Putting Cyber Infrastructure to Work for Combustion: Advantages from an Applications Perspective

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Motivation

- **Predictability: a key design concern for applications**
  - – Reduce number of design iterations
    - Reduce development cost
    - Reduce time to market (competitiveness)
  - – Avoid idling standing armies of engineers while solving unexpected problems

- **Recent example: alternative fuels**
  - – How will attempting to use them impact the enormous existing infrastructure?
    - Eg, emissions, combustion stability, etc

An Opportunity

- **A look into the future (in our lifetime):**
  - Project continued linear growth in experimental and diagnostic technologies, but *exponential* growth in computational capability.
  - On the brink of soon being able to routinely resolve large scale dynamic motions using methods such as LES.
    - This will enable a *significant* advancement in the ability to accurately calculate combustion flows, including engineering calculations

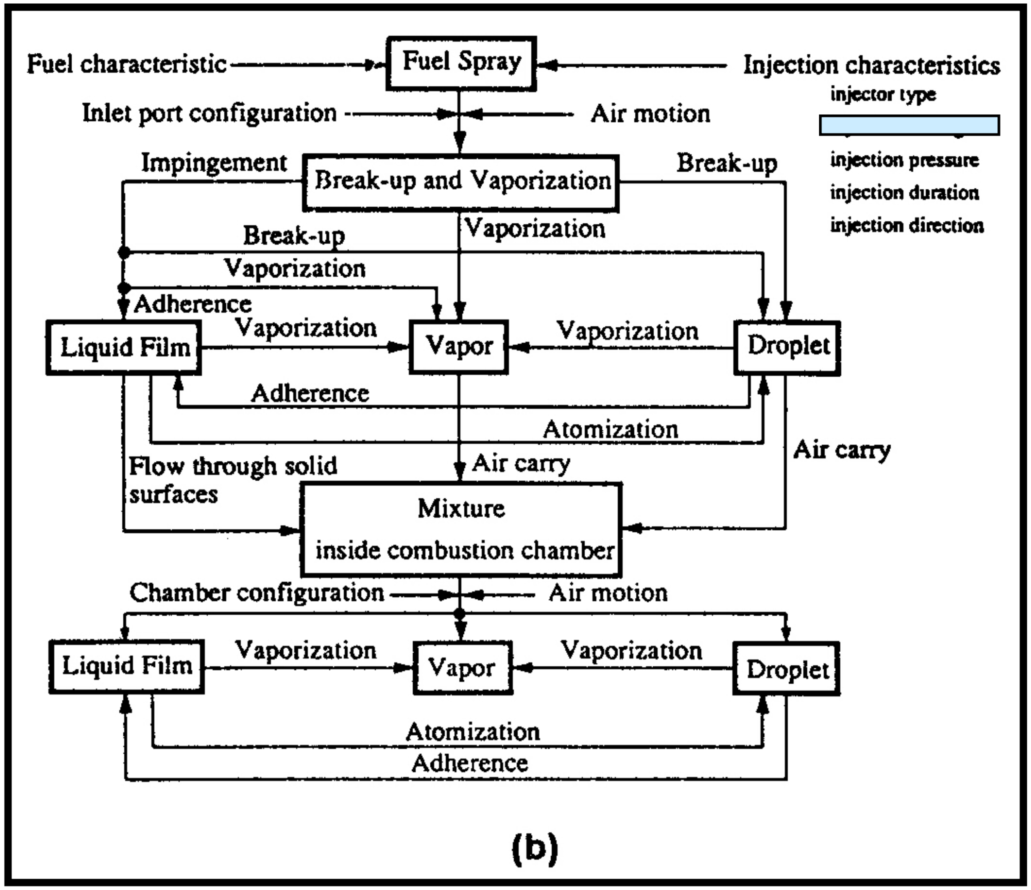
- **M&S must be a *key element* in combustion R&D strategy for any application**
  - But experiments will be a key cost driver

Another opportunity

- **Many applications share common problems**
  - Ex: combustion stability is a problem for liquid and solid rockets, gas turbines and augmentors, and land based power

