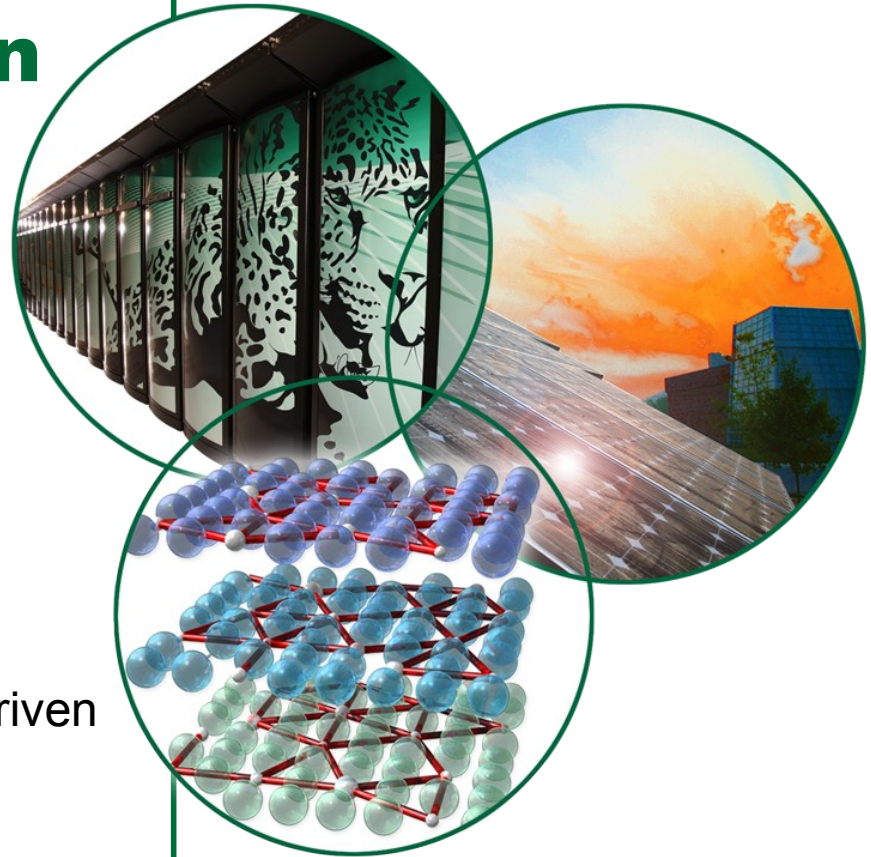# Computational Grand Challenges and Possibilities for Molten Fuel ADS Studies

Jay Jay Billings

1st International Workshop on Accelerator-Driven Sub-Critical Systems & Thorium Utilization

Virginia Tech

September 27, 2010

Disclaimer and Outline

Credit: xkcd

- **Nuclear Energy Modeling and Simulation**
  - **Current Efforts**
  - **Programmatic Challenges**
- **Computational Grand Challenges for a GEMSTAR system**
 - **Some things I've been pondering since a visit from Bruce...**

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Integrated Device-Level Modeling and Simulation

- ## Too costly to "random walk" to alternative energy sources

  - **A fully-crossed design with 10-factors at 2-levels requires 1024 experiments!**

  - **Impossible for "big devices"**

    - **A nuclear reactor**
    - **The energy grid**

2^3 Factorial Design

Three Independent Variables
Two Levels of Each Variable
Eight Test Conditions

Variable A, Level 2
Variable C, Level 2
Variable B, Level 1
Variable B, Level 2
Variable C, Level 1
Variable A, Level 1

Example Test Condition:
A1, B2, C1

- ## Must switch to a *predictive* science paradigm

  - **Accurately and precisely reproduce the behavior of known systems**

  - **Describe a NEW system, predict its behavior**

What is the payoff?

