TECHNICAL PROGRESS REPORT

A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes

GRANT DE-FG02-08ER54978

Feb. 15, 2014 - Feb. 14, 2015

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OFFICE OF SCIENCE - FUSION ENERGY SCIENCES PROGRAM

My original proposal for the period Feb. 15, 2014 through Feb. 14, 2017 called for an integrated validation and verification effort carried out by myself with collaborators. The validation component would require experimental profile and power-balance analysis. In addition, it would require running the gyrokinetic codes varying the input profiles within experimental uncertainties to seek agreement with experiment before discounting a code as invalidated. Therefore, validation would require a major increase of effort over my previous grant periods which covered only code verification (code benchmarking). Consequently, I had requested full-time funding. Instead, I am being funded at somewhat less than half time (5 calendar months per year). As a consequence, I decided to forego the validation component and to only continue the verification efforts.

There was also an unexpected change to the original proposed work. Despite a letter of support from the GEM group, attached to the proposal, the group informed me that they wished to terminate the collaboration. Fortunately, the proposal called for adding the GENE code, another Eulerian code, to the comparisons with GYRO and GS2. A major fraction of the past year I devoted to learning the GENE code and its associated IDL diagnostics GUI. I also wrote the necessary Python utility routines to translate a GYRO input file into a GENE input file, to set up the GENE runs, to consolidate the data, etc.

I made a deliberate effort to assimilate my benchmarking work into existing experimental programs to contribute to the physics goals of the programs. These experiments included

- A high-β_p, nearly noninductive, DIII-D H-mode discharge. This discharge was aimed at developing a scenario for long-pulse discharges on the EAST tokamak. Current results were recently presented in an IAEA paper by A. Garofalo et al.[1]
- A DIII-D plasma with electron-cyclotron heating (ECH) applied at r/a = 0.6 and/or 0.8. By adjusting the relative strengths of the heating at each location, the T_e profile could be modified in the intervening region (r/a = 0.7). This experiment was specifically aimed at studying this "outer core" region where some gyrokinetic codes under-predict the transport ("shortfall"). Results were recently presented in an IAEA paper by S. Smith et al.,[2] in which my GYRO results are featured.
- Two high-power, DIII-D H-mode discharges with differing degree of toroidal rotation from the beams. Primarily experimental results were recently presented in an IAEA paper by G. McKee et al.[3]

- The pedestal region of a long-pulse H-mode EAST discharge. Results were presented in a recent Phys. Rev. Lett.[4] My contribution to this work was at the invitation of X. Xu of LLNL and S. Ding of the Institute of Plasma Physics, Chinese Academy of Sciences, who desired linear results from codes other than GYRO.

Details of the physics results of my contributions to these experiments can be found in my poster for the recent APS/DPP conference accompanying this report. Summaries of the results are given below.

I should note that only collisionless linear results are presented near the plasma edge where the safety factor and/or shear are large. These effects act to highly localize the eigenfunctions in θ, introducing challenges into the GYRO collision algorithm. A new version of GYRO nearing completion, deemed CGYRO, will address this problem. The collisionless code comparisons will be extended to collisions when CGYRO becomes available.

I should also note that comparisons of linear eigenfunctions among codes, not only frequencies, is now a regular feature of my analysis.

- High-β_p, nearly noninductive, H-mode discharge: Here the analysis took place near the plasma edge, at *r/a* = 0.8, in a region of very flat n_e and T_e profiles. The linear frequencies, indicating an ITG mode, found by all three codes agreed ignoring collisions. Agreement between the codes capable of eigenvalue computations, GYRO and GENE, even extended to a sub-dominant "odd-parity" ITG mode. To my knowledge, this is one of the few, if only, benchmarking of sub-dominant modes.
- Analysis of the ECH-heated discharge was performed at *r/a* = 0.7 for 1) all six gyrotrons applied at *r/a* = 0.6, 2) all at *r/a* = 0.8, and 3) split between *r/a* = 0.6 and 0.8. For all three cases, the linear frequencies and eigenfunctions agreed well among codes. Agreement among the nonlinear fluxes was not clear for cases 2 and 3 because the fluxes from some of the codes, especially GS2, either did not converge, or were unsteady. I attribute this to the discharges being only marginally unstable at *r/a* = 0.7. The fluxes for case 1, however, were steady and in agreement among codes. As shown in Ref. 2, the electron energy flux agreed quite well with power balance, but the ion energy flux was significantly lower.
- Linear analysis of the two DIII-D H-mode discharges with differing rotation velocities found good agreement among the codes. The frequencies also agreed with independent analysis by C. Holland using GYRO. The discharge with higher rotation was found to have significantly higher growth rates, due to the steeper gradients. However, the larger **E**x**B** shearing rate is expected to compensate in determining the nonlinear fluxes (work yet to be performed).
- Good linear agreement of the fastest growing branch among codes, especially in the eigenfunctions, was found at the location of steepest gradient of the EAST pedestal ignoring collisions and assuming a local (Miller) equilibrium.

In closing, I believe that the last roughly eight months of work presented here at less than half time funding is substantial. It is also relevant to the broader fusion community.

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[3] G. R. McKee, C. Holland, Z. Yan, E. J. Doyle, T. C. Luce, A. Marinoni, C. C. Petty, T. Rhodes, L. Schmitz, W. M. Solomon, B. J. Tobias, G. Wang, and L. Zeng, Proc. of 25th IAEA Fusion Energy Conference, 2014, St. Petersburg, Russian Federation, paper EX/2-2.

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Project Title: A SYSTEMATIC METHOD FOR VERIFICATION AND VALIDATION OF GYROKINETIC MICROSTABILITY CODES	
Federal Award Identification Number: DE-FG02-08ER54978	
Agency Code: 8900	**Organization:** Office of Fusion Energy Sciences
Recipient Award Identification Number: Not Provided	**Project Period:** 02/15/2014 - 02/14/2017
Reporting Period: 02/15/2015 - 02/14/2016	**Budget Period:** 02/15/2015 - 02/14/2016
Report Term: Once per Budget Period	**Submission Date and Time:** 11/12/2015 04:29 PM ET
Principal Investigator Information: Dr. Ronald Victor Bravenec PI 503 Lockhart Dr. Austin, TX 78704-4335 **Email:** rvbravenec@4th-state.com **Contact:** (512) 800-3327	**Recipient Organization:** Fourth State Research 503 Lockhart Dr. Austin, TX 78704-4335 Country: USA **DUNS:** 808068469 **EIN:** 264021697
Submitting Official Information: Dr. Ronald Victor Bravenec PI 503 Lockhart Dr. Austin, TX 78704-4335 **Email:** rvbravenec@4th-state.com **Contact:** (512) 800-3327	

ACCOMPLISHMENTS

1. What are the major goals of the project?

The goal of this project is to verify the three gyrokinetic microstability codes GENE, GS2, and GYRO. By verify, I mean to demonstrate that the codes are solving their underlying equations correctly. For complex plasmas, this is accomplished by benchmarking, i.e., running the codes with identical input parameters and expecting identical results. If they all agree, it is likely that the codes are correct. If one code disagrees with the others and this persists after adjusting certain resolution parameters, it is likely that there is a problem in the code. It is then up to the code developer(s) to fix the code. To be convincing, this effort should be made using a variety of plasma conditions.
A secondary goal of the project is to provide gyrokinetic analysis to the community. Consequenlly, I perform the benchmarking exercises for discharges that are of general interest.

2. What was accomplished under these goals?

In the period between my last progress report in November of 2014 and the Transport Task Force (TTF) workshop in April of 2015, I performed linear benchmarking of the codes GENE, GS2, and CGYRO at the top of the pedestal of a DIII-D QH-mode discharge. (CGYRO is a new version of GYRO that is more accurate in treating collisions.) The discharge had EHO's (edge harmonic oscillations) that disappeared in time. The analysis was performed both with and without EHO's. The linear frequencies and eigenfunctions were found to be in agreement among all three codes. To my knowledge, this work represents the only benchmarking of CGYRO not performed by the code developers themselves.
The rest of the year was spent analyzing three JET discharges that had excellent ion energy confinement but different plasma parameters. The outstanding question was: What was responsible for the good confinement? Earlier GENE simulations indicated it was mainly due to electromagnetic effects rather than ExB flow shear. The JET researchers wanted to verify this conjecture using another code, hence my involvement in the project. I ran GS2 and GYRO for these discharges and came to the same conclusion. For one discharge, GYRO predicted complete stability. Details of this work can be found in my 2015 APS/DPP poster (attached document). I should note that none of the work includes nonlinear GS2 results. After an upgrade to the Hopper computer at NERSC, GS2 would not run nonlinearly. I have yet to determine the cause of the problem. Sorting it out represents a high priority of my future work.
In addition to these major projects, I also ran GENE nonlinearly for a DIII-D discharge including rotation. The results are featured in a figure in Darin Ernst's invited APS talk. I also contributed GENE linear results for a paper Emily Belli and Jeff Candy of General Atomics are writing.

3. What opportunities for training and professional development has the project provided?

Nothing to Report

4. How have the results been disseminated to communities of interest?

These results have been disseminated to the community via emails to selected individuals, my poster at the April 2015 Transport Task Force workshop, and a poster at the 2015 APS/DPP meeting this November. In addition, I presented a talk to JET researchers on Nov. 3 about a portion of my JET activities at a JET Task Force seminar (I attended remotely).

5. What do you plan to do during the next reporting period to accomplish the goals?

My immediate goal for the reporting period is to find and fix the problem in GS2 so I can include it in my nonlinear code comparisons. I will also be pursuing new projects. For instance, I plan to analyze a DIII-D discharge that was meant to simulate ITER startup. The analysis will be performed during the current ramp-up phase of the discharge. I will also be contacting members of the tokamak confinement community to identify discharges that would be good candidates for code benchmarking. This will satisfy two goals: benchmarking itself and identifying discharges that would benefit from such analysis.

The Relative Roles of Electromagnetic and ExB Stabilization in JET High-Performance Discharges

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M. J. Pueschel, *U. Wisconsin, Madison*

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Motivation

GYRO [1] simulations to verify the GENE [2] predictions that:
Fast-ion-enhanced electromagnetic stabilization is the main contributor to the low ion heat flux seen in selected JET discharges:

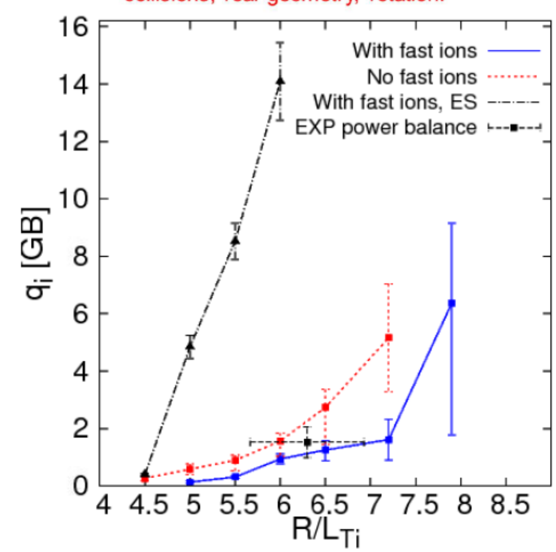
66404: Simplest test case. Imposed circular cross section, no impurities. Compare electrostatic (ES) and electromagnetic (EM) [3]

73224: Shaped plasma, EM. Compare 3 and 5 kinetic species (2 additional species are hot D beam and He3 ions). Benchmark fast ion enhanced EM-stabilization and relative impact of ExB [3,4]

75225: High performance hybrid scenario. Shaped, 4 kinetic species (including D fast ions). Compare ES and EM and relative impact of ExB [5]

This work is vital for verifying the physics basis for extrapolation of high-beta scenarios towards JET DT and reactors [6,7]

GENE nonlinear simulations of JET 75225 @ $\rho = 0.33$. 4 ion species, finite-β, collisions, real geometry, rotation.



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[2] F. Jenko et al., Phys. Plasmas 7, 1904 (2000); www.genecode.org
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[4] P. Mantica et al., Phys. Rev. Lett. 107, 135004 (2011)
[5] J.Citrin et al., Plasma Phys. Control. Fusion 57 (2015) 014032
[6] J. Garcia et al., Nucl. Fusion 55 (2015) 053007
[7] C. Challis et al., Nucl. Fusion 55 (2015) 053031

“Full Physics”

- $\delta B_\perp$ ($\delta B_{||}$ ignored except for shot 75225)
- trapped and passing electrons
- parametric plasma shaping: vertical elongation κ, triangularity δ, etc. (Miller model)
- electron collisions (Lorentz model)
- one dynamic impurity (C^{6+}), hot beam ions (shots 73224, 75225), and hot He3 (shot 73224)
- $E \times B$ rotation

JET Discharge Parameters

4th-State RESEARCH

- 3 discharges analyzed here:
  - Red indicates most significant differences among shots.
  - Circular cross-section, no impurities imposed on shot 66404

73224, 5 species:

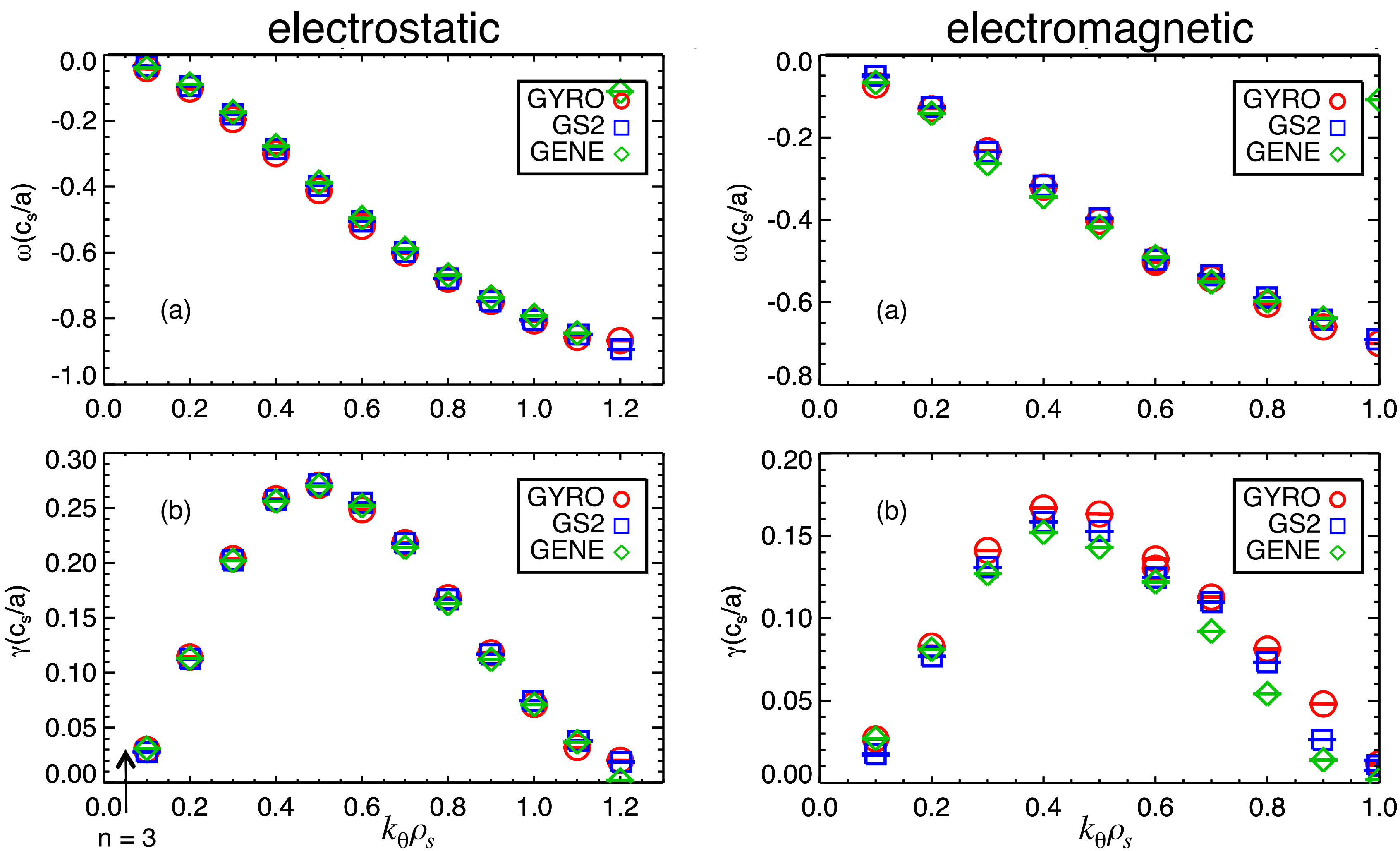
	fast D	He3
T/T_e	9.8	6.9
n/n_e	0.06	0.07
a/L_{Te}	1.0	7.4
a/L_{ne}	4.7	0.5

Device	JET	JET	JET
shot	66404	73224*	75225
r (m)	0.31	0.36	0.35
a (m)	0.94	0.96	0.94
n_e (10^{19} m^{-3})	2.3	2.95	3.92
T_e (keV)	4.0	3.2	4.8
n_i/n_e	1.0	0.648	0.79
n_{imp}/n_e	0.0	0.025	0.015
$T_i/T_e = T_{imp}/T_e$	1.0	1.0	1.19
$a/L_{ne} = a$ dln(n_e)/dr	0.924	0.422	0.906
$a/L_{ni} = a$ dln(n_i)/dr	0.924	0.006	0.760
$a/L_{nimp} = a$ dln(n_{imp})/dr	-	0.422	0.906
$a/L_{Te} = a$ dln(T_e)/dr	1.65	2.23	1.31
$a/L_{Ti} = a$ dln(T_i)/dr	2.84	3.56	2.51

Device	JET	JET	JET
shot	66404	73224	75225
$R_0(r)/a$	3.03	3.12	3.23
$\Delta = dR_0(r)/dr$	0	-0.14	-0.15
q	1.7	1.74	1.14
$s = r$ dln(q)/dr	0.2	0.523	0.159
κ	1.0	1.26	1.32
$s_\kappa = r$ dln(κ)/dr	0	0.030	-0.009
δ	0	0.030	0.036
$s_\delta = r\, d\delta/dr$	0	0.032	00.02
β_e	0.003	0.0033	0.018
Z_{eff}	1.0	1.9	1.45
$\nu_{ei}\, a/c_s$	0.015	0.032	0.019
$\gamma_{E\times B}\, a/c_s$	-	-	-

