Long-time scale simulation and V&V components of the ISEP* project

*Integrated Simulation of Energetic Particles in Burning Plasmas

Don Spong and the ISEP TEAM

Oak Ridge National Laboratory

2019 Scientific Discovery through Advanced Computing (SciDAC-4) Principal Investigator Meeting

Rockville, MD

July 16-18, 2019

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

Acknowledgements

Research sponsored by the Laboratory Directed Research and Development Pro- gram of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy and by U.S. Department of Energy, Office of Science Contract No. DE-AC05-00OR2

Motivations

- EP (**E**nergetic **P**article) confinement is a critical issue for self-heated ignition experiments such as ITER – ignition requires good EP confinement
- EPs can excite mesoscale EP instabilities => drive large EP transport.
- These can degrade overall plasma confinement and threaten the integrity of the wall and plasma-facing components
- EPs => significant fraction of the plasma energy density in ITER. EPs can influence microturbulence responsible for turbulent transport of thermal plasmas and macroscopic magnetohydrodynamic (MHD) modes potentially leading to disruptions
- Ignition regime plasma confinement with a-particle heating: one of the most uncertain issues in extrapolating from existing devices to ITER.

- ## Objectives
  - To improve physics understanding of EP confinement and EP interactions with burning thermal plasmas through exa-scale simulations
  - To develop a comprehensive predictive capability for EP physics
  - To deliver an EP module incorporating both first-principles simulation models and high fidelity reduced transport models to the fusion whole device modeling (WDM) project.

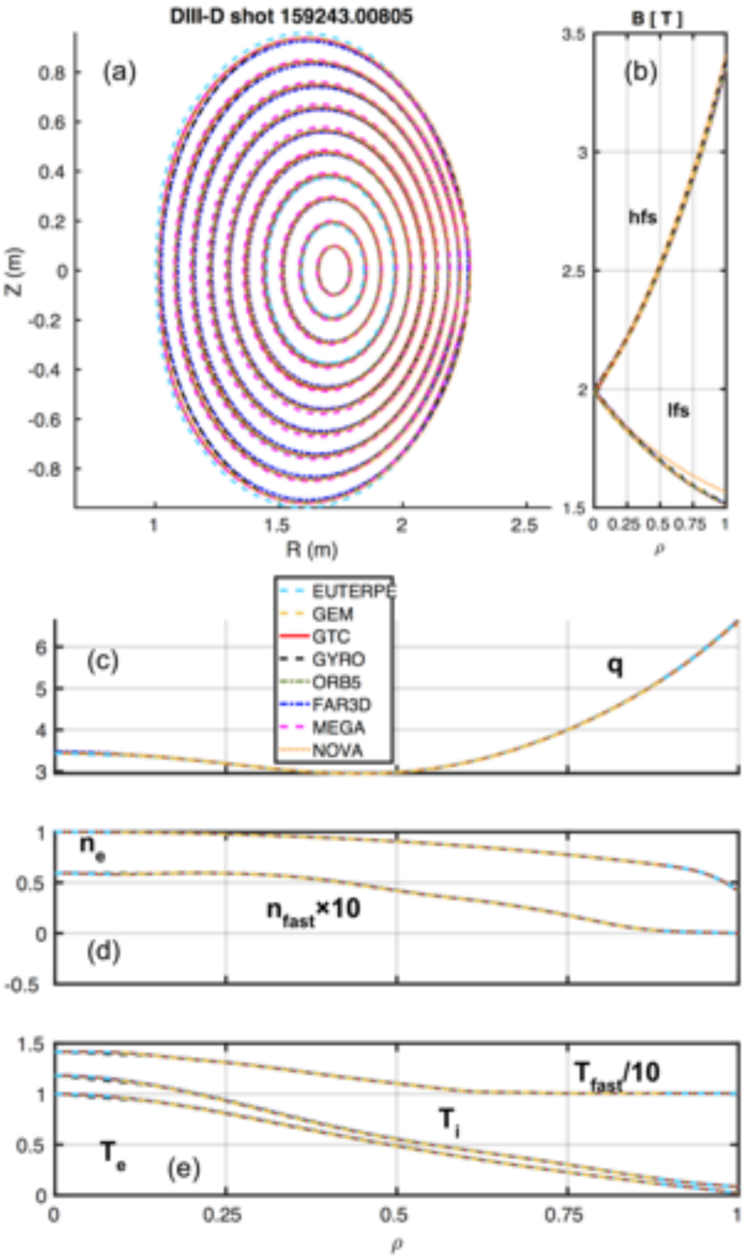
- ## Energetic particle instabilities – V&V challenges
  - The EP-driven Alfvén spectrum typically includes many unstable modes
  - The mode that dominates is model dependent and sensitive to profiles
  - A variety of different EP stability models have been developed (see below)
  - The most important profiles determining AE stability (n_{fast}, E_{fast}, q-profile) are not measured directly, but inferred from reconstruction or modeling
  - Fast ion distribution "sculpted-out" over time by AE instabilities

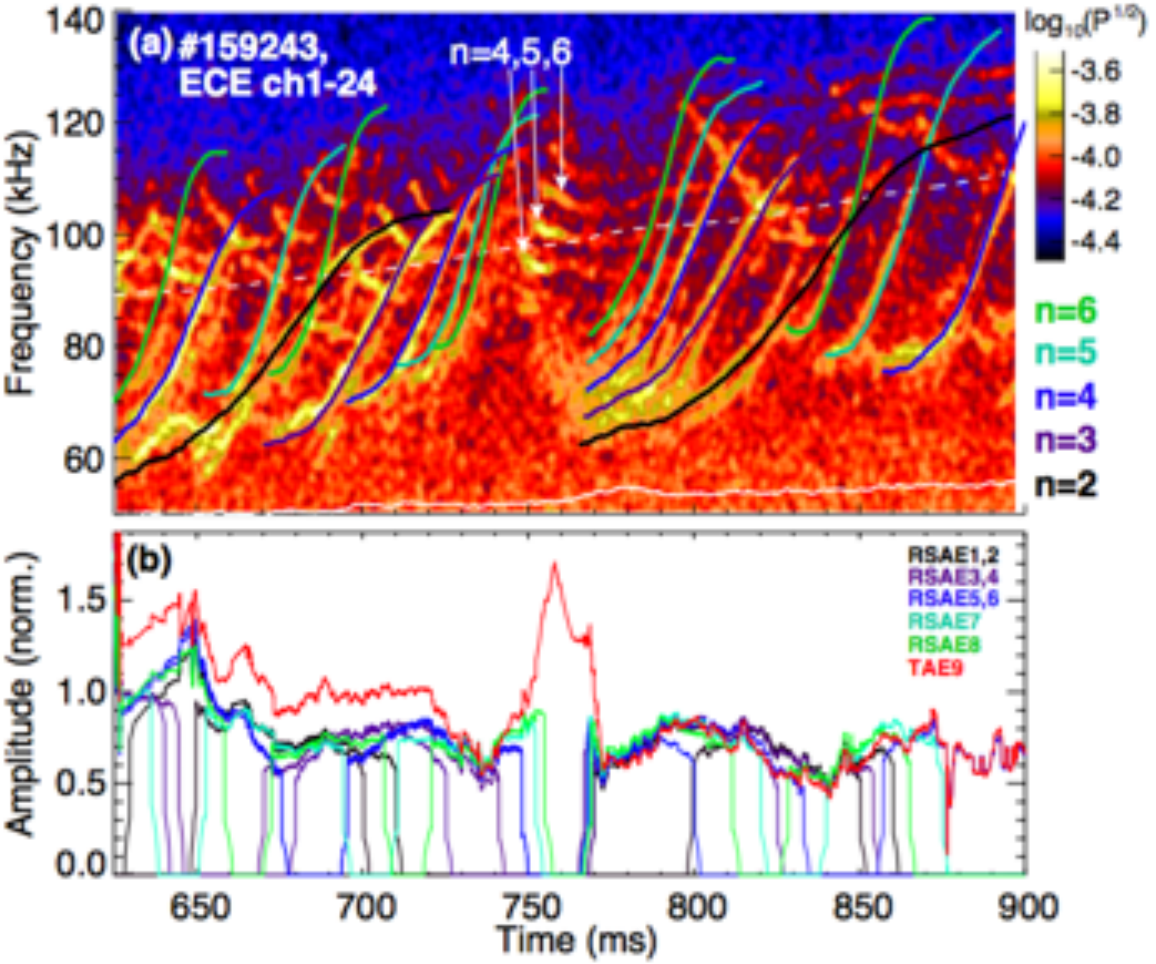
ISEP computational models

- ## GTC
  - First-principles, multi-physics, global gyrokinetic particle-in-cell (PIC) model with applications to microturbulence, meso-scale EP instabilities, MHD modes, RF (radio-frequency) heating and neoclassical transport
  - MPI, OpenMP and GPU parallelism, adapted to peta-scale and emerging exascale platforms
- ## GYRO
  - Comprehensive continuum (Eulerian) electromagnetic global δ*f* gyrokinetic model
  - Includes full physics features needed to realistically simulate turbulence and transport in experimental tokamak discharges
- ## FAR3D/TAEFL
  - High fidelity reduced stability model using Landau-fluid closures to include resonant drives and Padi approximations to include finite gyro-radius effects
  - Time evolution and direct eigen-solver options
- ## Collaborating models
  - **GEM** – gyrokinetic δf PIC; **EUTERPE** – global, electromagnetic gyrokinetic PIC; **ORB5** – linear/nonlinear gyrokinetic PIC; **MEGA** – kinetic/MHD hybrid; M3D-K - kinetic/MHD hybrid; **NOVA-K** – linear hybrid kinetic/MHD

