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Our Energy Future: The Role of High-End Computing …

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Simulation and Modeling at the Exascale for Energy, Ecological Sustainability & Global Security Town Hall Meeting

Argonne National Laboratory
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As a starting point, let's consider R.E. Smalley's view of Humanity's Top Ten Problems for the next 50 years …

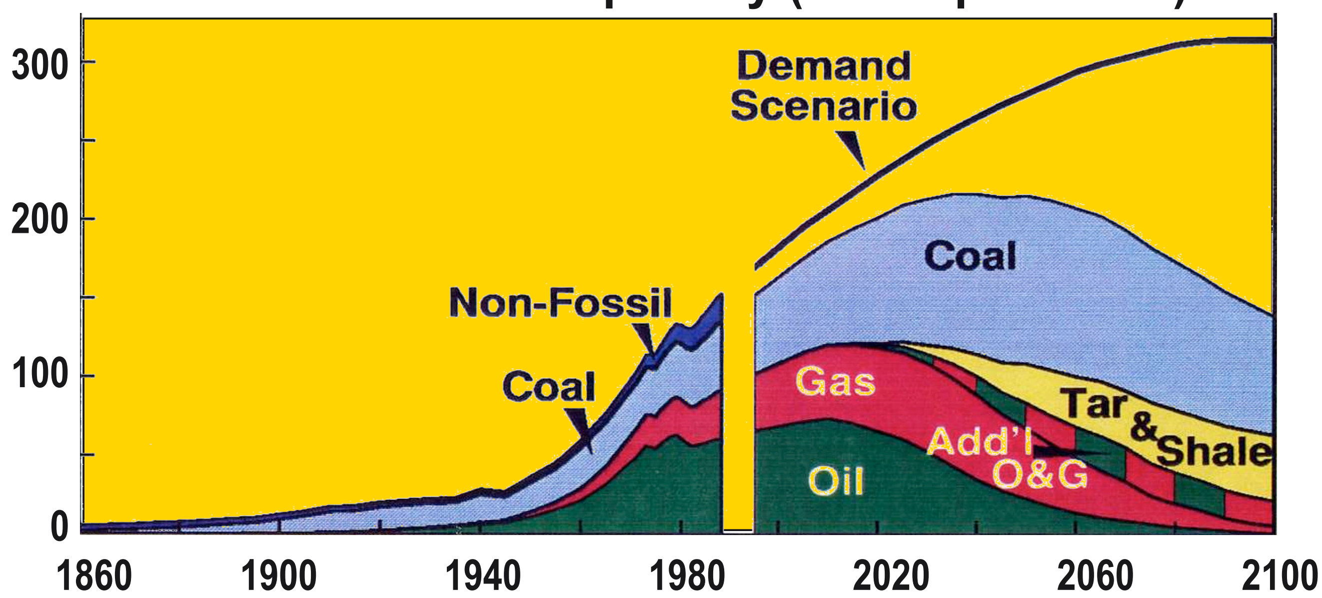
1. **ENERGY**
2. WATER
3. FOOD
4. ENVIRONMENT
5. POVERTY
6. TERRORISM & WAR
7. DISEASE
8. EDUCATION
9. DEMOCRACY
10. POPULATION

… that was the view in 2005 … and it hasn't changed a bit …

… and the context is, first, the economic world we live in, and the aspirations of the billions of folks who don't live here …

- Population growth projections
  - 2004: ~ 6.5 billion people
  - 2050: ~ 10 billion people
- Energy demand growth
  - Population increase
  - **Increased expectations**

Millions of Barrels per day ("Oil Equivalent")

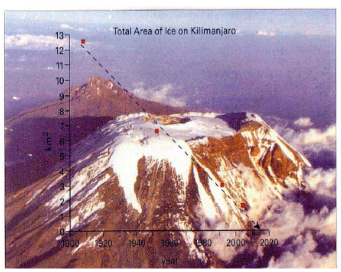


Source: John F. Bookout (President, Shell USA) ,"Two Centuries of Fossil Fuel Energy" International Geological Congress, Washington DC; July 10,1985. Episodes, vol. 12, 257-262 (1989).

