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SCI www.sci.utah.edu

Berkeley UNIVERSITY OF CALIFORNIA

BYU BRIGHAM YOUNG UNIVERSITY

NNSA National Nuclear Security Administration

CARBON CAPTURE MULTIDISCIPLINARY SIMULATION CENTER

http://ccmsc.utah.edu

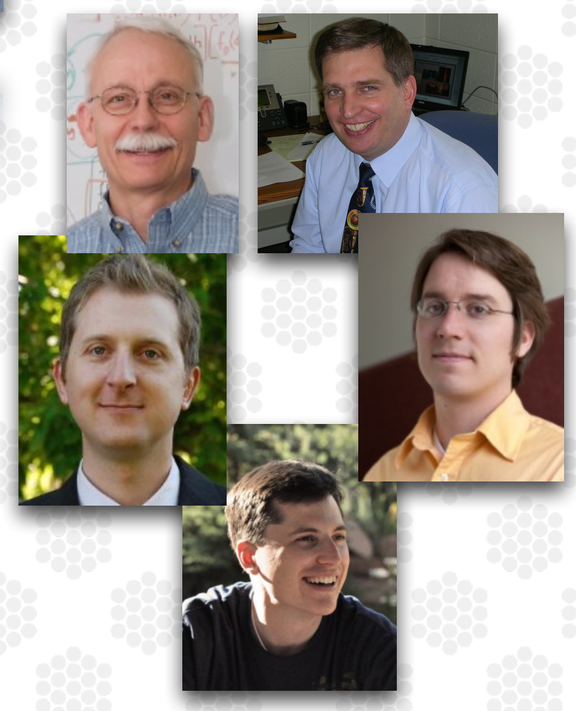
CCMSC

CARBON CAPTURE
MULTIDISCIPLINARY
SIMULATION CENTER

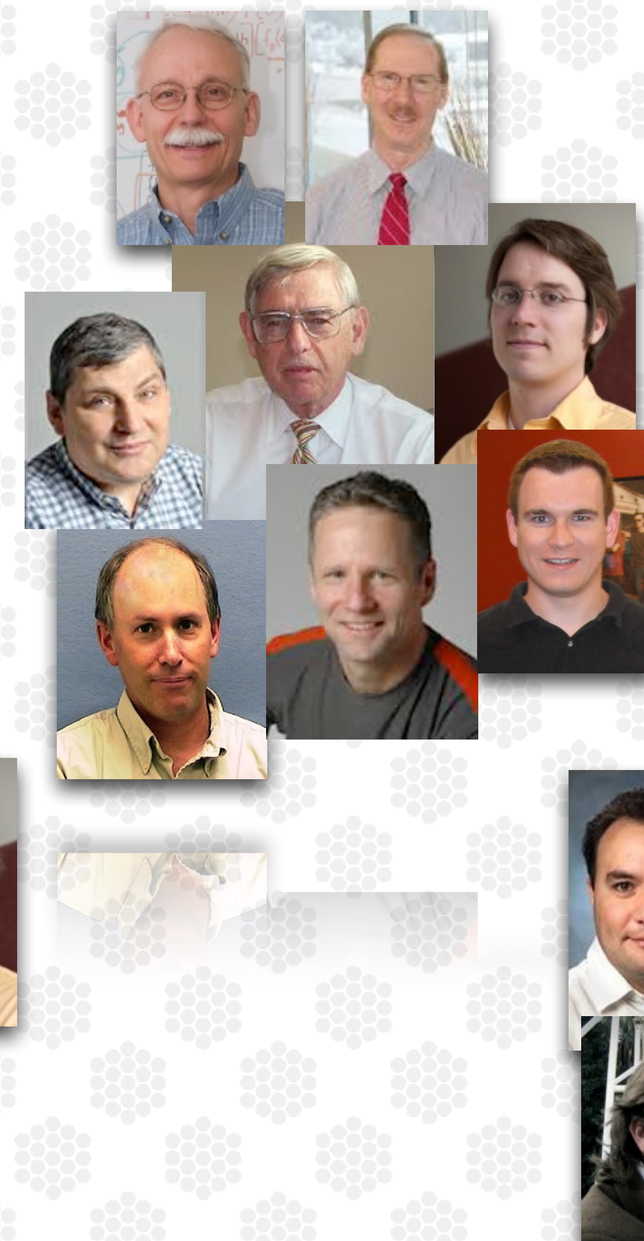
Executive Committee

Education and Outreach

Predictive Science



V&V/UQ



Exascale Computing & Software

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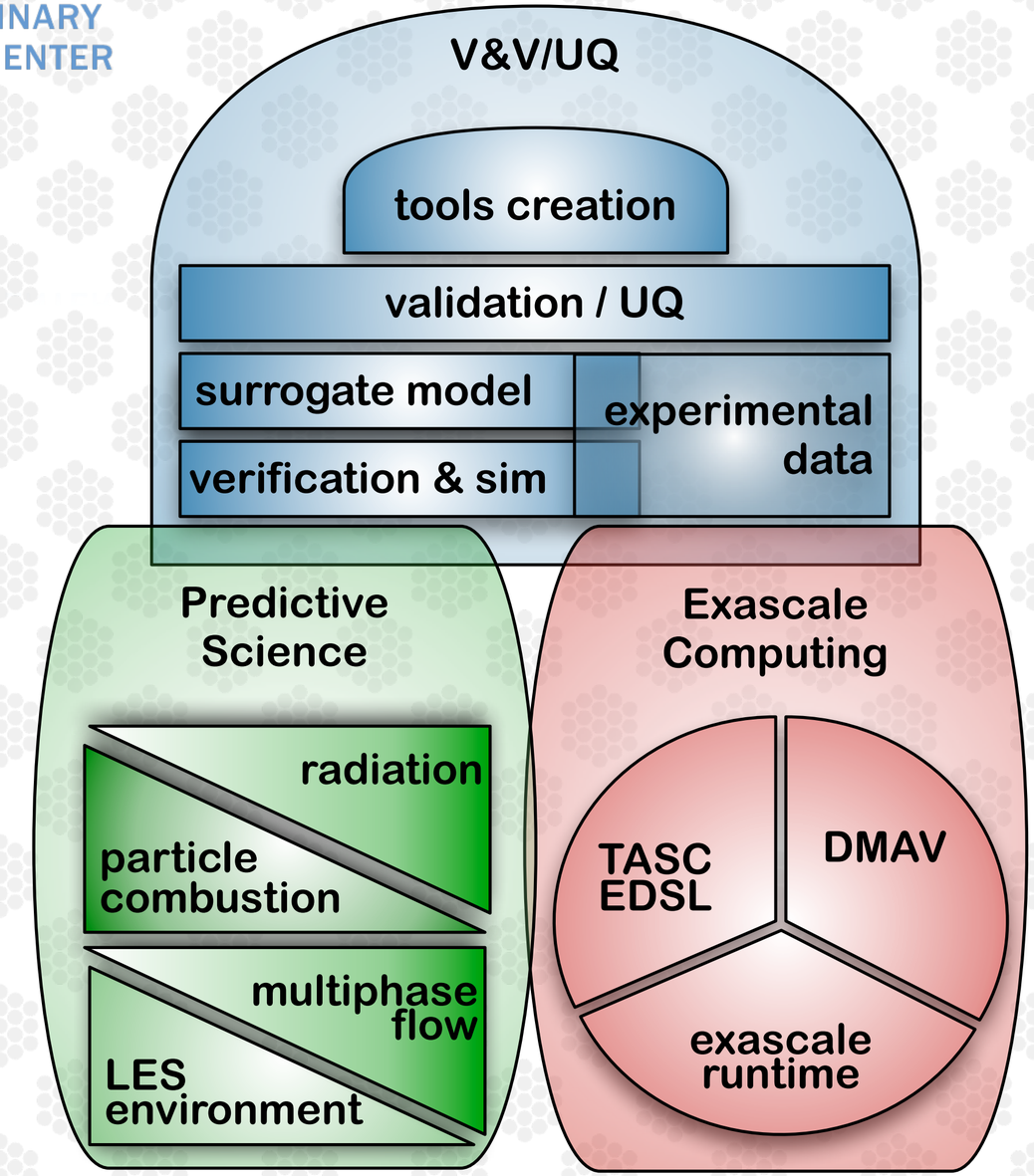

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Overarching Application

- high efficiency advanced ultra-supercritical (AUSC) oxy-coal tangentially-fired power boiler
  - *extreme computing*
  - *predictive science w hybrid validation/UQ*
    - expensive function evaluation
    - expensive data
  - *rapid design and deployment w Alstom*

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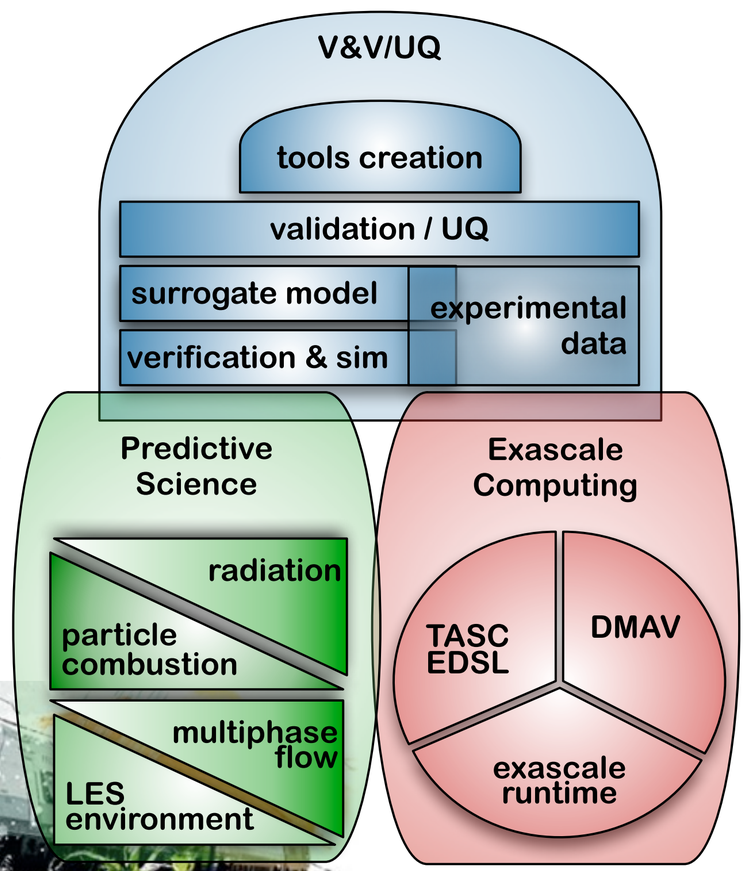
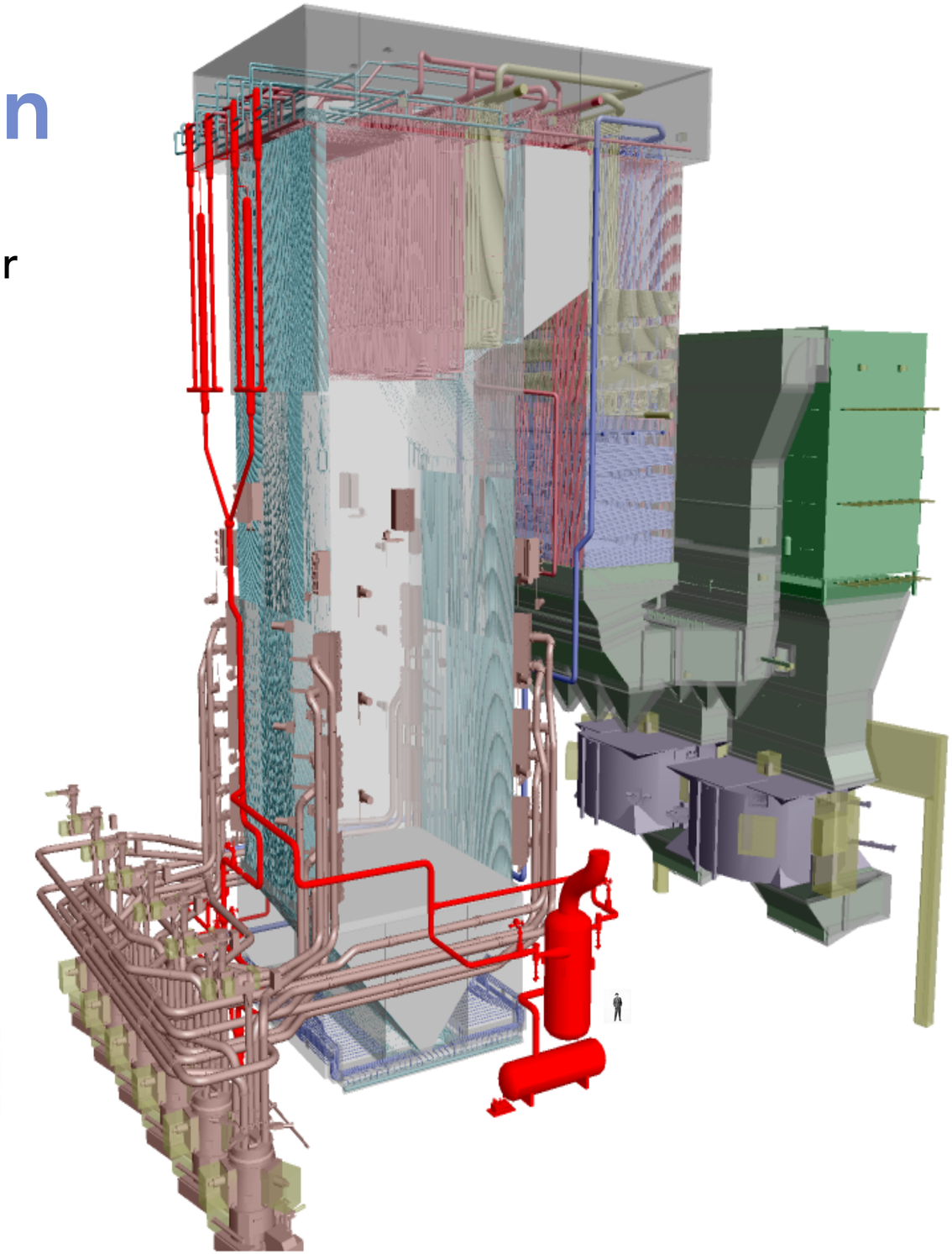
- *global reach: present in 100 countries*
- *2011/12 sales: $26.5 billion*
- *93,000 employees*

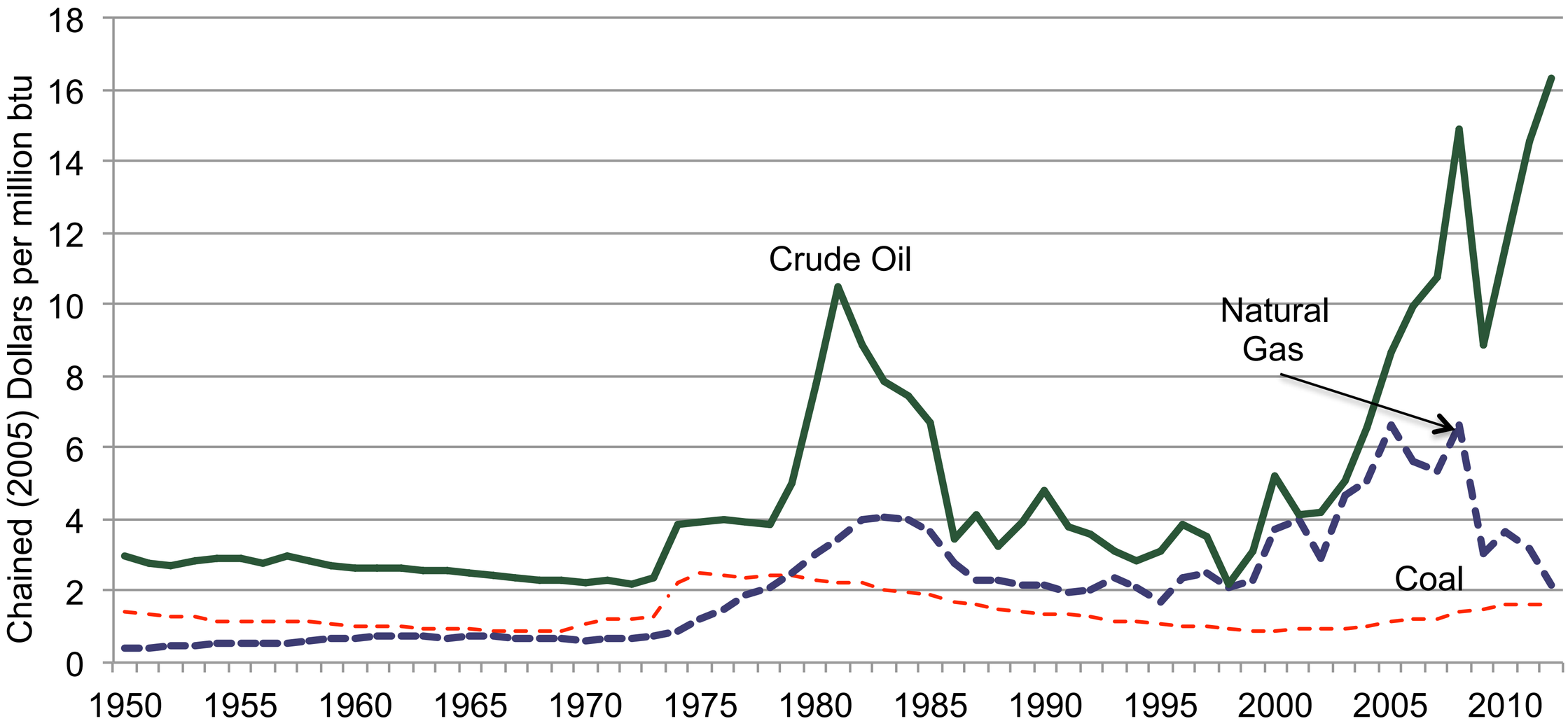




Why?