ISEP Verification/Validation: recent DIII-D case

S. Taimoruzadeh, et al., Nuclar Fusion (2019)

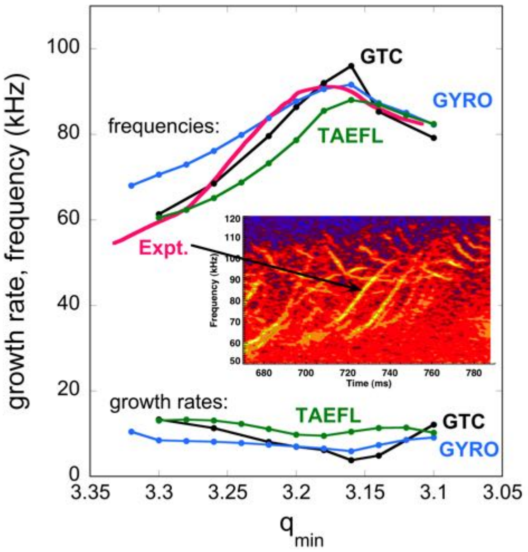




ISEP Verification/Validation

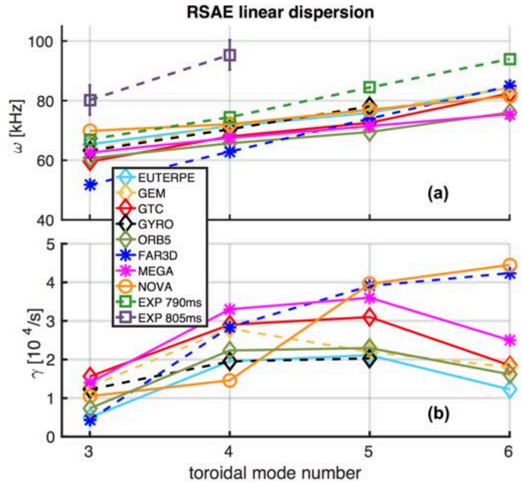
2012 V&V – growth rates/frequencies

D. Spong, et al., Phys. Plasmas (2012)

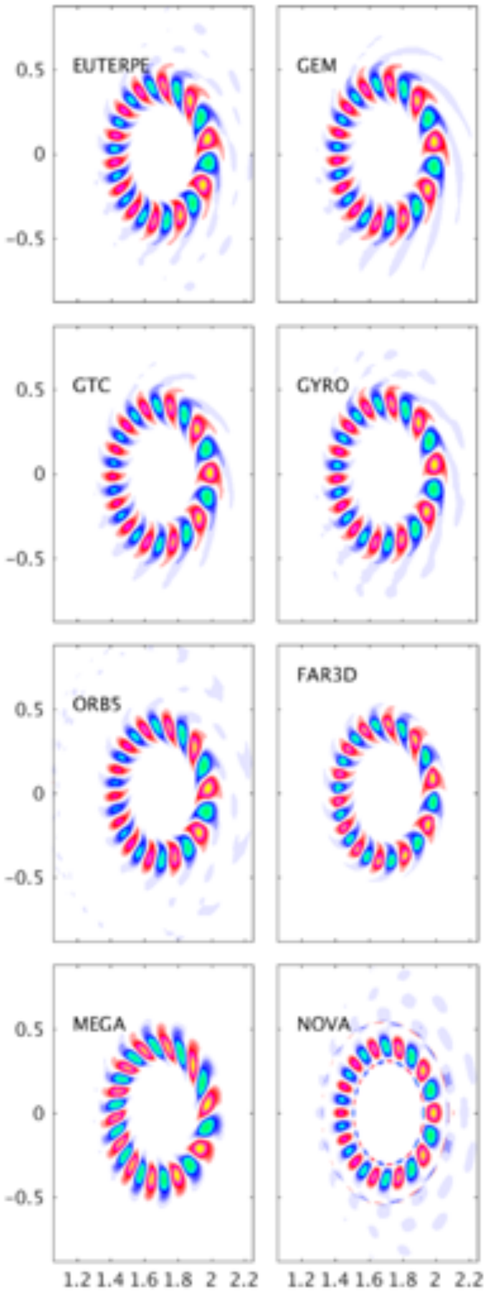


2019 V&V – growth rates/frequencies

S. Taimoruzadeh, et al., Nuclar Fusion (2019)



2019 V&V mode structures

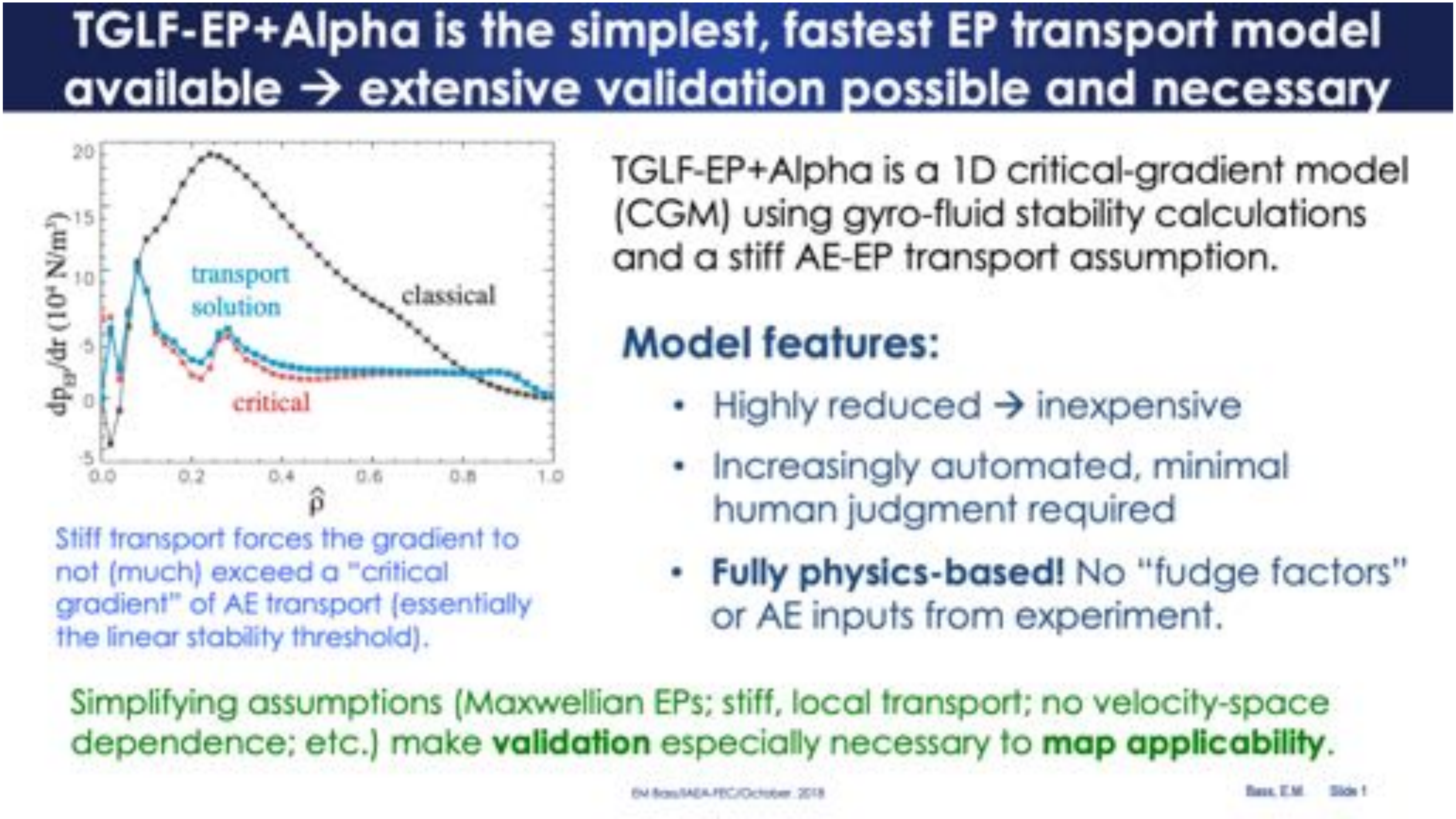


OAK RIDGE National Laboratory

Progress on reduced fidelity models for EP stability and transport is essential for whole device modeling

- **First step: need to rapidly evaluate Alfvén stability and mode structures**
  - Perturbative analysis (NOVA-K, AE3D-K)
  - Non-perturbative gyrofluid closure models (FAR3D, TGLF-EP)
- **Second step: must couple EP stability with energetic particle transport evaluation**
  - Critical gradient models (TGLF-EP)
  - Resonance-broadened quasilinear (RBQ) model
  - Perturbative phase space orbits (Kick model)
  - Rapid (GPU-based) fast ion Monte Carlo models with Alfvén mode structures (future versions of AE3D-K)

Critical gradient – reduced EP transport model



TGLF-EP+Alpha is the simplest, fastest EP transport model available → extensive validation possible and necessary

Stiff transport forces the gradient to not (much) exceed a "critical gradient" of AE transport (essentially the linear stability threshold).

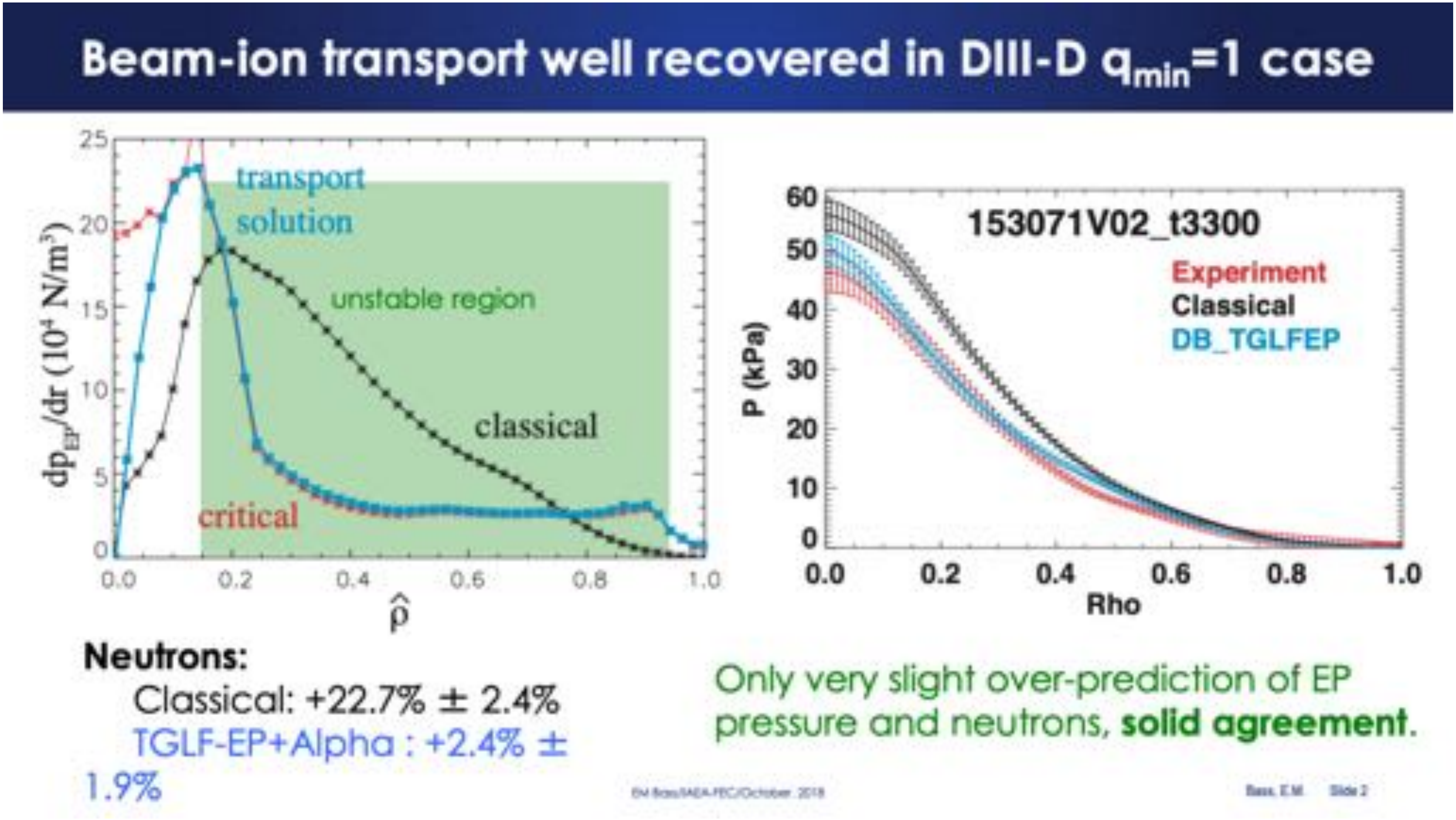
TGLF-EP+Alpha is a 1D critical-gradient model (CGM) using gyro-fluid stability calculations and a stiff AE-EP transport assumption.

Model features:

- Highly reduced → inexpensive
- Increasingly automated, minimal human judgment required
- **Fully physics-based!** No "fudge factors" or AE inputs from experiment.

Simplifying assumptions (Maxwellian EPs; stiff, local transport; no velocity-space dependence; etc.) make **validation** especially necessary to **map applicability**.