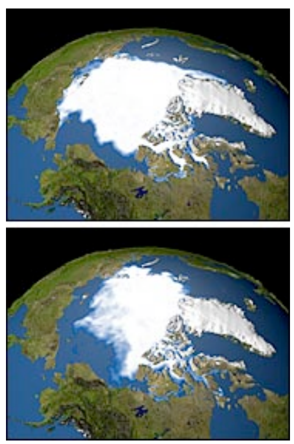
… and the context is, second, the environment we are creating …

- Surface, balloon & satellite temperature measurements agree: the mean temperature of the lower atmosphere is increasing
- Mean rates of evaporation & rainfall are increasing
- Coastal glaciers in most locations are retreating, Greenland’s ice cap is melting, sea ice is shrinking, and most mountain glaciers are disappearing
- Permafrost (in Canada and Siberia) is thawing
- Mean sea level is rising

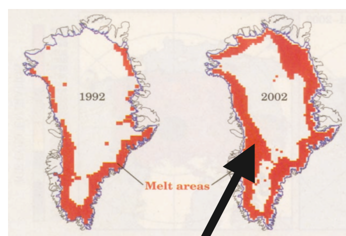
… and the evidence is becoming increasingly clear that much of these changes are the result of anthropogenic drivers



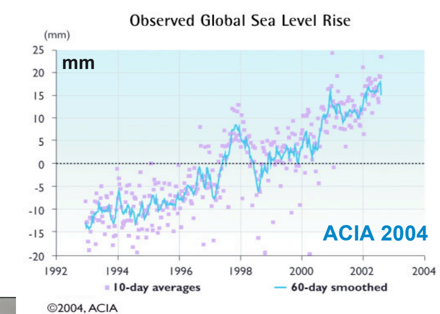
Ice cover on Mt. Kilimanjaro, 1912-2000

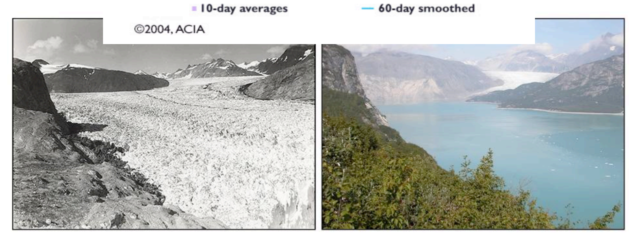


Arctic summer ice, 1979-2003



Greenland summer surface melt, 70 meters thinning in 5 years





Muir Glacier, Alaska, August 1941-2004

So what is the issue really?

- The "sustainability problem" with our current business-as-usual energy path is not that we're running out of energy.

- It's that we're running out of cheap and easy liquid fuels and running out of environment.

- So, the question really is: Are there sustainable solutions that
  - Don't bankrupt our economy, i.e., don't cause politically unpalatable changes in our quality of life?
  - Don't continue the destruction of our environment?

- And we need to remember: Solutions for the '1st World' may be irrelevant for the '3rd World' - and vice versa …

So, you might ask, why not just get going?

That is:

- Let's pick a few (1, 2, 3, … ?) plausible sustainable technologies …
- Invest heavily in R&D ("Manhattan Project"-style?), with the goals of
  - "Practical" deployment
  - "Reasonable" costs

- What could be wrong with that?

… after all, there are lots of plausible future energy supply options …

Type	Main Pros	Main Cons	Time frame
Conservation	Non-polluting; no global warming impacts; incremental	Does not solve base power problem or transport problem	Now
Wind/solar/tidal/ geothermal	Low or no pollution; no global warming impacts	Intermittent (need storage/R&D) and/or highly location-dependent; solar remains inefficient/expensive (R&D needed)	Now
Water ('hydro')	No pollution; no global warming impacts	Highly location-dependent; possible environmental damage	Now
Biodiesel	No global warming impact; positive for waste recycling; useful for transport	Non-carbon pollutants (NOx, particulates); possible agriculture impacts	Now
Ethanol	Little global warming impact; useful for transport	Agricultural impacts; current production methods energy-inefficient	Now
Coal/oil shale/tar sands	Very abundant; useful for transport	Major global warming impact in absence of effective/safe carbon sequestration	Now-50 years
Nuclear fission	Minimal global warming impact; potential long-term energy solution	Permanent waste storage in absence of closed fuel cycle; public perception concerns (safety, proliferation, …)	Now-50 years
Nuclear fusion	Minimal global warming impact	We don't know how to do this at present	?
Hydrogen	Depending on production mechanism, no global warming impact; transport fuel	Requires substantial primary energy source; production presently inefficient; storage and distribution major R&D issues	? for U.S.; now for Iceland (!)

