From: Martha Redi
To: M. Zarnstorff, NCSX Team
Date: 2/25/00
Re: Benchmarking of NEO code against other measures of transport

The purpose of this memo is to document the performance of the Nemov-Kernbichler NEO code (V. V. Nemov, S. V. Kasilov, W. Kernbichler, M. F. Heyn, Phys. Plas. **6**, 4622 (1999)) and the benchmarking of this code against other calculations of stellarator transport. It is found that NEO calculations follow the GTC and ORBIT results better than other methods used for rapidly calculating particle transport for QAS. This supports the incorporation of the NEO code into the stellarator optimizer.

1. Benchmarking the NEO code against other measures of Transport

Here are summarized the results of calculating neoclassical particle transport in a group of compact quasiaxial stellarators – three sets of thermal ion transport calculations and three measures of field line asymmetry, important for orbit confinement. As energetic particle loss ratios parallel the transport measures for thermal ions, these results are also included.

The measures used to estimate transport (in Tables I and II) are obtained from calculations of χ^2 (= ΣB_{mn}^2, for $n\neq0$, normalized by B_{oo}^2), chi2-J, a measure of the adiabatic invariant $J = \int v_{//} dl$ and the codes NEO, GTC, DKES and ORBIT3D. NEO calculates an estimate of trapped particle, non-axisymmetric transport only, with output being an effective ripple $\varepsilon^{1.5}$, proportional to the particle flux density crossing each surface. GTC (Ref. ?) is an enhanced, parallelized Monte Carlo code which calculates the global thermal ion particle flux, expressed as a confinement time, based on a δf method. DKES (Ref?) calculates the thermal particle flux from neoclassical analytic expressions. The GTC and DKES code results in the tables are specifically for transport in NCSX and both include a model electric field. Results for two values of ν/v are given. χ_J^2 is the deviation of J within a flux surface and its calculation as for NEO, is only for trapped particles and does not include the effects of electric fields. χ_J^2 weights the whole volume equally. ORBIT3D (White, Chance, Phys. Fluids **27**, 2455 (1984)) is a full Monte Carlo code that follows particles, with or without the collisional effects of pitch angle scattering. The ORBIT3D results in the tables are for energetic alpha particles, in a size-scaled reactor.

Four three-field-period QAS cases are used for comparison: QASC10, QASC93, QASC82, and QASI63. Figure 1 is a plot from Long-poe which shows χ^2. Figure 2 is a plot of the results of the NEO code, $\varepsilon^{1.5}$ for three of the stellarators, in addition to QAS2_40 (see Redi, Phys. Plas. **6**, 3509 (1999)). The tables summarize the data from these figures at the plasma edge, along with

summaries of GTC and DKES results reported in an earlier memo from Ku, χ_J^2 from the 1/11/00 Project Meeting (Spong) and results of ORBIT3D code calculations. Table I shows code results. Table II shows these results normalized to the C82 transport for each method.

Table I	C10	C93	C82	I63
GTC Flux	0.9	0.95	1.0	
χ^2	0.0032	0.0031	0.005	
NEO $\varepsilon^{1.5}$	0.009	0.012	0.002	0.05
χ_J^2	2550	3100	1850	
DKES, s=0.5, ν/v=0.0001	0.87	0.95	1.0	
DKES, s=0.5, ν/v=0.001	1.0	1.20	0.97	
ORBIT3D Eloss collisional	36%		36%	36%
ORBIT3D Eloss collisionless	23%		23%	25%

Table II	C10	C93	C82	I63
GTC Flux	0.9	0.95	1.0	
χ^2	0.64	0.62	1.0	
NEO $\varepsilon^{1.5}$	0.45	0.6	1.0	2.5
χ_J^2	1.4	1.7	1.0	
DKES, s=0.5, ν/v=0.0001	0.87	0.95	1.0	
DKES, s=0.5, ν/v=0.001	1.0	1.2	1.0	
ORBIT3D Eloss collisional	1.0		1.0	1.0
ORBIT3D Eloss collisionless	1.0		1.0	1.1

Figure 3 displays the trends. The GTC results represent our best estimate of neoclassical particle transport in these QAS, while χ^2 is presently used in the optimizer. Particle transport is best in QASC10 and becomes increasingly worse in C93 and C82.