Critical gradient – reduced EP transport model



Beam-ion transport well recovered in DIII-D $q_{min}=1$ case

Neutrons:

Classical: +22.7% ± 2.4%

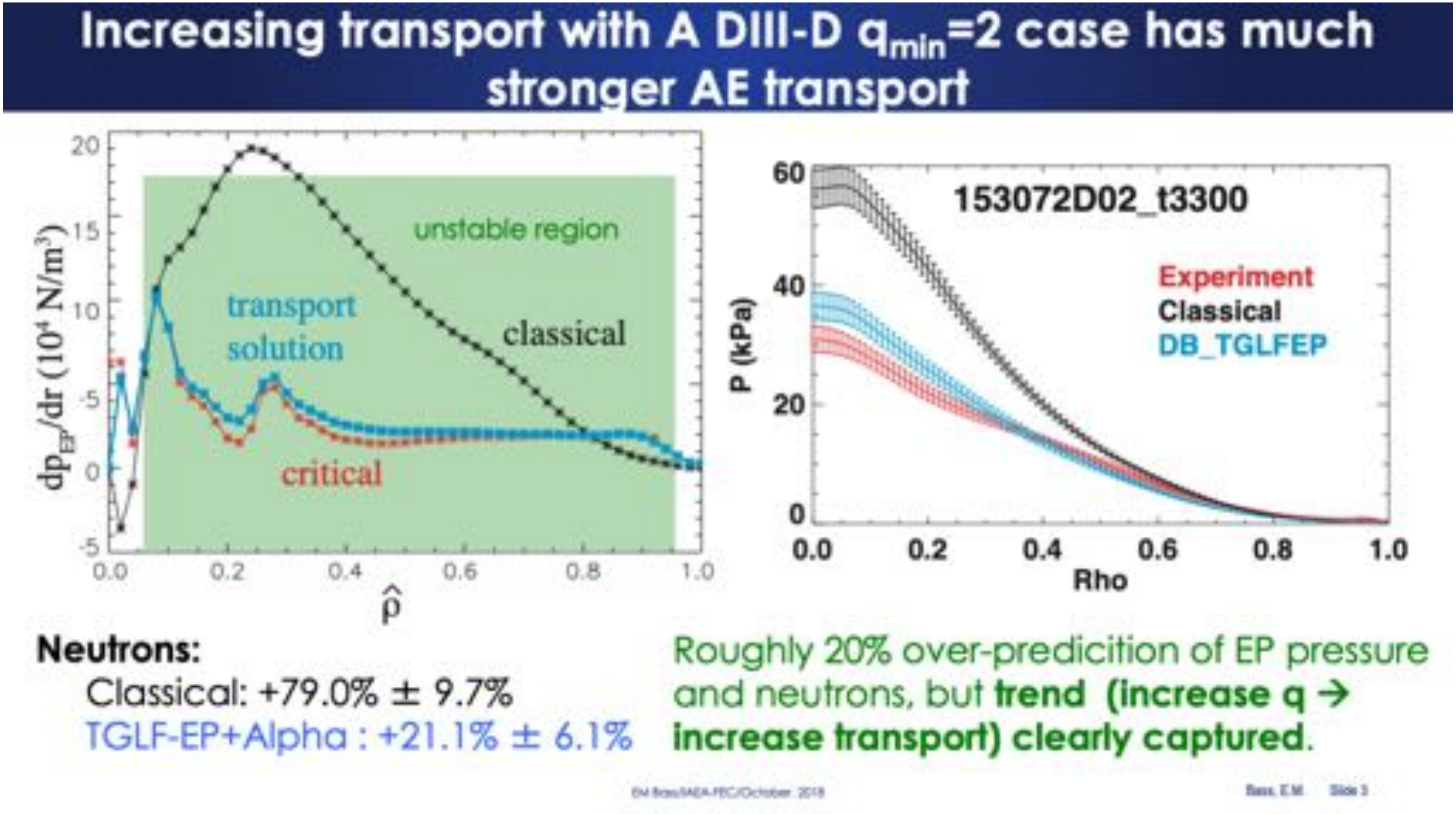
TGLF-EP+Alpha : +2.4% ± 1.9%

Only very slight over-prediction of EP pressure and neutrons, **solid agreement**.

EM Bass/IAEA-FEC/October 2018

Bass, E.M. Slide 2

Critical gradient – reduced EP transport model



Increasing transport with A DIII-D q_{min}=2 case has much stronger AE transport

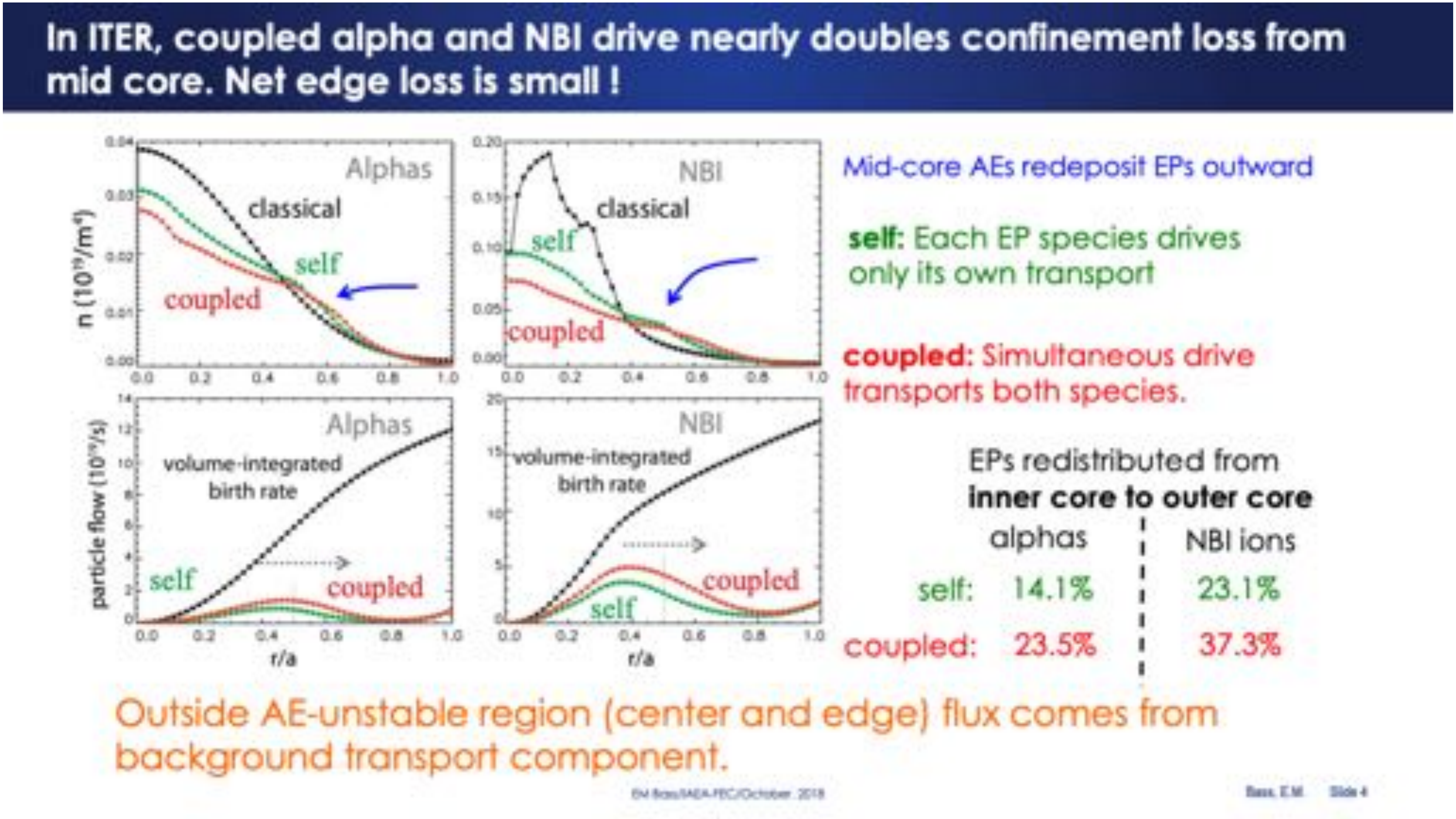
Neutrons:

Classical: +79.0% ± 9.7%

TGLF-EP+Alpha : +21.1% ± 6.1%

Roughly 20% over-predicition of EP pressure and neutrons, but **trend (increase q → increase transport) clearly captured.**

Critical gradient – reduced EP transport model



In ITER, coupled alpha and NBI drive nearly doubles confinement loss from mid core. Net edge loss is small !

Mid-core AEs redeposit EPs outward

self: Each EP species drives only its own transport

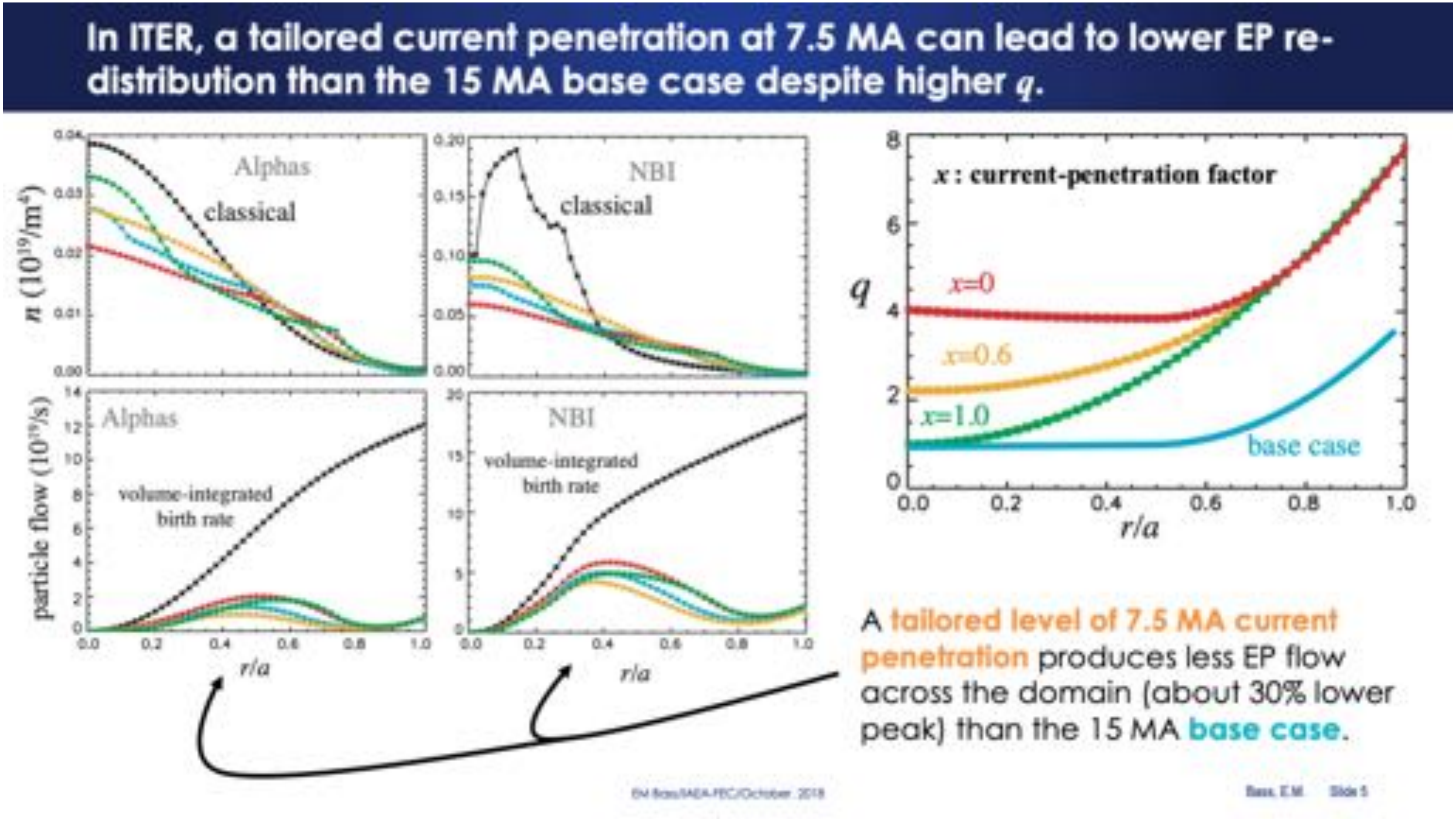
coupled: Simultaneous drive transports both species.

EPs redistributed from **inner core to outer core**

	alphas	NBI ions
self:	14.1%	23.1%
coupled:	23.5%	37.3%

Outside AE-unstable region (center and edge) flux comes from background transport component.

Critical gradient – reduced EP transport model



In ITER, a tailored current penetration at 7.5 MA can lead to lower EP re-distribution than the 15 MA base case despite higher q.

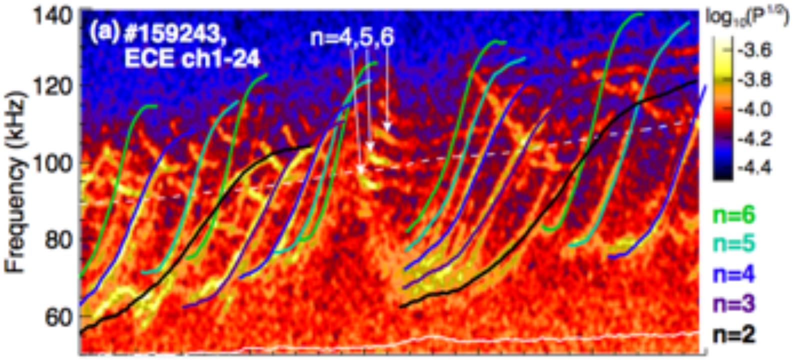
A **tailored level of 7.5 MA current penetration** produces less EP flow across the domain (about 30% lower peak) than the 15 MA **base case**.