*3 species

Linear Frequencies 66404

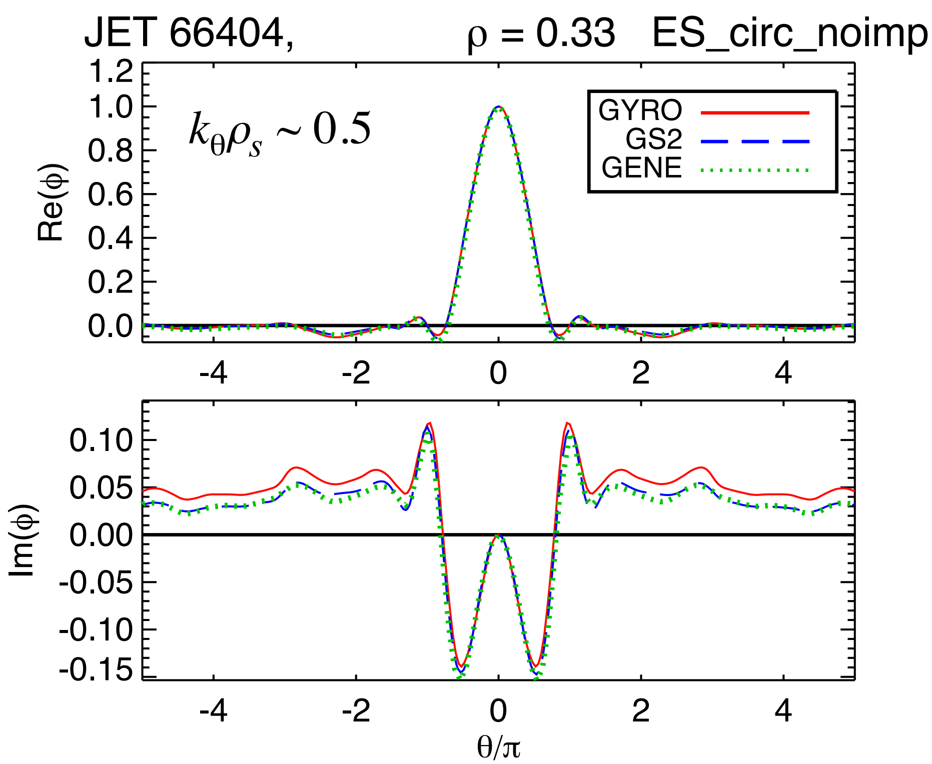


- Excellent agreement
- Good agreement except near stability boundary

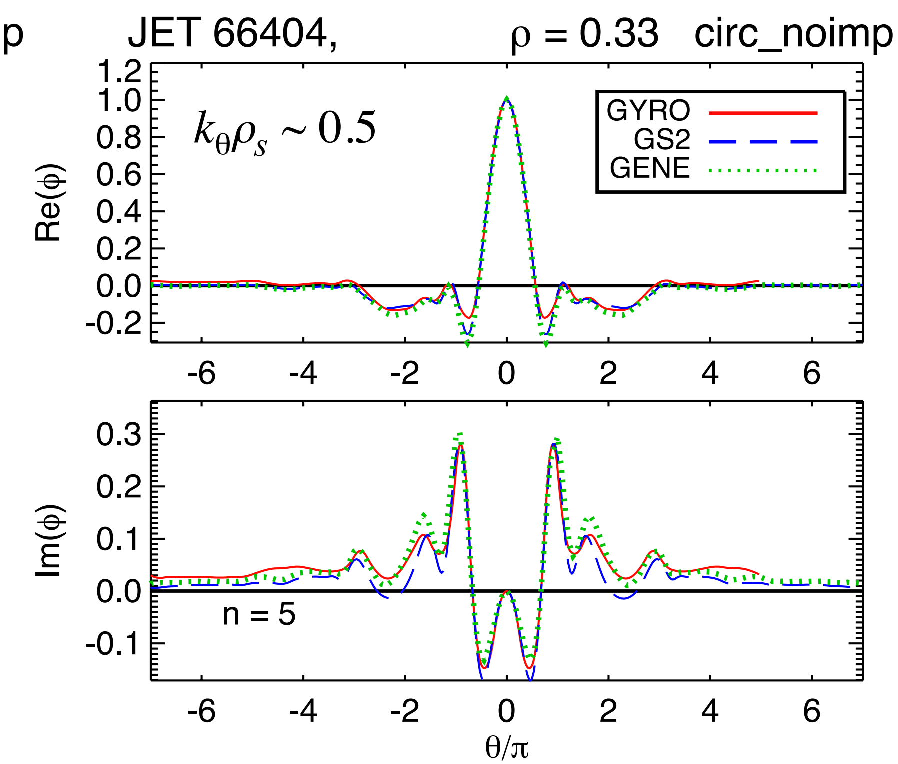
Bravenec_APS15.pdf

Eigenfunctions 66404

electrostatic

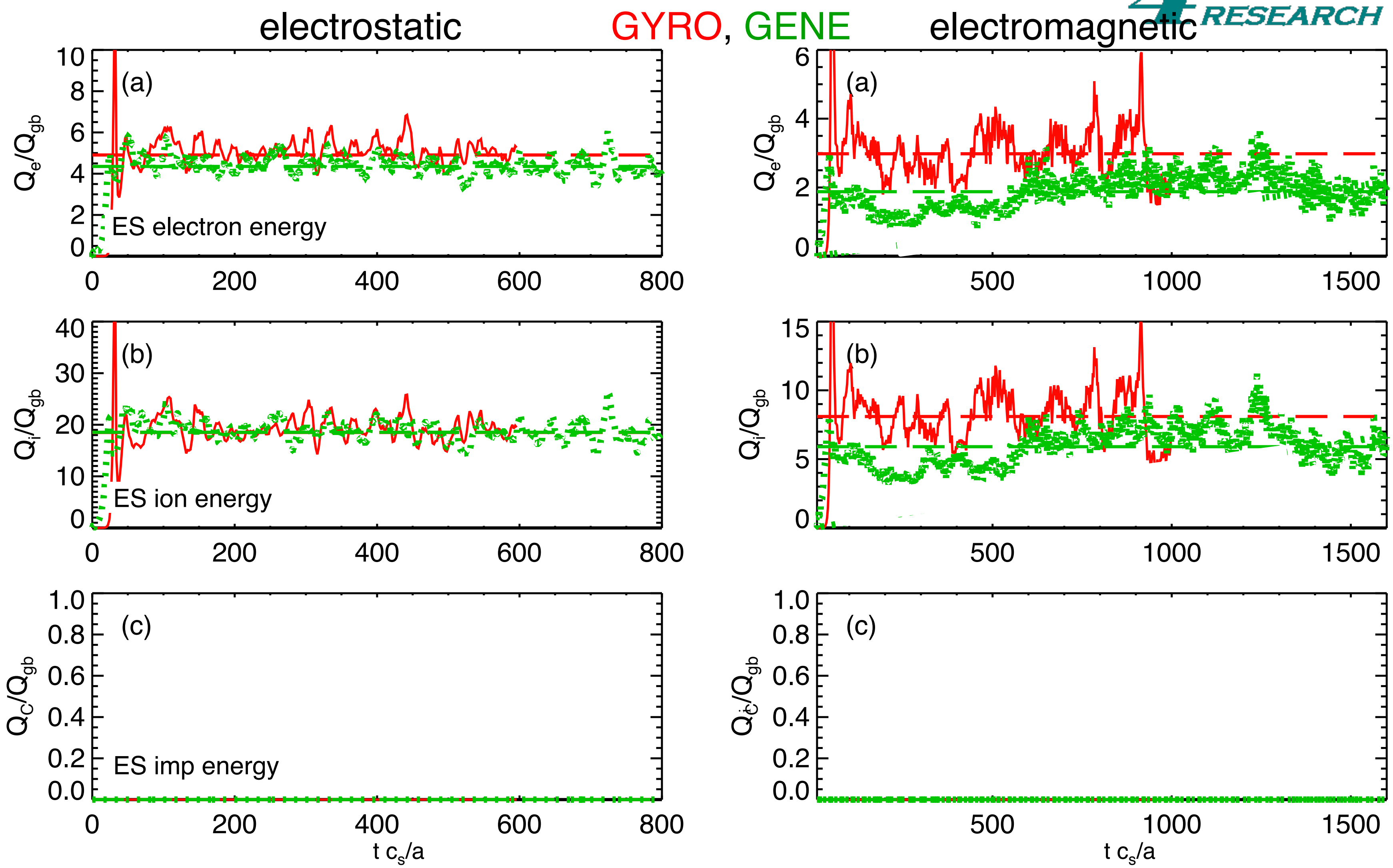


electromagnetic



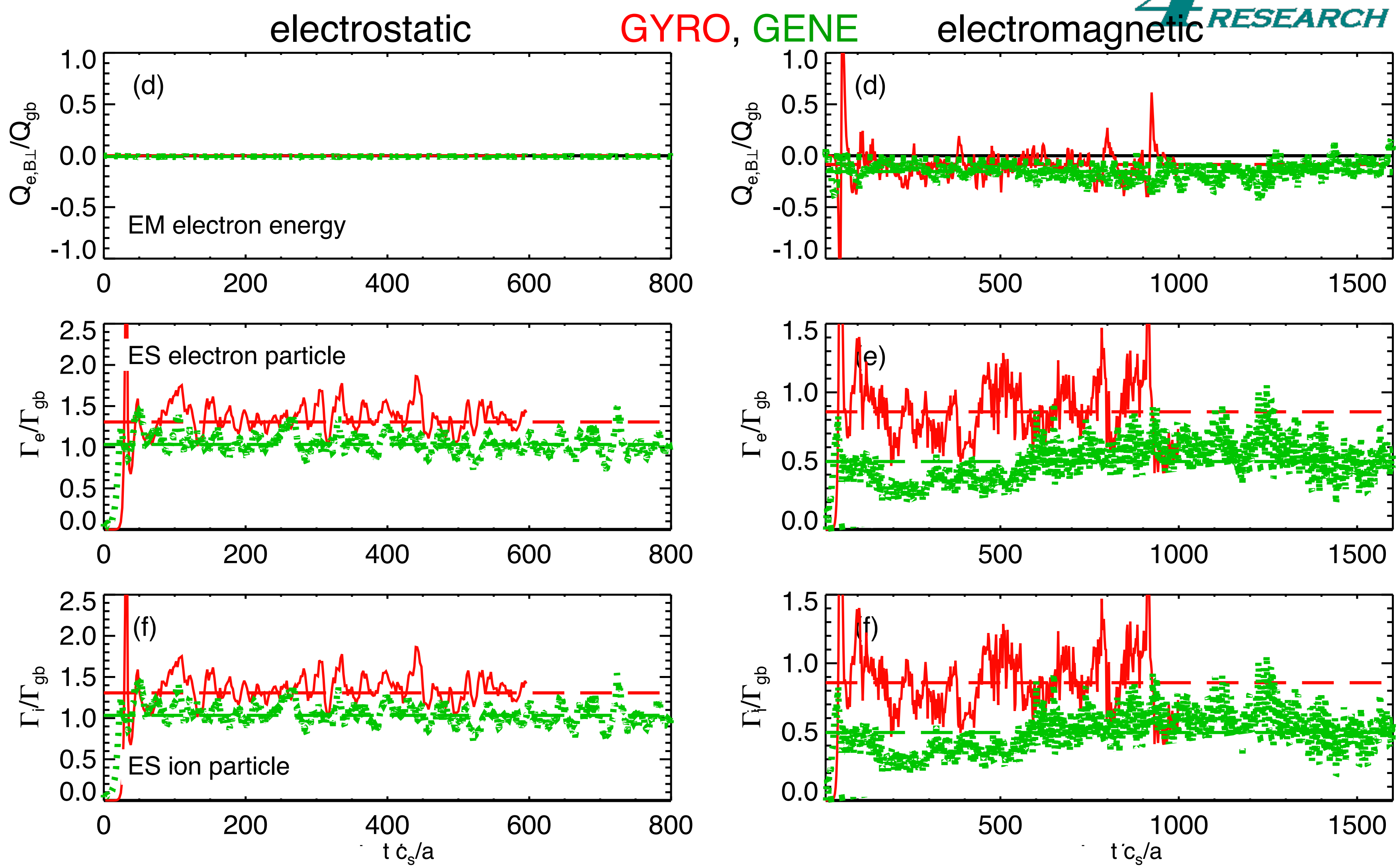
- Good agreement
- Good agreement

Energy Fluxes 66404



- Excellent agreement
- Fluxes reduced from ES case
- Significant difference between codes?

Particle Fluxes 66404



- Good agreement
- Significant difference between codes

Summary — 66404

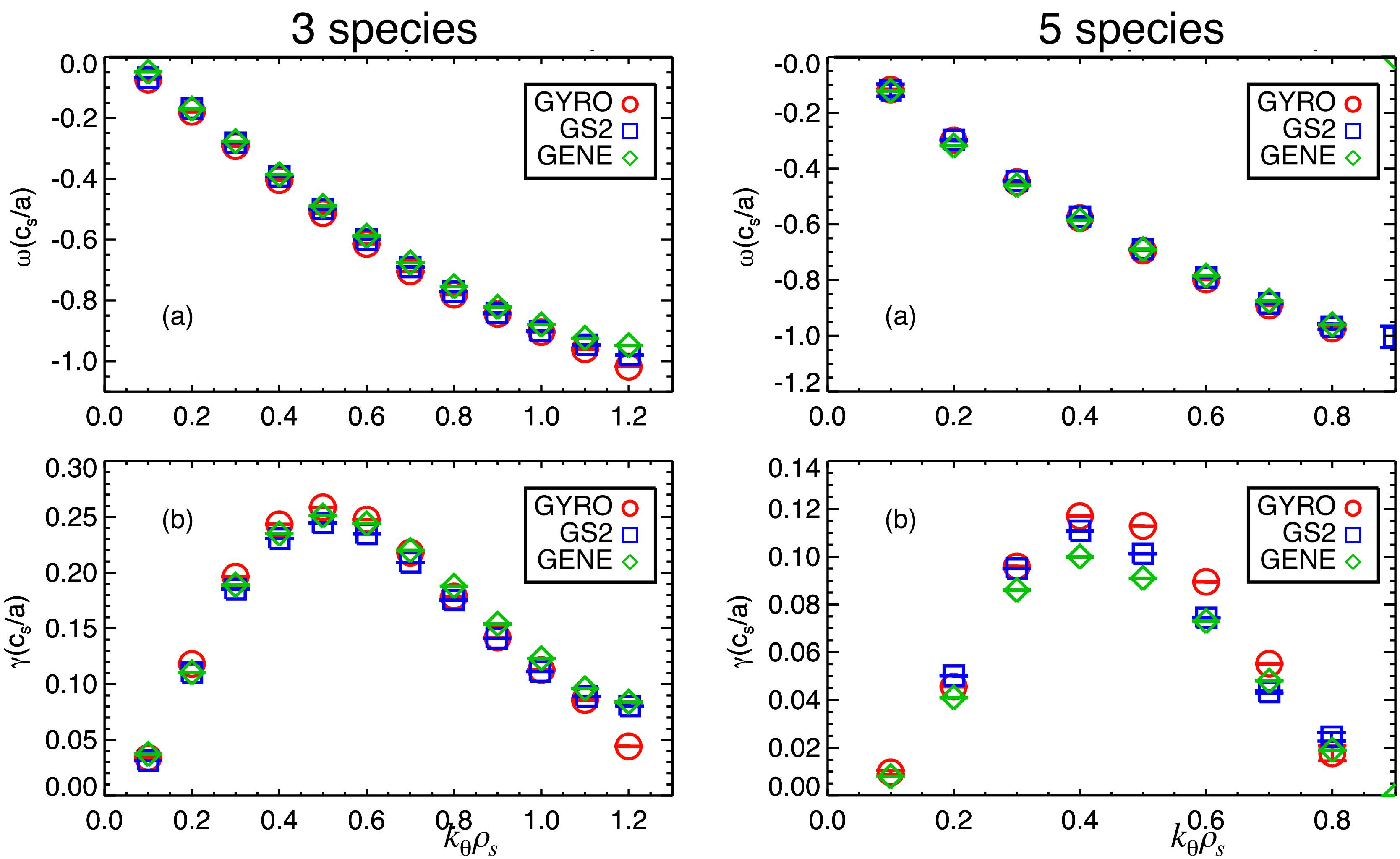
- Clear reduction in linear growth rates and nonlinear fluxes (esp. ion thermal) when electromagnetic effects included.

  Ratios of differences between ES and EM normalized to ES:

	GENE	GYRO	GS2
$\Delta\gamma_{max}/\gamma_{max}(ES)$	0.42	0.37	0.40
$\Delta Q_e/Q_e(ES)$	0.57 ± 0.12	0.41 ± 0.15	-
$\Delta Q_i/Q_i(ES)$	0.68 ± 0.08	0.58 ± 0.11	-
$\Delta\Gamma_e/\Gamma_e(ES)$	0.52 ± 0.15	0.38 ± 0.18	-

- Reduction in fluxes greater than in growth rates.

