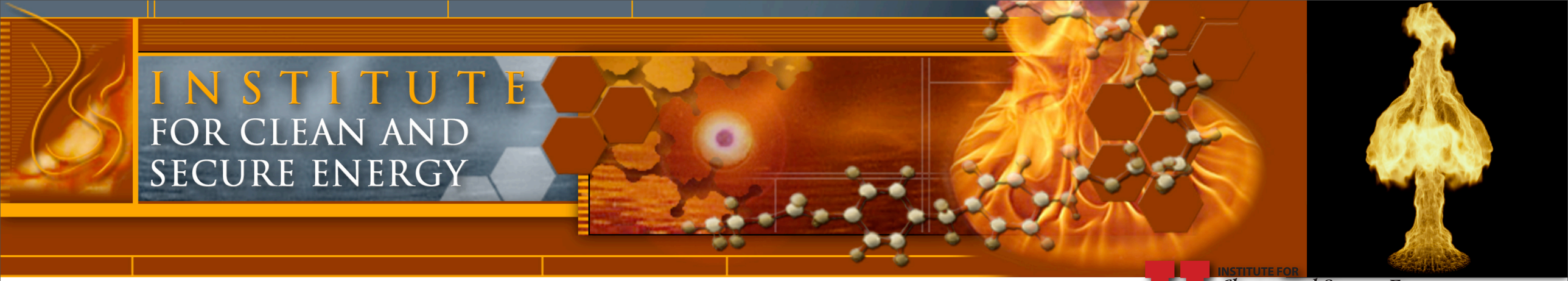


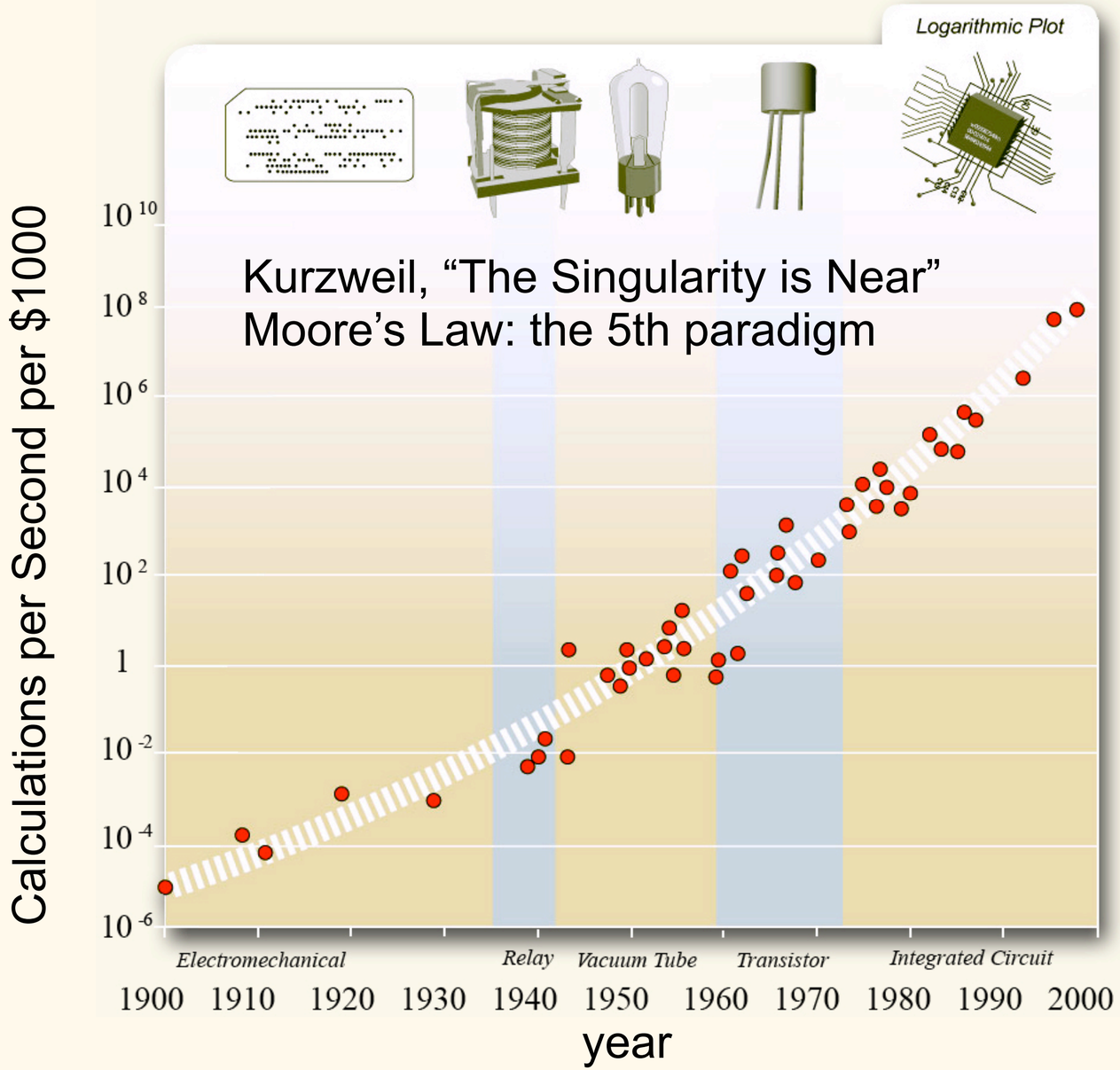
acknowledgement: funding from DOE (NNSA,NETL), ARC computational support from DOE-ASC

Chemically Reacting Flows: Using Manifold Methods to Achieve Predictivity from Large Eddy Simulations

Philip Smith, Jennifer Spinti, Jeremy Thornock

The University of Utah

Background / Context



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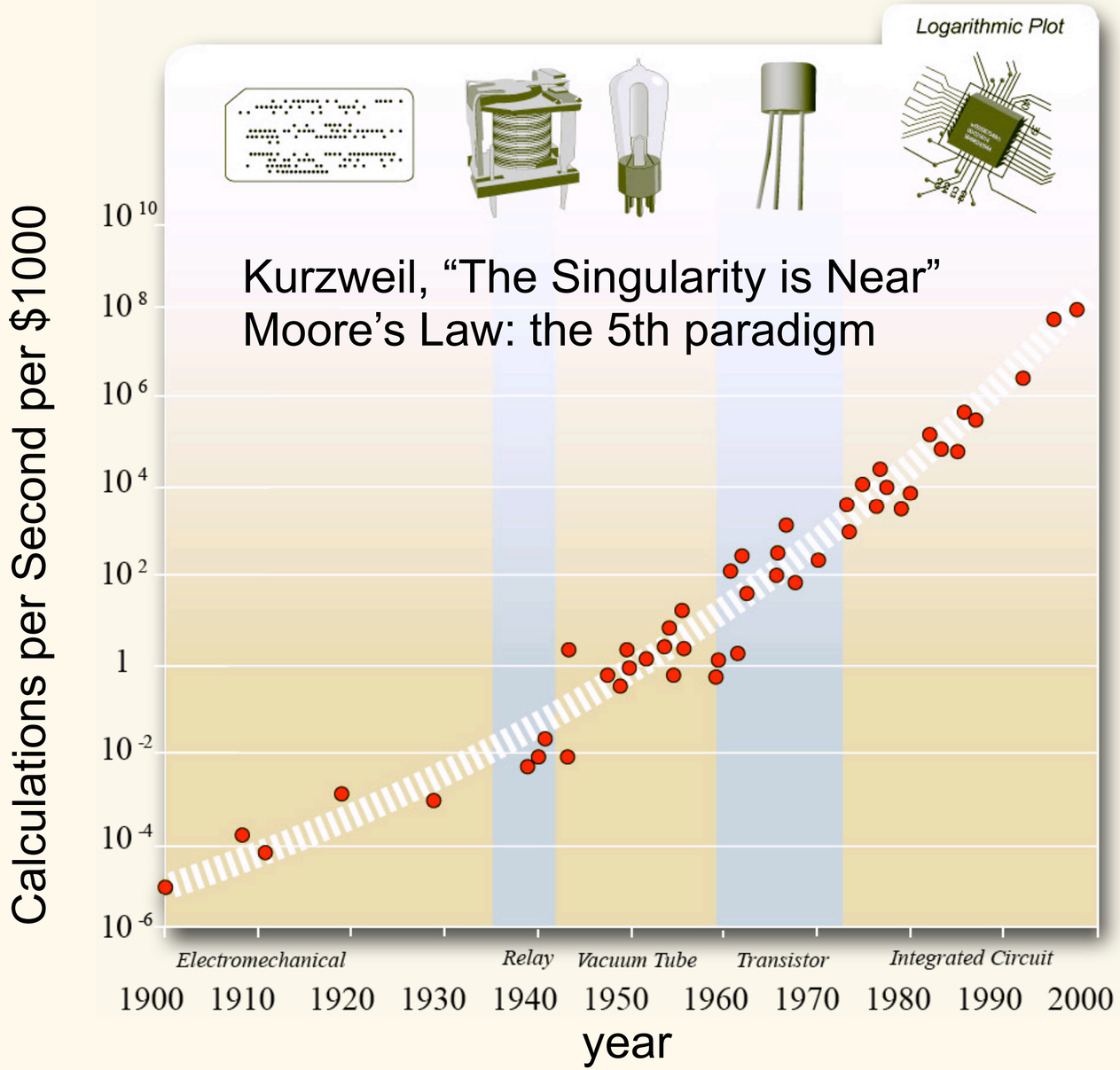

