A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes

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Background

- A few gyrokinetic microstability codes now include plasma shaping, trapped electrons, multiple kinetic species, collisions, magnetic fluctuations, and equilibrium $\boldsymbol{E}\times\boldsymbol{B}$ shear.
- Linear application of these codes is now routine for interpreting turbulence and/or transport measurements.
- The codes are beginning to be applied to predict confinement in ITER and next-step devices.
- **However, the codes have not been verified (much less validated) for linear analysis or nonlinear simulations of present-day experiments spanning a range of discharge conditions.**
- No analytical benchmarks exist for verification in such regimes – must resort to “cross-benchmarking”: code is “correct” if it agrees with others (unlikely all would produce exact same erroneous result).

History

Previous code-comparison (cross-benchmarking) efforts:

- "Numerical Tokamak": S. E. Parker, W. Dorland, R. A. Santoro, M. A. Beer, Q. P. Liu, W. W. Lee, G. W. Hammett, Phys. Plasmas **1**, 1461 (1994).
- "Cyclone Project": A. M. Dimits, G. Bateman, M. A. Beer, B. I. Cohen, W. Dorland, G. W. Hammett, C. Kim, J. E. Kinsey, M. Kotschenreuther, A. H. Kritz, L. L. Lao, J. Mandrekas, W. M. Nevins, S. E. Parker, A. J. Redd, D. E. Schumaker, R. Sydora, J. Weiland, Phys. Plasmas **7**, 969 (2000).
- "Plasma Microturbulence Project": abandoned early 2004, no publications.

➡ **No formal code benchmarking effort since.**

- Prior benchmarking plasmas were experimentally irrelevant (adiabatic electrons, circular plasmas, etc.).
- No informal code comparisons because code developers do not try to duplicate previously published results from other codes.

Why so little recent V&V??

Final report of the Energy Policy Act Task Group of the USBPO:

- “The *focus* of the U.S. Fusion Energy Sciences program is the development of a *predictive understanding* of the fusion plasma system ….”
- “Through participation in ITER, the U.S. will obtain the burning plasma knowledge that is needed ... to establish a path for practical fusion energy beyond ITER. *Predictive understanding*, embodied in theory and *simulation codes*, is a *key* to making this possible.”

OFES call for proposals under notice DE-PS02-07ER07-07 for

- “theory-based predictive transport modeling including *verification and validation (V&V) efforts*.”

OFES call for proposals under notice DE-PS02-07ER07-21 (SciDAC):

- “*A strong verification and validation (V&V) component is essential* for [development and application of high-performance nonlinear gyrokinetic simulation codes for the study of plasma turbulence and transport] …. In addition, … *cross-benchmarking of different codes* is an *indispensable* and often-used *verification tool* ….

Proposal

- An "**outsider**" develops **experimentally relevant** benchmarks through "**apples-to-apples**" comparisons among **GYRO, GS2, GKS**.
- "Experimentally relevant"?
  - Codes must be verified for actual discharges before applying to ITER and beyond.
  - Verification exercises double as
    - **analysis or simulation in support of experiments**
    - **validation exercises**
- Why (only) GYRO, GS2, and GKS?
  - personal experience
  - no sampling errors which can accumulate in PIC computations
  - user-friendly, extensively documented, in use by general fusion community, open source
  - **contain most, if not all, of the physics listed earlier**

GYRO	GS2 and GKS
Eulerian (continuum) gyrokinetic	same
linear or nonlinear	same (GKS - linear only)
local or global domain	local domain
periodic or non-periodic boundary conditions	periodic boundary conditions
s-α or Miller equilibria	same (GS2 - also numerical equilibria)
trapped electrons	same
electromagnetic ($\delta B_\perp$)	electromagnetic ($\delta B_\perp, \delta B_\parallel$)
quasi-neutrality not enforced	same
e-i collisions	e-i, i-i collisions
up to four dynamic species	up to five dynamic species
equilibrium E_r shear	GS2 - same?

Proposal (cont.)

- "Apples-to-apples"?
  - same plasma using Miller geometry (R. L. Miller, M. S. Chu, J. M. Greene, Y. R. Lin-Liu, and R. E. Waltz, Phys. Plasmas **5**, 973 (1998))
  - same physics (ES vs. EM, collisions, trapped electrons, etc.)
  - periodic (flux-tube) B.C.'s
  - sufficient temporal, spatial, pitch-angle, and energy resolutions
- Only one "outside" benchmarking "analyst"?

