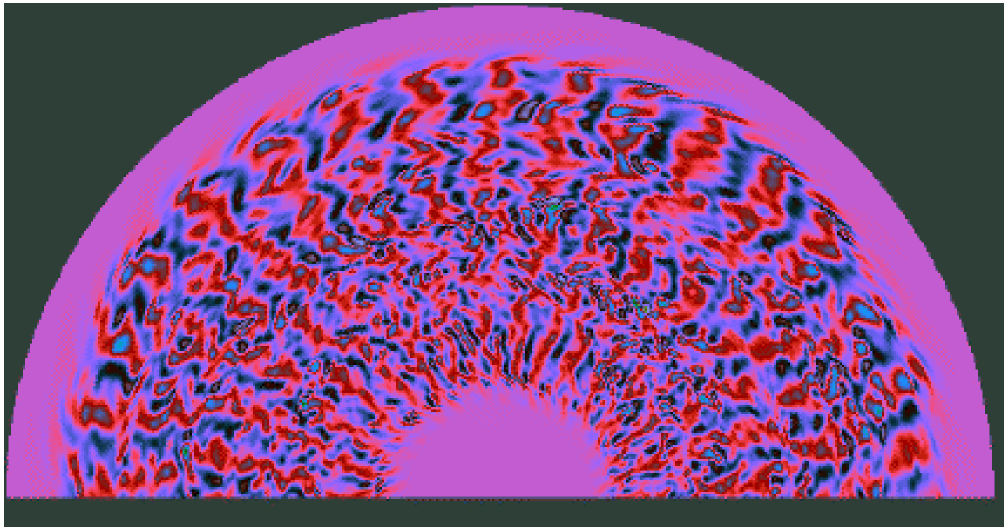
Validation for Magnetic Fusion:

Opportunities for Exploratory Plasma Research



Workshop on Exploratory Topics in Plasma and Fusion Research

February 12-15, 2013

M. Greenwald

Acknowledgements

This work builds on:

- The foundations set in the CFD community
- Activities by BPO and TTF working groups, including
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- A set of recent studies, mostly looking at models for plasma turbulence, that have tried to put these techniques into action

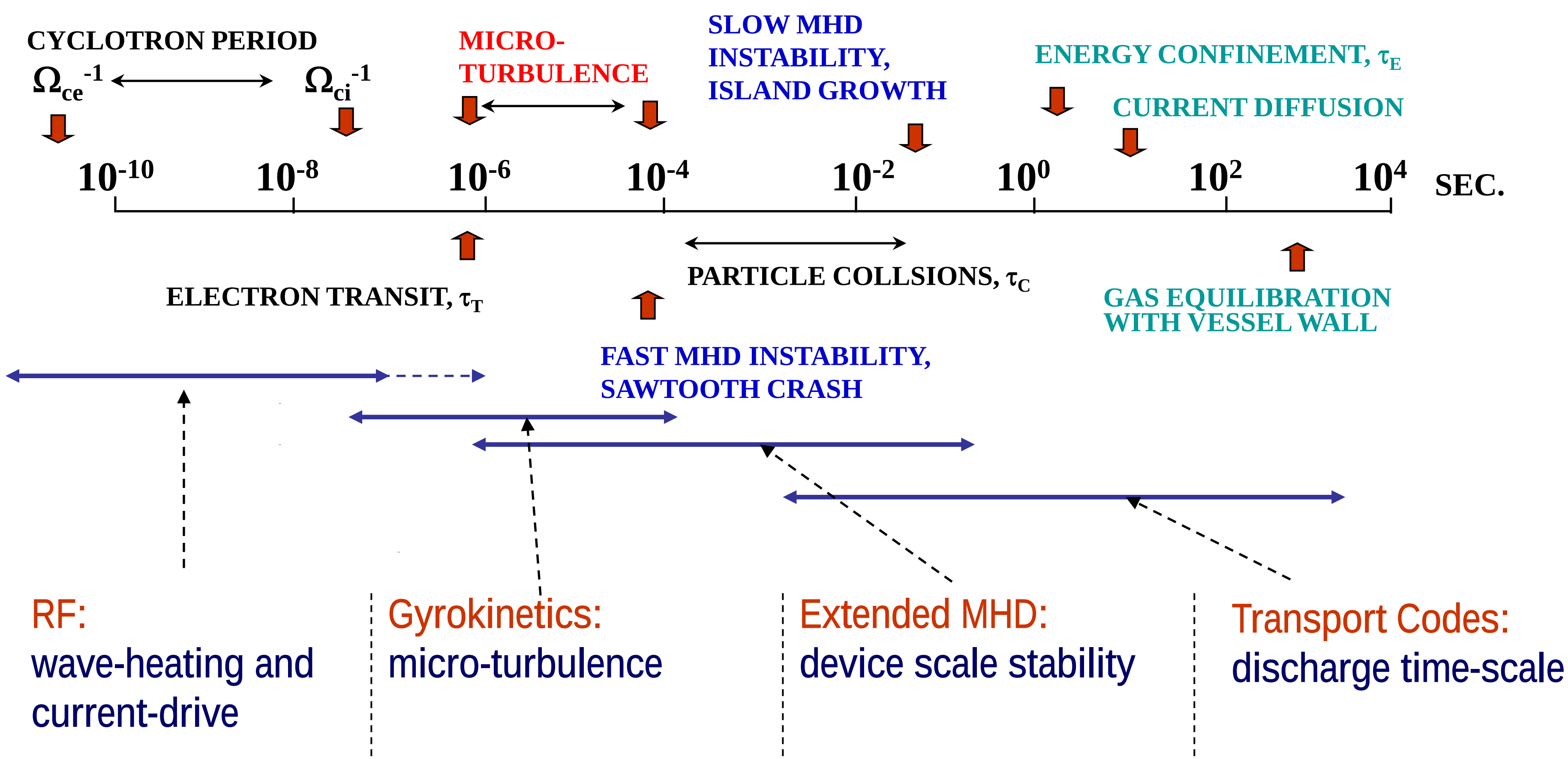
Verification, Validation & Uncertainty Quantification in Fusion Research

- Validation is an **extension of the scientific method** into areas where complex simulations are critical tools
- VVUQ are essentially **confidence building** activities – aimed at accumulating evidence that our codes are **correct and useful.**
  - Typically through accumulating instances of non-disagreement
- **Experience suggest that we, plasma and fusion research, need to make this process more systematic, quantitative, more rigorous and better documented**
- Validation can also be an important driver for our code development processes, identifying specific strengths and weaknesses in our models.

Let's Think About the Term "Model" In Our Context

- A **model** can be defined as "a representation of the essential aspects of some real thing, in an idealized or exemplary form, ignoring the inessential aspects" *(Huber)*
- The hard bit is identifying and demonstrating what is essential in each case
- Given the difficulty or our problems, the approach has been to develop **models** which…
  - obtain exact solutions to (very) approximate equations **or**
  - approximate solutions to (somewhat less) approximate equations
- We **test** the model to gain confidence that the approximations we've employed lack only "inessential" elements

As In CFD, We Need to Address Disparate Temporal and Spatial Scales, Extreme Anisotropy, Complex Geometry and Essential Non-linearities



We address different parts of the time domain with different **models**

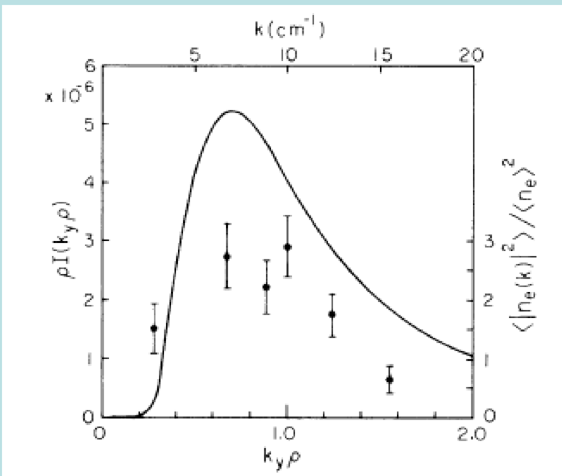
We Have to Confront the Significance of the Comparisons We Make

