Computational Modeling in Energy Science: Opportunities and Challenges

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Energy Technologies

Meeting world energy demands will require advances in many technology / science areas

- Combustion processes
- Fossil fuel exploration and production
- Fuel cells
- Renewable energy
- Fusion / nuclear energy

These are complex, nonlinear, multi-disciplinary problems that are beyond the scope of traditional theory and where experimentation is difficult and expensive if not impossible

Role of computational modeling

Traditional roles of computational modeling

- Engineering design
- “Science-based” interpolation
- Idealized subproblems

What is the potential for high-end computation?

- Fundamental new insights into key scientific issues
- Detailed quantitative, predictive engineering models

High-fidelity predictive simulation tools can have substantial impact on key energy applications

Components of a Computational Model

Mathematical model: describing the science in a way that is amenable to representation in a computer simulation

Approximation / discretization: approximating an infinite number of degrees of freedom with a finite number

Solvers and software: developing algorithms for solving the discrete approximation efficiently on high-end architecture

Mathematical Model

Mathematical model: describing the science in a way that is amenable to representation in a computer simulation

- Does the model have the fidelity to address the science question
- Is the model mathematically consistent: do solutions exist, are they unique, are they stable to small perturbations
- Qualitative properties: how smooth is the solution, what type of scaling behavior does it exhibit
- Is the system deterministic or stochastic

Approximation / Discretization

Approximation / discretization: approximating an infinite number of degrees of freedom with a finite number

- Stability + consistency $\longrightarrow$ convergence
- Are the assumptions for the discretization compatible with the mathematical model
- Do the resolution requirements vary either spatially or temporally
- Does the discretization strategy respect the coupling between different physical processes, time scales, …

Solvers and Software

Solvers and software: developing algorithms for solving the discrete approximation efficiently on high-end architecture

- Stability + conditioning $\longrightarrow$ precision
- Algorithmic efficiency: exploit the structure of the discretization / model while accommodating the structure of the architecture
- Software identifies and encapsulates recurring mathematical abstractions for reuse across multiple applications

Observations

There is a fundamental tension between these components

- Model fidelity versus discretization complexity
- Discretization complexity versus implementation complexity / performance

Computational modeling is an experimental science

- No general theory for numerical methods for complex nonlinear problems; design of numerical methods for such systems are based on rigorous analysis of model systems, asymptotic analysis (“physical reasoning”) and experimentation
- Obtaining good performance is inherently empirical

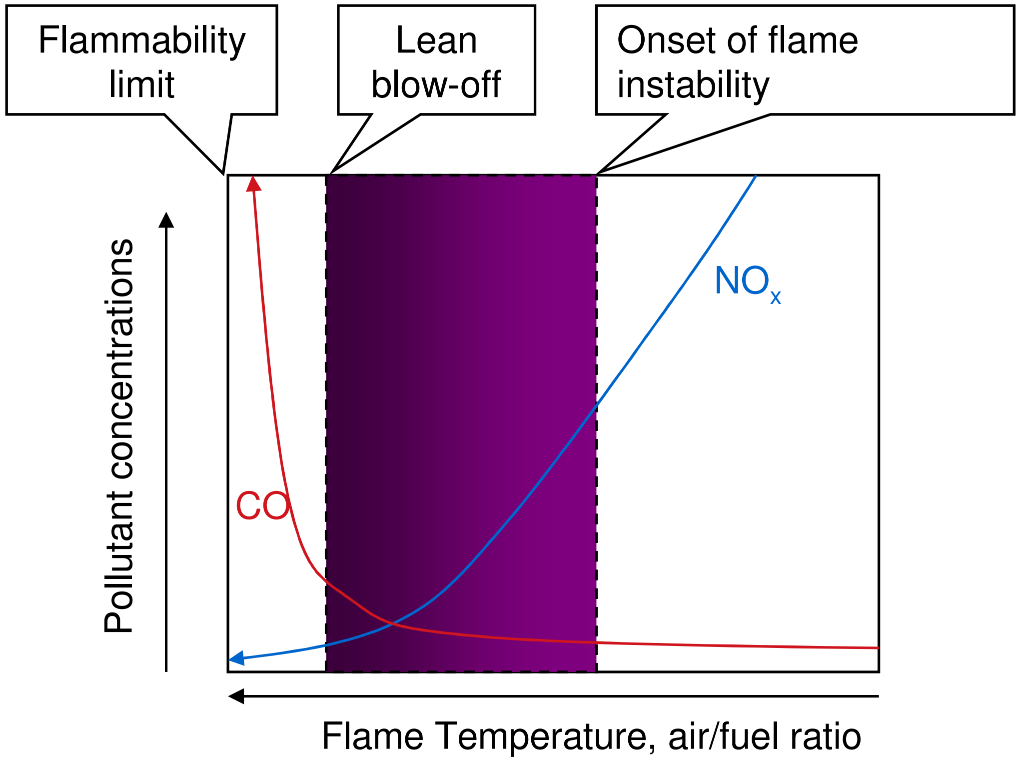
To make progress everything needs to be “on the table”