  (Code developers responsible for actual editing of their codes)
  - No time: Developers busy with physics projects; may not feel additional verification is necessary.
    - A coordinator would still be necessary.
  - "Outsider" is unaffiliated with any code group ⇒ objectivity.
  - More efficient: Dedicated "analyst" can write software to generate input files for all three codes, run them simultaneously.
  - Can verify that the codes are indeed starting with the same inputs.

Input Parameters

- Comparisons of three input-file generators (March 2006):

gradients defined using midplane radius r_mid/a			grads. defined by TRANSP r/a		
GS2 parameter					
Miller parameters:					
rhoc	0.9763	0.9750		0.9600	0.9600
rmaj	3.2968	3.2274		3.2086	3.2086
r_geo		3.2252		3.2065	3.2065
qinp	3.8978	3.9065		3.8849	3.8849
shift	-0.1729	-0.0908		-0.0639	-0.0973
akappa	1.3666	1.3668		1.3761	1.3761
akappri	1.9772	1.9536		1.2001	1.8268
tri	0.6512	0.3831		0.1935	0.1935
tripri	4.3775	1.4771		0.1612	0.2454
s_hat_input	5.3753	5.0821		6.7489	10.4471
beta_prime_input	-0.0210	-0.0187	-0.0129		-0.0197
electrons:					
temp	1.4027	1.4841	1.2969		1.2969
tprim	34.6131	21.4008	20.6518		31.4361
fprim	0.1413	0.1561	0.1102		0.1678
vnewk	2.3844	1.1047	2.3660		2.3660
main ion:					
dens	0.8422	0.8512	0.8507		0.8507
tprim	21.9361	15.8889	13.8542		21.0889
fprim	0.1413	0.1562	0.1102		0.1678
vnewk	0.0000	0.0713	0.1270		0.1270
impurity:					
dens	0.0147	0.0136	0.0137		0.0137
temp	1.0000	1.0036	1.0000		1.0000
tprim	21.9361	15.9209	13.8542		21.0889
fprim	0.1414	0.1552	0.1100		0.1675
vnewk	0.9504	0.9829	1.7536		1.7536
misc.					
beta	3.1107E-04	4.0655E-04	3.3136E-04		3.3136E-04
zeff	1.8246	1.7620	1.7648		1.7648
BT	5.2842	5.4666			

For edge ($\rho_{TF} = 0.96$) of C-Mod EDA H-mode

Differences among utilities noted in red

(found to be due to different fitting routines and default smoothing)

Now resolved.

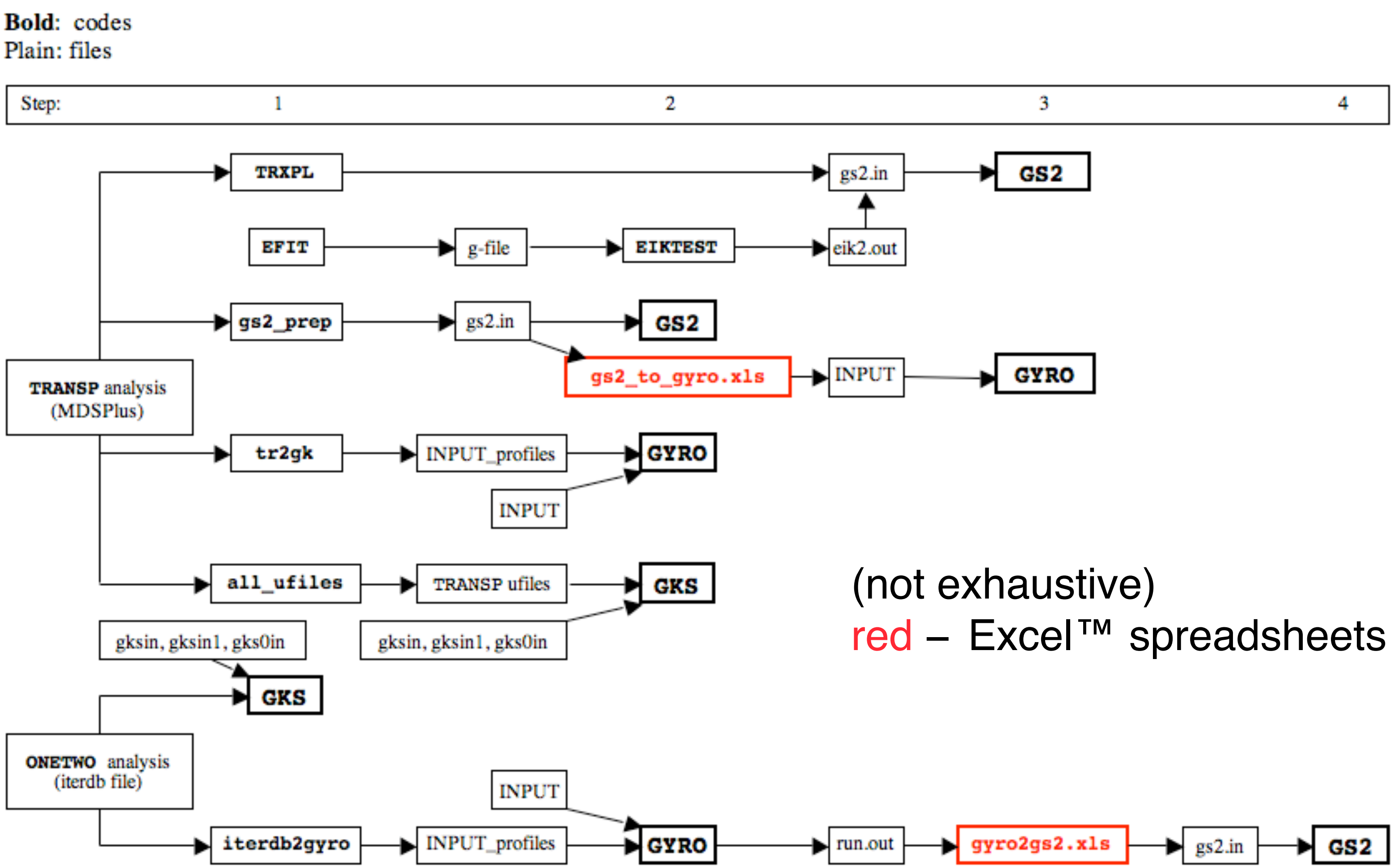
- Illustrates potential danger of using different input generators for each code.