the need for cheap clean energy

	2012	2013	2014
Natural gas	$3.39	$4.49	$4.64
Coal	$2.40	$2.36	$2.40



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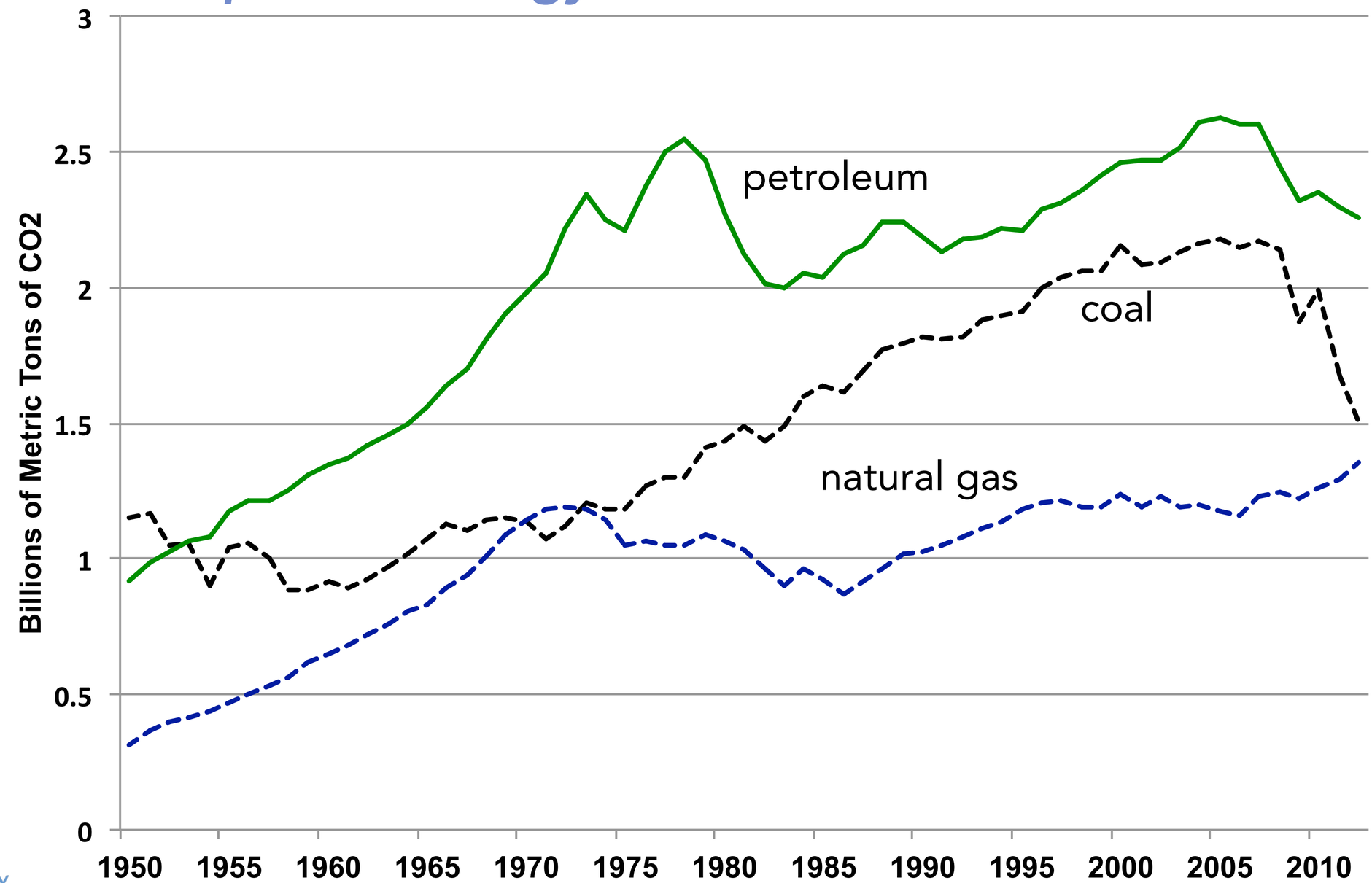
Why?

the need for cheap clean energy

	2012	2013	2014
Natural gas	$3.39	$4.49	$4.64
Coal	$2.40	$2.36	$2.40

- EPA: "new fossil fuel fired power plants meet an output based standard of 1,100 pounds of CO_2 per megawatt hour (lb CO_2/MWh gross)"



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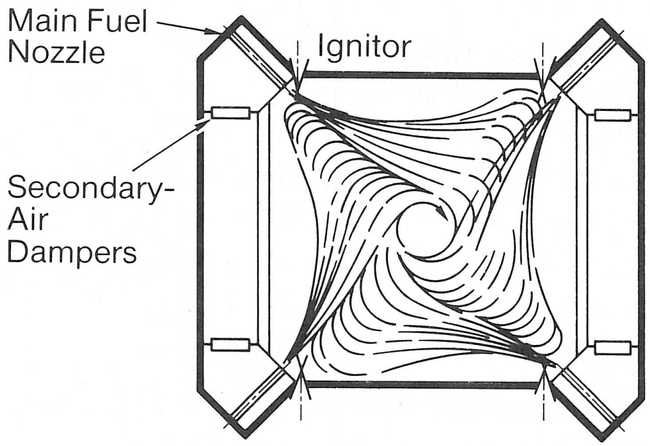
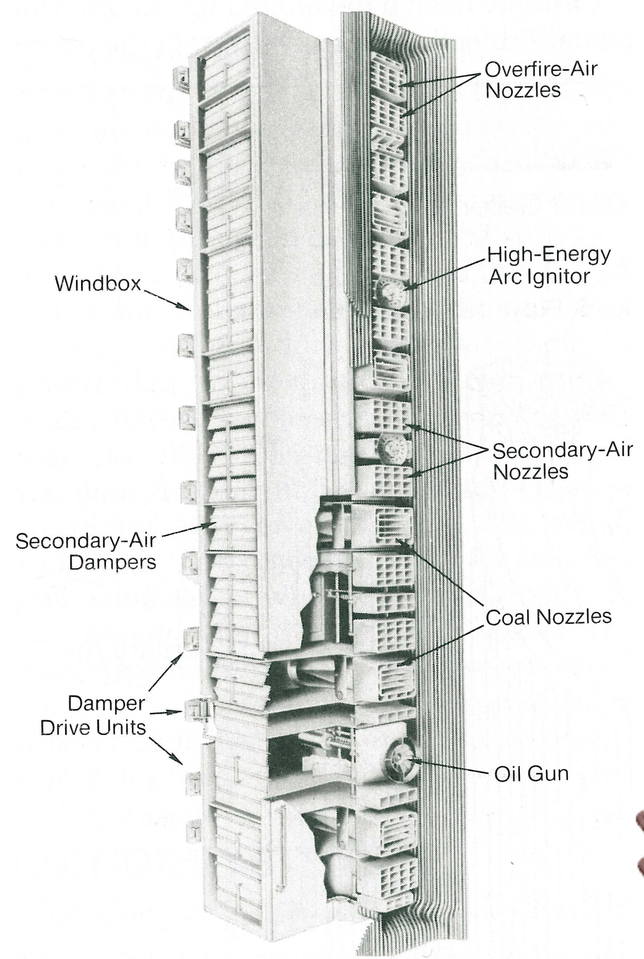
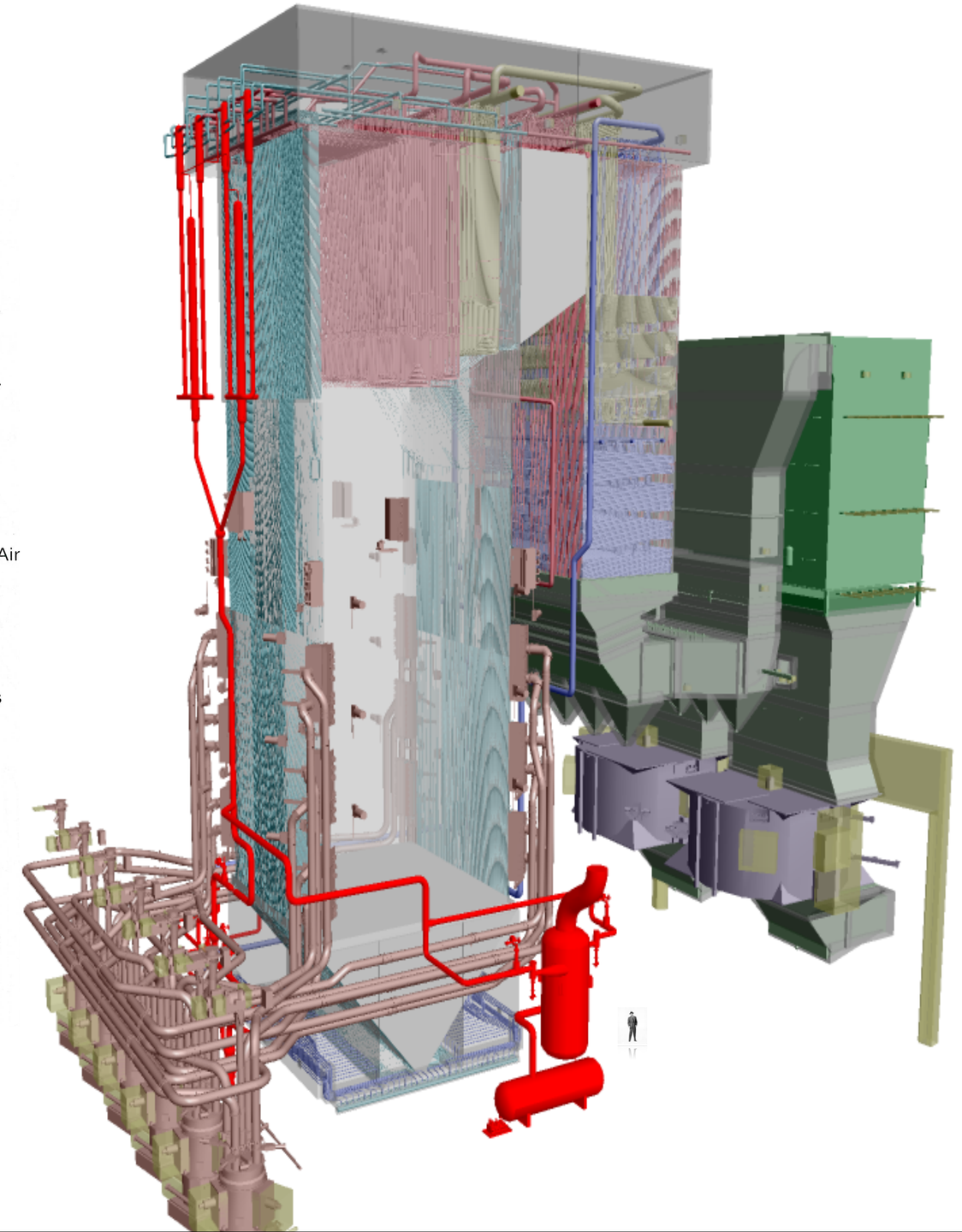
Pulverized Coal Power Generation







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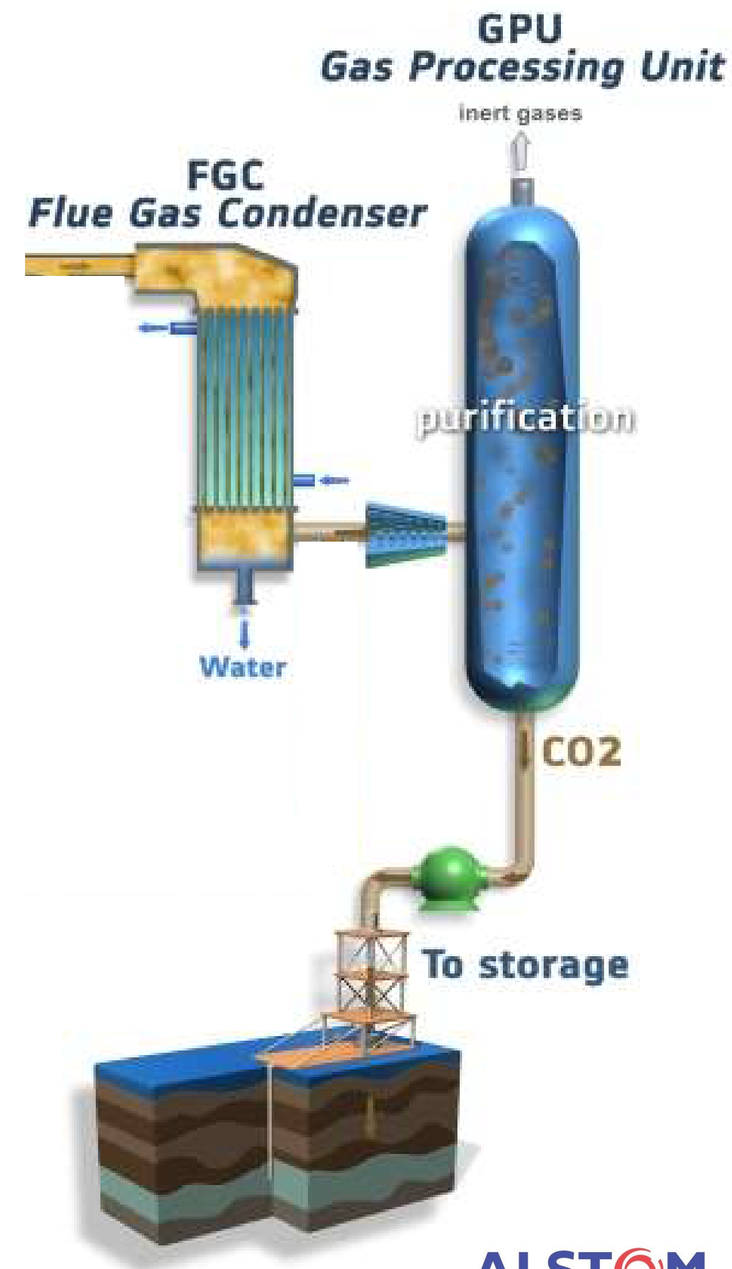
Carbon Capture, Utilization & Storage (CCUS)

typical flue gas	PC	NGCC	air
O_2	6%	14%	21%
N_2	76%	76%	78%
CO_2	11%	3%	0.04%
H_2O	6%	6%	?



