THRUST 6: Develop Validated Predictive Models

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Thrust 6: Develop Predictive Models for Fusion Plasmas, Supported by Theory and Challenged with Detailed Experimental Measurements

The thrust poses 4 related scientific questions

- *How well can the complex, multi-scale phenomena of fusion plasmas be reproduced and understood through first principles models, compared in detail to experimental measurements?*
- *What are the appropriate methods for integrating multi-physics and multi-scale effects needed to increase the fidelity of practical computer models?*
- *How can reliable, reduced, integrated models be constructed that allow for rapid exploration of operating scenarios on experiments, especially ITER?*
- *What innovations in measurement techniques or experiments should be pursued which would facilitate comprehensive tests of these models?*

Motivation

- Directly supports OFES mission
  - *Develop knowledge base for practical fusion energy*
- Enables maximum exploitation of existing and planned experiments, especially ITER
- Allows for more reliable design of new experiments
- Improves ability to transfer knowledge learned on one device or type of device to others (i.e. among toroidal magnetic confinement concepts)

Why Now?

- Programmatic need:
  - Be prepared for ITER operations
  - Increase confidence in design of future experiments
- Opportunity: Thrust builds on recent progress
  - Improved basic understanding and modeling
  - Better algorithms and faster computers
  - Significant improvements in measurement techniques
- Plays to U.S. strengths
  - Strong theory and modeling program
  - Best diagnosed experiments

What's New In The Thrust?

- Greater resources – progress is currently too slow to meet goals in a reasonable time.
  - Theory, modeling, applied math, computer science, software engineering
  - Experiments and diagnostics
    - New area of emphasis for laboratory-scale experiments
    - Additional run time and support on major experiments
    - Vigorous and innovative diagnostic development program
  - Dedicated analysts
    - More quantitative and systematic approach to model testing

- Unprecedented degree of cooperation and coordination among program elements
  - (theory, computation, large/small experiments also alternates, edge physics)

Elements of Thrust: Select Case Studies

- Choose set for focus of initial efforts
- Allows for rational prioritization and maximum impact on Fusion Program
- Criteria to include Importance, Urgency, Readiness
- Ideas include
  - PWI and SOL
  - Pedestal and Edge
  - Core: Transport and MHD
  - RF current drive and heating
  - Energetic particle physics
  - Physics of non-axisymmetric configurations
  - Integrated modeling – Reduced “whole" device models
- Much more discussion/debate required
- Scope will depend on resources

Elements of Thrust: Planning

- Ask some important questions
  - How will model predictions be used?
  - Which applications?
  - What are the impacts of predictions? (particularly of errors in predictions)
- Assess Current Status
  - Which areas are well understood? Where are they uncertain or controversial?
  - What new developments in physics or methodology are required?
- For each case study, map out research needs and directions in detail
  - Estimate resource requirements

Elements of Thrust: Model Development

- Develop strategy to address missing or inadequate physics
- Develop or improve existing codes
  - Foster innovation in algorithms and numerics – expand collaborations with applied math and computer science
  - Identify methods for physics and module integration (FSP mission)

Code Verification

- Does the code correctly implement the chosen physical model?
- Problems in code – coding errors, language or compiler bugs
- Problems in solution - Discretization errors, convergence, numerics or algorithms problems
  - Handle via comparison with theory, convergence tests, code to code comparisons
- Verify before comparing with experiments but don't wait until code is "complete" - Testing can and should guide development

Elements of Thrust: Validation

- Does the model correspond to reality?
  - Physical problem – compare code results to experimental measurements
  - Not a one-time exercise: approve or discard
  - Iterative – identify cause of discrepancies and improve models
- Focus on critical elements of model
- Define measurement needs
  - Diagnostic challenge can be formidable – **innovation required**
  - Make comparisons at multiple levels of integration (primacy hierarchy)
    - e.g. Fluctuation amplitudes, correlations, fluxes, profiles
  - Due consideration of uniqueness and sensitivity
- Requires attention to sources of error and uncertainty in both model and experiments
- Need a much more systematic and methodical approach (than currently)