EM Bass/IAEA-FEC/October 2018

Bass, E.M. Slide 5

Long time scale nonlinear: Alfvén instabilities are often observed to persist over 10^4 to 10^7 Alfvén times (R_0/v_A)

- **Observed time scales encompass many linear growth e-foldings** (~ 30 τ_A)
  - ➢ Nonlinear effects dominate

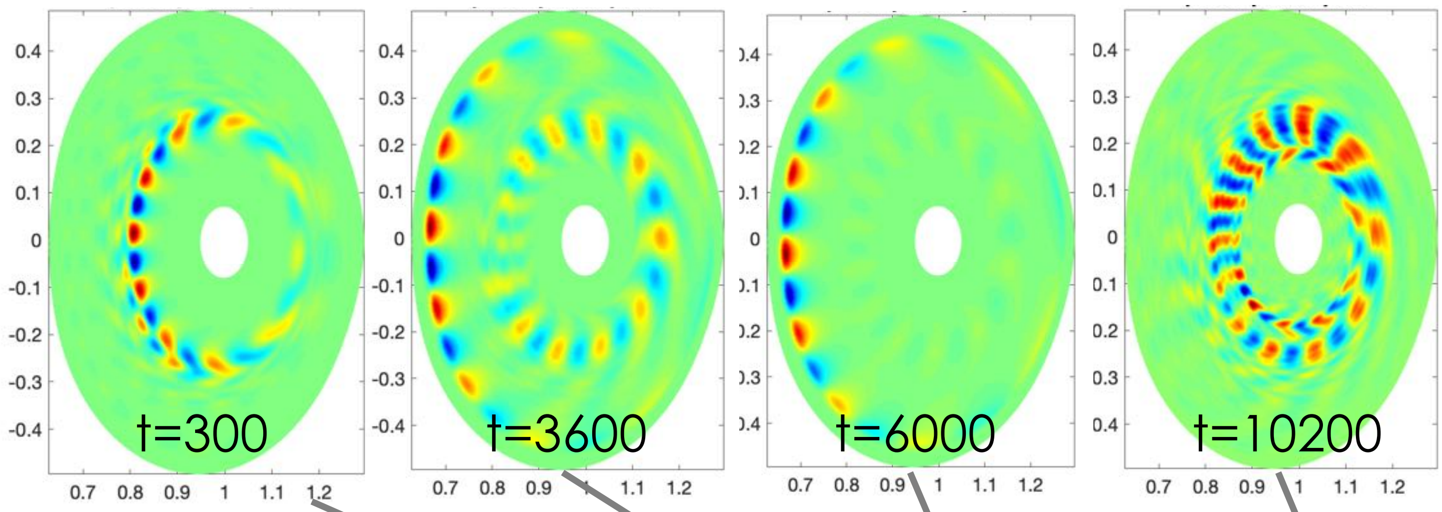


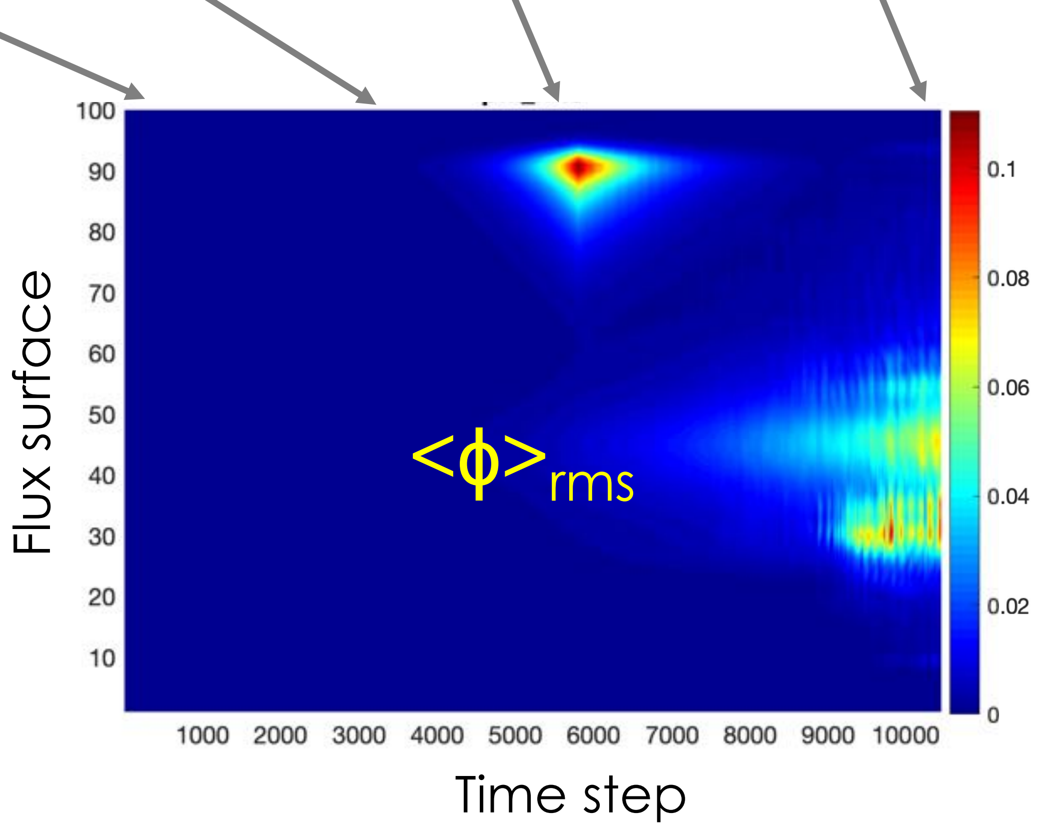
← ~ 1 million τ_A →

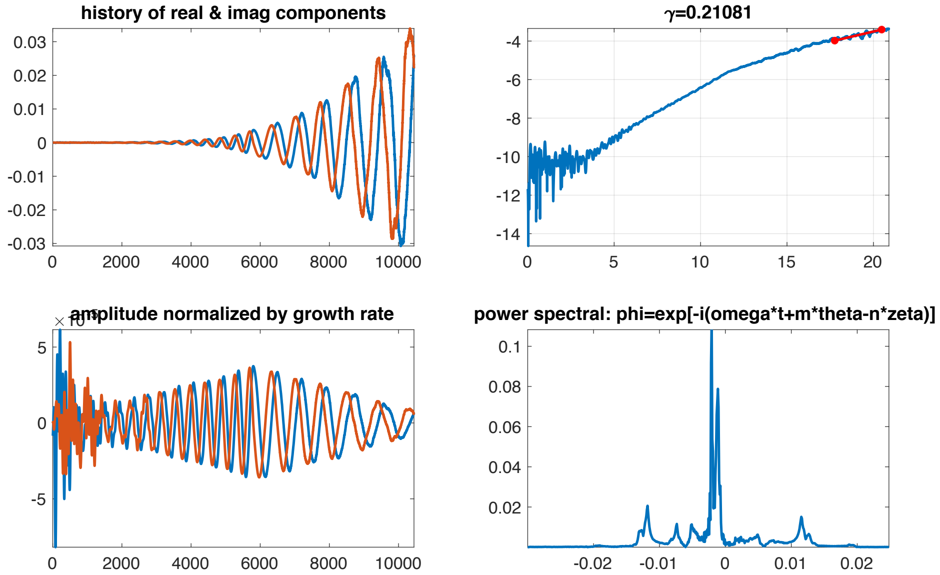
- **Intermittency also important**
  - ➢ As fast ion/wave system resolves imbalances
  - ➢ As changing plasma conditions change the mix of drive/damping
- **Studies of EP induced transport must account for conditions consistent with long-term sustainment**
  - ➢ Mode structure, equilibrium changes from zonal flows/currents
  - ➢ Dynamic adjustment in particle and energy flows
  - ➢ Fast ion distribution function imprinted by AE turbulence history

Long time-scale nonlinear: GTC gyrokinetic model

- New Summit version
  - Developed under CAAR program
  - Utilized GPU's
  - ~30x increase in performance
- Indicates bi-modal behavior
  - Switches from internal to edge mode and then back to internal mode