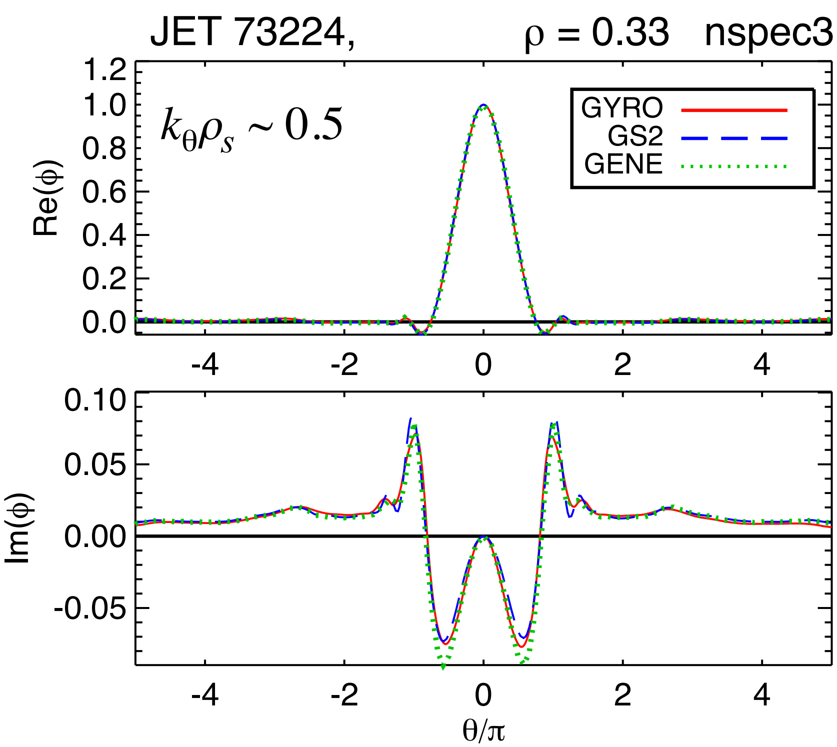
Linear Frequencies 73224



- Excellent agreement
- Good agreement
- Drop in growth rate from 3-species

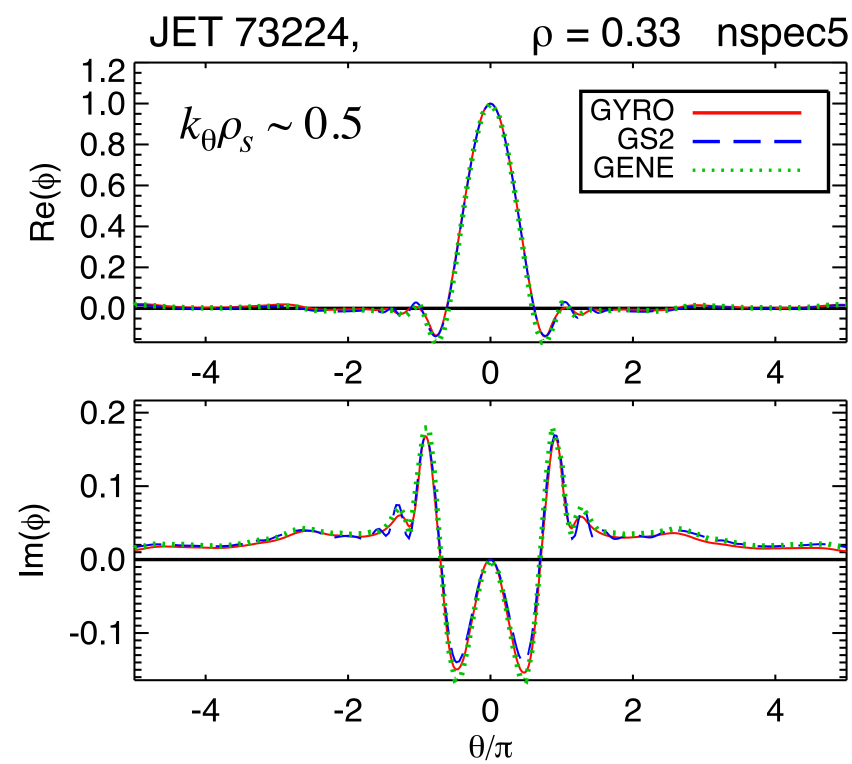
Eigenfunctions 73244

3 species



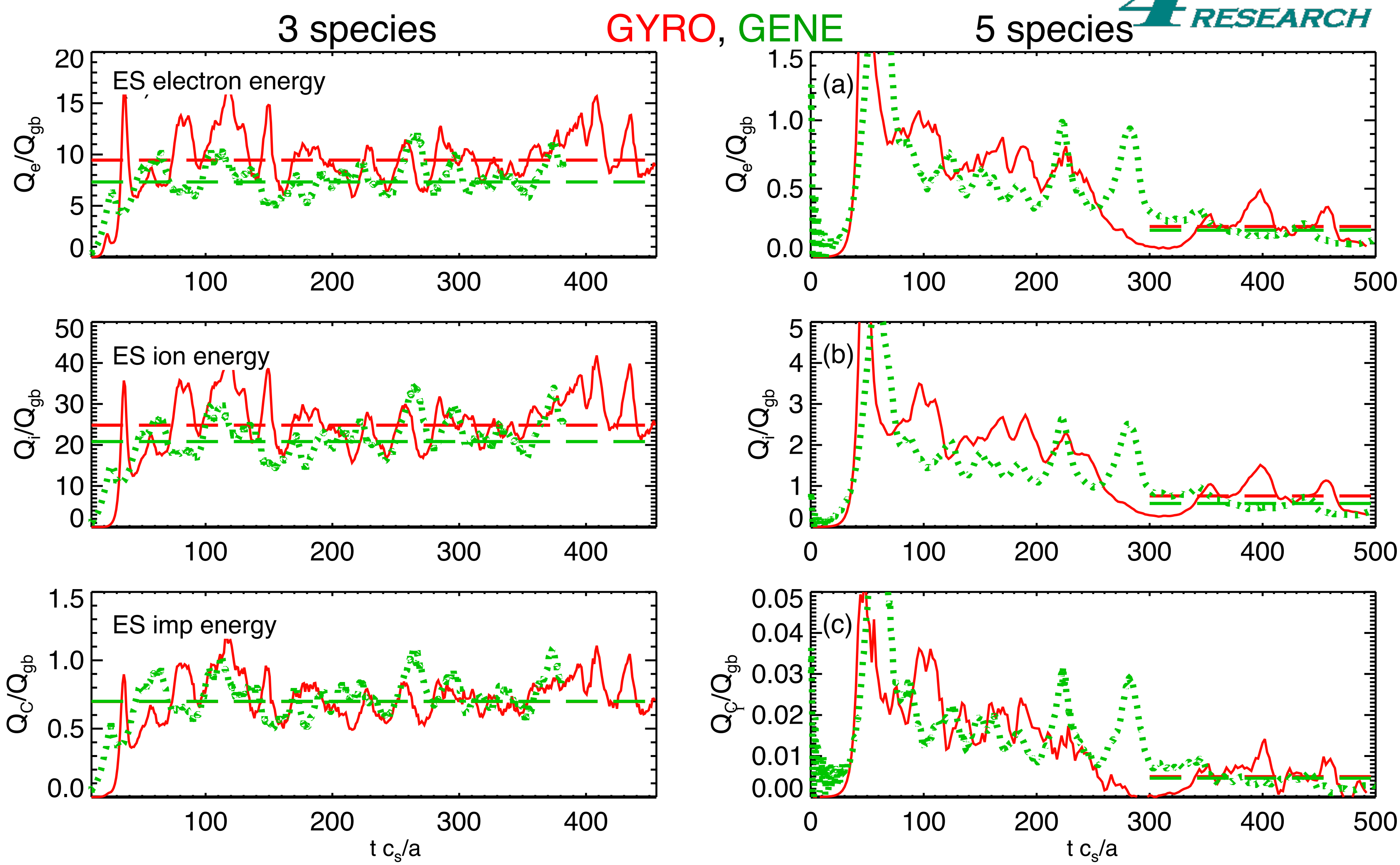
◆ Excellent agreement

5 species



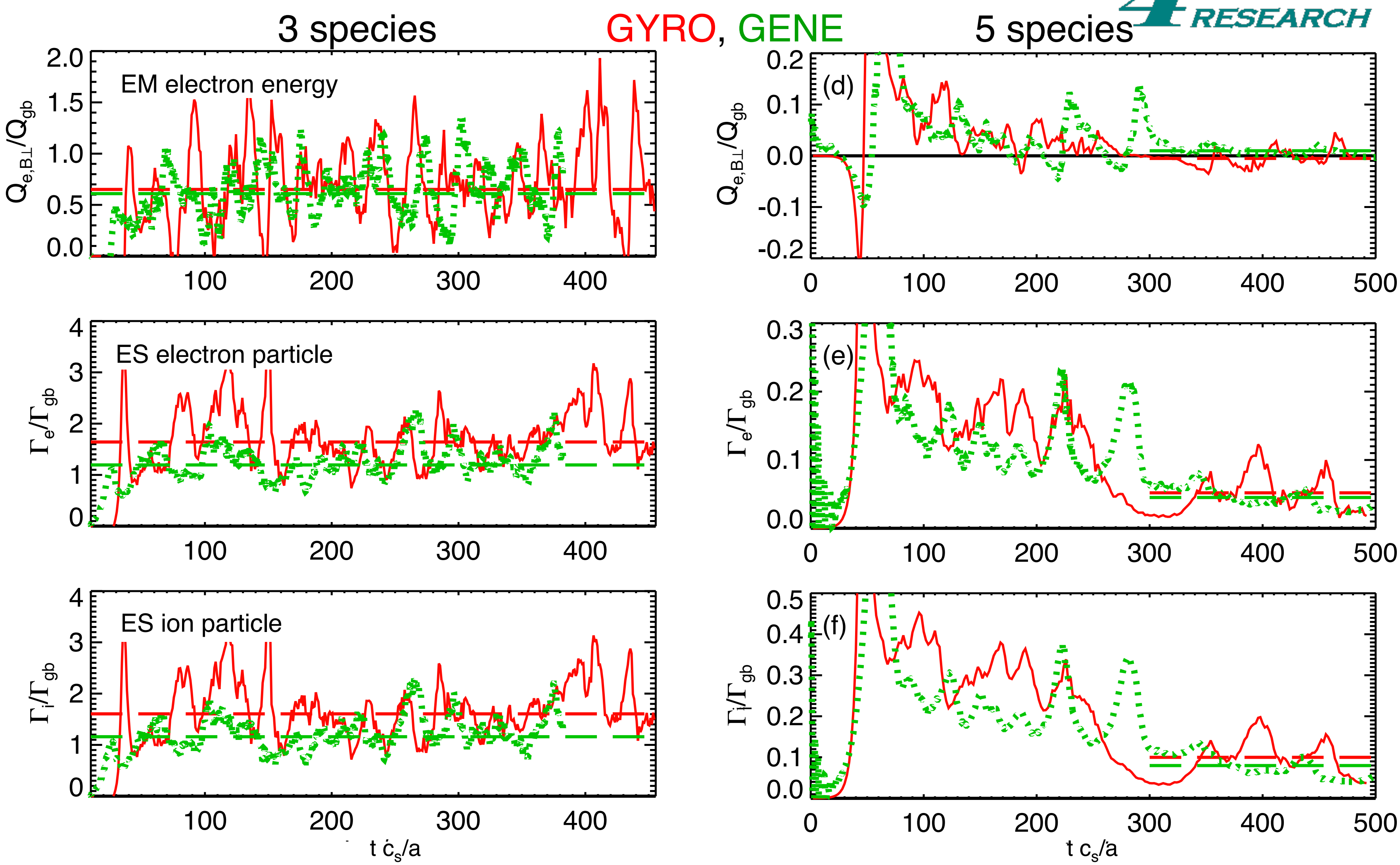
◆ Excellent agreement

Energy Fluxes 73224



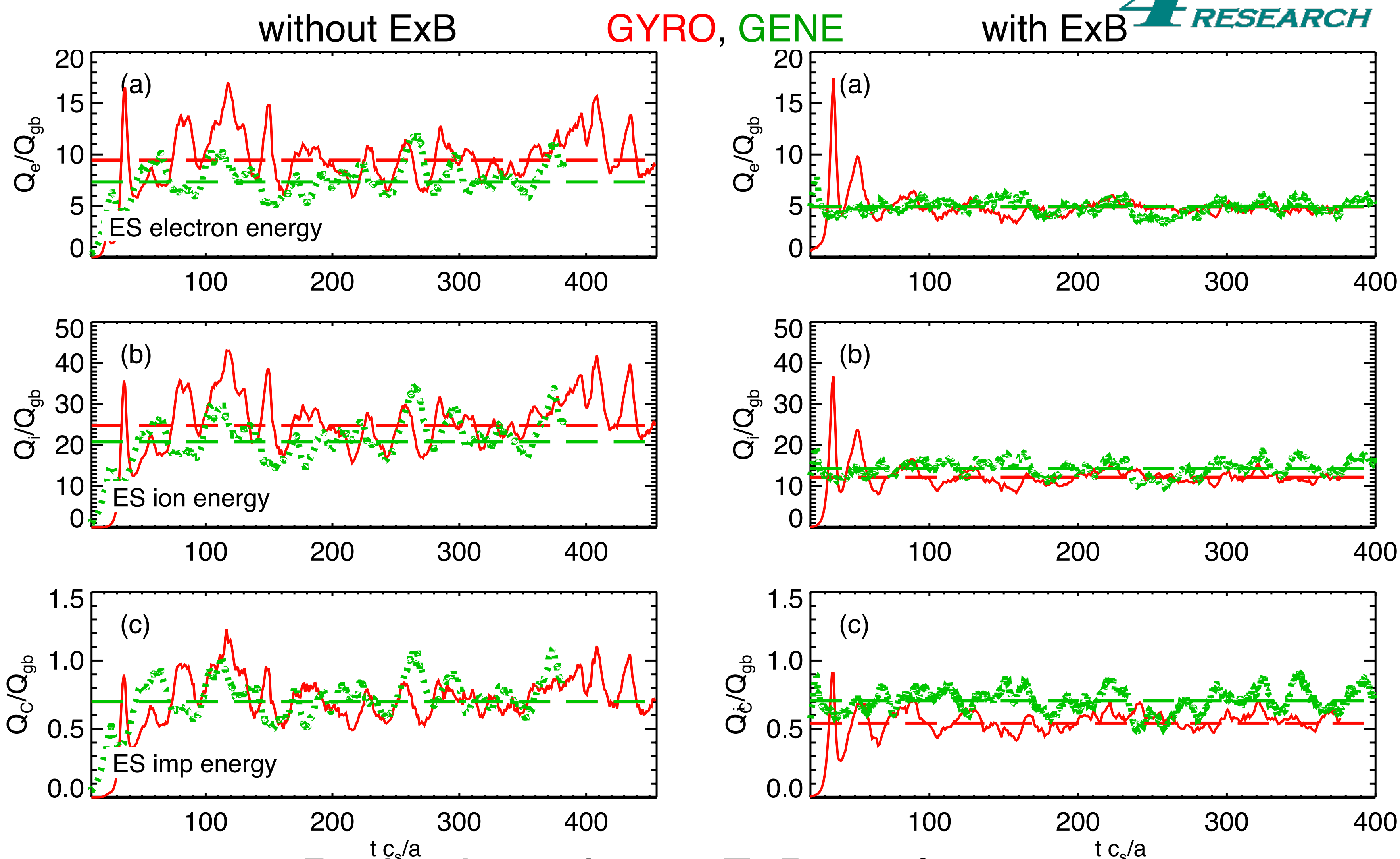
- Excellent agreement between GYRO, GENE
- Much reduced fluxes (factor > 10)
- Fluxes decay in time

Particle Fluxes 73224



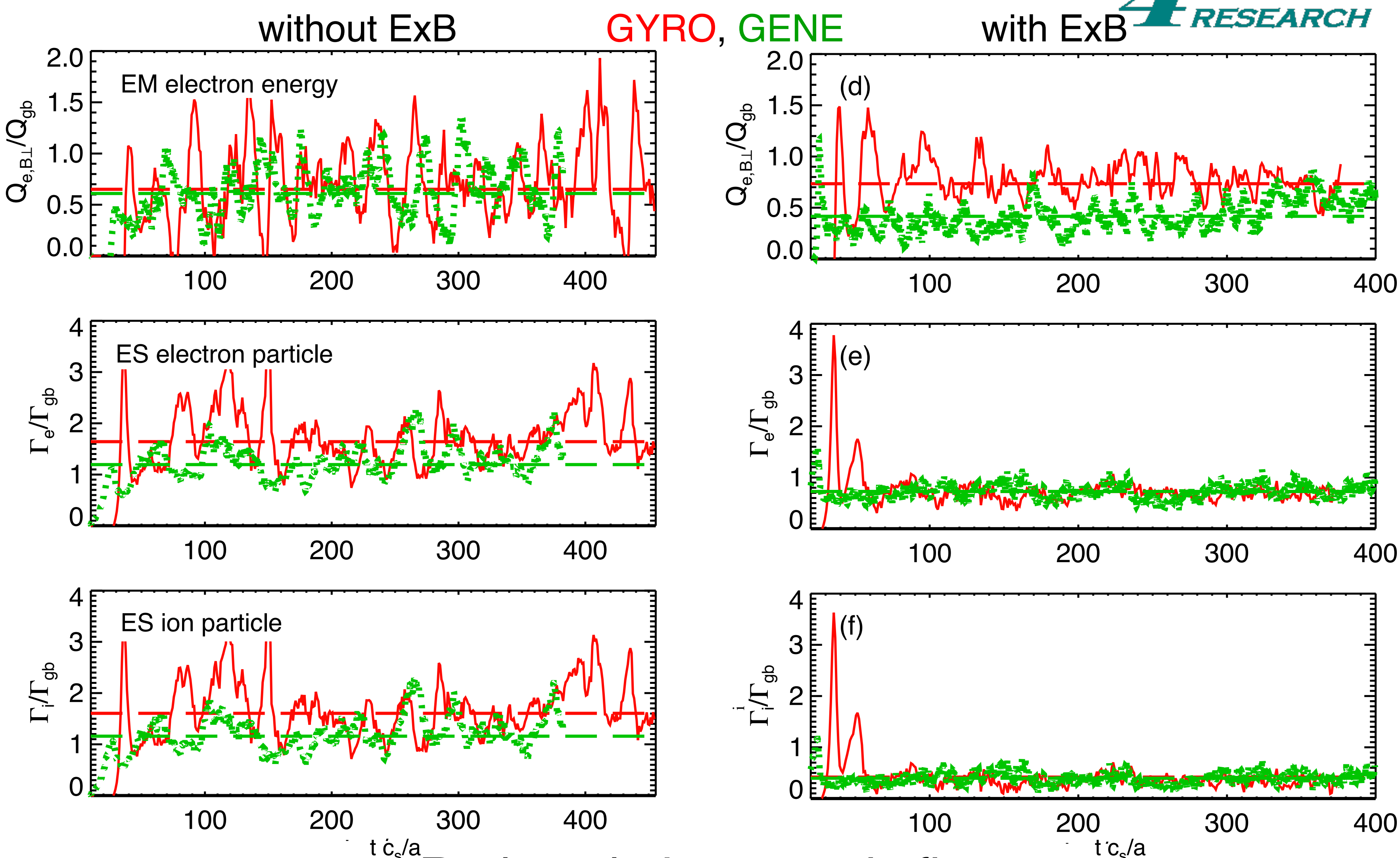
- Excellent agreement between GYRO, GENE
- Much reduced fluxes
- Fluxes decay in time

With ExB — 73224, 3 species



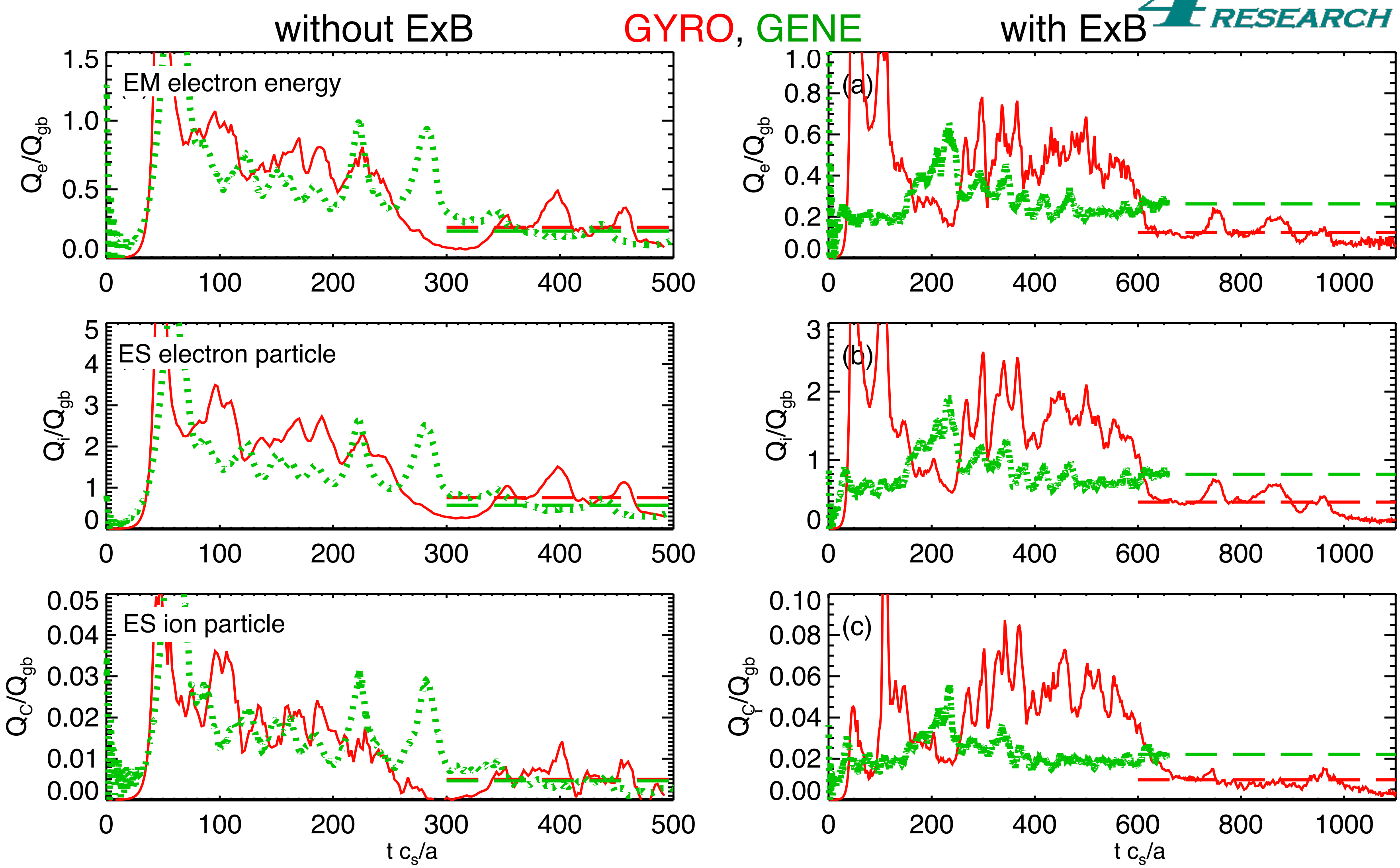
- Reductions due to ExB are factor > 1.5
- Good agreement between codes

With ExB — 73224, 3 species



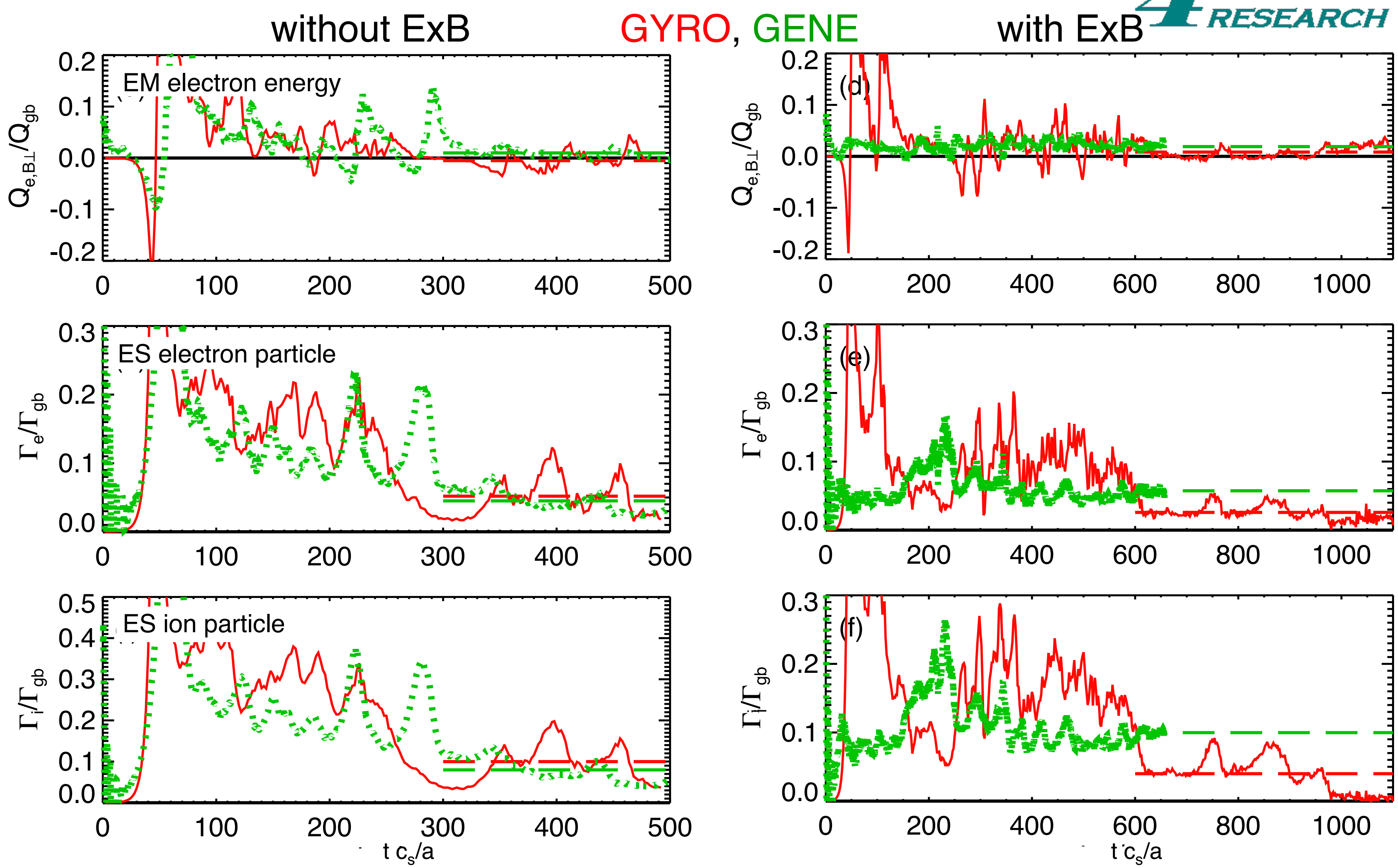
- Reduced electrostatic fluxes
- Good agreement between codes except EM flux

With ExB — 73224, 5 species



- No obvious reduction with ExB shear

With ExB — 73224, 5 species



- No obvious reduction with ExB shear

Summary — 73224

- Clear reduction in linear growth rates and nonlinear fluxes when hot ions (beam) included.