- What Constitutes agreement or non-agreement?
- What inferences can we draw?
- Challenges:
  - Uniqueness: Which measurements are important discriminators between models?
  - Sensitivity: Some measurable quantities vary strongly with certain input parameters
    - Agreement can be extremely difficult for some quantities and too easy for others
  - Measurement limitations
    - Measurements may be limited or indirect, “inversion” may not be accurate or unique

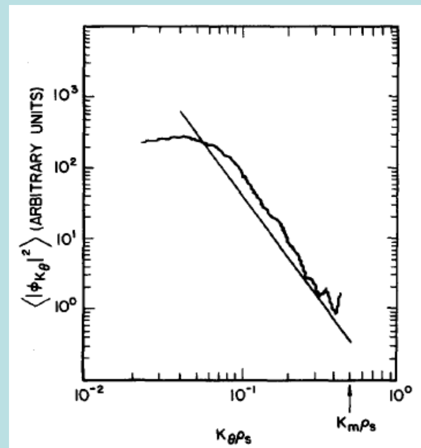
Prediction Uniqueness – Discrimination Between Models

- Physically, k spectrum arises from drive, dissipation and nonlinear coupling
- Very different models may predict essentially the same spectra

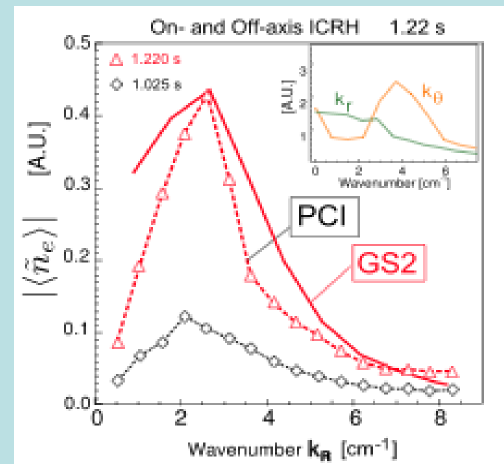
1976 ATC/theory



1985 PRETEXT/theory



2006 C-Mod/GS2



Increasing model complexity, analysis sophistication $\Rightarrow$

- **Try higher order moments (e.g. bicoherence) or other nonlinear statistics**
- **Though harder to measure, these may provide better discrimination**
- **Measure more quantities – primacy hierarchy**

Powerful Time Series Analysis Methods May Provide Better Sensitivity and Discrimination for Turbulence Models

Harmonic analysis techniques:

- Short-time Fourier transform
- Fractional Fourier transform (intermediate between time & space)
- Bispectral analysis
- Continuous wavelet transform
- Chirplet transform

Chaotic analysis

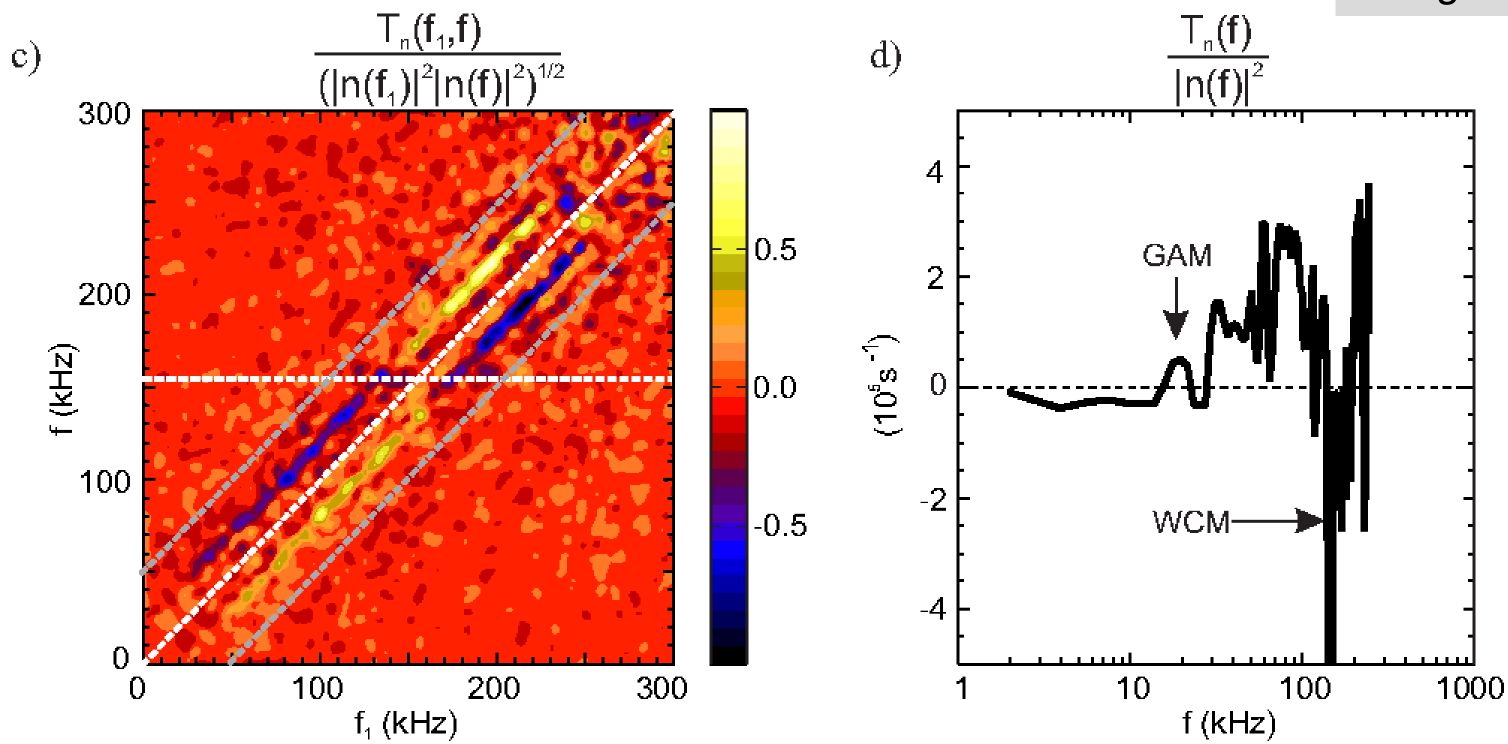
- Fractal dimension (correlation dimension)
- Recurrence analysis, periodicity or cyclic analysis
- Lyapunov exponents

Principal components analysis

And many others

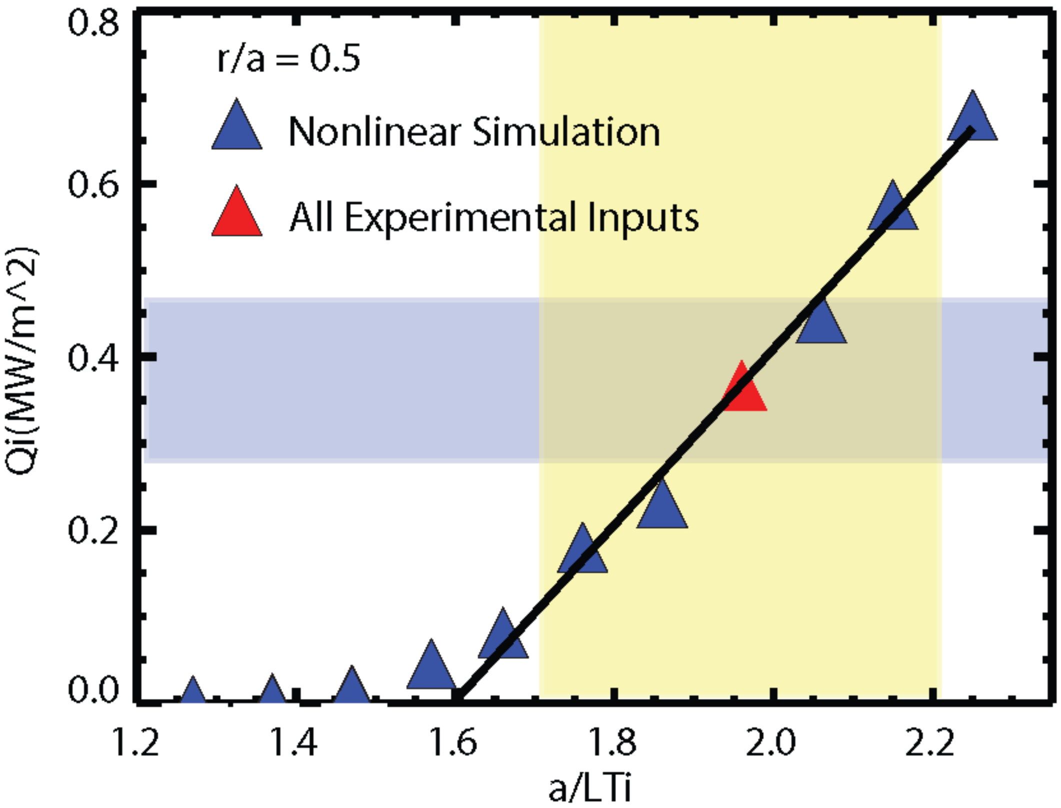
Validation Challenges & Opportunities: Nonlinear energy transfer and bicoherence techniques