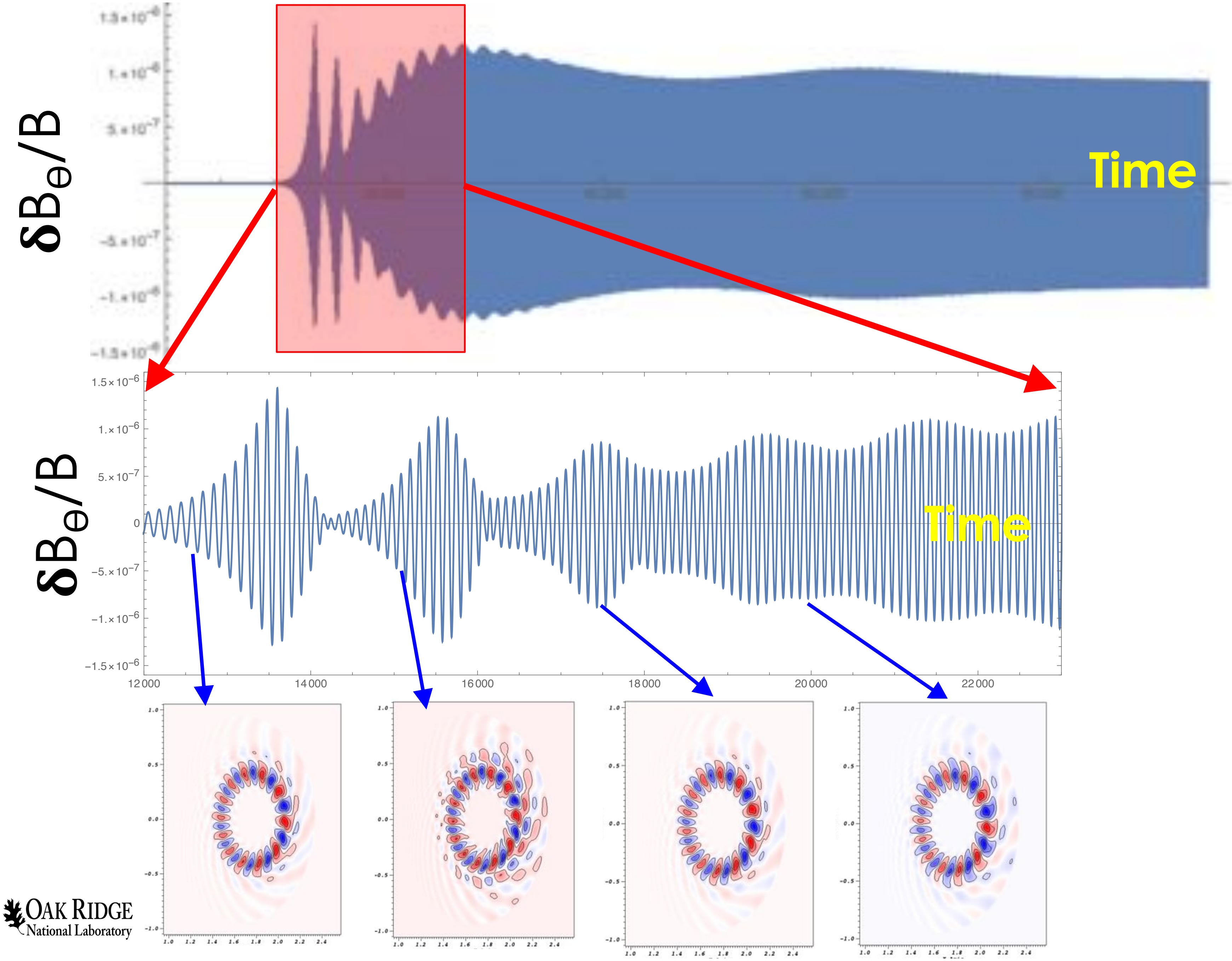




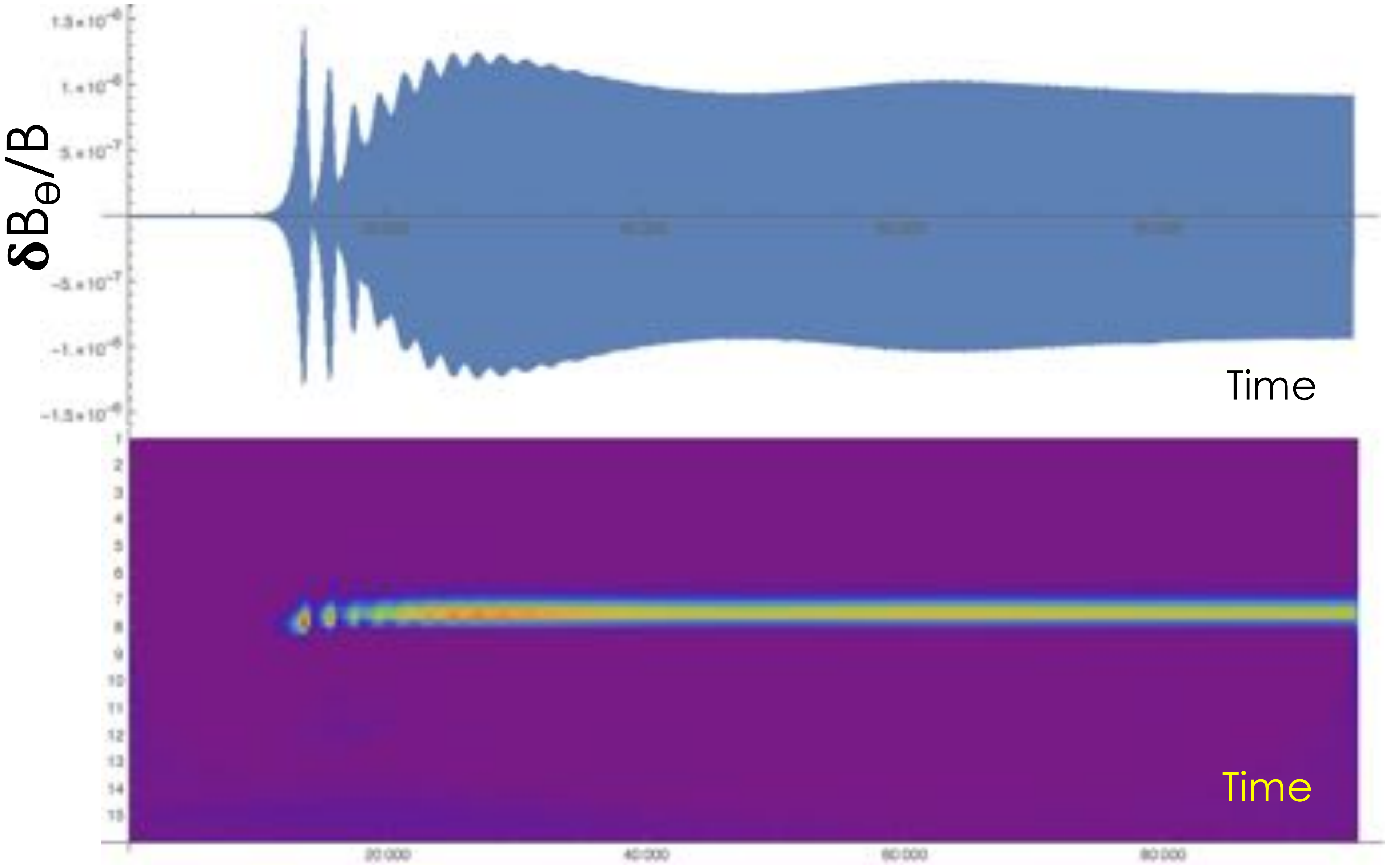


Oak Ridge National Laboratory

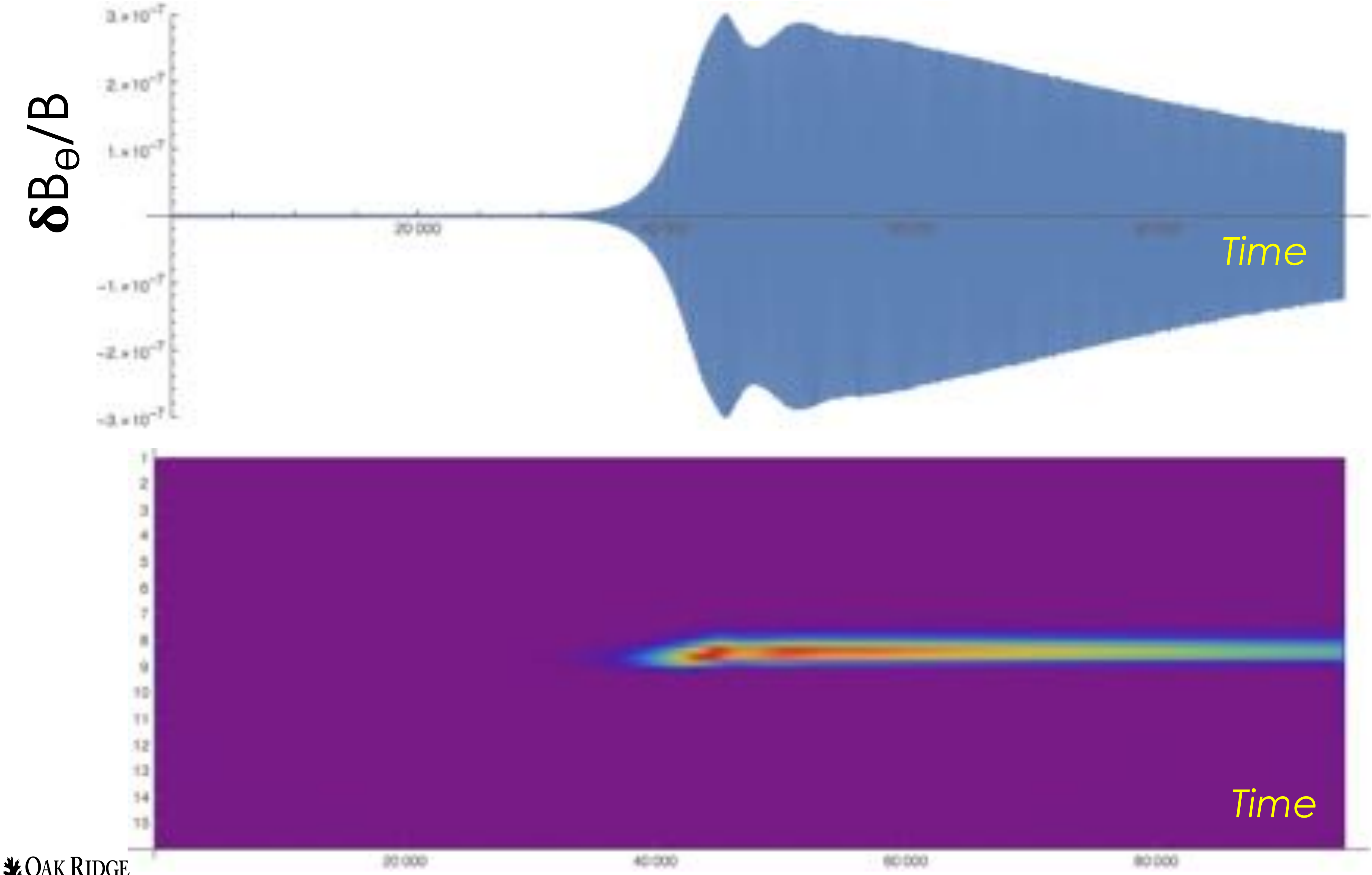
Long time scale nonlinear: this example is for n = 0, 4, 8 with all nonlinearities active



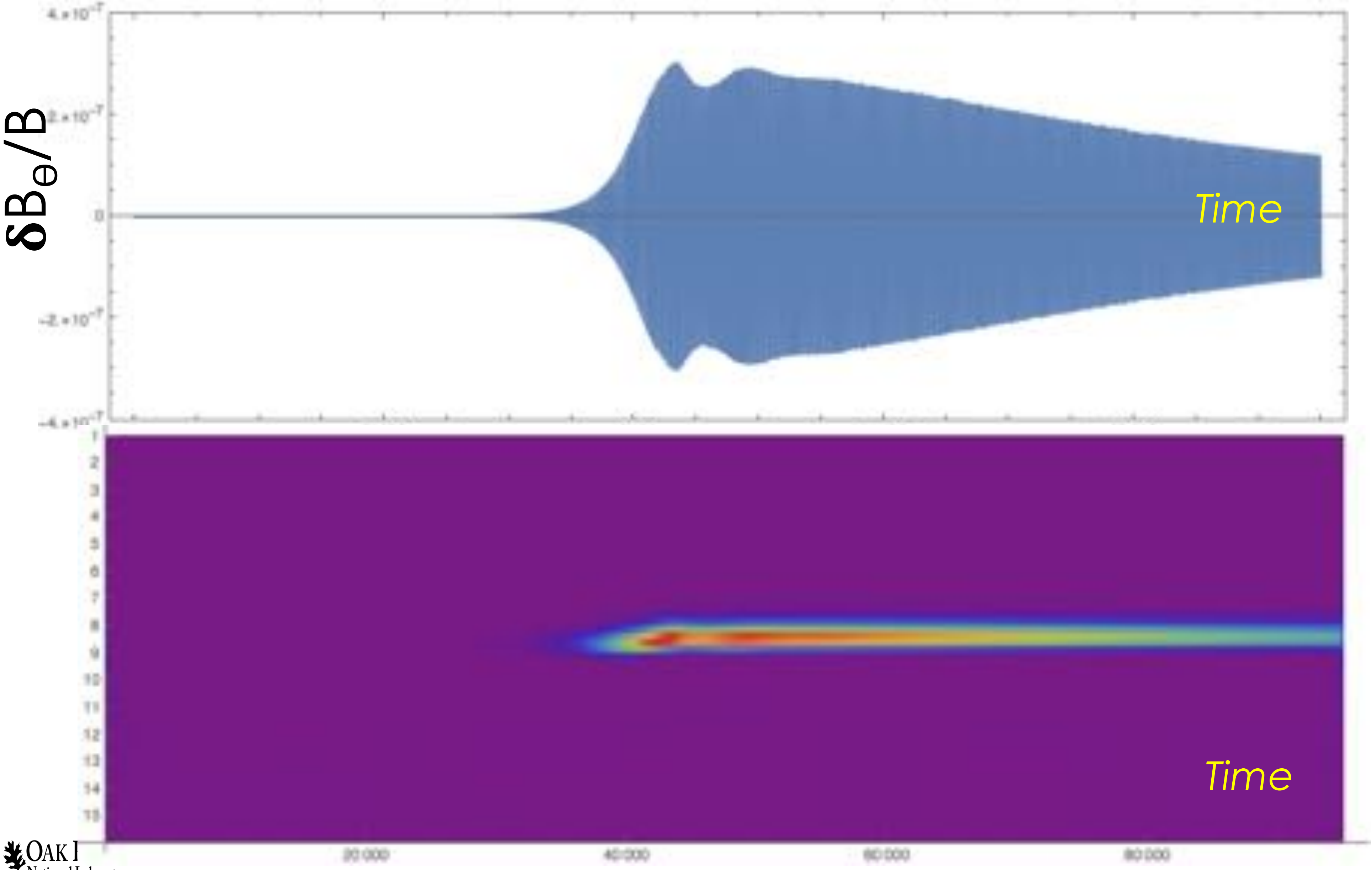
Long time scale nonlinear: n = 0, 4, 8 case with wavelet spectrogram