Elements of Thrust: Need for Range of Experiments

- Major fusion experiments have the greatest "realism" in physics and geometry
  - But they also have the greatest complexity and couplings
  - High temperature precludes "invasive" diagnostics
- Smaller experiments have been used effectively to study focused problems of "universal" importance – fusion relevance
  - (e.g. generation of flows by turbulent Reynold's stress)
  - Quantity and quality of data can be higher, more data on initial and boundary conditions
  - More flexibility, more experimental time and faster code runs
  - Can test some of the basic underpinnings which are critical but inaccessible on larger devices
- Requires adaptation of codes to relevant geometry and regime
- Requires adequate diagnostics and other resources

Elements of Thrust: Analysis

- In “high-consequence” applications, V&V is led by dedicated analysts
  - Weather prediction and climate modeling
  - Turbomachinery
  - Airframe design
- Not tied to code development groups
- Can serve as honest brokers, providing unbiased and dispassionate assessments
- Requires specialized skills
- Analysts would have leading role in designing and analyzing validation experiments
  - Close collaboration with theorists, computationalists and experimentalists
  - Help marshal the computational and experimental resources
  - Help develop post-processors, synthetic diagnostics

Resources Required
New and Augmented Capabilities Needed for Each Element

- Basic theory – conceptual models, mathematical formulations
- Small code teams – flexible, agile
- Large code teams – large, integrated efforts
- Multiple codes needed, including those that solve the same problem by different means
- Applied Mathematicians and Computer Scientists – numerics, algorithms, software frameworks and work flows
- Software engineering – make codes usable by larger community
- Computer time – requirements for verification and validation are substantial
- Innovative measurement techniques – developed and deployed
- Small scale experiments
- Run time and support on large experiments
- Dedicated analysts

Readiness for Thrust: Work Could Begin Now

- All of the elements, described above, could be addressed without waiting for future results or facilities.
  - FSP already in “program definition” phase
  - Other detailed planning would be required before new resources could be most effectively used, but some needs are already identified.
- Closer interaction between theory/computation and experiments requires new modes of collaboration.
  - Could we learn valuable lessons from other fields?
- Future developments will aid thrust
  - New experiments such as ITER or others proposed in this workshop could extend parameter ranges – useful for model testing
  - Innovation in diagnostics and analysis techniques
  - Alternates extend range to different magnetic geometries or parameter ordering
  - Faster computers will continue to be needed

Integration of Thrust Elements

- This thrust integrates in many dimensions
  - Theory, computation, experiments
  - Topical science areas (Transport, MHD, Wave-particle…)
  - Regions of plasma (Core, Edge, SOL, PWI)
  - Utilizes the full range of toroidal magnetic confinement concepts
  - Most ReNeW themes and thrusts
  - Plasma physics, applied math, computer sciences, software engineering
  - Small and large scale projects
- Impact (and burden) would be felt across entire program
  - Experiments would be more useful in guiding model development
  - Models would improve utilization of experiments – scenarios development
  - Resources would be required from all

Coordination and Management

- Interactions between theory, modeling and experimental efforts need to be stronger, more systematic and more immediate than they are now.
- Accomplish via “pull” and “push”
  - Pull = Modify rewards
    - Funding criteria
    - Reviews
    - Publications and invited talks
  - Push = some level of central coordination and management
- Analysts, who have not been adequately recognized in our community need stable and sufficient support – tied to experimental groups perhaps?
- For all elements (theory, computation, diagnostics, experiments, analysis), interdependence should be reinforced by consistent management decisions

Relation to Other Thrusts

- Validated predictive models would be essential for most/all of the other thrusts
- Many have a primary or secondary goal of improving modeling
- ITER, control and integration thrusts are particularly dependent on development of reliable models
- New facilities proposed by other thrusts can be platforms for validation in many cases. (Don't neglect diagnostics)

Other Scientific Benefits

- General scientific contributions to complex dynamics, turbulence etc.
- Specific contributions in areas like astrophysics, space physics where magnetized plasmas are important – "fusion" codes already in use.
- MFE has, for decades, provided leadership in use of computing and networking for enabling its science – this thrust will continue that tradition

