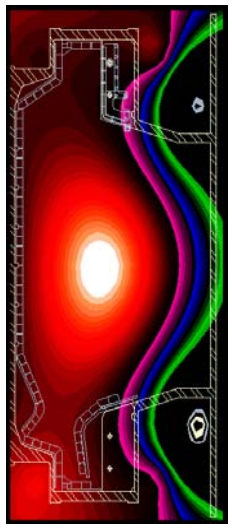
BEYOND BENCHMARKING: HOW EXPERIMENTS AND SIMULATIONS CAN WORK TOGETHER IN PLASMA PHYSICS



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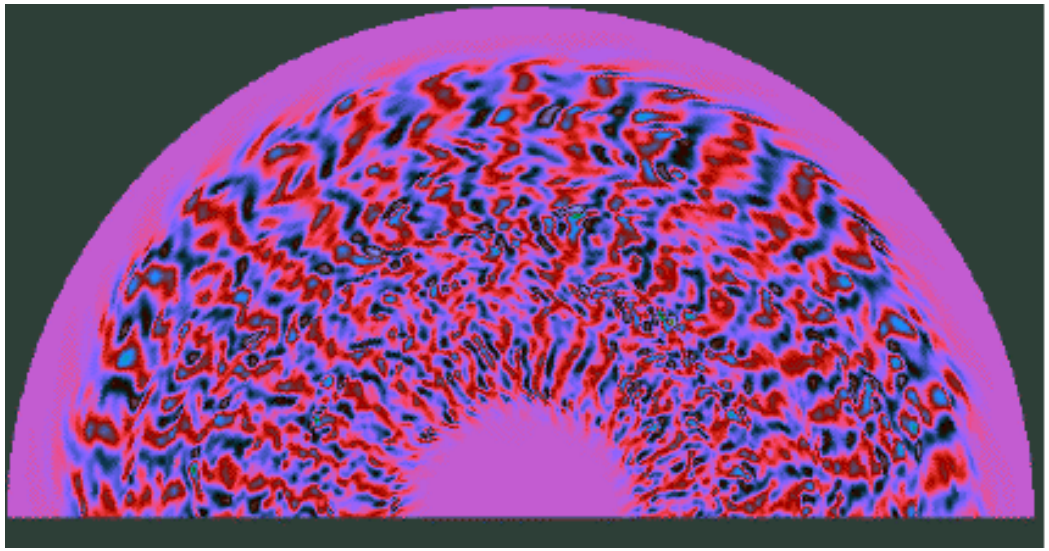
OUTLINE

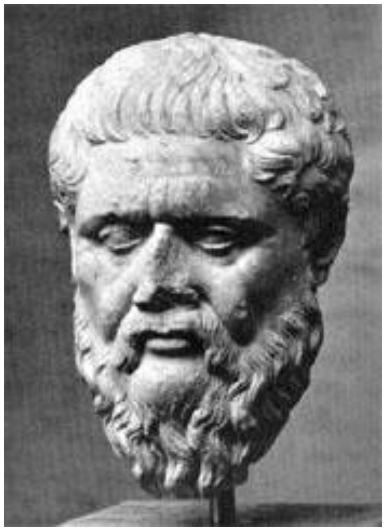
- Talk will be a combination of philosophic and practical issues
- Then examples, case studies
- Ideas for principles and practice
- Then discussion on how we could do things better

- This will be an experimentalist's view (from MFE).
- I won't make a sharp distinction between theory and computation
    - Simulation: an extension of theory by other means

BACKGROUND AND INTRODUCTION

- Dramatic advances in scope and power of numerical simulation
  - Advances in science/theory
  - Better algorithms
  - Moore's law
- But "virtual reality" from simulations is nowhere in sight.
- Computer "experiments" are a useful concept but shouldn't be confused with the real thing.
- Anticipate an ongoing collaboration.





Historical Note

Theory/modeling/experiments as distinguishable but mutually dependent activities have an important place in the history of philosophy and science.

Rationalism – logical development of a model based on indisputable axioms – pure logic

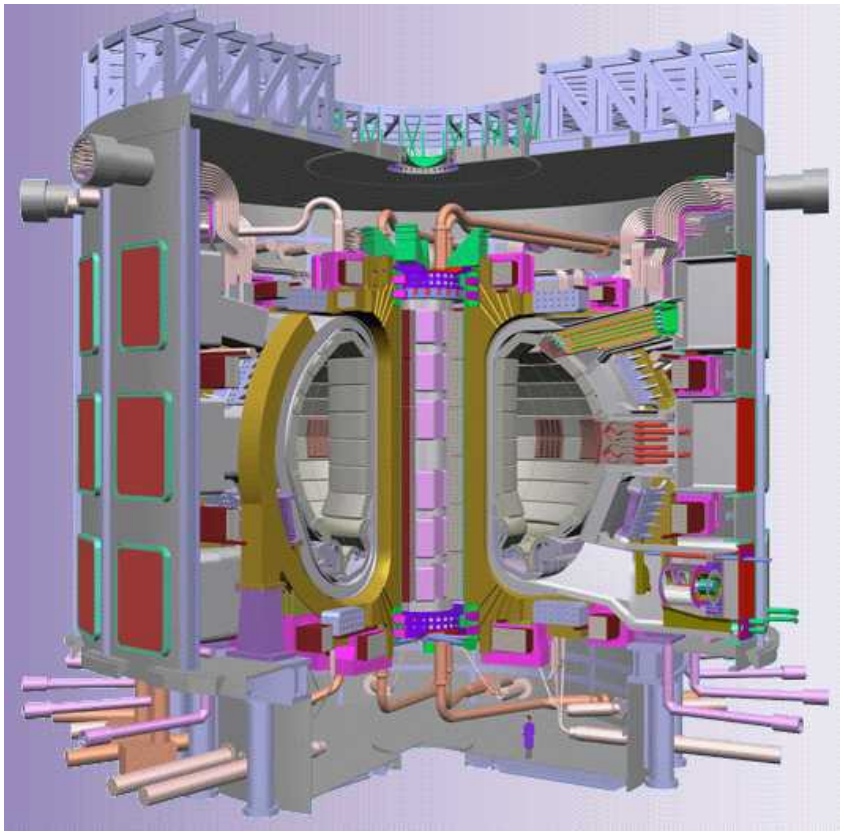
(knowledge gained through the senses is always confused and impure)

Empiricism – requires that every axiom, deduction, assumption or outcome be empirically confirmed

(only trust knowledge gained through the senses)