$$\$\$\$\$\$\$\$\$$$

SFR
Sodium-Cooled Fast Reactor
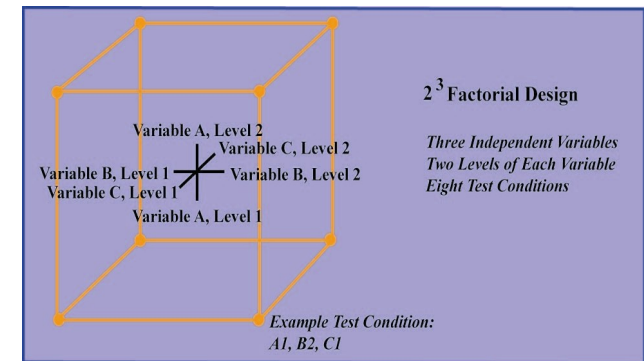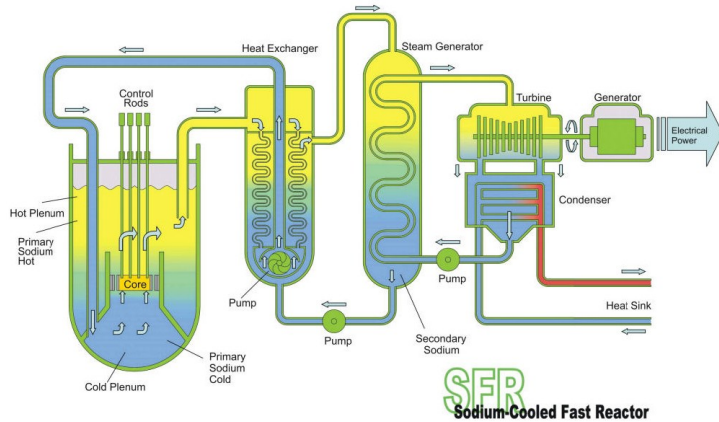
$15B/plant & maybe
$500M for research
reactors

$100M initially
+ $10M/yr +
FTEs

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Existing Programs

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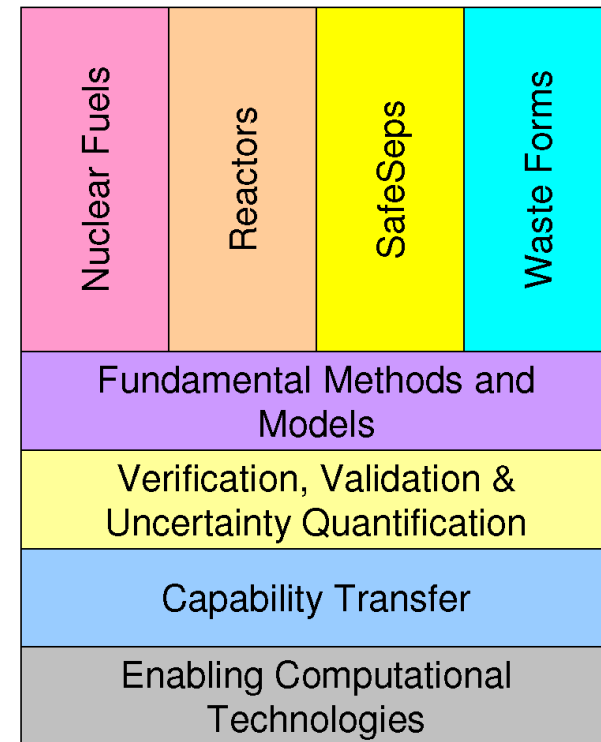# Existing Programs – Nuclear Energy Advanced Modeling and Simulation

Vision:

- To rapidly create and deploy "science-based" verified and validated modeling and simulation capabilities essential for the design, implementation, and operation of future nuclear energy systems with the goal of improving U.S. energy security
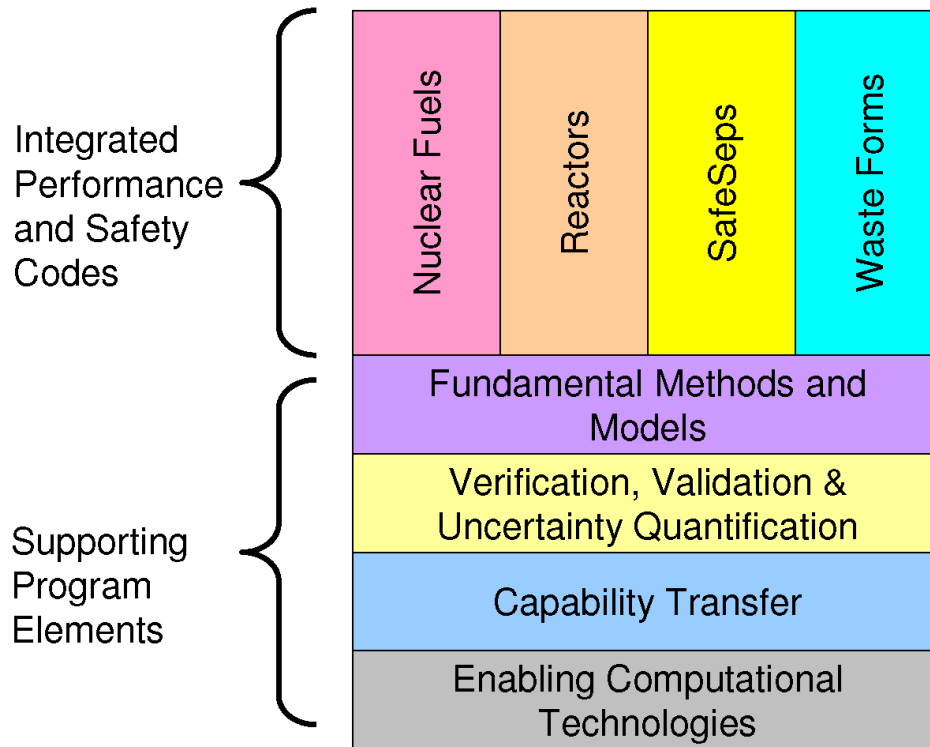
Integrated Performance and Safety Codes

- Nuclear Fuels
- Reactors
- SafeSeps
- Waste Forms

Supporting Program Elements

- Fundamental Methods and Models
- Verification, Validation & Uncertainty Quantification
- Capability Transfer
- Enabling Computational Technologies

- 3D, 2D, 1D
- Science Based Physical Behaviors
- High Resolution
- Integrated Systems
- Advanced Computing

Science Based Nuclear Energy Systems

NEAMS

- Low Dimensionality
- Test Based Physical Behaviors
- Low Resolution
- Uncoupled Systems
- Workstation Computing

Evolutionary

2008   2018   2030

NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

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Existing Programs – Nuclear Energy Advanced Modeling and Simulation - 2

Integrated Performance and Safety Codes

Nuclear Fuels	Reactors	SafeSeps	Waste Forms

Supporting Program Elements

Fundamental Methods and Models

Verification, Validation & Uncertainty Quantification

Capability Transfer

Enabling Computational Technologies

Please keep this in the back of your mind... I want to come back to it...

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Existing Programs – Consortium for Advanced Simulations of LWRS

First DOE Energy Innovation Hub

Task 1: Develop computer models that simulate nuclear power plant operations, forming a "virtual reactor" for the predictive simulation of light water reactors.