What's wrong is that we know so little, in a highly constrained environment …

- First, the 'energy problem' is itself highly complex, with many 'parts' whose interactions are very poorly understood …
  - Power for transport vs. power for stationary applications
  - Centralized power production vs. distributed power production
- Second, there are the environmental impacts/considerations, esp. of the 'unintended consequences' variety …
  - Global warming: We have no choice but to implement primary energy sources that do not continue to impact the Earth's atmosphere
    - *If carbon-based fuels, then sequestration or renewables, or*
    - *Non-carbon based energy sources*
  - Minimization of toxic waste streams
  - Land use policies
    - *Food vs power*
    - *Conflicting land/water uses*

November 3, 2006-10
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Exploding U.S. Grain Demand for Automotive Fuel Threatens World Food Security and Political Stability
Lester R. Brown

- Third, there are the costs, many of which are very poorly accounted for …
  - True costs include environmental costs and life cycle costs …
    - *Who pays for cleaning up our atmosphere? Decommissioning power plants? What are the hidden and not-so-hidden subsidies?*

Worse yet, the current economics of oil are biased against substantive change …

- Gasoline and oil products in general are amazingly efficient in packaging energy in an
  - easily obtained and
  - easily transportable way

  That is, they're cheap, and much of the current price volatility is driven by politics, not scarcity
- **All** of the alternatives - except for one, namely increased efficiency of energy use - are burdened with one or more relative disadvantages, which come in many flavors and are apparently expensive (or perhaps impossible) to fix …
  - Environmentally not benign, or
  - Costly to produce/store/distribute, or
  - Inefficient, or
  - Ineffective (despite the hype …), or
  - Does not really exist, or
  - …
- These disadvantages are the fundamental reason that oil still dominates …

Why are the ‘fixes’ so expensive to achieve?

- Much of energy engineering R&D remains highly phenomenological
  - Results tend not be be predictive, but postdictive: “Edisonian” science
  - Parameter space exploration tends to be very expensive, and hence is rarely fully exploited
    - *Optimization tends to be inefficient and ineffective*
- Resulting high R&D investment costs are viewed as especially risky, given
  - the high price volatility of the current energy market
  - uncertainties in the regulatory processes, for example:
    - *Nuclear (NRC, …)*
    - *Coal (EPA, …)*
    - *Biofuels (Land use, …)*
- What’s needed?
  - Changing the nature of energy engineering R&D
  - Enabling validated modeling of systems-level risk assessments

So what does computing have to do with all that?

In a nutshell …

- The ability to quantitatively predict the behavior of
  - materials (whether simple solids, liquids and gases, or complex ‘composites’, and their interactions),
  - radiation and its interaction with matter,
  - complex integrated systems,

  both reveals our fundamental understanding of the underlying science as well as greatly impacts the economics of design, manufacture, licensing and ultimate operations of complex energy systems and the environment in which they function.

- This capability is based on science-based predictive modeling.
- Savings accrue in time and cost, and if risks are reduced, because margins are improved.
  - Rapid prototyping/parameter space exploration …: risk reduction, with improved margins
  - ‘Design-to-build’: Boeing, Frank Gehry, …
  - Full life-cycle cost accounting/technology comparisons, …

So, let's consider an example …

- Rebuilding the US nuclear energy industry …

- … with thanks to Andrew Siegel, Paul Fischer, Pino Palmiotti, Dave Nowak, and friends …

Start w/ the economics: The Nuclear (New Build) Economics … part 1

What is the cost of the "first new unit" ($/KW)?