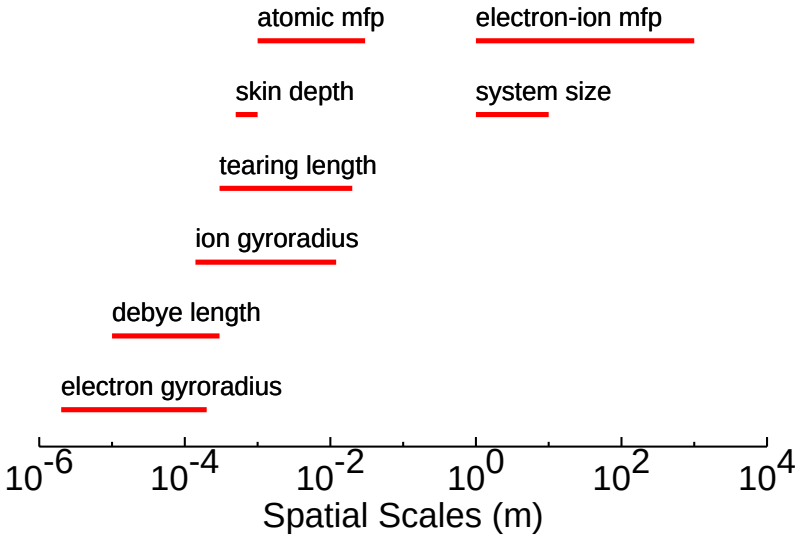
THEORY/SIMULATIONS ESSENTIAL FOR PREDICTION

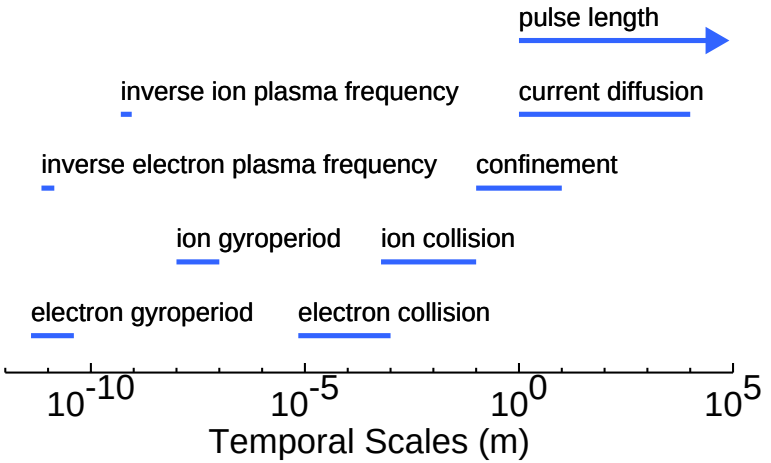
- Prediction
  - demonstrates fundamental understanding
  - design and/or optimization of new experiments or devices
  - operational support
- Predictive capability from purely statistical analysis of data (eg scaling laws) is not sufficient.
- For FES, prediction is embodied in programmatic goals
  - Snowmass I
  - IPPA (Integrated Program Planning Activity)
  - FESAC/DOE/OMB



PLASMA THEORY IS A FORMIDABLE CHALLENGE

- Theoretical problem is not tractable in straightforward manner
  - disparate time and spatial scales
  - extreme anisotropy
  - complex geometry
  - essential non-linearity
- instead
  - "obtain exact solutions to approximate equations" or
  - "approximate solutions to exact equations"
- this will be true for foreseeable future





Experiments and Computation Have Complementary Roles and Strengths

Theory/Simulation

- provides predictive capability and fundamental understanding

with

- near perfect diagnostics
- high degree of flexibility - computer "experiments"
- often cheaper and faster

but

- imperfect models or solutions

Experiments

- test theory/models/codes
- extend performance (fusion)
- discovery

with

- "perfect" model (reality)

but

- highly incomplete and imperfect measurements
- lower degree of flexibility

WE NEED TO STRENGTHEN MODES OF COLLABORATION

- Requires that both (all three) sides recognize that they are incomplete and insufficient by themselves

- Cooperation should permeate scientific process
  - Mutual identification of interesting or important phenomena
  - Validation of basic physical model
  - Validation of particular codes and calculations
  - Iteration and Co-development

- The benefits
  - For computationalists, experiments are the contact to physical reality
  - For experimentalists, more comprehensive involvement in scientific process

BOTTOM LINE

- Theory, simulation and experiments are complementary rather than competitive
- Scientific progress requires co-development involving all approaches
- not one-time benchmark exercise
- All needed for any foreseeable future

We all have ample reason to remain humble

"The greatest disaster one can encounter in computation is not instability or lack of convergence but results that are simultaneously good enough to be believable but bad enough to cause trouble" (Ferziger)

"No one believes the CFD results except the one who performed the calculation, and everyone believes the experimental results except the ones who performed the experiment." (Saying in aerodynamics community)

SYNERGIES

Codes

- Define critical experiments and diagnostics
- Help identify the critical physics in a given experiment
- Can explain long standing observations which are not consistent with simpler theories
- Can identify measurable quantities which are “proxies” for more fundamental but unmeasurable ones

Experiments

- Motivate development of physical models
- By accessing increasingly complex physics or geometry may be used to guide codes in their development
- Identify problems and confirm success
- Can search for phenomena predicted but as yet not observed
- Can be used to ‘calibrate’ models

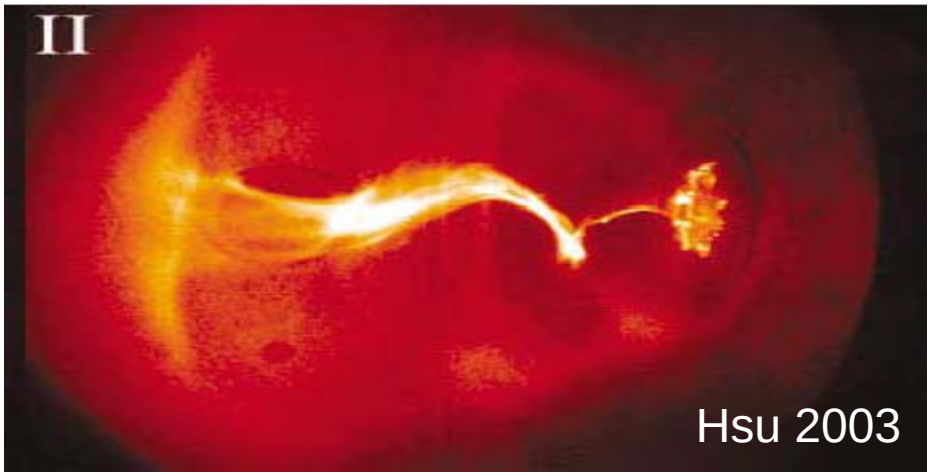
CASE STUDIES

HOW DOES THIS WORK OUT IN PRACTICE?