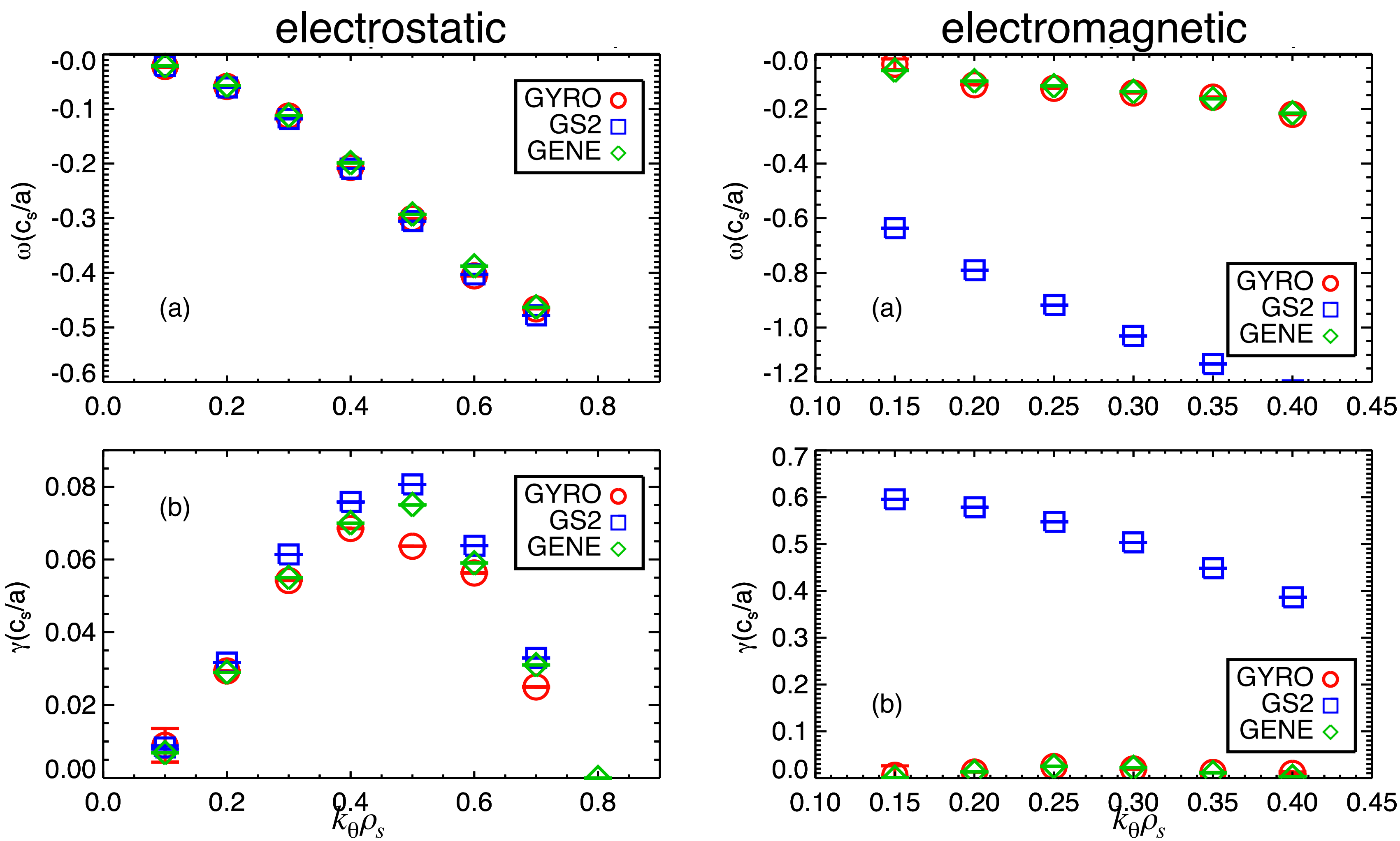
  Differences between 3 and 5 species normalized to 3 species:

	GENE	GYRO	GS2
$\Delta\gamma_{max}/\gamma_{max}(3spec)$	0.6	0.54	0.58
$\Delta Q_e/Q_e(3spec)$	0.95 ± 0.047	0.98 ± 0.012	-
$\Delta Q_i/Q_i(3spec)$	0.96 ± 0.045	0.97 ± 0.014	-
$\Delta\Gamma_e/\Gamma_e(3spec)$	0.94 ± 0.063	0.97 ± 0.018	-

- Agreement between GYRO and GENE for the factor >10 flux reduction when including fast ions.
- Agreement on smaller flux reduction when including ExB shear.

★ GYRO and GENE agree that fast-ion-enhanced EM stabilization dominates over ExB stabilization.

Linear Frequencies 75225

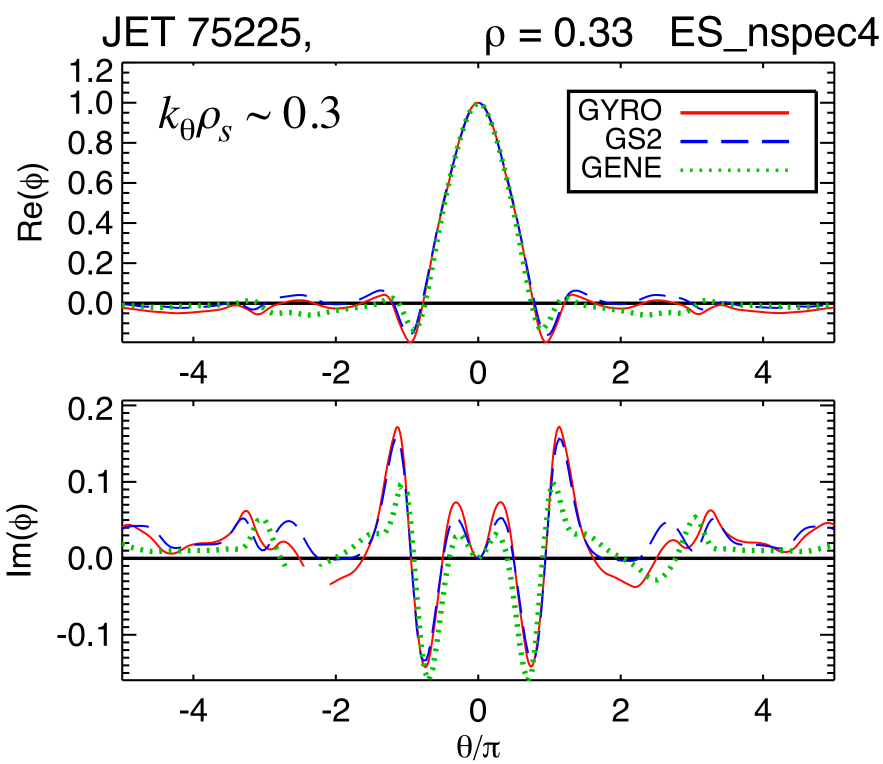


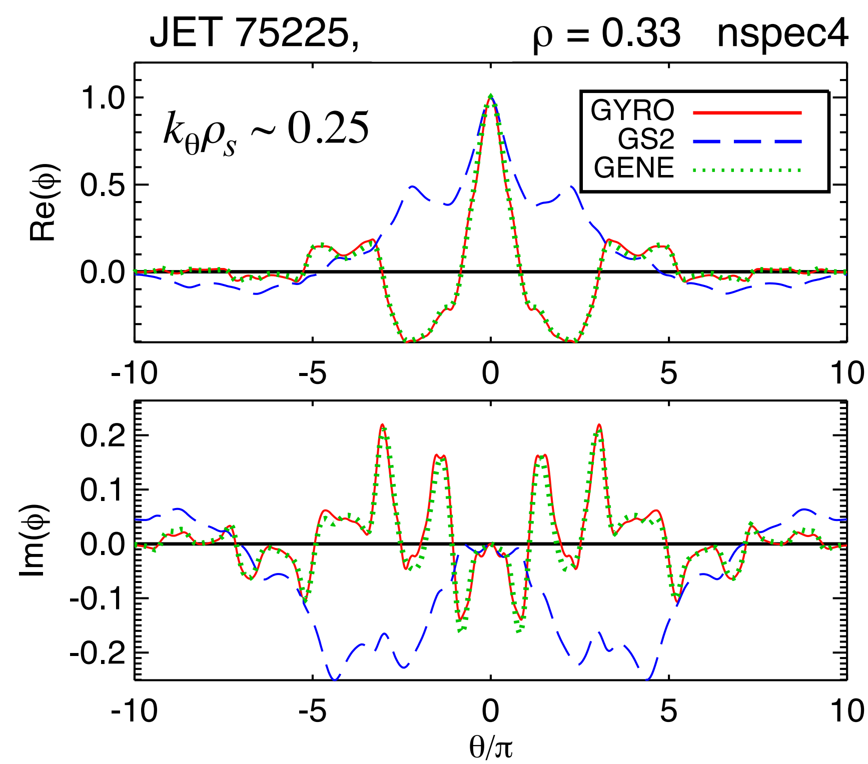
- Good agreement among codes
  (Stability above $k_\theta \rho_s \sim 0.75$)
- GS2 finds high-frequency modes

Eigenfunctions

electrostatic

electromagnetic



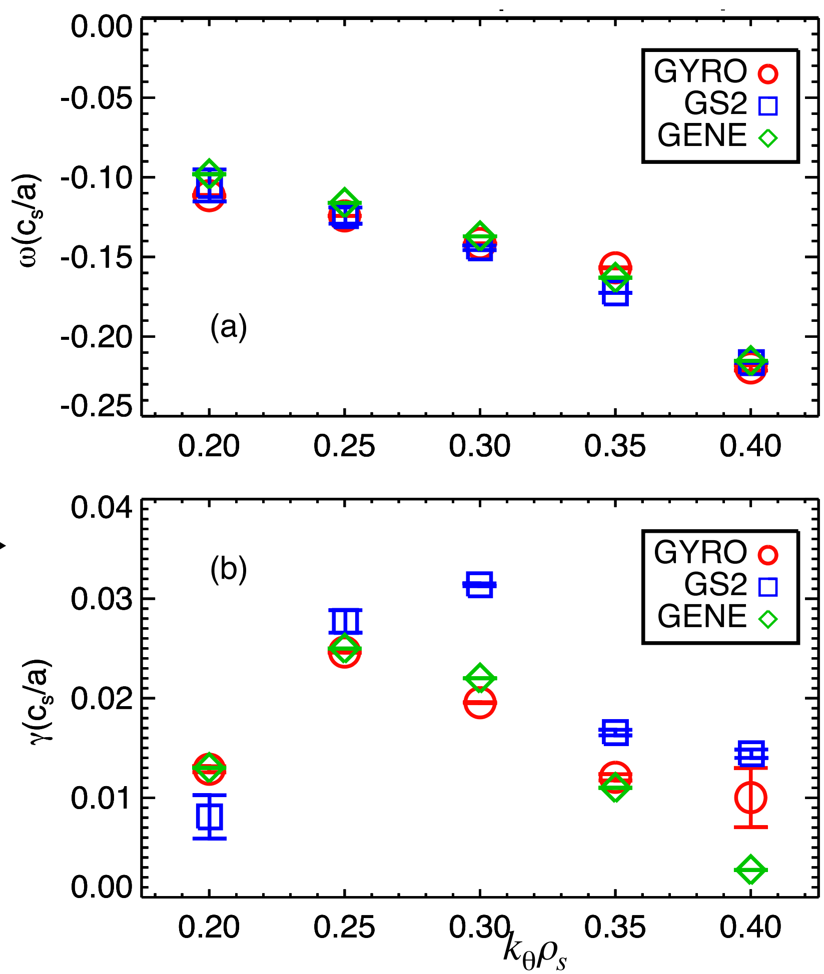


- Good agreement
- Excellent agreement GYRO/GENE
- Disagreement with GS2

Linear Frequencies 75225

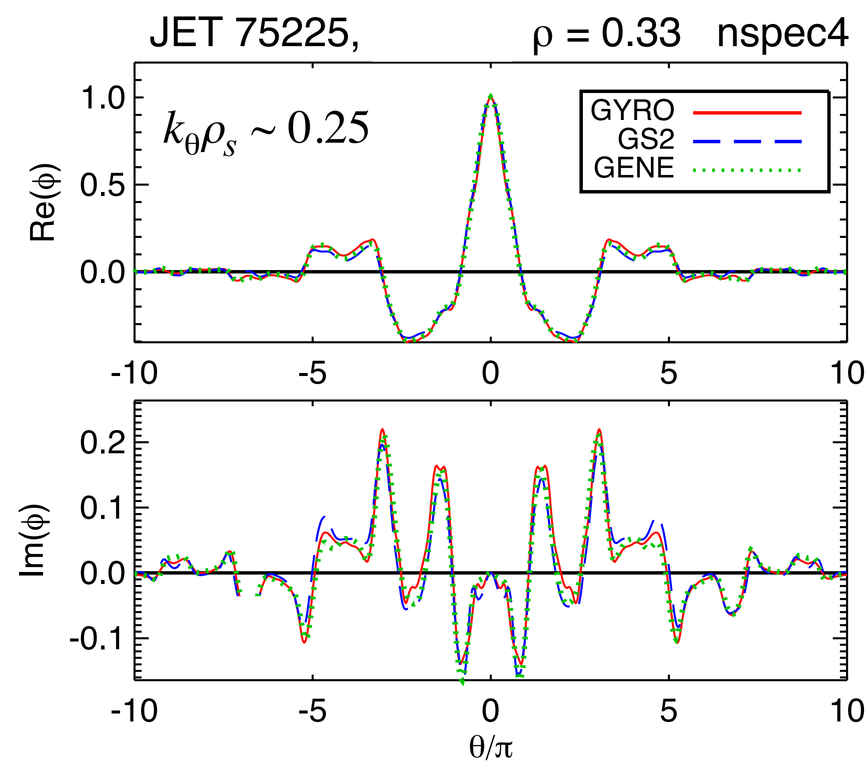
- Plasma profiles are near threshold from ITG modes to KBM-like modes.
- GYRO, GENE yield ITG modes while GS2 yields KBM-like modes (previous plots).
- Reduction of β in GS2 computation by 20% recovers ITG branch. ⟶

(GENE, GYRO also yield KBM modes at higher β.)