	Industry Quotes, All-in $2006/KW	$1,800 - $2,000
Overnight Costs	Plant Structures & Equipment	$1,500 - $2,000
	+ NRC Filing Fees	$30 - $50
	+ Permitting & Development	$150 - $250
	+ Owners Cost	$500 - $750
	+ Contingency	$300 - $500
	= Total, All-in $2006/KW	$2,400 - $3,500
	+ Escalation	$700 - $900
	+ Interest During Construction	$900 - $1,100
	= Total, All-in $2020/KW	$4,000 - $5,500

FPL GROUP

Source: Industry and internal estimates

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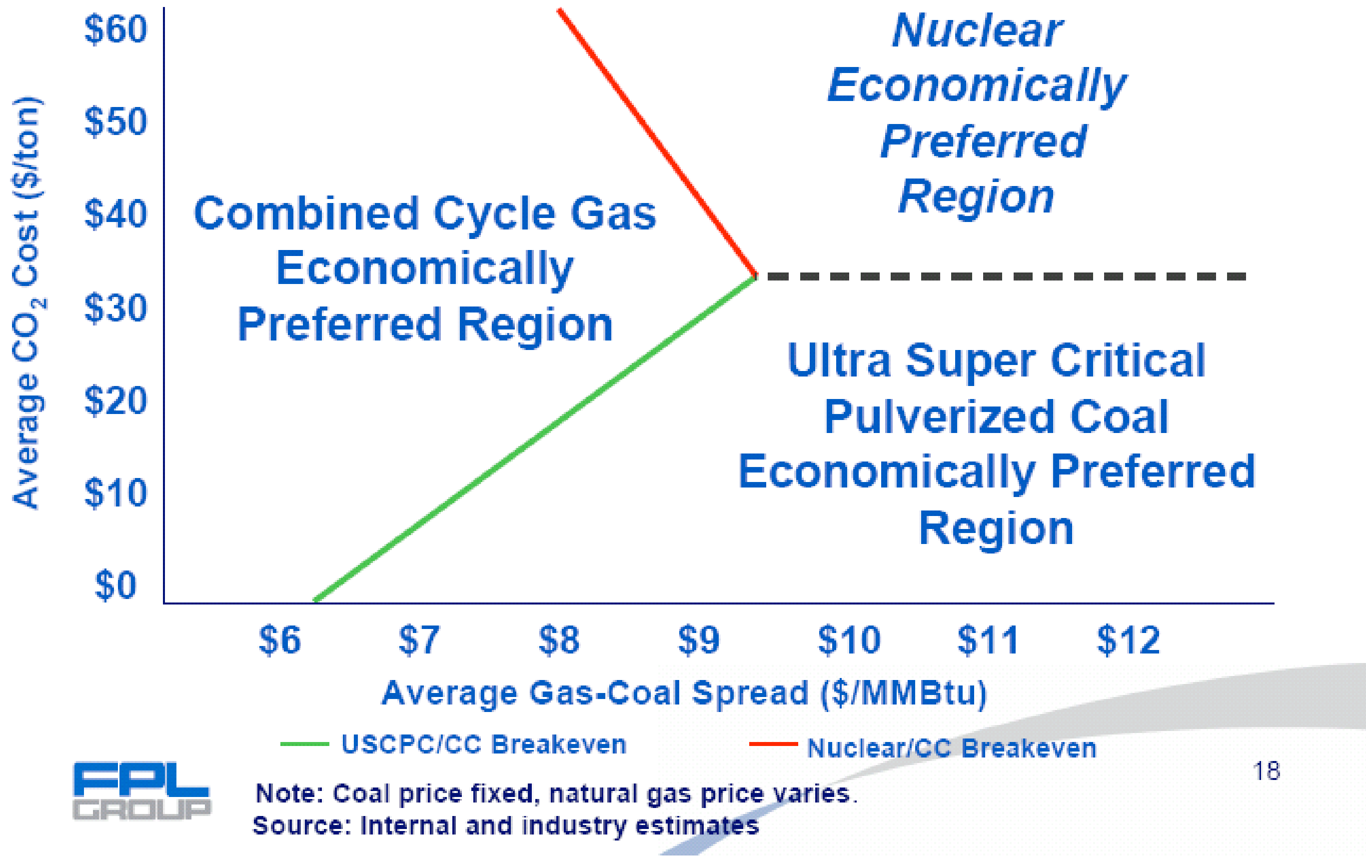
The Nuclear (New Build) Economics … part 2