Research is most effective when theory, computation and experiments work closely together in an iterative process.

Examples

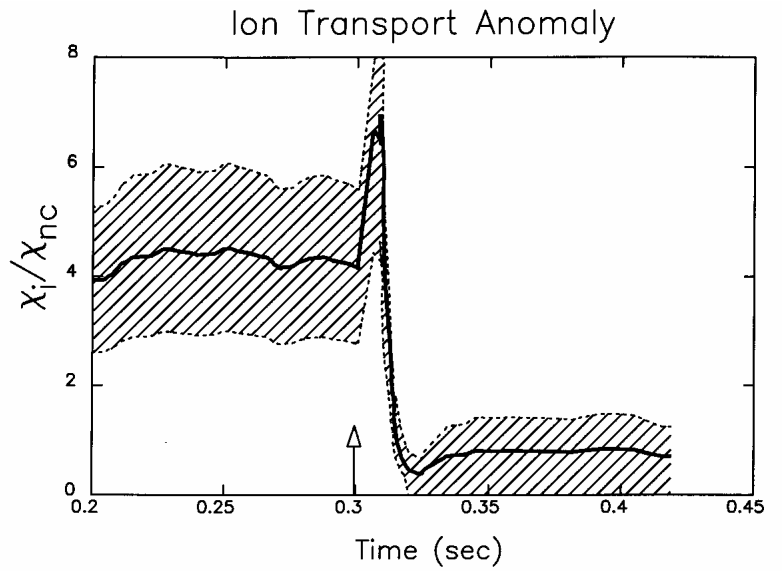
- MHD equilibrium and stability – theory and codes stimulated by dramatic instability of early experiments

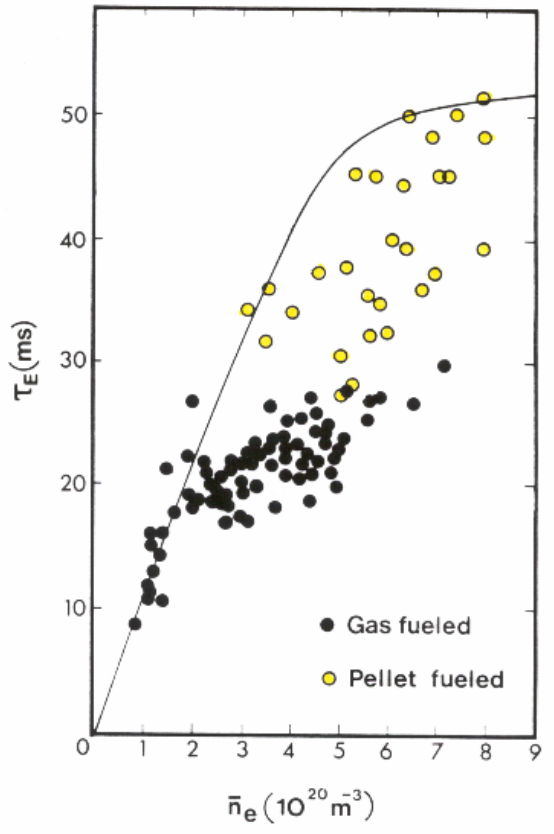


- η_i modes/ITG turbulence - example of prediction driving experiment
- Edge turbulence – pushing research into new directions
- ARM – experiment designed explicitly to provide inputs for code

η_i MODES/ITG TURBULENCE – PREDICTIONS DRIVE EXPERIMENTS

- Energy confinement time seen to scale with density (1976) then saturate – density profiles flat (1980-1982)
- Predictions from η_i calculations (slab) predicted ion turbulence could be stabilized with more peaked density profiles.

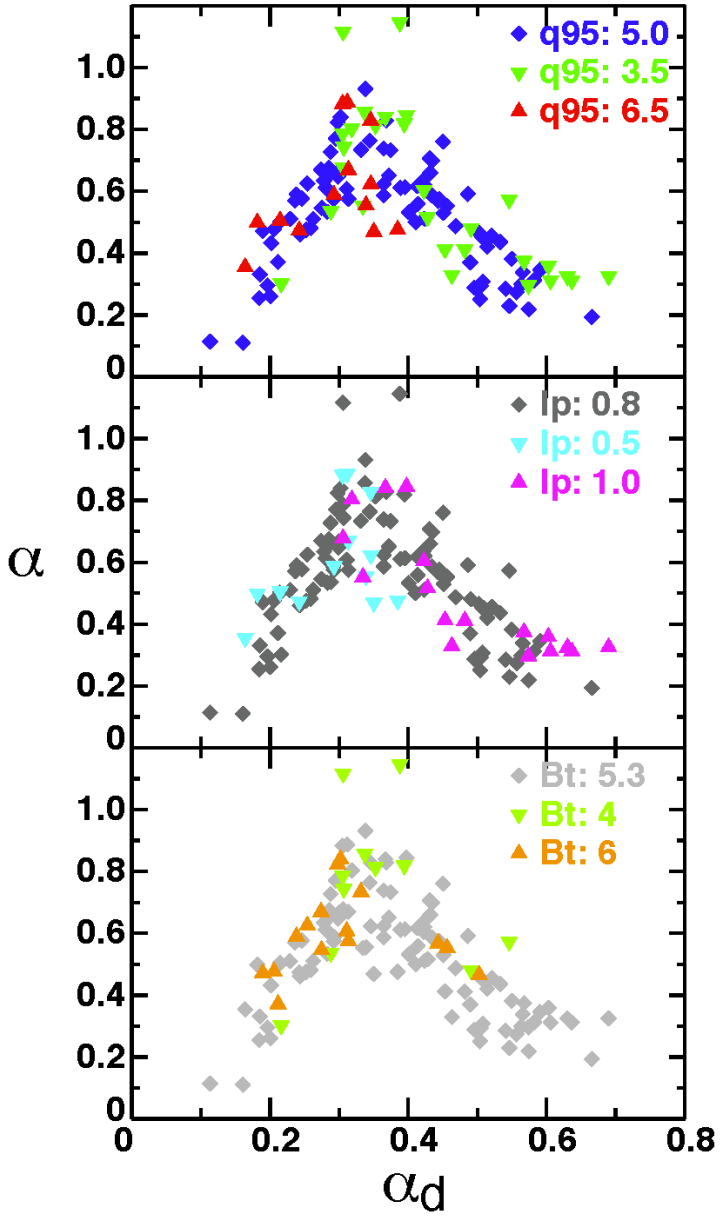




- Pellet injector built, experiments carried out
- Results – improved confinement, Lawson number reached, new regime (1983)