Ziegler 2012



- Issue: Linear analysis (power spectra) do not discriminate between models
- Experimental data with sufficient quality for nonlinear analysis exists

Sensitivity: Confined plasmas run near marginal stability most of the time



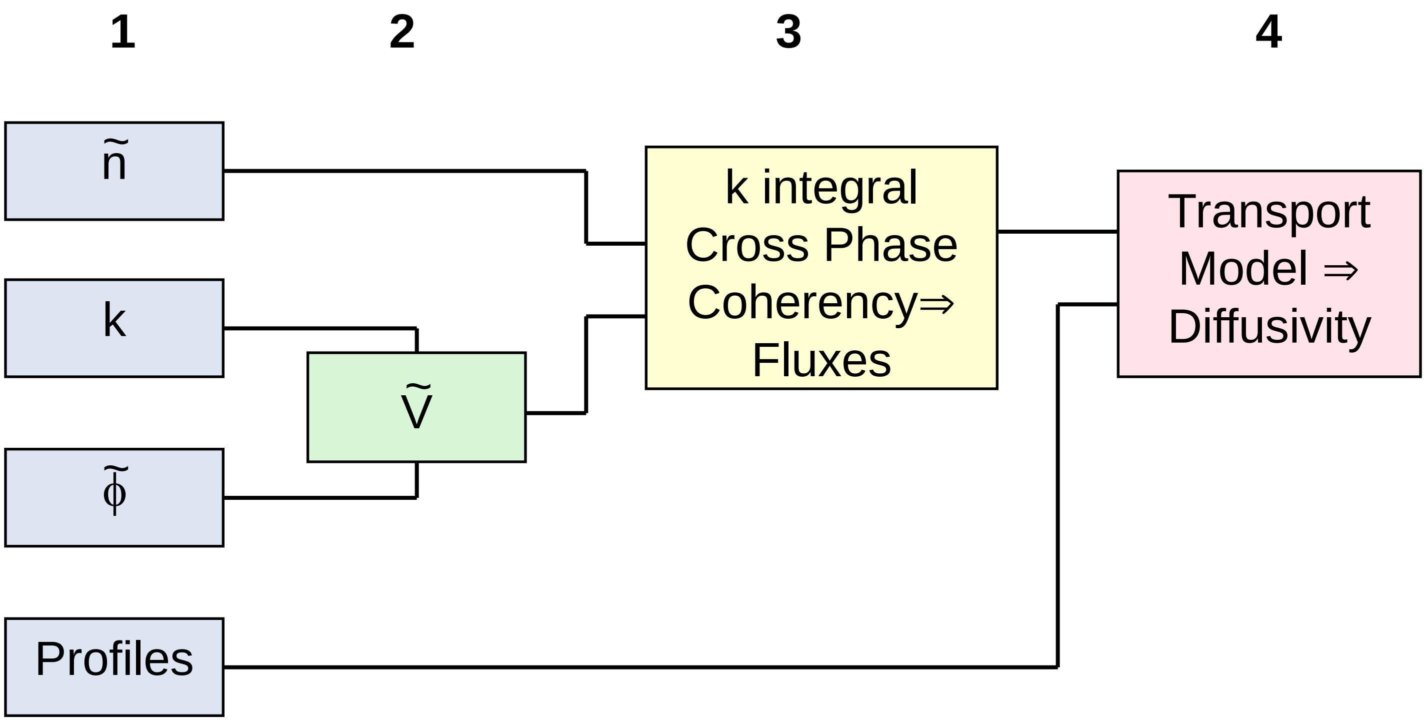
- Issue: critical gradients, extreme sensitivity
- Even with excellent measurements impact is substantial
- (There are also measurement and analysis challenges associated with extracting “experimental” heat flux and gradients)

Howard 2012

Primacy Hierarchy
Measure Multiple Quantities At Multiple Levels:

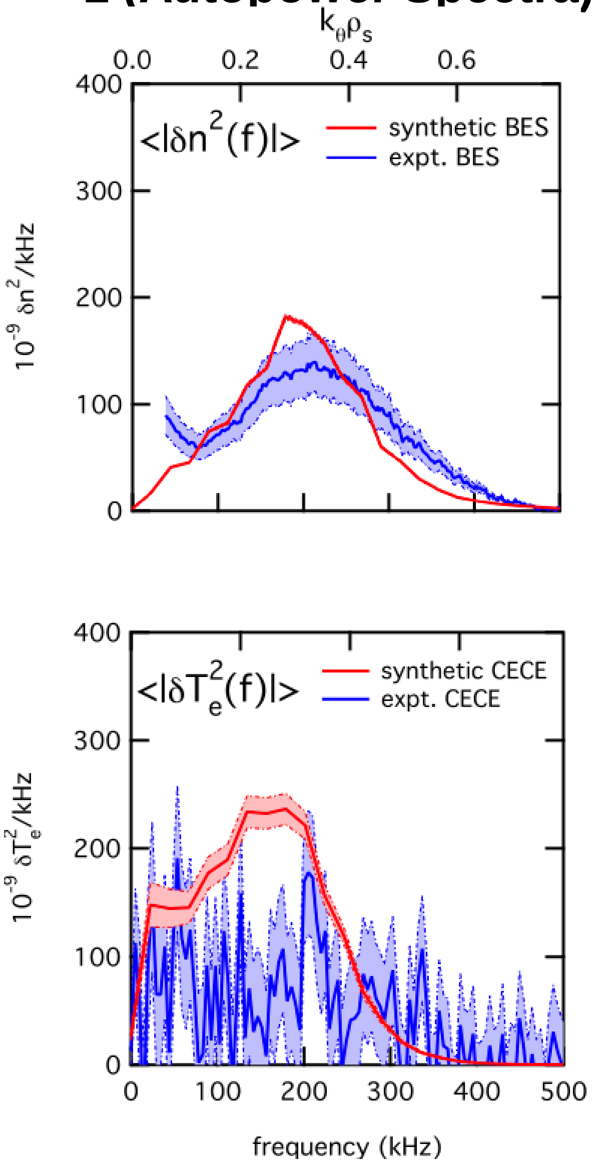
- We can try to distinguish between basic vs composite quantities
- Rank measured quantities in terms of the extent to which other effects combine