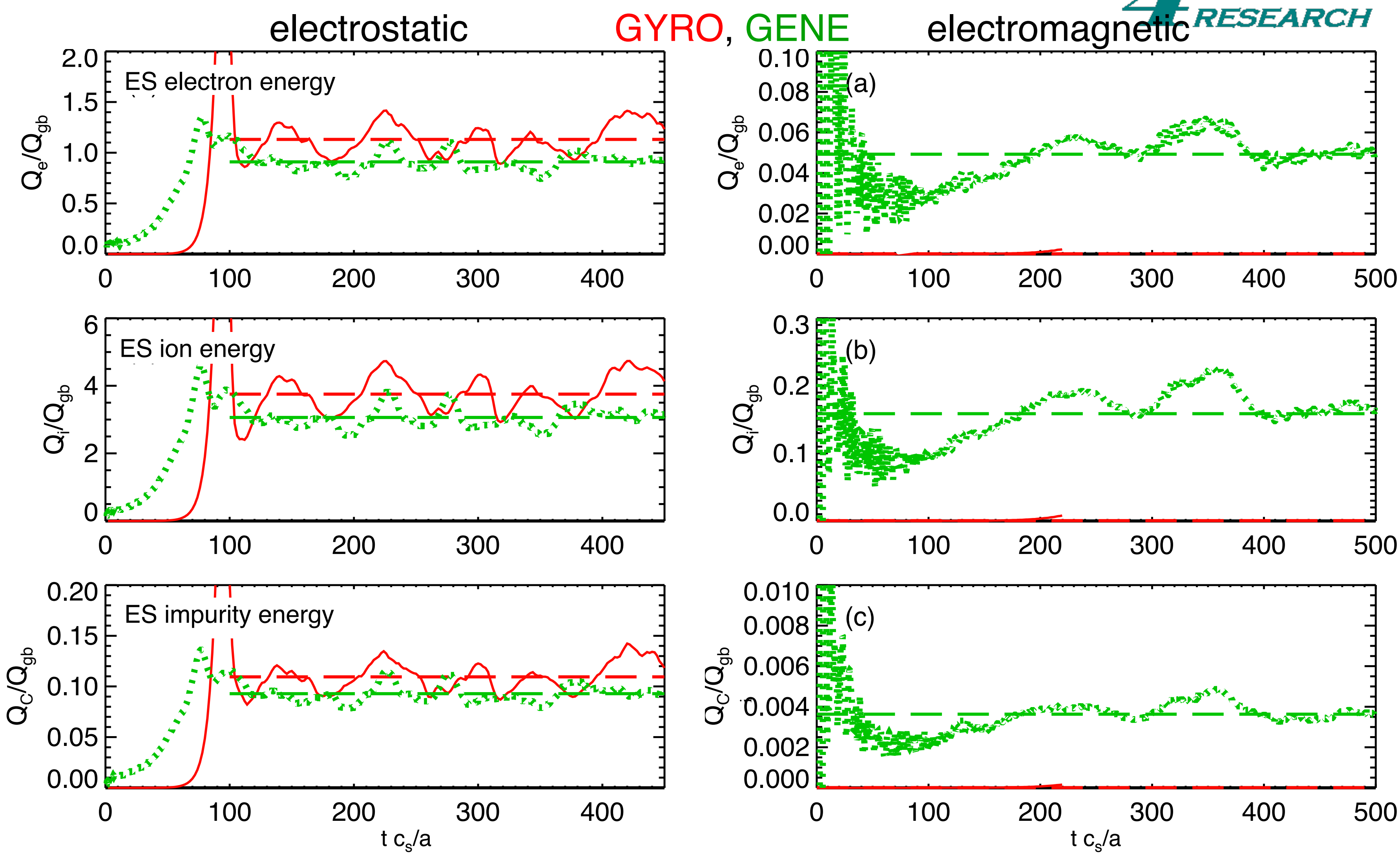
Eigenfunctions

electromagnetic, lower β



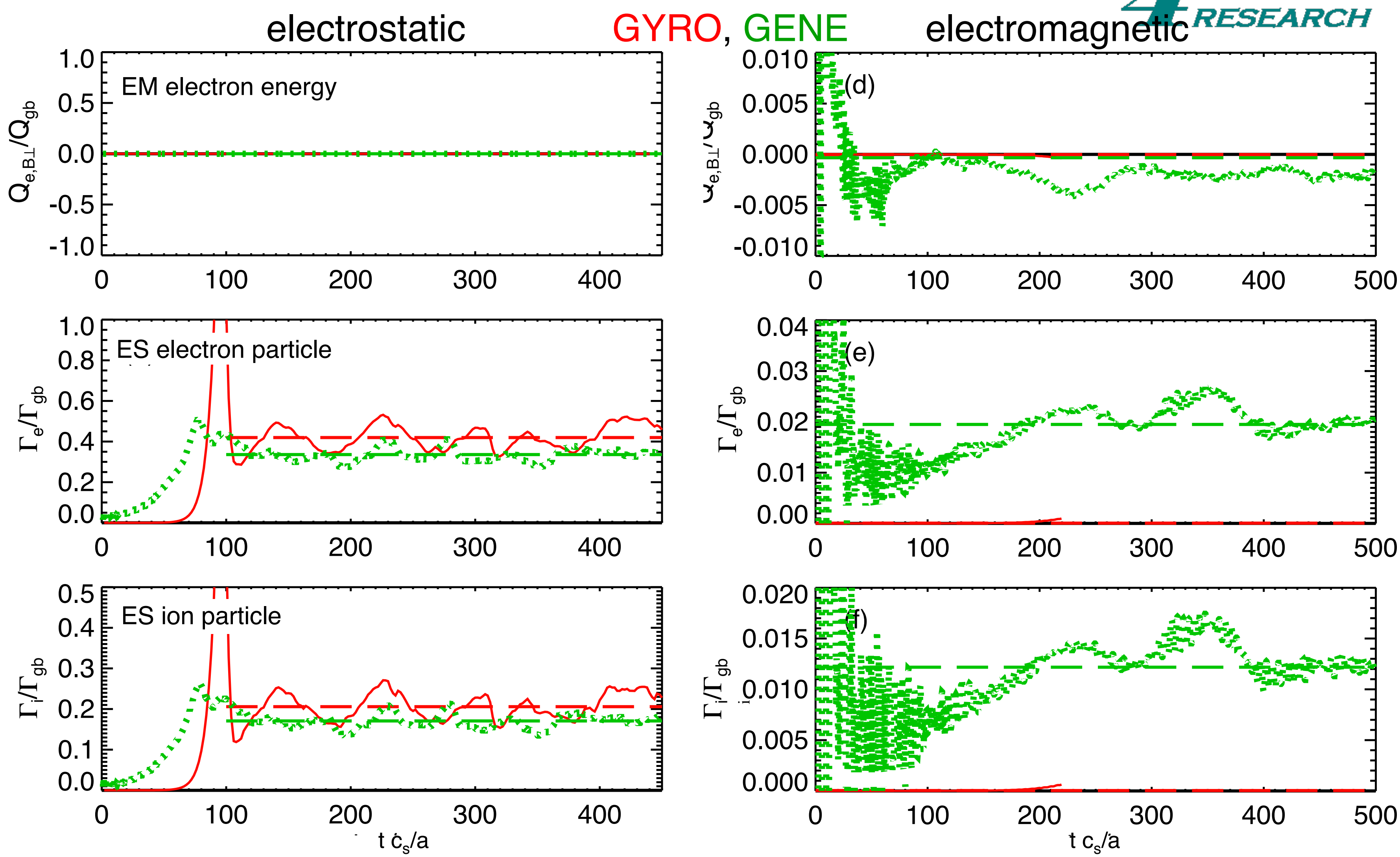
- Excellent agreement

Energy Fluxes 75225



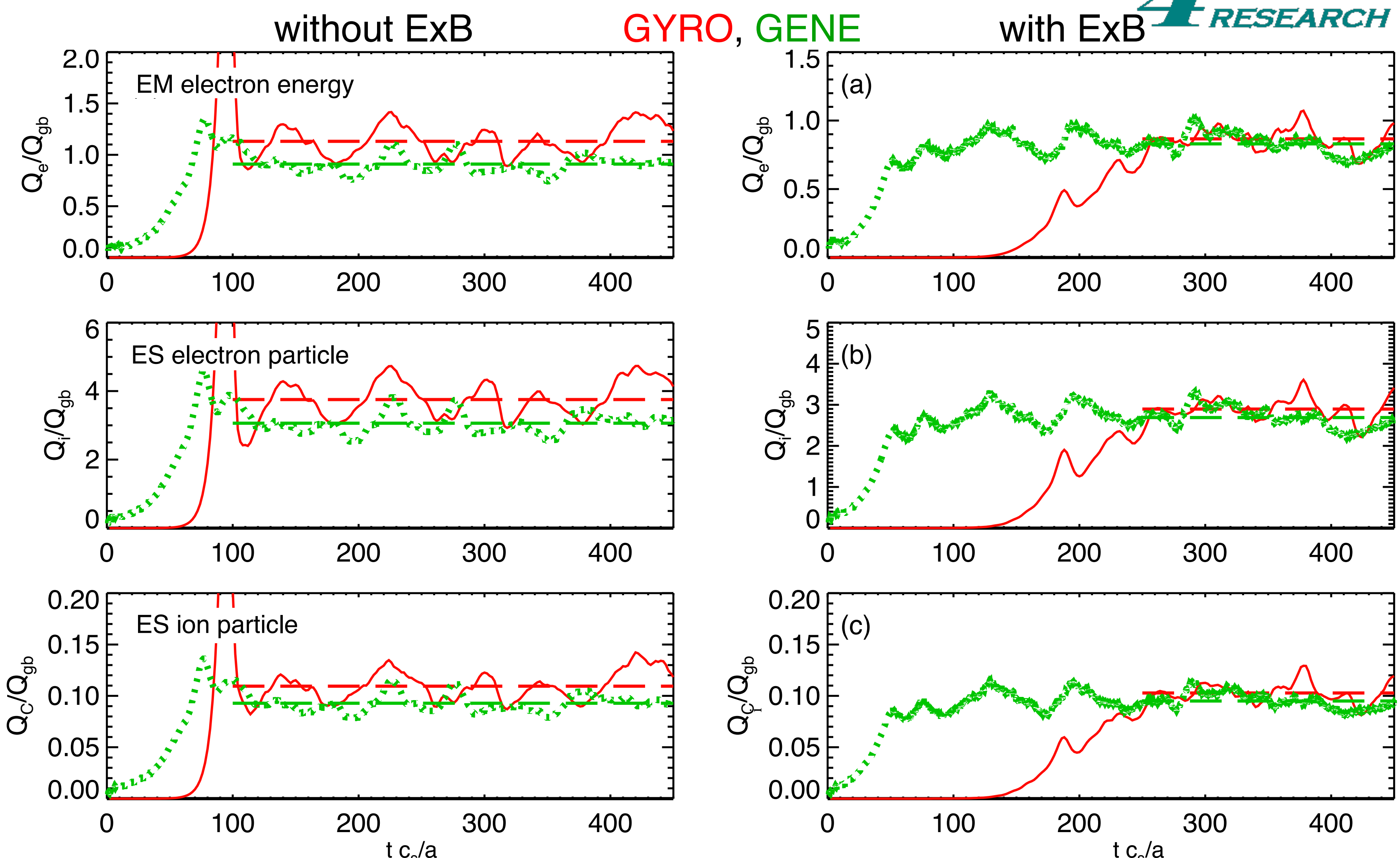
- Good agreement
- Much reduced fluxes
- GYRO fluxes negligible

Particle Fluxes 75225



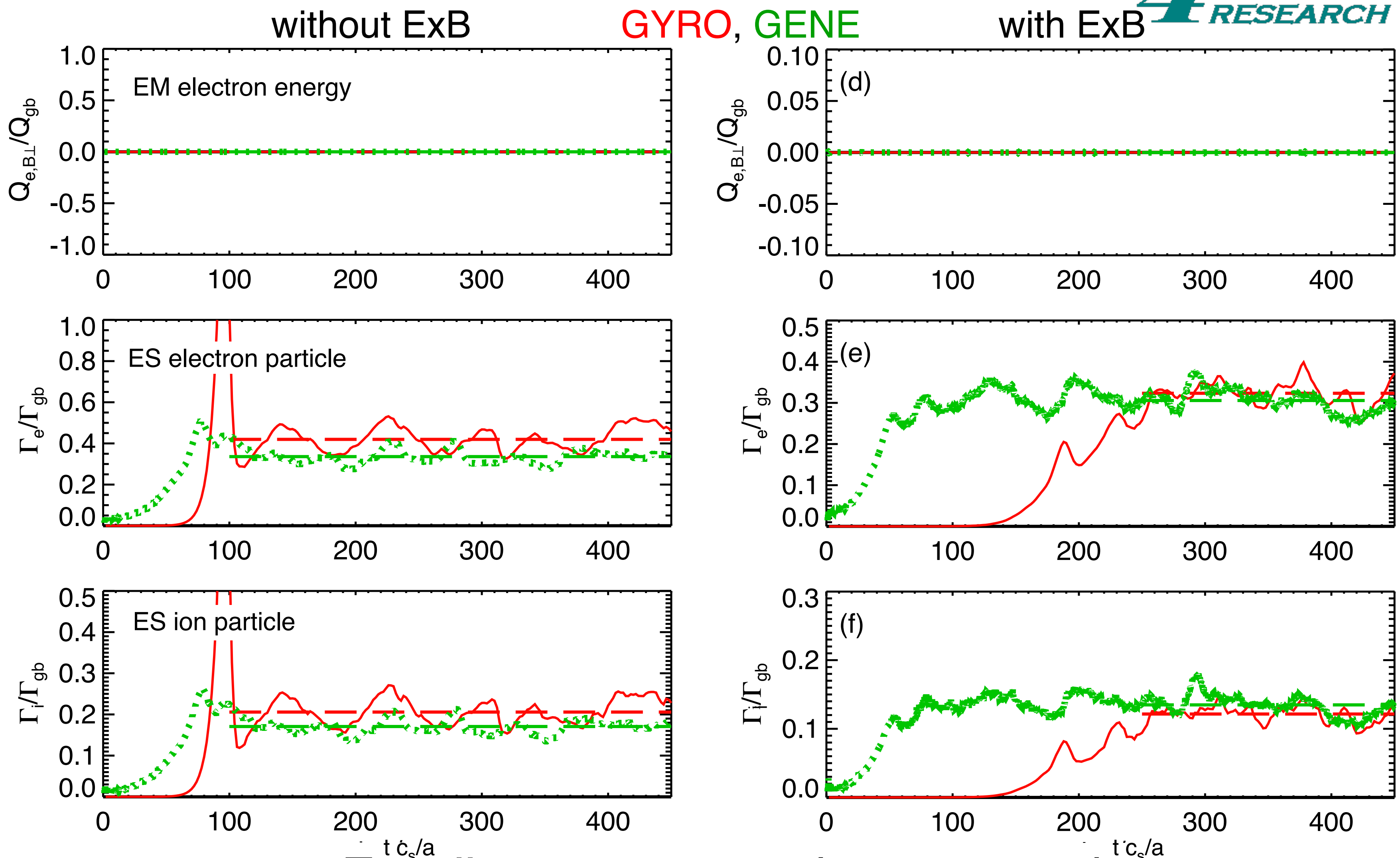
- Good agreement
- Much reduced fluxes
- GYRO fluxes negligible

With ExB — 75225, ES



- Excellent agreement between codes
- Little reduction with ExB shear

With ExB — 75225, ES



- Excellent agreement between codes
- Little reduction with ExB shear

Summary — 75225

- Excellent linear agreement
- Excellent ES agreement
- With EM stabilization, GENE fluxes are extremely small (in agreement with power balance). GYRO shows complete stabilization.

Conclusion and Next Steps

- Understand if nonlinear differences between codes for 66404 with EM effects are significant (now within error bars)
- Understand why some fluxes decay in 73224 case (GYRO with rotation, GENE without rotation)
- Understand why GS2 predicts KBM-like modes whereas GYRO, GENE predict ITG modes for 75225 EM.
- Add nonlinear GS2 simulations to code comparisons.

★ GYRO agrees with GENE on the physics picture for these discharges: EM-stabilization enhanced by fast ions is very significant, and much stronger than ExB stabilization.

PRODUCTS - DETAILS

PUBLICATIONS DETAIL

1. Journal Article: Electron temperature critical gradient and transport stiness in DIII-D	
Journal: Nuclear Fusion	
Publication Date: Not Provided	**Publication Status:** Published
Volume: 55	**First Page Number or eLocation ID:** 083011
Issue: Not Provided	**Publication Location:** Not Provided
Author(s): S.P. Smith1, C.C. Petty, A.E. White, C. Holland R. Bravenec, M.E. Austin, L. Zeng and O. Meneghini	
Publication Identifier Type: DOI	**Publication Identifier:** http://dx.doi.org/10.1088/0029-5515/55/8/083011
Acknowledgement of DOE Support: Yes	**Peer Reviewed:** Yes

INTELLECTUAL PROPERTIES DETAIL
There are no intellectual properties to report.

TECHNOLOGIES AND TECHNIQUES DETAIL
There are no technologies or techniques to report.

OTHER PRODUCTS DETAIL
There are no other products to report.

PARTICIPANTS AND OTHER COLLABORATING ORGANIZATIONS

PARTICIPANTS DETAIL

1. Participant: Dr. Ronald Victor Bravenec		
Project Role: Principal Investigator/Project Director	**Person Months Worked**: 5	**Funding Support (if other than this award)**: Not Provided
Contribution to the Project: Sole contributor funded by this grant		
International Collaboration: Yes		
#	**Country of Collaborator**	
1	Netherlands (NLD)	
2	Italy (ITA)	
3	France (FRA)	
4	Germany (DEU)	
5	United Kingdom (GBR)	
International Travel: No		

PARTNERS DETAIL

There are no partners to report.

OTHER COLLABORATORS DETAIL

1. Description of the Contribution:
Jeff Candy of General Atomics -- help with running GYRO and interpreting results.

2. Description of the Contribution:
Michael Barnes of Oxford Univ. -- help with running GS2 and interpreting results

3. Description of the Contribution:
Tobias Goerler of Max Planck Institute for Plasma Physics, Garching, Germany -- help with running GENE and interpreting results

4. Description of the Contribution:
M. J. Pueschel of Univ. of Wisconsin, Madison -- help with running GENE and interpreting results.

5. Description of the Contribution:
Jonathan Citrin of FOM Institute DIFFER, The Netherlands, and CEA Cadarche -- chief collaborator on project reported in APS/DPP poster: provided guidance and GENE results

6. Description of the Contribution:
Emily Belli of General Atomics -- discussions about GYRO runs

7. Description of the Contribution:
Gary Staebler of General Atomics -- discussions about general transport issues

IMPACT

1. What is the impact on the development of the principal discipline(s) of the project?
Gyrokinetic microinstability codes are used routinely to interpret experimental data and to predict transport in existing or future devices. Benchmarking (verifiification) is necessary to instill confidence in the codes' predictions.
2. What is the impact on other disciplines?
Nothing to Report
3. What is the impact on the development of human resources?
Nothing to Report
4. What is the impact on physical, institutional, and information resources that form infrastructure?
Nothing to Report
5. What is the impact on technology transfer?
Nothing to Report
6. What is the impact on society beyond science and technology?
Nothing to Report
7. Foreign Spending
Not Provided

CHANGES - PROBLEMS

1. Changes in approach and reasons for change
Nothing to Report
2. Actual or anticipated problems or delays and actions or plans to resolve them
After an upgrade to the Hopper computer at NERSC, I could not run GS2 nonlinearly ("segmentation faults," etc.). Plans to resolve this issue are to first download the most recent version of the code and compile it. If running the executable is unsuccessful, I will consult with the code developers.
3. Changes that have a significant impact on expenditures
Nothing to Report
4. Significant changes in use or care of human subjects, vertebrate animals, and/or biohazards
Nothing to Report
5. Change of primary performance site location from that originally proposed
Nothing to Report
6. Carryover Amount
Estimated carryover amount for the next budget period: $ 5,000.00

Proposal #
0000225539

U.S. Department of Energy
Office of Science

GrantsGov #
GRANT12197477

APPLICATION/PROPOSAL COVER SHEET

THE ATTACHED APPLICATION/PROPOSAL IS FOR YOUR REVIEW & APPROPRIATE ACTION

INSTITUTION: Fourth State Research, Austin, Texas

TYPE OF REQUEST: Renewal

P.I.: Bravenec, Ronald

DATE RECEIVED: 6/17/2016 4:28:38 PM

AWARD NO: DE-FG02-08ER54978

SOLICITATION NO: DE-FOA-0001560

TITLE: A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes

TOTAL NUMBER OF PAGES SUBMITTED: 35

ERROR LIST: No Errors

Table Of Contents

OMB Number: 4040-0001
Expiration Date: 6/30/2016

APPLICATION FOR FEDERAL ASSISTANCE
SF 424 (R&R)

3. DATE RECEIVED BY STATE:

State Application Identifier:

1. TYPE OF SUBMISSION

☐ Pre-application ☒ Application ☐ Changed/Corrected Application

4. a. Federal Identifier: DE-FG02-08ER54978

b. Agency Routing Identifier:

2. DATE SUBMITTED:

Applicant Identifier:

c. Previous Grants.gov Tracking ID:

5. APPLICANT INFORMATION

Organizational DUNS: 808068469

Legal Name: Fourth State Research

Department:

Division:

Street1: 503 Lockhart Dr.

Street2:

City: Austin

County / Parish: Travis

State: TX: Texas

Province:

Country: USA: UNITED STATES

ZIP / Postal Code: 78704-4335

Person to be contacted on matters involving this application

Prefix: Dr.

First Name: Ronald

Middle Name: Victor

Last Name: Bravenec

Suffix: Ph.D

Position/Title: owner

Street1: 503 Lockhart Dr.

Street2:

City: Austin

County / Parish: Travis

State: TX: Texas

Province:

Country: USA: UNITED STATES

ZIP / Postal Code: 78704-4335

Phone Number: 512-800-3327

Fax Number:

Email: rvbravenec@4th-state.com

6. EMPLOYER IDENTIFICATION *(EIN) or (TIN):* 26-4021697

7. TYPE OF APPLICANT: R: Small Business

Other (Specify):

Small Business Organization Type ☐ Women Owned ☐ Socially and Economically Disadvantaged

8. TYPE OF APPLICATION:

☐ New ☐ Resubmission

☒ Renewal ☐ Continuation ☐ Revision

If Revision, mark appropriate box(es).

☐ A. Increase Award ☐ B. Decrease Award ☐ C. Increase Duration ☐ D. Decrease Duration

☐ E. Other (specify):

Is this application being submitted to other agencies? Yes ☐ No ☒ What other Agencies?

9. NAME OF FEDERAL AGENCY: Office of Science

10. CATALOG OF FEDERAL DOMESTIC ASSISTANCE NUMBER: 81.049

TITLE: Office of Science Financial Assistance Program

11. DESCRIPTIVE TITLE OF APPLICANT'S PROJECT:

A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes

12. PROPOSED PROJECT:

Start Date: 02/15/2017

Ending Date: 02/14/2020

13. CONGRESSIONAL DISTRICT OF APPLICANT: 21

SF 424 (R&R) APPLICATION FOR FEDERAL ASSISTANCE

14. PROJECT DIRECTOR/PRINCIPAL INVESTIGATOR CONTACT INFORMATION

Prefix: Dr. First Name: Ronald Middle Name: Victor
Last Name: Bravenec Suffix: Ph.D
Position/Title: Owner
Organization Name: Fourth State Research
Department: Division:
Street1: 503 Lockhart Dr.
Street2:
City: Austin County / Parish: Travis
State: TX: Texas Province:
Country: USA: UNITED STATES ZIP / Postal Code: 78704-4335
Phone Number: 512-800-3327 Fax Number:
Email: rvbravenec@4th-state.com

15. ESTIMATED PROJECT FUNDING

a. Total Federal Funds Requested	225,000.00
b. Total Non-Federal Funds	0.00
c. Total Federal & Non-Federal Funds	225,000.00
d. Estimated Program Income	0.00

16. IS APPLICATION SUBJECT TO REVIEW BY STATE EXECUTIVE ORDER 12372 PROCESS?

a. YES ☐ THIS PREAPPLICATION/APPLICATION WAS MADE AVAILABLE TO THE STATE EXECUTIVE ORDER 12372 PROCESS FOR REVIEW ON:

DATE:

b. NO ☒ PROGRAM IS NOT COVERED BY E.O. 12372; OR

☐ PROGRAM HAS NOT BEEN SELECTED BY STATE FOR REVIEW

17.

17. By signing this application, I certify (1) to the statements contained in the list of certifications* and (2) that the statements herein are true, complete and accurate to the best of my knowledge. I also provide the required assurances * and agree to comply with any resulting terms if I accept an award. I am aware that any false, fictitious. or fraudulent statements or claims may subject me to criminal, civil, or administrative penalties. (U.S. Code, Title 18, Section 1001)

☒ **I agree**

**The list of certifications and assurances, or an Internet site where you may obtain this list, is contained in the announcement or agency specific instructions.*

18. SFLLL (Disclosure of Lobbying Activities) or other Explanatory Documentation

Add Attachment | Delete Attachment | View Attachment

19. Authorized Representative

Prefix: Dr. First Name: Ronald Middle Name: Victor
Last Name: Bravenec Suffix: Ph.D
Position/Title: Owner
Organization: Fourth State Research
Department: Division:
Street1: 503 Lockhart Dr.
Street2:
City: Austin County / Parish: Travis
State: TX: Texas Province:
Country: USA: UNITED STATES ZIP / Postal Code: 78704-4335
Phone Number: 512-800-3327 Fax Number:
Email: rvbravenec@4th-state.com

Signature of Authorized Representative	Date Signed
Ronald Bravenec	06/17/2016

20. Pre-application Add Attachment | Delete Attachment | View Attachment

21. Cover Letter Attachment Add Attachment | Delete Attachment | View Attachment

RESEARCH & RELATED Other Project Information

OMB Number: 4040-0001
Expiration Date: 6/30/2016

1. Are Human Subjects Involved? ☐ Yes ☒ No
   1.a. If YES to Human Subjects
   Is the Project Exempt from Federal regulations? ☐ Yes ☐ No
   If yes, check appropriate exemption number. ☐ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6
   If no, is the IRB review Pending? ☐ Yes ☐ No
   IRB Approval Date:
   Human Subject Assurance Number:
2. Are Vertebrate Animals Used? ☐ Yes ☒ No
   2.a. If YES to Vertebrate Animals
   Is the IACUC review Pending? ☐ Yes ☐ No
   IACUC Approval Date:
   Animal Welfare Assurance Number:
3. Is proprietary/privileged information included in the application? ☐ Yes ☒ No

4.a. Does this Project Have an Actual or Potential Impact - positive or negative - on the environment? ☐ Yes ☒ No

4.b. If yes, please explain:

4.c. If this project has an actual or potential impact on the environment, has an exemption been authorized or an environmental assessment (EA) or environmental impact statement (EIS) been performed? ☐ Yes ☐ No

4.d. If yes, please explain:

5. Is the research performance site designated, or eligible to be designated, as a historic place? ☐ Yes ☒ No

5.a. If yes, please explain:

6. Does this project involve activities outside of the United States or partnerships with international collaborators? ☒ Yes ☐ No

6.a. If yes, identify countries: The Netherlands, Italy, England

6.b. Optional Explanation:

7. Project Summary/Abstract 1235-Bravenec_Summary_Abstract.pdf Add Attachment Delete Attachment View Attachment

8. Project Narrative 1236-Bravenec_Project_Narrative.pdf Add Attachment Delete Attachment View Attachment

9. Bibliography & References Cited Add Attachment Delete Attachment View Attachment

10. Facilities & Other Resources Add Attachment Delete Attachment View Attachment

11. Equipment Add Attachment Delete Attachment View Attachment

12. Other Attachments Add Attachments Delete Attachments View Attachments ☐

OMB Number: 4040-0010
Expiration Date: 9/30/2016

Project/Performance Site Location(s)

Project/Performance Site Primary Location

☐ I am submitting an application as an individual, and not on behalf of a company, state, local or tribal government, academia, or other type of organization.