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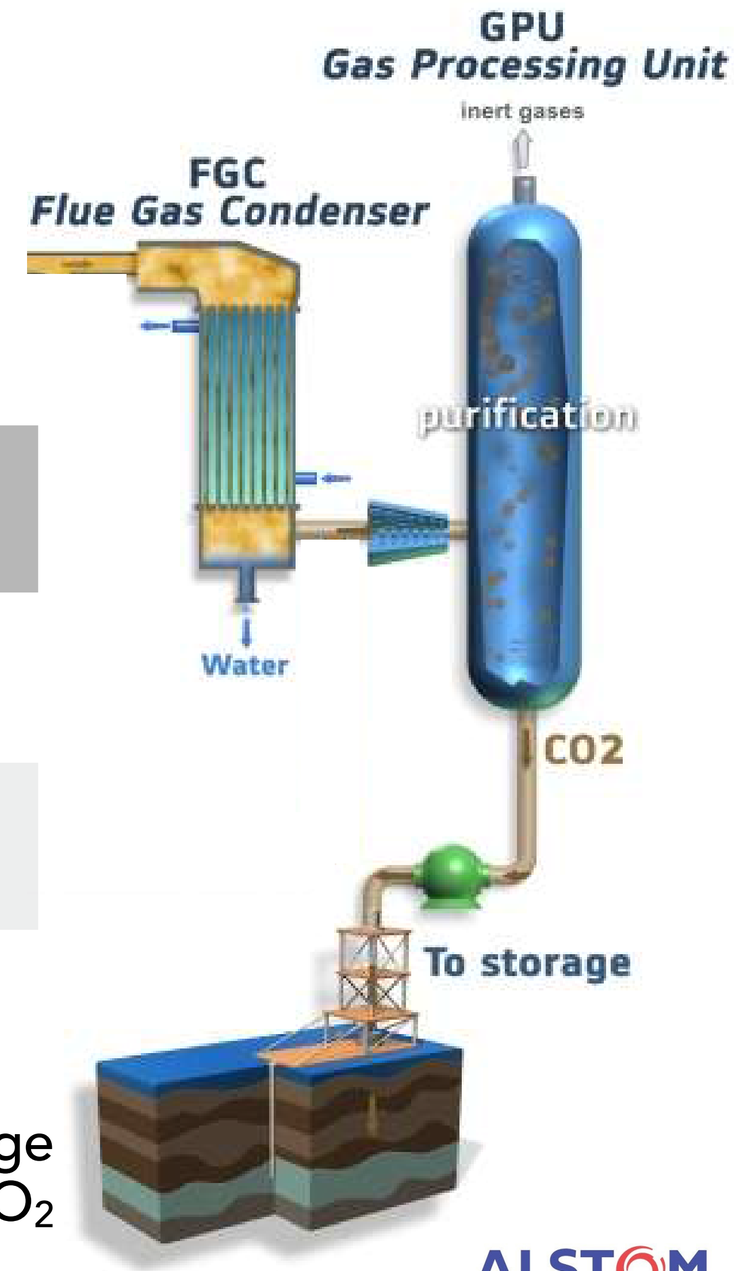
Carbon Capture, Utilization & Storage (CCUS)

David & Herzog, MIT, 2012

cost of post combustion carbon capture	PC 2010	PC 2012	NGCC 2010	NGCC 2012
incremental cost of electricity (¢/kWh)	3.3	2.2	1.6	1.2
energy penalty (%)	25	15	13	10
mitigation cost: capture vs reference ($/tonne of CO_2 avoided)	49	32	49	41

cost of CO_2 transportation and storage (sequestration): $15/tonne of CO_2



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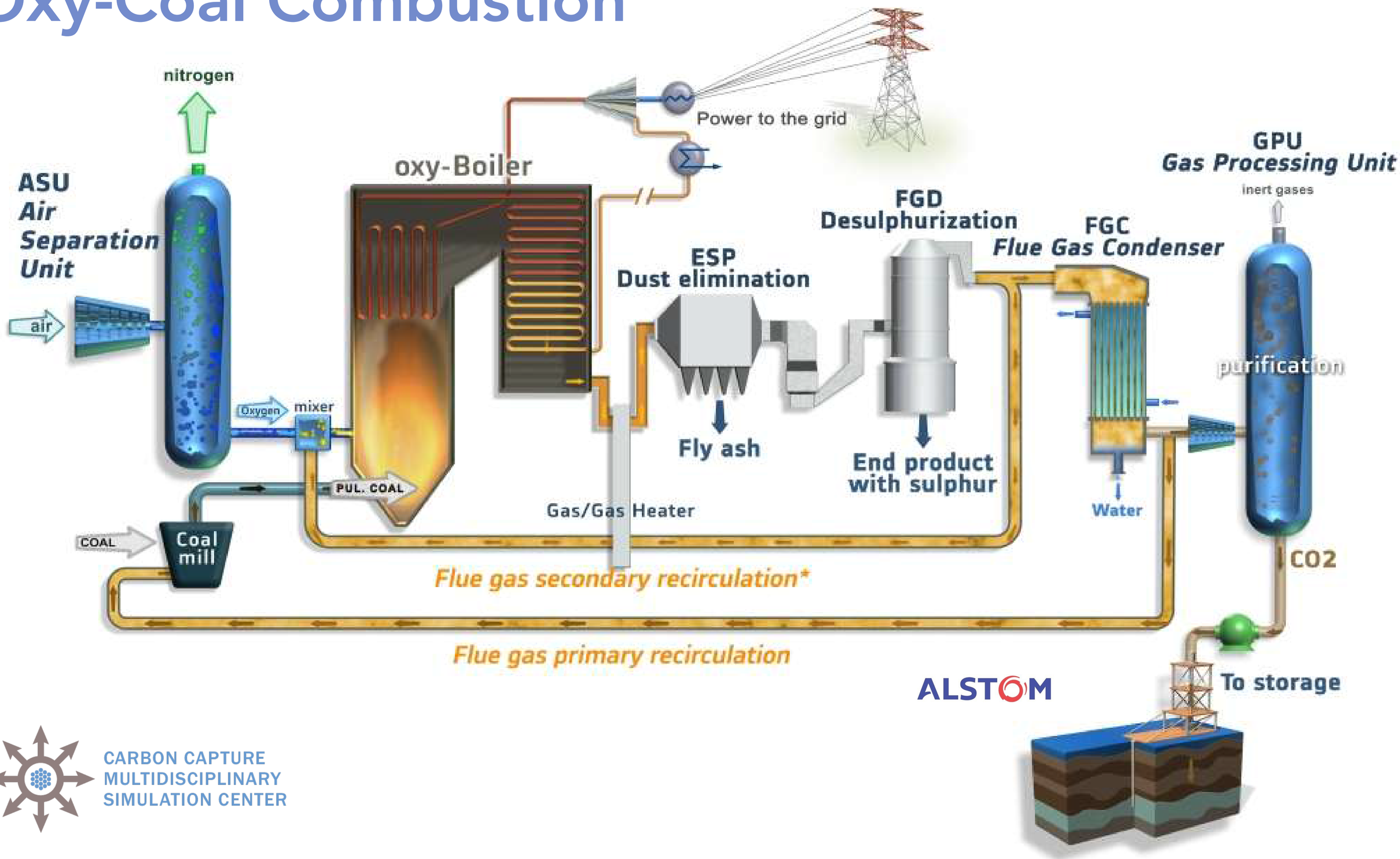
Oxy-Coal Combustion



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Why exascale?

- dynamics
  - *pulverized-coal fuel*
  - *mixing & reaction*
  - *deposition*
- multi-phase radiation
  - *participating media*
  - *absorbing/emitting/scattering*
- resolved physics
  - *1mm spatial resolution*
  - *30 seconds of real time*
  - *1microsecond temporal resolution*
- validation
  - *quantify degree of consistency w mmts.*
  - *reduce risk for rapid deployment*
  - *expensive function evaluation ➟ exascale*

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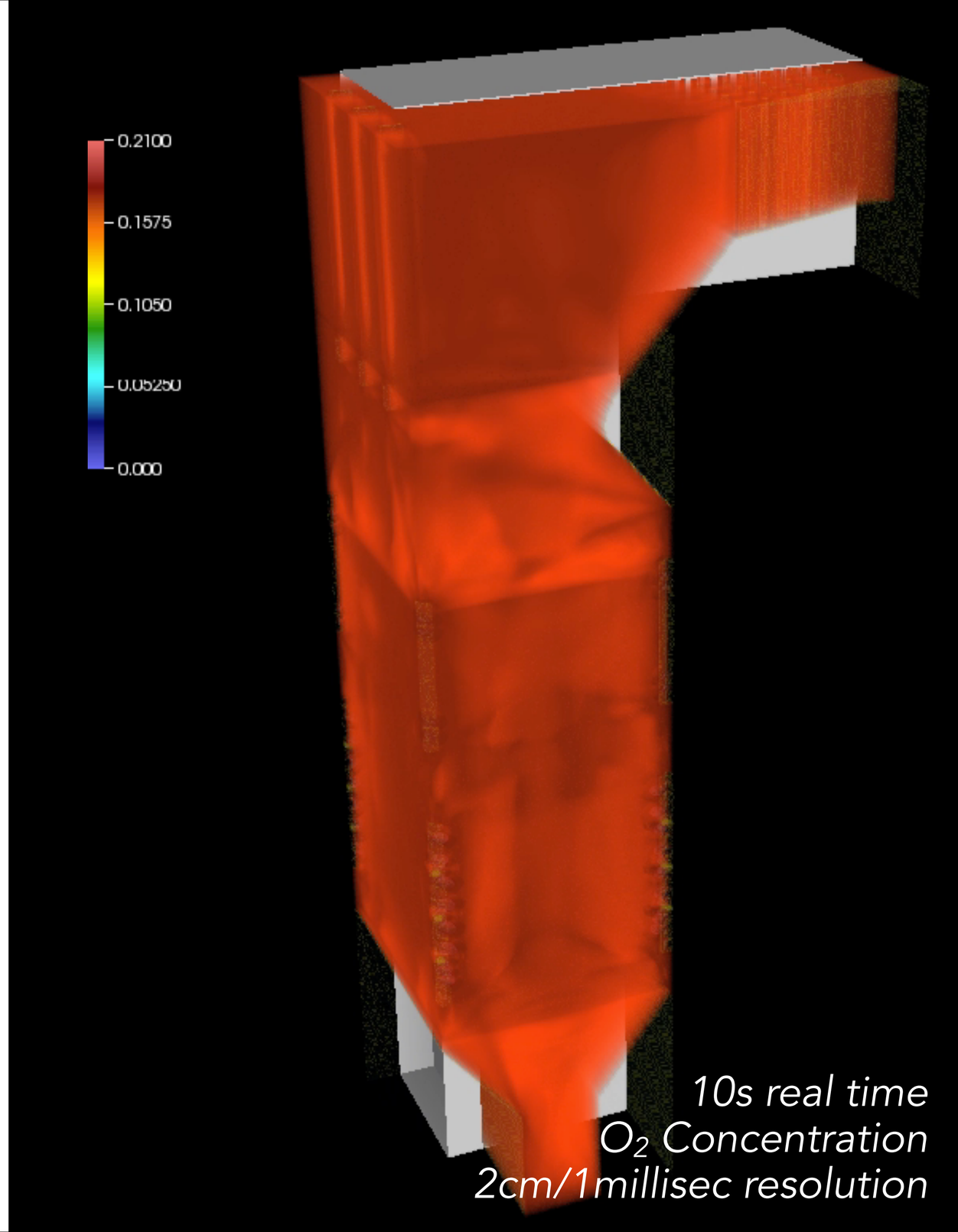
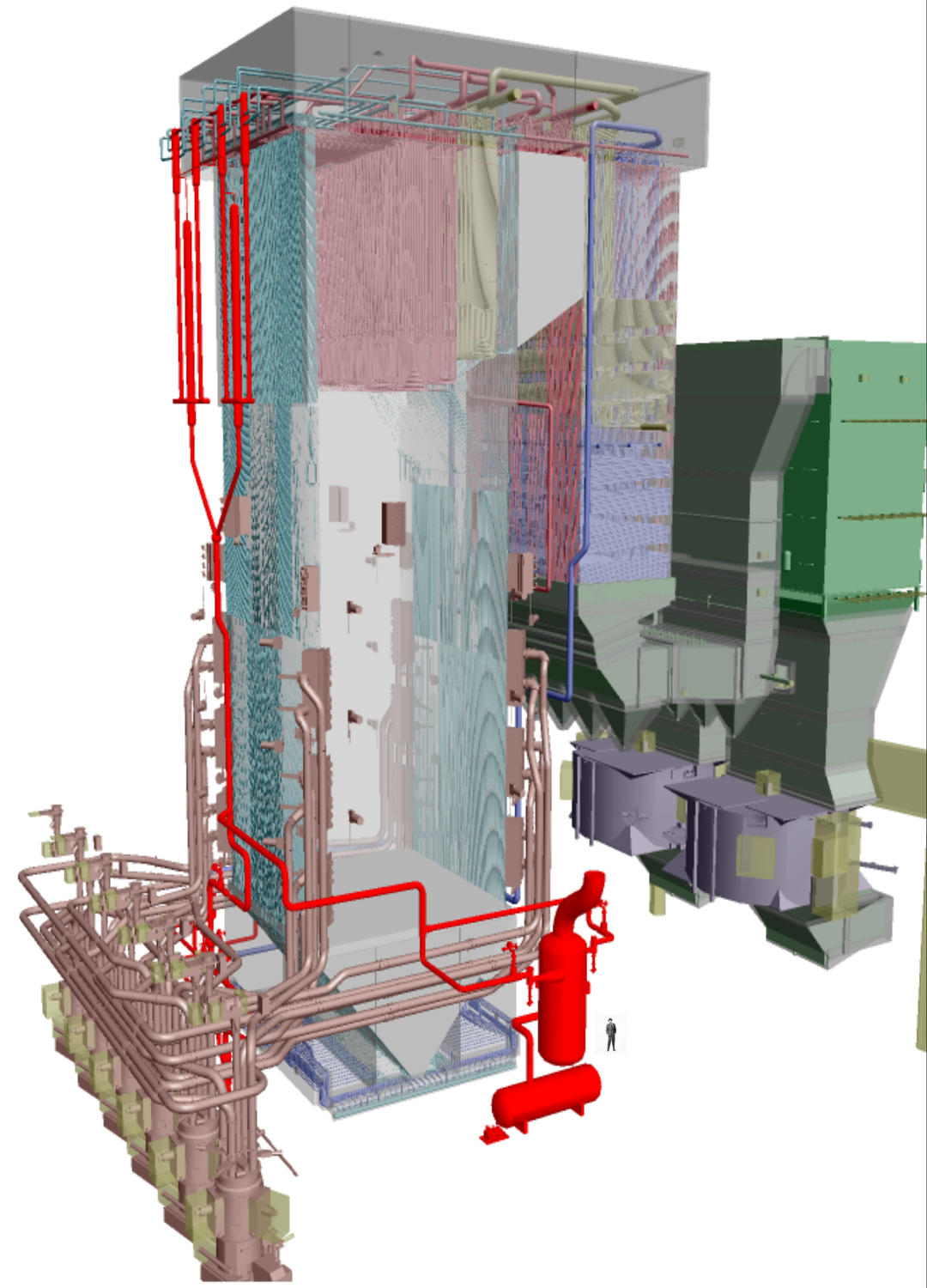


10s real time
O_2 Concentration
2cm/1millisec resolution

Specific Goal

overarching prediction

- predict *heat flux profile* for 350MW oxy-coal AUSC
  - *no experimental data @ demonstration scale*
  - *UQ predictive design: produce uncertainty in QOI that is 'consistent' with all experimental observations in hierarchy*
- secondary QOIs:
  - *boiler efficiency*
  - *exhaust NOx*
  - *unburned carbon in ash*
- "embrace uncertainty"
  - *quantify uncertainties in mmts. & sims.*
  - *V/UQ process for decision making in the presence of uncertainty*
- accelerate the deployment of a new technology:
  - *high efficiency carbon capture for pc power generation*



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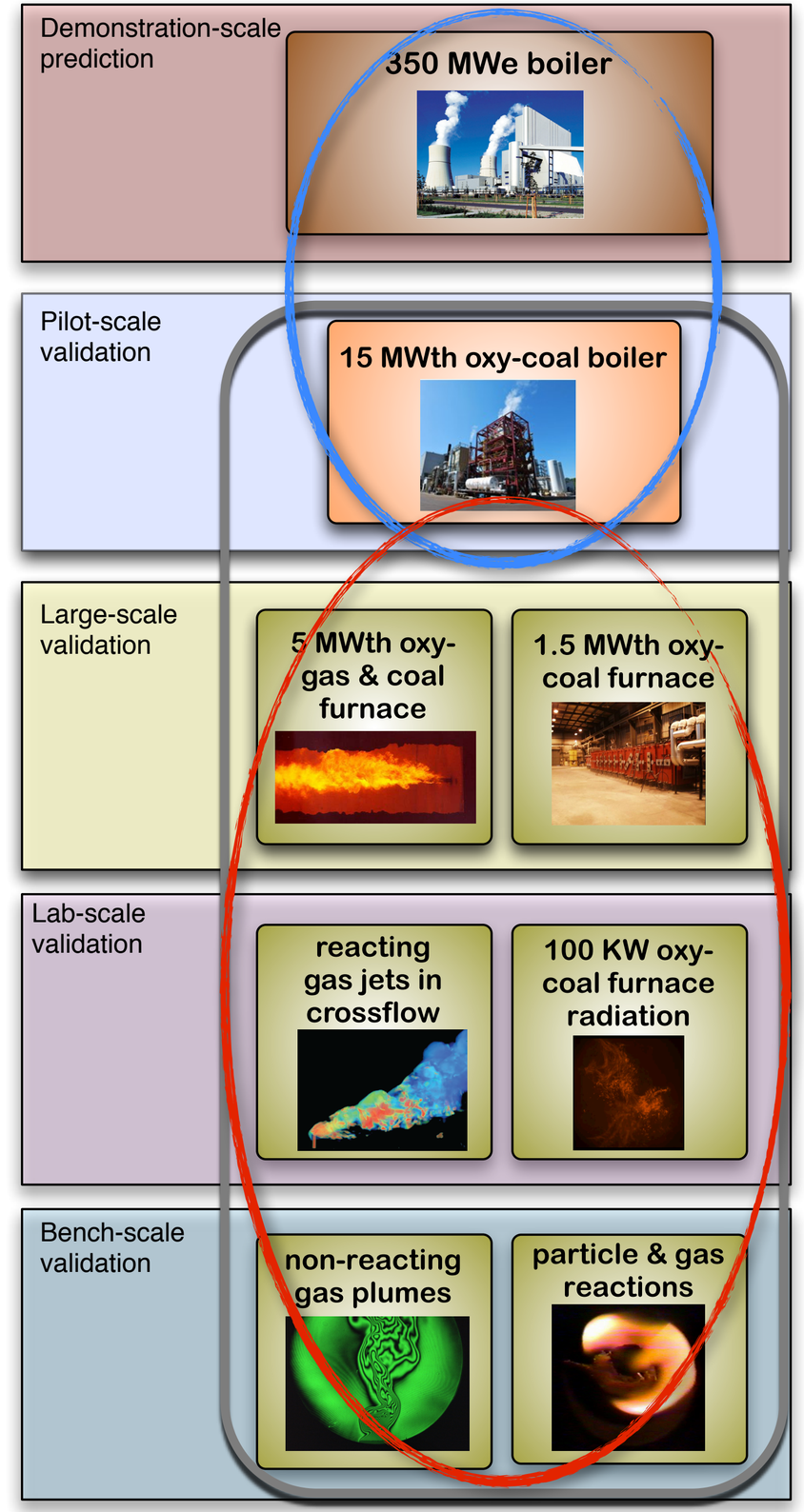