Primacy Level For Turbulent Transport

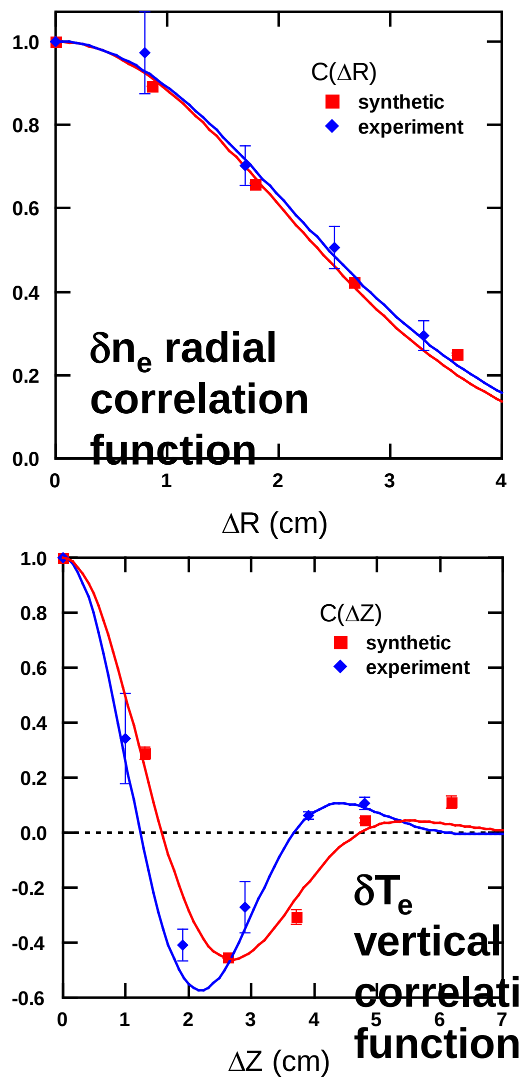


Example 1: Turbulence and Transport

1 (Autopower Spectra)



2 (Correlation Lengths)

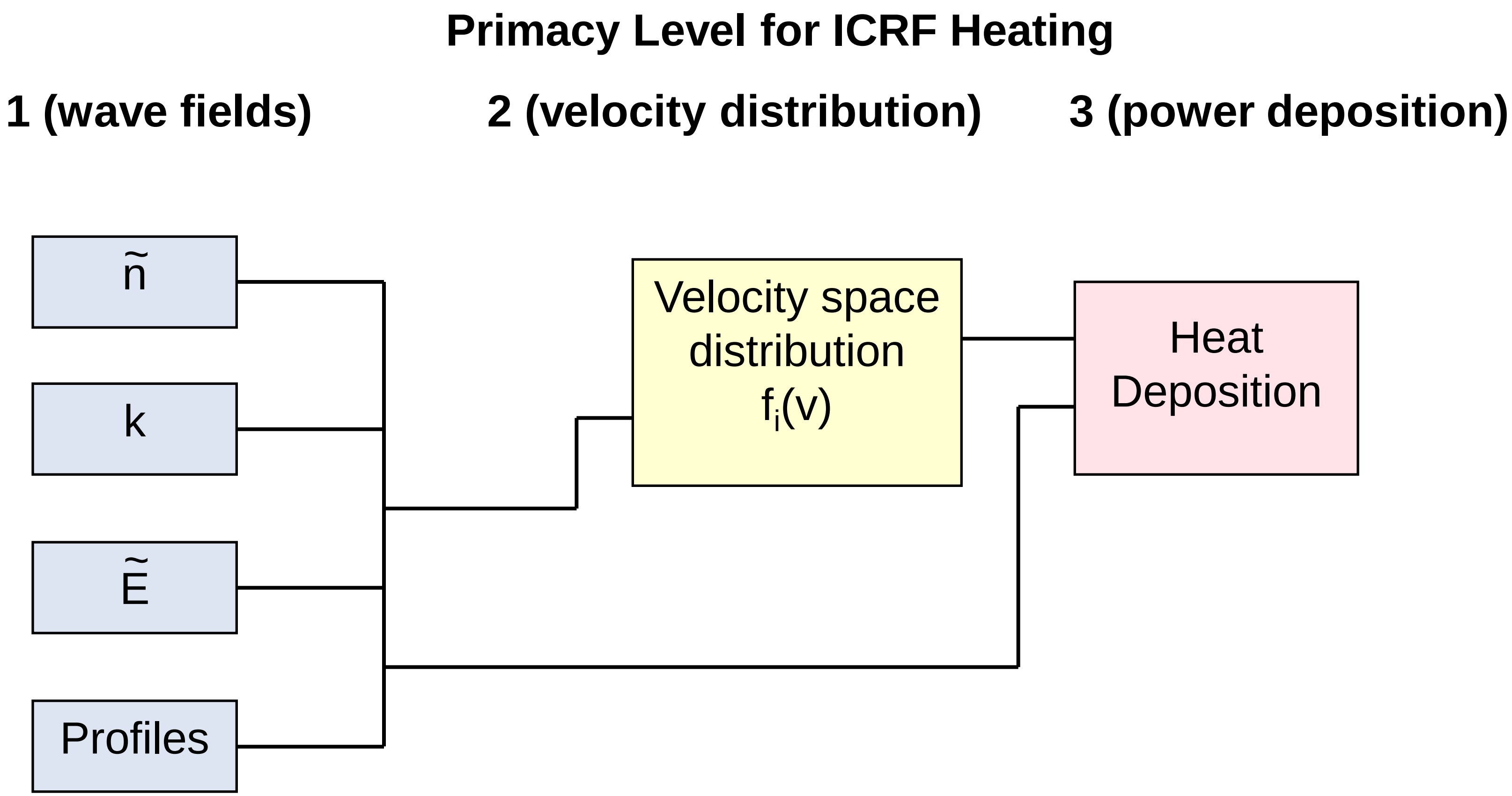


3 (Heat Flux)

(C. Holland, et al.)

D3D 128913 1300-1700 ms r/a = 0.5	Expt.	GYRO
Q_i (kW/m^2)	32 ± 6	38 ± 7
Q_e (kW/m^2)	26 ± 7	34 ± 7
RMS δn_e (%)	0.6 ± 0.1	0.56 ± 0.01
RMS δT_e (%)	0.4 ± 0.2	0.66 ± 0.02