Input Parameters (cont.)

- GS2/GYRO input parameter translation table (circulated among developers for comment): page 1 of 3

GS2		GYRO	
Parameter	Definition	Parameter	Definition
Important: Paired parameters not necessarily equal			
Plasma Parameter s			
a	half-width of LCFS at z of magnetic axis	a	Same
r_geo	R/a at center of LCFS	none	
rmaj	R/a of magnetic axis if iflux = 1, R/a of center of flux surface of interest otherwise	R_0	major radius of center of flux surface
		ASPECT_RATIO	Same as GS2 rmaj for iflux $\neq 1$
ρ	irho=1: sqrt[$\phi/\phi(a)$], ϕ is toroidal flux per 2π irho=2: $r_{\rm mid}/a$, where $r_{\rm mid}$ is half-width of flux surface at z of magnetic axis	ρ	sqrt($2\phi/B_0$), B_0 = vacuum B at location dependent on input source
		$\hat{\rho}$	$\rho/\rho(\mathrm{a})$
		r	Same as GS2 ρa for irho=2
rhoc	ρ of center of computation box	RADIUS	r/a of center of computation box
$v_{\rm ref}$	sqrt($T_{\rm ref}/m_{\rm ref}$) at rhoc for "t_over_m" norm.	c_s	sqrt(T_e/m_i) at RADIUS
$B_{\rm geo}$	vacuum B at r_geo	$B_{\rm unit}$	$B_0(\rho/r)(\mathrm{d}\rho/\mathrm{d}r)$ at r
$\rho_{\rm ref}$	$v_{\rm ref}/[eB_{\rm geo}/(m_{\rm ref}c)]$	$\rho_{\rm s,unit}$	$c_s/[eB_{\rm unit}/(m_i c)]$
none		RHO_STAR	$\rho_{\rm s,unit}/a$ (arbitrary for flux-tube runs)
qinp	safety factor q at rhoc	SAFETY_FACTOR	Same
s_hat_input	ρ/q dq/dρ at rhoc	SHEAR	r/q (dq/dr) at RADIUS
shift	d$rmaj$/dρ at rhoc	SHIFT	dR_0/dr at RADIUS
akappa	elongation κ at rhoc (assumes up-down symmetry)	KAPPA0	Same
akappri	dκ/dρ at rhoc	S_KAPPA0	$r/KAPPA0 \times$ d$KAPPA0$/dr at RADIUS
tri	asin[($rmaj$-R(z_max))/$r_{\rm mid}$] at rhoc (assumes up-down symmetry)	DELTA0	[R_0-R(z_max)]/r at RADIUS
tripri	dtri/dρ at rhoc	S_DELTA0	r dDELTA0/dr at RADIUS
beta	403e-5*ne_19*$T_{\rm ref}$(kev)/$B_{\rm geo}$(T)^2 at rhoc (not total beta)	BETAE_UNIT	403e-5*ne_19*T_e(kev)/B_$unit$(T)^2 at RADIUS
beta_prime_input	total dβ/dρ at rhoc used in equilibrium	none (computed internally)	Same
zeff	used only for electron collisionality	Z_EFF	Same