CO_2 Pricing Impact …

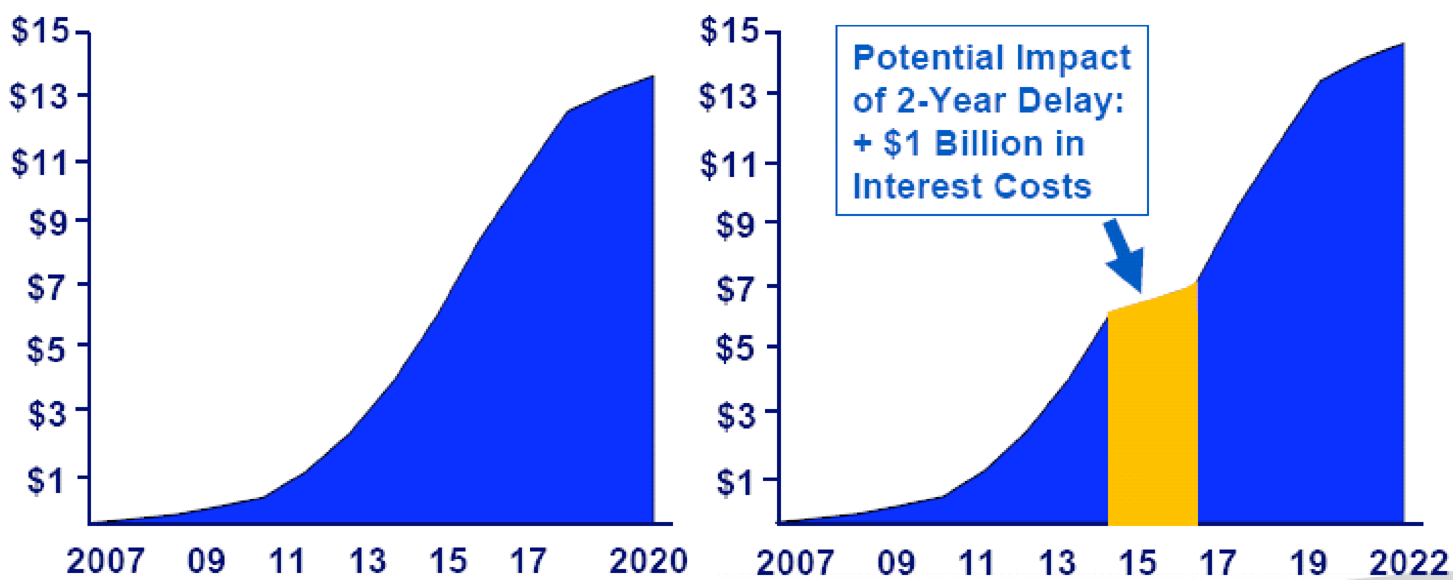


Note: Coal price fixed, natural gas price varies.
Source: Internal and industry estimates

The Nuclear (New Build) Economics … part 3

Cumulative All-In Spend Curve - Impact of Delays …

Total Cost: $13.5 Billion ($4,500/KW) | Total Cost: $14.5 Billion ($4,850/KW)



Source: Internal estimates based on 3,000 MW facility

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From what we know today, we can conclude …

- We know (now!) how to operate nuclear plants safely and effectively
  - Operating capacities ~90%
  - Production costs currently below $0.02/kWh (2005)

- Public perceptions of nuclear energy remain mixed (though changing!)