The trends of the ratios of the NEO edge $\varepsilon^{1.5}$ and from DKES at s=0.5, ν/v=0.0001 are in agreement with GTC as are the trends of the ORBIT3D ratios. The trends of the ratios of the edge values of χ^2 are not in agreement with GTC, nor are the trends of χ_J^2, nor the trends of the DKES results at s=0.5, ν/v=0.001.. GTC calculations for confinement times at radii inside the last closed flux surface at present (for 4000 particles) have error bars too large to discriminate among the three QAS C10, C82 and C93.

While the NEO results show the same trends as GTC, the variation of $\varepsilon^{1.5}$ is stronger than for the GTC τ_E. This is presumably due to the electric field in the GTC and DKES calculations, and due to NEO only calculating the $1/\nu$ contribution. Thus, it may be that the quantitative variation of $\varepsilon^{1.5}$ is more similar to the variation of χ_e .

Why include energetic ion transport in the Tables? Neoclassical energetic ion transport differs from thermal because of the larger Larmor radius, ρ_L. Comparing birth energy alphas to thermal deuterium ions (at 10 keV) the ratio of Larmor radii is 13. Bad first orbit and stochastic ripple losses are increased for larger ρ_L/a. Neoclassical energetic ion losses can also differ from thermal losses because energetic ions sample a larger fraction of the plasma volume. The rates of pitch angle scattering are also different. Nevertheless, a rough correlation has been found between thermal ion diffusion coefficients and energetic ion loss rates for QAS with ORBIT3D. Figure 4 (Redi, Phys. Plas **6**, 3509 1999) shows that the thermal ion diffusion coefficients and parallel beam ion loss rates have qualitatively the same dependence on edge poloidal flux for five different compact QAS and two related tokamaks. Table II and Figure 3 show also that ORBIT3D results for energetic ion transport are similar, but do not exactly parallel the trends of thermal ion transport from GTC.

2. Suggested use of NEO code in optimizer.

Figure 2 shows the effective $\varepsilon^{1.5}$ for 4 stellarators. The relative effective ripple at the outermost flux surfaces parallels the thermal particle flux from GTC evaluated at the edge. The curves cross so that the relative values of the effective ripple at r/a=0.5 do not reproduce the relative global flux from GTC.

The choice of flux surfaces for NEO output should be parametrized in the optimizer. Initially I'd suggest minimizing the effective ripple at the last closed flux surface in the optimizer, as the figure of merit to keep transport low.

It is important to make sure that the surfaces on which $\varepsilon^{1.5}$ is evaluated are not low order rationals, as the method breaks down and gives rise to small anomalous bumps at those sufaces (see Figure 5). Figure 5 shows results for two QAS based on Paul Garabedian designs, for W7X and for C82.

With respect to reactor performance: the electric field effect relied on by W7X for reduction of alpha collisional losses has been shown not to be effective for alpha particles, so that alpha losses in the Helias reactor appear to be ~7%. SInce ITER's limit was 5%, our configuration optimization goal should be particle losses lower than the W7X level.

3. Structure of NEO code

The code was written by W. Kernbichler and S. Nemov. The source code has been run at PPPL on the MARS DEC alpha and gives identical results to those sent from Graz in December, 1999. Time of calculations is roughly 30 seconds per flux surface on a DEC alpha.

