A brief introduction to GENE

Gene Development Team

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WARNING

This tutorial aims at providing the basics for installing and running GENE. Please check

- the website http://genecode.org
- the website http://genecode.org

the documentation

for more recent or more detailed information regarding required libraries, input parameters, file formats etc.!

Outline

- What is GENE?
- Property and Appendix and Ap
- Setting up a simulation
- Analyzing and post-processing
- The Diagnostics Tool

What is GENE?

GENE = **G**yrokinetic **E**lectromagnetic **N**umerical **E**xperiment

- designed for numerical investigations of plasma microturbulence
- ullet solving the δf -splitted gyrokinetic system of equations using a Eulerian approach (fixed grid) in 5D phase space
- initial value or eigenvalue computations
- radially local^a (flux tube) or global (up to full torus) simulation domain
- various interfaces to MHD equilibrium codes and transport solvers
- massively parallelized using (mainly) MPI and OpenMP

^aaddressed in this tutorial

Gyrokinetic system of equations I

Gyrokinetic Vlasov equation per species σ with collisions

$$\frac{\partial f_{\sigma}}{\partial t} + \dot{\mathbf{X}} \cdot \nabla f_{\sigma} + \dot{\mathbf{v}}_{\parallel} \frac{\partial f_{\sigma}}{\partial \mathbf{v}_{\parallel}} + \dot{\mu} \frac{\partial f_{\sigma}}{\partial \mu} = C(f_{\sigma}, f_{\sigma'})$$
(1)

gyrocenter position X

$$\dot{\mathbf{X}} = v_{\parallel} \mathbf{b}_0 + \frac{B_0}{B_{0\parallel}^*} \mathbf{v}_{\perp}$$

with the combined drift velocities

$$egin{aligned} \mathbf{v}_{\perp} &\equiv & rac{c}{B_0^2} ar{\chi}_1 imes \mathbf{B}_0 + rac{\mu}{m_{\sigma}\Omega_{\sigma}} \mathbf{b}_0 imes
abla B_0 \ &+ rac{v_{\parallel}^2}{\Omega_{\sigma}} (
abla imes \mathbf{b})_{\perp} \end{aligned}$$

and the generalized potential

$$\bar{\chi} = \bar{\phi}_1 - \frac{v_{\parallel}}{c} \bar{A}_{1\parallel} + \frac{\mu}{q_{\sigma}} \bar{B}_{1\parallel}$$

parallel velocity v_{\parallel}

$$\dot{v}_{\parallel} = rac{\dot{\mathbf{X}}}{m_{\sigma}v_{\parallel}} \cdot \left(q_{\sigma}ar{\mathbf{E}}_{1} - \mu
abla(B_{0} + ar{B}_{1\parallel})
ight)$$

with the electric field

$$\mathbf{E}_1 = -\nabla \phi_1 - \frac{\mathbf{b}_0}{c} \frac{\partial}{\partial t} A_{1\parallel}$$

 $\operatorname{magnetic} \operatorname{moment} \mu$

$$\dot{\mu} = 0$$

... which is δf -splitted in GENE

Gyrokinetic system of equations II

Gyrokinetic field equations

Poisson equation

$$\nabla_{\perp}^2 \phi_1 = -4\pi \sum_{\sigma} q_{\sigma} n_{1\sigma}$$

Ampère's law

$$\nabla_{\perp}^{2} A_{1\parallel} = -\frac{4\pi}{c} \sum_{\sigma} j_{1\parallel\sigma}$$

$$B_{1\parallel} = -4\pi \sum_{\sigma} \frac{p_{1\perp,\sigma}}{B_{0}}$$

... all in all a nonlinear, 5D partial integro-differential system of equations

Relevant moments (in local approx./Fourier space)

$$\begin{split} n_{1\sigma,\mathbf{k}} &= \frac{2\pi B_0}{m_\sigma} \! \int \! \mathrm{d}\nu_\parallel \mathrm{d}\mu \left[J_0 h_{1\sigma,\mathbf{k}} - q_\sigma \phi_{1,\mathbf{k}} \frac{F_{0\sigma}}{T_{0\sigma}} \right] \\ j_{1\parallel\sigma,\mathbf{k}} &= & q_\sigma \frac{2\pi B_0}{m_\sigma} \! \int \! \mathrm{d}\nu_\parallel \mathrm{d}\mu \ \nu_\parallel \left[J_0 h_{1\sigma,\mathbf{k}} - q_\sigma \phi_{1,\mathbf{k}} \frac{F_{0\sigma}}{T_{0\sigma}} \right] \\ p_{1\perp\sigma,\mathbf{k}} &\equiv & \frac{2\pi B_0}{m_\sigma} \! \int \! \mathrm{d}\nu_\parallel \mathrm{d}\mu \ \mu B_0 I_1 h_{1\sigma,\mathbf{k}} \end{split}$$