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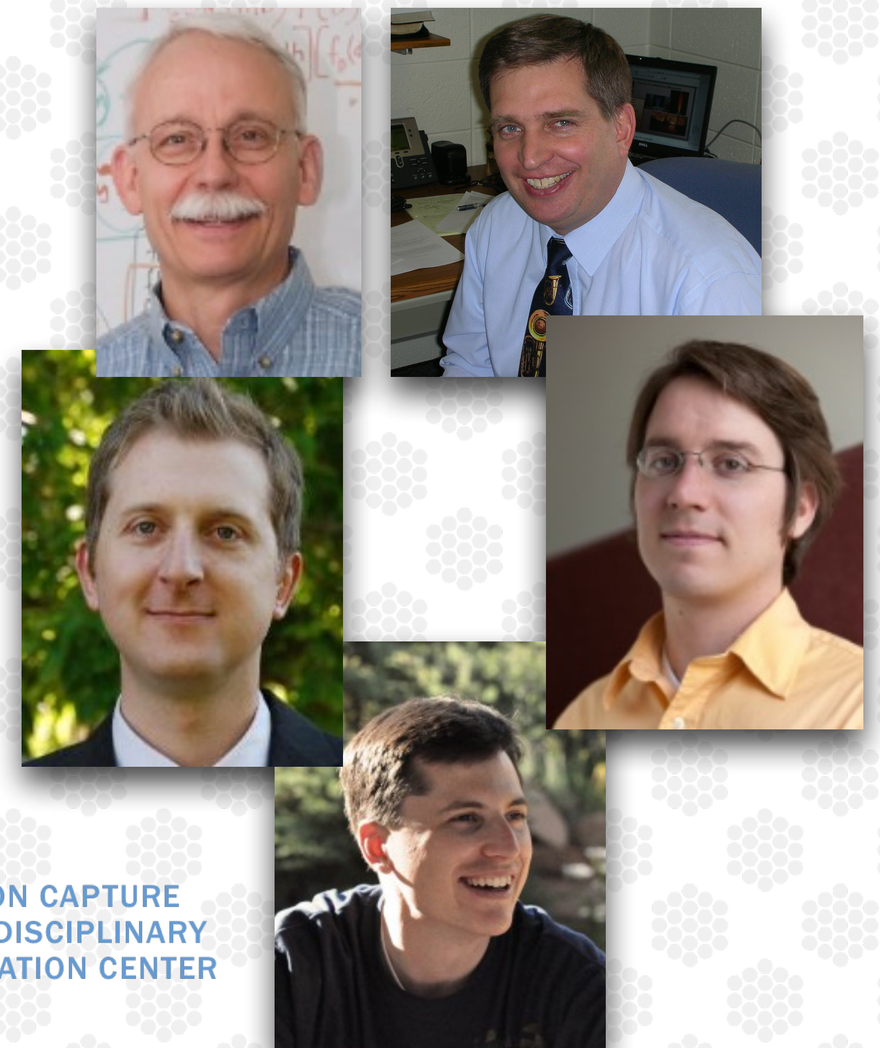
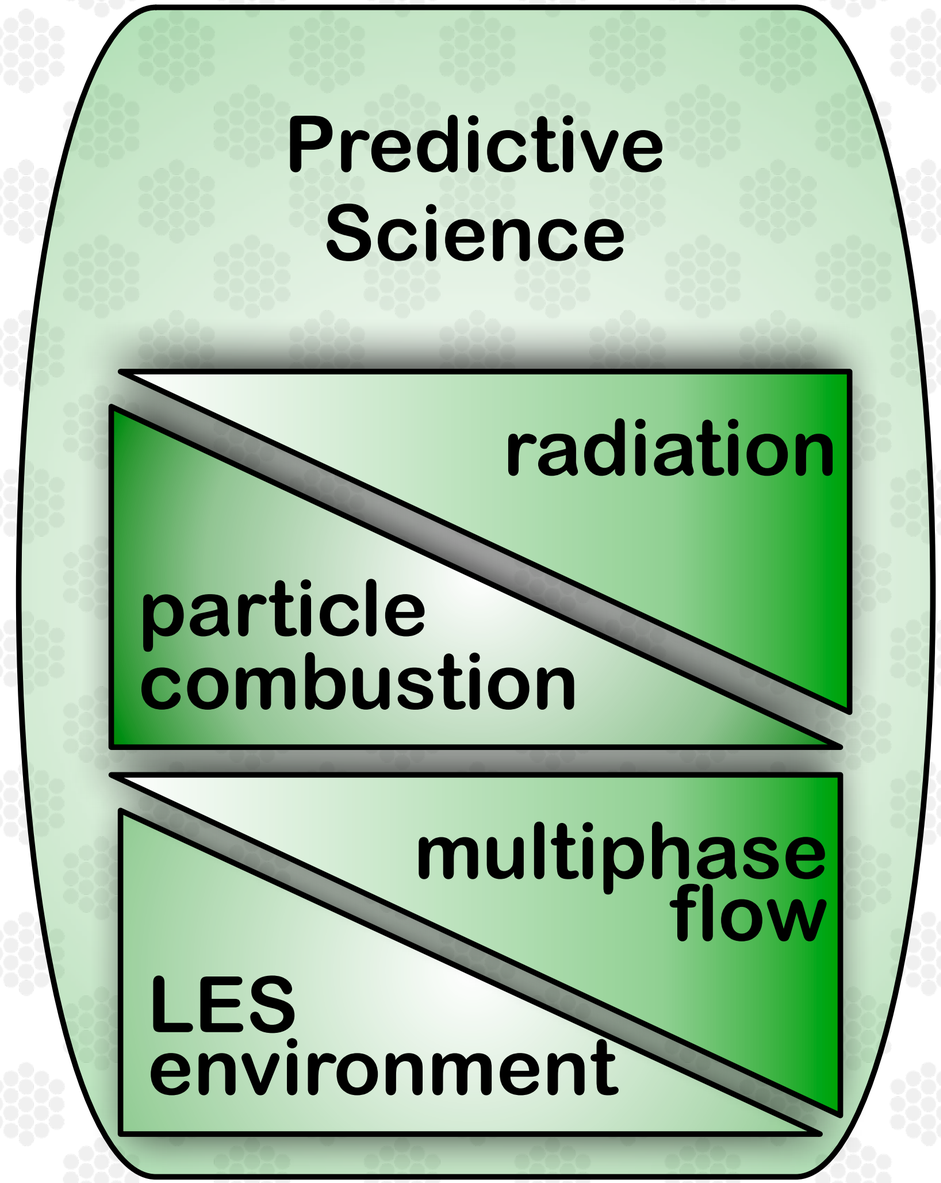
Predictive Science (Physics) Team





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Resolution (spatial & temporal)

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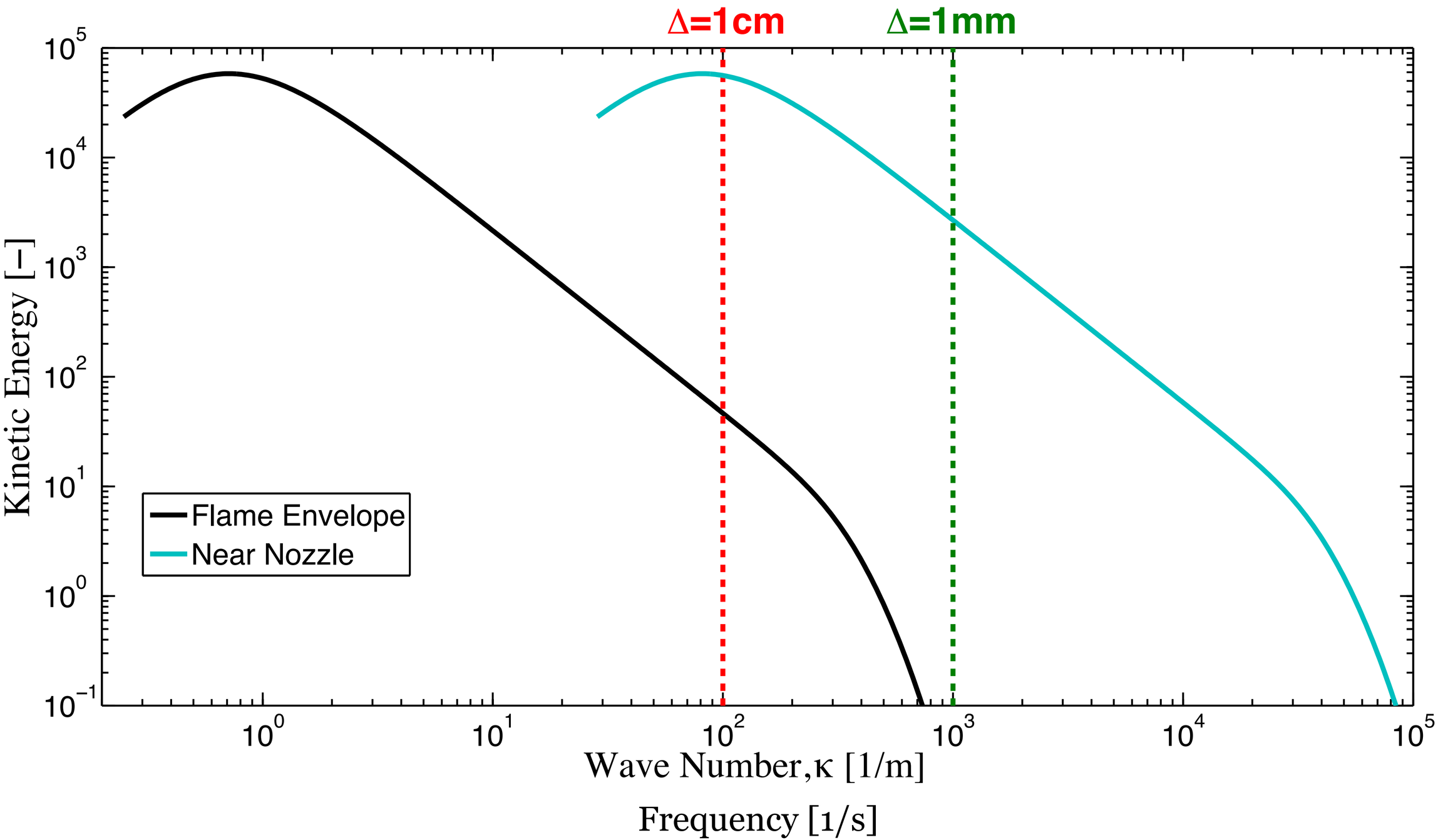
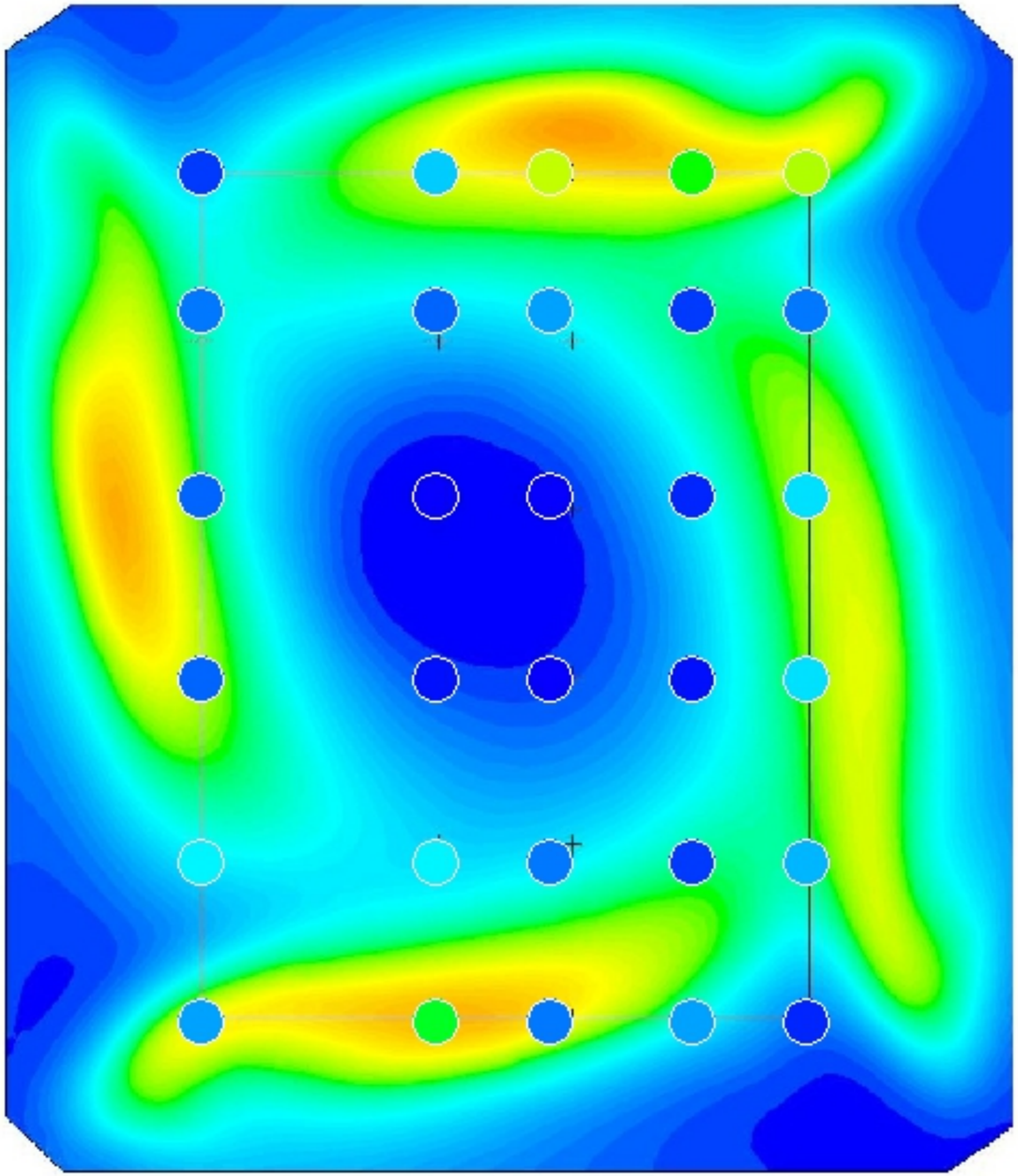
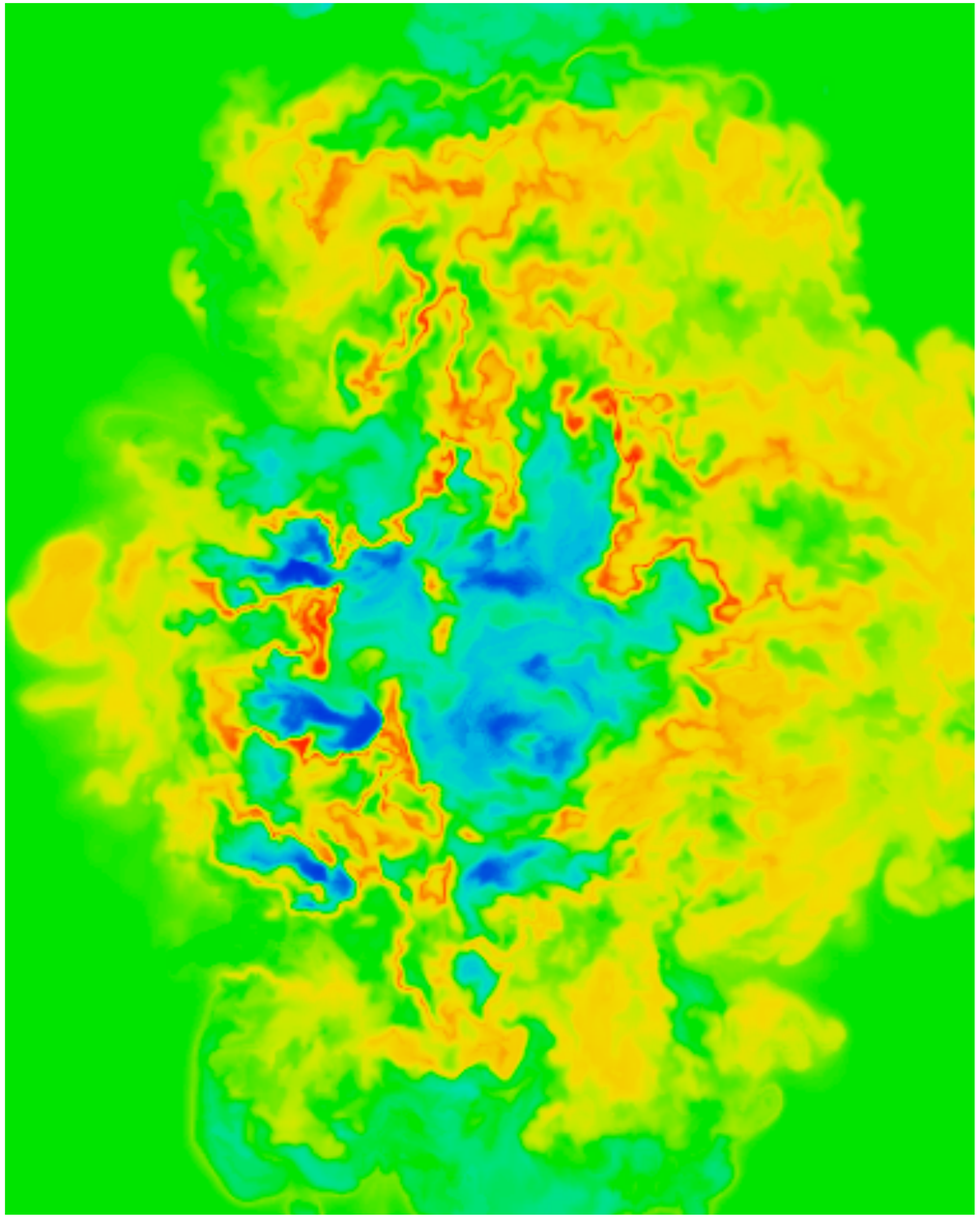