Many applications share common processes

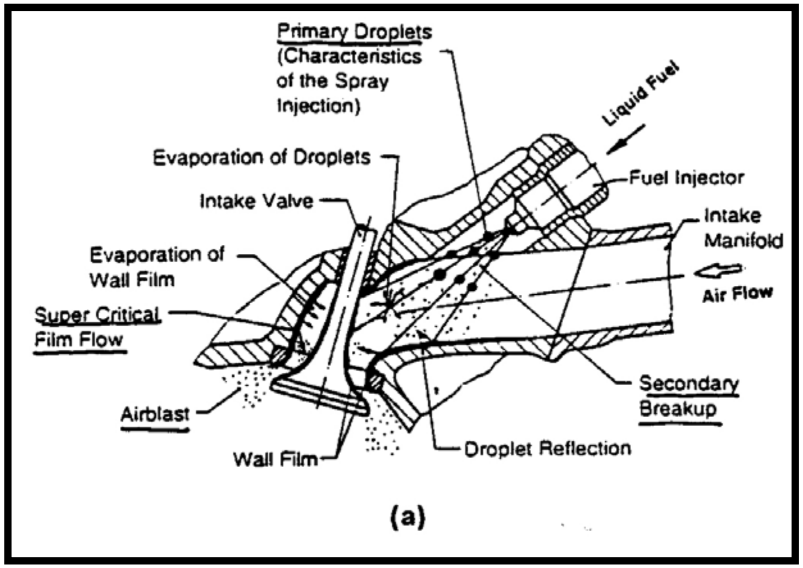
- **What application does this process describe?**

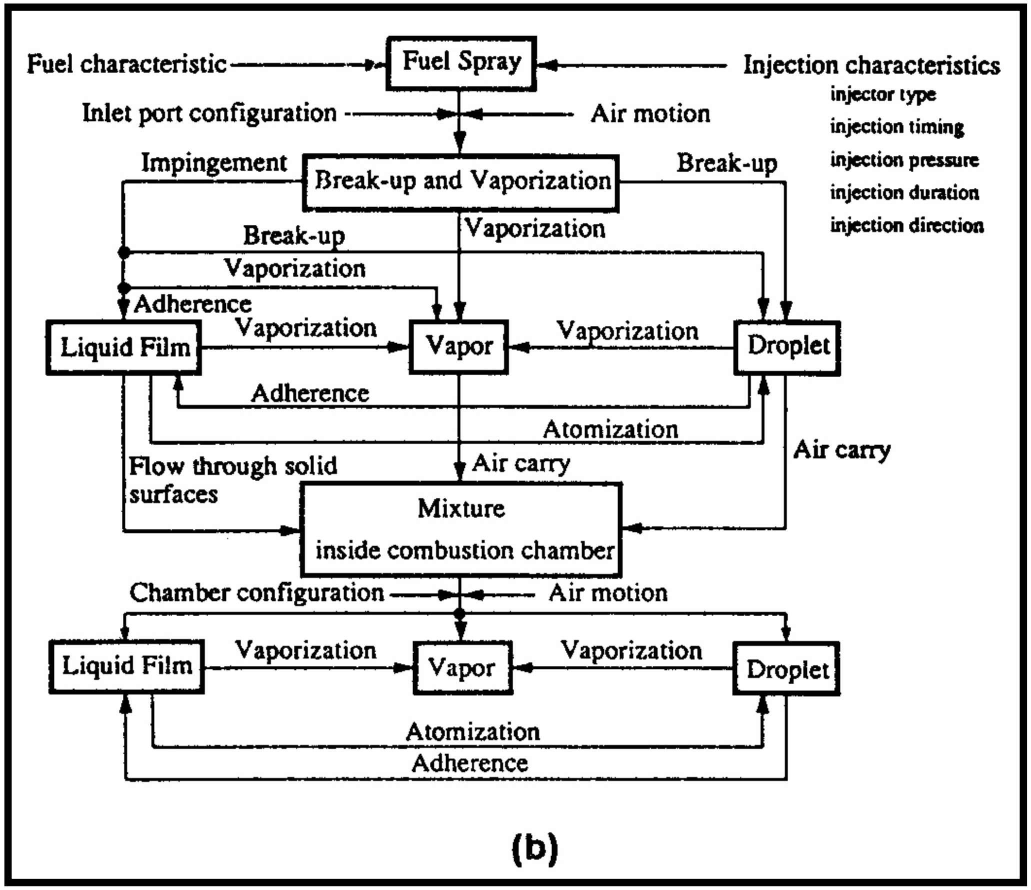


(b)