with the nonadiabatic part of f_1

$$h_{1\sigma} \equiv f_{1\sigma} + \left[q_{\sigma} J_0 \phi_1 + \mu I_1 B_{1\parallel} \right] \frac{F_{0\sigma}}{T_{0\sigma}}$$

and the Bessel functions

$$J_0 = J_0(k_{\perp}\rho)$$

 $I_1 = I_1(k_{\perp}\rho) = 2J_1(k_{\perp}\rho)/(k_{\perp}\rho)$

How to get and install GENE

How to get and compile the code

- visit http://genecode.org, fill and submit the short form in "Get GENE"
- download the code as indicated via email
- git clone https://<USER>@gitlab.mpcdf.mpg.de/GENE/gene.git -b release-<X.Y> <genedir>
- ochange to the <genedir> directory
- call make doc or gmake doc to create the documentation to be found in <genedir>/doc/gene.pdf
- o call make mach_wrapper and check resulting string <mach>
 - if <mach> is other than new_machine and clearly related to your machine, check the header of makefiles/<mach>/<mach>.mk for modules to be loaded on some machines you may also run make get_required_modules (skip the next slide)
 otherwise, you need to set up the machine dependent part of the makefile (see next slide)
- finally, type make (or make -j for parallel compilation); the resulting binary can be found in <genedir>/bin/gene_<mach>

Setting up the makefile for an unknown machine

- define a meaningful name for your machine (<mach> in the following)
 - either by adding an appropriate identification in <genedir>/makefiles/machine.def (preferred; one time change only)
 - or by permanently setting the environment variable MACHINE
- copy and rename the makefile template from

```
<genedir>/makefiles/new_machine/new_machine.mk to
<genedir>/makefiles/<mach>/<mach>.mk
```

- open <genedir>/makefiles/<mach>/<mach>.mk, search for and fill at least the following tokens (check the documentation for details)
 - ▶ the Fortran compiler COMPILER (e.g., intel, gnu, cray, pgi, etc.)
 - FFTLIB (fftw, mkl or essl) and the corresponding block
 - ▶ the compiler flag for double precision (search for DOUBLE_PREC)
 - the complex versions of PETSC and SLEPC via PETSC_DIR, SLEPC_DIR, PETSC_ARCH; set SLEPC = yes
- compile, run the test suite and optionally send modifications to support@genecode.org

note: changes to makefiles/<mach>/<mach.mk> require gmake distclean

Setting up a simulation

Running GENE

Example

This would be the way how to call GENE in a shell or batch script with 8 MPI processes $mpiexec -n 8 ./gene_<mach>$ where mpiexec -n might need to be substituted by mpirun, aprun, poe. ...

The input file

The simulation parameters are set in the parameters input file which must be located in the same directory & will be read upon simulation start

Remarks

- a strategy to organize your simulations is to create individual prob (~ problem)
 directories containing parameters, a link to the executable, batch scripts, etc. for
 each of them
- the command . /newprob in <genedir> will automatically perform those steps

The parameters input file

Setting up the parameters input file is the crucial part when attempting to run a simulation. As this file uses formatted data and Fortran namelists, it can either be modified with

(a) the text editor of your choice

or

- (b) the graphical launcher
 - ... which furthermore tries to automatically resolve inconsistencies and assist with job submission

The parameters file - parallelization namelist

```
&parallelization
n_procs_s = 1 !divisor of n_spec
n_procs_v = 1 !divisor of nv0 (max: 0.5*nv0)
n_procs_w = 8 !divisor of nw0
n_procs_y = 1 !divisor of nky0 (keep low)
n_procs_z = 1 !divisor of nz0 (maximum: 0.5*nz0)
/
```

- This namelist sets the number of MPI processes in each dimension.
- Set to \leq 0 if the appropriate value is unknown and should be detected by GENE (will increase the initialization time); Lower (upper) bounds for the automatic parallelization tests can be specified by $\min_{n} pA \pmod{max_npA}$ where A=s,v,w,y or z.