Mathematics is central to the development of high-end computational models

Case Study -- Combustion

Lean premixed turbulent combustion

Courtesy of R. K. Cheng



Low emissions

Compact design

Flames are subject to a variety of instabilities making flame stabilization difficult

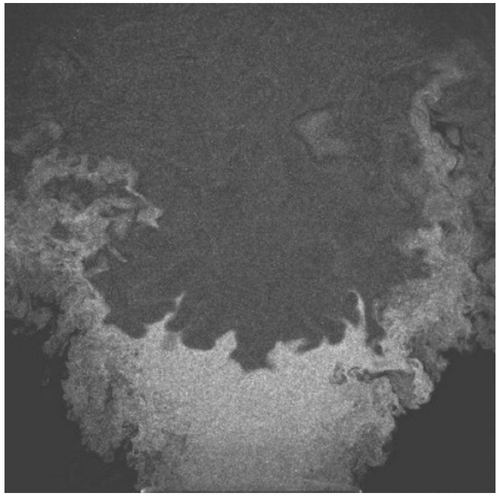
Problem features

Multi-scale

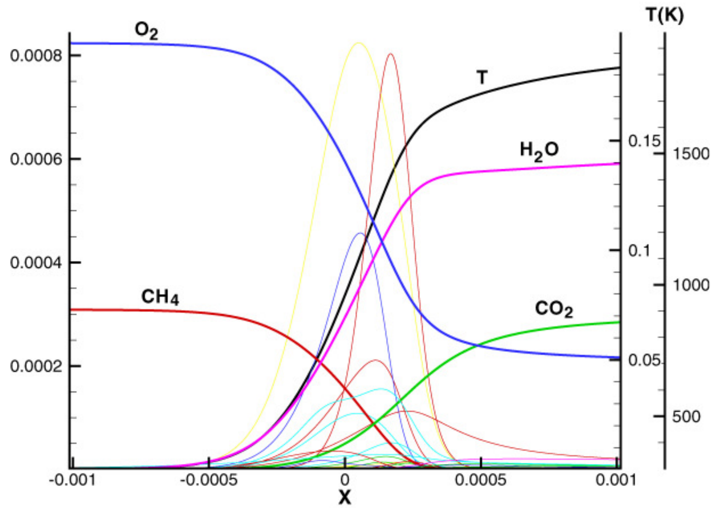
- Length scale O(10) cm
- Time scale O(1) sec
- Flame thickness O(10^{-2}) cm
- Sound speed O(10^{5}) cm/sec
- Chemical time scale O(10^{-6}) sec

Multi-physics

- Fluid mechanics
- Chemistry
- Multicomponent species transport
- Thermal radiation and conduction



PIV showing flame



Approach

Combustion simulation is multi-scale and multi-physics

Traditional approach

- Discretize reacting compressible Navier Stokes
- Determine time step from fastest time scale
- Determine mesh spacing from smallest spatial scale

This approach is computationally intractable

Exploit multi-scale character of the problem to reduce computational cost

- Flames are low speed (Mach number)
- Flames are localized in space

Mathematical Model

Natural separation between flame speed and sound speed

Asymptotic analysis in Mach number shows that

$$p(\vec{x},t) = p_0(t) + \pi(\vec{x},t) \qquad \pi/p_0 \sim \mathcal{O}(M^2)$$

Low Mach number combustion equations

- Coupled system of PDE's evolving subject to a constraint
- Analytically removes acoustic time scale
- Fundamental change to mathematical structure of the system