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- **11 year ASC university alliance partner**
- **multidisciplinary, multiscale simulation science**

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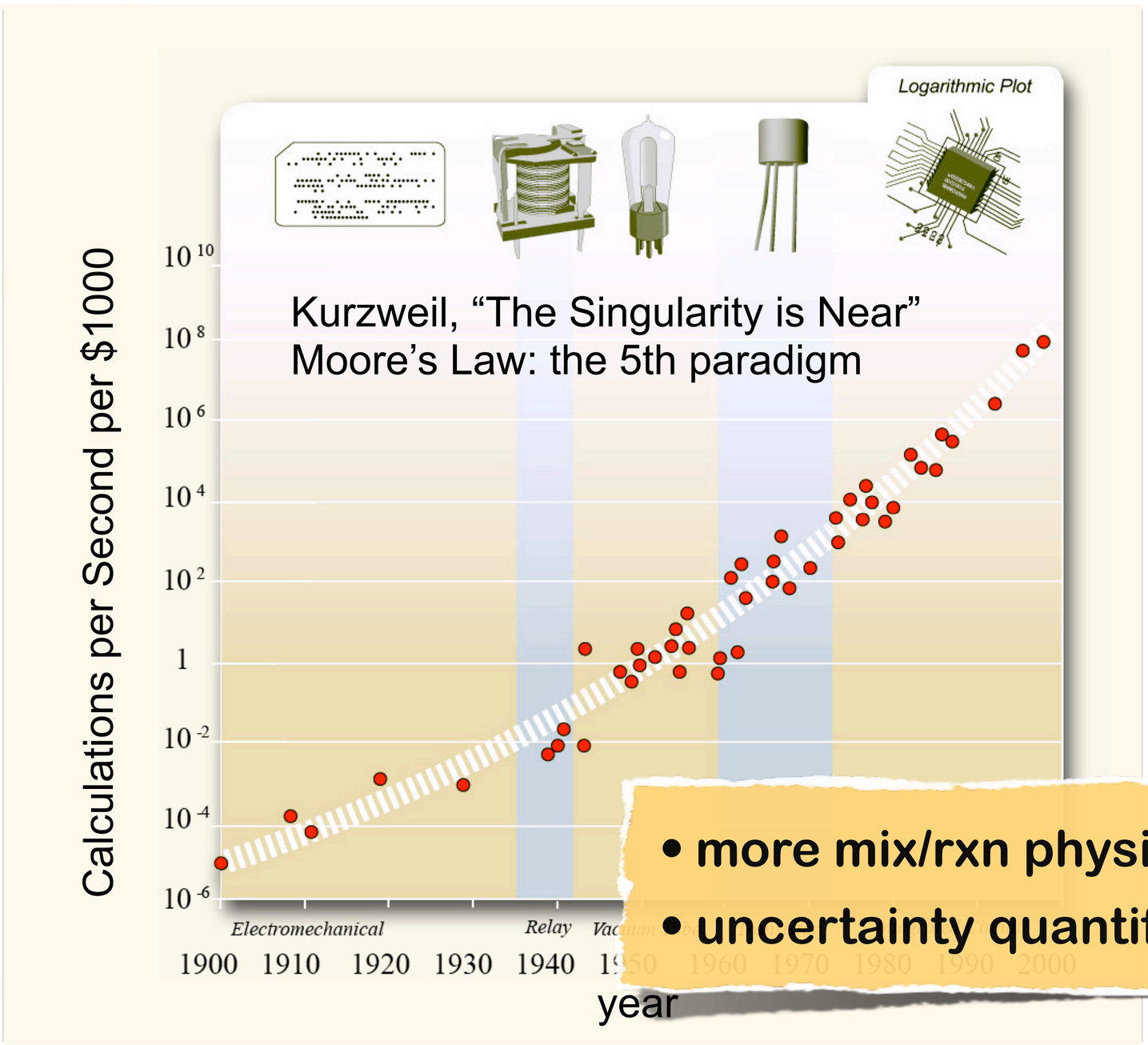

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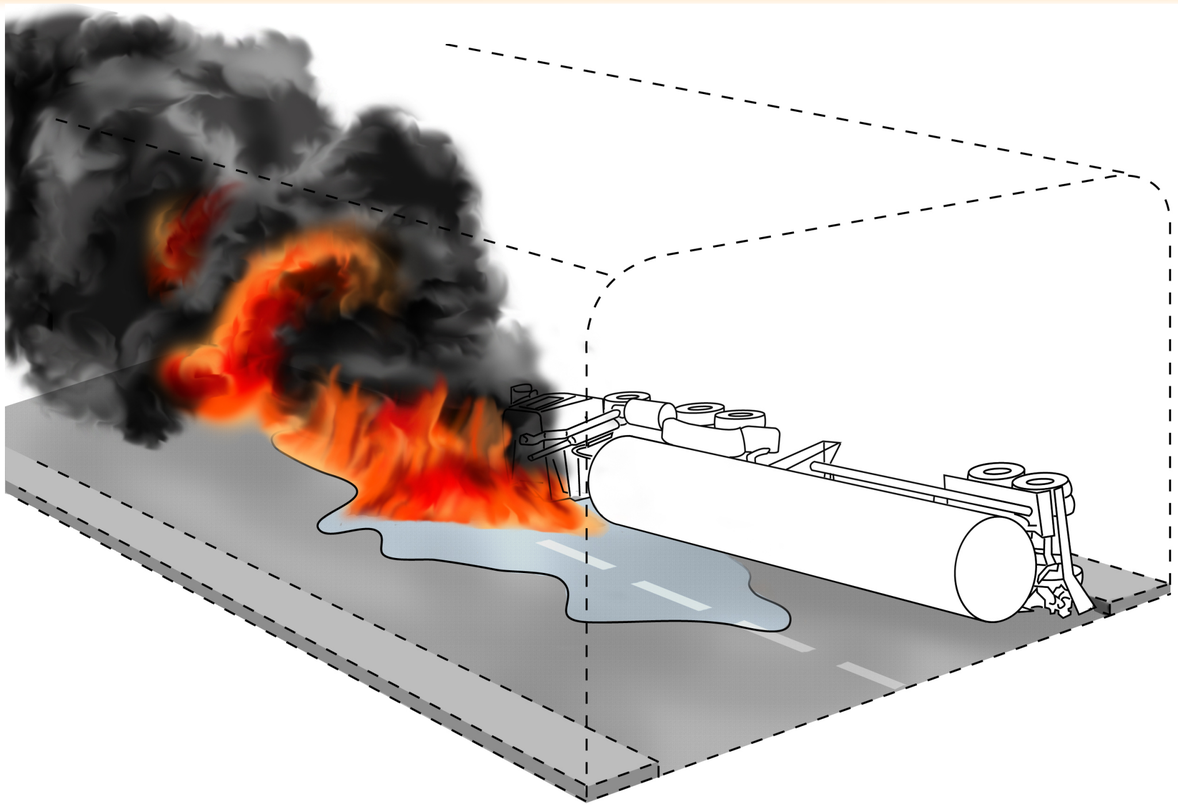

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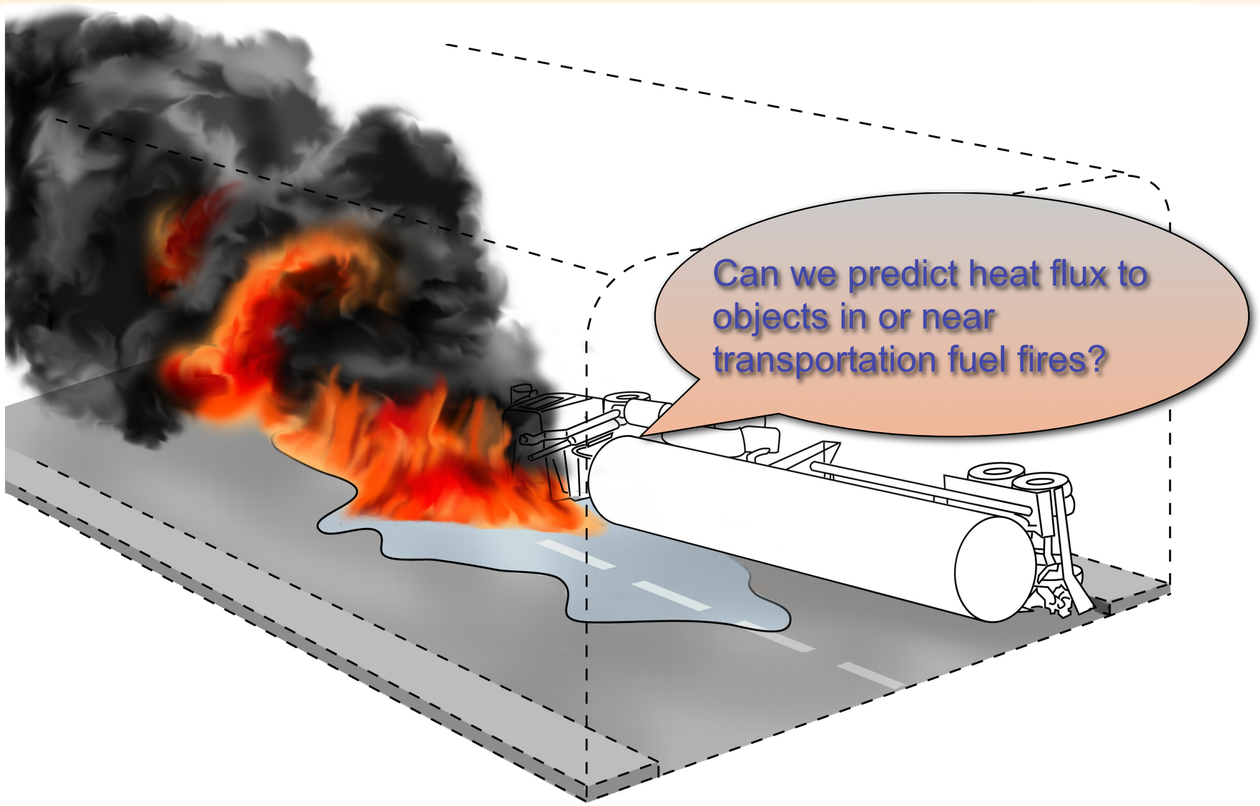