The code package includes

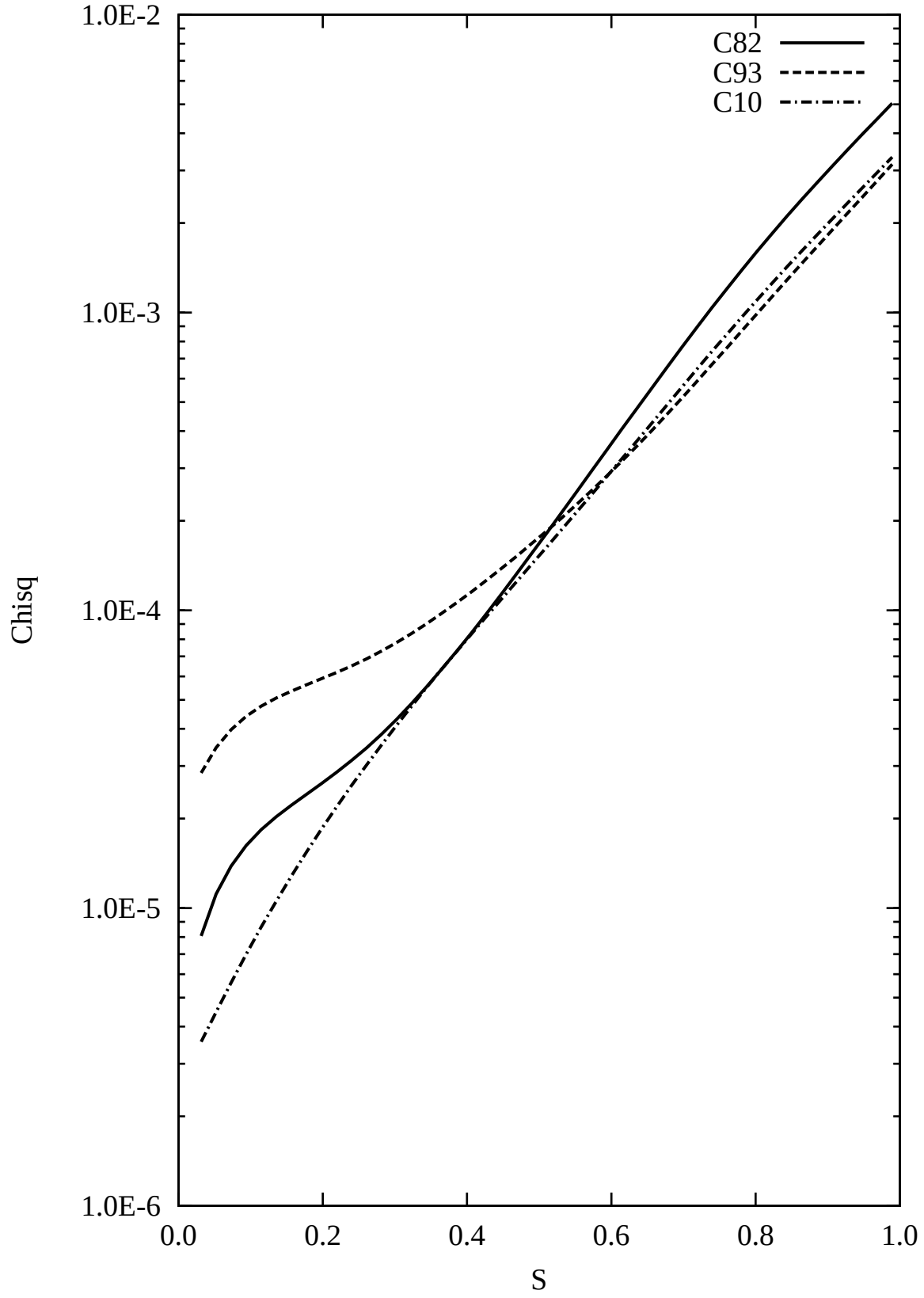
- *.f90 files - Fortran 90 code
- Makefile - a make file, which worked on DEC Alpha and two different Linux compilers
- neo.in - an Input file with remarks
- Bmn* - one of our Bmns files
- *.m - some Matlab files for plotting

There is some documentation in the f90 files.

