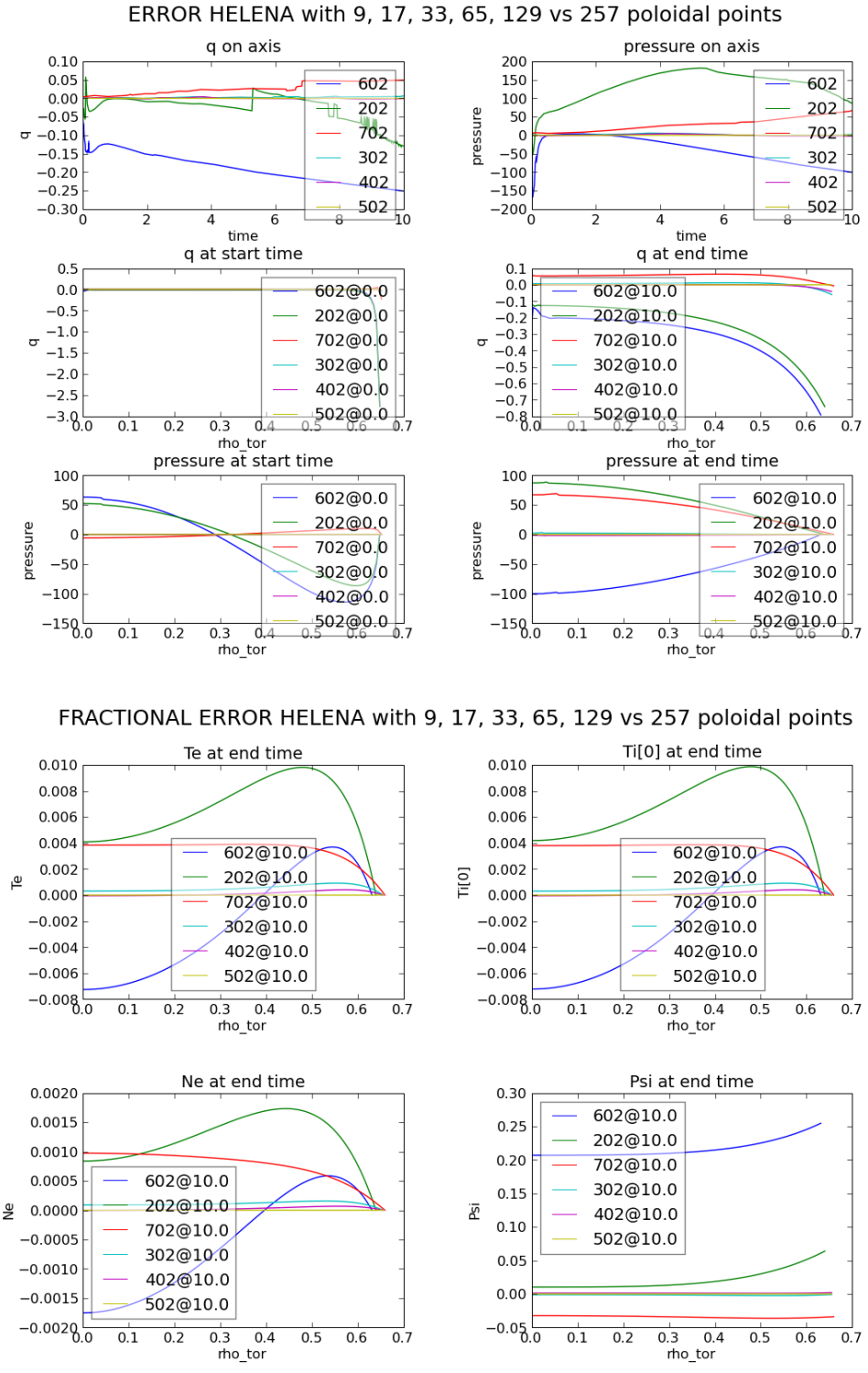

Figure 79: Comparison of the results of a JET simulation for 20116 for the NP resolution scan (no physics other than the equilibrium!).

12 Generic sources

Generic source routines have been created using the schema `sources.xsd`.

Flag	Description
parameters	GLOBAL: parameters for generic source modules (ECRH, ICRH, NBI)
coresource	BLOCK: specify parameters for the coresource CPO
j	expression for j as a function of a normalized radial coordinate [A/m$\hat{2}$]
qe_exp	expression for the explicit part of the electron heating as a function of a normalized radial coordinate [W/m$\hat{3}$]
qe_imp	expression for the implicit part of the electron heating as a function of a normalized radial coordinate [W/m$\hat{3}$/eV ??]
qi_exp	NION expressions for the explicit part of the ion heating as a function of a normalized radial coordinate [W/m$\hat{3}$]
qi_imp	NION expressions for the implicit part of the ion heating as a function of a normalized radial coordinate [W/m$\hat{3}$/eV ??]
si_exp	NION expressions for the explicit part of the ion particle source as a function of a normalized radial coordinate [/m$\hat{3}$/s]
si_imp	NION expressions for the implicit part of the ion particle source as a function of a normalized radial coordinate [/m$\hat{3}$/s.m$\hat{3}$??]
ui_exp	NION expressions for the explicit part of the toroidal velocity source as a function of a normalized radial coordinate [??]
ui_imp	NION expressions for the implicit part of the toroidal velocity source as a function of a normalized radial coordinate [??]
j_int	desired integral of j as a function of a normalized radial coordinate [A/m$\hat{2}$] (not yet implemented)
qe_exp_int	desired integral of the explicit part of the electron heating as a function of a normalized radial coordinate [W/m$\hat{3}$]
qe_imp_int	desired integral of the implicit part of the electron heating as a function of a normalized radial coordinate [W/m$\hat{3}$/eV ??] (not yet implemented)
qi_exp_int	NION desired integrals of the explicit part of the ion heating as a function of a normalized radial coordinate [W/m$\hat{3}$]
qi_imp_int	NION desired integrals of the implicit part of the ion heating as a function of a normalized radial coordinate [W/m$\hat{3}$/eV ??] (not yet implemented)
si_exp_int	NION desired integrals of the explicit part of the ion particle source as a function of a normalized radial coordinate [/m$\hat{3}$/s]
	continued

continued	
Flag	**Description**
si_imp_int	NION desired integrals of the implicit part of the ion particle source as a function of a normalized radial coordinate [/m3̂/s.m3̂ ??] (not yet implemented)
ui_exp_int	NION desired integrals of the explicit part of the toroidal velocity source as a function of a normalized radial coordinate [??]
ui_imp_int	NION desired integrals of the implicit part of the toroidal velocity source as a function of a normalized radial coordinate [??] (not yet implemented)

Three instances have been created for NBI, ECRH and ICRH.