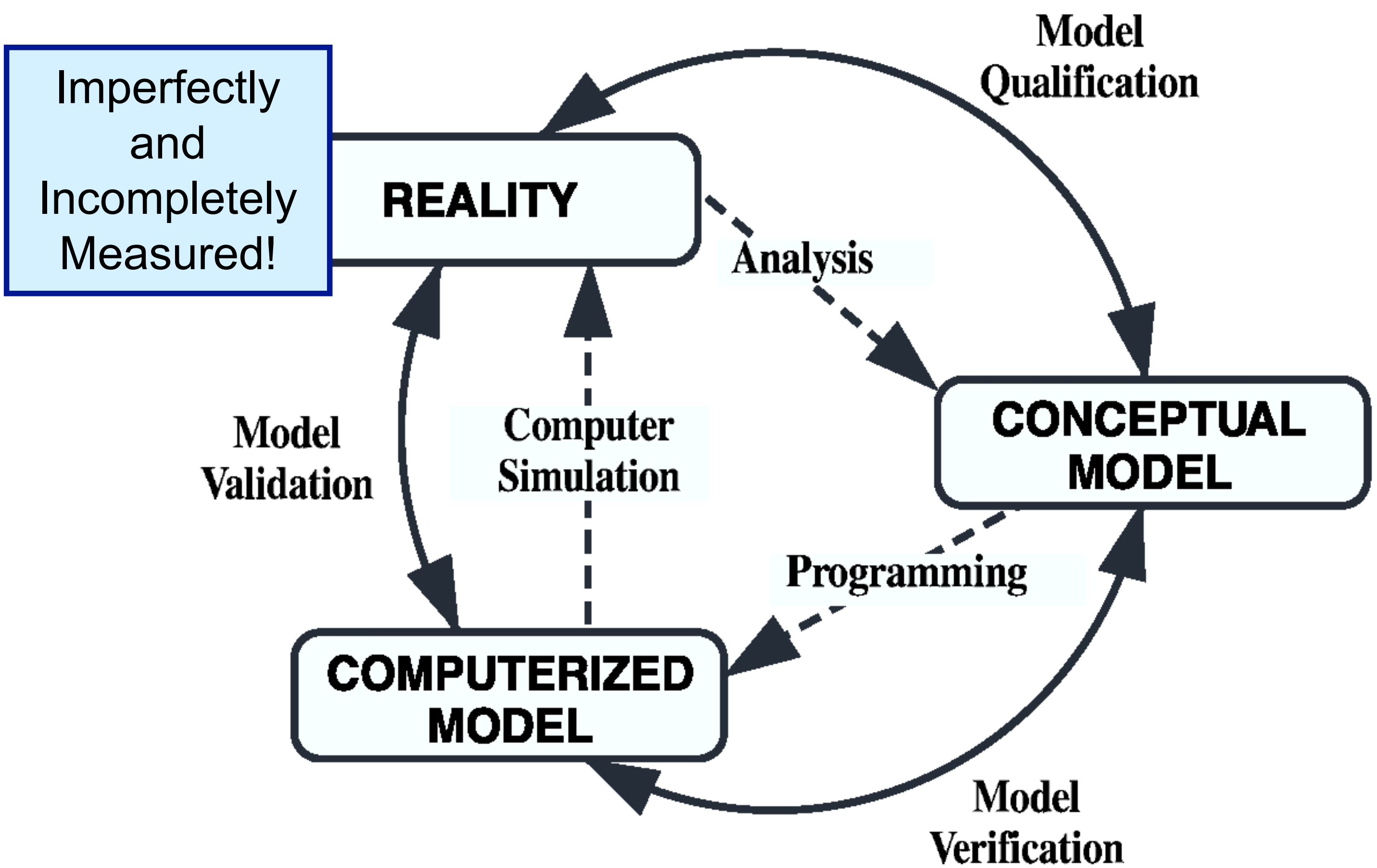
Summary of Proposed Actions

- Strengthen the basic theory program to address areas where current physical models are inadequate or incomplete.
- Develop a spectrum of powerful, robust, well-verified computer models shared by a large user community.
- Innovate in diagnostic techniques to enable measurements critical for validation.
- Provision a spectrum of experiments including both large and small facilities, a range of confinement concepts and adequate run time dedicated to model testing.
- Conduct a rigorous set of validation activities - assess critical elements of physical models through careful comparison with experiments.
- Recruit and support dedicated analysts to bridge the gap between theorists, code developers and experimentalists, providing unbiased assessments.
- Provide substantial computer time for code verification and model validation.

END

Additional Material

Elements of Thrust: Relation of Processes



Schlesinger 1979