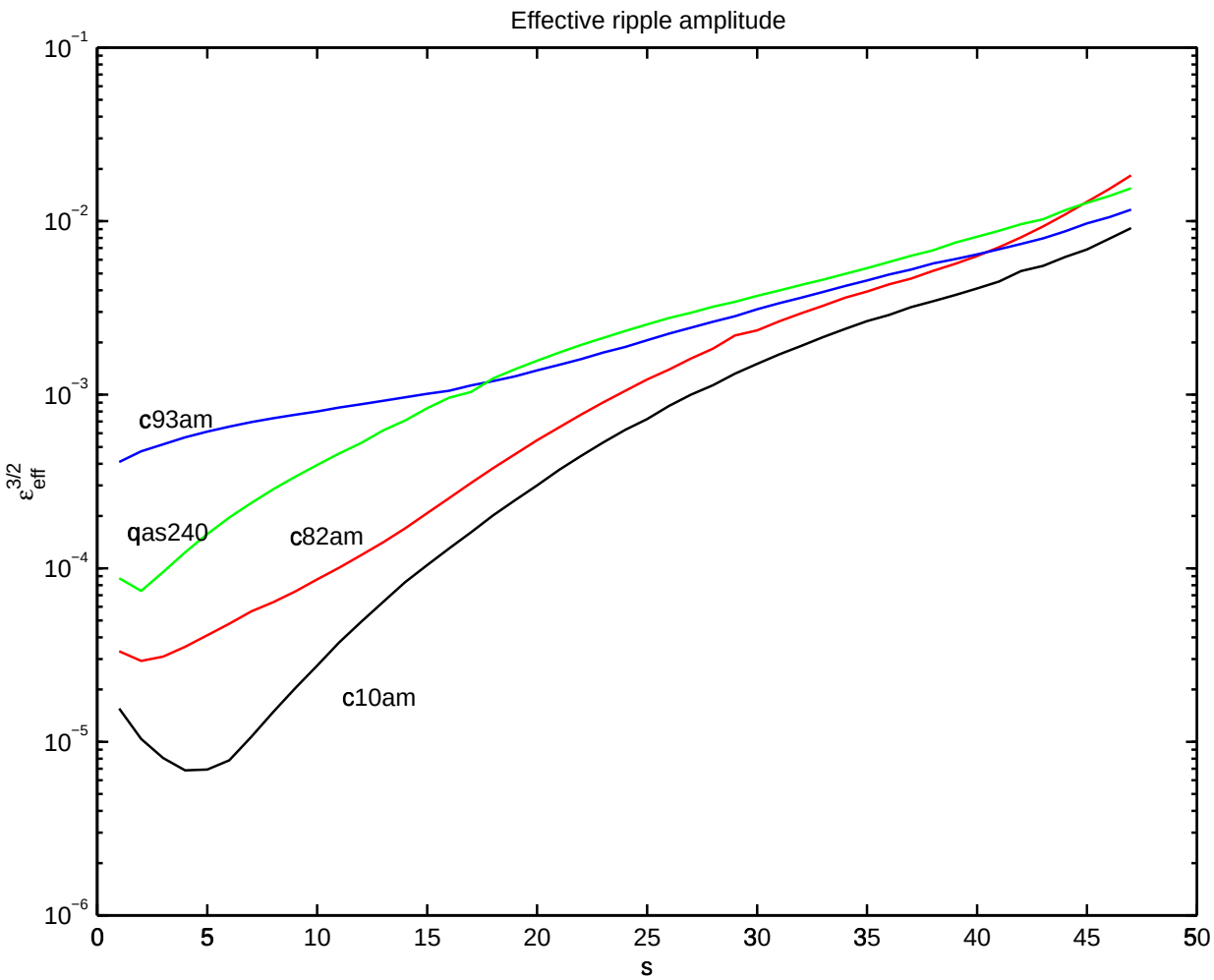
- The whole code uses the modules in neo_modules.f90 for definitions and for data exchange between different routines.
- neo: main routine, loop for flux surfaces
- neo_sub: a collection of subroutines for reading, Fourier summation, spline handling, ...
- pspline: collection of spline routines (1-D, 2-D, periodic and non-periodic). 2-D periodic spline is used for 4 quantities for speed.
- flint_bo: contains the integration according to the paper
- rk4d_bo: differential equation solver
- rhs_bo: right hand side of differential equation.