RANS of O_2 inT-fired coal boiler simulation: desktop



LES of O_2 inT-fired coal boiler simulation: Titan 1cm resolution

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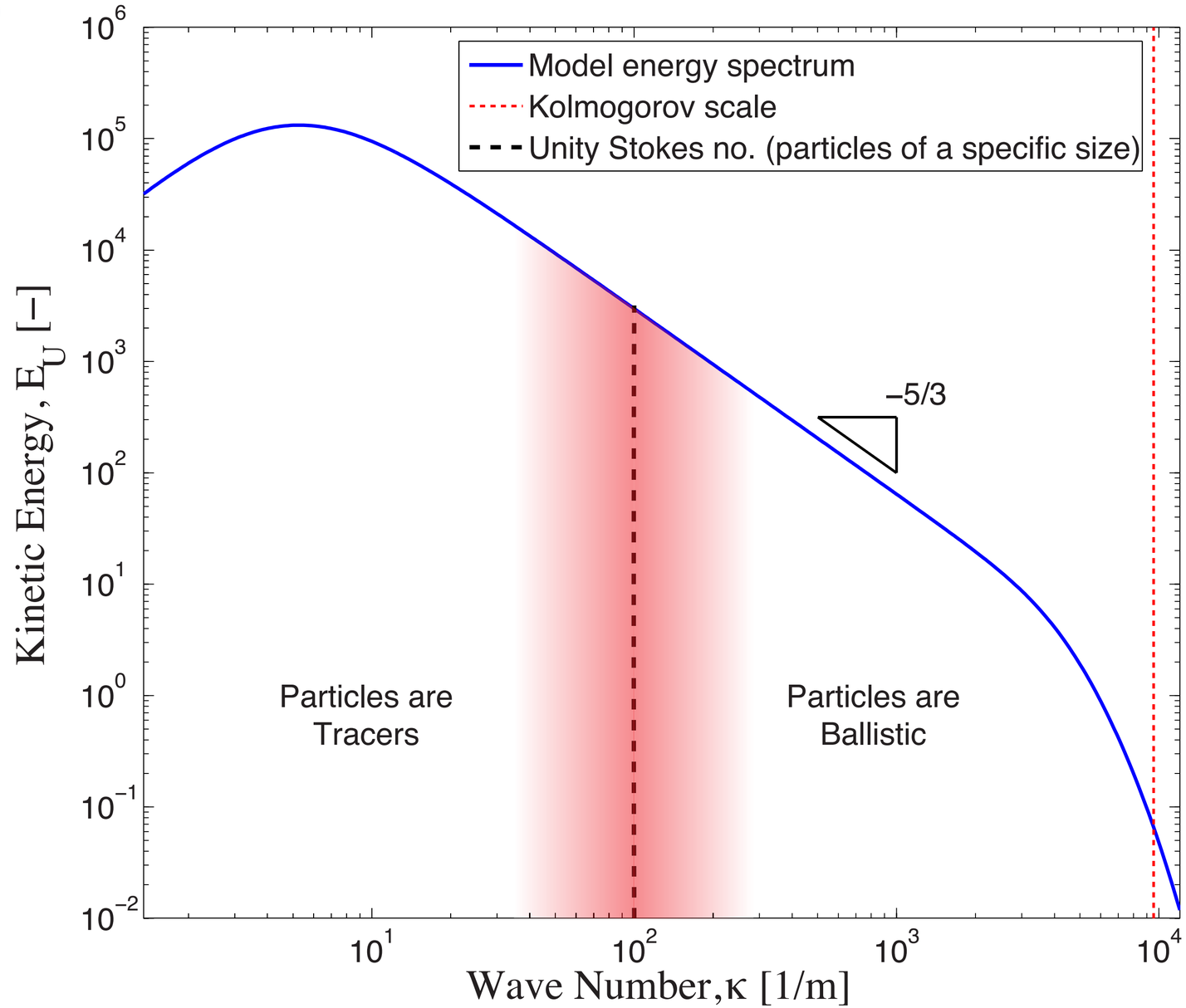
the particles

$$St = \frac{\tau_p}{\tau_f}$$



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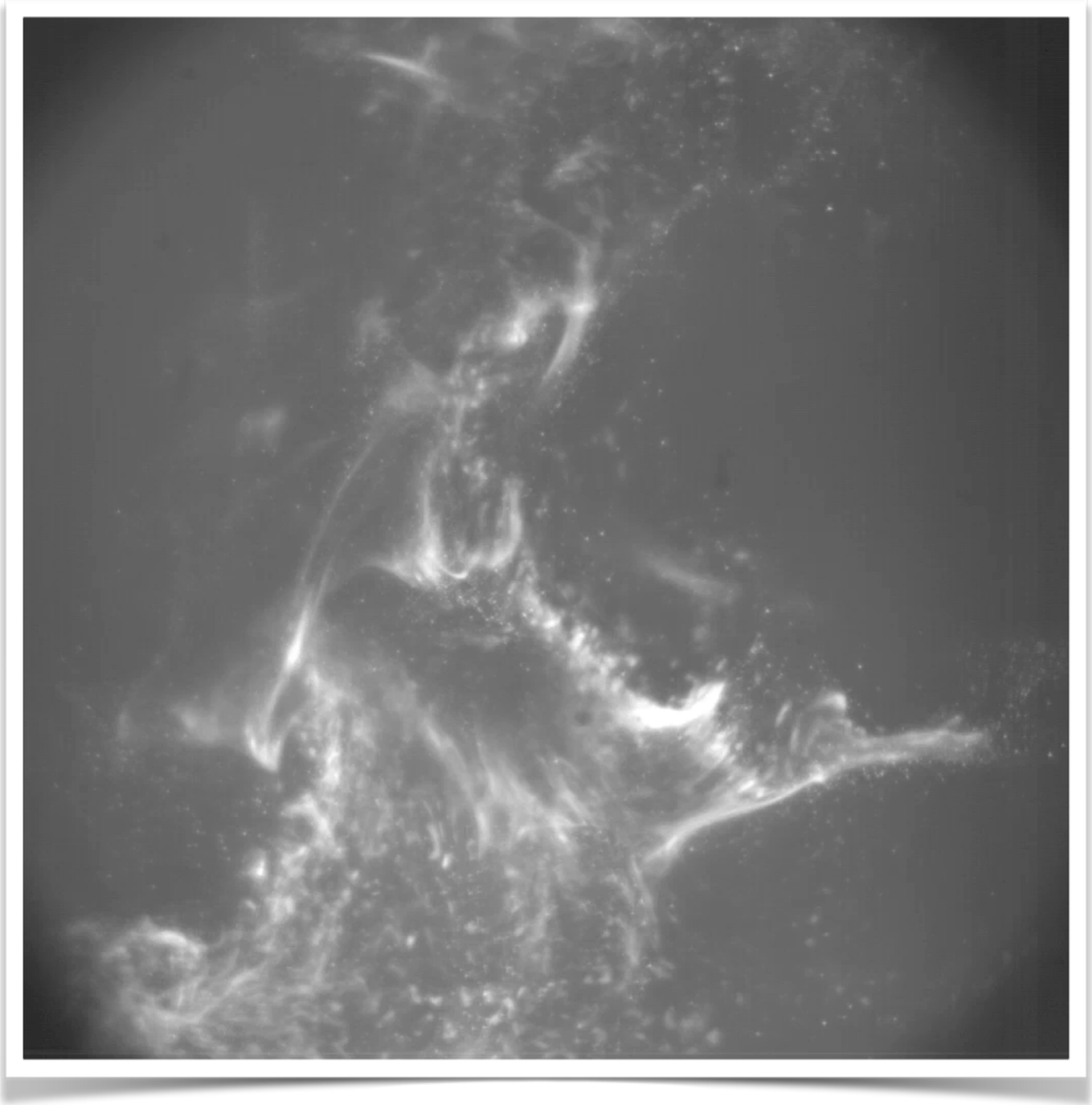

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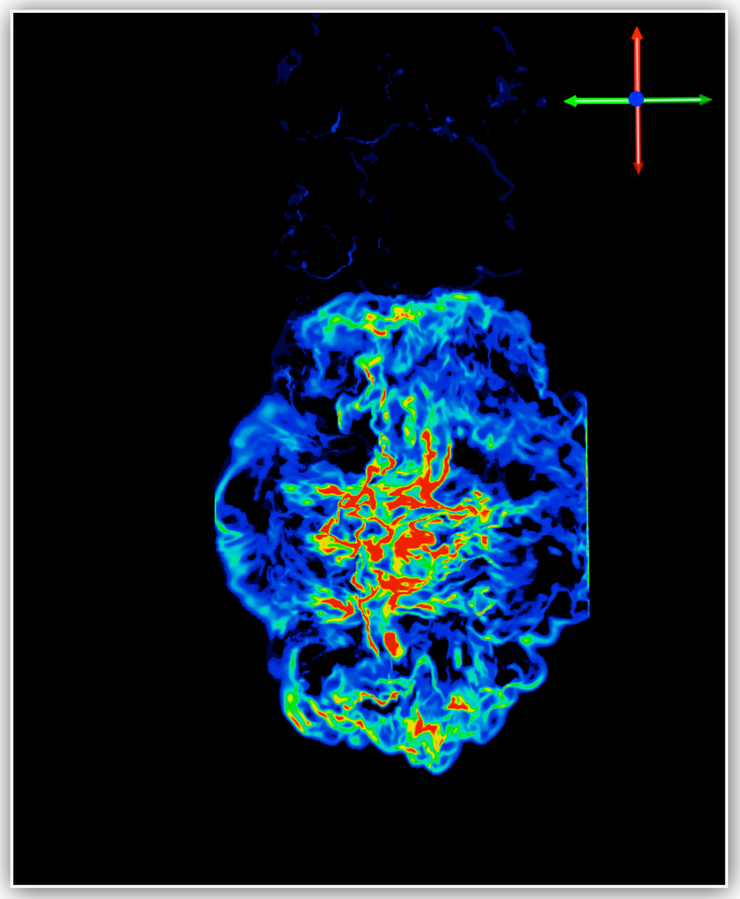
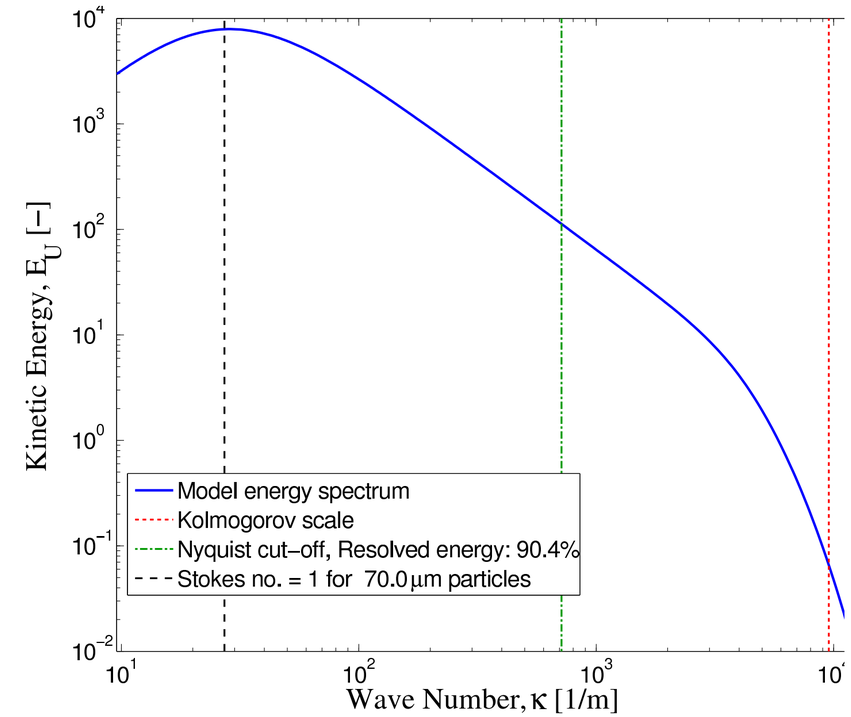
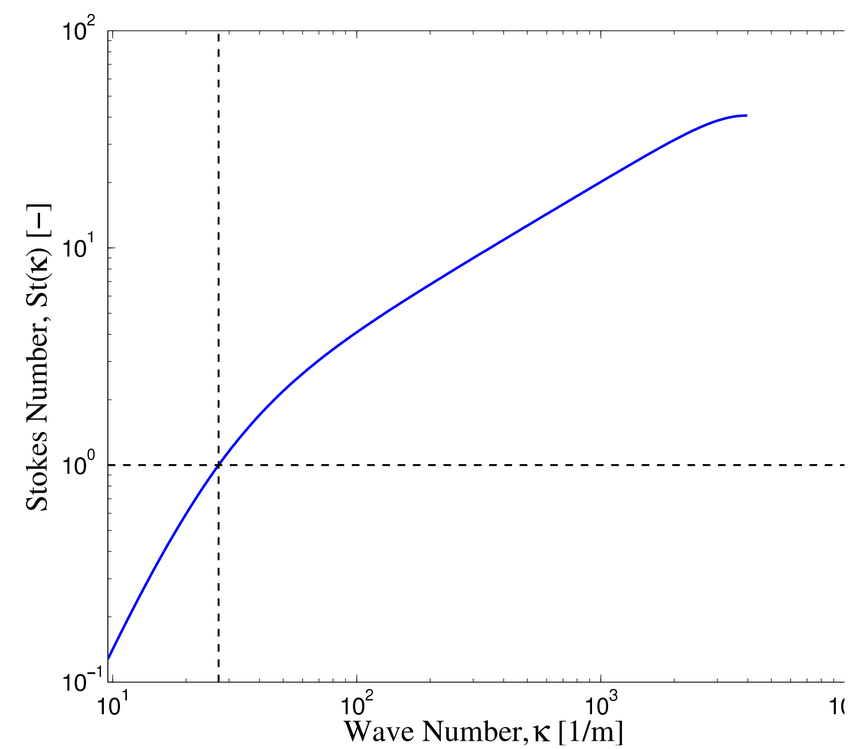
the particles





(b)