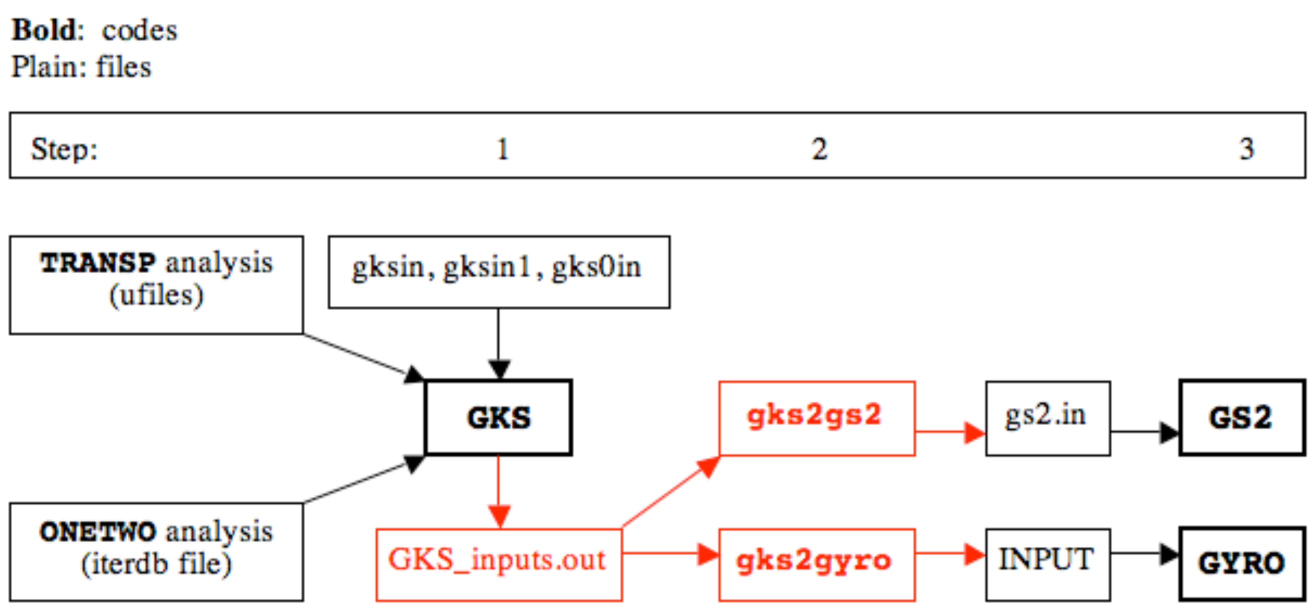
Present Flowchart



(not exhaustive)
red – Excel™ spreadsheets

- Complex – typically requiring multiple steps
- Different input-file generators for each code

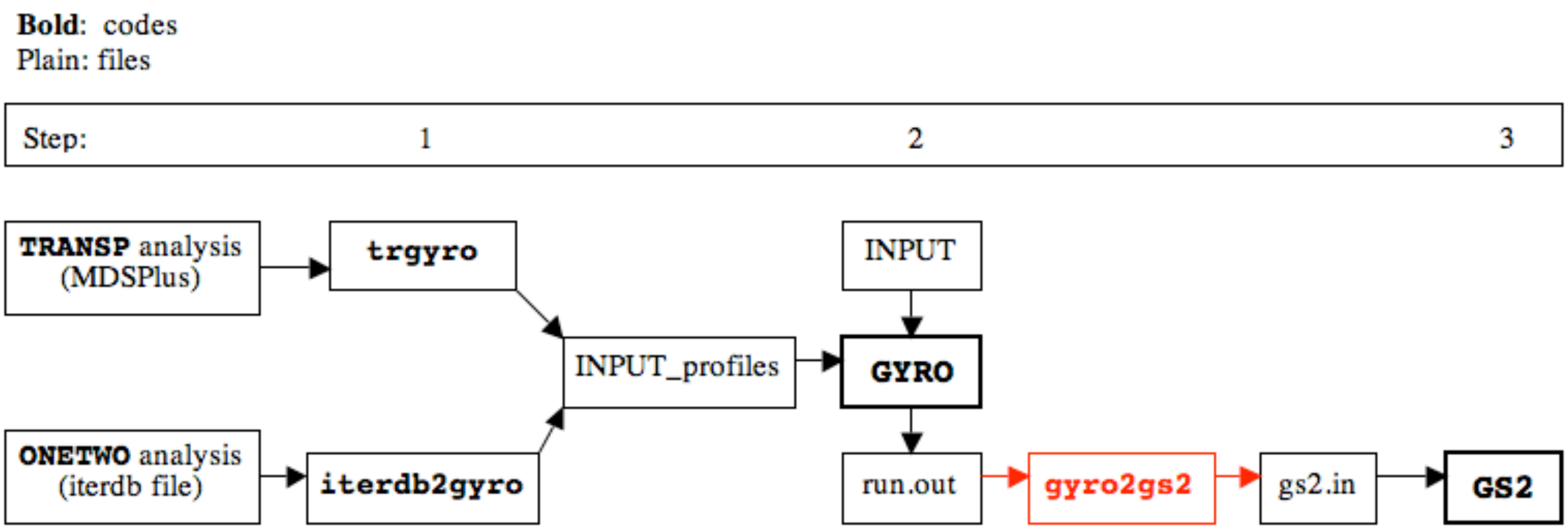
Proposed Flowchart (linear)