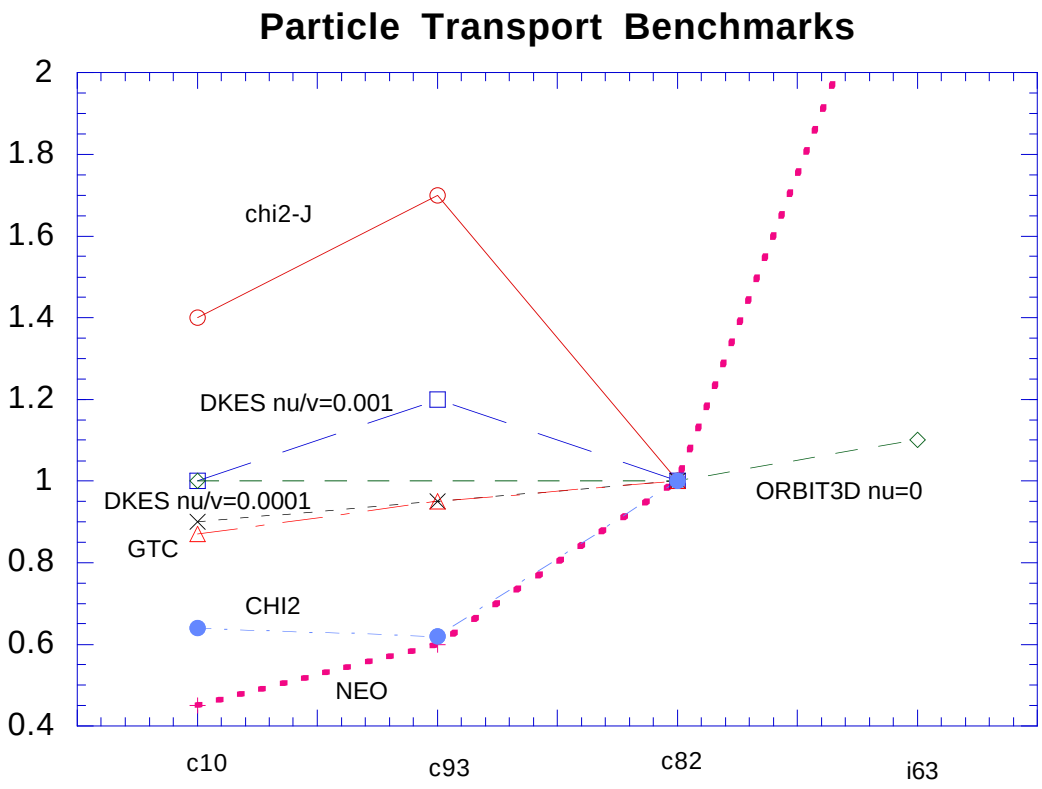
4. How to run the code on MARS:

   - Edit neo.in so that first two lines refer to “Bmns…” file for equilibrium of interest.
   - Edit neo.in to select the flux surfaces of interest: psi_is is the start index, psi_ie is the end index, psi_id is the delta index [0 gives all surfaces]
   - Delete all files *.o
   - type “gmake”
   - type “neo”. Produces an output file called “Bmns….”.dat giving on each line: the flux surface #, an effective radius, the effective $\varepsilon^{1.5}$, and several other quantities. Evaluation of $1/\nu$ transport will require for each flux surface of interest, only the flux surface number and the effective $\varepsilon^{1.5}$.