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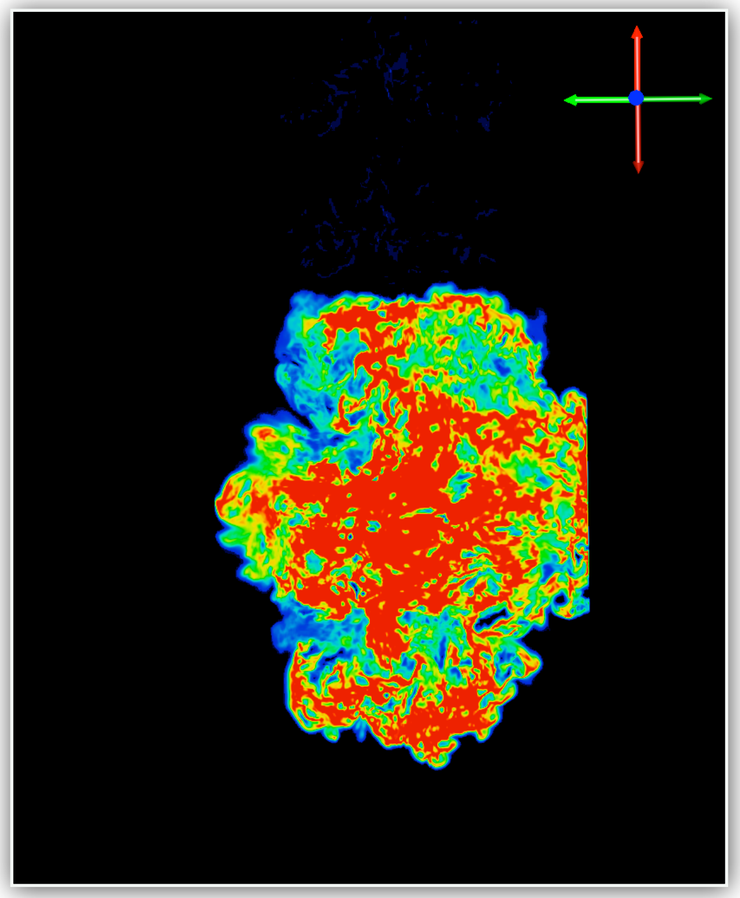
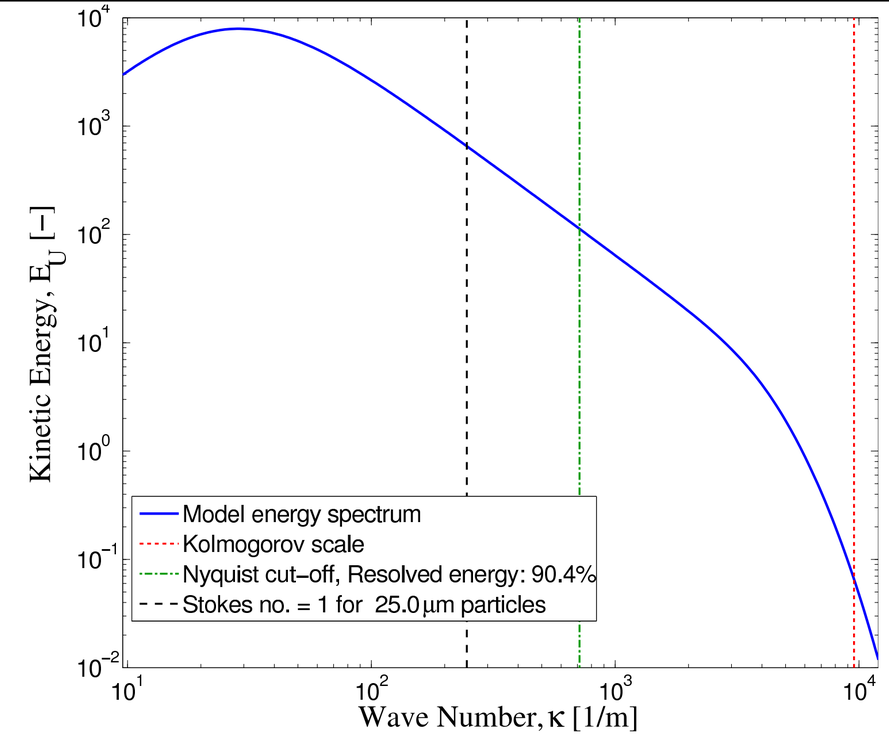
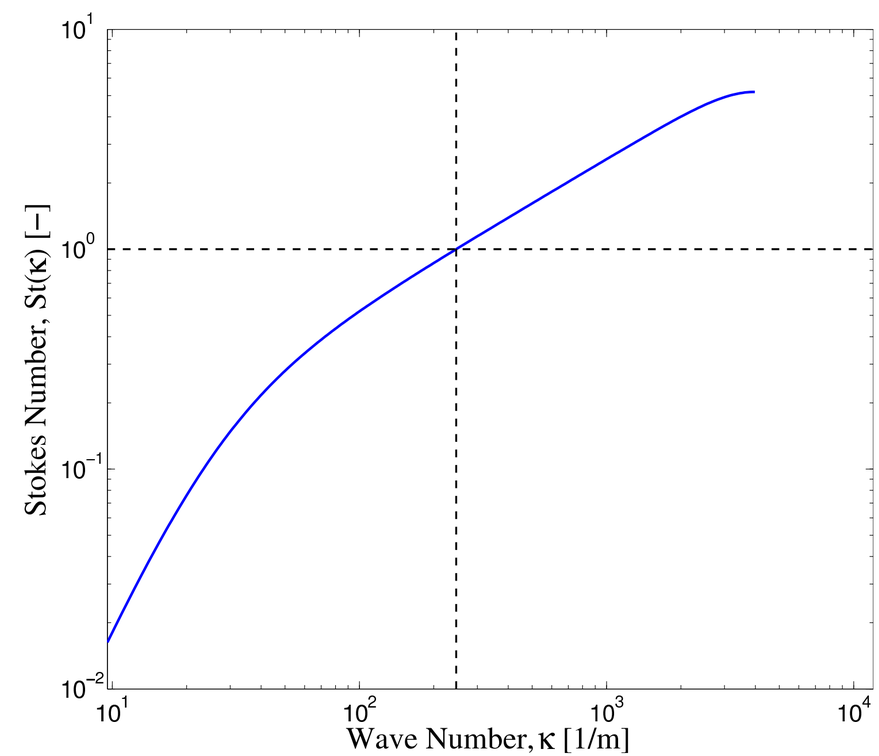
the particles





(a)



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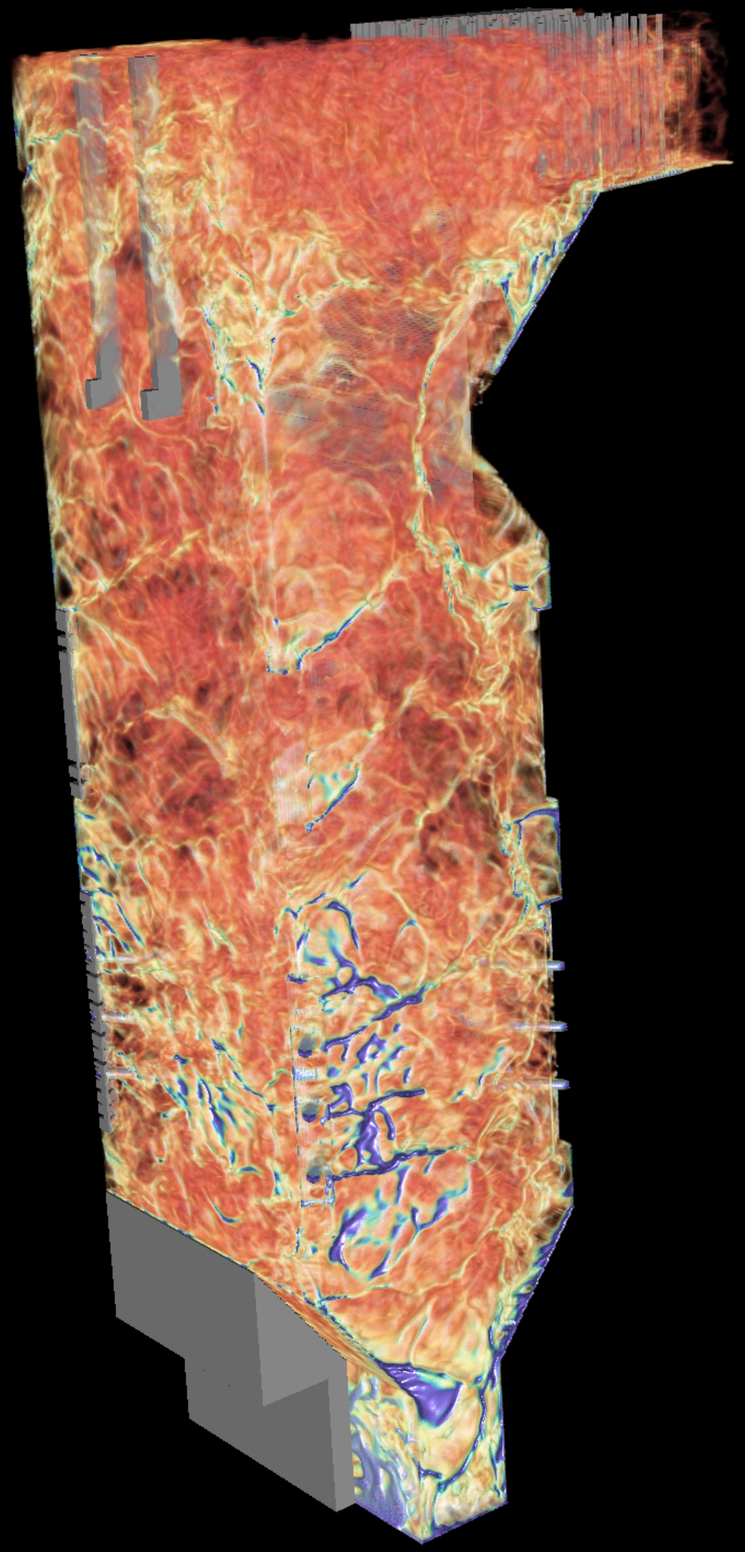
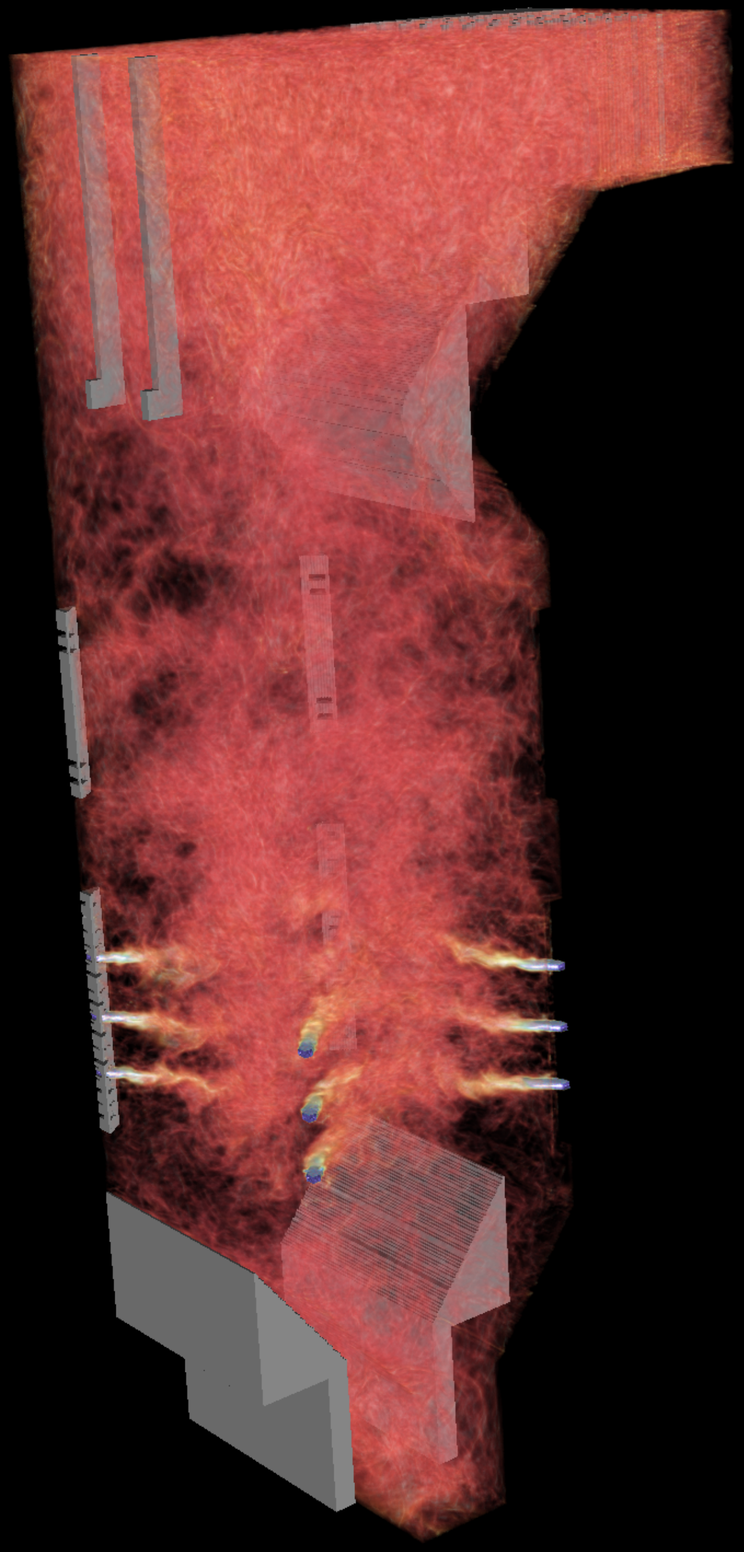
the particles

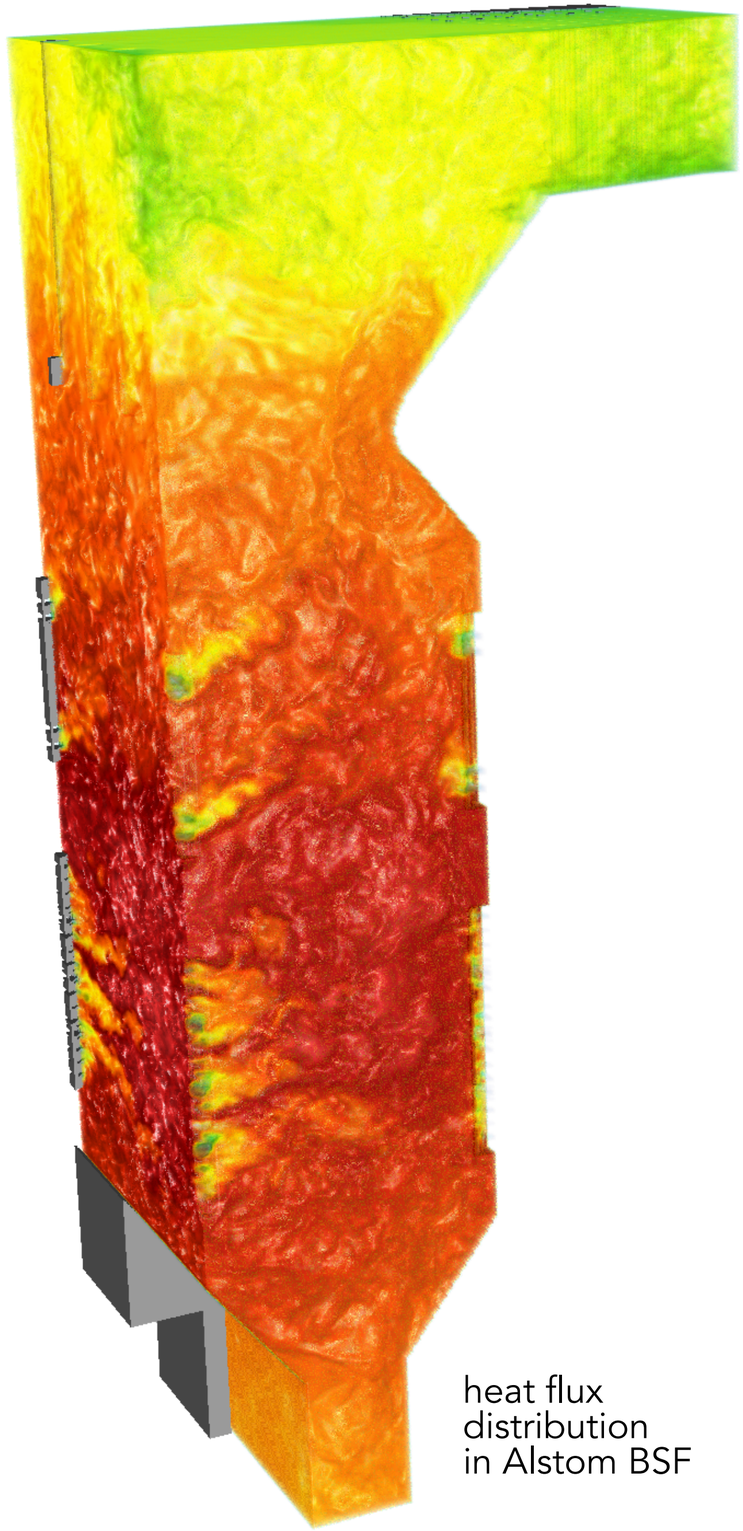




Heat Transfer

- QOI: heat flux distribution
- radiation dominated
- particle laden, scattering, absorbing, emitting participating media
  - *coal particles*
  - *soot*
  - *CO_2 & H_2O (and other minor gases)*
  - *spectral*
  - *specular*
  - *walls & tubes with deposits*