Approximation / Discretization

Temporal discretization should respect different types of behavior

- Different physical processes
- Constrained evolution

Fractional step projection algorithm

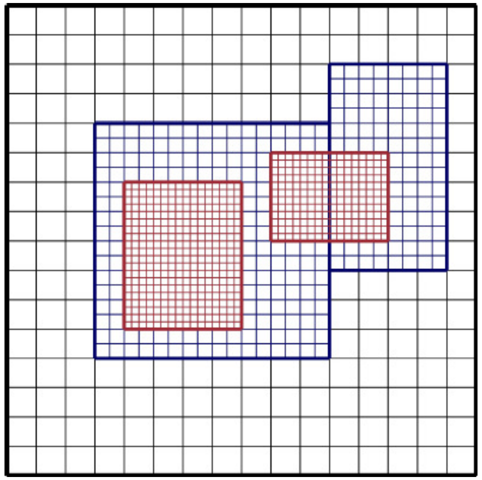
- Semi-implicit discretization of advection / diffusion
- Stiff ODEs for chemistry
- Implicit elliptic discretization to enforce constraint

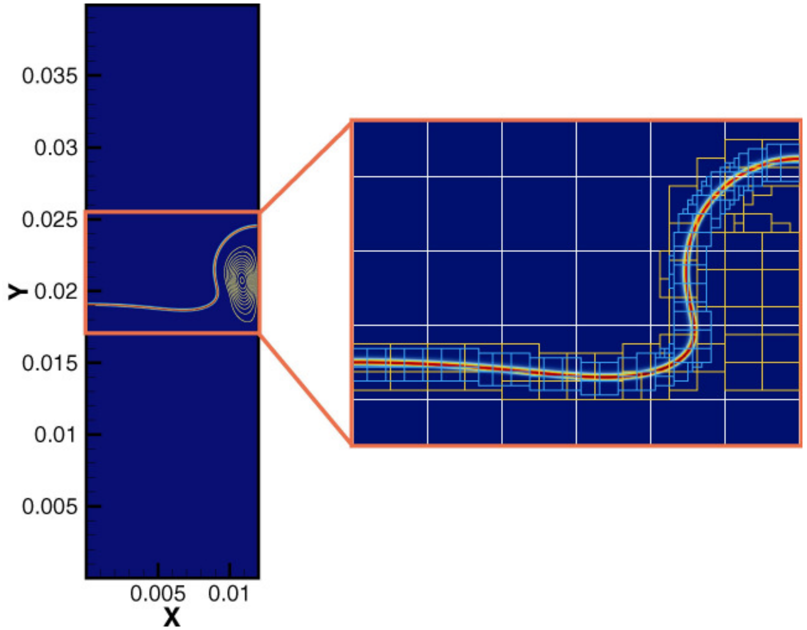
Approximation / Discretization

Spatial discretization should exploit flame locality

Structured adaptive mesh refinement

- Hierarchical patches of data
- Dynamically created and destroyed





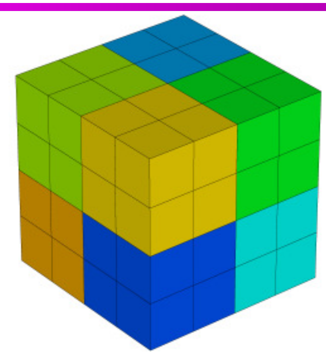
Solvers and Software

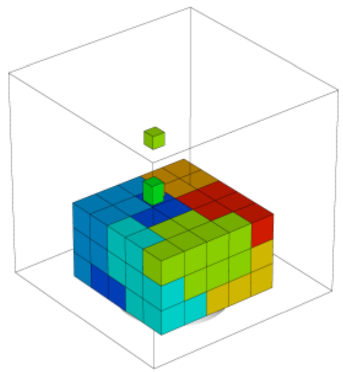
Implementation in BoxLib, a framework to support parallel implementation of structured AMR

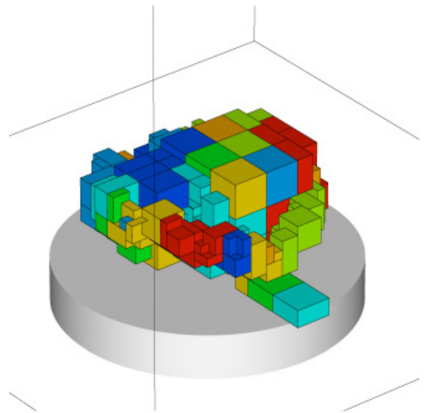
- Data distribution
- Parallel communication
- Dynamic load balancing