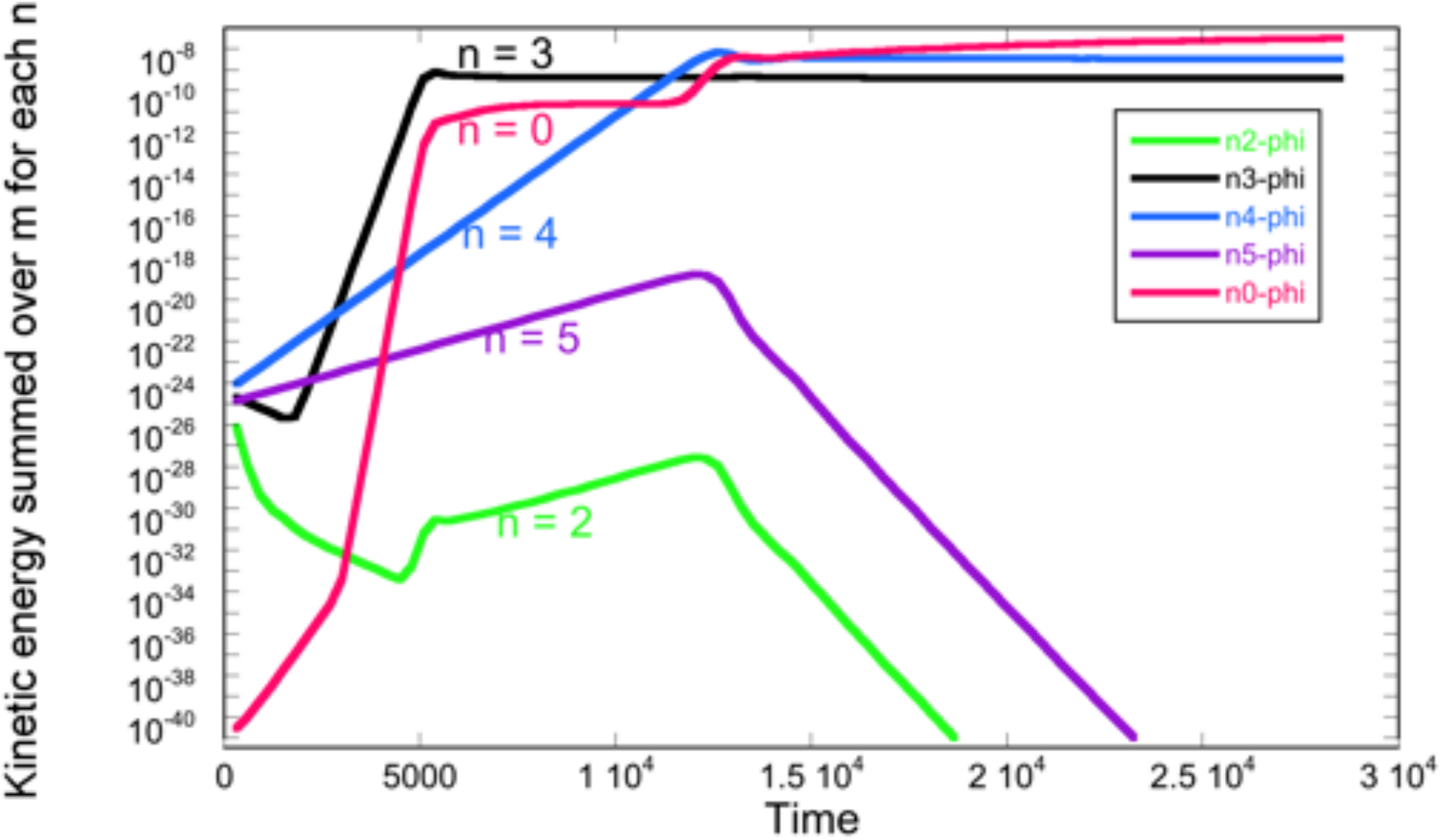
Long time scale nonlinear: n = 0, 4 case with wavelet spectrogram



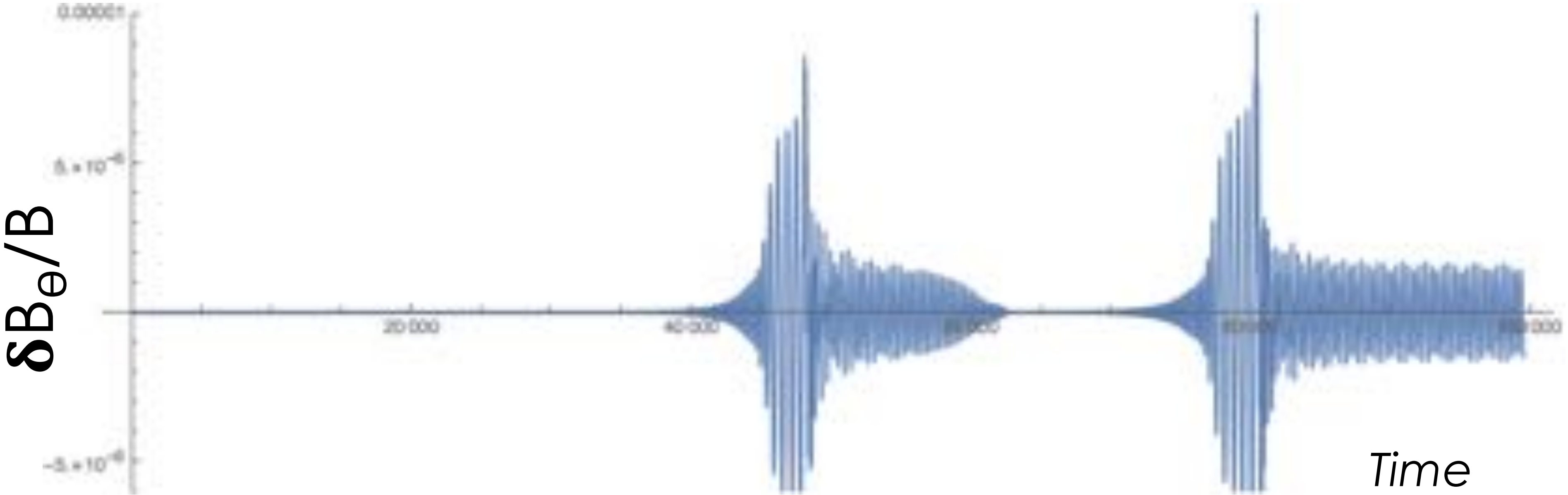
Long time scale nonlinear: n = 0, 2, 3, 4, 5 case with wavelet spectrogram

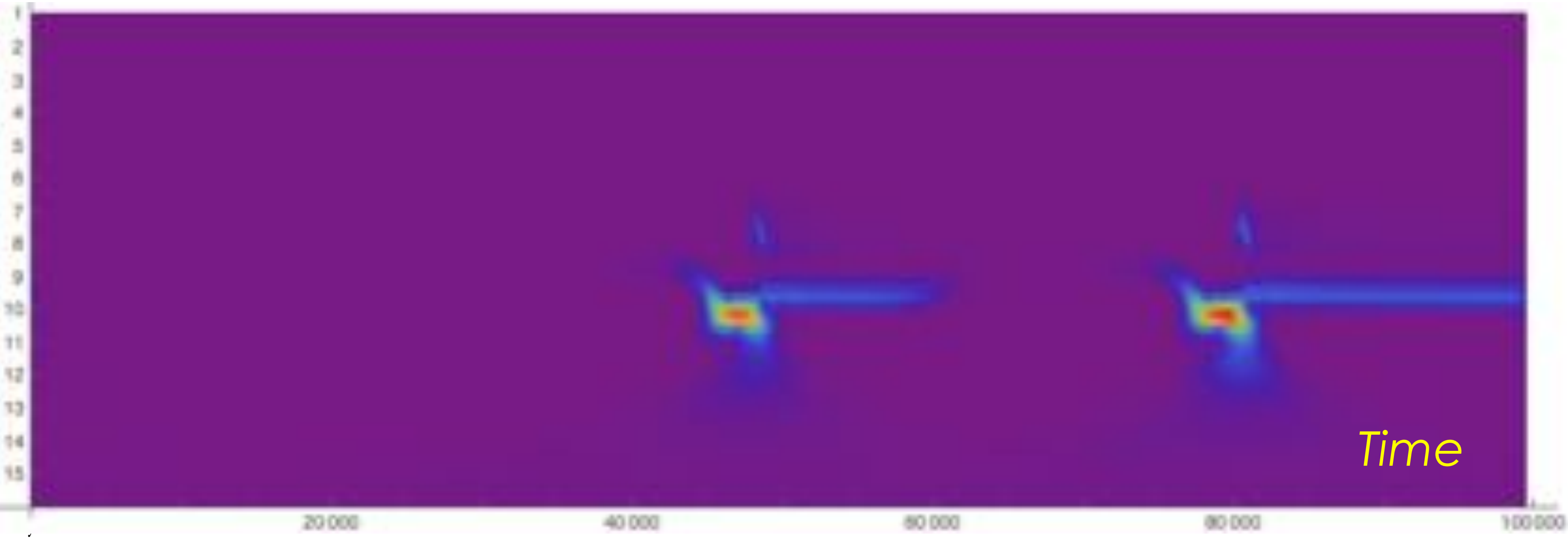


Long time scale nonlinear: energy evolution for the different toroidal modes shows role of n = 0 in regulating saturation stages

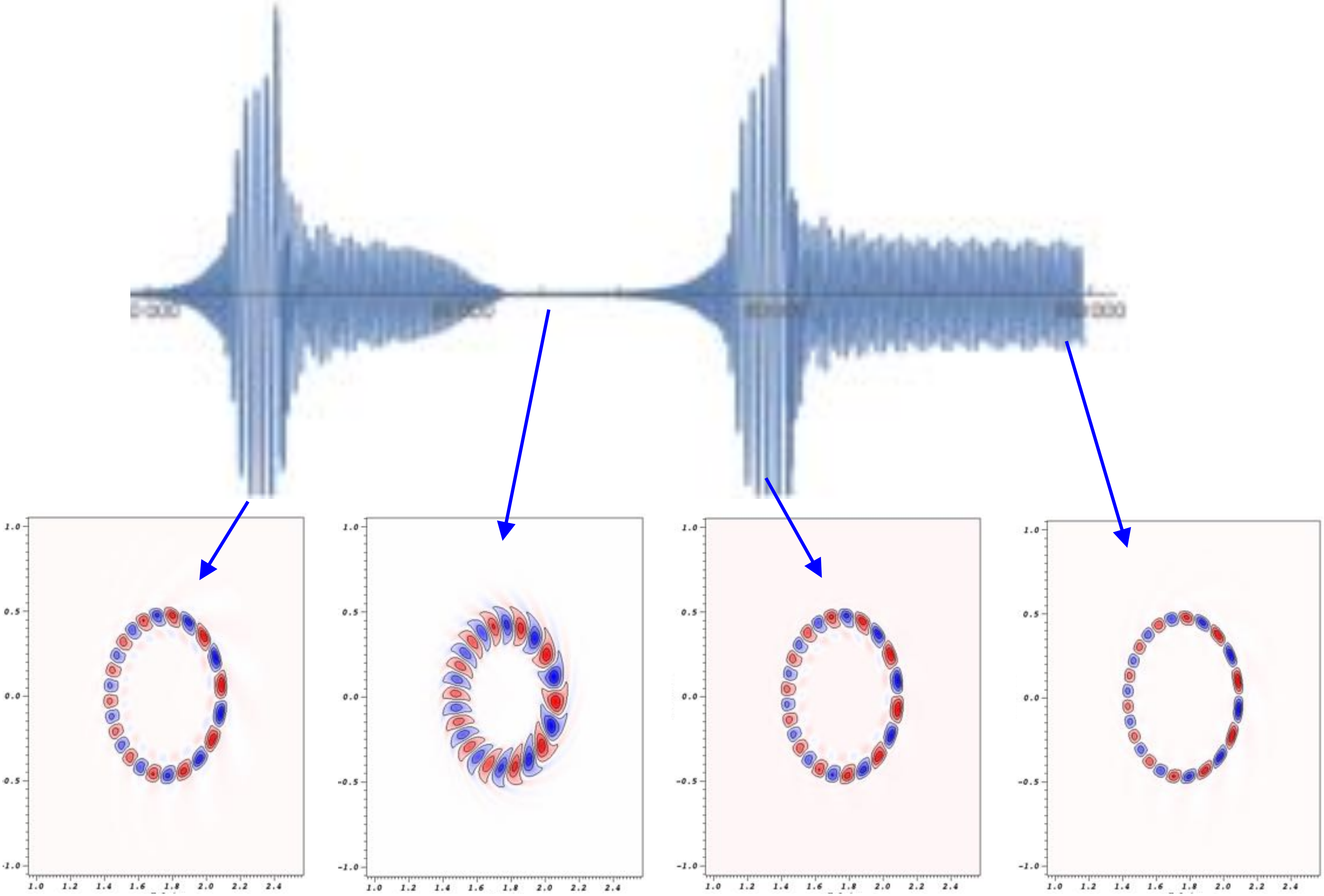


This includes n = 0, 4, and 8, but with the fast ion nonlinearities turned off => no profile flattening – only zonal flows/currents. Source instantly fills in losses.