Task 2: Use computer models to reduce capital and operating costs per unit of energy, extend the lifetime of the existing U.S. Reactor fleet, and reduce nuclear waste volume
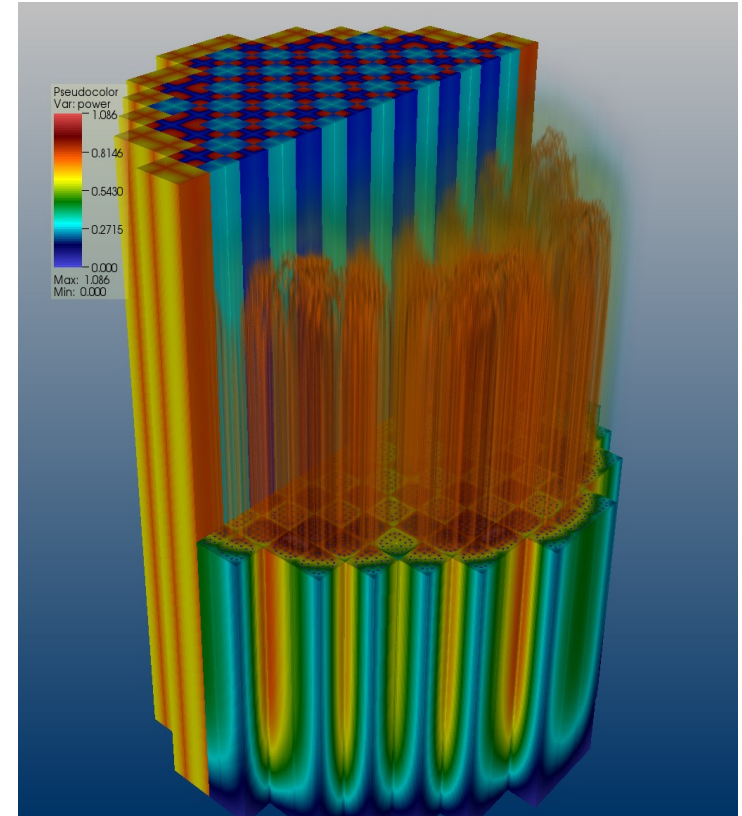
# Why is this challenging?

- **Scientifically**
  - Much new scientific research and development is required, at multiple levels
  - New software under constant development

- **Organizationally**
  - Large geographically distributed teams of *domain* scientists
 - Different teams has different schedules, approaches

- **Computationally**
  - Must run on laptops & supercomputers, Windows, Mac, Linux
  - Parallelism: 1-2 cores to 1million-1 billion cores, GPUs, and more

SFR
Sodium-Cooled Fast Reactor

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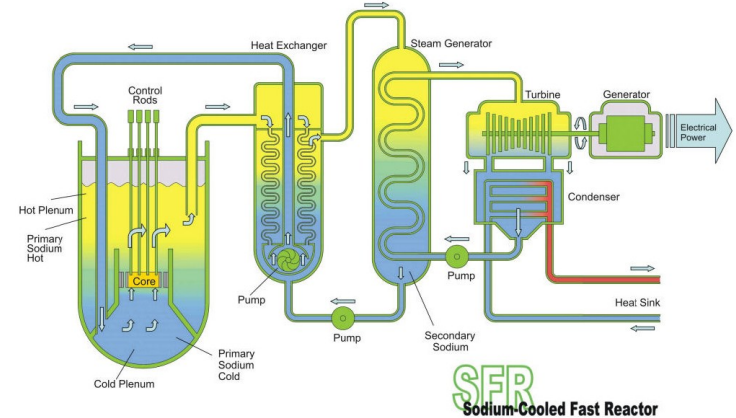
Similar Possibilities for Molten Fuel ADS