Many applications share common processes

- **What application does this process describe?**





Port fuel injector

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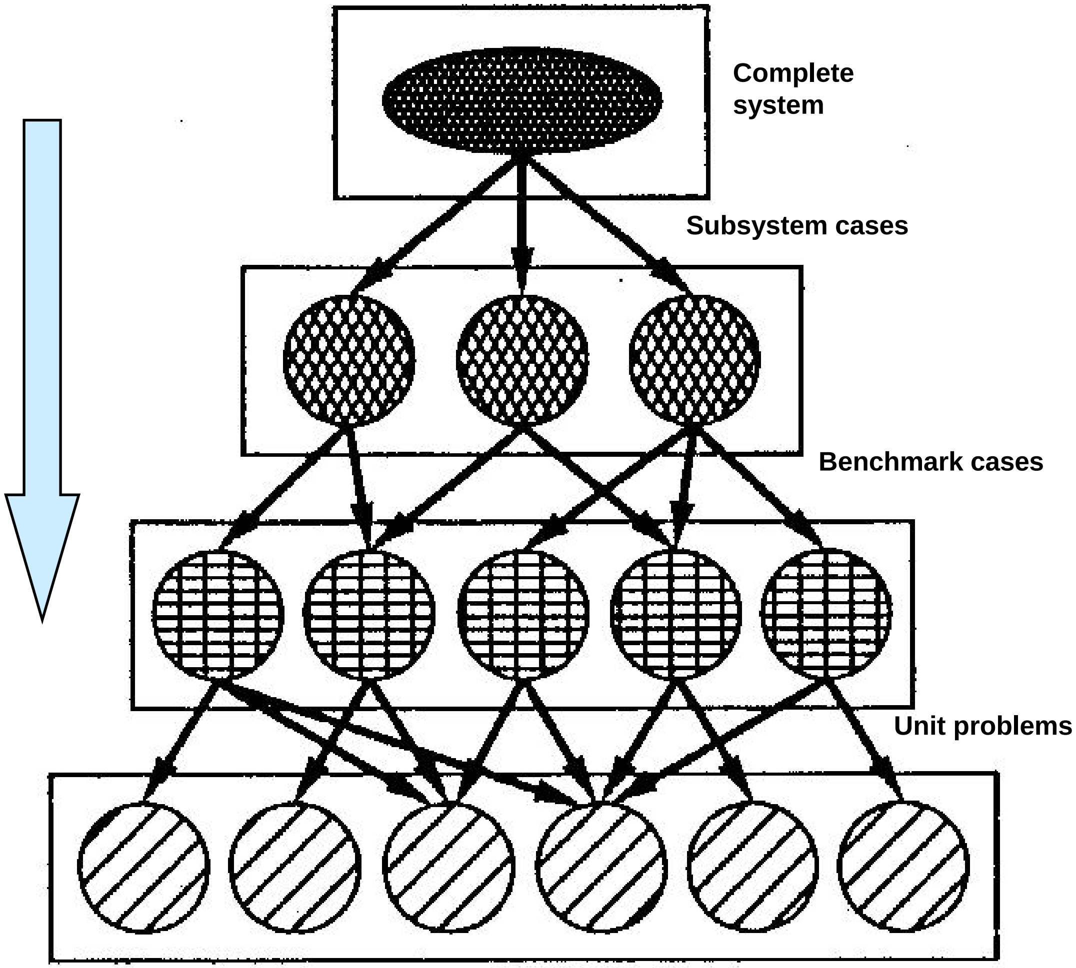
To date, applications have not collaborated very well with each other. Is there a way cyber infrastructure can help foster closer and more cost effective collaboration?

A model for collaboration



- Work units break the problem up into its component parts.
- Opportunities to collaborate between applications increase at successively lower levels of the tree

Figure from Oberkampf and Trucano, Verification and Validation in Computational Fluid Dynamics," Progress in Aerospace Sciences 38 (2002) 209-272

Recent initiatives

- **Formation of the Multi-Agency Coordinating Committee on Combustion Research (MACCCR).**

- **Organization of a workshop on the Future of Modeling and Simulation for Combustion Applications, held 21-23 February 2006 in Pittsburgh, PA.**
  - Co-sponsored by AFRL and DOE
  - General objective to understand requirements applications have in common
  - Five applications represented: liquid rockets, solid rockets, gas turbines and augmentors for propulsion, stationary gas turbines, and ramjets/scramjets.
  - 120 participants from across many organizations: AFRL, AFOSR, Army, Navy, NASA (GRC, MSFC, LaRC), NSF, NIST, DOE-NETL, DOE-CRF, industry, small businesses, and academia.