- We know how to build new nuclear plants, but
  - Rigorous safety and performance analyses of reactors, waste disposal, fuel fabrication, … , remain mostly phenomenological
    - *Trial-and-error — not science — still forms the basis for much of the discipline*
    - *Dated analytical tools handicap both design & regulation*
  - Major alterations in reactor design, fuel assemblies, waste forms, … , currently require extensive phenomenological R&D - making optimization, especially at the integrated systems level, prohibitive
  - These issues largely drive both construction and operations costs … and affect public perceptions …

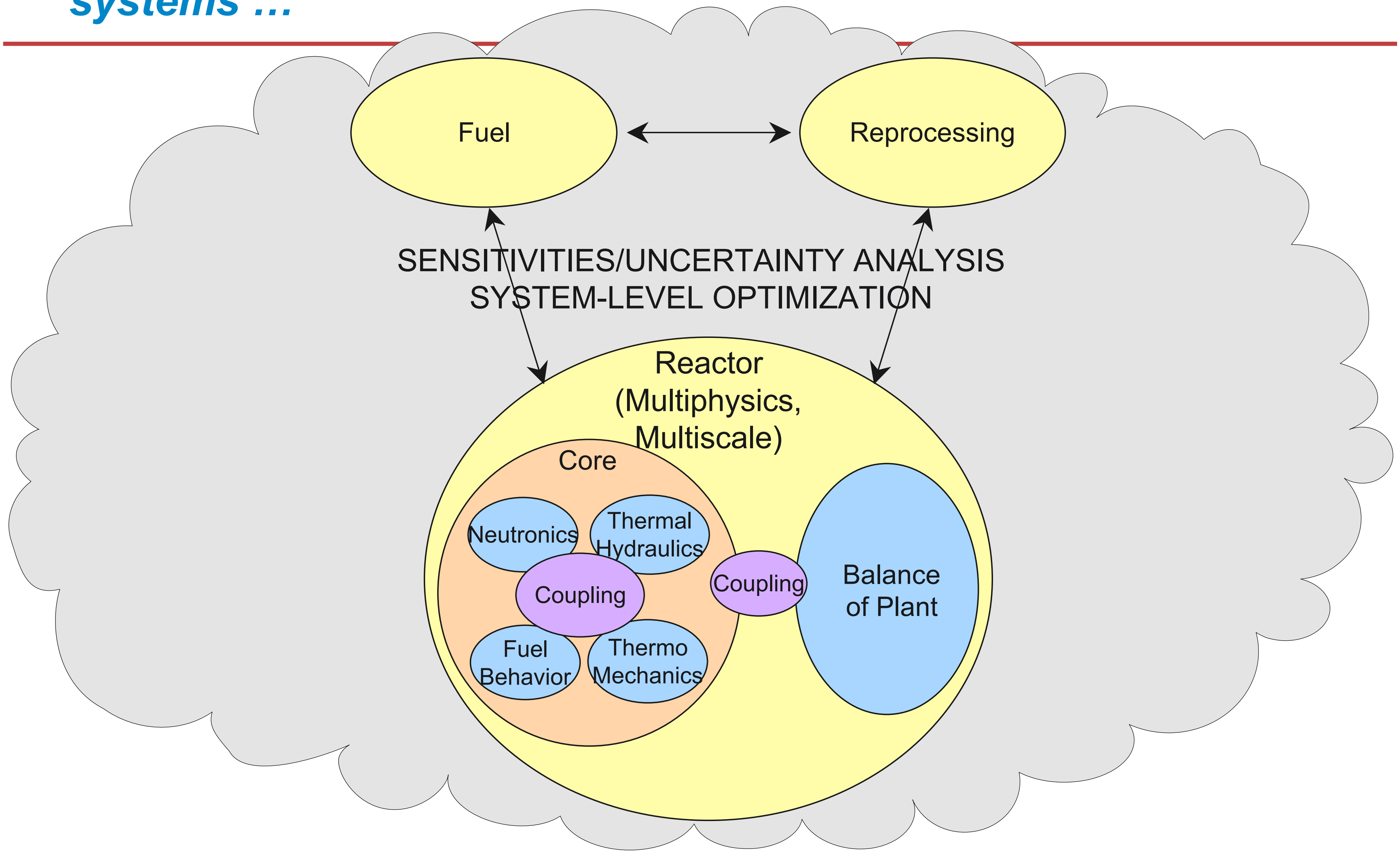
What needs to change?