#1 Non-Computational Grand Challenge for Molten Fuel ADS

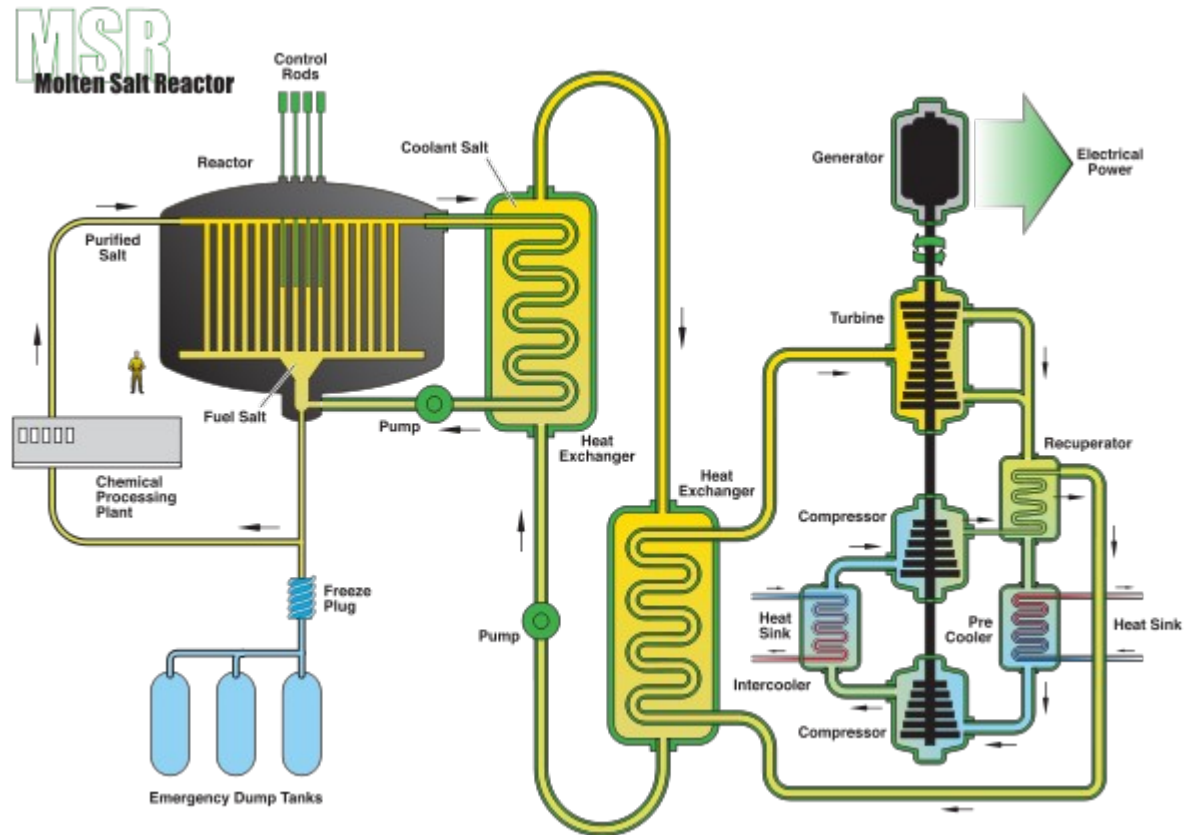