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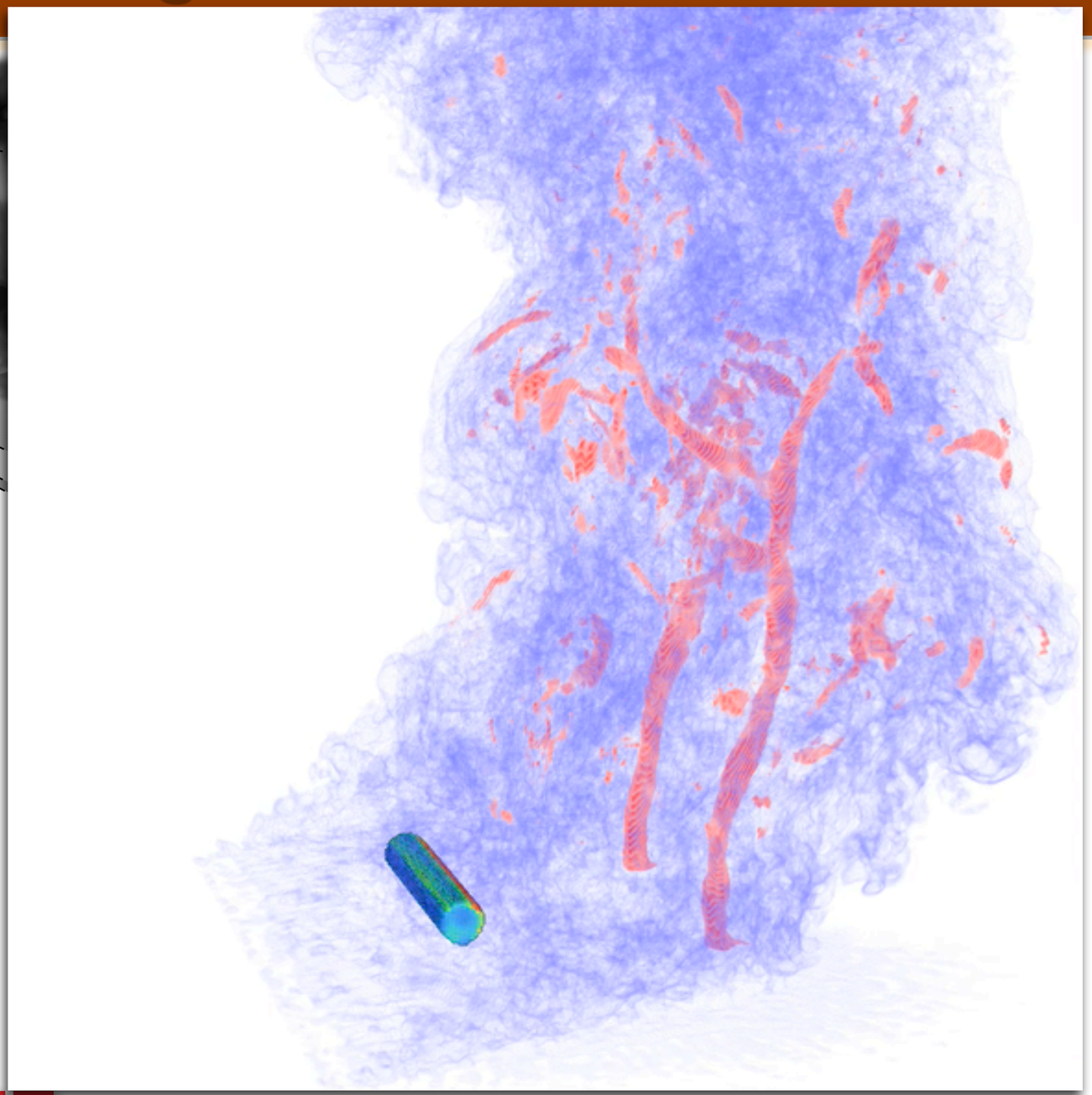