12.1 case_5_118

The NBI module uses the input:

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./ets.xsl" charset="ISO-8859-1"?>

<parameters>

  <coresource>
    <j>
0.0
    </j>
    <qe_exp>
exp(-((x-0.0)/0.4)^2)
    </qe_exp>
    <qe_imp>
0.0
    </qe_imp>
    <qi_exp>
exp(-((x-0.0)/0.4)^2)
    </qi_exp>
    <qi_imp>
0.0
    </qi_imp>
    <si_exp>
exp(-((x-0.0)/0.4)^2)
    </si_exp>
    <si_imp>
0.0
    </si_imp>
    <ui_exp>
0.0
```

```
    </ui_exp>
    <ui_imp>
0.0
    </ui_imp>
    <j_int>          0.0     </j_int>
    <qe_exp_int>   10.0e6    </qe_exp_int>
    <qe_imp_int>    0.0      </qe_imp_int>
    <qi_exp_int>   10.0e6    </qi_exp_int>
    <qi_imp_int>    0.0      </qi_imp_int>
    <si_exp_int>    1.25e20  </si_exp_int>
    <si_imp_int>    0.0      </si_imp_int>
    <ui_exp_int>    0.0      </ui_exp_int>
    <ui_imp_int>    0.0      </ui_imp_int>
  </coresource>

</parameters>
```

The ECRH module uses the input:

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./ets.xsl" charset="ISO-8859-1"?>

<parameters>

  <coresource>
    <j>
0.0
    </j>
    <qe_exp>
exp(-((x-0.5)/0.05)^2)
    </qe_exp>
    <qe_imp>
0.0
    </qe_imp>
    <qi_exp>
0.0
    </qi_exp>
    <qi_imp>
0.0
    </qi_imp>
    <si_exp>
0.0
    </si_exp>
    <si_imp>
0.0
    </si_imp>
    <ui_exp>
0.0
```

```
    </ui_exp>
    <ui_imp>
0.0
    </ui_imp>
    <j_int>          0.0     </j_int>
    <qe_exp_int>   20.0e6    </qe_exp_int>
    <qe_imp_int>     0.0     </qe_imp_int>
    <qi_exp_int>     0.0     </qi_exp_int>
    <qi_imp_int>     0.0     </qi_imp_int>
    <si_exp_int>     0.0     </si_exp_int>
    <si_imp_int>     0.0     </si_imp_int>
    <ui_exp_int>     0.0     </ui_exp_int>
    <ui_imp_int>     0.0     </ui_imp_int>
  </coresource>

</parameters>
```

The ICRH module uses the input:

```
<?xml version="1.0"?>

<?xml-stylesheet type="text/xsl" href="./ets.xsl" charset="ISO-8859-1"?>

<parameters>

  <coresource>
    <j>
0.0
    </j>
    <qe_exp>
0.0
    </qe_exp>
    <qe_imp>
0.0
    </qe_imp>
    <qi_exp>
exp(-((x-0.2)/0.20)^2)
    </qi_exp>
    <qi_imp>
0.0
    </qi_imp>
    <si_exp>
0.0
    </si_exp>
    <si_imp>
0.0
    </si_imp>
    <ui_exp>
0.0
    </ui_exp>
```

```
    <ui_imp>
0.0
    </ui_imp>
    <j_int>          0.0     </j_int>
    <qe_exp_int>     0.0     </qe_exp_int>
    <qe_imp_int>     0.0     </qe_imp_int>
    <qi_exp_int>    20.0e6   </qi_exp_int>
    <qi_imp_int>     0.0     </qi_imp_int>
    <si_exp_int>     0.0     </si_exp_int>
    <si_imp_int>     0.0     </si_imp_int>
    <ui_exp_int>     0.0     </ui_exp_int>
    <ui_imp_int>     0.0     </ui_imp_int>
  </coresource>

</parameters>
```

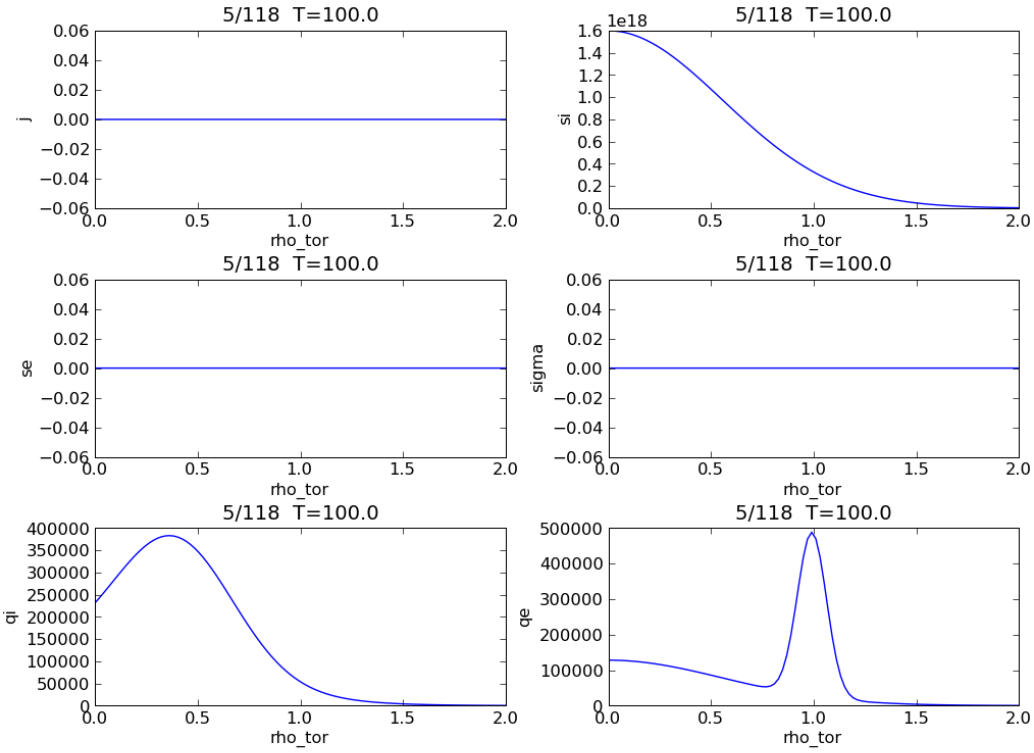

Figure 80: Resultant coresource from NBI, ECRH and ICRH.