The parameters file - box namelist I

Perpendicular box sizes

&box kymin = 0.05 ! min. binormal Fourier mode adapt_lx = .t. ! adapt lx to to ky mode (in linear sim's) lx = 128. ! radial box width (determines Δk_x)

- ullet typical kymin value $\lesssim 0.1$ (ly $\gtrsim 60\,
 ho_{
 m ref}$) for nonlinear sim's
- adapt_lx = .t. replaces lx by 1/(ky·shat) to maximize number of poloidal connections nexc in linear sim's
- 1x should be $\gtrsim 60 \, \rho_{\rm ref}$ and will be adjusted to kymin \cdot shat \cdot lx \in N; alternatively, the number of poloidal connections nexc can be specified

```
kx_center = 0.0 ! kx center value for linear studies
```

• typically, linear investigations are considering the dominant nonlinear mode which is typically $k_x = 0$ (+connections); however, particularly in strongly shaped geometries other k_x values might be interesting, as well.

The parameters file - box namelist II

Perpendicular grid points

```
n \times 0 = 128 !number of grid points in x direction n \times y = 16 !number of Fourier modes in y direction
```

guideline for perpendicular grid points:

- linearly:
 - ▶ at least $nx0 \gtrsim 4$ (if adapt_lx is true)
 - nky0 = 1 individual simulations per ky are recommended!
 - $k_v = \text{kymin}$ (and multiples if nky0>1)
 - nonlinearly:
 - radial resolution lx/nx0 < 1 (down to $\mathcal{O}(0.1)$);
 - number of Fourier modes in binormal (y) direction should be $kymin \cdot nky0 \gtrsim 1.0$ (check for vanishing growth rate with linear sim's);
 - powers of low prime numbers are recommended (better FFT performance)
 - $k_y = 0$, kymin, ..., kymin · (nky0 1)

remark: number of y grid points in real space ny0 = 2 nky0

The parameters file - box namelist III

Velocity space grid

```
lv = 3.0 ! box size in \nu_{\parallel} direction lw = 9.0 ! upper simulation box end in \mu direction
```

- Iv should be ≥ 3.0 (in units of $v_{T\sigma} = (2T_{\sigma 0}/m_{\sigma})^{1/2}$, σ : species index)
- the parallel velocity points span the range from $-v_{T\sigma}$ to $v_{T\sigma}$
- Iw should be ≥ 9.0 (in units of $T_{\sigma 0}/B_{\rm ref}$)

```
nv0 = 32 !v_{\parallel} grid points (usually 32, 64)

nw0 = 8 !\mu grid points (typically 8, 16)
```

• equidistant grid in v_{\parallel} , Gauss-Laguerre knots for μ grid

The parameters file - box namelist IV

```
nz0 = 16 !grid points in z(\parallel) direction
```

- simple circular geometries: 16 or 24 parallel grid points sufficient
- realistic MHD-equlibria: up to 100 grid points needed

```
n_spec = 1 !number of particle species
```

n_spec = 1: oppositely charged species is assumed to be adiabatic!

```
x0 = 0.5 !macroscopic radial position of box center in L_{\rm ref}
```

• req'd only if some parameters are set by MHD or profiles interfaces; often given as normalized $\rho_{\rm tor}$

The parameters file - in_out namelist

Usually, no changes are needed in this namelist except for the following parameters:

```
&in_out
diagdir = '/ptmp/exampledir' ! output file dir
read_checkpoint = .f.
```

- output files (e.g. nrg, mom, field) are written to diagdir;
 make sure to use a high performance I/O file system
- to continue an old simulation set read_checkpoint to .t. to read an existing checkpoint file from chptdir (=diagdir by default) when starting the next simulation

The parameters file - general namelist I

```
&general nonlinear = .t. !switch on/off nonlinear terms
comp_type = 'IV' !initial(IV) or eigenvalue(EV) comput.
```

```
comp_type = 'IV' calc_dt = .t. !switch on/off !dt_max calculation dt_max = 0.0385 !maximum time step !in L_{\rm ref}/c_{\rm ref}
```

```
comp_type = 'EV' (lin. only)
n_ev = 1 !no. of EVs
```