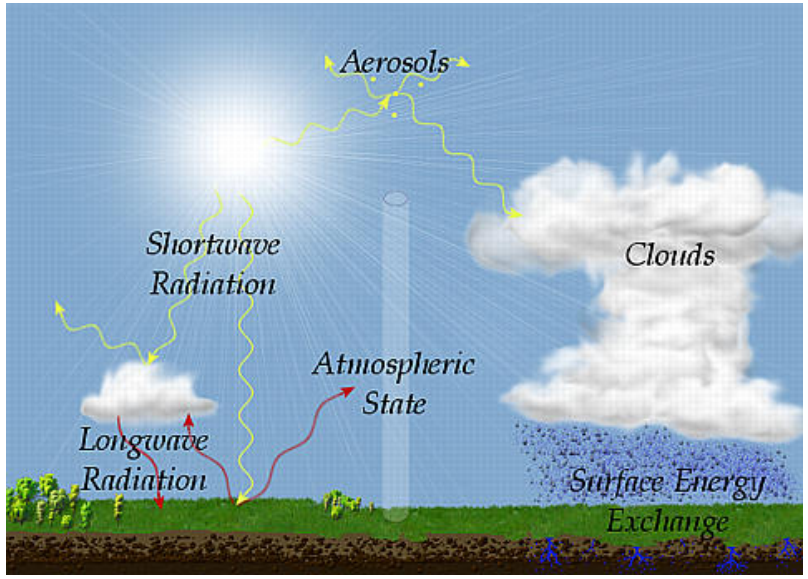
EDGE TRANSPORT AND MODELING

- Lots of sophisticated modeling - UEDGE, DEGAS, B2, EIRENE, etc.
  - Parallel physics, radiation and neutrals well treated, naïve models for perpendicular transport.
- At the same time, lots of measurements of edge fluctuations and profiles
- Evolving simulations of edge turbulence (Rogers, Drake, Zeiler, Scott, Xu, Nevins, Hallatschek, etc.)
- Bringing these threads together is leading to new understanding
  - L/H transition
  - neutral and impurity sources
  - density limit



ARM (Atmospheric Radiation Measurement)

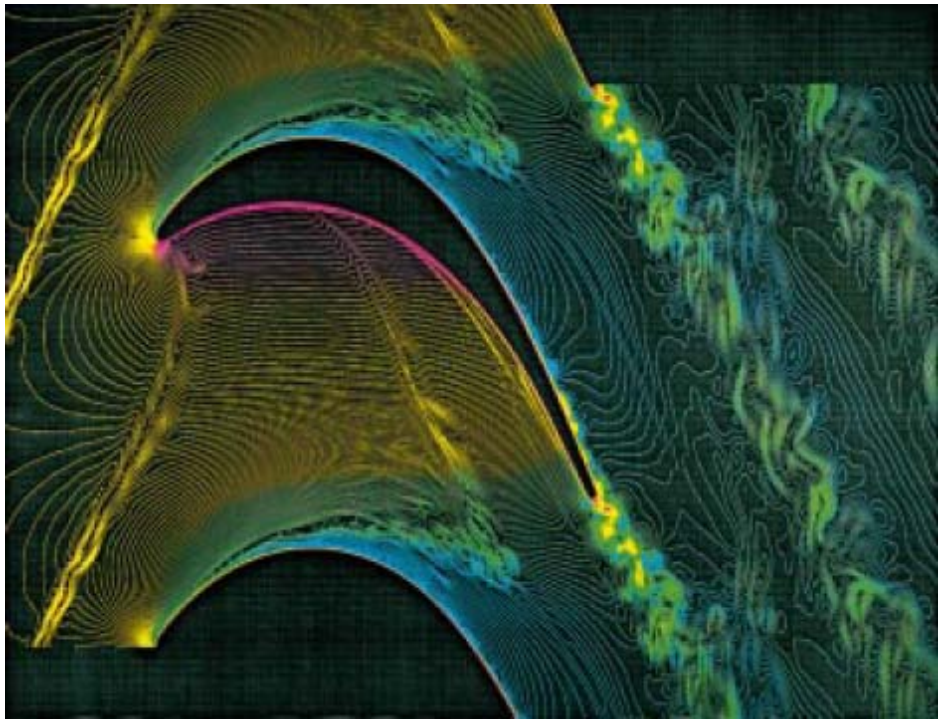
- Almost uniquely, a large-scale experiment was designed in direct response to needs of simulation community
- During 70's, 80's powerful climate modeling codes developed and tested
- Disconcertingly, predictions varied dramatically
- Key issue/difference was treatment of clouds and radiative heat transfer
- About 10 years ago, ARM program initiated
  - Learn as much as possible about interaction between clouds and radiative heat flux
  - Embody that knowledge in simulation codes



LESSONS FROM CFD (COMPUTATIONAL FLUID DYNAMICS)