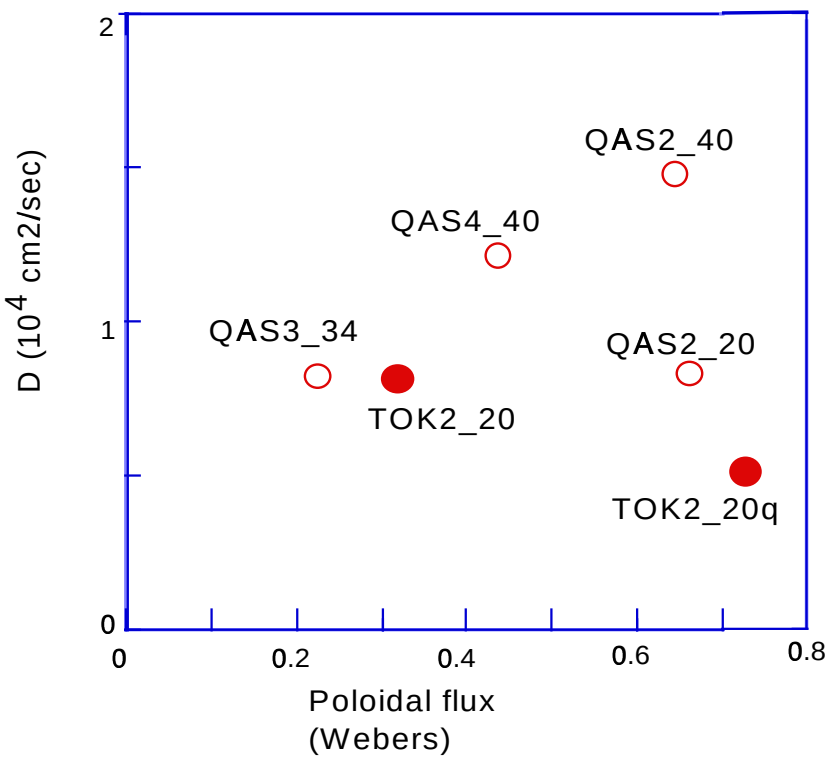

1.0E-2
1.0E-3
1.0E-4
1.0E-5
1.0E-6
Chisq
0.0
0.2
0.4
0.6
0.8
1.0
S
C82
C93
C10

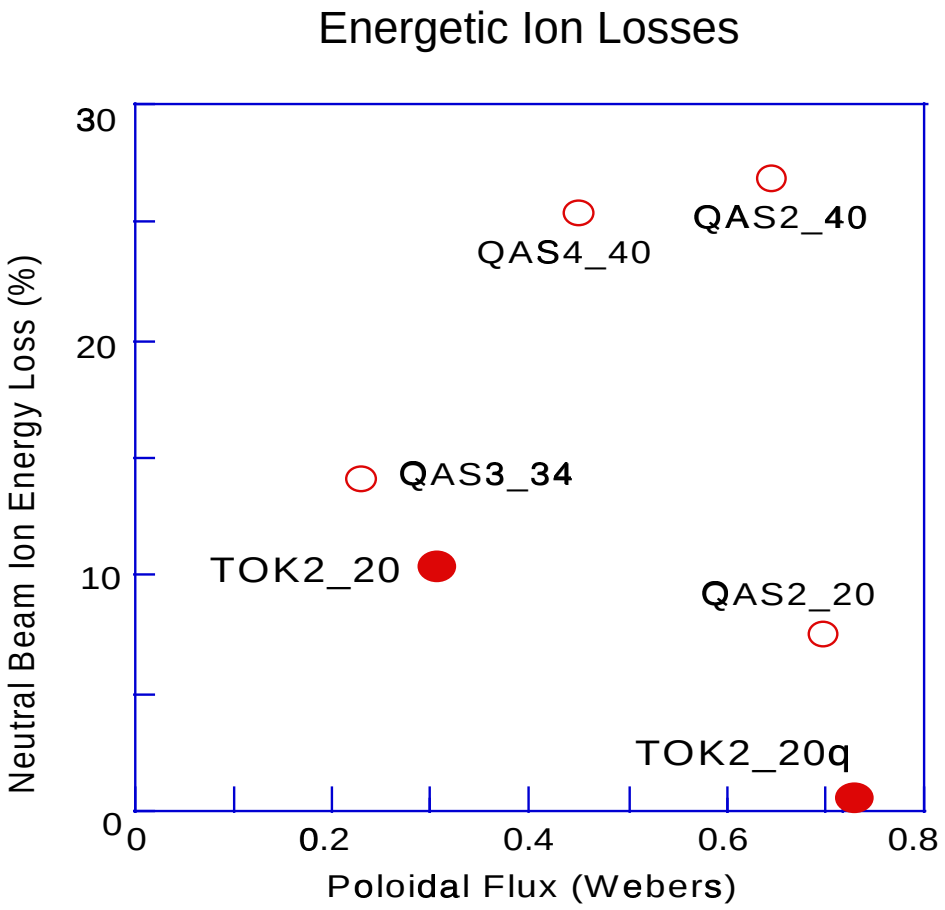
NEO calculations of effective ripple on log plot