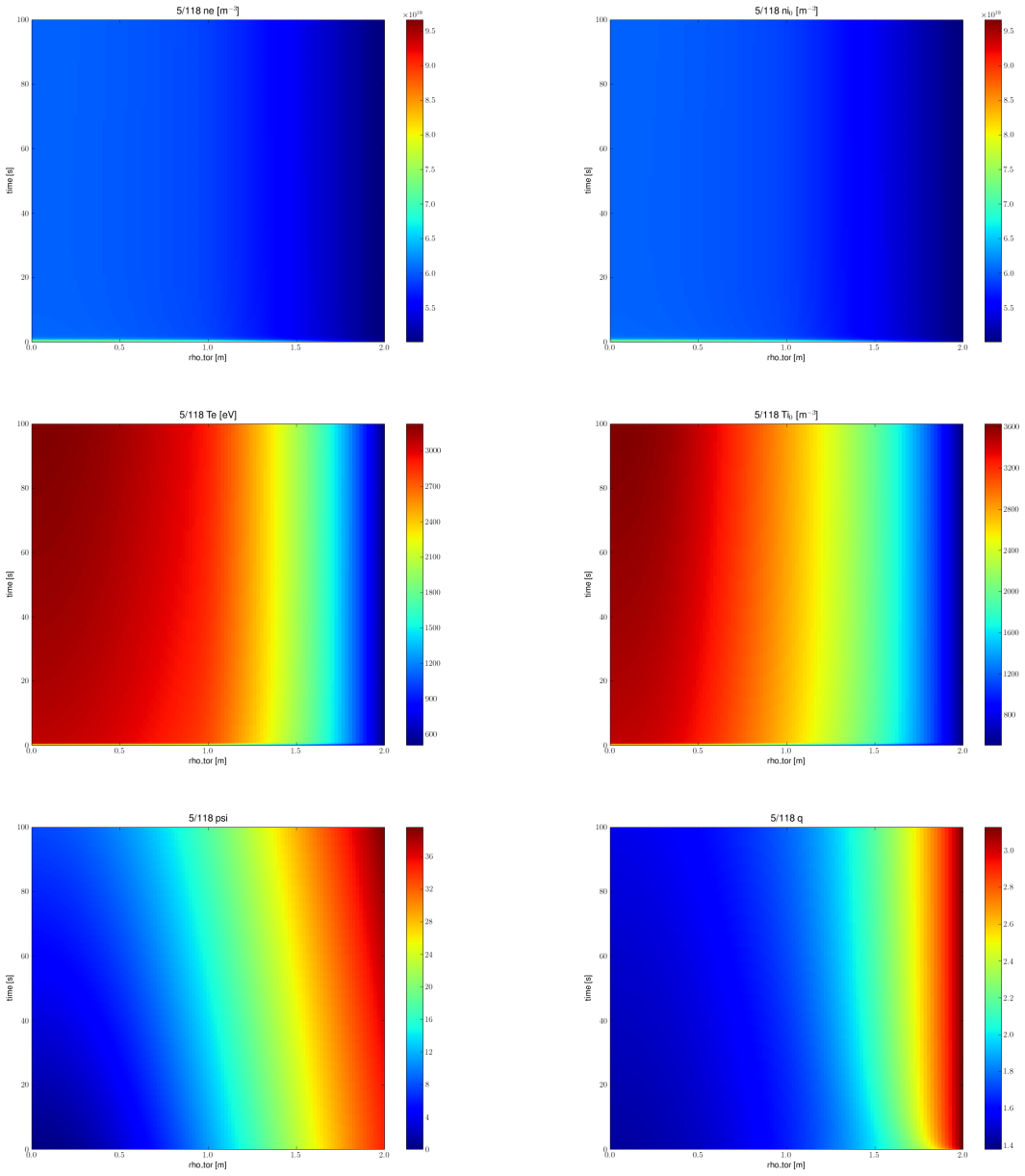

Figure 81: Results of using the NBI, ECRH and ICRH core sources.

13 Equilibrium augmentation

In order to calculate $\psi(R,Z)$ as well as $B_R(R,Z)$, $B_Z(R,Z)$ and $B_\phi(R,Z)$ when only $R(\psi,\theta)$ and $Z(\psi,\theta)$ are present, a short routine was wriiten to calculate a spline repersentation of $\psi(R,Z)$ (using the dierckx routine "surfit"), which is then used to calculate $\psi(R,Z)$ (using "bispev") as well as $B_R(R,Z)$ and $B_Z(R,Z)$ (using "parder"). Similarly $B_\phi(R,Z)$ is calculated from the spline of F_{dia}.

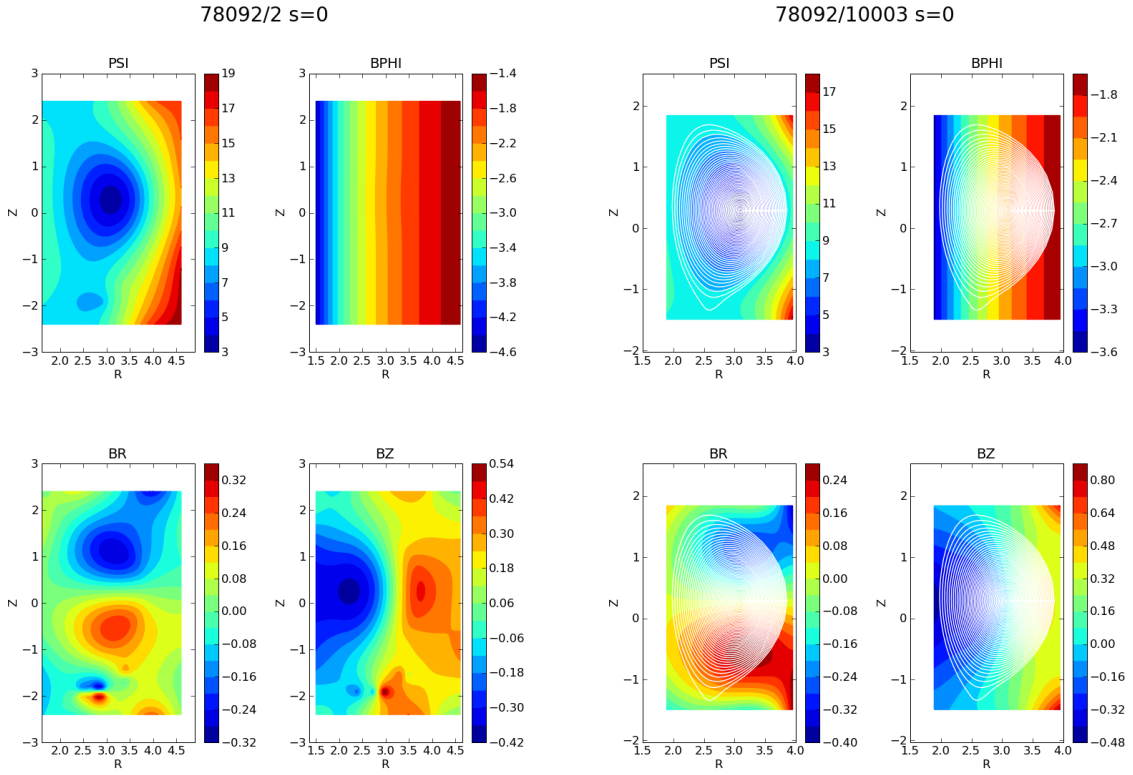

Figure 82: On the left the original data from the EQUAL simulation. On the right the reconstruction of $\psi(R,Z)$, B_R, B_Z and B_ϕ arising from a HELENA simulation based on the EQUAL simulation.