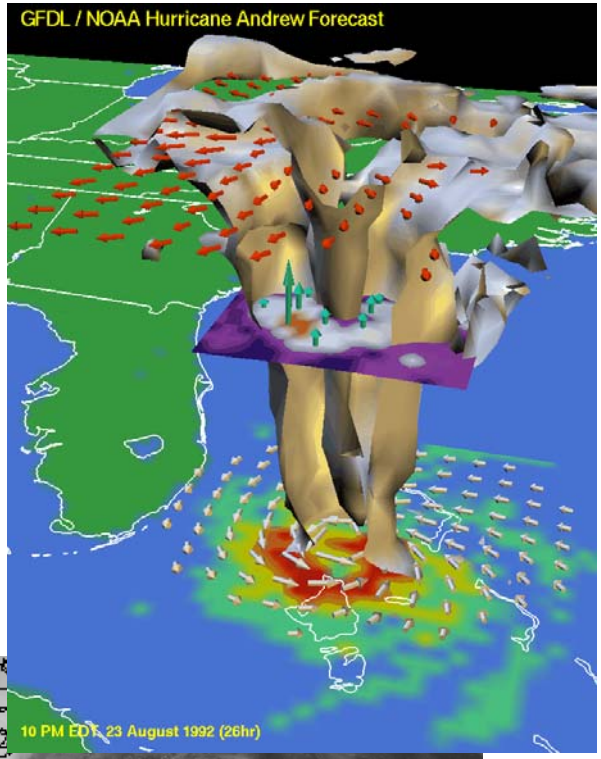
- Physics has many similarities to ours

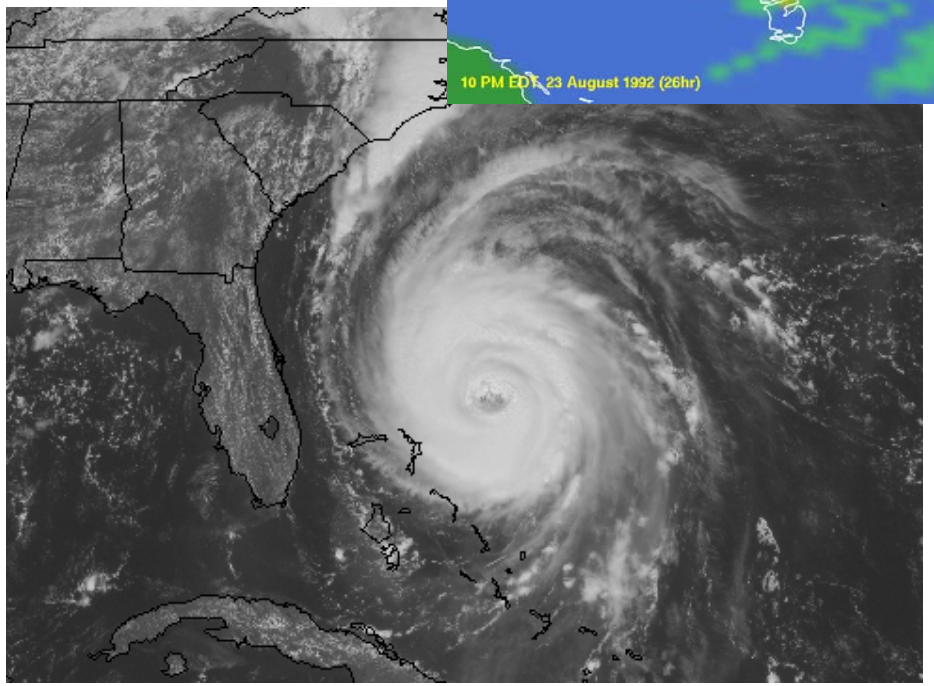
- Applications:
  - Airplane, automobile, ship design
  - Architecture
  - Turbomachinery
  - Noise reduction
  - Weather
  - Air and water cooling
  - Acoustics/noise
  - Pollution effects/dispersal – air, land and water



ACCURACY AND RELIABILITY OF CODES HAVE IMPORTANT CONSEQUENCES

- Impacts
  - safety
  - economic
  - environmental
  - legal
- Tests of code reliability can be part of regulatory scheme



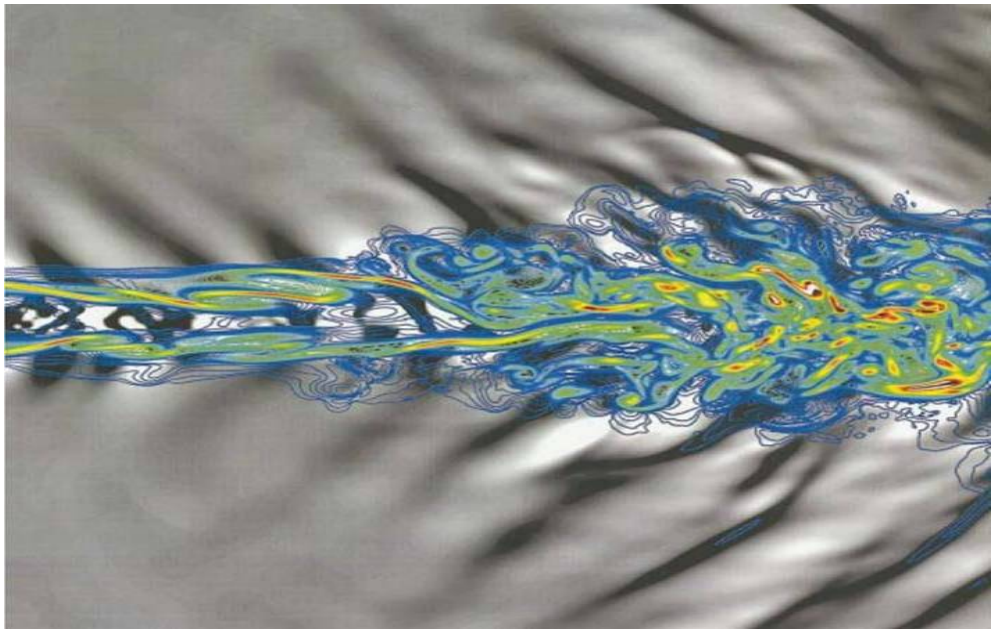


Realistic Fluid Simulations Require Significant Approximations to Navier-Stokes Equations

- DNS – Direct Numerical Simulation
  - Limited to low (typically non-physical) Reynolds numbers
  - Boundary conditions (walls) problematic
  - Not used for many realistic problems

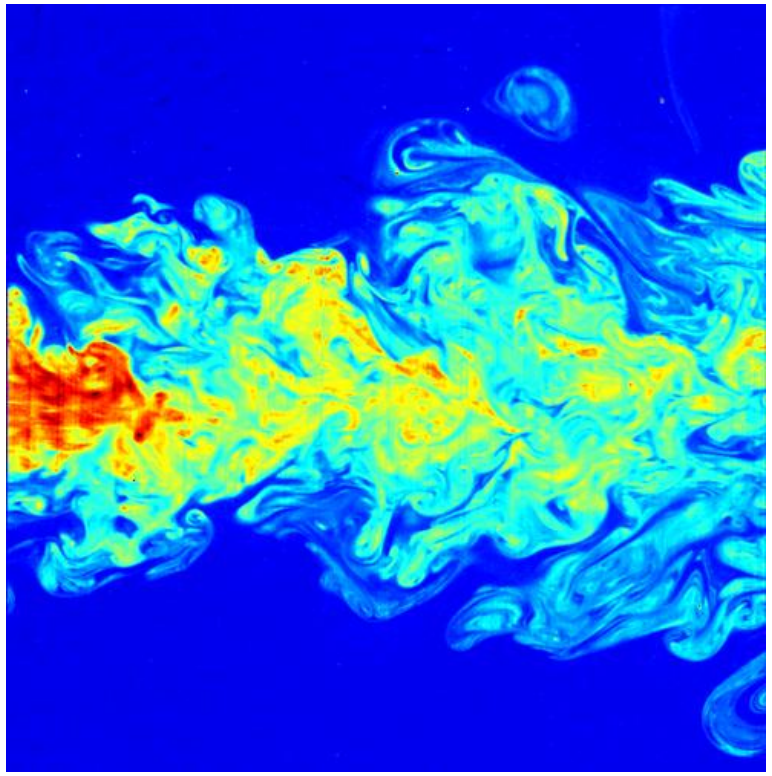
- RANS – Reynold's Averaged Navier-Stokes
  - Fine structure averaged over, leaving equations for fluctuation amplitude and transport

- LES – Large Eddy Simulation
  - Treat large eddies by direct simulation
  - Use averaging for smaller scales



CFD Researchers Have Had to Confront Reliability Issues

- Origins early in 20th century *(Richardson 1910)*, accelerated dramatically in 60's with advent of powerful (and usable) computers
- "Computer Experiments in Fluid Dynamics" *(Harlow and Fromm, Sci Am 1965)*
- Demise of wind tunnels predicted *(Chapman, Mark and Pirtle 1975)* (Assertion vigorously challenged at time)
- Stanford turbulence olympics *1981*
    - o "quality of the solutions was so poor that it was impossible to draw meaningful conclusions about the relative merits of the various models"



- Limitations on simulations and their complexity led to formalism for verification and validation of codes – embodied in editorial policies of leading journals
- Despite improvements in computing beyond those assumed by CM&P, talk of simulation approach "supplanting" experiments has effectively ceased.