Linear solvers for block-structured hierarchical grids

- Parabolic and elliptic operators
- Parallel multigrid



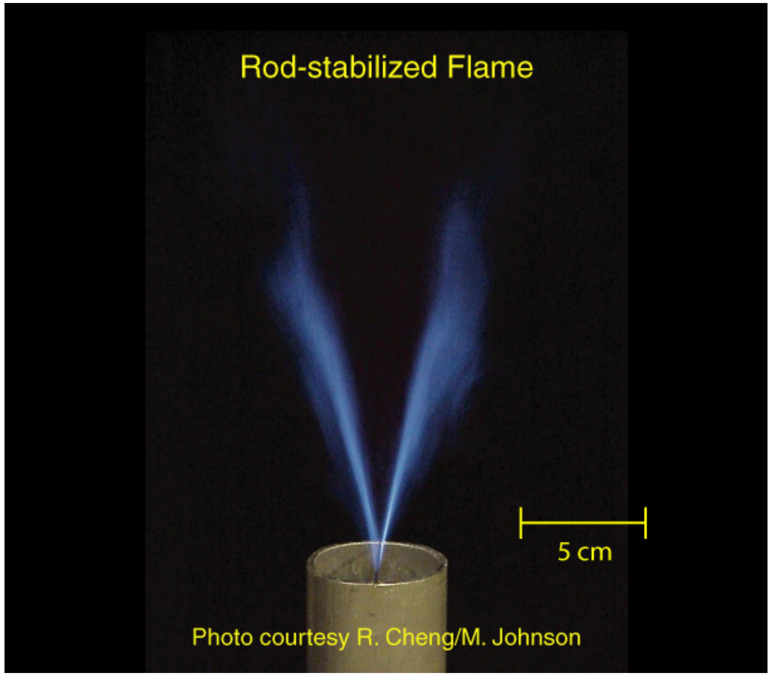




Configuration

Laboratory-scale V-flame

- Detailed chemistry (20 species)
- Mixture-averaged transport properties
- Characterization of turbulence generation