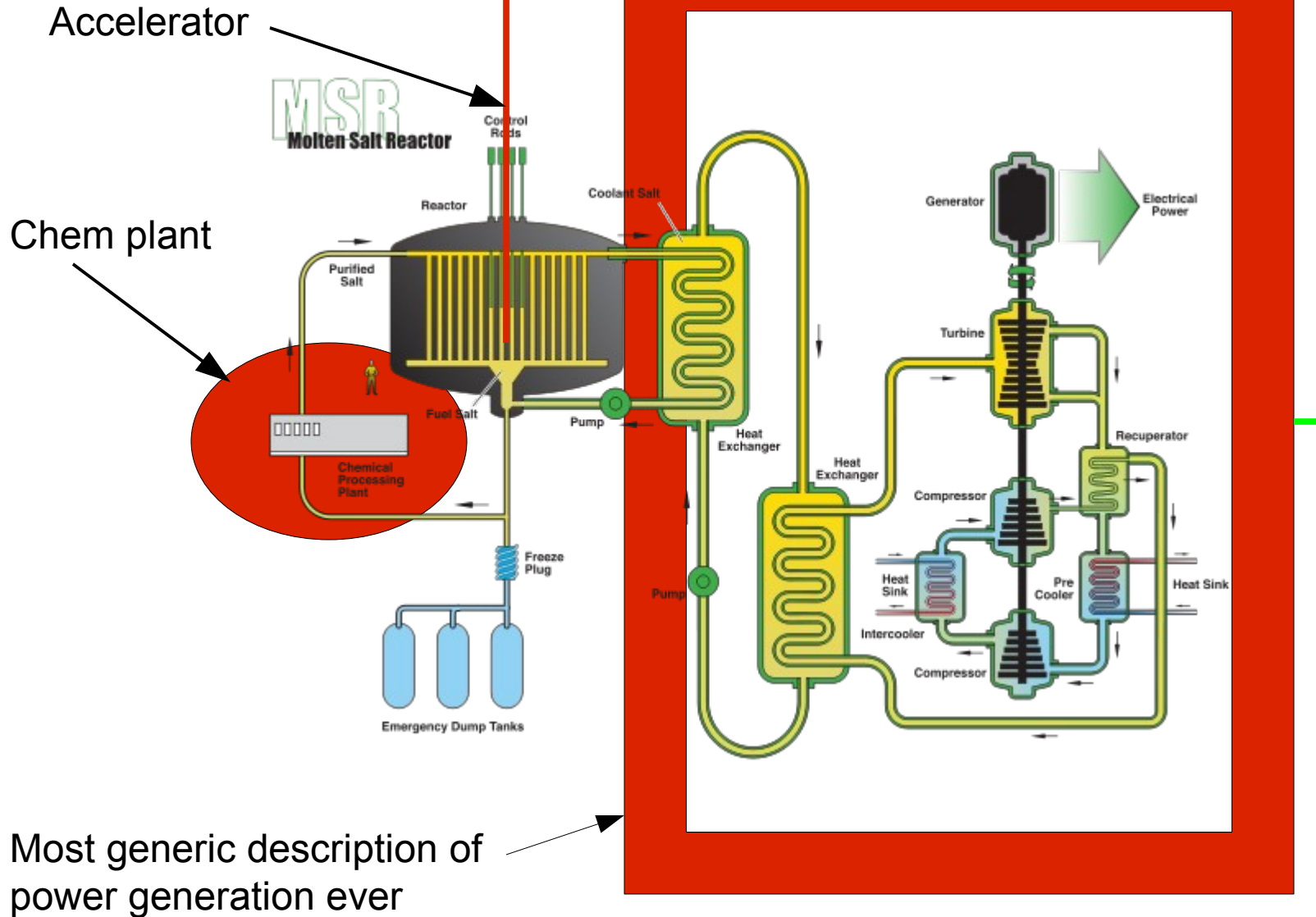Consider GEMSTAR...
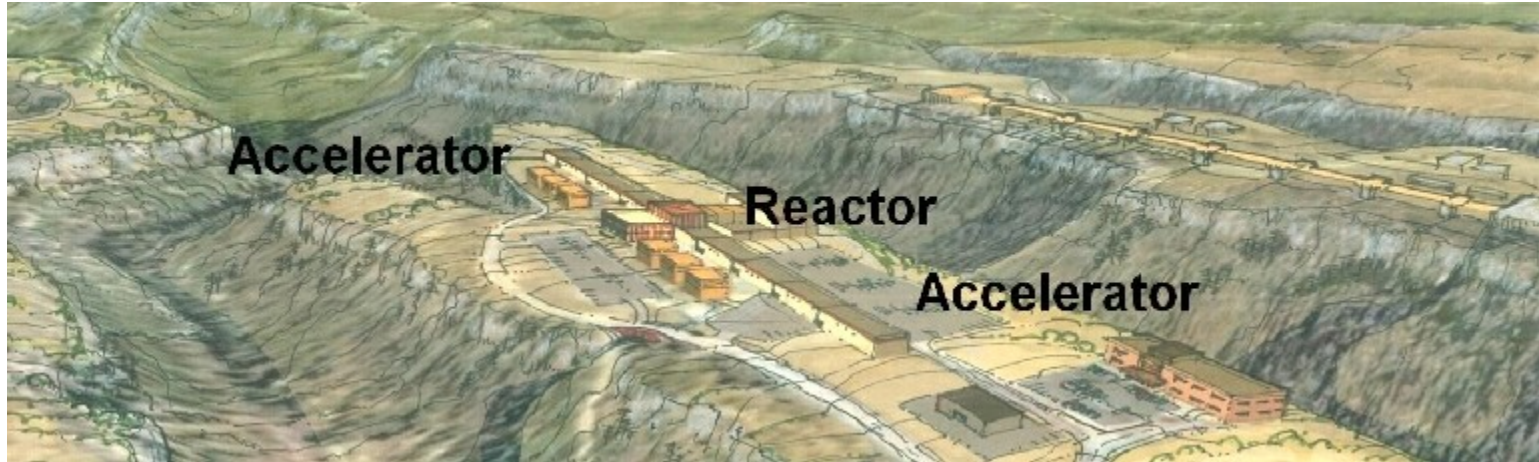
I bet the NRC says....