VERIFICATION – "SOLVING THE EQUATIONS RIGHT"

"Verification: substantiation that a computerized model represents a conceptual model within specified limits of accuracy" (Schlesinger 79)

- Essentially a mathematical problem
- Possible sources of error
  - algorithms,
  - numerics,
  - spatial or temporal gridding,
  - coding errors,
  - language or compiler bugs,
  - convergence difficulties
- Methodology
  - Theory to code comparisons
  - Formal convergence tests
  - Code to code comparisons
- Logically should precede validation

VALIDATION – "SOLVING THE RIGHT EQUATIONS

"Validation: substantiation that a computerized model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model" *(Schlesinger 79)*

- Essentially a physical problem
- No clearly defined end point - ongoing activity.
- Verification and validation – "confidence building activities"
- Overall, the goal of validation and verification is an assessment of the extent to which a simulation represents true system behavior sufficiently to be useful.

CONDITIONAL NATURE OF VALIDATION

- No absolute or unambiguous meaning to validation
- At best, validity is defined
  1. for a class of nearby problems
  2. for a set of specified variables
  3. at a specified level of accuracy

note on 1. "nearby" hard to define – transition boundaries crucial.

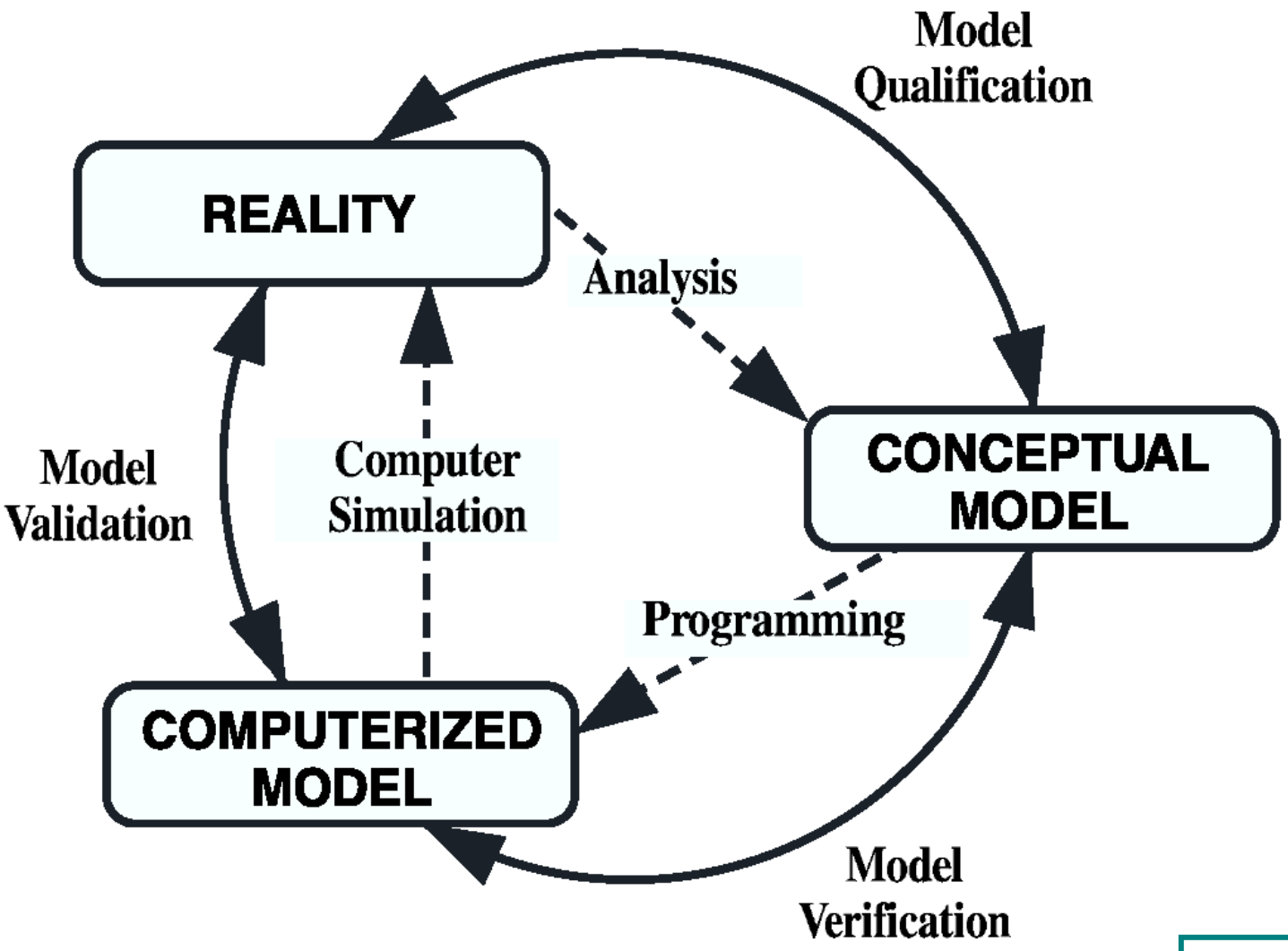
note on 2. This is especially true if these variable are on very different spatial or temporal scales. Example – predicting gradients vs predicting turbulence and dynamics.