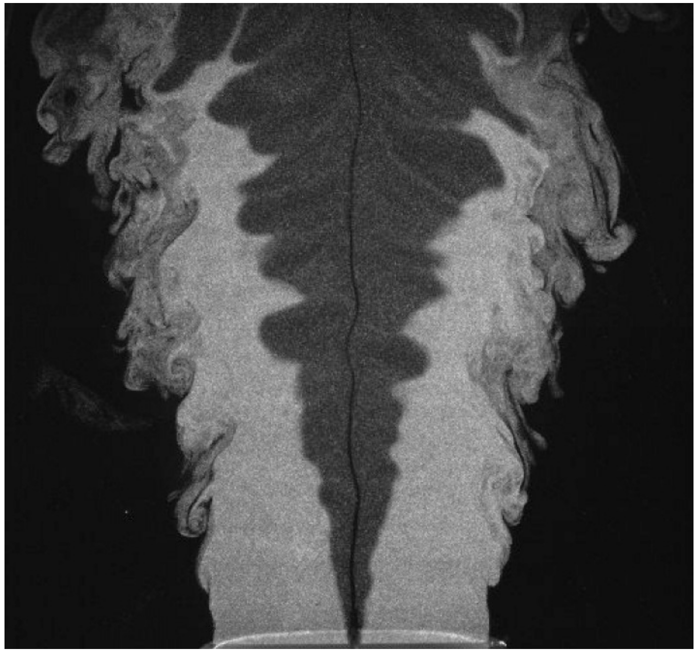
Domain is 12 cm x 12 cm x 12 cm

Effective resolution at finest level is 156 microns

Low Mach number + AMR saves $10^3 – 10^4$

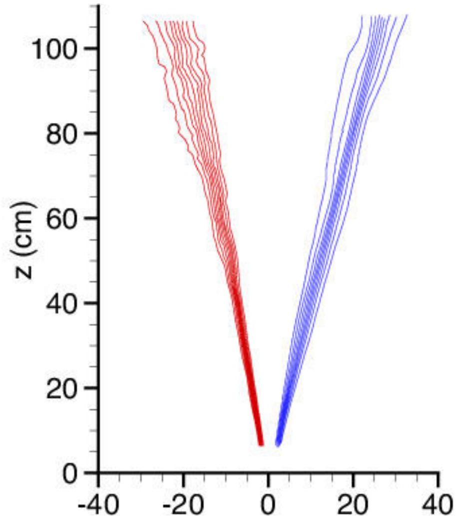
Results: Computation vs. Experiment

CH4 from simulation

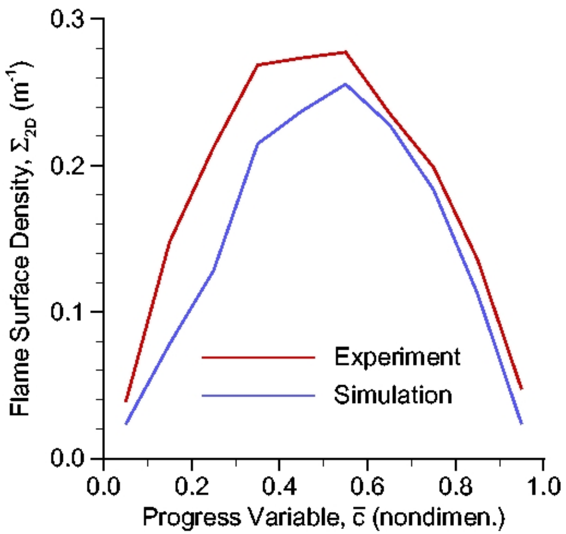


PIV from experiment

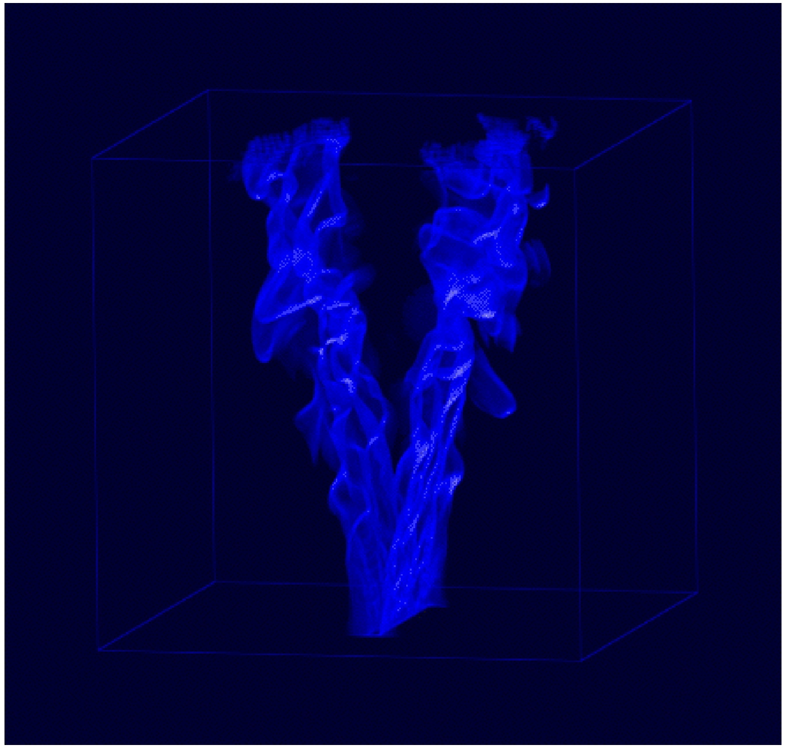
Additional comparisons



Flame brush



Flame surface density



Animation of instantaneous flame surface

Reservoir Modeling

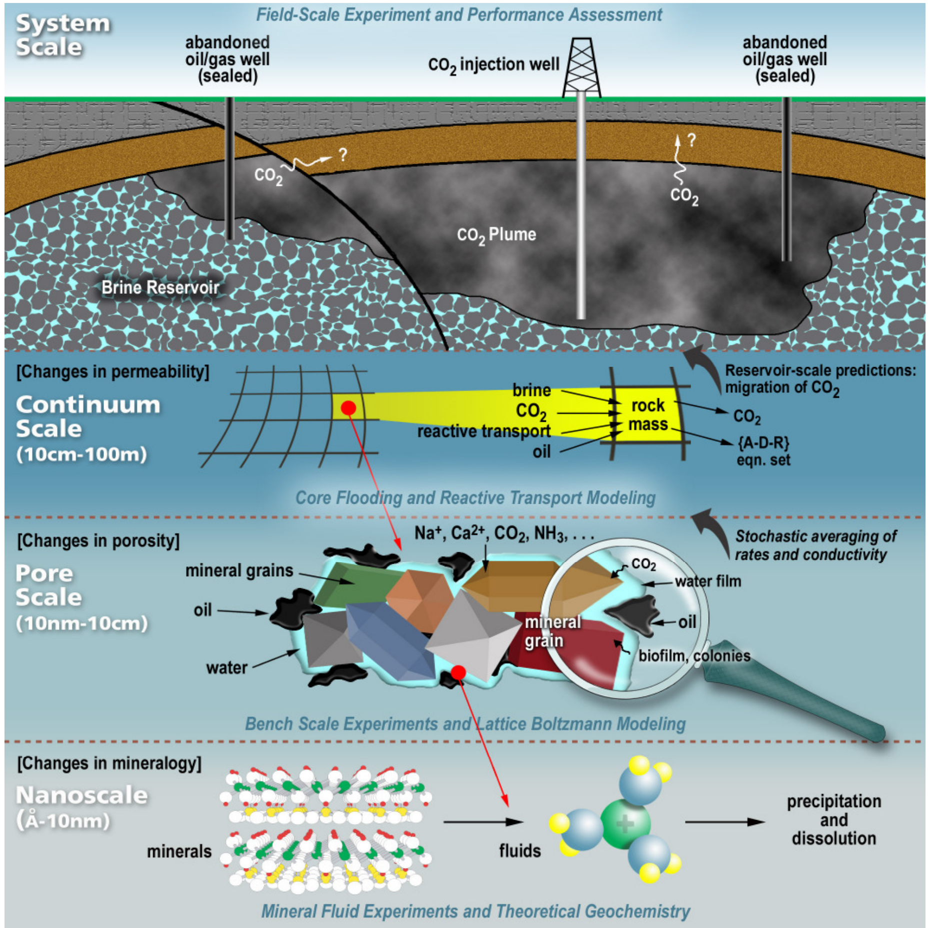
Multiple scales

- Chemical scales
- Pore scales
- Continuum scales

Anisotropy

Inherently noisy

- Limited data
- Statistical characterization of media



Report of the First Multiscale Mathematics Workshop

Magnetic Fusion

Kinetic equations are fundamental; everything else is derived (MHD, edge fluid, transport)