- **The public perception and acceptance**
  - Reactor safety and domestic nuclear waste disposal
    - *Demonstrated capabilities for constraining safety and proliferation risks*
    - *Demonstrably defusing the domestic 'spent fuel' issue - it's not 'spent'!!!*
  - International nonproliferation
    - *Demonstrating an end-to-end fuel cycle that sustains nuclear energy expansion without increasing (indeed, hopefully decreasing) proliferation risks*
  - The role of nuclear energy in addressing global warming
    - *Demonstrably affecting current atmospheric CO_2 balance (as USA is 20% nuclear)*
    - *Demonstrably affecting future atmospheric CO_2 balance*
  - The role of nuclear energy in US energy security
    - *Demonstrably impacting overall US energy economics and energy use*
    - *Demonstrably impacting US competitiveness in energy industrial sector*
- **The economics**
  - Dramatically reduce the economic penalty imposed by regulatory systems that produce archaic design margins
  - Allow for effective 'local' and systems-level optimization

… and that is how HPC enters the picture …

- There are three highly interconnected methodologies that can get us there
  - Experiment/phenomenology
  - Theory
  - Simulations
- Modern scientific enquiry entails these three critical axes of investigation, that together provide as complete a picture as possible of the relevant physics/engineering phenomena.
  - Experiment, theory, and simulation do not compete, and none alone is without its flaws
    - ***Experiment*** *is expensive, is sometimes dangerous, and is very difficult to get precise answers at more than a few spatial or temporal locations.*
    - ***Theory*** *is limited to very idealized cases, and does not work well for highly non-linear phenomena, detailed geometries, etc.*
    - ***Simulation****'s issues relate to the fidelity of the models, numerical instability, etc., but is extremely inexpensive, predictive, and can give incredibly detailed data sets.*
  - We want to do fewer, cheaper, and smarter experiments, augment our theories (such has been done in combustion community), guide our judgment, ...

What we are aiming for — Full coupling of nuclear energy systems …



To illustrate, consider how we can respond to this 'vision': SHARP (Simulation-based High-efficiency Advanced Reactor Prototyping)

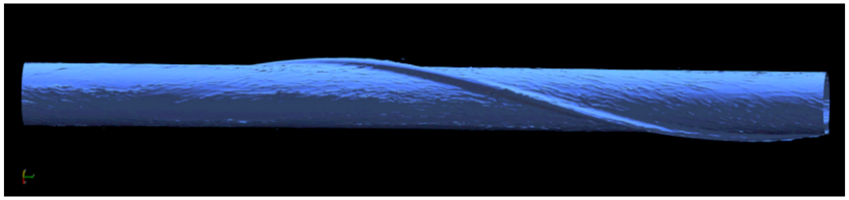
- **Long-Term Objectives (~ 5 years):**
  Exploit DOE's Petascale computing facilities (P > 100,000 processors) and state-of-the-art simulation capabilities for dynamic coupled thermal-hydraulics (TH)-neutronics-fuel/structural material predictive capabilities at the design level
  - Planned capability includes fast transient response for coupled TH/neutronics
  - Provide validated *predictive* capabilities, based on a fidelity hierarchy
  - Allow for distinct modeling capabilities (DNS, LES, RANS, …), based on the level of detail/fidelity required
- Provide coupled simulation capability (e.g., allow for systems-level optimization)
- Ultimately (=10 years), cover all aspects of reactor (balance of plant) **& "I/O"**

E.g., aim to answer the questions that industry wants answered

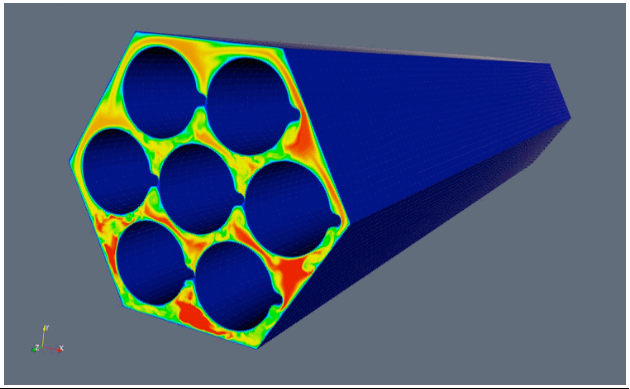
- **Short-term objectives (= this year):**
- Beginning with the core, establish high-fidelity TH baselines for multi-pin subassemblies – seeking to understand peak temperature limitations within a single subassembly
- Provide steady-state coupled TH/neutronics simulation capability