note on 3. what defines "agreement"? - depends on end use of calculation

VALIDATION OF A MODEL VS CODE OR CALCULATION

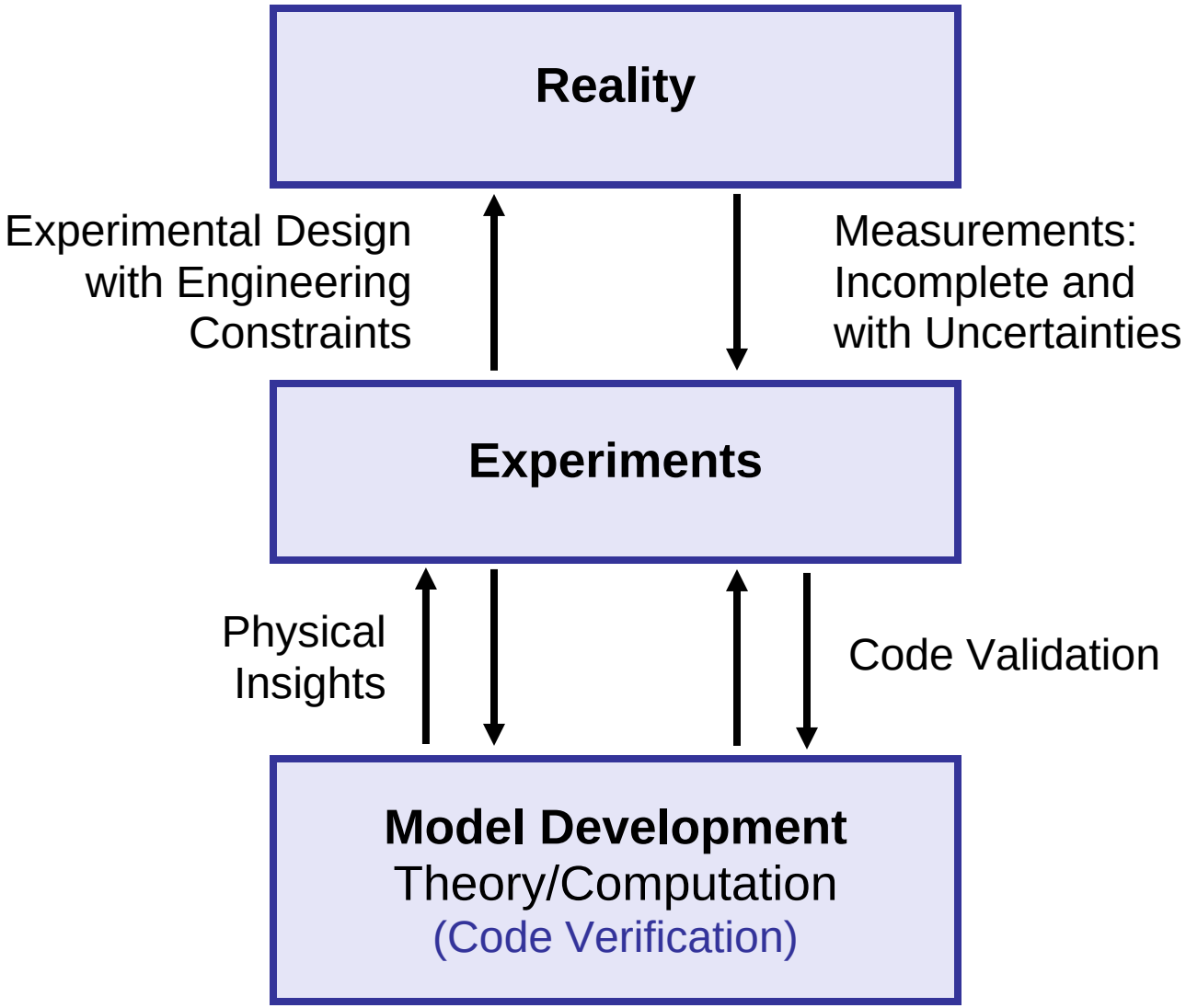
- Model Validation: Basic affirmation that the important physical principles have been identified and characterized
- Still leaves problems with sensitivity to boundary conditions, initial conditions, geometry, intermittency/time averaging, etc. which are critical for a predicting a particular outcome.
- For the latter, much greater attention to errors and statistics are necessary.
- As before, nature of validation depends on end use.

VARIOUS AUTHORS HAVE ATTEMPTED TO SHOW THESE RELATIONSHIPS GRAPHICALLY



Schlesinger

EXPERIMENTS ARE THE INTERMEDIARY WITH REALITY



MEASUREMENTS AND PREDICTIONS MAY NOT AGREE FOR A NUMBER OF REASONS

- Validation will "fail" due to:
  - numerical solution errors due to discretization, initial or boundary conditions
  - measurement errors and scarcity
  - formulation errors – missing or incorrect physics
- Clearly this last point is the critical one – try to eliminate the others
- Assessment of trends may be more important than quantitative comparisons
  - typically repeatability better than absolute accuracy

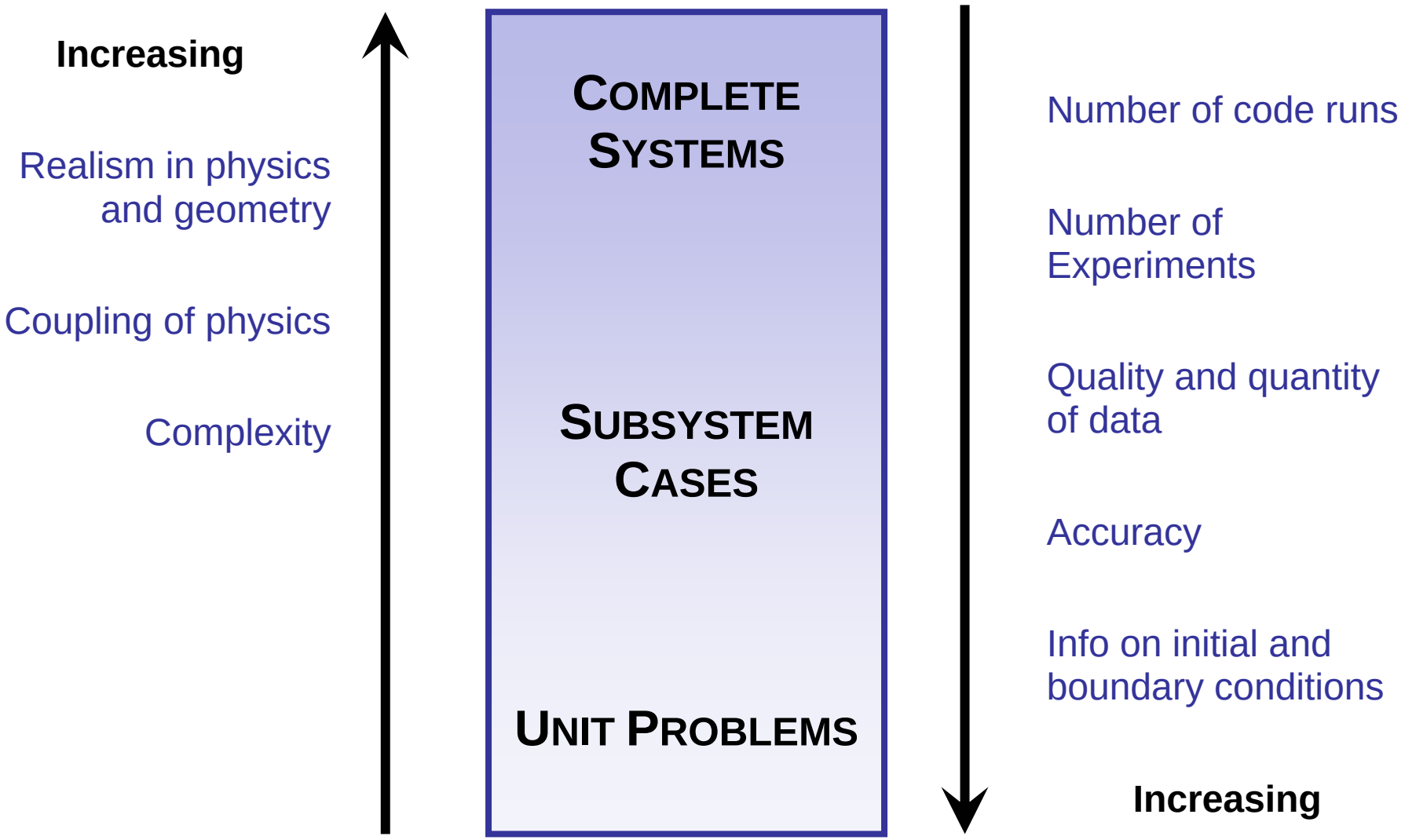
Sources of error in experiments – validation errors