- conjugate heat transfer
  - *radiation & convection*



heat flux distribution in Alstom BSF

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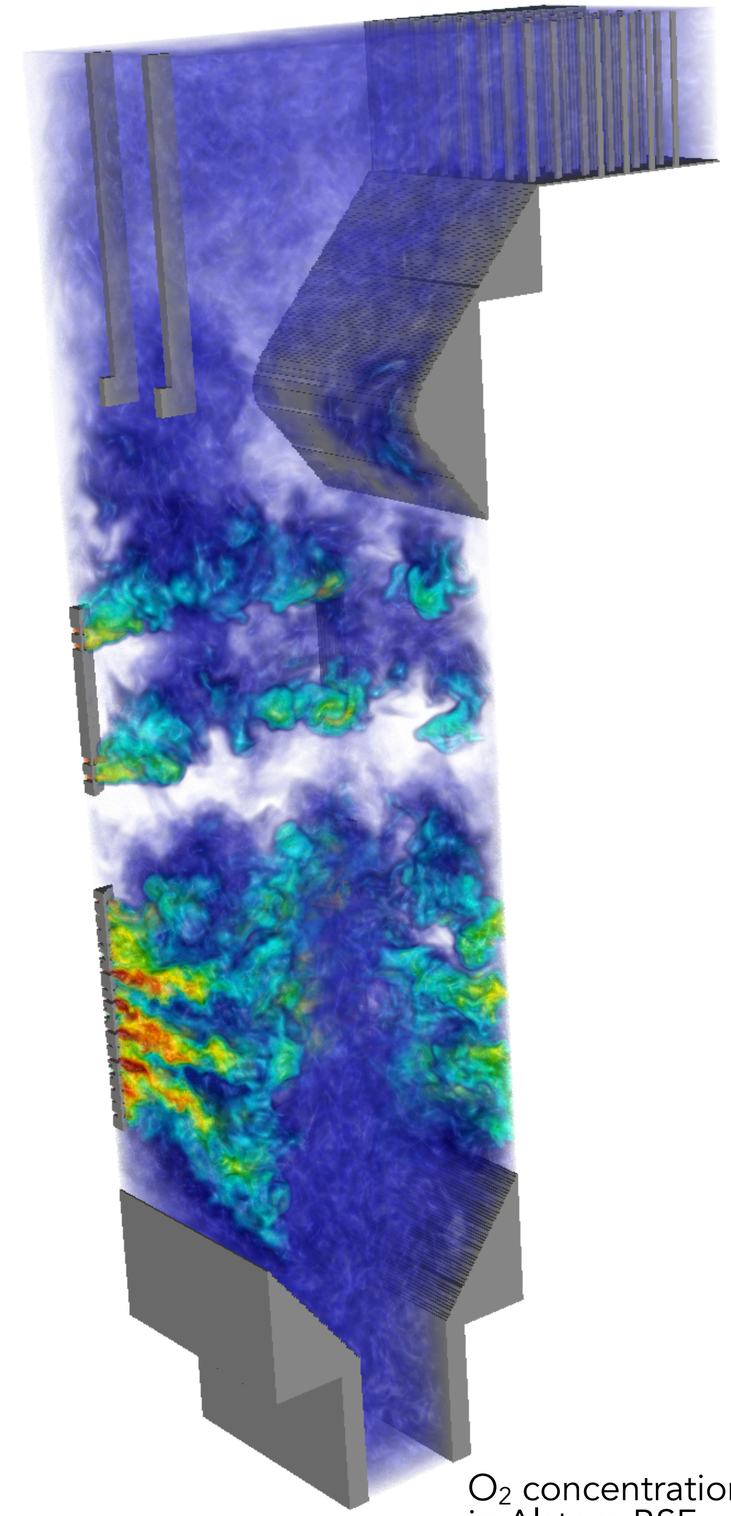
Radiation

- RTE:
  - *Discrete Ordinates Method (DOM)*
  - *Reverse Monte Carlo Ray Tracing (RMCRT)*
  - *spectral*
  - *specular*

- Properties:
  - *full spectrum k-distributions to compute spectrally-resolved absorption coefficients as a function of state space*

- Parallelism:
  - *multi-level, asynchronous, adaptive mesh*
  - *GPU*



O_2 concentration in Alstom BSF

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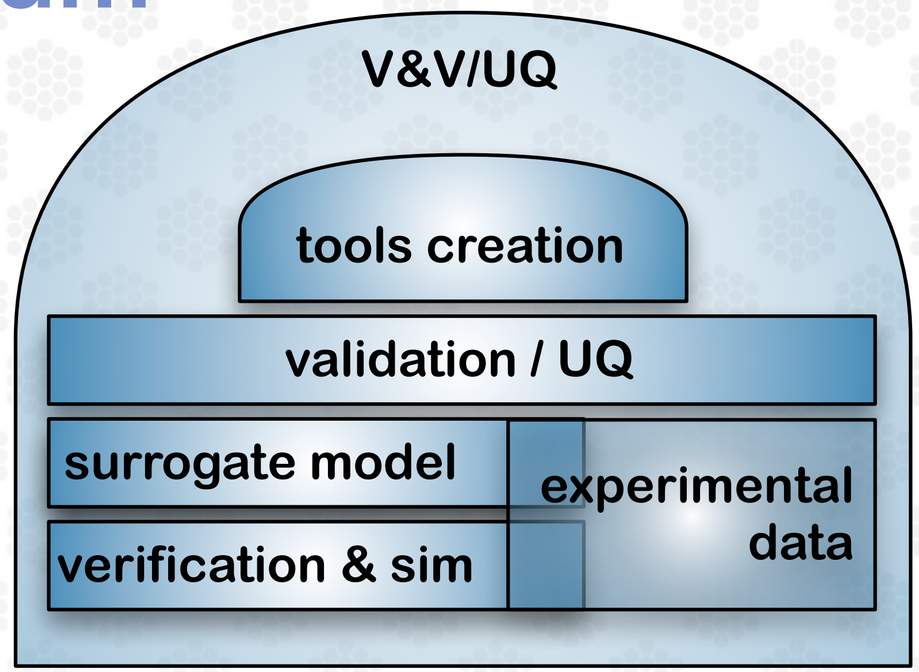
Verification & Validation/UQ Team



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V/UQ methodology .....develop hybrids

Statistical Formulation (K-O)

(Kennedy-O'Hagan, Berger, Sacks, … 2001–present)

$$y = y_m(\mathbf{x}) + \mathbf{B} + \varepsilon$$

y	$y_m(\mathbf{x})$	$\mathbf{B}$	ε
observed QOI	*computer model of QOI*	*discrepancy between $y_m(x)$ and true QOI*	*error in the measured QOI*

The K-O formulation addresses the inherent confounding between model discrepancy and unknown model parameters and is the approach widely adopted in the statistics community.

Bound to Bound Data Collaboration (B2B)

(Frenklach, Packard, … 2002–present)

- optimize objective, subject to:

$$\beta_i \geq x_i \geq \alpha_i, \quad \text{for } i = 1, \ldots, n$$

- all parameters are within prior bounds

$$u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e, \text{ for each } e \in \mathcal{E}$$

B2B is closely related to "structured singular value analysis", a workhorse for 30+ years in robustness analysis (i.e., UQ) of feedback control systems. It is used ubiquitously worldwide by thousands, at major industrial sites (like Boeing, NASA, Toyota, Caterpillar, Toshiba, Honeywell, United Technologies, Siemens, General Electric, Raytheon, Lockheed, and many others)

Validation:
consistency constraint

x_m model parameters
x_s scenario parameters
x_n numerical parameters

$$u_e \geq [y_m(\mathbf{x}) - y_e] \geq l_e,$$

$$\beta_i \geq x_i \geq \alpha_i, \quad \text{for } i = 1, ..., n$$

$$\text{for each } e \in \mathcal{E}$$

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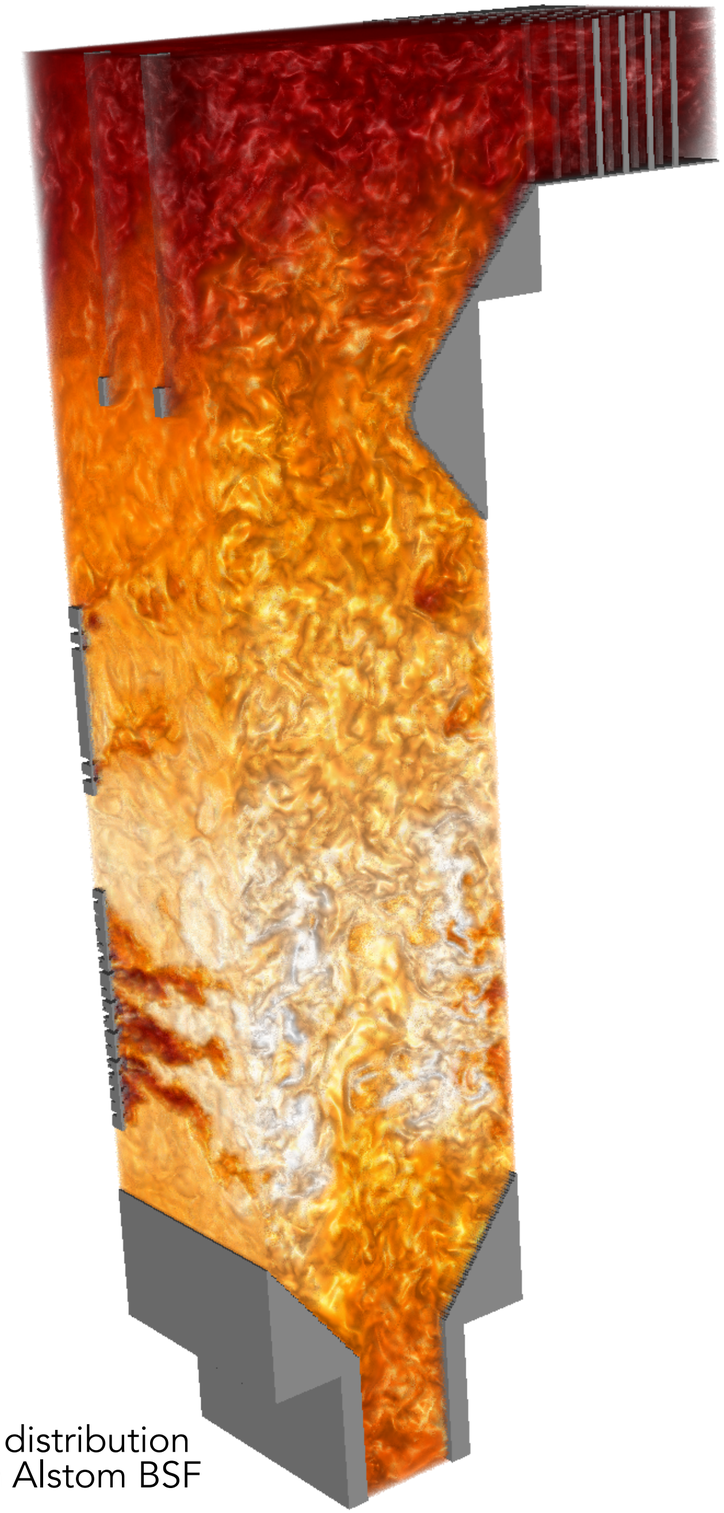
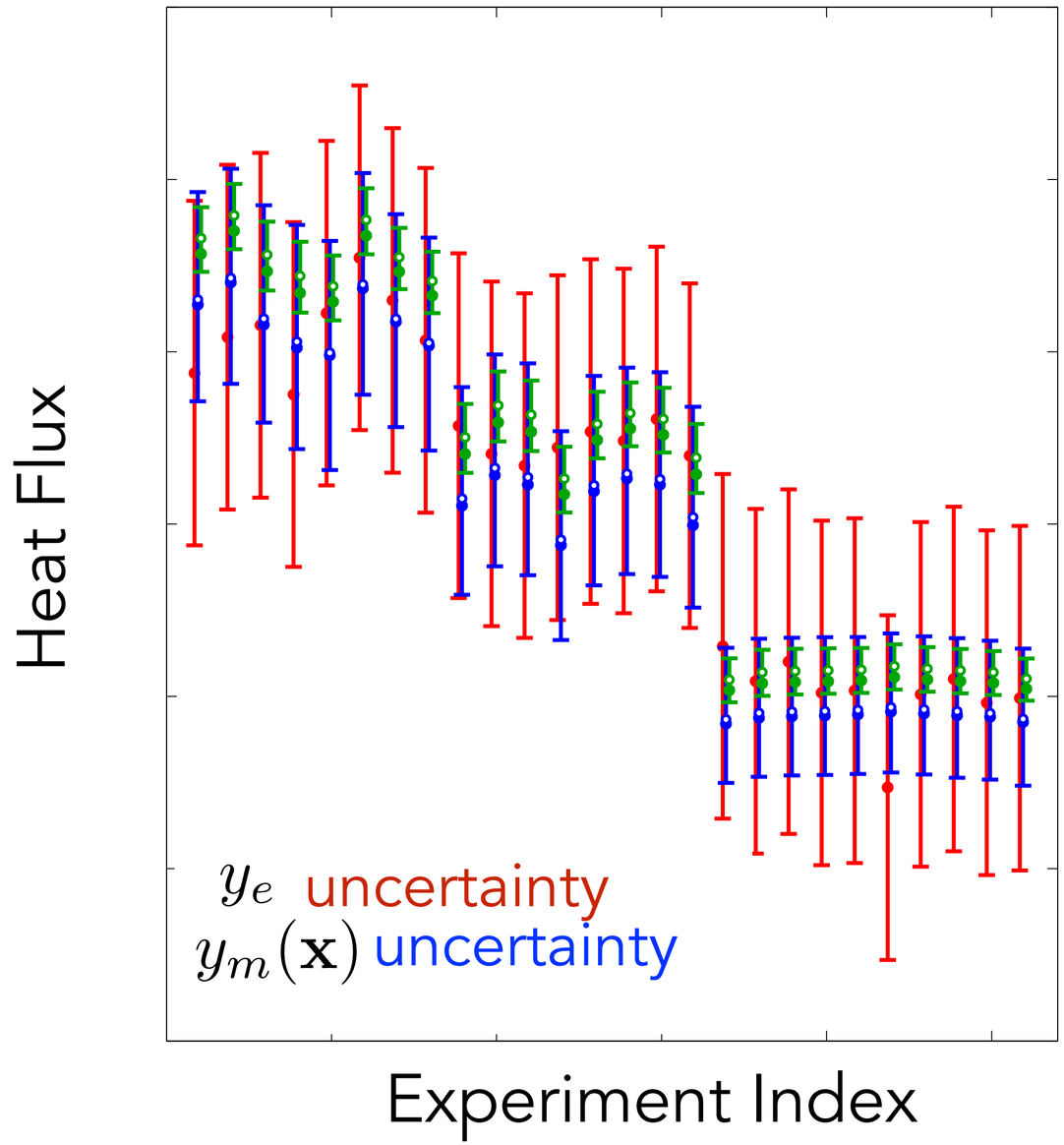
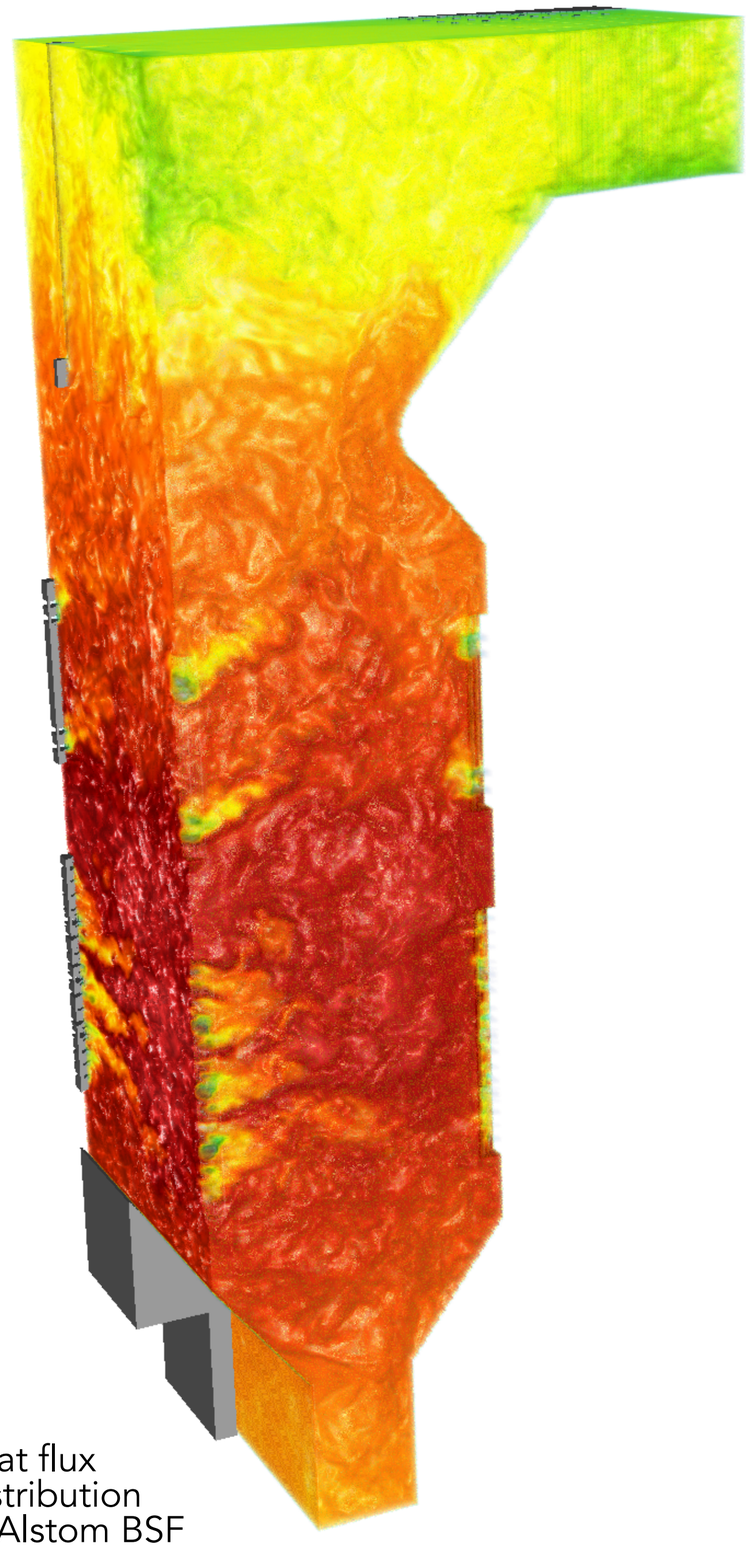
V/UQ example results