In figure 82 the results of this procedure are shown, and a more detailed comparison is shown in 83: in blue data from the original EQUAL run are shown, and in red the results of the equilibrium augmentation applied to a HELENA run based on the EQUAL data.

The results for an AUG and a JET shot are shown in 84.

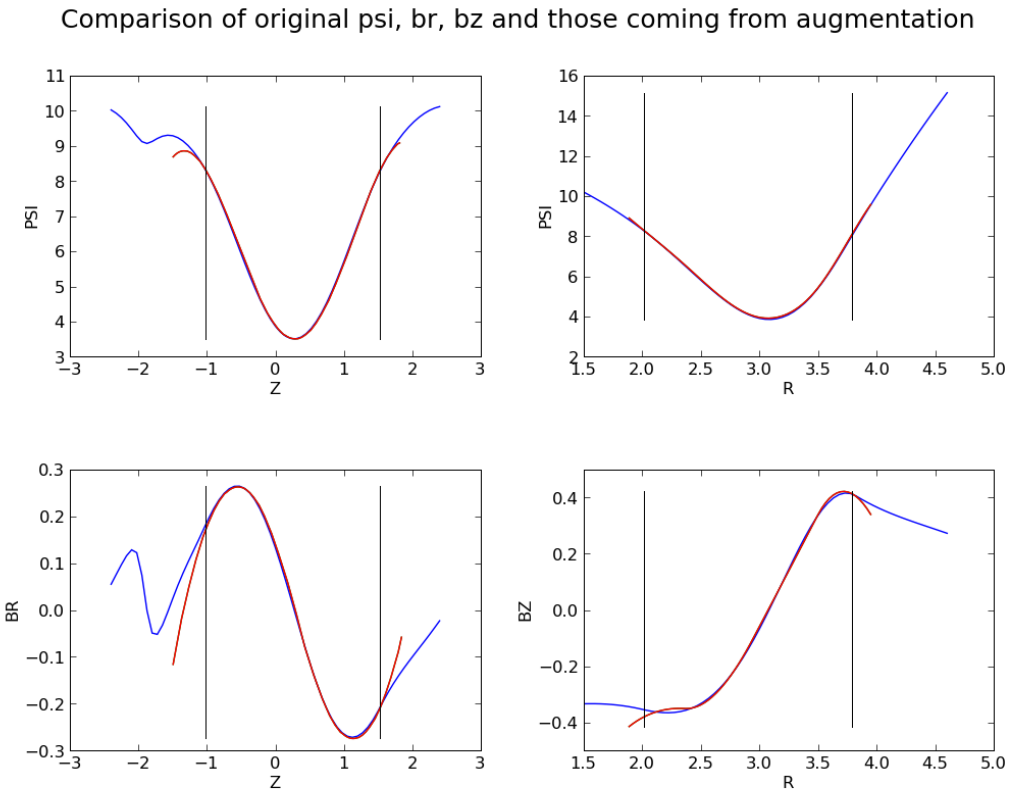

Figure 83: Comparison of ψ, B_R, B_Z arising from equilibrium augmentation and the original.

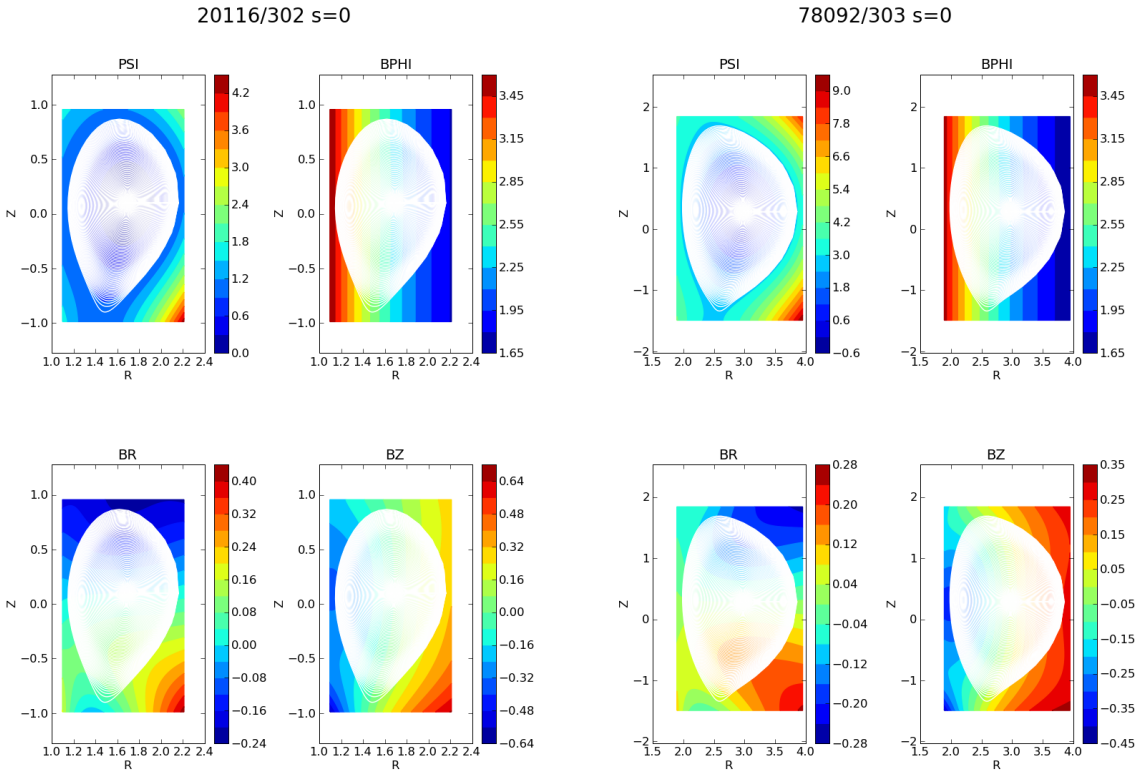

Figure 84: Reconstruction of $\psi(R, Z)$, B_R, B_Z and B_ϕ for an AUG and a JET ETS simulation.

14 Kepler ETS Workflow

The result of the Kepler implementation of the ETS is shown in 85 with the workflow depicted in figures 86, 87, 88, 89, 90, 91, 92, 93, 94, 95 and 96.

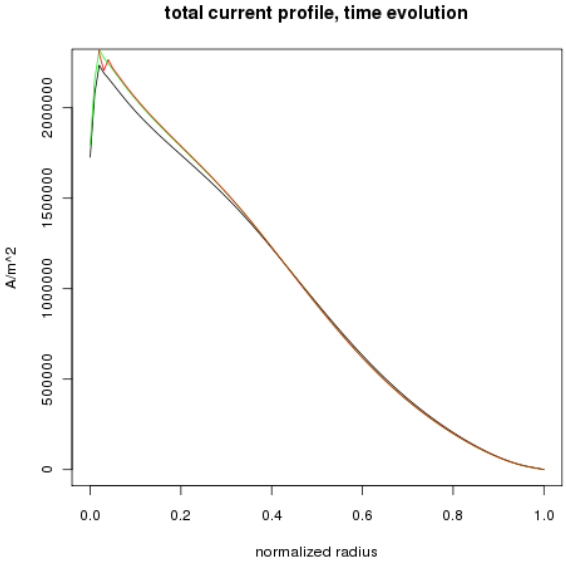

Figure 85: Kepler ETS workflow result.