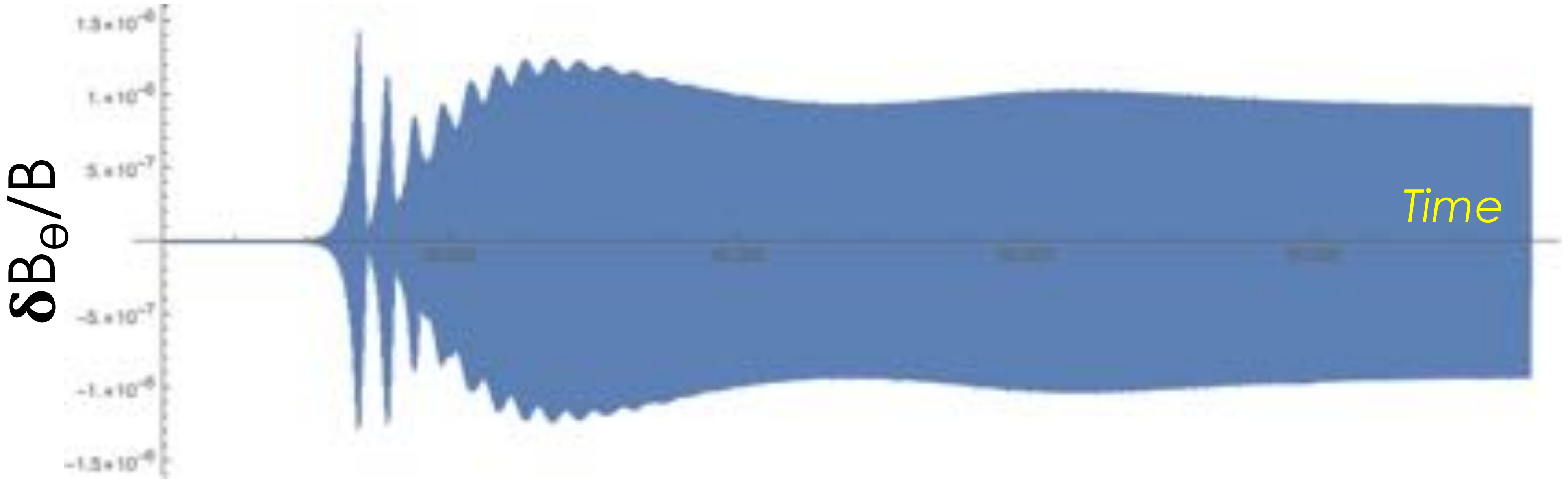


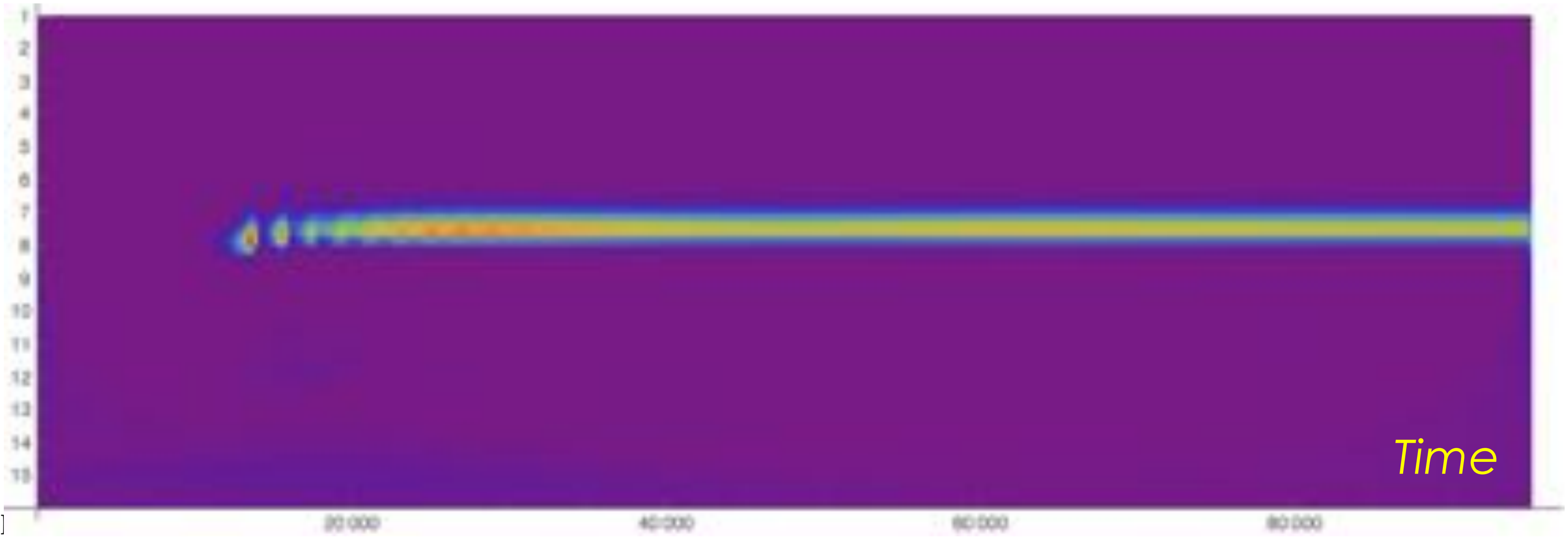


Long time scale nonlinear: the 2D mode structure evolves with time:

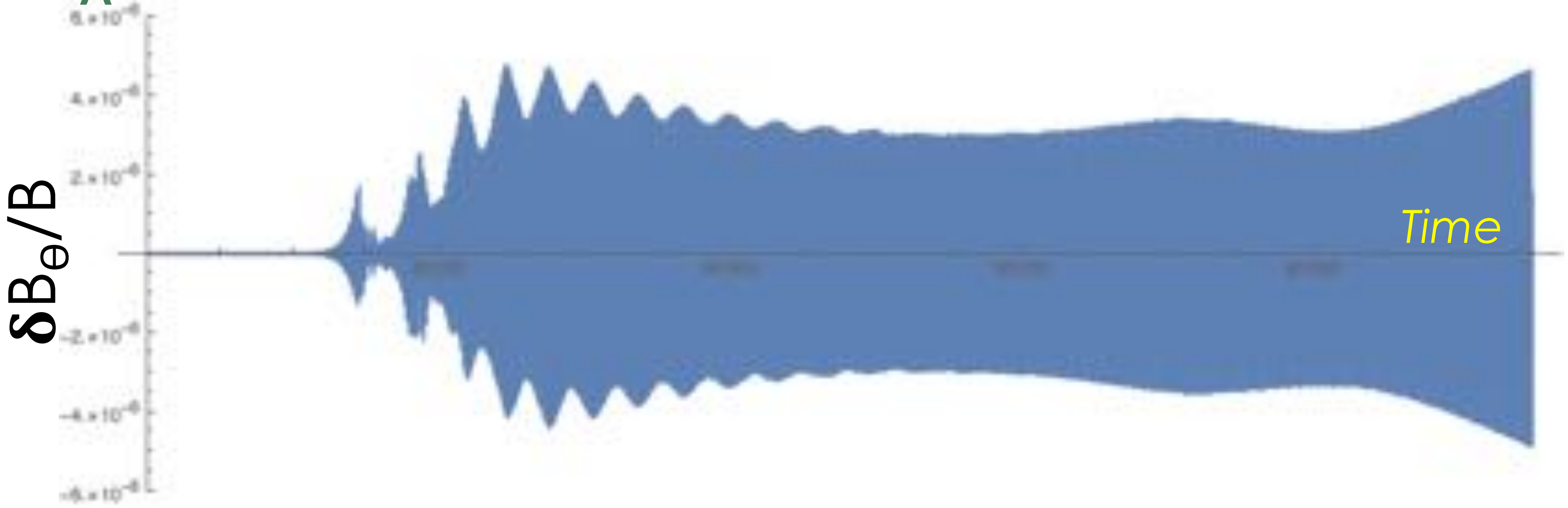


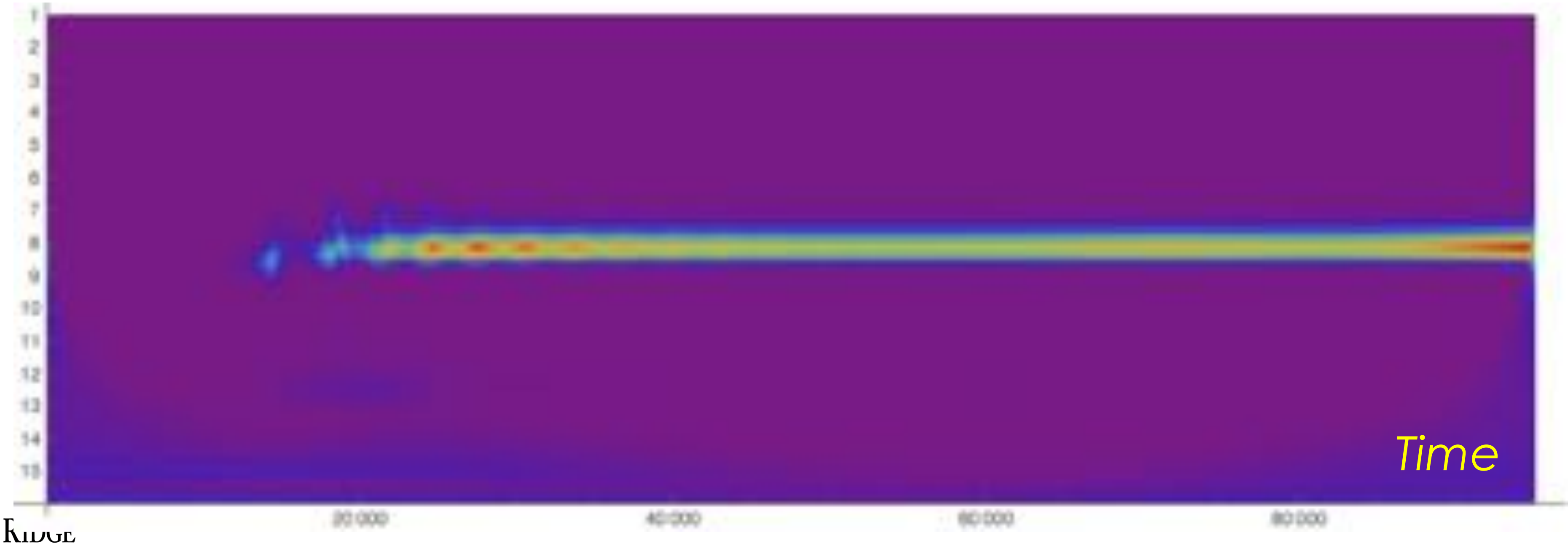
Long time scale nonlinear: Diffusion coefficients x $\tau_A/a^2 = 1 \times 10^{-5}$, n = 0, 4, 8