- calc_dt = .t.
 - PETSc/SLEPc linked → exact determination of dt_max
 - not linked → approximated by CFL
- calc_dt = .f.
 - ▶ use dt max

The parameters file - general namelist II

Termination conditions

```
ntimesteps = 100000 !maximum number of time steps
timelim = 64500 !(system) time limit in sec
simtimelim = 5000 !simulation time limit
omega_prec = 1e-3 !convergence precision (absolute value)
```

- simulation will stop in a controlled way, if
 - number of time steps exceeds ntimesteps
 - ▶ simulation runs longer than timelim seconds; set < wallclock limit!
 - ightharpoonup simulation time in $L_{\rm ref}/c_{\rm ref}$ reaches simtimelim
 - growth rates and real frequencies are converged up to a precision of omega_prec (only for linear simulations and istep_omega > 0).

The parameters file - general namelist III

Physics parameters

```
beta = 0.71E-02 !\beta_{\rm ref} \approx 403 \cdot 10^{-5} n_{\rm el9} T_{\rm ref,keV}/B_{\rm ref,\it{T}}^2 coll = 0.68E-02 !normalized collision frequency collision_op = 'landau' !'landau','sugama', or 'none' debye2 = 0.0 !normalized \lambda_{\rm Debye}^2/\rho_{\rm ref}^2
```

Hyper diffusion

```
hyp_x = 0.0 !radial hyper diffusion (keep small)

GyroLES = T !nl. sims only! adaptive perp. hyper diffusion

hyp_z = 2.0 !parallel hyper diffusion

hyp_v = 0.2 !\nu_{\parallel} hyper diffusion (collisionless sims only)
```

- If parallel profiles show zig-zag patterns and nx0 and/or nz0 cannot be increased try hyp_z = -1 for automatic adjustment
- to avoid recurrence effects, we recommend to set hyp_v to a value $\sim 0.1-0.5$ in **collisionless** simulations and to 0 or small values else

The parameters file - geometry namelist

Geometry

analytic models: s_alpha, circular, miller, slab

```
q0 = 1.4 !safety factor q shat = 0.796 !magnetic shear parameter amhd = 0.0 !\alpha_{\rm MHD} = -q^2 R \left(d\beta/dr\right) (-1 for automatic) trpeps = 0.18 !r/R at flux tube position r major R = 1.0 !major radius with respect to L_{\rm ref}
```

interfaces: chease, tracer_efit, gist

minimum requirement:

```
geomfile = 'examplefile' !declaration of interface file
```

Optional: enforce plasma current (Ip) / toroidal magnetic field (Bt) orientation (see documentation)

```
sign_Ip_CW = -1 !counter-/clockwise (-1/1)
sign_Bt_CW = 1 !counter-/clockwise (-1/1)
```

The parameters file - species namelist(s)

Add a species namelist for each species:

check documentation for interfaces to profile files (e.g., prof_type iterdb file, etc.)

The parameters file - units namelist

Optional(!) namelist for

- denormalisation in post-processing routines
- ullet consistent and automatic calculation of physics parameters as, e.g., eta

• check documentation for automatic calculation in profile file interface cases

The parameters file - automatic computations

Recommended/helpful settings if all ref. value are filled/requested(*) in units:

```
&hox
n0 \text{ global} = -1111 \text{ !find min. toroidal mode number closest}
                  !to given kymin or force a given value
adapt_ly = T !adapt kymin to n0_global for given rhostar;
             !recommended for applications to expt.
&general
beta = -1! beta consistently from ref. values
coll = -1 !coll consistently from ref. values
debye2 = -1 !debye2 consistently from ref. values
zeff = -1 ! zeff from data base(*)
&geometry
amhd = -1 !amhd consistently from gradients and beta
rhostar = -1 !rhostar consistently from ref. values
dpdx_pm = -2 !pressure gradient from equilibrium (amhd)
&external_contr
ExBrate = -1111 !ext. shear flow rate from data base(*)
pfsrate = -1111 !parallel flow shear rate from data base(\star)
```

(*) requires active data base interface (see documentation/prof_type)

The parameters file

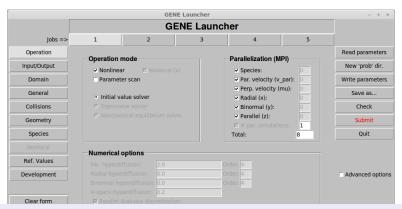
Some remarks

• Information on further parameters, e.g. concerning the initial condition, numerical schemes, frequency of data ouput, etc. can be found in the GENE documentation located in the /doc/ subdirectory of your GENE installation.