Requires writing codes to

- extract inputs from GKS and write to file (`GKS_inputs.out`),
- read file and generate input files to GS2 and GYRO.

Proposed Flowchart (nonlinear)



Requires writing code to

- read file generated by GYRO and generate input file to GS2.

Proposed Procedure

1. Use **one** utility code to extract experimental data from analysis by TRANSP or ONETWO and to produce input files for all three codes. First run three codes linearly.
2. If differences found between codes, remove shaping, collisions, etc. until agreement is reached $\Rightarrow$ **basic benchmark**.
3. Reinstate shaping, collisions, etc., one at a time:

   agreement $\Rightarrow$ successively **more complex benchmarks**

   disagreement $\Rightarrow$ source(s) of problem, e.g., collisions
4. Present to code developers who must first concur with findings, then seek resolution $\Rightarrow$ yet **more complex benchmark**.
5. Return to 3 until all terms are included $\Rightarrow$ **"full physics" benchmark**.
6. Run codes including nonlinear terms (exit GKS). Repeat 2-5.
7. Repeat 1-5 for different radius and/or plasma.

Example Benchmarking Discharges

- DIII-D plasmas with added ECH
  - benchmarks at significant β, low collisionality
  - analysis and simulation of ongoing experiments (turbulence measurements and transport).
- C-Mod EDA H-mode plasmas
  - benchmarks at high densities, low β, moderate collisionality
  - analysis and simulation of ongoing experiments (ITB's, strong TEM activity, etc.)
- NSTX plasmas
  - benchmarks at low aspect ratio, high β, large trapped-electron fraction, etc.
- Any near edge
  - benchmarks for strong shaping, high collisionality, high shear
  - insight into role of $\boldsymbol{E}\times\boldsymbol{B}$ shear in determining pedestal width?

➡ **No dedicated discharges required**

Summary – Deliverables

- Benchmarks, linear and nonlinear, at various levels of complexity over range of radii, plasma conditions
  - Other codes should meet these benchmarks in stages as they develop increased capabilities.
  - Other code developers could contest the benchmark(s) but should be willing to work with GYRO, GS2, GKS developers and “analyst” to resolve disagreement(s).
- Verification of GYRO, GS2, GKS over same radial ranges, plasma conditions
- Portable, user-friendly routines (red boxes in previous flowcharts) for use by general community
- Analysis and simulations in support of experiments
- **Validation** of codes in some cases (because plasmas are from actual experiments)

➡ **A clear, systematic, efficient V&V effort geared toward developing a predictive capability for ITER and next-step devices**

Summary (cont.)

Why me as benchmarking "analyst?"

- Experience with GYRO, GS2, GKS:
  - Know individual definitions of input parameters.
  - Have run all three codes (GYRO, GS2 on Seaborg).
  - Have delved into source code, found errors.
- Experience since 1998 with comparing nonlinear simulations with experiment (incl. fluctuations).
- Familiarity with experimental data and analysis (TRANSP, ONETWO, GAPROFILES, etc.), esp. **uncertainties**
- Familiarity with relevant programming languages (IDL, Fortran)
- Unaffiliated with any code group $\Rightarrow$ objectivity
- Experimentalist $\Rightarrow$ different perspective
- Excellent working relationships with code groups and users