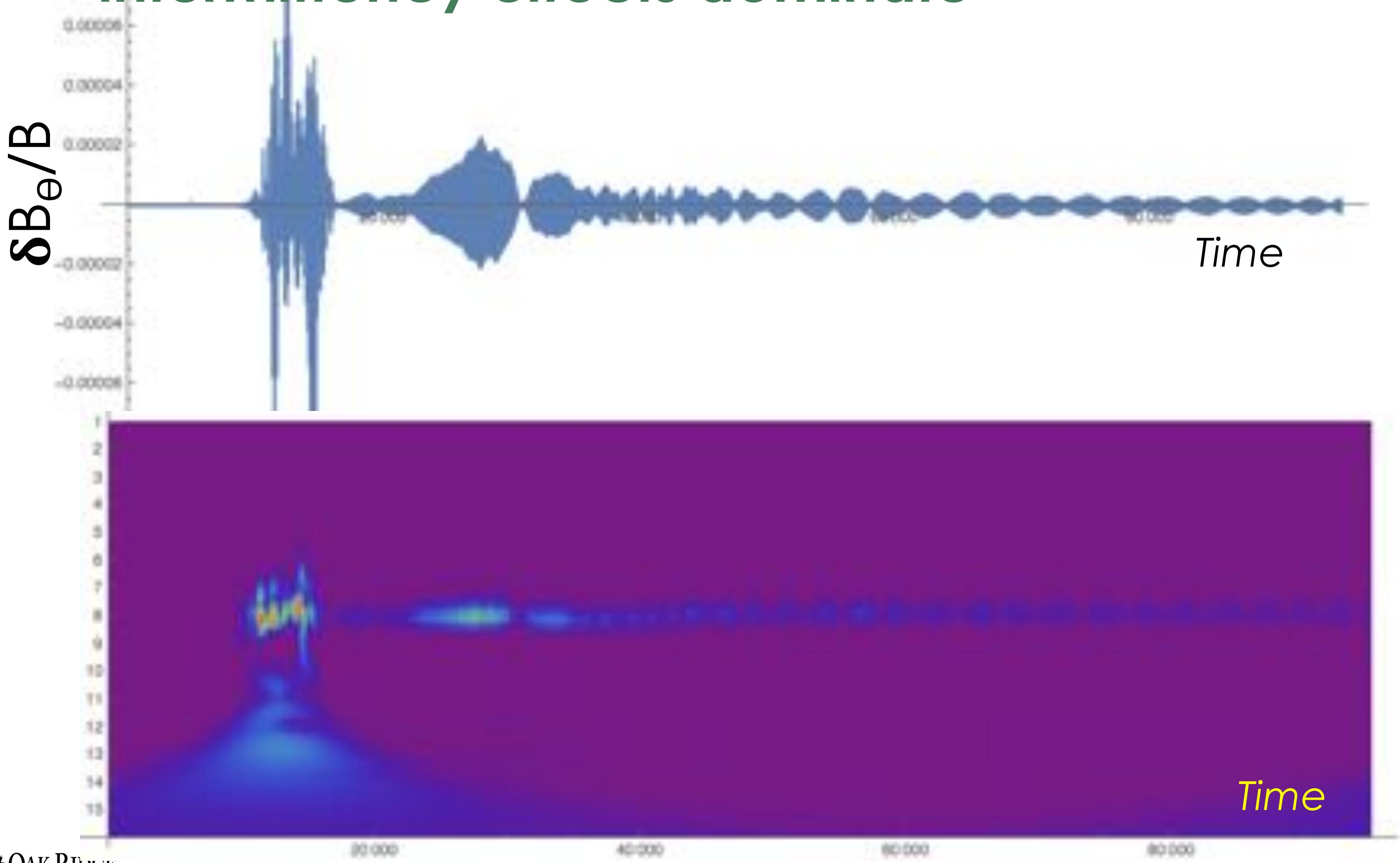


Long time scale nonlinear: Diffusion coefficients x $\tau_A/a^2 = 7 \times 10^{-6}$, n = 0, 4, 8



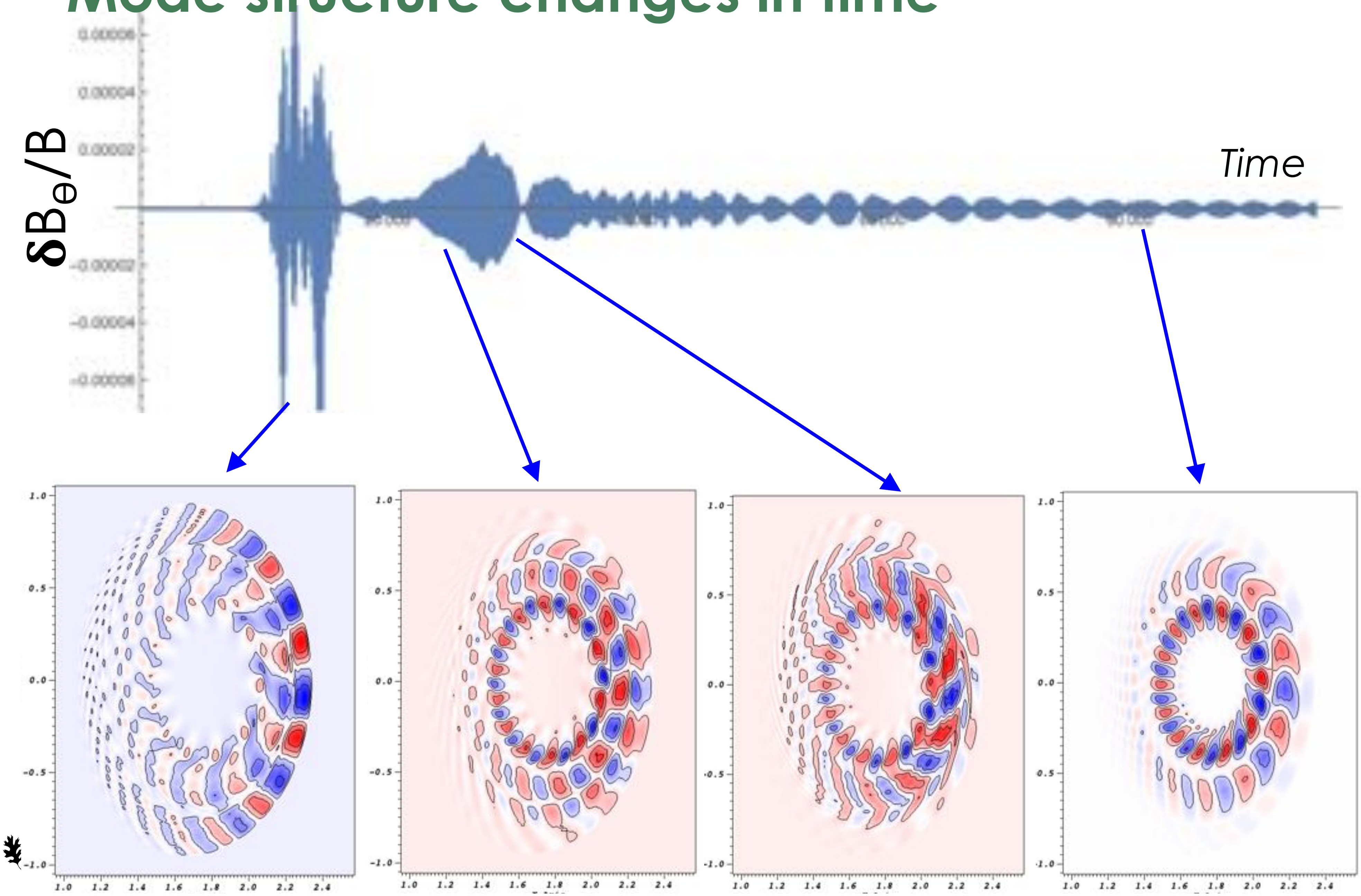


Long time scale nonlinear: Diffusion coefficients x $\tau_A/a^2 = 3 \times 10^{-6}$, n = 0, 4, 8 => intermittency effects dominate



Long time scale nonlinear: Diffusion coefficients x $\tau_A/a^2 = 3 \times 10^{-6}$, n = 0, 4, 8

- Mode structure changes in time

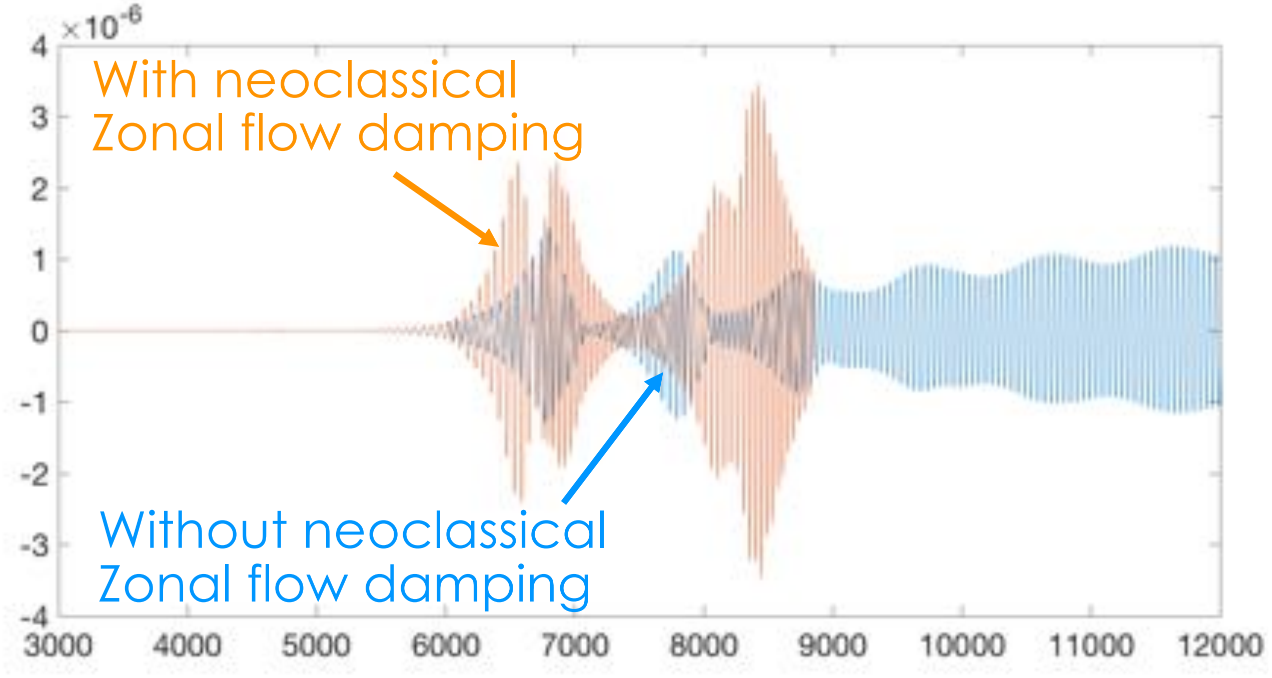


Long time scale nonlinear: neoclassical flow damping (Hinton/Rosenbluth) increases amplitude and intermittency

- Zonal flows are damped by a factor of:

$$\epsilon^{1/2}/1.6\ q^2$$

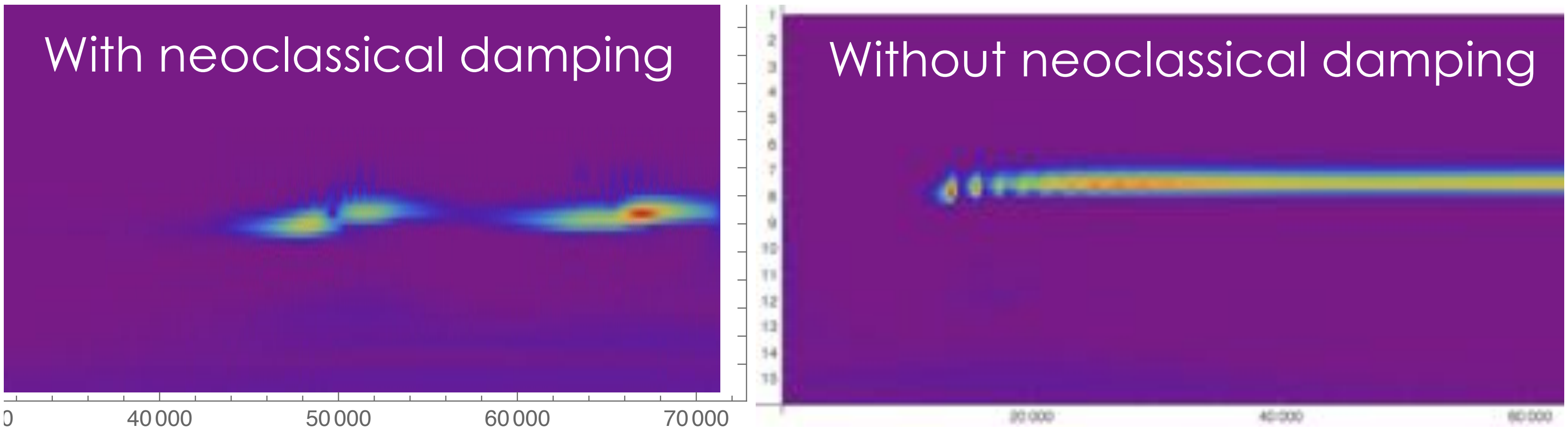
- Introduced into gyrofluid model through vorticity nonlinearity



With neoclassical Zonal flow damping

Without neoclassical Zonal flow damping

Diffusion coefficients x $\tau_A/a^2 = 1 \times 10^{-5}$, n = 0, 4, 8



With neoclassical damping

Without neoclassical damping

Summary

- ## Verification and Validation
  - ISEP and the previous GSEP projects have developed close connections with fusion experiments, such as DIII-D => successful V&V activities
  - In addition to the primary ISEP models, we have engaged with outside EP modeling codes
  - Recent linear stability verification will be extended to the nonlinear regime

- ## Long-term nonlinear simulations
  - Multiple AE modes have been followed for 10,000 Alfvén times
  - Extension to recent DIII-D transport analysis case
  - Connection with critical gradient modeling
  - Source/sink balancing models will be further developed