Convergence

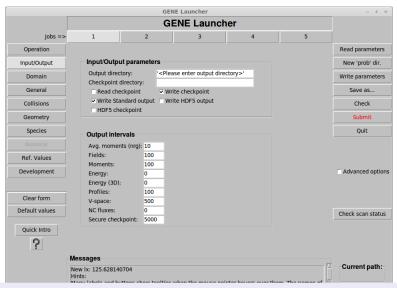
 In principle, each simulation has to be carefully checked for convergence with regard to numerical parameters that is e.g. doubling box sizes and/or grid resolution for testing purposes.

Setting parameters with the launcher I



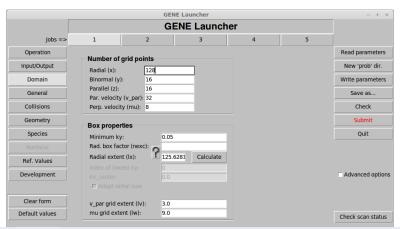
- start python based GUI by calling ./GENE-GUI.py in <genedir>
- click on Default values to fill with Cyclone-like parameters
- set a least the number of total MPI processes and check all parallelization choices if not sure what to do here
- click on New 'prob' dir. for creating a new problem directory
- ... and finally save your parameters here

Setting parameters with the launcher II



fill at least the Output directory

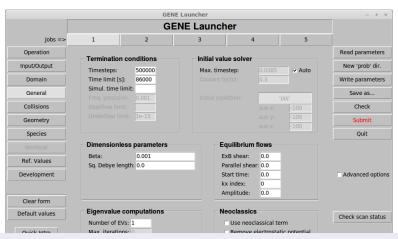
Setting parameters with the launcher III



- fill proper grid numbers (rules of thumb in previous section)
- note that the number of poloidal connections (nexc) can be entered directly and consistently with the radial box extension (lx)

Many labels and buttons show tooltips when the mouse pointer hovers over them. The names of the actual parameters can also be found there.

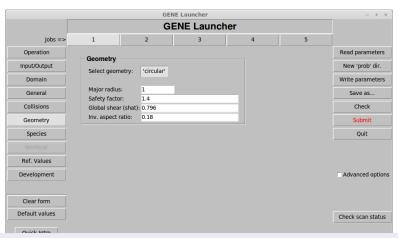
Setting parameters with the launcher IV



- set time limit according to your batch system
- fill dimensionless physical parameters as needed

Hints:
Many labels and buttons show tooltips when the mouse pointer hovers over them. The names of the actual parameters can also be found there.

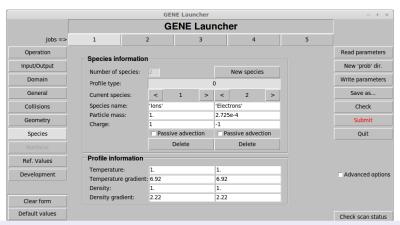
Setting parameters with the launcher V



- choose MHD equilibrium
- fill the requested fields

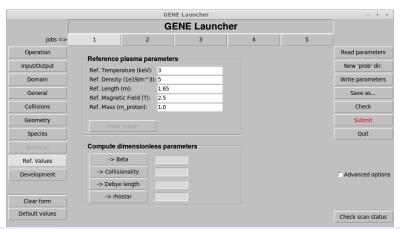
Hints:
Many labels and buttons show tooltips when the mouse pointer hovers over them. The names of the actual parameters can also be found there.

Setting parameters with the launcher VI



- add and remove species using the 'New species' and 'Delete' buttons
- fill the corresponding list for each species
- to read numerical profiles select the appropriate profile type, and fill the requested fields

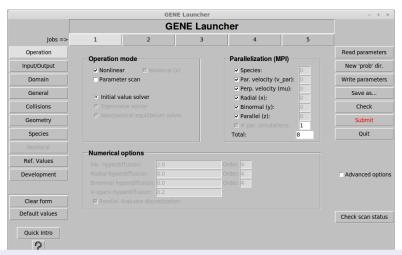
Setting parameters with the launcher VII



- optionally fill reference values for denormalization in the post-processing
- optionally set dependent dimensionless input parameters self-consistently by clicking the buttons

Many labels and buttons show tooltips when the mouse pointer hovers over them. The names of the actual parameters can also be found there.