The GOTChA process was used at the Pittsburgh workshop to translate requirements into recommended work units

- **Goals**
- **Objectives**
- **Technical Challenges**
  - What is preventing us from achieving our objectives today?
- **Approach**
  - Fundamental work units, can and does include basic research

- **GOTChA analysis of the workshop proceedings follows**

Legend

- **LR – liquid rockets**
- **PGT&A – propulsion gas turbines and augmentors**
- **SGT – stationary gas turbines**
- **SR – solid rockets**
- **R/S – ramjets / scramjets**

- **X – an item was explicitly mentioned by an application**
- **O – an item is judged to apply to an application even though it was not explicitly mentioned**
- ***Italics* means the workshop did not carry the analysis further in the GOTChA tree**

Customer Goals - three nested levels
Top level

CG	Customer Goal	LR	PGT &A	SGT	R/S	SR
1	Cost	X	O	X	O	O
2	Operability	X	O	X	X	O
3	Reliability	X	X	X	O	O
4	Satisfy emissions requirements		X	X		
5	Meet performance requirements	X	X	O	X	X
6	*Low observables*		X			
7	*Weight*	O	X		O	O

Customer Goals – all levels

CG	Customer Goal	LR	PGT &A	SGT	R/S	SR
1	Cost	X	O	X	O	O
1a	*Product cost*	X	O	X	O	O
1b	*Operations costs*	X	O	X	O	O
1c	Development cost	X	X	X	O	O
2	Operability	X	O	X	X	O
2a	Static stability		O	X	O	
2b	Dynamic stability	O	O	X	O	O
2ba	Reduce risk of developing combustion instabilities	X	O	O	O	O
2c	Control response		O		O	
3	Reliability	X	X	X	O	O
3a	Life	X	X	X	X	
4	Satisfy emissions requirements		X	X		
5	Meet performance requirements	X	X	O	X	X
5a	Thrust, power	O	O	O	O	X
5b	Efficiency, Isp, Sfc	O	O	O	O	X
6	*Low observables*		X			
7	*Weight*	O	X		O	O

Technical goals

- **For any design configuration, including but not limited to new concepts, revolutionary combustion concepts including those that capitalize on unsteady reacting flow, and for each point in the operating envelope, including start up, shut down, turndown, throttle setting, part load, base load, flight regime, variable geometry, and fuel / oxidant composition:**

Technical Goals - five nested levels
Top level

CG	TG	Technical Goal	LR	PGT&A	SGT	R/S	SR
1	1	Reduce cost	O	O	X	X	O
2	2	Accurately predict operability limits	O	O	O	O	O
3	3	Accuately predict reliability	X	X	X	X	X
4	4	Accurately predict emissions at (high / low) power		X	X		
5	5	Accurately predict performance	X	O	O	X	X

Technical goals

- **All five levels contained 63 technical goals**
- **Below is an example from predicting life**

TG	Technical Goal	LR	PGT&A	SGT	R/S	SR
3	Accuately predict reliability	X	X	X	X	X
3a	Accurately predict life	X	X	X	X	X
3aa	Accurately predict thermal loads (short term)	X	O	X	O	O
3aaa	Predict heat flux variations for steady state conditions	X	O	O	O	O
3aaaa	Global	X	O	O	O	O
3aaab	Local	X	O	O	O	O
3aab	Predict heat flux variations for transient conditions	X	O	O	O	O
3aaba	Global	X	O	O	O	O
3aabb	Local	X	O	O	O	O
3ab	Accurately predict thermal loads (long term)	X	X	X	X	X
3aba	Predict heat flux variations for steady state conditions	X	O	O	O	X
3abaa	Global	X	O	O	O	X
3abab	Local	X	O	O	O	X
3abb	Predict heat flux variations for transient conditions	X	O	O	O	O
3abba	Global	X	O	O	O	O
3abbb	Local	X	O	O	O	O

Objectives – four nested levels

- **All objectives could be expressed in four general categories**

O	Objectives	LR	PGT &A	SGT	R/S	SR
1	Predict statistically stationary quantities	X	O	X	O	O
2	Predict incoherent rms quantities	X	O	X	O	O
3	Predict coherent, non-acoustic quantities, for each dominant peak in the power spectra	X	O	X	O	O
4	Predict acoustic quantities, for each dominant peak in the power spectra	X	X	X	O	O