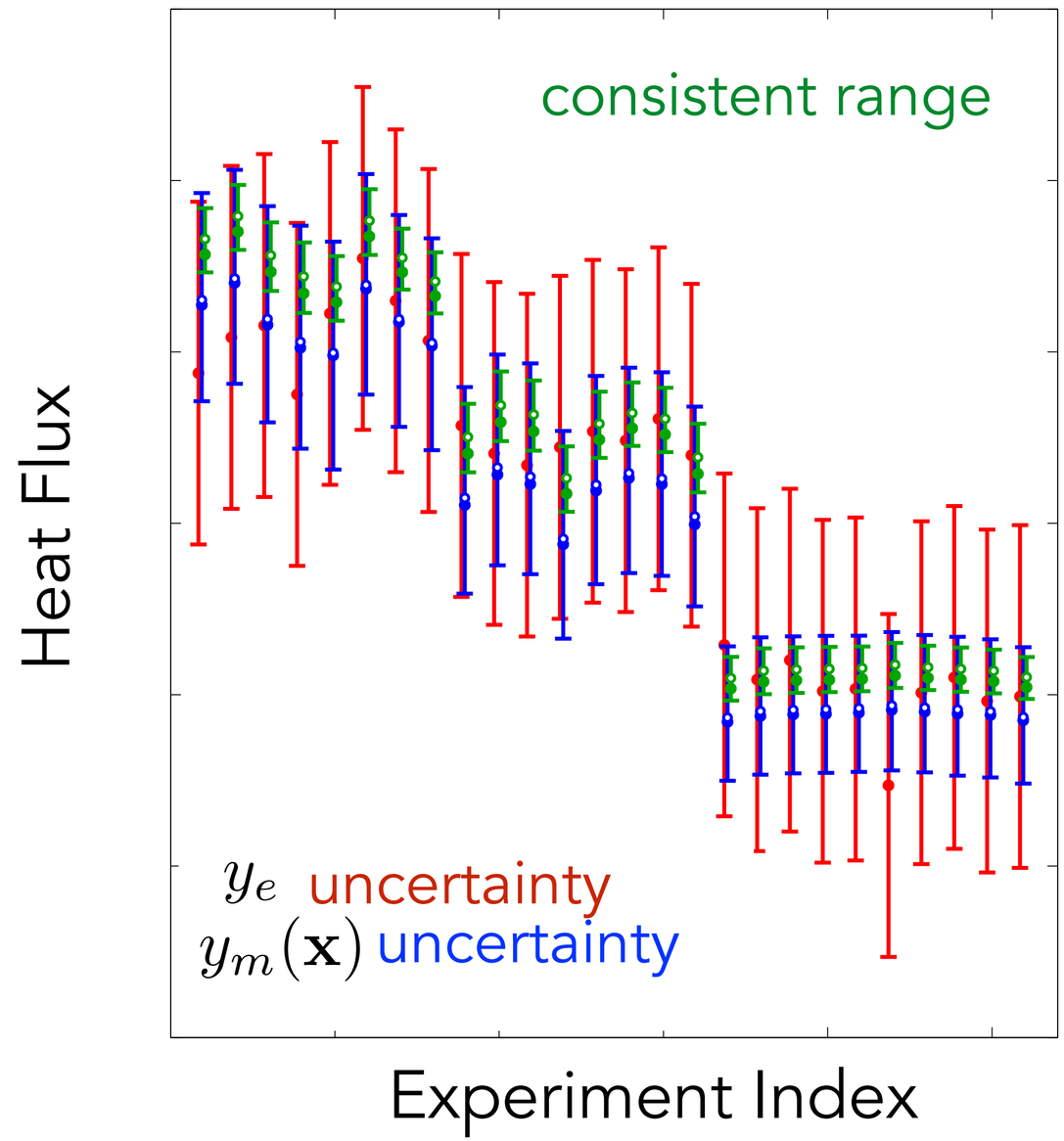
T distribution
in Alstom BSF

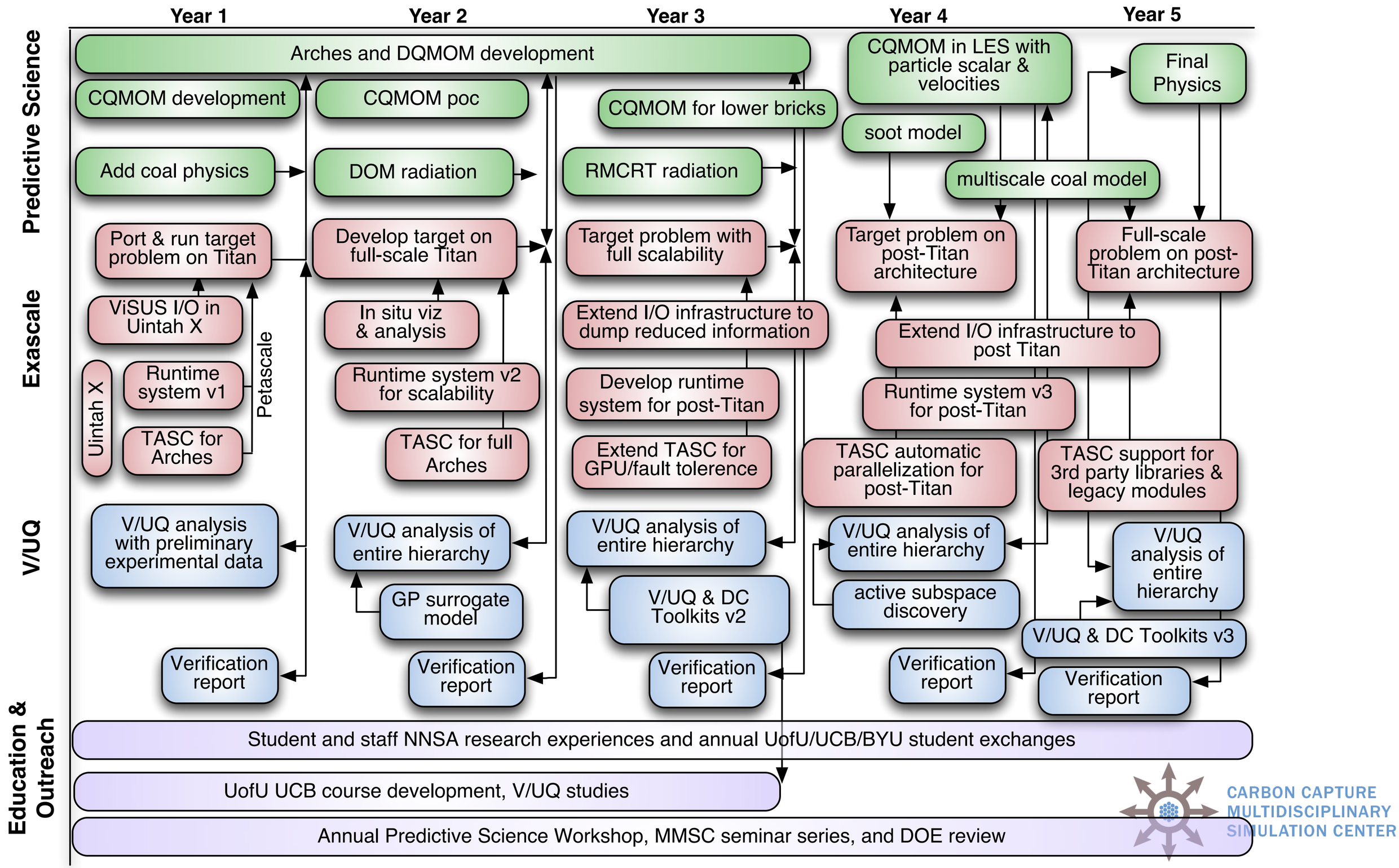


V/UQ example results



heat flux
distribution
in Alstom BSF




Year 1
Year 2
Year 3
Year 4
Year 5
Predictive Science
Exascale
V/UQ
Education & Outreach
Arches and DQMOM development
CQMOM development
CQMOM poc
CQMOM for lower bricks
CQMOM in LES with particle scalar & velocities
Final Physics
soot model
Add coal physics
DOM radiation
RMCRT radiation
multiscale coal model
Port & run target problem on Titan
Develop target on full-scale Titan
Target problem with full scalability
Target problem on post-Titan architecture
Full-scale problem on post-Titan architecture
ViSUS I/O in Uintah X
In situ viz & analysis
Extend I/O infrastructure to dump reduced information
Extend I/O infrastructure to post Titan
Uintah X
Runtime system v1
Petascale
Runtime system v2 for scalability
Develop runtime system for post-Titan
Runtime system v3 for post-Titan
TASC for Arches
TASC for full Arches
Extend TASC for GPU/fault tolerence
TASC automatic parallelization for post-Titan
TASC support for 3rd party libraries & legacy modules
V/UQ analysis with preliminary experimental data
V/UQ analysis of entire hierarchy
V/UQ analysis of entire hierarchy
V/UQ analysis of entire hierarchy
GP surrogate model
V/UQ & DC Toolkits v2
active subspace discovery
V/UQ & DC Toolkits v3
Verification report
Verification report
Verification report
Verification report
Verification report
Student and staff NNSA research experiences and annual UofU/UCB/BYU student exchanges
UofU UCB course development, V/UQ studies
Annual Predictive Science Workshop, MMSC seminar series, and DOE review
CARBON CAPTURE MULTIDISCIPLINARY SIMULATION CENTER

Scientific Questions

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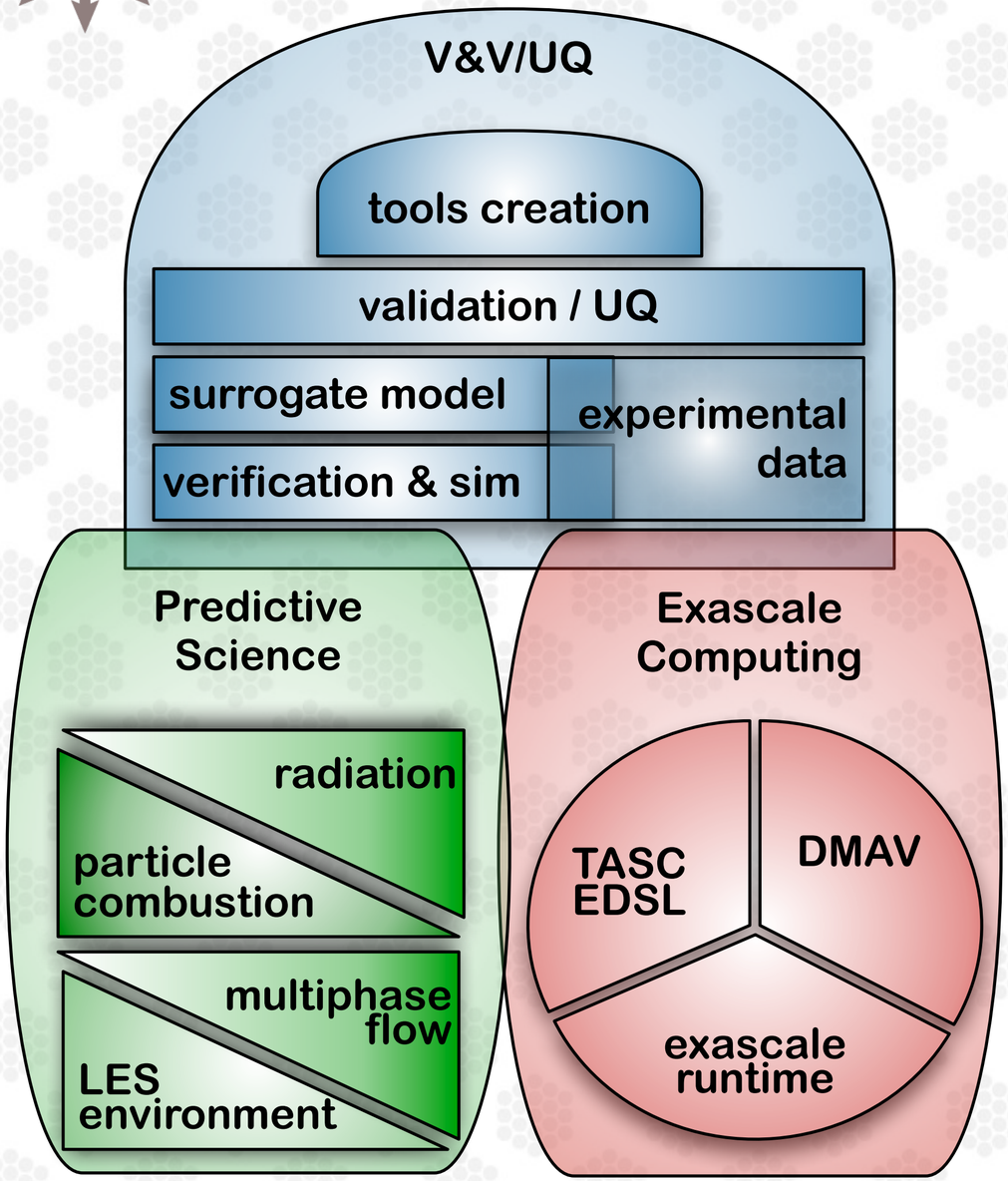
Can extreme computing accelerate deployment of a low-cost, low-carbon energy solution for power generation: AUSC oxy-coal ?



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BYU BRIGHAM YOUNG UNIVERSITY

NNSA National Nuclear Security Administration

Scientific Questions

- turbulent reacting particle laden flows:
  - *can exascale resolve a pc-boiler to 1mm resolution?*
- scale separation:
  - *can we construct dynamic models that separate resolved physics and modeled physics?*
- radiative transport:
  - *will exascale computing make ray tracing possible?*
- DMAV:
  - *how to use cache, memory and IO at exascale?*
- TASC EDSL:
  - *can programmer productivity be increased while going to exascale?*
- exascale runtime:
  - *can we get to exascale?*
- validation:
  - *will prediction of QOI uncertainties lead to faster technology deployment?*

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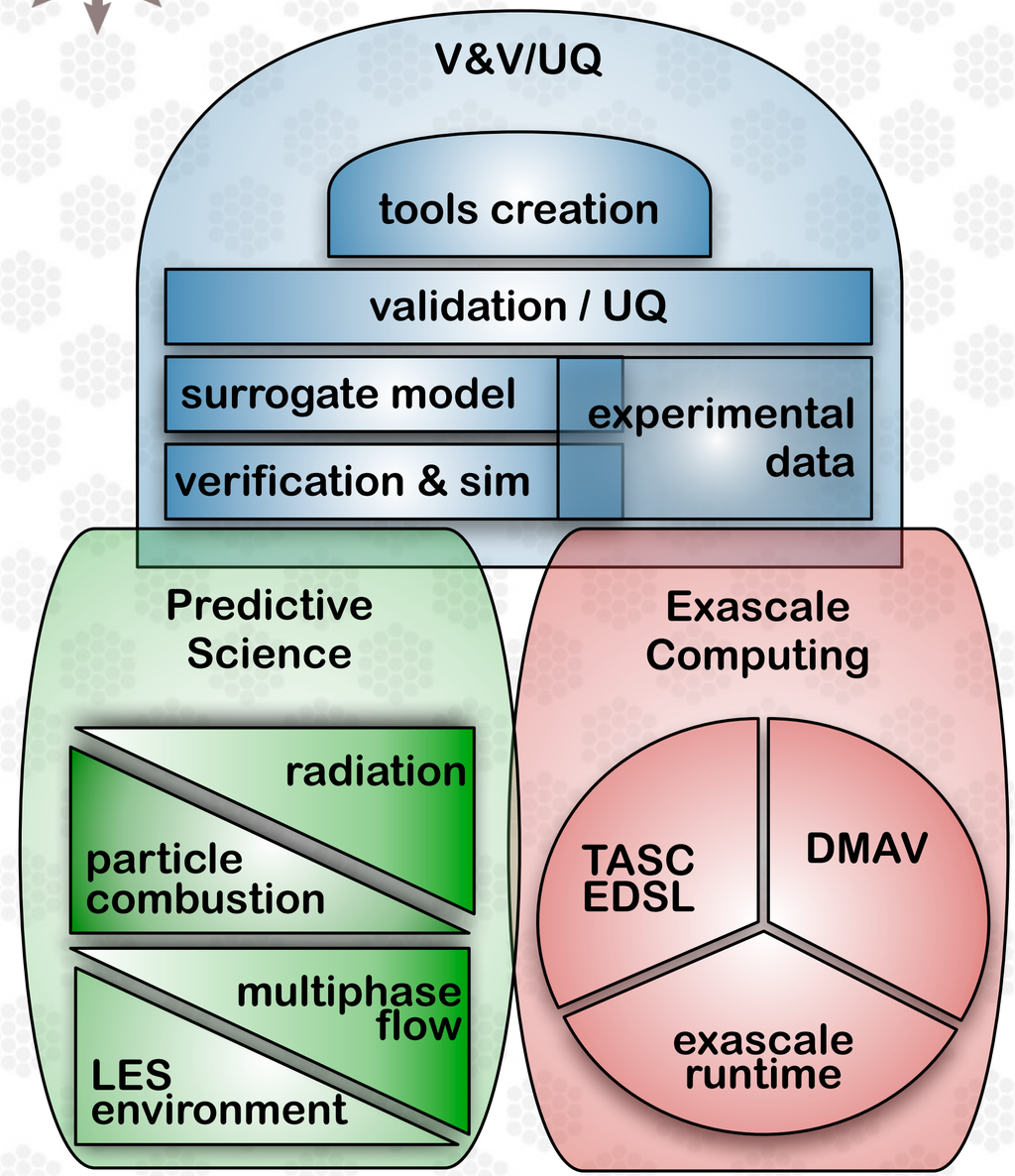

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