Setting parameters with the launcher VIII



- Check
- and Submit
 (this requires a launcher.cmd batch script template in makefiles/<mach>/)

The scanscript

A well known problem ...

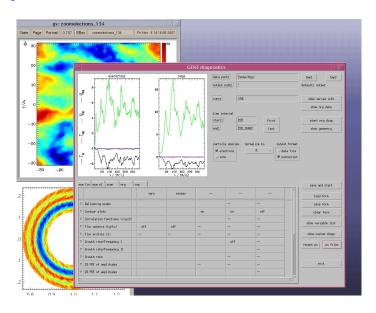
The need to scan over multiple parameter values, e.g., to determine a threshold

Solution

- add Fortran comments as follows to the desired parameters, e.g.,
 - omt = 6.9 !scanlist: 0.0, 3.0, 4.0, 5.0, 6.9
 - ... representing a scan over a list of temperature gradient values. This also works in the launcher tool!
- use the proper system call!
 - either just activate *parameter scan* in the launcher
 - or replace mpiexec -n <NMPI> ./gene_<mach> in your batch script by
 ./scanscript -np <NMPI> -ppn <MINPROCS>
 - <NMPI>: total number of mpi processes
 - <MINPROCS>: minimum number of processors per simulation (scanscript might run several simulations in parallel for optimum efficiency)
- (linear) scan results will be collected in diagdir/scanfiles<ID>/scan.log at the end of the job; call ./scanscript --mks in the directory where the job has been launched for a manual update of scan.log at runtime
- check ./scanscript --help and the documentation for further options and output file arrangement

Analyzing and post-processing

The Diagnostics Tool



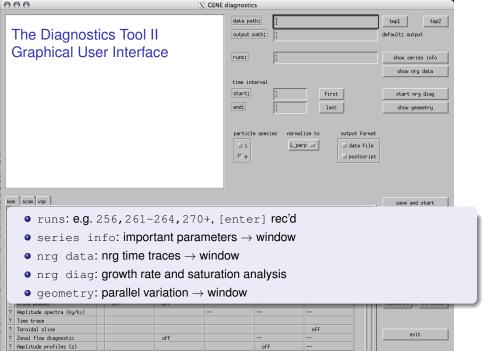
The Diagnostics Tool I

Starting

- regular IDL version (requires IDL licence): full functionality, user can customize diagnostics
- IDL Virtual machine version:
 no manipulation of source possible; IDL VM is free
- Both versions: platform-independent (Unix, Mac OS, Win32; for latter, see documentation)
- IDL: start idl in diagnostics directory, then run @diag
- IDL VM: start idl -vm=vm_diag.sav

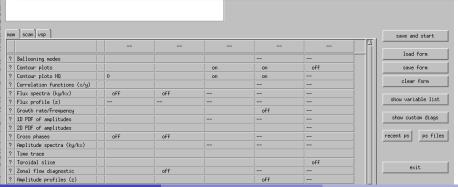
Warning

The diagnostics tool needs to be run on a platform from which one's data is accessible via the file system!





- diag table: labs: analyze mom/scan/vsp files
 - ?: help text
 - activation status: if active, X
- save and start: selected mom/scan/vsp diags
- variable list: variable ↔ number for diag table par's
- recent ps: ps files in gv after save and start
- ps files: open dialog, output directory
- exit: close, GUI state not saved



The Diagnostics Tool III

Using the Diagnostics Tool

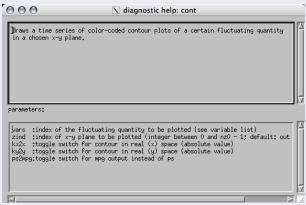
- preliminaries (to check run parameters and/or time evolution): run number, [enter], normalization, show series info/show nrg data
- full nrg analysis: time window, species, normalization, output format, start nrg diag, (hourglass cursor), recent ps
- full mom/scan/vsp analysis: time window, species, normalization, output format, select diags in table (check third column with X), fill in diag parameters, repeat this with other diags, save and start, wait for completion dialog, recent ps

mon	om scan vsp						
			vans	zind	kx2x	ky2y	
?	Ballooning modes						
?	Contour plots	Х	1:3,5		on	on	0