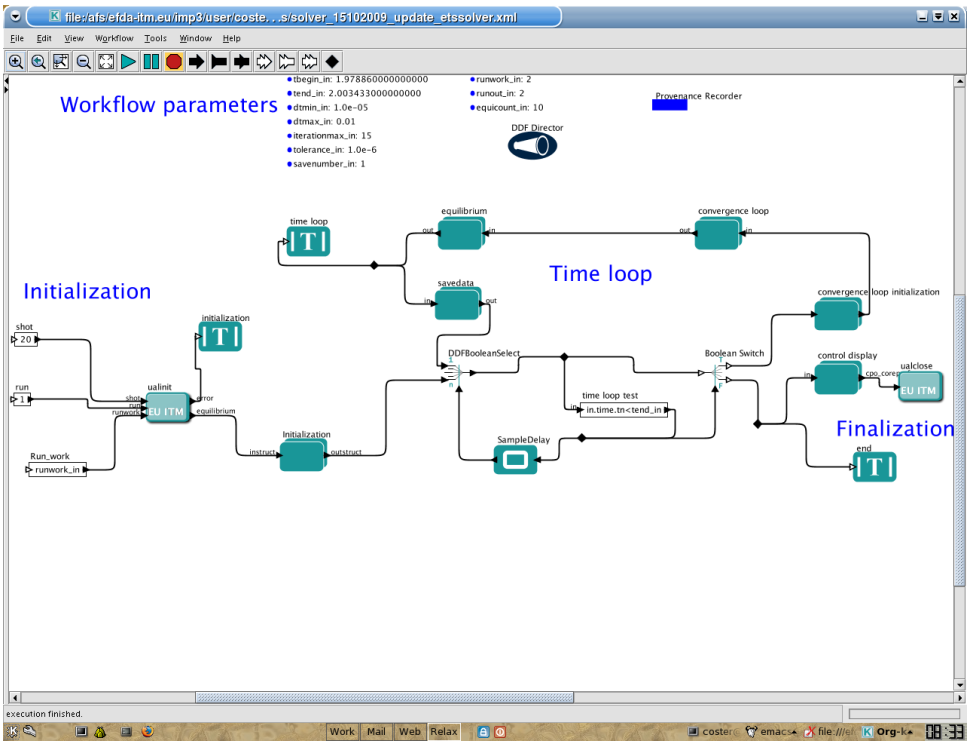

Figure 86: Kepler ETS workflow.

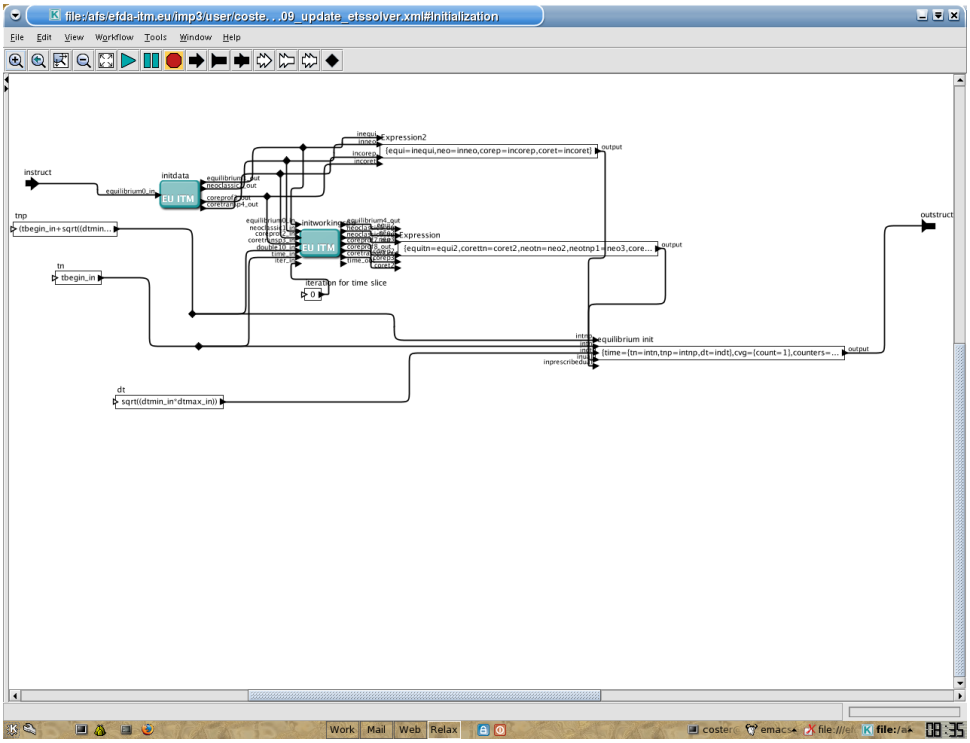

Figure 87: Zoom in of the composite actor “Initialization” in the Kepler ETS workflow.

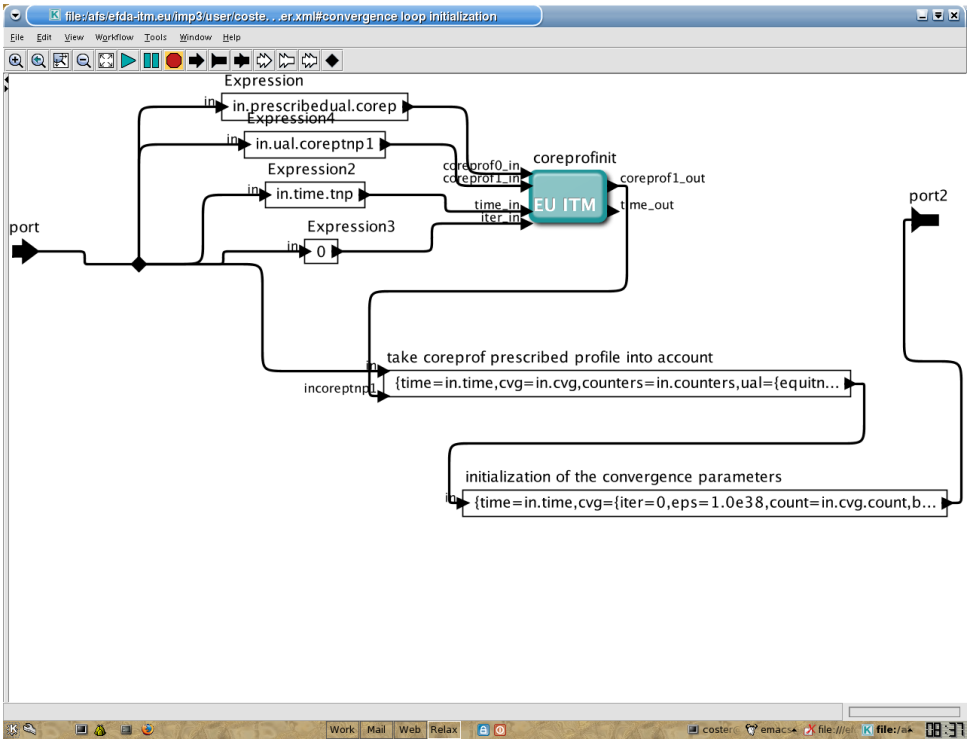

Figure 88: Zoom in of the composite actor “convergence loop initialization” in the Kepler ETS workflow.