Organization Name: Fourth State Research

DUNS Number: 8080684690000

* Street1: 503 Lockhart Dr.

Street2:

* City: Austin

County: Travis

* State: TX: Texas

Province:

* Country: USA: UNITED STATES

* ZIP / Postal Code: 78704-4335

* Project/ Performance Site Congressional District: TX-021

Project/Performance Site Location 1

☐ I am submitting an application as an individual, and not on behalf of a company, state, local or tribal government, academia, or other type of organization.

Organization Name: Fourth State Research

DUNS Number: 8080684690000

* Street1: 503 Lockhart Dr.

Street2:

* City: Austin

County: Travis

* State: TX: Texas

Province:

* Country: USA: UNITED STATES

* ZIP / Postal Code: 78704-4335

* Project/ Performance Site Congressional District: TX-021

Additional Location(s) Add Attachment Delete Attachment View Attachment

Budget Period: 1 Duration: 12 months	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested ($) (Salary+Fringe)
A. Senior Personnel: PI/PO, Co-PI's, Faculty and Other Senior Associates — **Total Senior Personnel (1-8)**				69,785.00
1. Bravenec, Ronald Victor	5	0	0	69,785.00
2.				
3.				
4.				
5.				
6.				
7.				
8.				
9. Others (See Attachment for Details)				0.00
B. Other Personnel (Number in Brackets) — **Total Other Personnel**				0.00
(0) Post Doctoral Associates				0.00
(0) Graduate Students				0.00
(0) Undergraduate Students				0.00
(0) Secretarial / Clerical				0.00
Total Personnel Costs — **Total Salaries and Wages (A+B)**				69,785.00
C. Permanent Equipment — **Total Permanent Equipment**				0.00
D. Travel — **Total Travel**				4,915.00
1. Domestic Travel Costs (including Canada, Mexico, and U.S. possessions)				4,915.00
2. Foreign Travel Costs				0.00
E. Trainee/Participant Costs (Total Participants: 0) — **Total Trainee/Participants**				0.00
1. Tuition/Fees/Health Insurance				0.00
2. Stipends				0.00
3. Trainee Travel				0.00
4. Subsistence				0.00
5. Other				0.00
F. Other Direct Costs — **Total Other Direct Costs**				300.00
1. Materials and Supplies				10.00
2. Publication Costs/Documentation/Dissemination				290.00
3. Consultant Services				0.00
4. Computer (ADP) Services				0.00
5. SubAwards/Consortium/Contractual Costs				0.00
6. Equipment or Facility Rental/User Fees				0.00
7. Alterations and Renovations				0.00
8.				0.00
9.				0.00
10.				0.00
G. Direct Costs — **Total Direct Costs (A through F)**				75,000.00
H. Indirect Costs — **Total Indirect Costs**				0.00
		Indirect Cost Rate	**Indirect Cost Base**	
I. Direct and Indirect Costs — **Total Direct and Indirect Costs (G+H)**				75,000.00
J. Fee — **Total Fee**				0.00
K. Cost of Project — **Total Cost of Project (I+J)**				75,000.00

Budget Period: 2 Duration: 12 months	DOE Funded Person-mos.			Funds Requested ($) (Salary+Fringe)
	CAL	ACAD	SUMR	
A. Senior Personnel: PI/PO, Co-PI's, Faculty and Other Senior Associates — **Total Senior Personnel (1-8)**				69,926.00
1. Bravenec, Ronald Victor	5	0	0	69,926.00
2.				
3.				
4.				
5.				
6.				
7.				
8.				
9. Others (See Attachment for Details)				0.00
B. Other Personnel (Number in Brackets) — **Total Other Personnel**				0.00
(0) Post Doctoral Associates				0.00
(0) Graduate Students				0.00
(0) Undergraduate Students				0.00
(0) Secretarial / Clerical				0.00
Total Personnel Costs — **Total Salaries and Wages (A+B)**				69,926.00
C. Permanent Equipment — **Total Permanent Equipment**				0.00
D. Travel — **Total Travel**				5,013.00
1. Domestic Travel Costs (including Canada, Mexico, and U.S. possessions)				5,013.00
2. Foreign Travel Costs				0.00
E. Trainee/Participant Costs (Total Participants: 0) — **Total Trainee/Participants**				0.00
1. Tuition/Fees/Health Insurance				0.00
2. Stipends				0.00
3. Trainee Travel				0.00
4. Subsistence				0.00
5. Other				0.00
F. Other Direct Costs — **Total Other Direct Costs**				61.00
1. Materials and Supplies				10.00
2. Publication Costs/Documentation/Dissemination				51.00
3. Consultant Services				0.00
4. Computer (ADP) Services				0.00
5. SubAwards/Consortium/Contractual Costs				0.00
6. Equipment or Facility Rental/User Fees				0.00
7. Alterations and Renovations				0.00
8.				0.00
9.				0.00
10.				0.00
G. Direct Costs — **Total Direct Costs (A through F)**				75,000.00
H. Indirect Costs — **Total Indirect Costs**				0.00
		Indirect Cost Rate	**Indirect Cost Base**	
I. Direct and Indirect Costs — **Total Direct and Indirect Costs (G+H)**				75,000.00
J. Fee — **Total Fee**				0.00
K. Cost of Project — **Total Cost of Project (I+J)**				75,000.00

Budget Period: 3 Duration: 12 months	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested ($) (Salary+Fringe)
A. Senior Personnel: PI/PO, Co-PI's, Faculty and Other Senior Associates — **Total Senior Personnel (1-8)**				69,574.00
1. Bravenec, Ronald Victor	5	0	0	69,574.00
2.				
3.				
4.				
5.				
6.				
7.				
8.				
9. Others (See Attachment for Details)				0.00
B. Other Personnel (Number in Brackets) — **Total Other Personnel**				0.00
(0) Post Doctoral Associates				0.00
(0) Graduate Students				0.00
(0) Undergraduate Students				0.00
(0) Secretarial / Clerical				0.00
Total Personnel Costs — **Total Salaries and Wages (A+B)**				69,574.00
C. Permanent Equipment — **Total Permanent Equipment**				0.00
D. Travel — **Total Travel**				5,114.00
1. Domestic Travel Costs (including Canada, Mexico, and U.S. possessions)				5,114.00
2. Foreign Travel Costs				0.00
E. Trainee/Participant Costs (Total Participants: 0) — **Total Trainee/Participants**				0.00
1. Tuition/Fees/Health Insurance				0.00
2. Stipends				0.00
3. Trainee Travel				0.00
4. Subsistence				0.00
5. Other				0.00
F. Other Direct Costs — **Total Other Direct Costs**				312.00
1. Materials and Supplies				10.00
2. Publication Costs/Documentation/Dissemination				302.00
3. Consultant Services				0.00
4. Computer (ADP) Services				0.00
5. SubAwards/Consortium/Contractual Costs				0.00
6. Equipment or Facility Rental/User Fees				0.00
7. Alterations and Renovations				0.00
8.				0.00
9.				0.00
10.				0.00
G. Direct Costs — **Total Direct Costs (A through F)**				75,000.00
H. Indirect Costs — **Total Indirect Costs**				0.00
		Indirect Cost Rate	**Indirect Cost Base**	
I. Direct and Indirect Costs — **Total Direct and Indirect Costs (G+H)**				75,000.00
J. Fee — **Total Fee**				0.00
K. Cost of Project — **Total Cost of Project (I+J)**				75,000.00

Cumulative Total	Subtotal	Totals ($)
Section A, Senior/Key Person		209,285.00
Section B, Other Personnel		0.00
Total Number Other Personnel	0	
Total Salary, Wages and Fringe Benefits (A+B)		209,285.00
Section C, Equipment		0.00
Section D, Travel		15,042.00
1. Domestic	15,042.00	
2. Foreign	0.00	
Section E, Participant/Trainee Support Costs		0.00
1. Tuition/Fees/Health Insurance	0.00	
2. Stipends	0.00	
3. Travel	0.00	
4. Subsistence	0.00	
5. Other	0.00	
Number of Participants/Trainees	0	
Section F, Other Direct Costs		673.00
1. Material and Supplies	30.00	
2. Publication Costs	643.00	
3. Consultant Services	0.00	
4. ADP/Computer Services	0.00	
5. Subawards/Consortium/Contractual Costs	0.00	
6. Equipment or Facility Rental/User Fees	0.00	
7. Alterations and Renovations	0.00	
8. Other 1	0.00	
9. Other 2	0.00	
10. Other 3	0.00	
Section G, Direct Costs (A thru F)		225,000.00
Section H, Indirect Costs		0.00
Section I, Total Direct and Indirect Costs (G+H)		225,000.00
Section J, Fee		0.00
Section K, Total Cost of Project (I+J)		225,000.00

Budget Justification – Year 1	
A. Senior Personnel	
Ronald Bravenec: a rate not unreasonable for researchers of his experience and seniority.	$57,493
C. Fringe Benefits	
Dental insurance $30.87/mo.	$154
Employer share of FICA/Medicare (7.65% of earnings)	$4,398
Paid absences (2 weeks sick, 3 weeks vacation, 2 weeks holidays)	$7,739
E. Travel	
Transport Task Force Workshop – unknown location	
Purpose: To present results from this project, to interact with collaborators, and to keep abreast of other work in the field	
One person, four nights	
Airfare: $400, hotel: $600, MIE: $315, registration: $275, taxis to and from Austin airport: $60	$1,650
Visit to General Atomics	
Purpose: To interact with collaborators	
One person, three nights	
Airfare: $400, hotel: $480, rental car: $130, MIE: $183, taxis to and from Austin airport: $60	$1,253
APS/DPP Conference - Milwaukee, WI	
Purpose: To present results from this project, to interact with collaborators, and to keep abreast of other work in the field	
One person, five nights	
Airfare and hotel: $1150, MIE: $352, registration: $450, taxis to and from Austin airport: $60	$2,012
G. Other Direct Costs	
1. Materials and Supplies	
Office supplies: pens, paper tablets	$10
2. Publication Costs/Documentation/Dissemination	
Article charge ($20), page charge ($55/pg), in four-page article (Phys. Plasmas rate)	$240
Poster material	$50
Total:	$75,000

Budget Justification – Year 2		
A. Senior Personnel		
	Ronald Bravenec: a rate not unreasonable for researchers of his experience and seniority.	$57,610
C. Fringe Benefits		
	Dental insurance (same as Year 1)	$154
	Employer share of FICA/Medicare (7.65% of earnings)	$4,407
	Paid absences (2 weeks sick, 3 weeks vacation, 2 weeks holidays)	$7,755
E. Travel		
	Transport Task Force Workshop – Unknown location	
	Purpose: To present results from this project, to interact with collaborators, and to keep abreast of other work in the field	
	One person, four nights	
	Costs estimated as 2% above Year 1	$1,683
	Visit to MIT	
	Purpose: to interact with collaborators	
	One person, three nights	
	Costs estimated as 2% above Year 1	$1,278
	APS/DPP Conference - Portland, OR	
	Purpose: To present results from this project, to interact with collaborators, and to keep abreast of other work in the field	
	One person, five nights	
	Costs estimated as 2% above Year 1	$2,052
G. Other Direct Costs		
	1. Materials and Supplies	
	Costs estimated as 2% above Year 1	$10
	2. Publication Costs/Documentation/Dissemination	
	Poster material 2% higher than Year 1	$51
	Total:	$75,000

Budget Justification – Year 3		
A. Senior Personnel		
	Ronald Bravenec: a rate not unreasonable for researchers of his experience and seniority.	$56,984
C. Fringe Benefits		
	Dental insurance (same as Year 1)	$154
	Employer share of FICA/Medicare (7.65% of earnings)	$4,359
	Paid absences (2 weeks sick, 3 weeks vacation, 2 weeks holidays)	$7,671
E. Travel		
	Transport Task Force Workshop – Unknown location	
	Purpose: To present results from this project, to interact with collaborators, and to keep abreast of other work in the field	
	One person, four nights	
	Costs estimated as 2% above Year 2	$1,431
	Foreign: EPS, IAEA, or European TTF	
	Purpose: To present results from this project, to interact with collaborators, and to keep abreast of other work in the field	
	One person, five nights	
	Costs estimated as 2% above Year 2	$1,168
	APS/DPP Conference - Unknown location	
	Purpose: To present results from this project, to interact with collaborators, and to keep abreast of other work in the field	
	One person, five nights	
	Costs estimated as 2% above Year 2	$2,041
G. Other Direct Costs		
	1. Materials and Supplies	
	Costs estimated as 2% above Year 2	$10
	2. Publication Costs/Documentation/Dissemination	
	publication charges same as Year 1	$1,130
	Poster material 2% higher than Year 2	$52
	Total:	$75,000

A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes

Ronald V. Bravenec, PI

A number of nonlinear gyrokinetic microstability codes are now able to compute particle, energy, and momentum fluxes in the core of tokamak plasmas with realistic shaping, kinetic electrons (passing and trapped), multiple gyrokinetic impurities, collisions, magnetic fluctuations, and equilibrium toroidal rotation shear. These codes are being applied to predict the performance of ITER and future devices. Such important applications are premature, however, until the codes are shown to unambiguously and consistently predict transport in existing tokamak experiments ("validation"). As a prerequisite to validation, the codes must be shown to correctly solve the gyrokinetic-Maxwell equations upon which they are based ("verification"); otherwise, validation efforts have no legitimacy and the codes have no sound theoretical foundation from which an understanding and prediction of transport can emerge.

Although both are required, verification and validation (V&V) need not be independent activities. My verification efforts have always used experimental data so that the benchmarks are more relevant for interpreting or simulating experiment. It is therefore straightforward to integrate verification into a validation exercise by adding other codes to the code being validated, all using the same input plasma profiles.

I propose to continue systematic verification through cross-code comparisons (benchmarking) among the Eulerian codes GYRO, CGYRO, GS2 and GENE. The premise is that the codes will not converge to the same wrong answer. All these codes contain the physics capabilities listed above. The computations must have sufficient spatial and temporal resolutions and velocity-space resolution for the results to have converged. I propose to continue code comparisons for disparate plasma conditions — important to ensure that agreement for a particular condition is not simply fortuitous — that are being used in existing validation efforts or are of interest to the community.

I will work closely with existing validation groups by introducing other codes to the efforts. I will similarly consult with the code developers. There are many validation activities that are of interest to me and the community and to which I can contribute. The order in which I will address these activities will be determined by priority as judged by the community. The folding in of verification into existing validation efforts will provide for a systematic, coordinated, and efficient V&V program.

A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes

Proposal submitted to the DOE Office of Science, Office of Fusion Energy Sciences
Funding Opportunity Number DE-FOA-0001560
Research area: Confinement and Transport

by

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DOE Office of Science Program Office Technical Contact: Dr. John Mandrekas
DOE Grant Number DE-FG02-08ER54978
PAMS Letter of Intent tracking number: LOI-0000014634

Background/Introduction

The state of the art in plasma microstability theory is represented by complex nonlinear gyrokinetic codes that run on massively parallel supercomputers. The codes GYRO,[1] GS2,[2] GEM,[3] PG3EQ,[4] GTC,[5] GENE,[6] and recently CGYRO, among others, are able to compute the saturated fluctuations in not only the electrostatic potential, but also in the electromagnetic potentials and in the densities and temperatures of multiple ion species in the tokamak core plasma. CGYRO is an offshoot of GYRO especially designed to treat the plasma edge where the safety factor q and collisionality are high. The codes include kinetic electrons (passing and trapped) and gyrokinetic impurities with interspecies collisions. Plasma shaping is modeled assuming a local equilibrium[7,8] or actual numerical equilibria are employed. Equilibrium $\mathbf{E}\times\mathbf{B}$ rotation shear − important for turbulence stabilization[9] and crucial for realistic nonlinear simulations in some regimes − is functional in all the codes listed above. Therefore, these codes have the capability of computing the turbulence-induced particle and energy fluxes thought to dominate radial transport. Linear application of the codes has become routine for interpreting experimental results, while nonlinear simulations are being applied to predict performance in ITER and other future devices.

Before one can believe the predictions of these codes, they must be validated. Validation is “the process by which it is determined that the mathematical model faithfully represents stipulated [nonlinear] physical processes [e.g., electron and ion heat fluxes, particle fluxes, fluctuation parameters] within prescribed limits.”[10] Although there has been considerable work,[11-44] with some success, robust agreement of all code results with experimental measurements has not been consistently found in studies to date.

More fundamentally, the codes have not been convincingly verified — “the process by which it is determined that a numerical algorithm correctly solves a mathematical model [here, gyrokinetic-Maxwell] within a set of specified, predetermined tolerances.”[10] The code developers have performed their own individual nonlinear verification exercises in addition to debugging, but only indirectly by comparing t analytical instability threshold conditions, nonlinear saturation estimates, etc. Verification for more realistic plasma conditions must therefore rely on favorable comparisons among codes, i.e., benchmarking, the idea being that it is highly unlikely for all codes to yield the same erroneous results. The common results would serve as benchmarks for other codes to meet.

It is important to realize that validation does not supersede verification, i.e., a “validated” code is not necessarily verified. Rigorous validation requires variation of the input plasma profiles within their experimental uncertainties to seek code agreement with as much data as possible. Regardless of the outcome of this exercise, there is no way to distinguish between code fidelity and optimal adjustment of the plasma profiles. Nevertheless, comparisons among codes[45-52] are much fewer than comparisons between code and experiment.

To be apples-to-apples comparisons, a local equilibrium (dictated by GS2) is taken using Miller parameterization of plasma shape with up-down symmetry (sufficient for analysis of core plasmas), and ignore i-i collisions (typically small). Computations include trapped electrons and gyrokinetic ions (including one impurity) and finite ratio of plasma pressure to magnetic field pressjre β. Linear high-k_θ comparisons include gyrokinetic electrons. However, none of the nonlinear simulations do, so electron-scale fluctuations are not treated so far. The inclusion of all these physics features is hereafter referred to as “full physics.” (**E**×**B** rotation shear is considered an add-on.) The same data reader is employed for all the codes; otherwise, differences between the readers (fitting functions, smoothing technique and degree) often provide significantly different inputs to each code.[53]

Implicit in this procedure is that the code results have converged, i.e., that they change minimally when the spatial, temporal, and velocity-space resolutions are increased. The same applies when the simulation box is expanded. These tests add greatly to the work load but are absolutely necessary. The verification procedure therefore requires keeping track of linear and nonlinear computations with different resolutions in addition to computations for each physics model at multiple times, radii, discharges, and devices. I have developed a directory structure and Python routines to automate setting up and executing the computations and organizing the results.

This work is intended to deliver benchmarks — linear and nonlinear — at various levels of physical realism and over a wide range of plasma conditions. Other codes should be able to reproduce these benchmarks in order to be considered verified. Because the benchmarks span a range of physics complexity, codes that are not as advanced can still compare to some of them. If another code differs with a benchmark, its developer can certainly challenge it, but he/she should be willing to work with GYRO, GS2 and GENE developers and me to resolve the disagreement. Because this work is performed using experimental data, it can be integrated into validation exercises. These do not necessarily require full physics because collisions, finite β, impurities, equilibrium **E×B** rotation shear, etc., may not play important roles in some plasmas.

Recent Accomplishments

Important to this proposal is the requirement that the code comparisons should be made for a broad range of discharge conditions. Otherwise, agreement among the codes for a particular discharge could simply be coincidence. CGYRO was employed at the plasma edge ($r/a > 0.8$) when retaining collisions.