"They want to do WHAT!?"

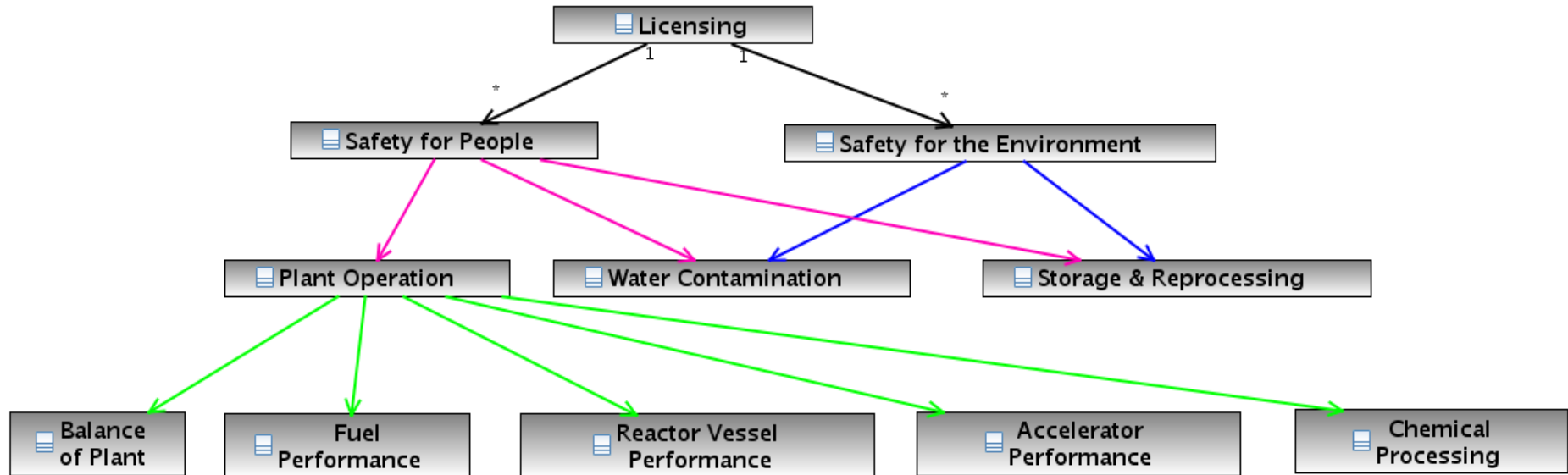**High-Performance Computing can help with the "WHAT!?"**

Reactor by parts

Reactor by parts - 2

Accelerator

Chem plant

MSR
Molten Salt Reactor

Control Rods

Reactor

Coolant Salt

Generator

Electrical Power

Purified Salt

Fuel Salt

Pump

Heat Exchanger

Turbine

Recuperator

Chemical Processing Plant

Heat Exchanger

Compressor

Pump

Freeze Plug

Heat Sink

Pre Cooler

Heat Sink

Intercooler

Compressor

Emergency Dump Tanks

Most generic description of power generation ever

Decomposing the problem

Improving the Science with HPC

- **What are the "pain points?"**
  - The accelerator
  - The fuel
  - The chemical processing
  - Balancing the Plant (including Accelerator)

- **M&S can…**
  - Simulate the *WHOLE* plant
  - Investigate the ADS-MSR coupling in detail
  - "Specialize" the accelerator
  - Optimize the chemical processing
  - Paint a prettier picture to answer the "WHAT!?"