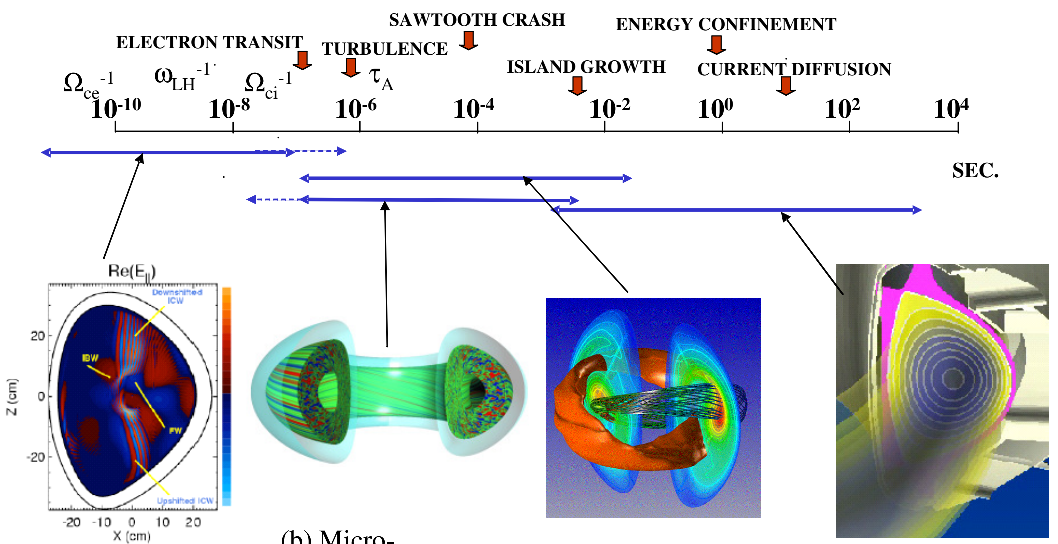
- Model depends on scale and question

Strong anisotropy

Multiscale nature

- Closure methods
- Hybrid methods

Relevant timescales for a burning plasma experiment



(a) RF codes

(b) Micro-turbulence codes

(c) Extended-MHD codes

(d) Transport Codes

Report of the First Multiscale Mathematics Workshop

Conclusions

Computational modeling has the potential for substantial impact on key energy applications

- Mathematics is central to the development of methodology
- Sustained focused effort leads to scientific and technological impact (10-15 years)

Barriers to progress

- Machine architectures increasingly difficult to use
- Extracting knowledge from the data poses major challenges
- Who will train the people needed to build these types of simulation capabilities