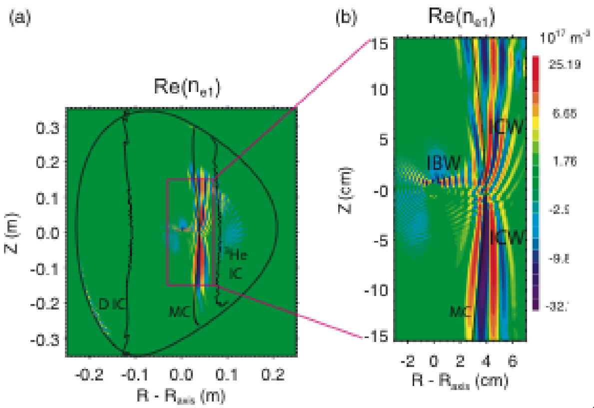
Example 2: ICRF Heating

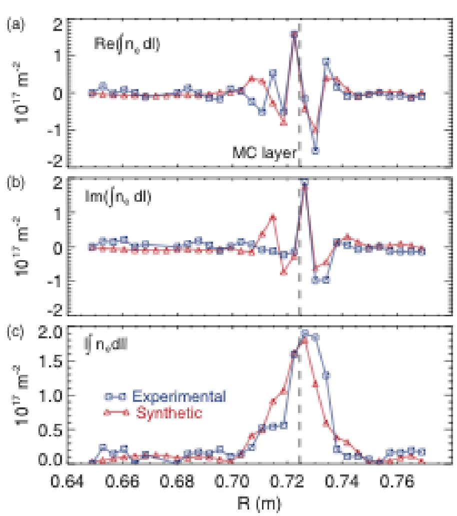


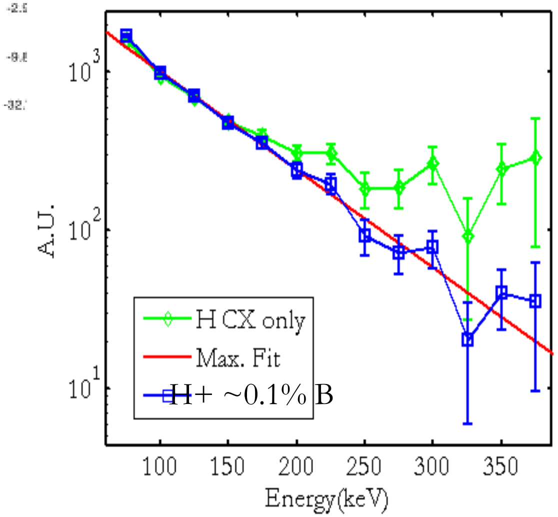
Example 2: ICRF Heating - Results

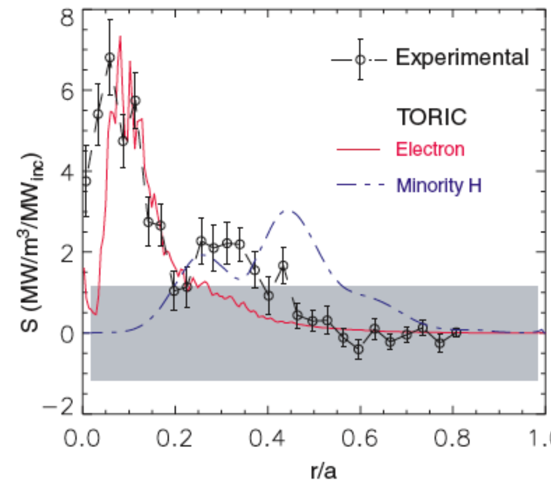
Primacy Level

1 (wave fields) **2 (velocity distribution)** **3 (power deposition)**









Lin

Tang

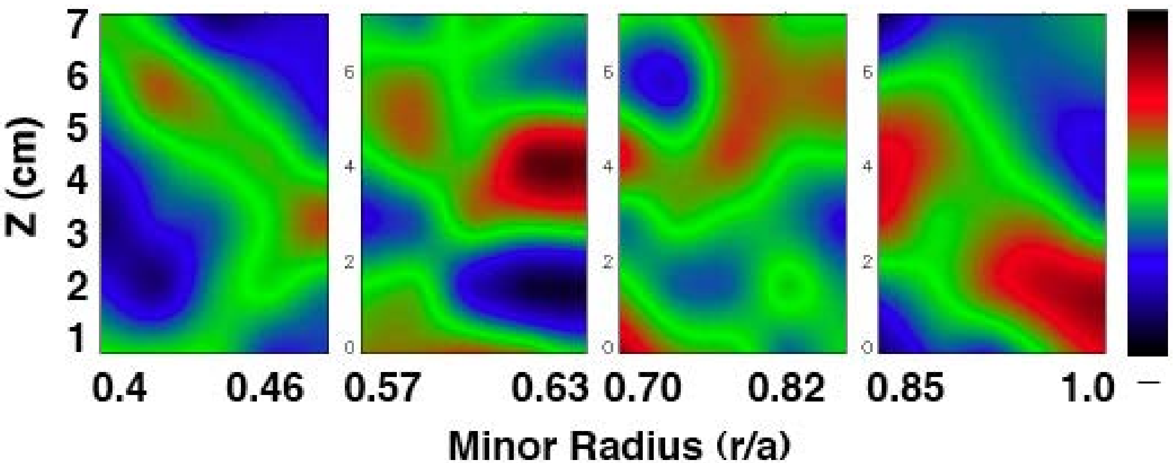
Nelson-Melby PCI synthetic diagnostic for TORIC code

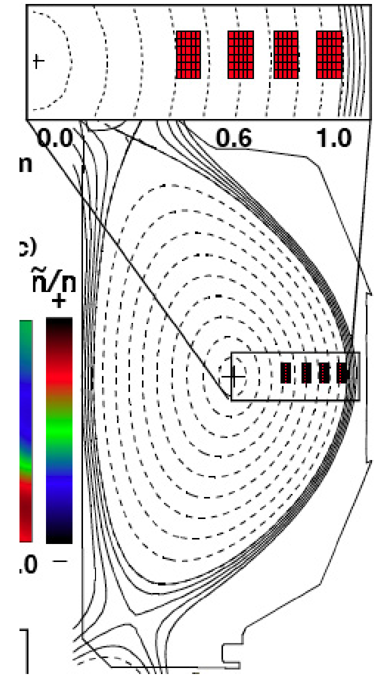
The Primacy Hierarchy Helps Address The Issue Of Discrimination

- Comparison at several levels in the hierarchy is best practice
- In general, discrimination between models is reduced as one goes up the primacy hierarchy
- It may be possible to identify ways in which physics cause uncertainties and errors to cancel
- The form of the hierarchy is not necessarily unique – the important thing is to come to grips with the issue

The Measurement Challenge: Diagnostics Are Critical For Validation of Fusion Codes

- Turbulence visualization (BES, GPI) and innovative probe diagnostics are providing unprecedented views into plasma dynamics

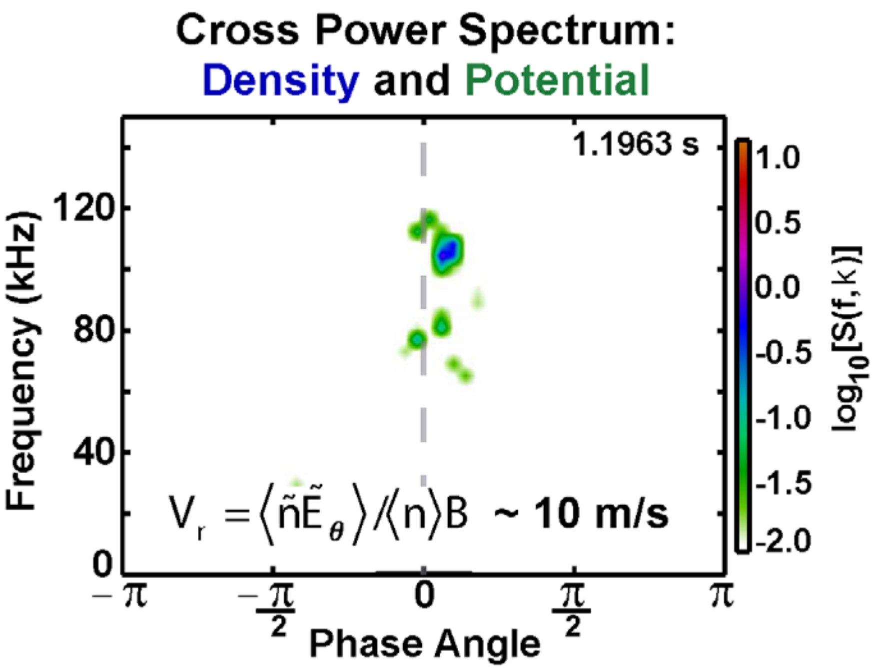




McKee

- **How to use these capabilities for quantitative comparisons with codes?**

Probes Can Measure Many of the Quantities Of Interest With Exceptional Spatial and Temporal Resolution



LaBombard 2012

- “Mirror” probe systems allows accurate measurement of $\tilde{n}_e, \tilde{T}_e, \tilde{\phi}$ with a single probe. (LaBombard 2012)
- This allows computation k resolved heat and particle flux
- Other probe systems have allowed measurement of magnetically induced particle transport (Stoneking 1994, Ding 2007) and energy transport (Fiksel 1994)
- Where probes can be used, they provide measurements unavailable by other diagnostics

Synthetic Diagnostics Enable More Direct Comparisons

- Validation requires comparison of identical quantities
  - Diagnostics often can't make local measurements of fundamental quantities
  - Inverting the data may be impossible or may introduce artifacts
- To help with this problem, synthetic diagnostics have been developed as post-processors for many codes
- The synthetic diagnostic attempts to replicate, numerically, the physical processes and geometry along with any temporal or spectral averaging – essentially an exercise in phase-space geometry.
  - Comparison between the synthetic diagnostic and data is direct (but at a cost - some power of discrimination may be lost)
  - Thorough and careful characterization of diagnostic is required.
  - The synthetic diagnostic code may be quite complex and must be carefully tested.