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Improving the Comfort Level with HPC

- **Verification and Validation, Uncertainty Quantification**
    - Take the high-ground on testing… (use SCALE first!)
    - Parameter studies: consider 250,000 cpus per hour
    - In-depth Physics & Chemistry investigations:
        - Computation + Experiment

- **"Operational Clarity"**
    - Model & Simulate the operational systems
        - Things observed by sensors
        - Simulate the Instrumentation and Control systems

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Back to that NEAMS Picture...
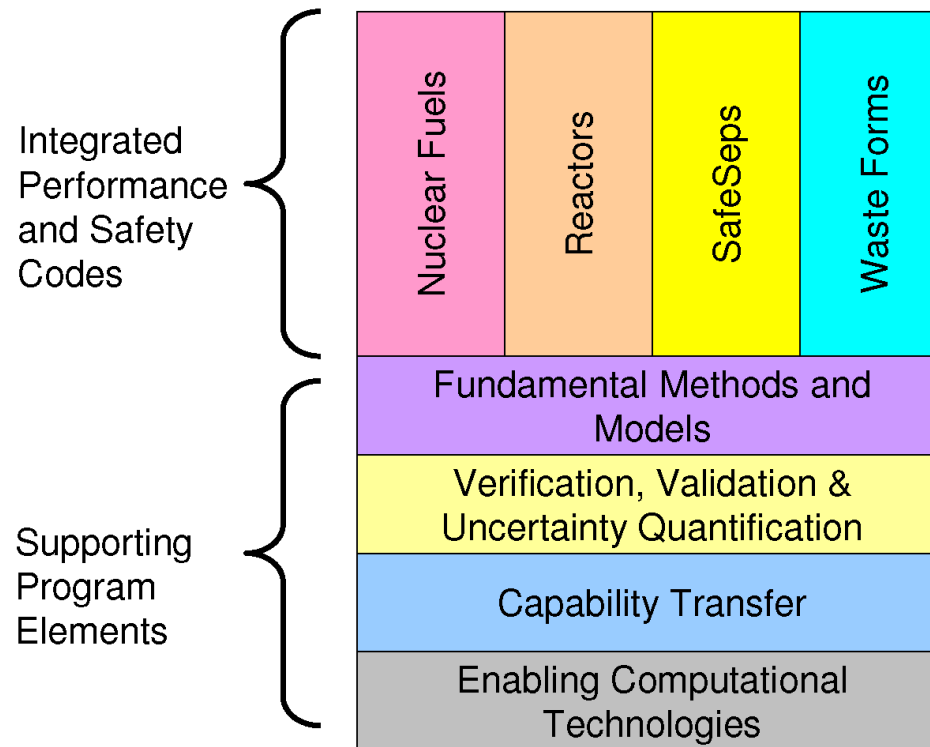
Where's our ADS column?

Final Thoughts

- **Challenges**
  - **Figure out as much as possible about that accelerator without building a bunch of them!**
  - **Learn about the chemical processing!**
  - **Assist plant designers with information gathering and I&C concerns**
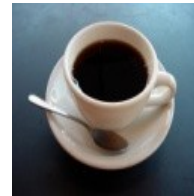- **Possibilities**
  - **Measure twice, cut once with a *virtual* liquid-fuel ADS system**

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Special Thanks

Thanks very much to the organizers and to the members of the audience for attending!

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