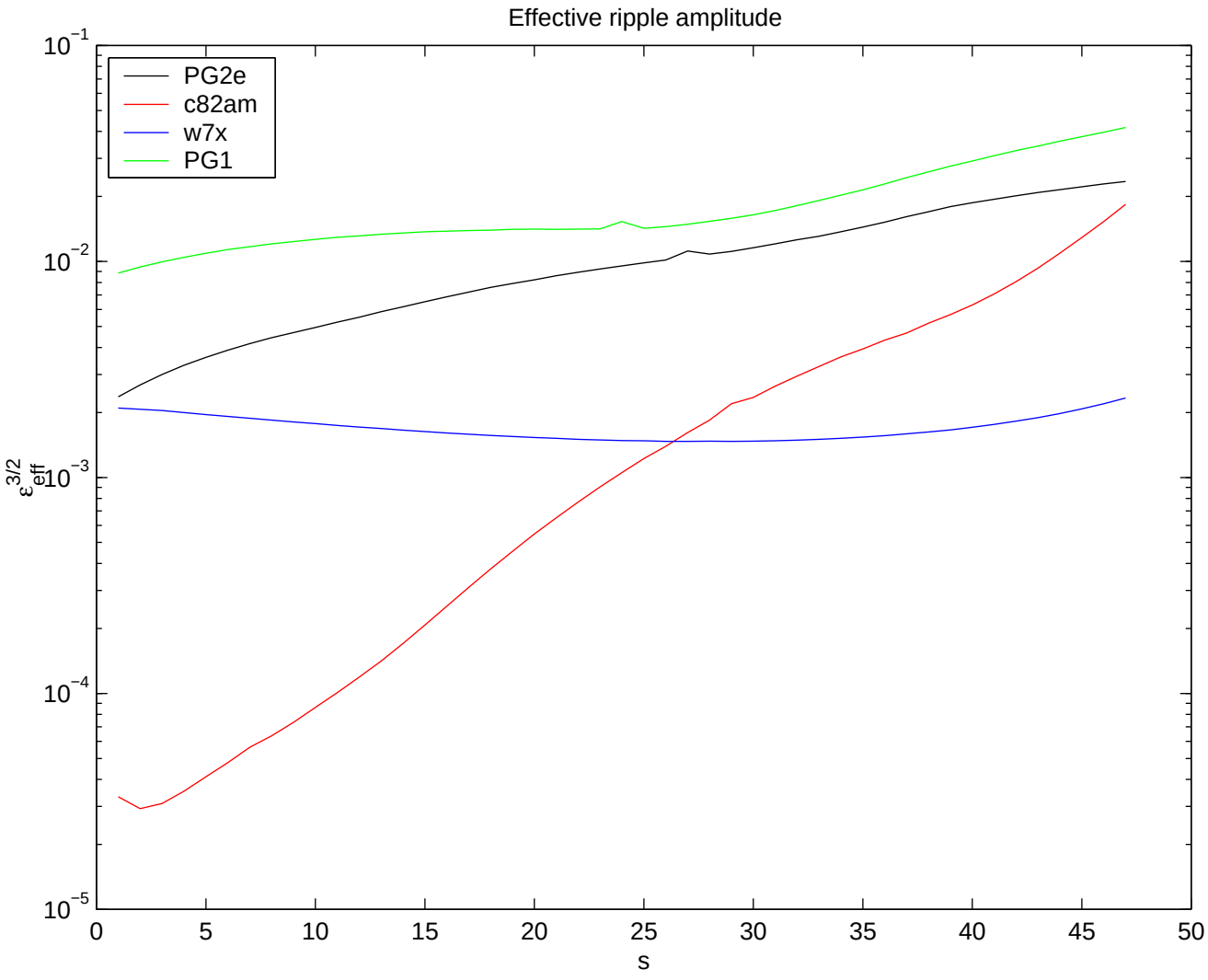



Particle Transport Benchmarks
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
chi2-J
DKES nu/v=0.001
DKES nu/v=0.0001
GTC
CHI2
NEO
ORBIT3D nu=0
c10
c93
c82
i63

Thermal Ion Diffusion Coeffiecients




Energetic Ion Losses
Neutral Beam Ion Energy Loss (%)
30
20
10
0
0
0.2
0.4
0.6
0.8
Poloidal Flux (Webers)
QAS2_40
QAS4_40
QAS3_34
TOK2_20
QAS2_20
TOK2_20q


Effective ripple amplitude
PG2e
c82am
w7x
PG1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
$\varepsilon_{eff}^{3/2}$
0
5
10
15
20
25
30
35
40
45
50
s