Synthetic Diagnostics Example

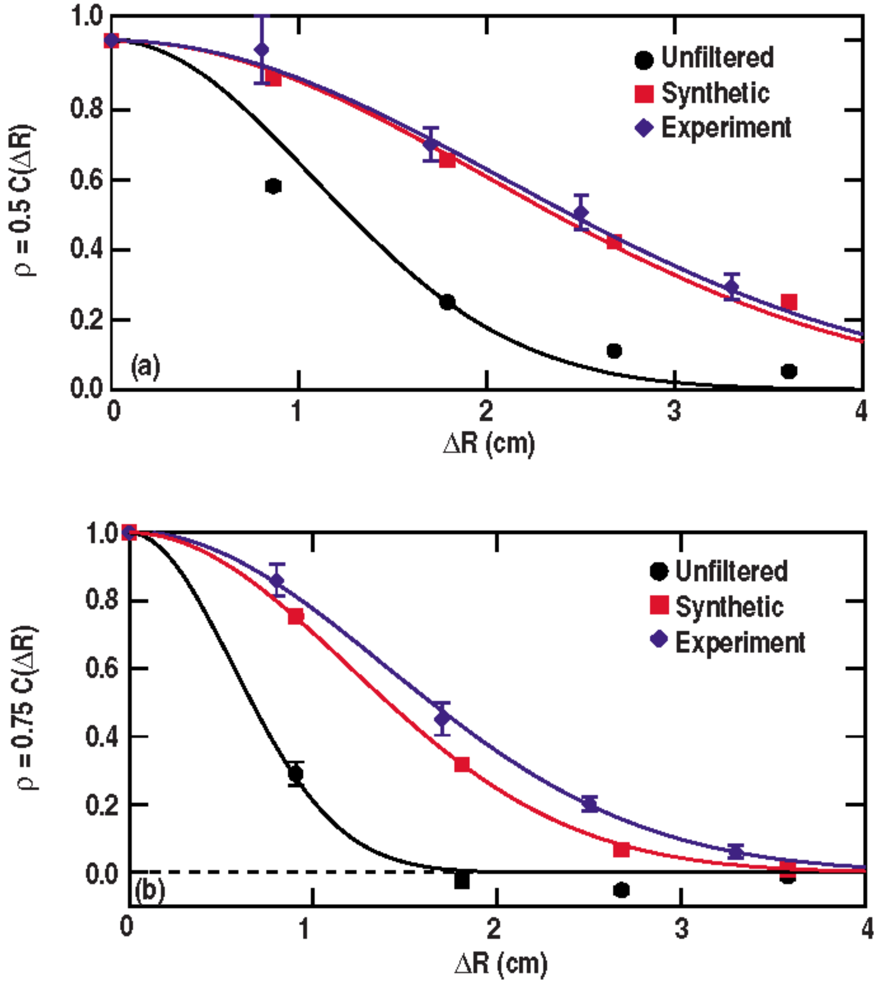


FIG. 12. (Color online) Comparison of density fluctuation radial correlation functions calculated for the unfiltered GYRO data (●), the synthetic BES data (■), and experimental data (♦) at (a) $\rho = 0.5$ and (b) 0.75.

- Comparison of radial correlation of density fluctuations
- Proper treatment of diagnostic resolution brings simulation into reasonable agreement with experiment.
- *From Holland et. al. PoP 2009*

UQ - Quantitative Analysis, Data Quality and Sources of Error and Uncertainty

- Validation requires careful **quantitative** consideration of uncertainties and errors in both experiments and simulations
- Some simulation codes - GK PIC codes in particular - are so compute intensive that “ensemble” computing to estimate parameter sensitivity and overall uncertainties are prohibitive.
- Sources of errors in experiments – systematic and random (reducible and irreducible)
  - Statistical or counting errors
  - Calibration errors
  - Electronic noise and data acquisition errors
  - Differences arising from temporal or spatial averaging
  - **Conceptual errors with measurement techniques**
  - **Data reduction errors**

UQ: Estimation of "Experimental" Quantities Is Often Model Dependent Itself

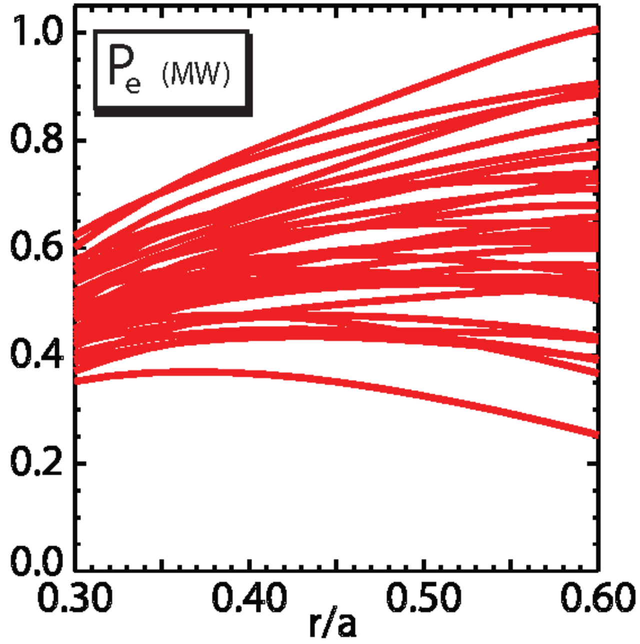
This seems to be a particular challenge for plasma fusion, where needed experimental quantities are derived with :

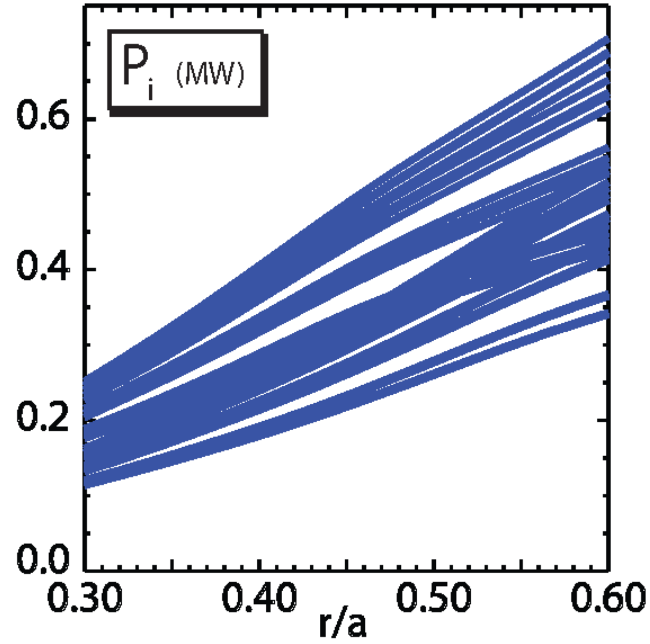
- Important quantities, for example heat flux or impurity profiles, are derived from raw measurements using complex physics codes
  - (and even simple quantities like gradients depend on fitting models)
- For example
  - Heat flux usually computed by TRANSP
  - Impurity profiles, transport coefficients, etc. via STRAHL
- We're beginning to apply formal UQ methodology to extraction of derived quantities

UQ: TRANSP Calculation of Heat Fluxes

- TRANSP - ~2,000,000 lines of code, running time = 30 min-4 weeks
- Includes physics for power input (OH, ICRF), losses (Radiation, CX), electron-ion equilibration
- Run ensemble of cases, varying inputs