Objectives

- **All four levels contained 55 objectives**
- **An example from acoustics is given below**

O	Objectives	LR	PGT &A	SGT	R/S	SR
4	Predict acoustic quantities, for each dominant peak in the power spectra	X	X	X	O	O
4a	Frequency	X	X	O	O	O
4b	Pressure	X	X	O	O	O
4ba	Amplitude	X	O	O	O	O
4bb	Phase	X	X	O	O	O
4c	Velocity magnitude	X	O	X	O	O
4ca	Amplitude	X	O	X	O	O
4cb	Phase	X	O	X	O	O
4d	Velocity direction	O	O	O	O	O
4e	Heat release	X	X	X	O	O
4ea	Amplitude	X	X	X	O	O
4eb	Phase	X	X	X	O	O
4f	Temperature	O	O	O	O	O
4fa	Amplitude	O	O	O	O	O
4fb	Phase	O	O	O	O	O
4g	Major species	X	O	O	O	O
4ga	Amplitude (as MR, LR value is for near walls)	xx	O	O	O	O
4gb	Phase	O	O	O	O	O
4h	Minor species					
4ha	Amplitude					
4hb	Phase					

Note no requirement for minor species

- **In some instances where more than one application gave a quantitative number, the numbers were very close despite having been developed by completely independent groups**

Technical Challenges – five nested levels

- **Most had to do with predictability (focus of the workshop). Only these are shown here**
- **156 technical challenges were given at all levels**
- **The eight top level technical challenges are given below**

TC	Technical challenges	LR	PGT &A	SGT	R/S	SR
2	The fidelity of combustion predictions is not high enough.	X	X	X	X	X
2a	Lack of the required experiments and measurements in relevant conditions	X	X	X	X	X
2b	Models / approaches to predict phenomena at relevant conditions are inadequate	X	X	X	X	X
2c	High fidelity may require tremendous computational power or long solution times	X	X	X	X	X
2d	Existing numerical algorithms are inadequate	X	O	O	O	O
2e	Difficult to scale from sub-scale to full scale	X	O	O	X	X
2f	*Computations are useful for tends only and are not truly predictive*	O	O	O	X	O
2g	*Strong sensitivites to boundary conditions and flow characteristics*	O	O	O	X	O
2h	*Difficult to handle large amounts of data*	O	O	O	X	O

- **The importance developing technical challenges was emphasized at the workshop**

Approaches

- **143 Approaches were given in 8 nested levels**

- **Many instances of “weak” approaches:**
  - TCh: Difficult to do X
  - Approach: Develop better ways to do X

Example of the best grouping of technical challenges and approaches into a research plan

- **One application provided a matrix filled out in detail:**
  - Each process considered to be important, eg
    - Injection
    - Ligament formation
    - Drop formation
    - etc.
  - The technical barrier for each process
  - The model improvement needed
  - Technical effort required
  - Measurements required under what relevant conditions

An opportunity for Cyber infrastructure?

- **Address fundamental problems**
  - R&D tool
- **Tackle a few larger problems with common interest**
  - Establish some large practical cases worth doing for the whole community
- **Note many combustors share common and repeated calculations**
  - What is different?
    - Boundary conditions
    - Fuel type
  - Can we store what is repeated and use it again?
    - Existing ISAT methods do this in one problem
    - Continuation methods for parametric studies