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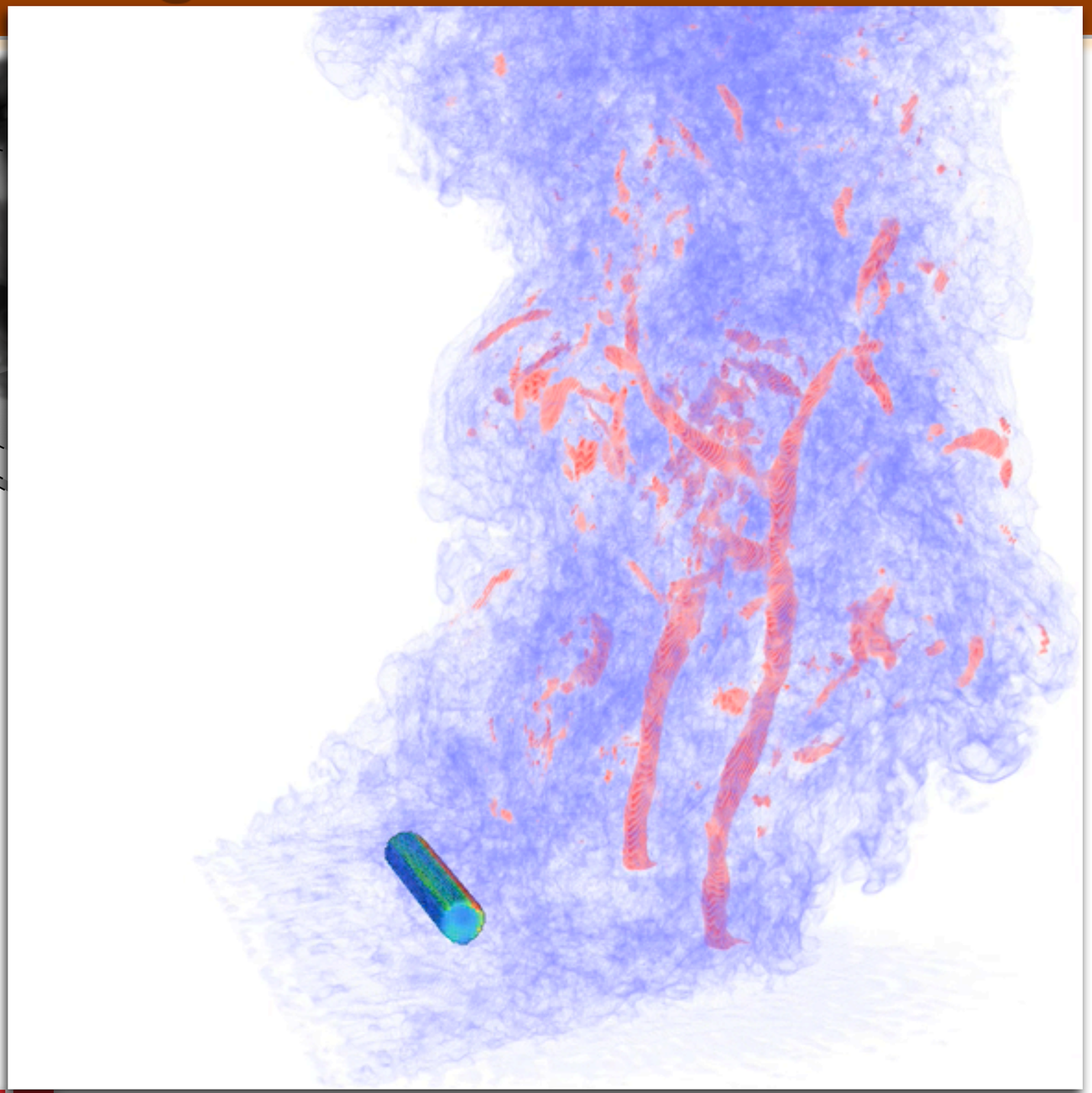
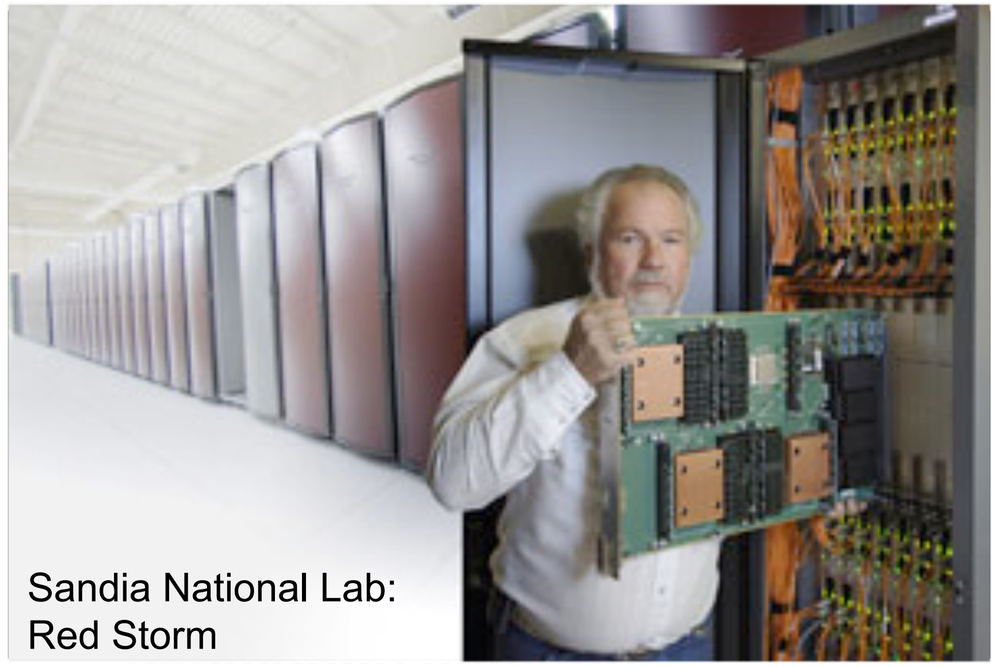
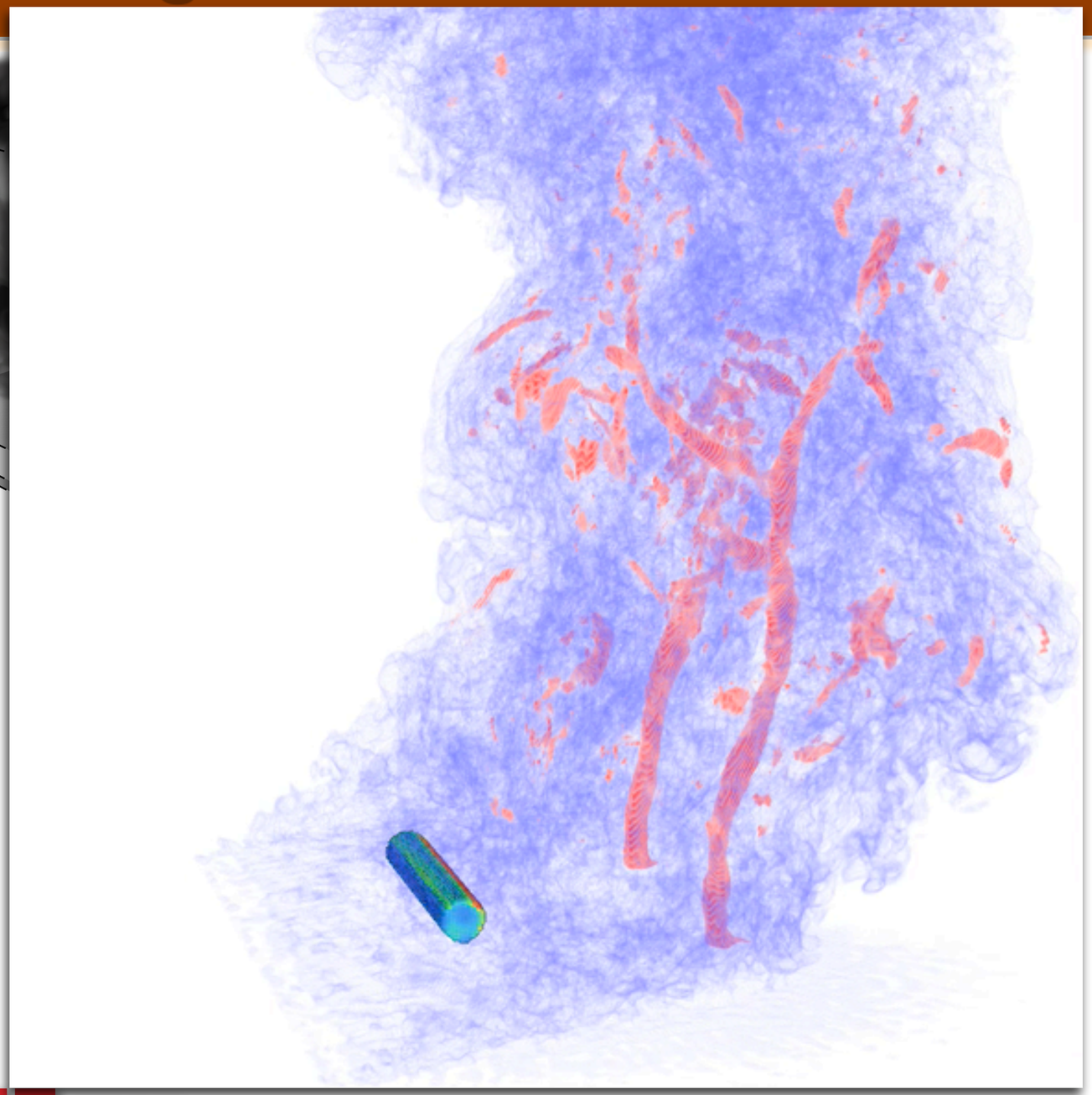
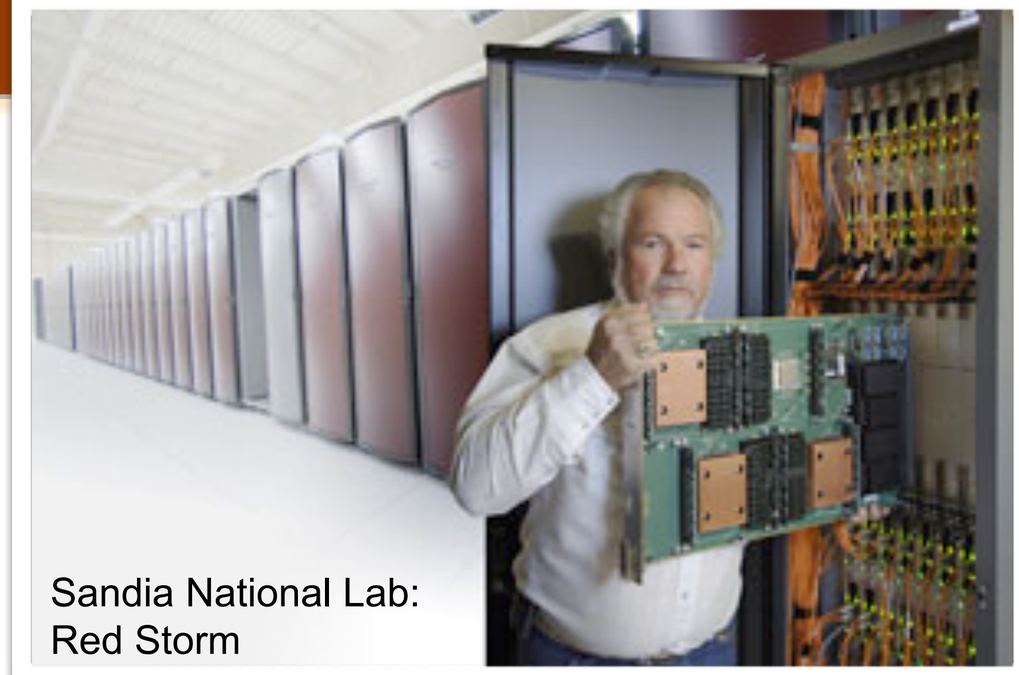