The principal result for the first months of the grant period was analysis of a high bootstrap-current H-mode discharge near the edge where the electron density and temperature profiles were relatively flat. The linear frequencies of the fastest growing modes are shown in Fig.1 plotted versus the poloidal wave

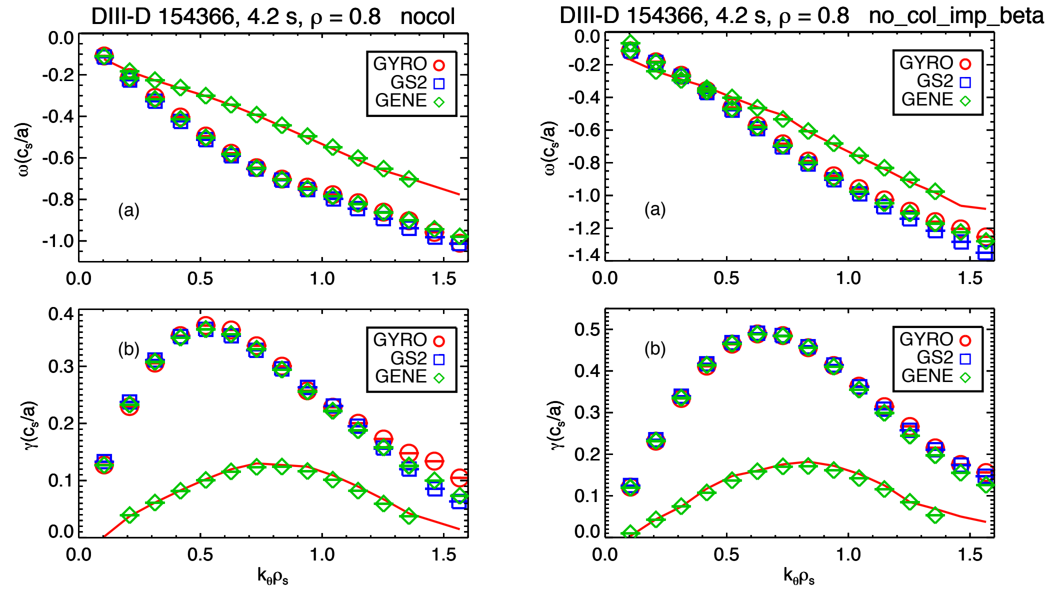

Fig. 1. Real (top) and imaginary (bottom) normalized frequencies for high-bootstrap-fraction discharge at flat spot near edge (*r/a* = 0.8) ignoring collisions. Plots on left are otherwise full physics while plots on right ignore impurities and electromagnetic effects (β = 0). Solid red lines indicate GYRO eigenmode results for sub-dominant mode.

numbers normalized to the gyroradius at the sound speed ρ_s. Collisions were ignored because GYRO was not expected to perform well in a region of high q and collisionality (motivation for CGYRO). We see excellent agreement among the codes, not only with respect to the fastest growing modes, but also to a sub-dominant (smaller growth rate) branch. Eigenfunctions of plasma potential are shown in Fig. 2,

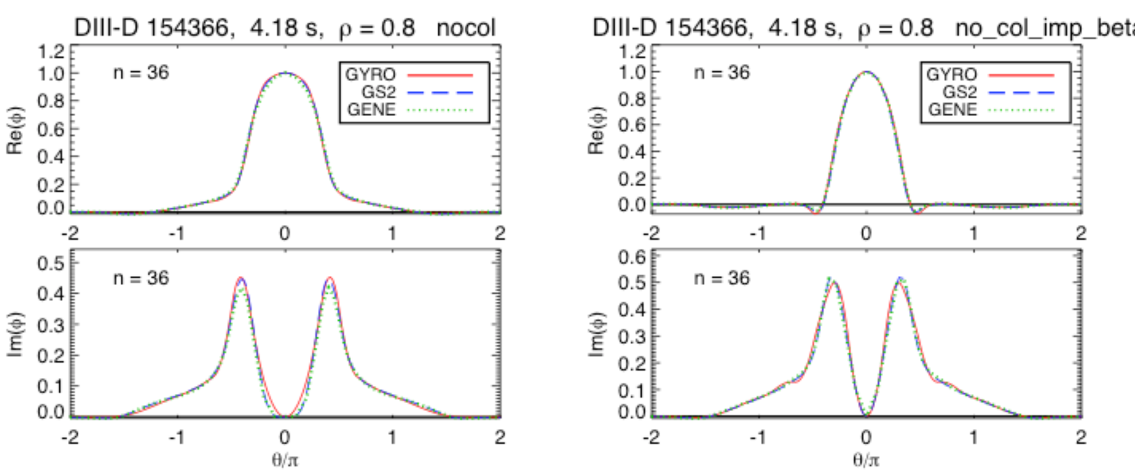

Fig. 2. Real (top) and imaginary (bottom) components of the potential eigenfunctions for the same conditions as in Fig. 1 and for fastest-growing modes. Here *n* = 36 corresponds to $k_\theta\rho_s = 0.656$.

where again there is excellent agreement. The negative frequencies (in the ion diamagnetic direction) and the even-parity eigenmodes are evidence of ITG (ion temperature gradient) modes.

Next are results for ECRH (electron cyclotrons resonance heating) localized on either side of *r/a* = 0.7 of a set of DIII-D discharges. There are three cases: heating at *r/a* = 0.6, at *r/a* = 0.8, and at both *r/a* = 0.6 and *r/a* = 0.8. The intent was to change the electron temperature gradient at *r/a* = 0.7. Shown in Fig. 3 are the linear frequencies (top) and growth rates (bottom) for the three cases. We first see that agreement among the codes is good. The character of the turbulence changes from ITG-domimant to TEM-dominant as the T_e profile is steepened (left to right). Note the doubling of the maximum growth rate.

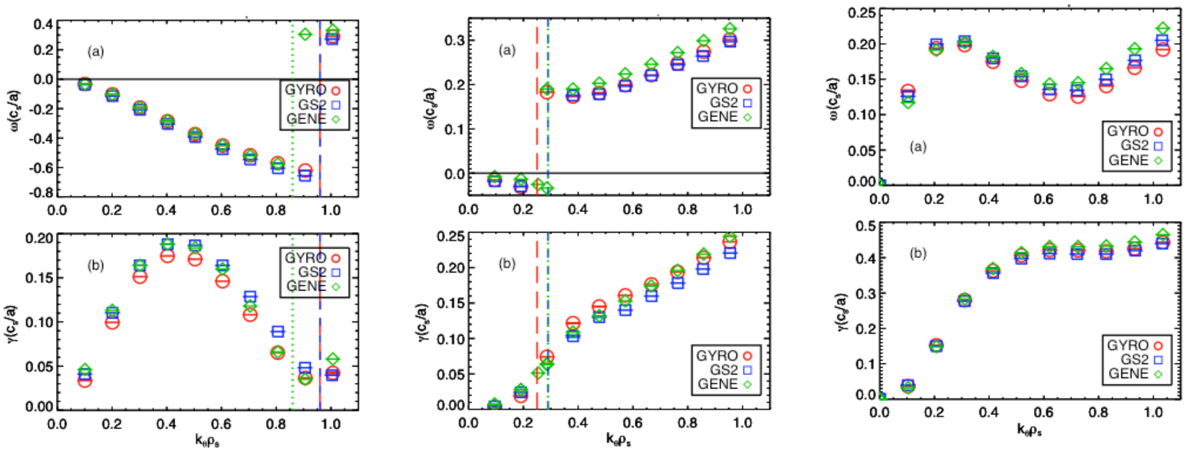

Fig. 3. Linear (a) frequencies and (b) growth rates at *r/a* = 0.7 for ECRH applied (left to right) at *r/a* = 0.8, at *r/a* = 0.8 and 0.6, and at *r/a* = 0.6. Dashed lines indicate locations of branch transition.

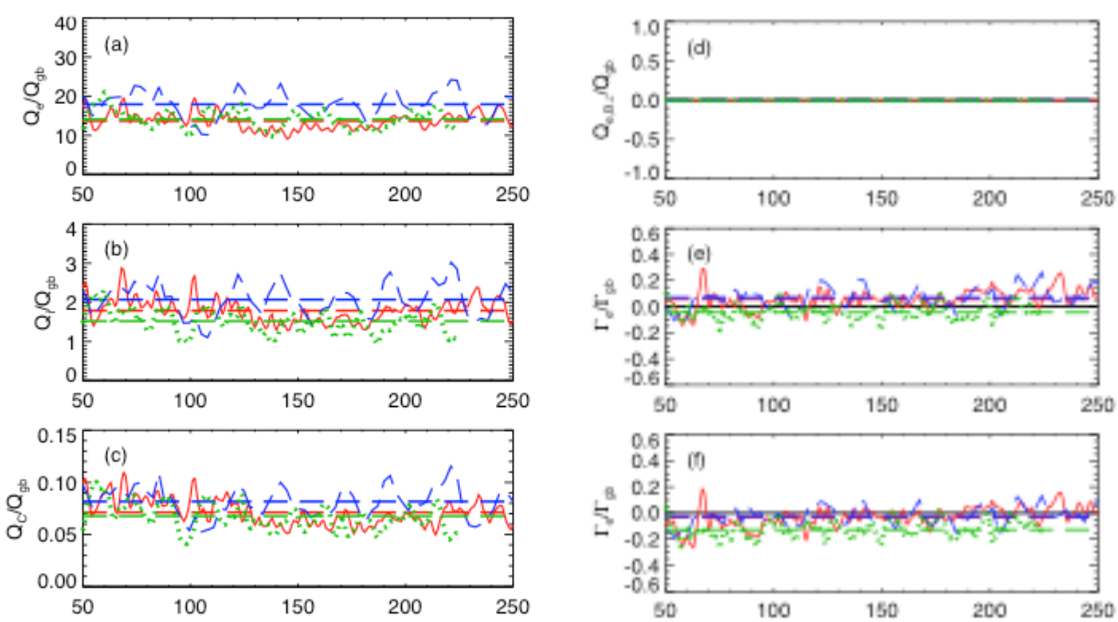

Fig. 4. Gyro-Bohm-normalized (a) electron, (b) main ion (D), (c) impurity ion (C^{6+}) electrostatic energy fluxes, (d) electromagnetic electron energy flux, and (e) electron and (f) main ion electrostatic particle fluxes vs time normalized to a/c_s at *r/a* = 0.7 with ECRH applied at *r/a* = 0.6. GYRO (red), GS2 (blue) and GENE (green). Dashed lines indicate time averages.

Nonlinear simulations of the three cases were performed next. Shown in Fig. 4 are the normalized fluxes versus normalized time at r/a = 0.7 for the case with all the ECRH applied at r/a = 0.6. These simulations ignored electromagnetic effects and **E×B** shear, which were small. There is good overall agreement among the codes. The simulated fluxes for the other two cases were problematic in that the fluxes were unsteady and small, making it difficult to compare the codes. In particular, the case with ECRH applied on both sides of r/a = 0.7 exhibited substantial activity at $k_\theta \rho_s \sim 1$, indicating electron-scale fluctuations (ignored here) are important. The GYRO results above have been published in Ref. 54.

In keeping with the intent to compare codes over a broad range of parameters, Fig 5 shows the linear frequencies in the steep gradient region of the edge pedestal of an EAST H-mode discharge. The calculations neglected impurities and collisions for historical reasons. We see there is fair agreement among the codes in this challenging region.

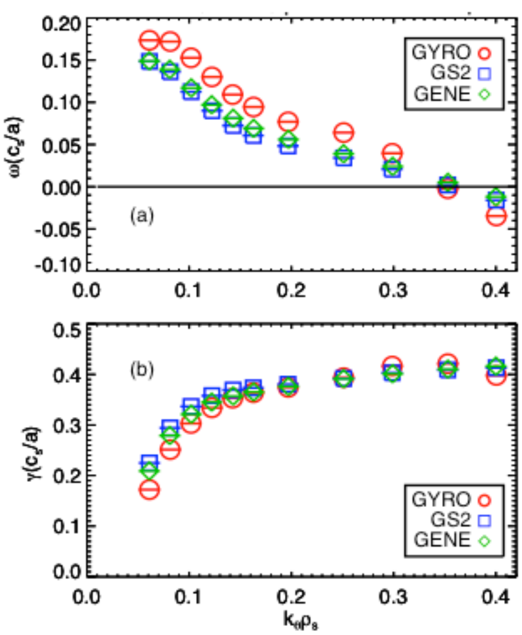

Fig. 5. Normalized linear frequencies (top) and growth rates (bottom) vs normalized poloidal wave number for the steepest location in the H-mode pedestal for EAST discharge 38300. Impurities and collisions were neglected.

Linear comparisons were also made for two DIII-D discharges as similar as possible, but one with much higher toroidal rotation. The case with higher rotation exhibits higher growth rates, a conundrum considering that the transport is less. The explanation is that the **E×B** shearing rate is about equal to the maximum linear growth rate, whereas it is smaller in the no-rotation case. The real frequencies compare favorably code to code, whereas the growth rates are greater than 10% different for the slower rotation case. The fact that the growth rates are smaller for the slower plasma perhaps explains the larger relative difference. The eigenfunctions, however, are in excellent agreement in both cases.

Analysis of a DIII-D discharge exhibiting edge harmonic oscillations (EHO's) was carried out at two different times into the discharge: one with EHO's present, one without. The linear results are shown in Fig. 6. Here CGYRO was utlized because of high q and inclusion of collisions. (I believe that this is the first third-party benchmarking of CGYRO.) We note good agreement again among the codes. The eigen-functions (not shown) were likewise in good agreement.

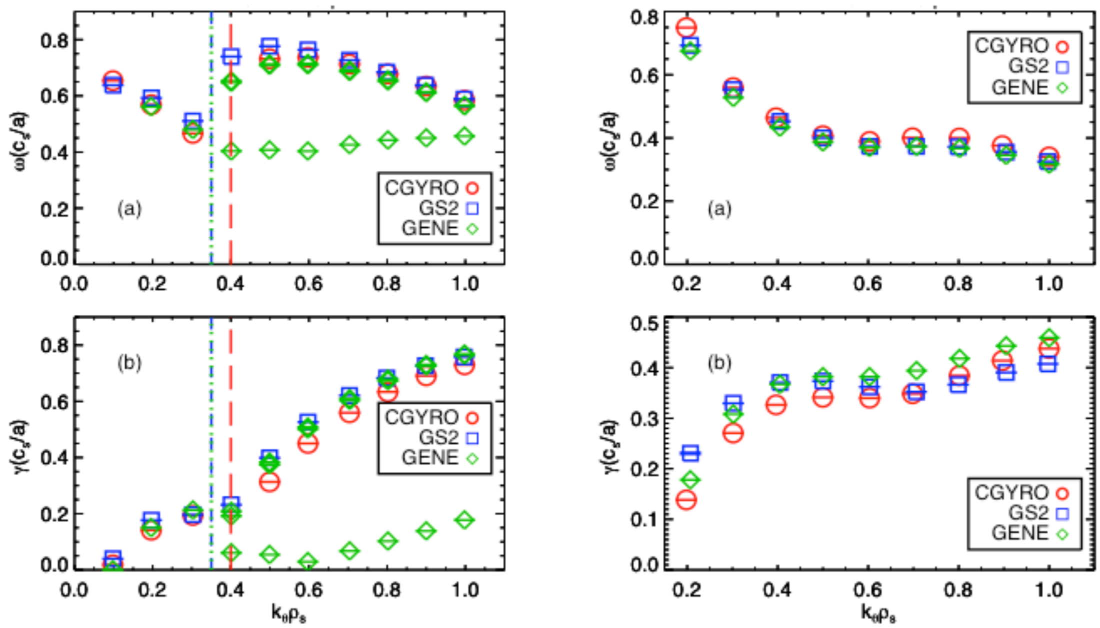

Fig. 6. Normalized real frequencies (top) and growth rates (bottom) versus normalized wave number for a QH-mode DIII-D discharge at the top of the edge pedestals. Plots on left are at a time with EHO's (edge harmonic oscillations) while plots on right are without. Dashed lines on left indicate mode transition. Lower points from GENE are for a subdominant branch.

A high-density Alcator C-Mod discharge was analyzed for which GYRO greatly underpredicts the electron energy transport at *r/a* ~ 0.7.[37] Shown in Fig. 7 are the linear frequencies *r/a* ~ 0.7 both with (left) and

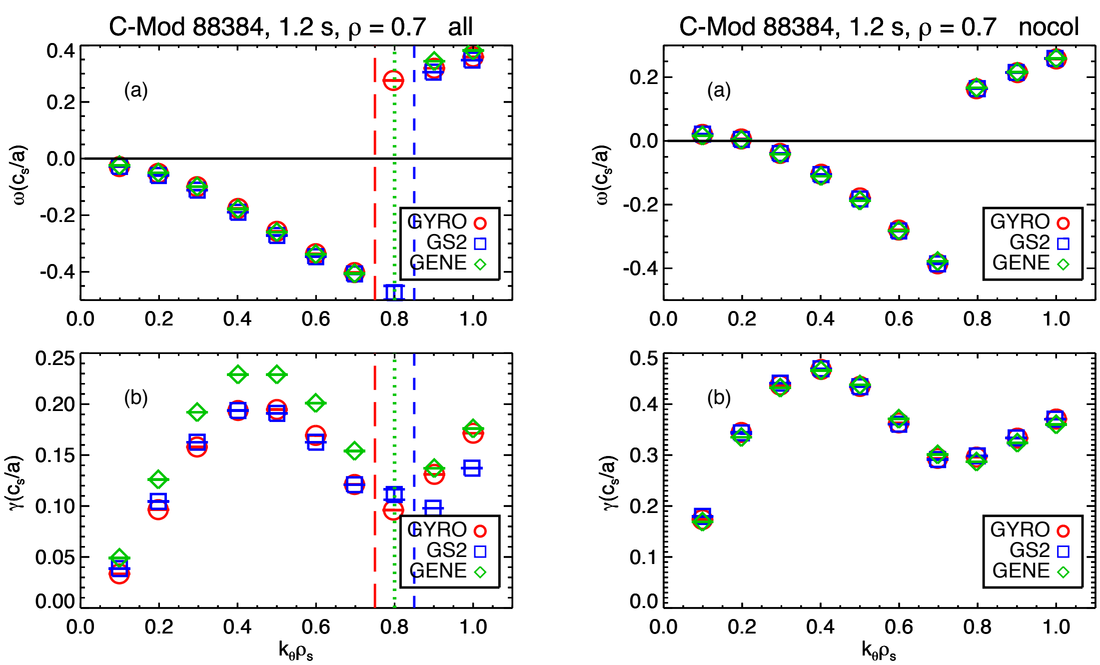

Fig. 7. Normalized real frequencies (top) and growth rates (bottom) versus normalized wave number for a Alcator C-Mod discharge at *r/a* = 0.7. Plots on left are with collisions while those of the right are collisionless. Dashed lines on left indicate wave number of mode transition.

without (right) collisions. Because the codes agree almost perfectly without collisions, we can deduce from the collisional results that there are real differences among the basic collision operators that manifest themselves for these particular plasma profiles. Such a comparison is warrented by the fact that for both cases the modes do not change character, i.e., the modes are ITG transitioning to TEM as k_θ increases.

We next look at the nonlinear fluxes ignoring electromagnetic effects (small in this low-β plasma). Shown in Fig. 8 are the powers exiting the flux surface at r/a = 0.7. The experimental values of the electron and ion energy fluxes are denoted. As mentioned earlier, the electron power fluxes from all three codes are much less than the experimental value. Much of the missing electron power flux has been attributed to electron-scale fluctuations.[39] Comparing codes, GENE predicts greater power fluxes and more outward particle fluxes than GYRO or GS2, consistent with the linear results for growth rates.

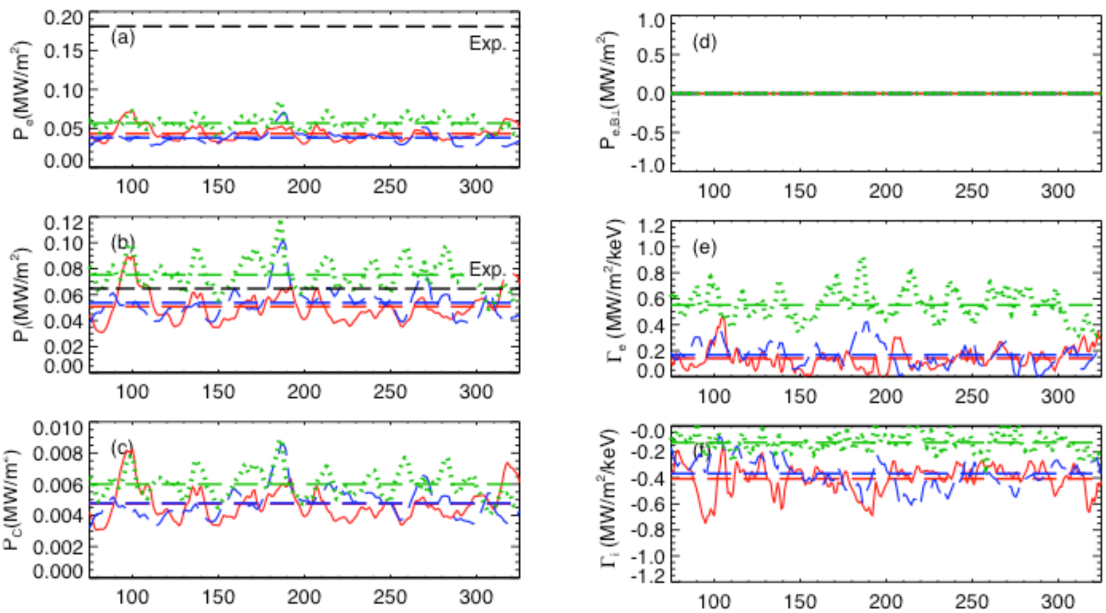

Fig. 8. (a) Electron, (b) main ion (D), (c) impurity ion (C^{6+}) electrostatic energy fluxes, (d) electromagnetic electron energy flux, and (e) electron and (f) main ion electrostatic particle fluxes at r/a = 0.7 versus time normalized to a/c_s for an Alcator C-mod discharge. GYRO (red), GS2 (blue) and GENE (green). Dashed straight lines indicate time averages.