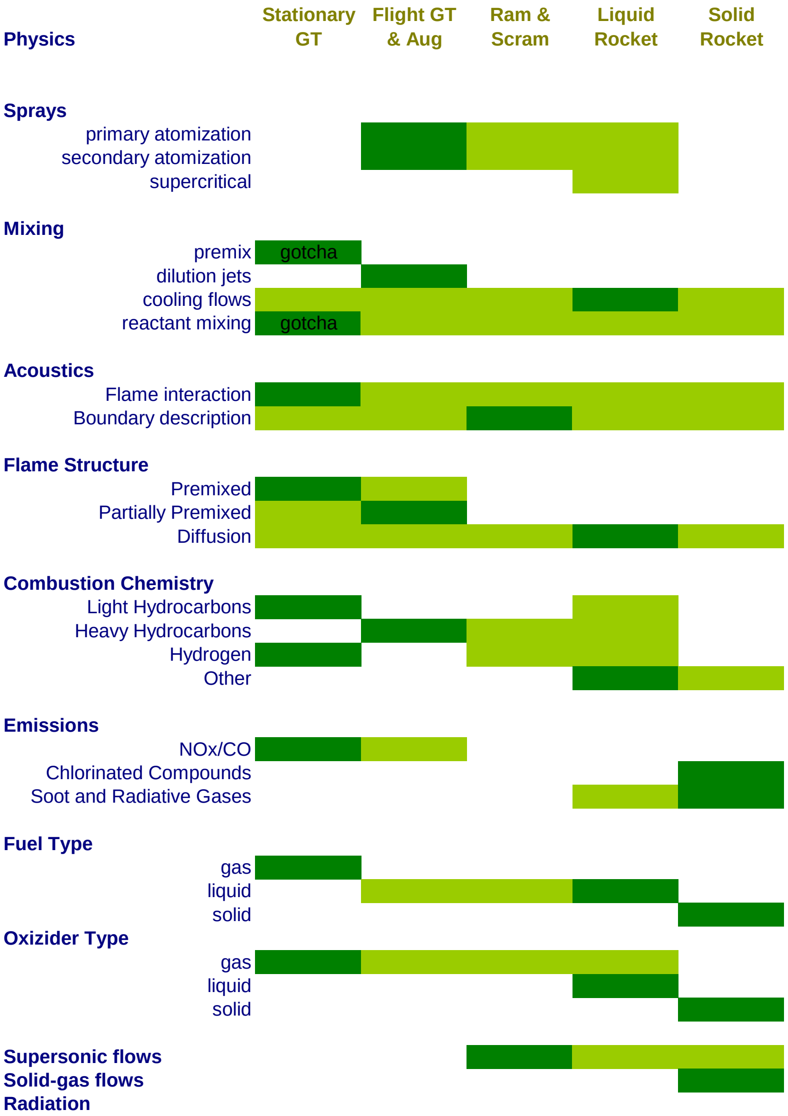
An opportunity for Cyber infrastructure? (cont.)

- **Can we gather validation data in an organized way ?**
  - Hard to develop a common format for aerothermal information

- **Can we use it to organize efforts on a larger scale and across applications?**

- **Ex: jet in a cross flow**
  - Propulsion gas turbines need to do sprays
    - Can’t do the spray problem if the gas problem can’t be done
  - Stationary power only cares about the gas problem
    - May not care at all about sprays
  - Concl: propulsion gas turbines has a bigger stake in stationary power than stationary power has in propulsion gas turbines.
    - *Make propulsion gas turbines a process owner*

Notional Shared and Common Processes



Physics	Stationary GT	Flight GT & Aug	Ram & Scram	Liquid Rocket	Solid Rocket
Sprays					
primary atomization		🟩	▨	▨	
secondary atomization		🟩	▨	▨	
supercritical				▨	
Mixing					
premix	🟩 gotcha				
dilution jets		🟩			
cooling flows	▨	▨	▨	🟩	▨
reactant mixing	🟩 gotcha	▨	▨	▨	▨
Acoustics					
Flame interaction	🟩	▨	▨	▨	▨
Boundary description	▨	▨	🟩	▨	▨
Flame Structure					
Premixed	🟩	▨			
Partially Premixed	▨	🟩			
Diffusion	▨	▨	▨	🟩	▨
Combustion Chemistry					
Light Hydrocarbons	🟩			▨	
Heavy Hydrocarbons		🟩	▨	▨	
Hydrogen	🟩		▨	▨	
Other				🟩	▨
Emissions					
NOx/CO	🟩	▨			
Chlorinated Compounds					🟩
Soot and Radiative Gases				▨	🟩
Fuel Type					
gas	🟩				
liquid		▨	▨	🟩	
solid					🟩
Oxizider Type					
gas	🟩	▨	▨	▨	
liquid				🟩	
solid					🟩
Supersonic flows			🟩	▨	▨
Solid-gas flows					🟩
Radiation					

🟩 Indicates possible process lead

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Summary: Putting Cyber Infrastructure to Work for Combustion: Advantages from an Applications Perspective

- **An opportunity to consolidate, organize, facilitate, and improve initiatives that have already been initiated.**
- **An opportunity to better bridge the gap between combustion research and the requirements of combustion applications.**
- **An opportunity to foster more effective collaborative combustion R&D across applications.**
- **An opportunity to promote higher quality combustion R&D.**
- **An opportunity to develop more effective advocacy for the combustion community.**