- massive parallelism

Background / Context



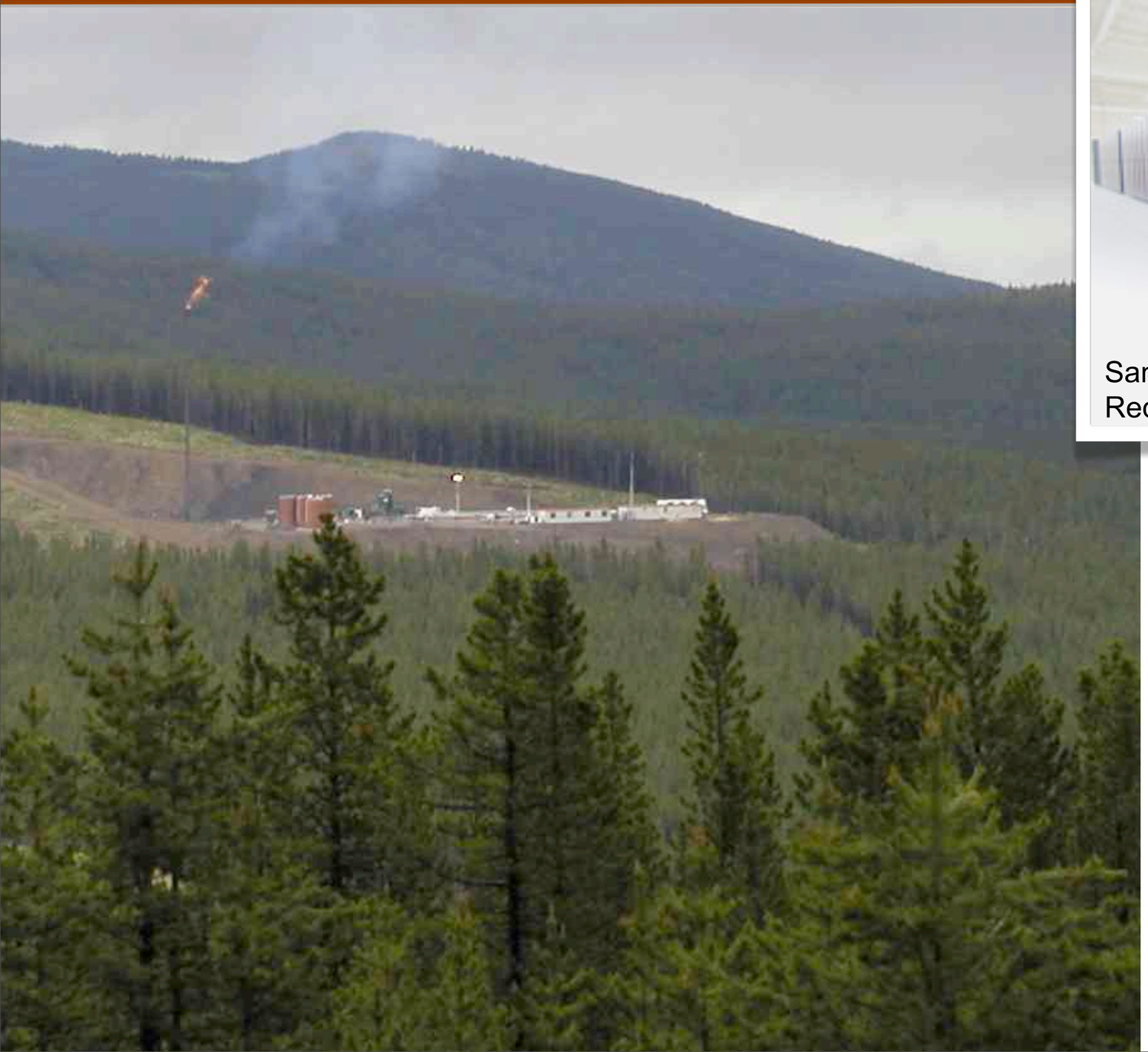


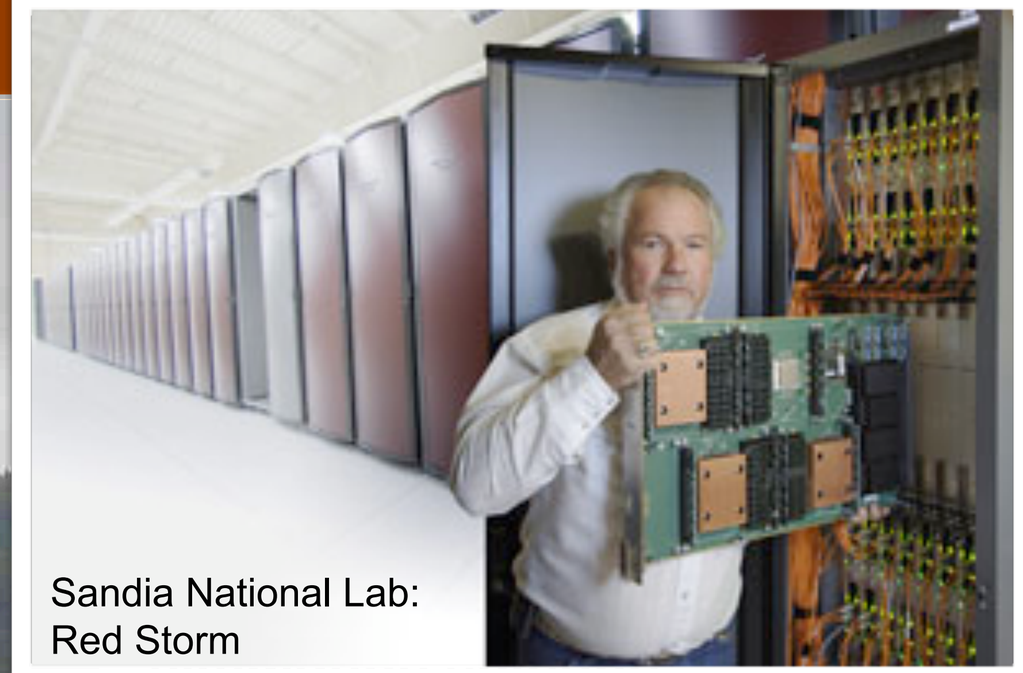
- massive parallelism

2000 cores for 10 days per simulation

> 56 cpu years per simulation

Background / Context



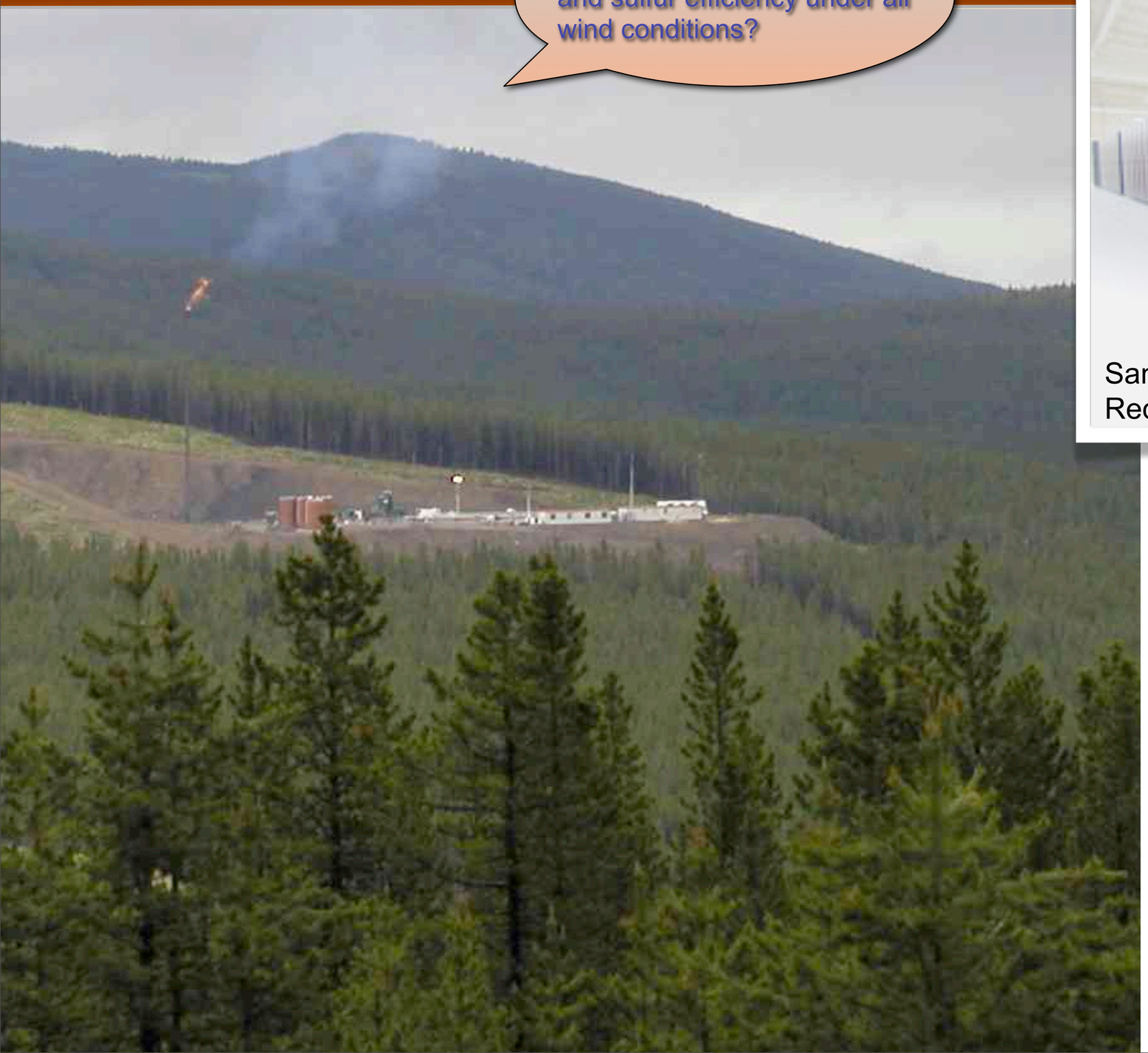


Sandia National Lab:
Red Storm

massive parallelism

Background / Cor

Can we predict combustion and sulfur efficiency under all wind conditions?