- conceptual errors with measurement technique
- differences arising from temporal or spatial averaging
- statistical or counting errors
- calibration errors
- electronic noise and data acquisition errors
- data reduction errors

PHASES OF VALIDATION - CO-DEVELOPMENT

- Begins during code development stage
  - Perform small-scale, well diagnosed experiments dedicated to purpose
  - Validate building blocks
  - Isolate features and physics as much as possible
  - (Comparison to analytic solutions may be possible at this stage)
- Move to more complex systems and geometries as experience and confidence is gained
  - Complexity increases and data availability and accuracy decreases through the progression
- Final tests involve full scale experiments and simulations

VALIDATION HIERARCHY



PRINCIPLES - DESIGN AND EXECUTION OF VALIDATION EXPERIMENTS (1)

1) Verify codes first.

2) Plan a hierarchy of experiments beginning with the simplest physics and geometry.

3) Conduct dedicated experiments – not enough to mine archives
   - Older Data is usually incomplete, not sufficiently documented or characterized
   - In any case, direct interaction between simulators and experimentalists is essential to the process

PRINCIPLES - DESIGN AND EXECUTION OF VALIDATION EXPERIMENTS (2)

4) Design experiments should be jointly by experimentalists and computationalists.

- Should be designed to test critical physics and to measure parameters critical to model, especially boundary or initial conditions
- Physics assumptions must be well documented and tested
- Perturbing effects should be minimized.
- What measurements are needed
  - i) At what accuracy
  - ii) At what resolution
  - iii) In what regimes
  - iv) At what range of parameters
- Openness and candor about limitations and sources of error is essential

5) Document code predictions well in advance.

PRINCIPLES - DESIGN AND EXECUTION OF VALIDATION EXPERIMENTS (3)

6) While jointly designed, carry out experiments and code runs independently.

7) Make as complete measurements as possible

- Multiple diagnostics to measure the same quantities is desirable.
- Statistically sufficient data sets should be collected, repeating runs as required.
- Conduct experiments at more than one facility if practical.

8) Pay special attention to analysis of errors and uncertainties.

- Use modern statistical techniques to design experiments and to identify random and bias errors.

9) When analyzing results, don't paper over differences. The goal is not to prove that a code is correct, but to assess it's reliability and point the way towards improvement.

10) Document process and results, including data reduction techniques and error analysis

DISCUSSION TOPICS

- More emphasis on basic physics experiments
- Use of synthetic diagnostics and advanced statistical techniques
- Computer infrastructure
- Focused Workshops
- Co-development model

STRENGTHEN COMPARISONS WITH BASIC EXPERIMENTS

- Most resources go to simulations and comparisons with the largest most complicated systems (For fusion research at least).
- This situation compromises attempts to develop validated codes.
- Significant resources should be allocated to smaller scale experiments designed to test basic physical phenomena (eg, ITG identification and properties, self-generated flows, etc).
- These experiments would need to be extensively diagnosed and extensively modeled (opportunities for multi-institutional collaborations).
- Codes would be configured to work in relevant geometry and regimes
- Successful comparisons would provide needed confidence in models
- This would require **significant** restructuring of the (fusion) program!

SYNTHETIC DIAGNOSTICS, ADVANCED STATISTICAL TECHNIQUES

- Synthetic diagnostics
  - o Experimental measurements are often quite indirect.
  - o As data is reduced to obtain basic quantities, errors propagate
  - o Comparison can be much more direct with synthetic diagnostics applied to simulation results
  - o Data from simulations processed in a manner which is as close to physical diagnostic as possible
  - o Also - advanced time series for fluctuation/turbulence data
- Statistical techniques
  - Improve estimates of random and systematic errors
  - Quantify confidence in prediction
- Need to share data and tools
- Common API's (Application Program Interface, eg MDSplus)

SHARED DATABASES

- Contains both experimental and simulation data
- Must be dynamic and interactive
- Must be complete and self descriptive
- Must contain all auxiliary data, assumptions, geometry, boundary and initial conditions
- Must contain estimations of error
- Regimes well defined
- Can be updated, annotated, appended
- Searchable by content or by address
- Browsable
- Linked to publications

WORKSHOPS

- Should be on well defined and relatively narrow subject
- Valuable for both code to code comparisons and validation exercises
- Places to discuss nuts and bolts of comparisons
  - Sources of error
  - Data structures and archives
- Importance of reasonably rigorous statistical analysis
- Planning
  - experiments
  - code developments
  - code runs

How to Move Toward Co-Development Model

- Integrate validation approaches into work flow for experiments and simulations
  - Significant change in how we work
- How do we foster this?
  - Rewards systems
  - Publications, program committees, etc
  - Recognition at home institution

SUMMARY

- Despite dramatic advances in computational plasma physics, we are still far from solving the problem.
- Experiments and simulation are complementary rather than competitive approaches – and should be viewed that way.
- Science benefits from a continuous and ongoing collaboration between them.
- A more concerted effort to validate codes and calculations should be undertaken.
- This effort should include tests on a range of systems from the simplest to the most complex.
- Requires new modes of collaboration - openness about uncertainties, errors and limitations of methods is essential.