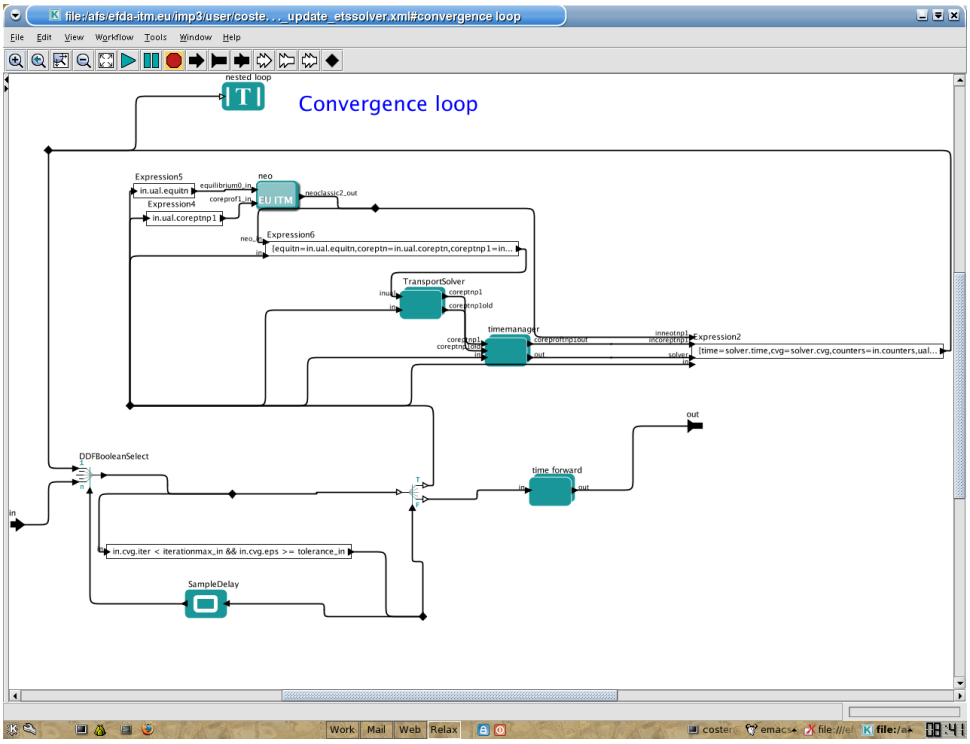

Figure 89: Zoom in of the composite actor "convergence loop" in the Kepler ETS workflow.

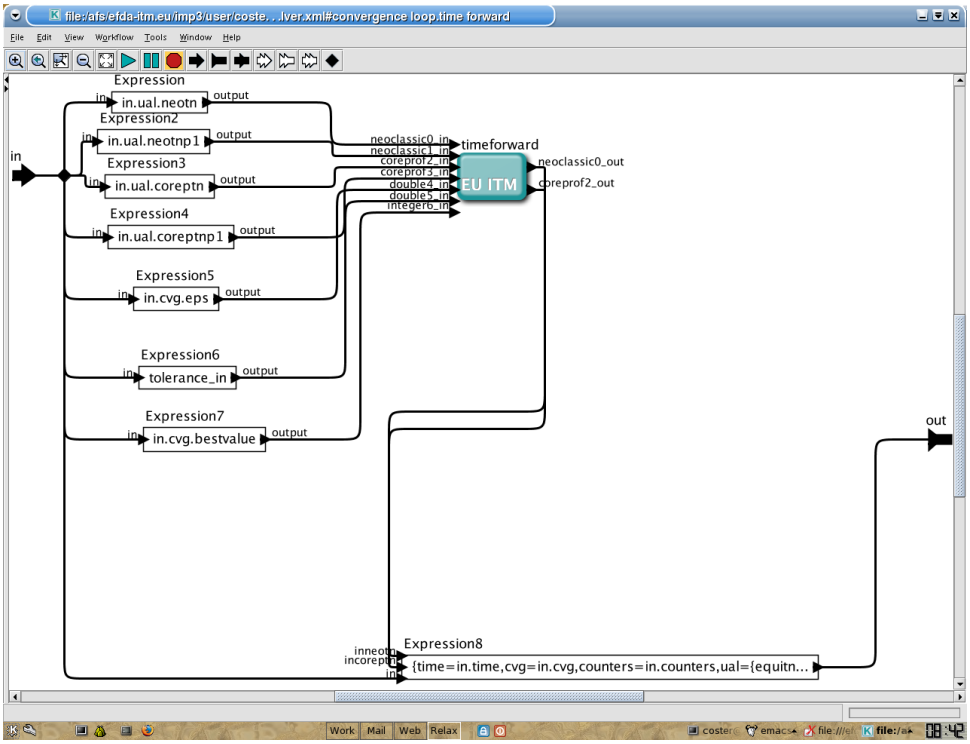

Figure 90: Zoom in of the composite actor "time forward" in the composite actor "convergence loop" in the Kepler ETS workflow.