What the ANL group has accomplished to date …

- Single pin thermal hydraulics calculation …
  - First detailed study of the effects of wire wrap on flow near a pin
  - Demonstrated significant variations in the effects of the wire wrap on the nearby flow, quite different from previous expectations
  - This is important because the wire wrap is intended to promote mixing between channels adjacent to pins

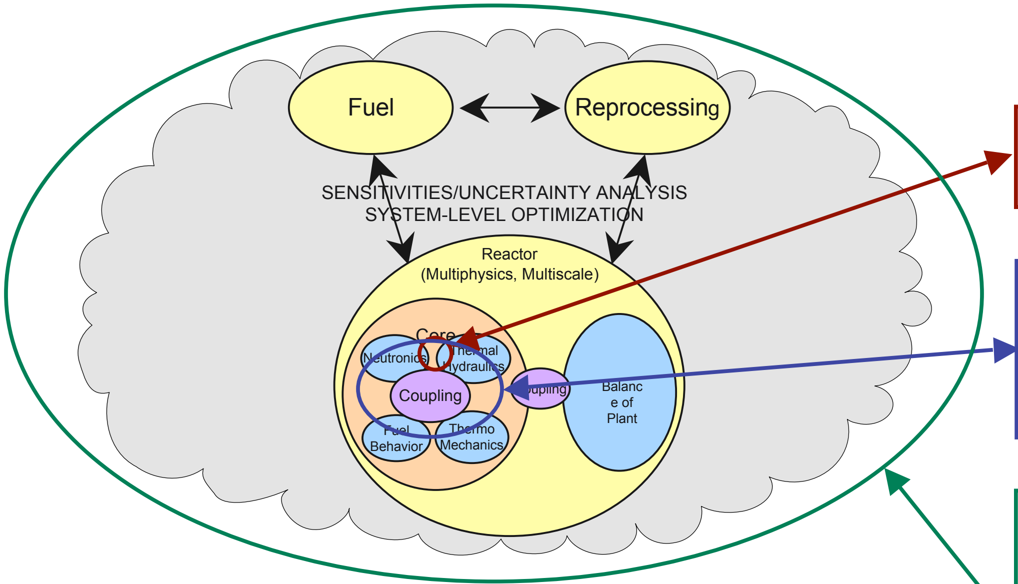


- LES-based simulation of 7-pin configuration with wire wrap
  - DOE 2007 INCITE award for 1 million node hours on BG/L for this task
  - More pins possible with BG/P after October 2007
  - Allows us to explore (undesired) temp. fluctuations
  - Will allow study of bypass flow in side channels
  - Will allow systematic optimization of structural geometry
  - That is: **rapid prototyping**



Axial velocity distribution, start-up flow in 7 pin subassembly 18 subchannels

… so where does exascale computing enter?



This is what we did.

Petascale computing will get us this far …

Exascale computing and beyond will be needed to complete the picture …

- … and this is only for the case of nuclear energy, where the ‘existence proof’ has been pretty much understood …

… and many similarly-scaled energy problem areas exist to challenge our computing abilities

- Science-based engineering of renewable energy technologies
- Full life-cycle cost and environmental impact comparisons for competing energy technologies
- Coupling energy systems, climatic and econometric analyses
- …
- In all these cases, the way we do 'business' must transition to a modern science and computations-based discipline
  - *High fidelity (science-based) integrated simulations must form the core of the design efforts and allow for rapid prototyping*
  - *Science-based, validated modeling at both the detailed (small-scale) and systems-level must be part of the core capabilities*
  - *The field must generate internal technical excitement to attract the "best and the brightest"*
- … and all this can only be realized by appropriate investments, including a roadmap to exascale computing and beyond …

… which brings us to questions and discussion

By Michael Ramirez, *Investor's Business Daily*, Copley News Service