The Diagnostics Tool III

Using the Diagnostics Tool

- \bullet for help with specific diags, press ? next to diag name \to general description, parameters info
- custom diags: can modify with Diagnostics Tool open, auto-recompiled on save and start (only with full IDL)



The Diagnostics Tool IV

Scans and Data Output

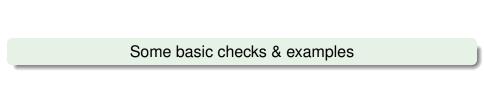
Scan analysis: runs - ignored; sort method - 0 Data output:

- (plain text) data files with predefined output
- for modification/specific info, change source: prog/[diag].pro
 - → search for dat=
 - → modify content (e.g., variables) to be written to file

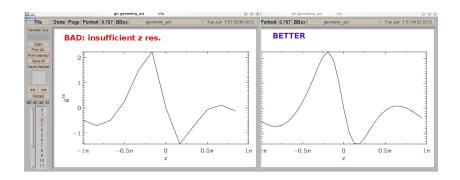
Reality Check: Which Diags Are Essential?

- linear runs: Growth rate/Frequency, Amplitude spectra, Amplitude profiles
- nonlinear runs: Contour plots, Flux spectra, Flux profile

Note: for eigenvalue analysis, enter - [EV number] as time window

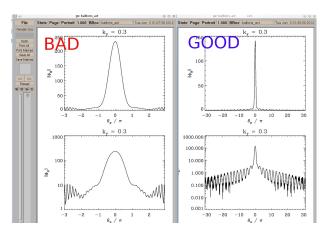


Check the metric coefficients for realistic geometries



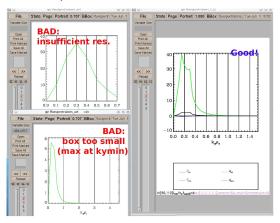
- click "show geometry"
- check smoothness
- if jagged, increase nz0

Linear: Check ballooning structure



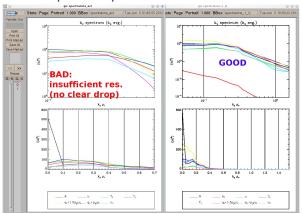
- select "Ballooning modes" for the last time steps
- mode structure should significantly fall off; if not increase nx0
- if still jagged afterwards, increase nz0 or (carefully) apply hyp_z

Nonlinear: Check flux spectra



- select "Flux Spectra (ky/kx)"
- (!)use long time windows beyond the overshoot for nonlinear analysis(!)
- transport should be small at highest k_y , k_x , otherwise increase nx0, nky0
- transport should not peak at lowest k, increase box size lx/decrease kymin else

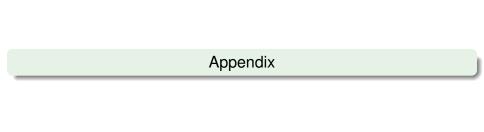
Nonlinear: Check amplitude spectra



- select "Amplitude spectra (ky/kx)"
- (!)use long time windows beyond the overshoot for nonlinear analysis(!)
- ullet observables should be small at highest k_y, k_x and a power law should typically develop
- otherwise increase nx0, nky0

Happy computing!

Feel free to contact support@genecode.org if you have questions or comments



The parallel boundary condition

Standard flux tube (flux bundle) parallel boundary condition

$$F(\rho, \nu, \chi + 2\pi) = F(\rho, \nu - 2\pi q, \chi)$$

with flux surface label ρ , field line label ν , and straight field line angle χ .

In GENE coordinates and Fourier transformed in 2nd dimension

$$F(x, k_y, z + L_z) = F(x, k_y, z) \exp\left(-2\pi i n q(x)\right)$$

with toroidal mode number n, and radial/binormal/parallel coordinates $x/k_y/z$.

Local limit: Fourier transformed in 1st dimension and linearized safety factor

$$F(k_x,k_y,z+L_z) = F(k_x',k_y,z)(-1)^{\mathcal{N}j} \text{ with } k_x'=k_x+k_x^{\min}\mathcal{N}j \text{ and } \mathcal{N}=\hat{s}k_y^{\min}L_x.$$

Here, \hat{s} corresponds to shat, \mathcal{N} to the optional input parameter nexc and j denotes the index in k_v .

Note that k_x wave numbers become coupled due to the parallel b.c.! A mode might require several connections, see ballooning diagnostic!