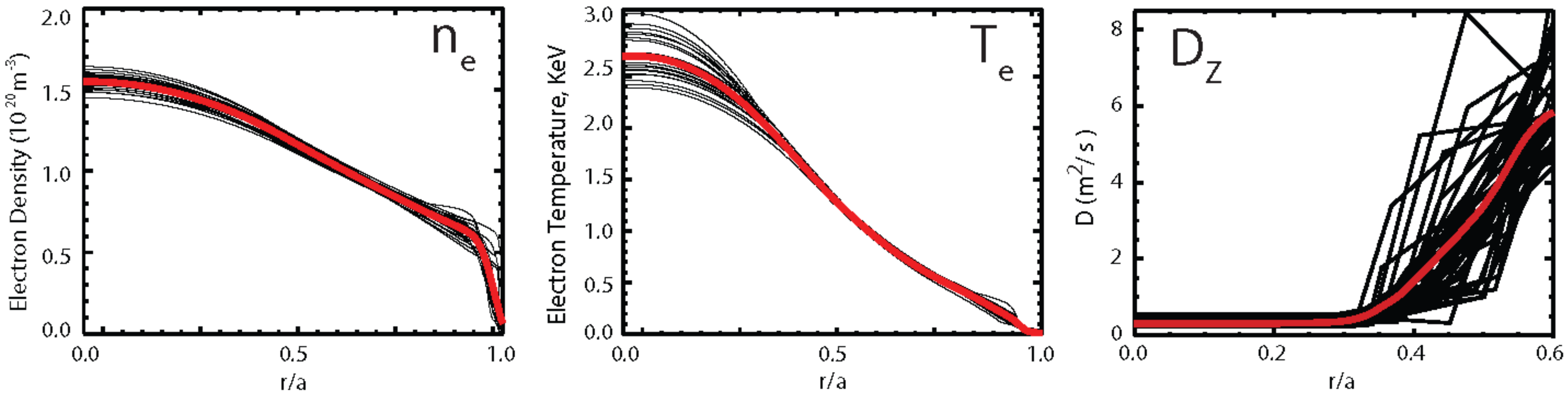
  - $\delta n_e = \pm 10\%$
  - $\delta T_e = \pm 10\%$
  - $\delta T_i = \pm 10\%$
  - $\delta Z_{EFF} = \pm 20\%$
  - $\delta f_{ICRF} = \pm 10\%$





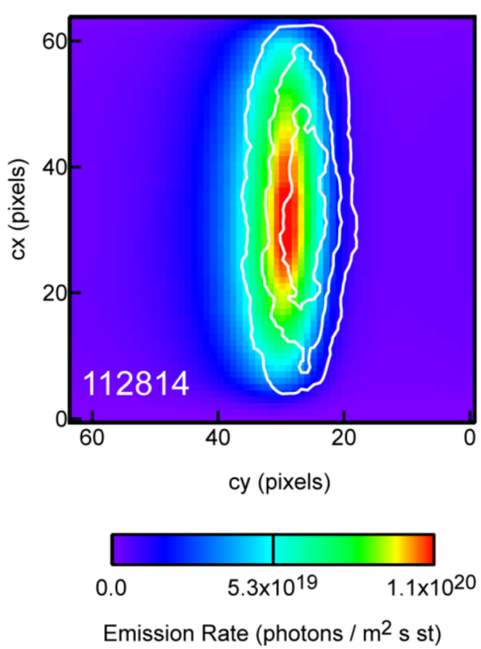
UQ: STRAHL Used To Compute Impurity Transport

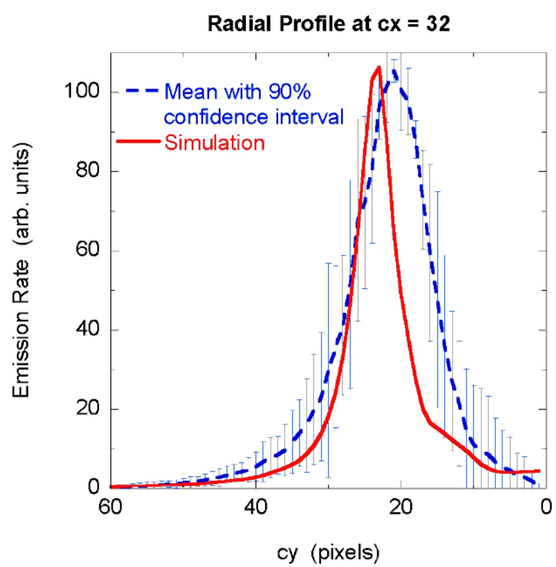
- STRAHL computes impurity profiles for all ionization states based on ADAS atomic physics data and assumed D, V transport profiles
  - We then carry out a carry out a minimization procedure, comparing computed brightnesses with spectroscopic profiles (x-rays)
- The atomic physics imposes a strong sensitivity to plasma T_e and n_e
  - Compute for an ensemble of profiles, then estimate errors

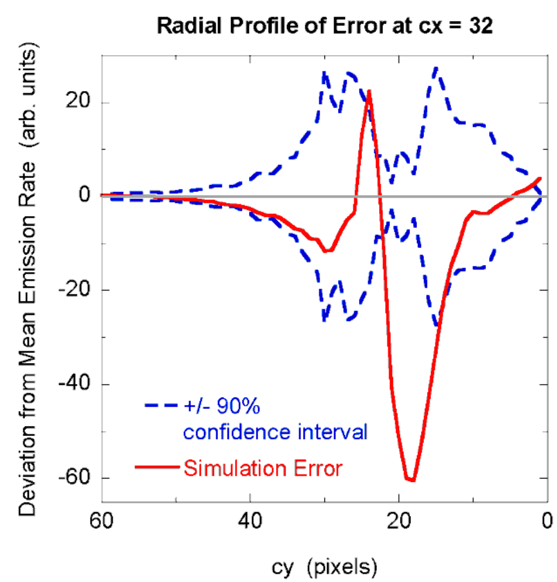


A Few Words About Graphical Methods

- We've stressed here quantitative techniques – the "vugraph norm" is often deprecated in discussion of validation
- However, the power of good graphical techniques should not be underestimated – especially for data exploration.
- The best practice probably combines both approaches
- Example:

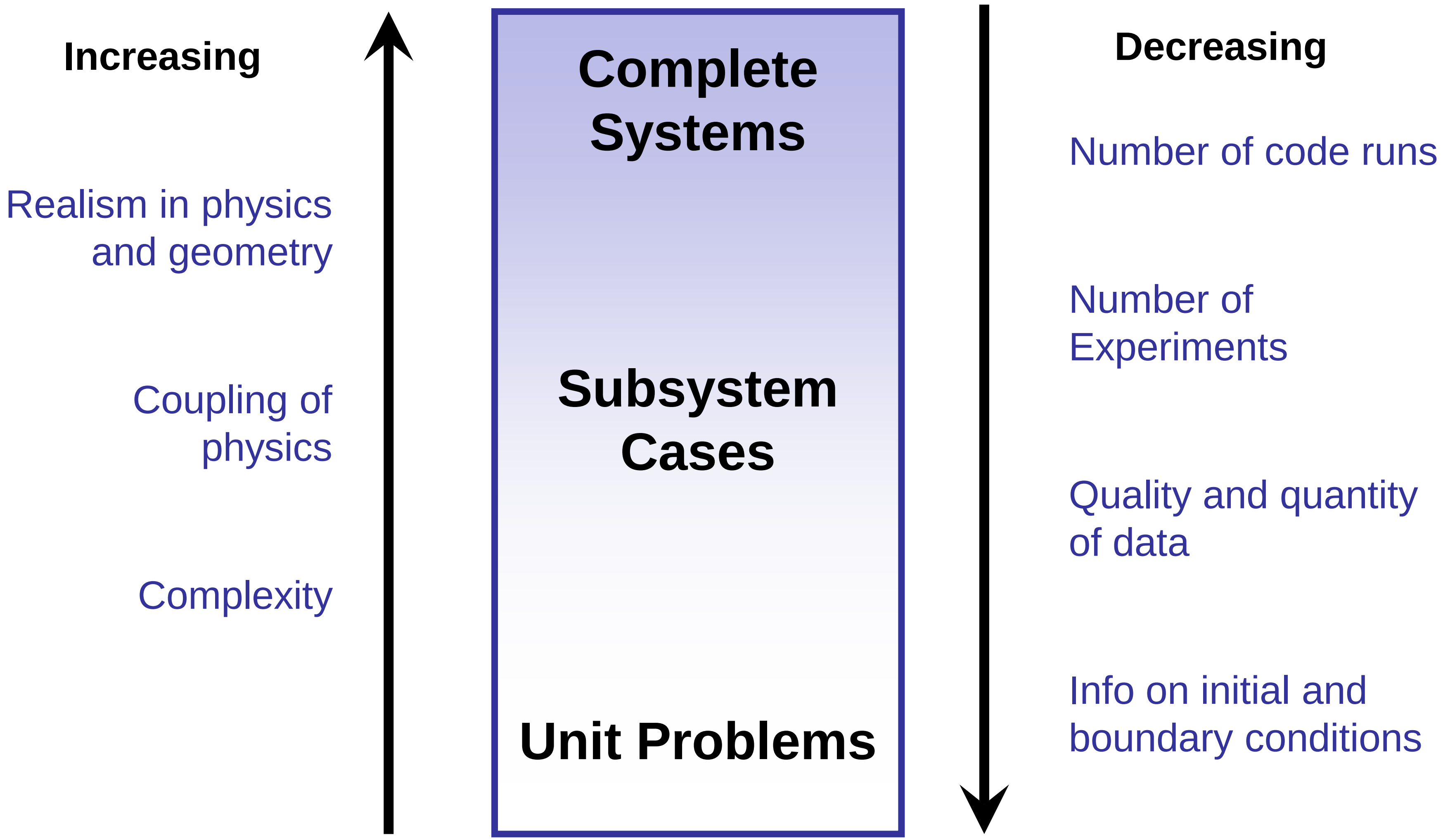






Stotler TTF 2007

Validation Hierarchy – The Principle



Validation Hierarchy For Fusion Experiments

- A good deal of linear theory was validated decades ago on linear plasma machines
- However, for nonlinear or strongly coupled physics, true “unit” problems are hard to come by in our domain
  - Simpler geometry – often leads to degraded confinement, cold ions, larger neutral effects
  - Simpler magnetic topologies – can lead to line tying, greater importance of sheaths, change in connection length, etc.
  - Scale reduction – different ρ^*, ν^* can cause different physics to dominate
- Limitations must be dealt with in experimental design
  - Make unwanted effects smaller or less critical
  - Focus on physics that is less sensitive to unwanted effect

Is There a Special Role for EPR Experiments?

- Progress could be accelerated with experiments that:
  - Simplify or vary the magnetic geometry
  - Have key parameters in regimes of simpler physics (e.g. fluid vs kinetic)
  - Integrate fewer disparate effects
  - Freeze quantities that vary in other experiments
  - Allow enhanced diagnostic access (e.g. probes accessible because of lower plasma pressure or shorter discharge time)
- Obstacles?
  - Completeness of diagnostics
  - Codes not available for relevant geometry or regime

State of the Art Codes Are Becoming Available For Wider Range of Magnetic Geometries

A few examples:

- NIMROD (nonlinear, extended MHD) has been applied to Tokamaks, RFPs, FRCs, Spheromaks, Stellarators, Dipoles among others
- Fluid turbulence codes (BOUT/BOUT++, GBS, ESEL, SOLT, CYTO, NLD, TORB) have been written and/or applied for both toroidal and linear machines
- Nonlinear gyrokinetic turbulence continuum code gs2 has been adapted for linear devices
- Same for several nonlinear GK PIC codes
- The amount of effort varies, but is often carried out as part of student thesis work

Collaborations Between "Main-line", EPR and Basic Experiments Could Yield Important New Results

Cross cutting physics include:

- Fluid or GK turbulence at or near plasma boundary
- Plasma-Wall interactions
- Reconnection
- 3D physics
- Role of magnetic fluctuations (break 2D geometry)
- RF-edge plasma interactions
  - RF sheath production
  - Non-linear process (e.g. PDI)

Summary

- Despite dramatic advances in computational plasma physics, we are still far from solving the critical problems.
- **Validation can provide a framework for carrying out the collaboration between simulation and experiments in a methodical and systematic way – to the benefit of both**
- This will require new modes of interaction – openness about uncertainties, errors and limitations of methods is essential
- The technical challenges, some particular to fusion experiments, must be overcome, but in most cases there are paths forward
- EPR experiments can play a unique role if they can commit the resources

Bibliography 1

N.T. Howard, M. Greenwald, D.R. Mikkelsen, M.L. Reinke, A.E. White, D. Ernst, Y. Podpaly and J. Candy, *"Quantitative Comparison of Impurity Transport Measurement and Nonlinear Gyrokinetic Simulation in an Alcator C-Mod L-Mode Plasma"*, Nucl. Fusion 52, 063002(2012)

P. Ricci, C. Theiler, A. Fasoli, I. Furno, K. Gustafson, D. Iraji, and J. Loizu, *"Methodology for turbulence code validation: Quantification of simulation-experiment agreement and application to the TORPEX experiment"*,Phys. Plasmas 18, 032109 (2011)

M. Greenwald, *"Tutorial: Verification and validation for magnetic fusion"*, Phys. Plasmas 17, 058101, 2010.

Oberkampf, W.L. and C. J. Roy (2010), Verification and Validation in Scientific Computing, Cambridge University Press, Cambridge, UK.

C. Holland, A. E. White, G. R. McKee, M. W. Shafer, J. Candy, R. E. Waltz, L. Schmitz, and G. R. Tynan, *"Implementation and application of two synthetic diagnostics for validating simulations of core tokamak turbulence*", Phys. Plasmas 16, 052301 (2009)

A. E. White, L. Schmitz, G. R. McKee, C. Holland, W. A. Peebles, T. A. Carter, M. W. Shafer, et al., *"Measurements of core electron temperature and density fluctuations in DIII-D and comparison to nonlinear gyrokinetic simulations* ", Phys. Plasmas 15, 056116 (2008)

Bibliography 2

J. Weathers, R. Taylor, J. Weathers, "Computational Fluid Dynamics Simulation of a Mesoscale Combuster: An Exercise in Verification and Validation" J. of Thermal Science and Eng. Applications **1**, 011008-1, 2009

P.W. Terry et al., *"Validation In Fusion Research: Towards Guidelines And Best Practices"*, Physics of Plasmas **15**, 062503, 2008

W. Oberkampf and T. Trucano, *"Verification and Validation Benchmarks",* Nuclear Eng. And Design **238**, 716, 2008

L. Schwer, *"Validation metrics for response histories: perspectives and case studies"*, Engineering with Computers **23**, 295, 2007

W.L. Oberkampf and M.F. Barone, *"Measures Of Agreement Between Computation And Experiment: Validation Metrics",* J. Comp. Phys. **217**, 5 2006.

M. Greenwald, "*Beyond Benchmarking – How Experiments and Simulations Can Work Together in Plasma Physics*" Computer Physics Communications, **164**, 1-8, 2004.

Bibliography 3

T. Trucano, M. Pilch, W. Oberkampf, *“On The Role Of Code Comparisons In Verification And Validation”* Sandia Report SAND2003-2752, 2003

W.L. Oberkampf and T.G. Trucano, “*Verification And Validation In Computational Fluid Dynamics*”, Progress Aerospace Sci **38**, 209 2002.

T. Trucano, M. Pilch, W. Oberkampf, *“General Concepts For Experimental Validation Of Asci Code Applications”* Sandia report SAND2002-0341, 2002

B. Thacker, et al., “*Concepts Of Model Verification And Validation*” Los Alamos Report LA-14167-MS 2002

R. Sargent *“Some Approaches And Paradigms For Verifying And Validating Simulation Models”,* Proceedings of the 2001 Winter Simulation Conference, B.A. Peters editor.

W. Oberkampf in “*Verification and Validation of Computational Fluid Dynamics*”, F. Grasso, J. Perlaux, H. Deconinck editors, von Karman Institute for Fluid Dynamics publishers, Belgium, (2000).

D.P. Aeschliman and W.L. Oberkamf, AIAA Journal **36**, (1998), pp. 733.

Bibliography 4

Rizzi, J. Vos, *"Towards Establishing Credibility In CFD Simulations"* AIAA Journal **36**, (1998), pp. 668.

Roache, P. J. *Verification and Validation in Computational Science and Engineering*, Hermosa Publishers, Albuquerque, NM. (1998)

Schlesinger S. et al., *Terminology for model credibility*, Simulation **32**(3), 103–104 (1979).