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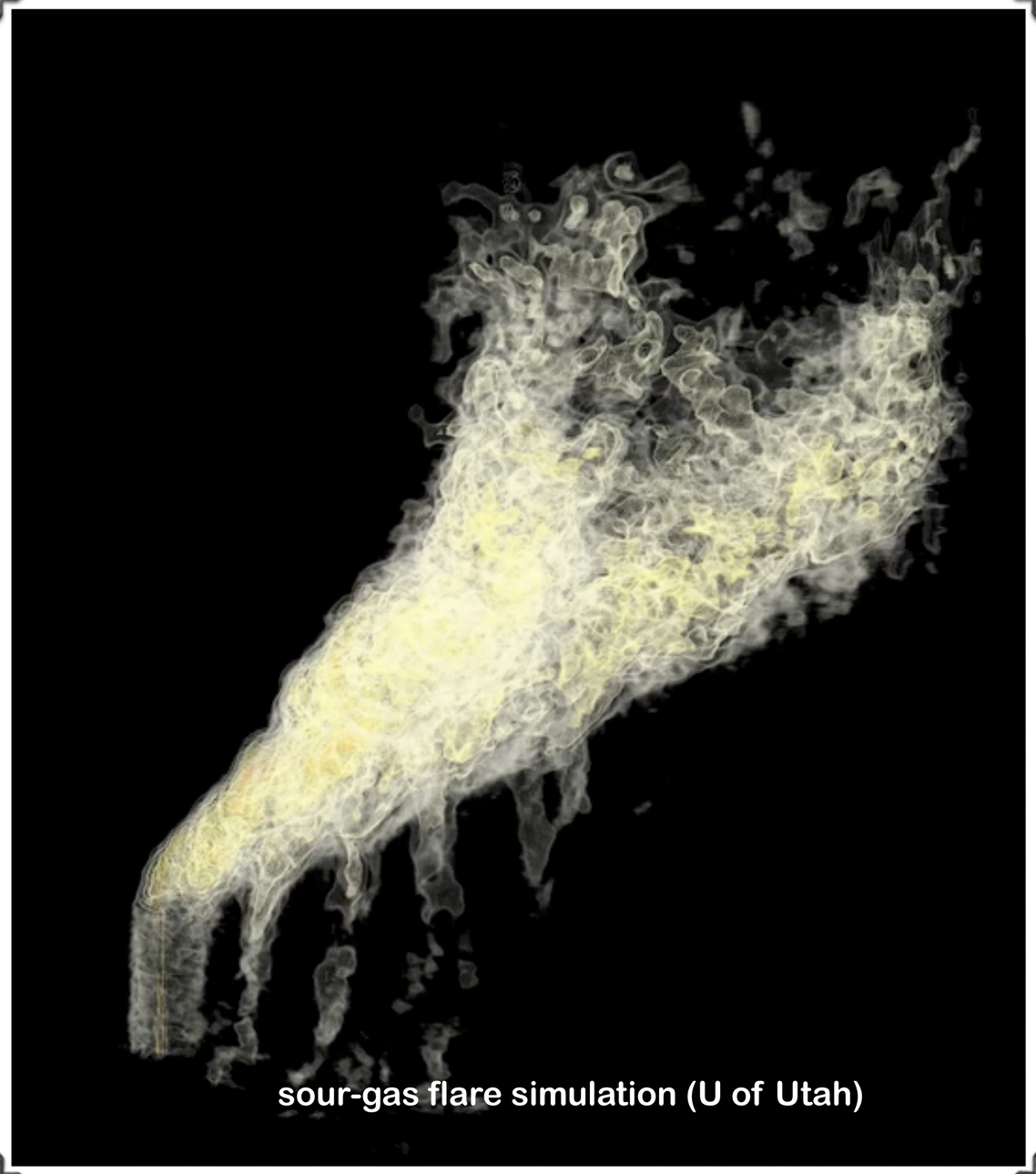
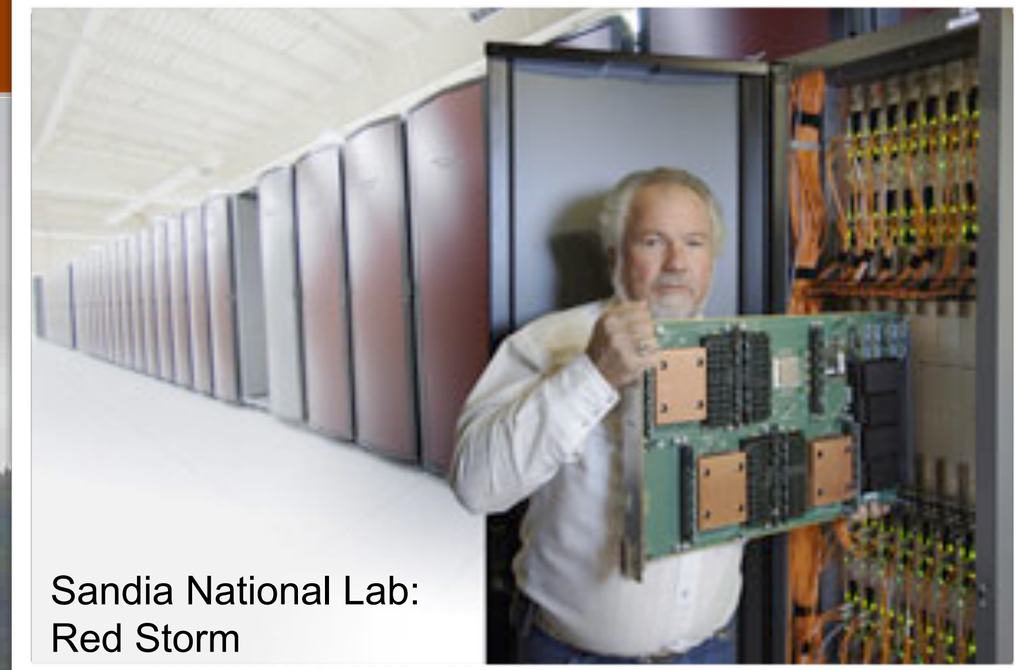


sour-gas flare simulation (U of Utah)



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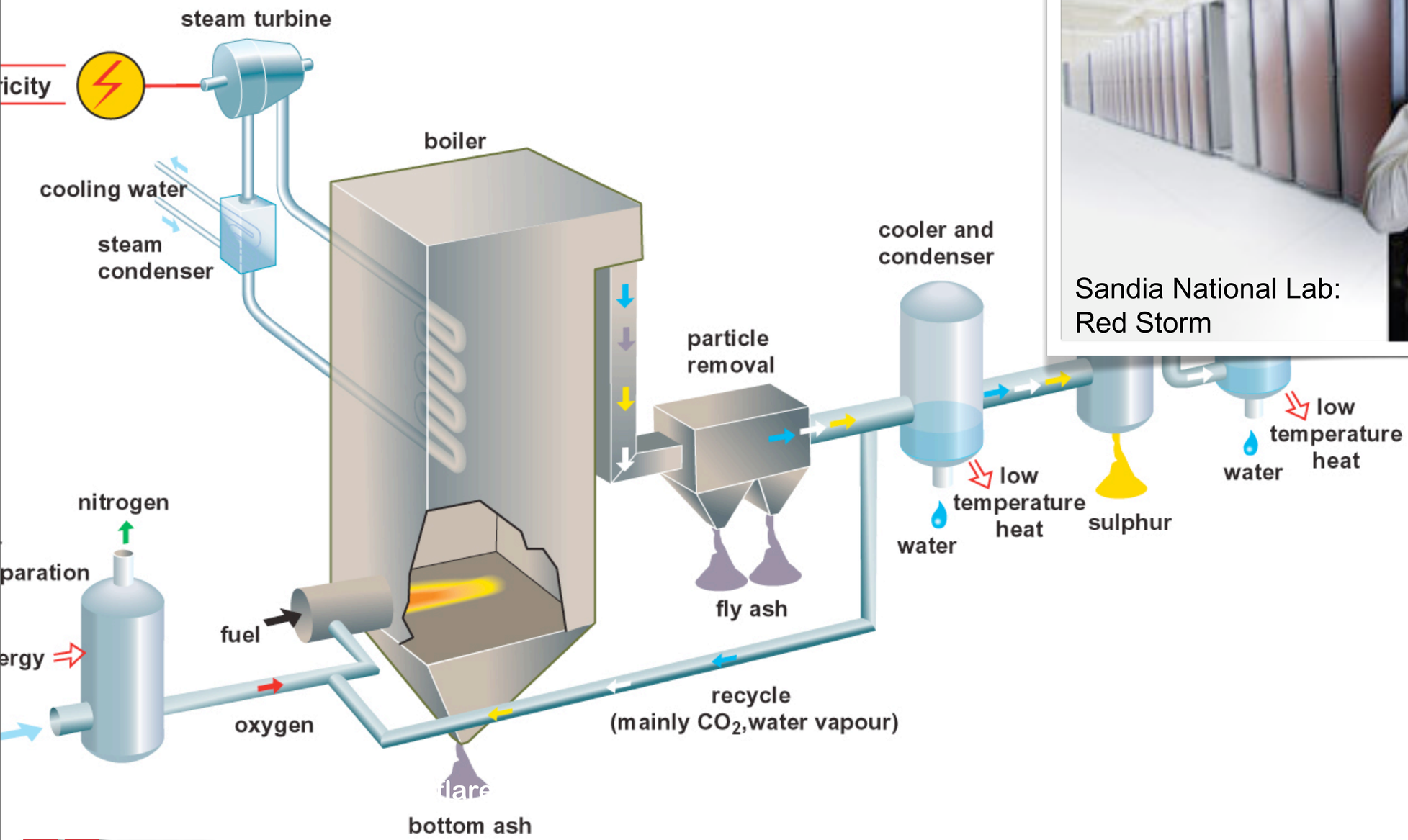