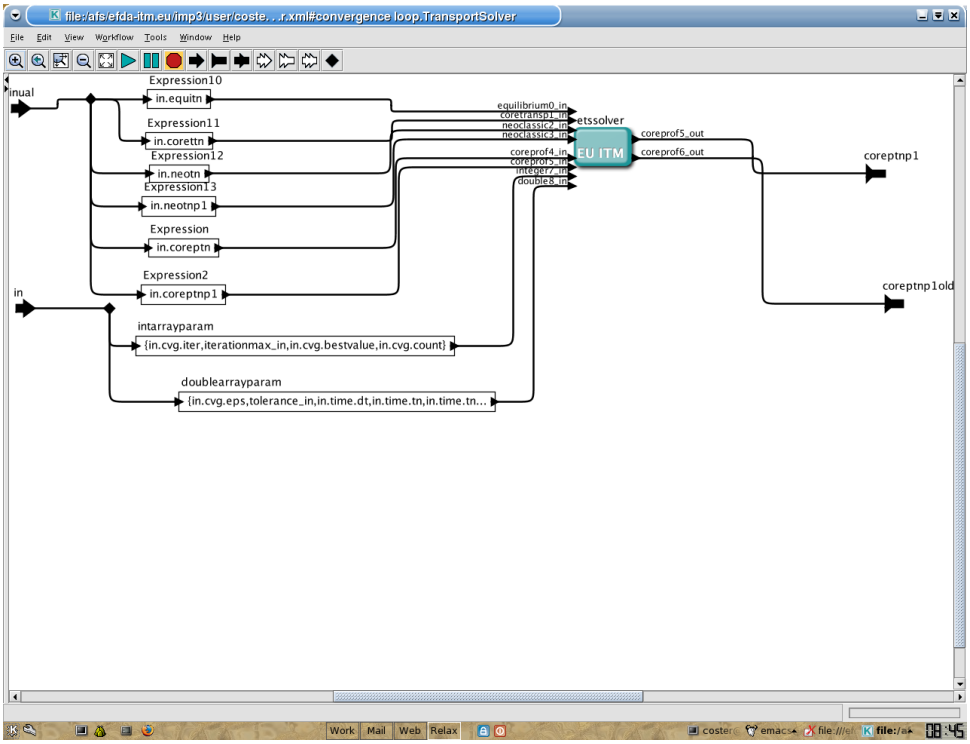

Figure 91: Zoom in of the composite actor "transport solver" in the composite actor "convergence loop" in the Kepler ETS workflow.

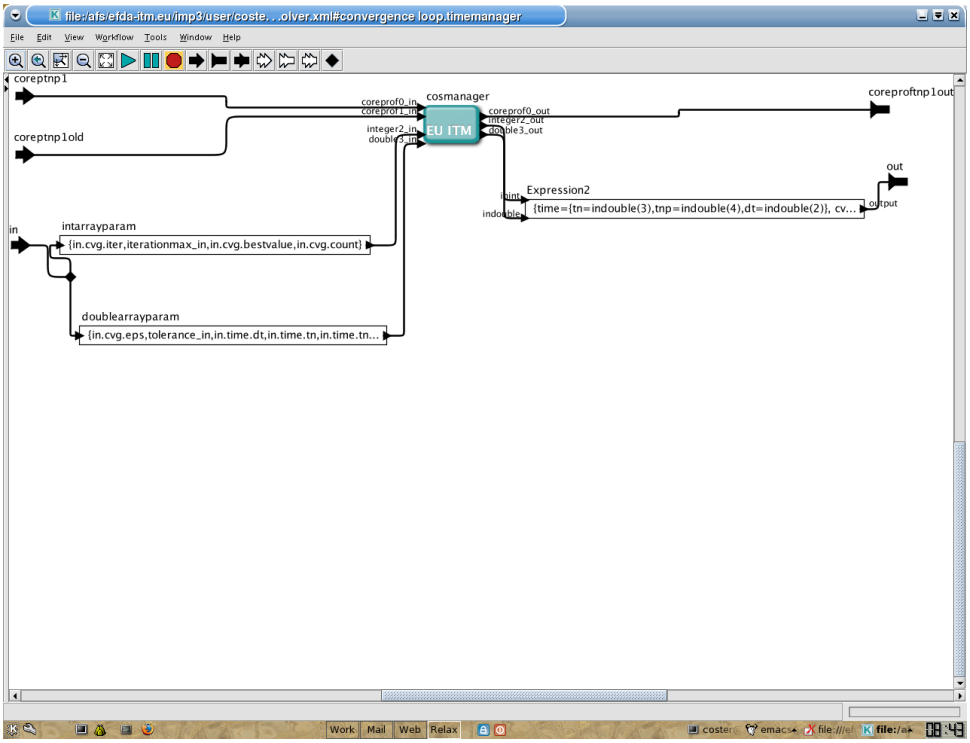

Figure 92: Zoom in of the composite actor "time manager" in the composite actor "convergence loop" in the Kepler ETS workflow.

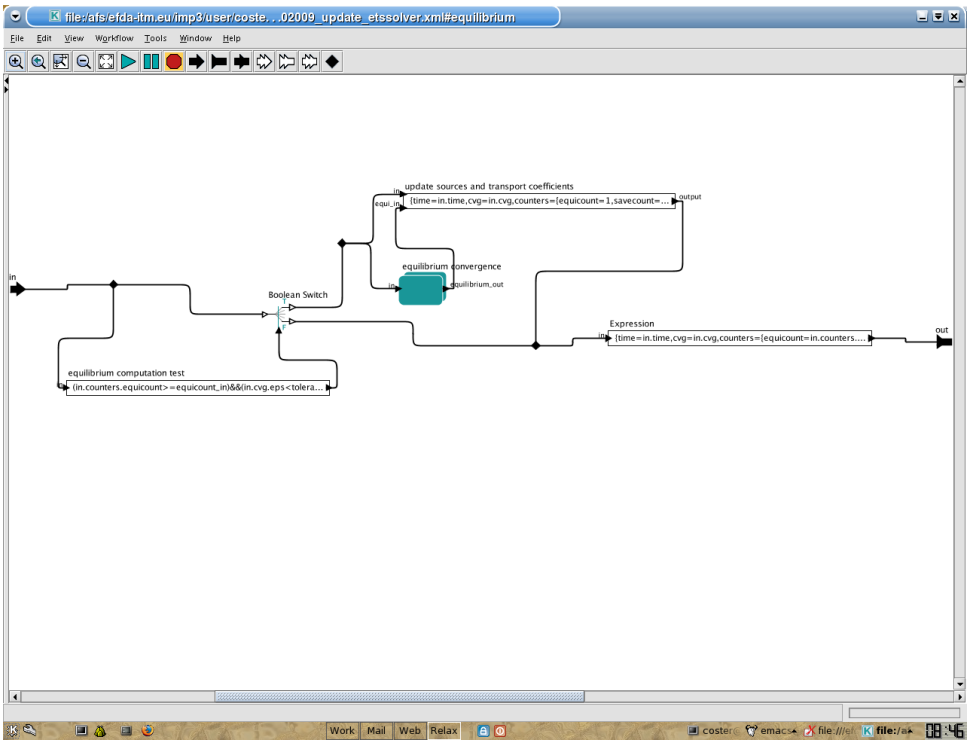

Figure 93: Zoom in of the composite actor "equilibrium" in the Kepler ETS workflow.