The remainder of the grant period was spent studying three high-performance JET discharges. (GS2 was not a part of this study because the machine it ran on, Hopper, was retired, and attempts to compile on either Edison or Cori have been unsuccessful.) The goal was to gauge the importance of electromagnetic stabilization relative to **E×B** stabilization. The first was a JET shot simplified by assuming a circular cross section and ignoring collisions. Including electromagnetic effects reduced the fluxes by more than half. On this the codes were in agreement.

Next was a discharge with significant densities of fast particles (D beam ions, He3). Prior GENE simulations had already shown that electromagnetic effects had a stronger stabilizing influence including the fast ions as dynamic species than the case ignoring them. We performed a code comparison of the electromagnetic cases with and without fast ions. The linear results were in good agreement, both for the frequencies (see Fig. 9) and the eigenfunctions (see Fig. 10). The growth rates were reduced by a factor of ~ 2.5 while the flux reduction was large (see Fig. 11) — much larger than the reduction due to **E×B** shear. A large reduction of the fluxes due to electromagnetic effects was also found for a high-β hybrid discharge. This JET analysis was recently submitted for publication in Plasma Physics and Controlled Fusion.

In addition to these accomplishments are nonlinear GENE results including plasma rotation shown in a recently published work.[55]

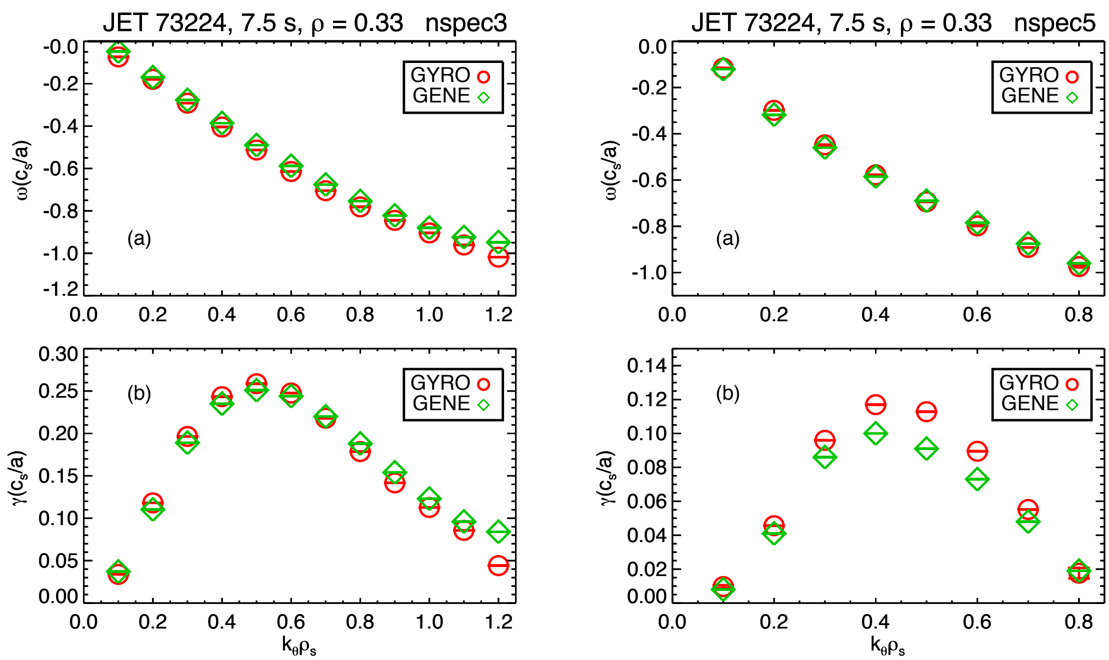

Fig. 9. Real (top) and imaginary (bottom) normalized frequencies versus normalized wave number for JET discharge 74224 at *r/a* = 0.33. Plots on left are with three dynamic species (main ions, electrons, impurity) while those on the right include fast ions (D, He3).

Proposed Research

Important to this proposal is the fact that verification and validation need not be independent activities. Other codes may be run simultaneously with the code being validated. Therefore, this project can piggyback on concurrent validation efforts. Also important to this proposal is the fact that the verification effort employs profiles from actual discharges, thereby making the effort more relevant.

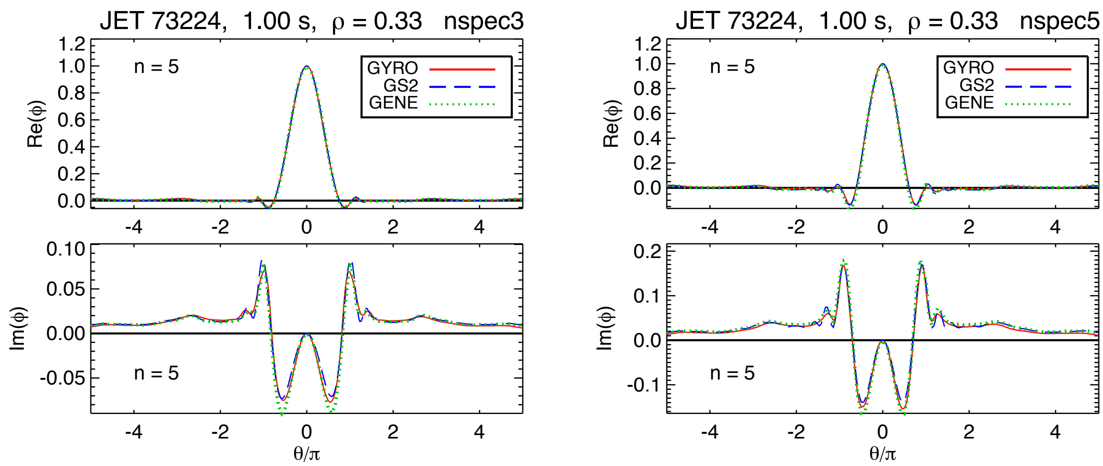

Fig. 10. Real (top) and imaginary (bottom) components of the potential eigenfunctions for the same conditions as in Fig. 9. Here $n = 5$ corresponds to $k_\theta\rho_s \sim 0.6$.

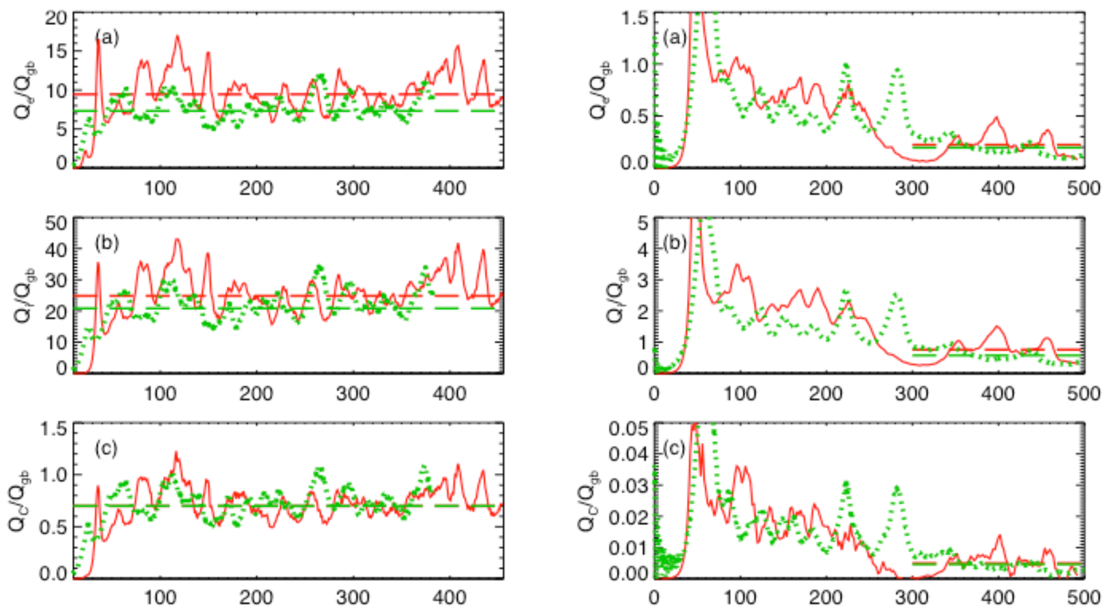

Fig. 11. Gyro-Bohm-normalized (a) electron, (b) main ion (D), and (c) impurity ion (C^{6+}) electrostatic energy fluxes at r/a = 0.7 versus normalized time from GYRO (red) and GENE (green). On the left are the 3-species fluxes while those on the right include gyrokinetic beam (D) and He3. Dashed lines indicate time averages. Time axis is normalized to a/c_s.

There are many validation activities that are of interest to the community and to which I can contribute, some of which are:

- Comparing simulations of “Quiescent H-mode” and “Improved-mode” discharges.
- H-mode core transport: How does one account for all the mechanisms other than turbulence that influence transport, e.g., tearing modes, edge-localized modes, etc., in the comparisons of codes and experiment? Assuming one can, how well do the models work?

- Predicting transport, especially electron, during current ramp-up (important for ITER).
- Transport and turbulence suppression in internal transport barriers, especially at small radii and weak or negative magnetic shear: How well do gyrokinetic codes do here, and do the reduced models accurately reproduce experiment or gyrokinetics for those conditions?
- How important are intermediate- and high-*k* modes? Do they simply add electron transport without much impact on the ions, or is there significant nonlinear coupling between the scales, e.g, a significant inverse cascade, that needs to be accounted for?

This may appear to be a laundry list, but the point is that there are enough topics to consume the resources of the proposed funding level. Adding to these are the multitude of other experiments on which a code comparison can piggyback on. Prioritization of the tasks will be in consultation with the community. (Presently we are beginning to address the current ramp issue.) Therefore, it is difficult to apply a time line to this work.

I should note that work up to now has dealt with cases for which there was small apparent flux for $k_\theta \rho_s > 1$, as evident by a decay with k_θ of the low-k_θ flux spectra. However, there are cases when the fluxes from electron-scale turbulence can be significant,[34-43] such as for the DIII-D discharge with ECRH applied on either side of r/a = 0.7. All four codes referred to (including CGYRO) in this proposal have the capability to treat gyrokinetic electrons. Therefore, subject to available processor hours, I expect to be able to include electron-scale turbulence in the simulations if necessary. Another major goal is to verify CGYRO, which has only recently been released to the community. Benchmarking would be most interesting in the edge, where q is largest and collisionality is high.

All that is needed to start a benchmarking exercise is the file "input.profiles" from which input files for all four codes can be generated by Python routines. This file is produced trivially during plasma profile analysis, but not by me. Therefore, collaboration with others is a necessity for this effort. So far, obtaining the file for discharges that were subsequently analyzed has not been an issue.

Closing

Verification and validation ("V&V") of gyrokinetic microstability codes is a major research topic in the tokamak transport community. Early on, there were invited talks on the subject at the 2004 and 2005 Transport Task Force (TTF) meetings,[56,57] and dedicated sessions since then. The importance of V&V is recognized by the DoE Office of Fusion Energy Sciences in this Funding Opportunity Announcement for proposals in which "Verification and validation (V&V) work will be considered, provided it has a strong theory component and it is not predominately a data analysis or evaluation effort." Verification and validation is a component of The Center for the Study of Plasma Microturbulence (CSPM)[58] — a collaboration of code developers and users. The first goal of the FES program listed on the home page of its web site[59] is to "Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source." Clearly, V&V of the predictive codes is necessary to accomplish this.

I have excellent working relationships with the code developers: J. Candy of GA (GYRO), W. Dorland of Univ. of Maryland (GS2), and T. Görler of Max Planck Institute for Plasma Research, Garching, Germany, D. Told of UCLA, and M.J. Pueschel of U. Wisconsin, Madison (GENE). I have collaborated with researchers already involved in validation efforts, such as C. Holland and N. Howard of Univ. Calfornia, San Diego. Furthermore, I have the support of representatives of the DIII-D and Alcator C-Mod facilities. I am recognized in the area of V&V by the tokamak transport community: Before dedicating myself to verification, I gave an oral presentation on V&V and summarized the V&V presentations at the 2005 TTF meeting.[60] I have indicated through my current grant period that I am qualified to formulate benchmarks using the nonlinear gyrokinetic codes GYRO, GS2, and GENE for a variety of plasma conditions.

If this renewal proposal is funded, I will continue to be one of few performing verification of nonlinear gyrokinetic codes. The verification effort can proceed concurrently with validation by introducing other codes into ongoing validation exercises, thereby leading to a systematic and efficient V&V effort.

Appendix I: Biographical Sketch

EDUCATION AND TRAINING:

B.S., Electrical Engineering, The University of Texas at Austin, 1975

Ph.D., Electrical Engineering, Major: Plasmas, University of California at Berkeley, 1982

RESEARCH AND PROFESSIONAL EXPERIENCE

Feb. 2008 – present	Principal Investigator, DoE/OFES grant DE-FG02-08ER54978: Verification of gyrokinetic microstability codes
July 2007 – Dec. 2010	Researcher, Tokyo Electron America, Inc., Austin, TX: Analysis, PIC simulations, and design of microwave plasma etcher
2004 – June, 2007	Research Scientist, Fusion Research Center, The University of Texas at Austin TEXT tokamak operator, solid-state bolometer design and operation, analysis of fluctuation data and transport, designer and operator of Alcator C-Mod BES system, profile analysis on DIII-D, verification and validation of GS2 and GYRO codes
1994 – 2004	Research Associate, Fusion Research Center, The University of Texas at Austin: TEXT tokamak operator, bolometer operation, analysis of fluctuation data and transport, validation of PPPL/IFS and GS2 codes
Fall 1988	Lecturer, Physics Department, The University of Texas at Austin
1982 – 1994	Research Engineer/Scientist Assoc. IV, Fusion Research Center, The University of Texas at Austin: TEXT tokamak operator, author of transport analysis code, analysis of fluctuation data and transport

PUBLICATIONS (10 MOST CLOSELY RELATED TO PROPOSAL)

R.V. Bravenec, J. Citrin, J. Candy, P. Mantica, T. Görler, and JET contributors, “Benchmarking the GENE and GYRO codes through the Relative Roles of Electromagnetic and E×B Stabilization in JET High-Performance Discharges,” submitted to Plasma Phys. Contr. Fusion, April, 2016.

E. Belli, J. Candy, R. Bravenec, “A High-Accuracy Eulerian Gyrokinetic Solver for Collisional Plasmas,” to be published in J. Comput. Physics, July, 2016.

R. V. Bravenec, Y. Chen, J. Candy, W. Wan, and S. Parker, “A verification of the gyrokinetic microstability codes GEM, GYRO, and GS2,” Phys. Plasmas **20**, 104506 (2013).

R. V. Bravenec, J. Candy, M. Barnes, and C. Holland, "Linear and nonlinear verification of gyrokinetic microstability codes," Phys. Plasmas **18**, 122505 (2011).

R. V. Bravenec and W. M. Nevins, "System for simulating fluctuation diagnostics for application to turbulence computations," Rev. Sci. Instrum. **77**, 015101 (2006).

T. L. Rhodes, J.-N. Leboeuf, D. W. Ross, J. Candy, G. R. McKee, R. Bravenec, E. J. Doyle, R. J. Groebner, W. A. Peebles, R. D. Sydora, L. Zeng, and G. Wang, "Quantitative Comparisons of DIII-D Turbulence Measurements to Gyro-Kinetic and Gyro-Fluid Turbulence Simulations," in *Fusion Energy 2002*, paper EX/C4-1Rb (International Atomic Energy Agency, Vienna, 2002).

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R. V. Bravenec, "Effects of Finite Sample Volumes on Fluctuation Measurements," in *Transport, Chaos and Plasma Physics 2*, edited by S. Benkadda, F. Doveil, Y. Elskens (World Scientific, River Edge, New Jersey, 1996), pp. 350-357.

R. V. Bravenec and A. J. Wootton, "Effects of Limited Spatial Resolution on Fluctuation Measurements (invited)," Rev. Sci. Instrum. **66**, 802 (1995).

POTENTIAL CONFLICTS OF INTEREST OR BIAS

COLLABORATORS:

W. Dorland, University of Maryland, College Park
J. Candy, General Atomics, San Diego
C. Holland, N. Howard, University of California, San Diego
Darin Ernst, Plasma Science and Fusion Center, MIT
T. Görler, Max Planck Institute for Plasma Physics, Garching, Germany
M. J. Pueschel, University of Wisconsin, Madison

Appendix II: Current and Pending Support

CURRENT

Project/Proposal Title: A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes

Source of Support: U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences

Total Award Amount: $195,000

Total Award Period Covered: Feb. 15, 2014 – Feb. 14, 2017

Location of Project: Fourth State Research, 503 Lockhart Dr., Austin, TX 78704

Person-Months Per Year Committed to the Project: Cal: 5

PENDING (THIS PROPOSAL)

Project/Proposal Title: A Systematic Method for Verification and Validation of Gyrokinetic Microstability Codes (Renewal)

Source of Support: U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences

Total Award Amount: $225,000

Total Award Period Covered: Feb. 15, 2017 – Feb. 14, 2020

Location of Project: Fourth State Research, 503 Lockhart Dr., Austin, TX 78704

Person-Months Per Year Committed to the Project: Cal: 5

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Appendix IV: Facilities & Other Resources

COMPUTATIONAL:

- Access to internet
- MacBook Pro laptop computer
- Access to General Atomics Linux clusters, DIII-D data and software for analysis
- Access to MIT PSFC Linux clusters, Alcator C-Mod data and software for analysis (subject to future DoE support of Alcator C-Mod database)
- Account at NERSC, access to computational systems via ERCAP allocation to gc3 repository − the Magnetic Fusion Plasma Microturbulence Project, PI: B. Cohen. Anticipated allocation: 2 million processor-hours per year (current allocation)

OFFICE:

- Home office with wifi ink-jet printer/copier/scanner.

PRODUCTS - DETAILS

PUBLICATIONS DETAIL

1. Journal Article: Benchmarking the GENE and GYRO codes through the Relative Roles of Electromagnetic and E×B Stabilization in JET High-Performance Discharges	
Journal: Plasma Physics and Controlled Fusion	
Publication Date: Not Provided	**Publication Status:** Under Review
Volume: Not Provided	**First Page Number or eLocation ID:** Not Provided
Issue: Not Provided	**Publication Location:** Not Provided
Author(s): R. Bravenec, J. Citrin, J. Candy, P. Mantica, T. Goerler, and JET contributors	
Publication Identifier Type: Not Provided	**Publication Identifier:** Not Provided
Acknowledgement of DOE Support: Yes	**Peer Reviewed:** Yes

2. Journal Article: Electron temperature critical gradient and transport stiness in DIII-D	
Journal: Nuclear Fusion	
Publication Date: Not Provided	**Publication Status:** Published
Volume: 55	**First Page Number or eLocation ID:** 083011
Issue: Not Provided	**Publication Location:** Not Provided
Author(s): S.P. Smith1, C.C. Petty, A.E. White, C. Holland R. Bravenec, M.E. Austin, L. Zeng and O. Meneghini	
Publication Identifier Type: DOI	**Publication Identifier:** http://dx.doi.org/10.1088/0029-5515/55/8/083011
Acknowledgement of DOE Support: Yes	**Peer Reviewed:** Yes

3. Journal Article: Role of Density Gradient Driven Trapped Electron Mode Turbulence in the H-mode Inner Core with Electron Heating	
Journal: Physics of Plasmas	
Publication Date: Not Provided	**Publication Status:** Awaiting Publication
Volume: Not Provided	**First Page Number or eLocation ID:** Not Provided
Issue: Not Provided	**Publication Location:** Not Provided
Author(s): D. Ernst, K. H. Burrell, W. Guttenfelder, T. L. Rhodes, A. M. Dimits, R. Bravenec, B. A. Grierson, C. Holland, J. Lohr, A. Marinoni, G. R. McKee, C. C. Petty, J. C. Rost, L. Schmitz, G. Wang, S. Zemedkun, L. Zeng, and the DIII-D Team	
Publication Identifier Type: Not Provided	**Publication Identifier:** Not Provided
Acknowledgement of DOE Support: Yes	**Peer Reviewed:** Yes

INTELLECTUAL PROPERTIES DETAIL

There are no intellectual properties to report.

TECHNOLOGIES AND TECHNIQUES DETAIL

There are no technologies or techniques to report.

OTHER PRODUCTS DETAIL

There are no other products to report.