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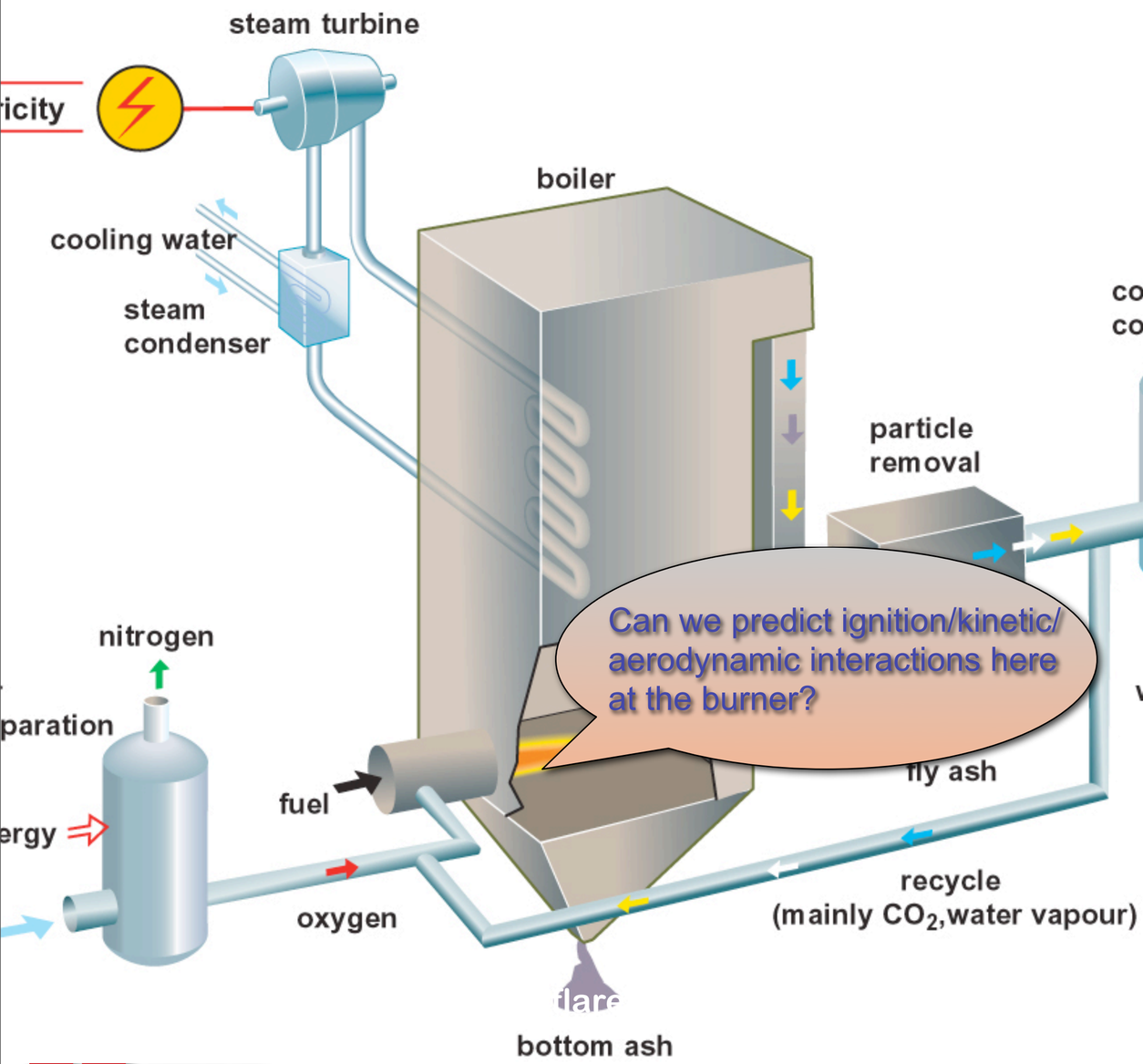


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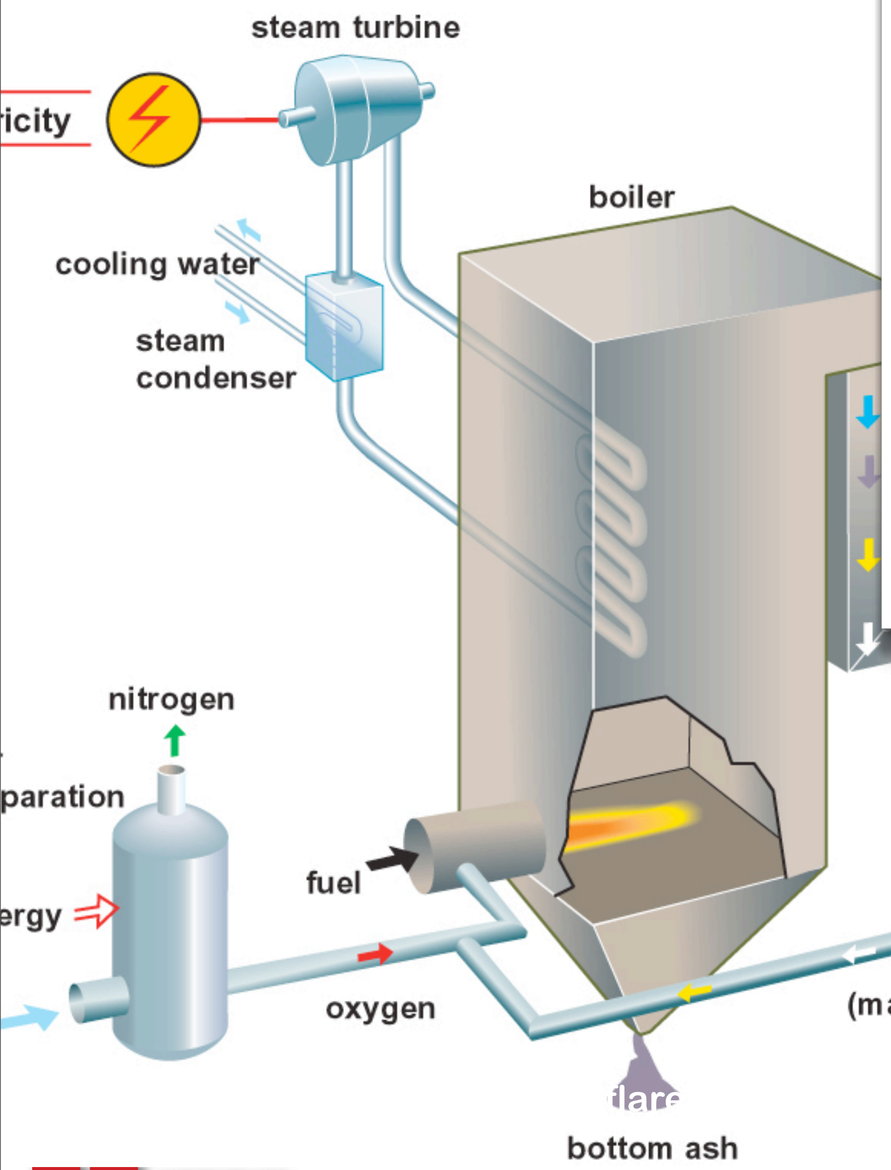