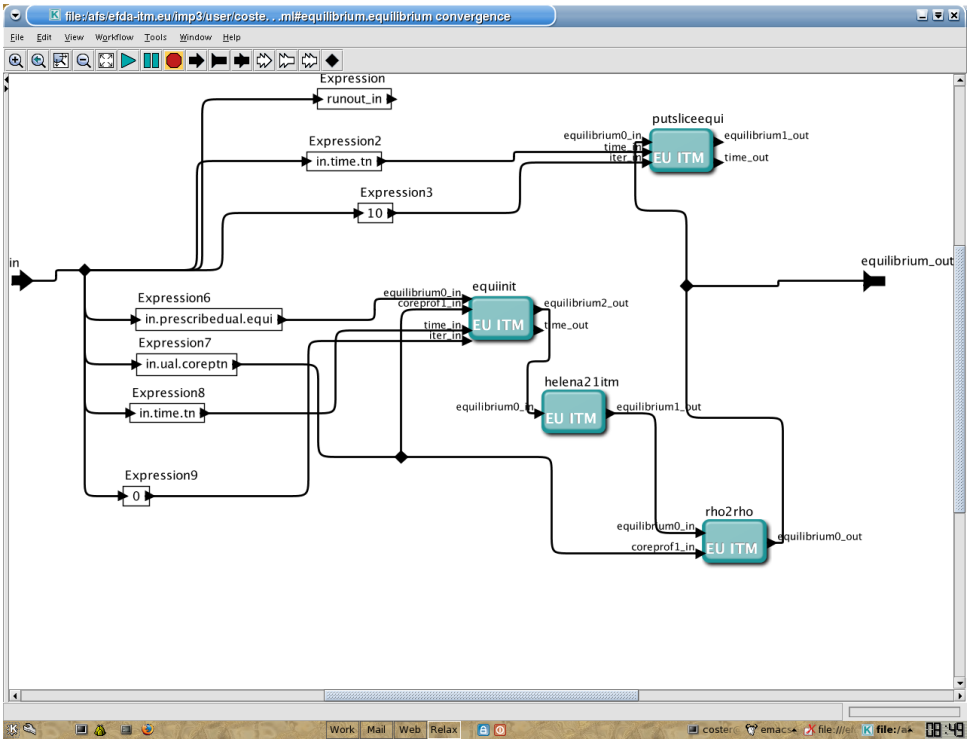

Figure 94: Zoom in of the composite actor "equilibrium convergence" in the composite actor "equilibrium" in the Kepler ETS workflow.

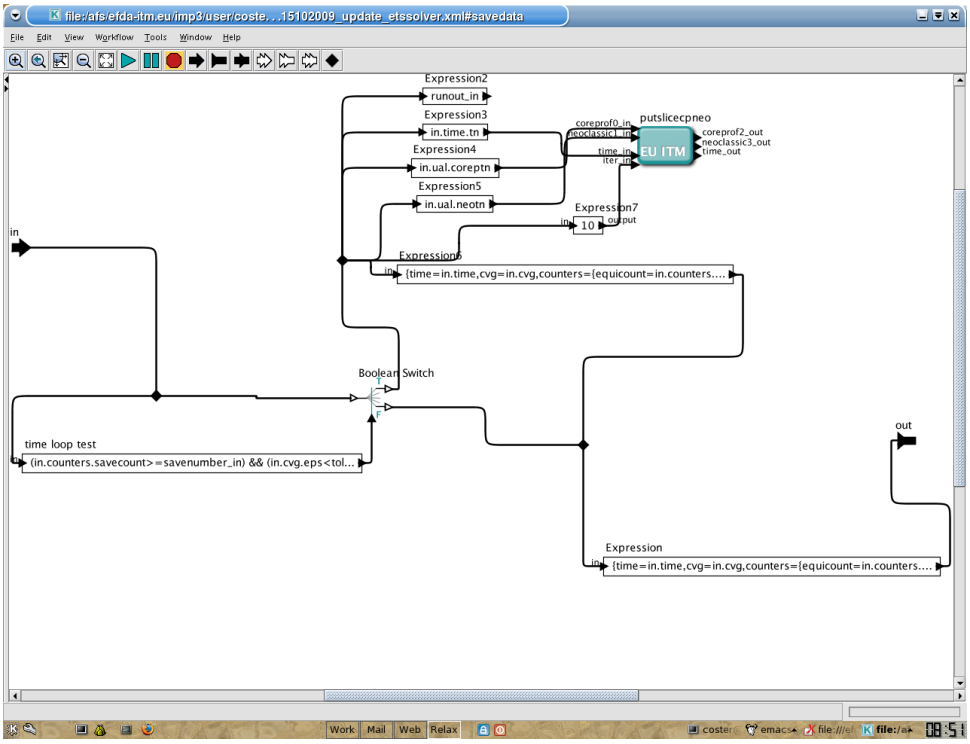

Figure 95: Zoom in of the composite actor “save data” in the Kepler ETS workflow.

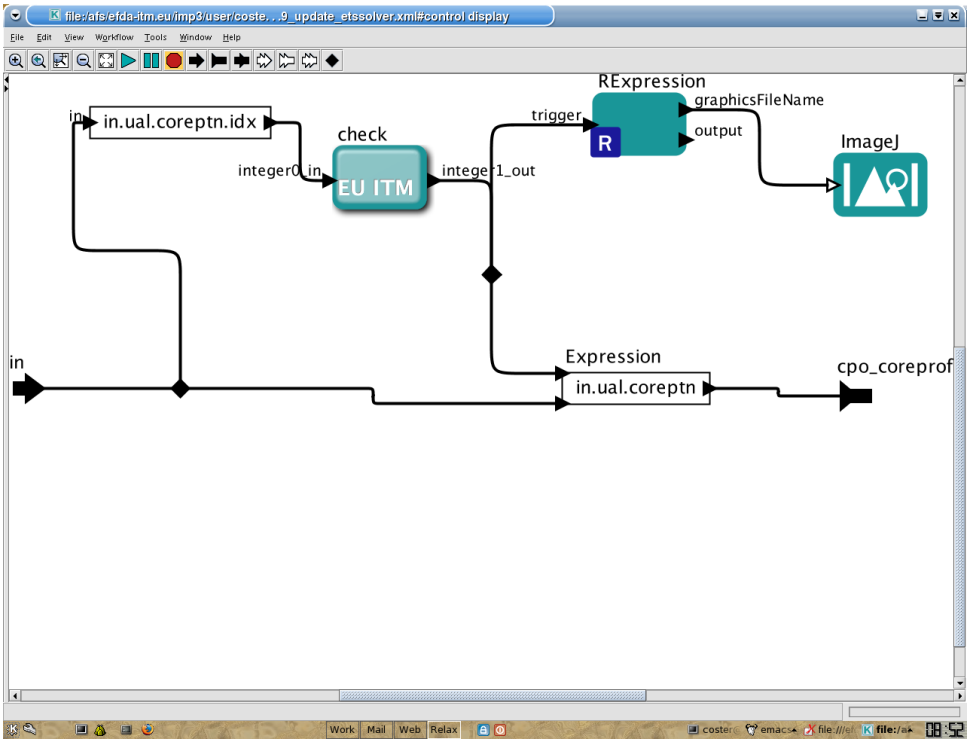

Figure 96: Zoom in of the composite actor “control display” in the Kepler ETS workflow.