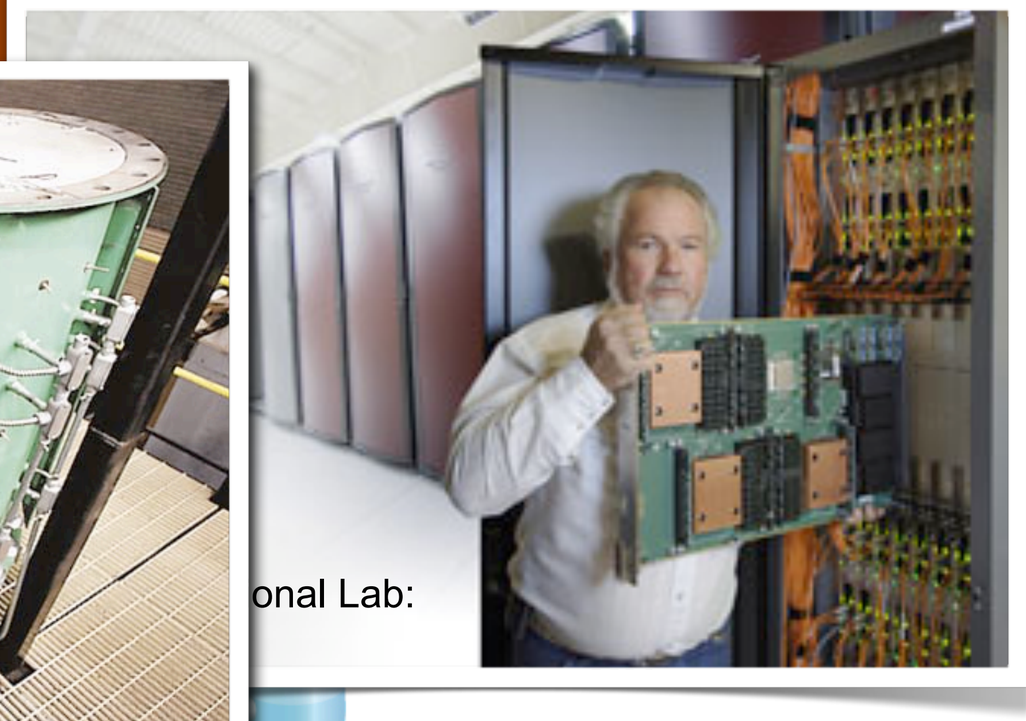

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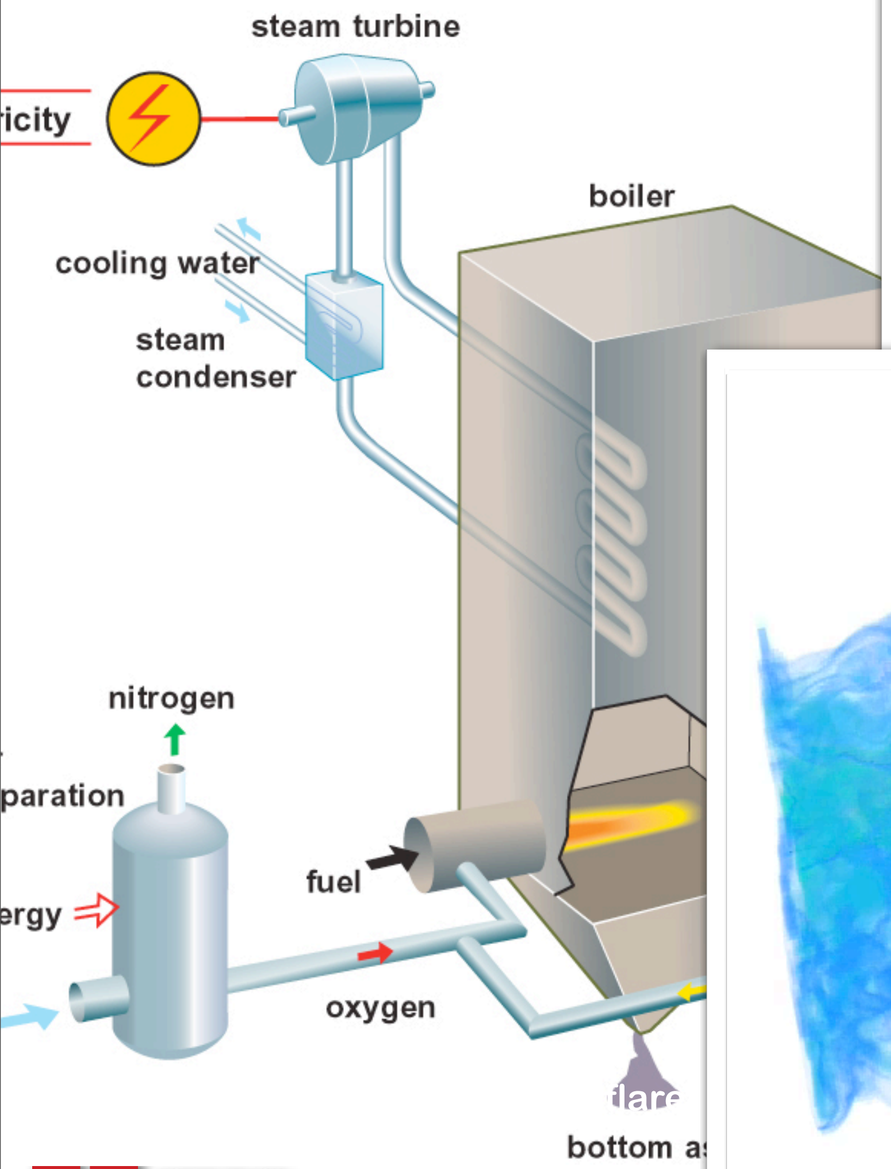

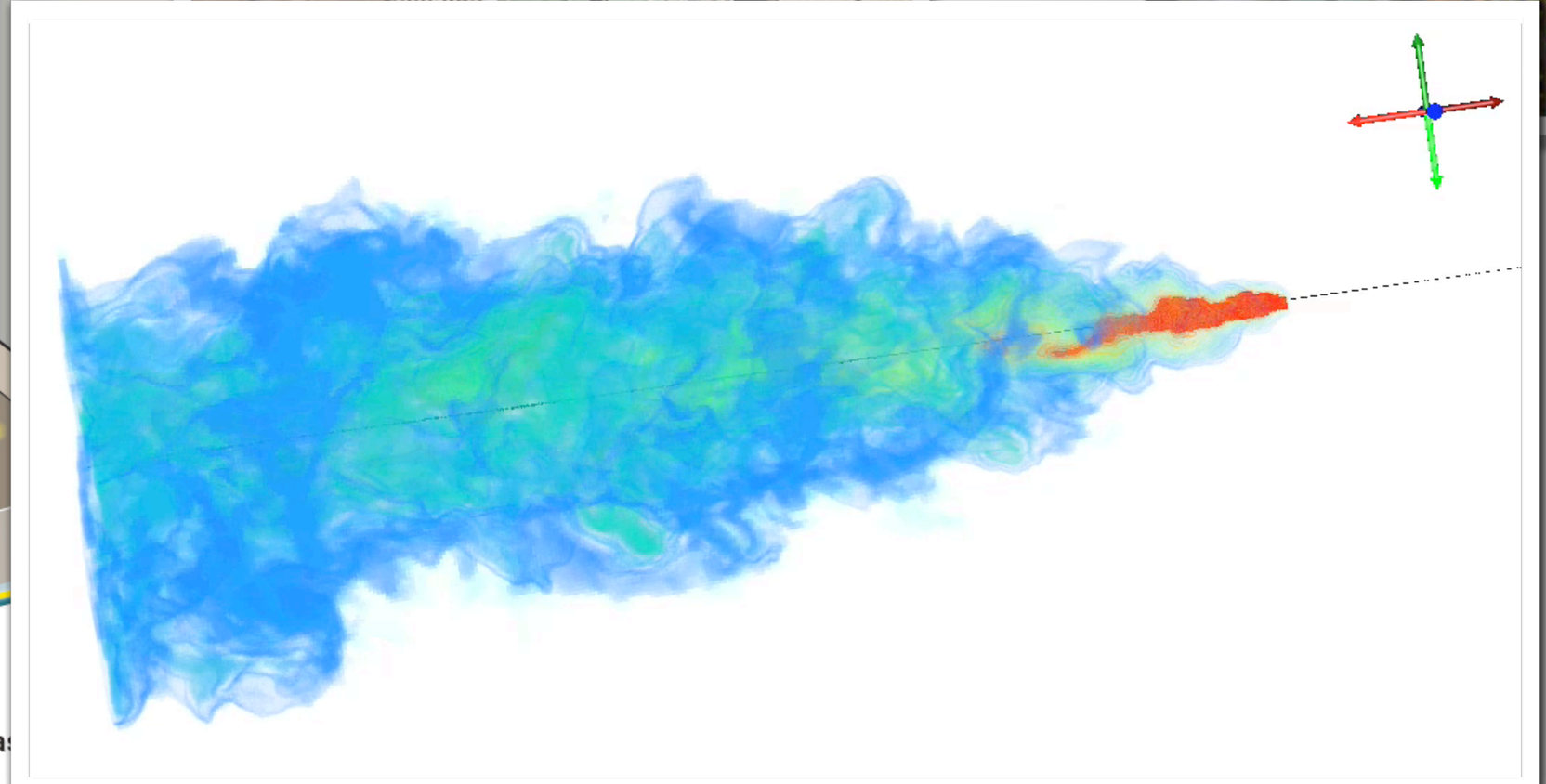

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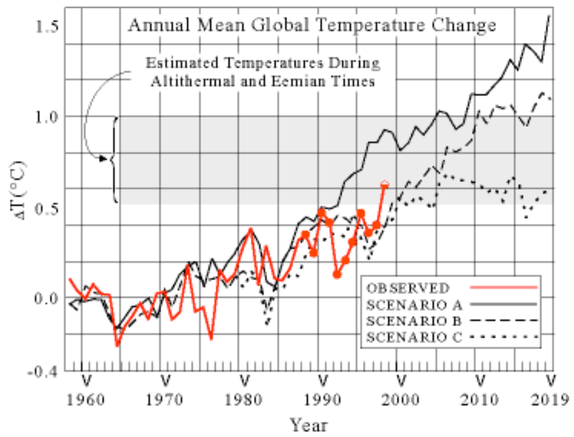
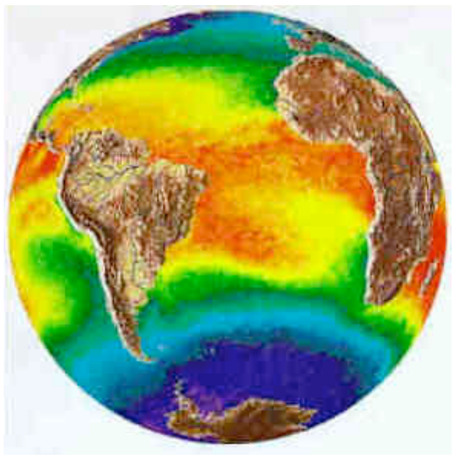
Simulation & Experiment: quantifiable predictivity

source: GeographyAcademy

- **simulation is increasingly being called upon to provide predictive capability for decision making**
- **multidisciplinary problems** *(expensive function evaluations)* **that require communication between stake-holders (risk assessment)**
- **need measurements & simulation together to produce quantified predictivity with uncertainty assessment (trends not enough)**





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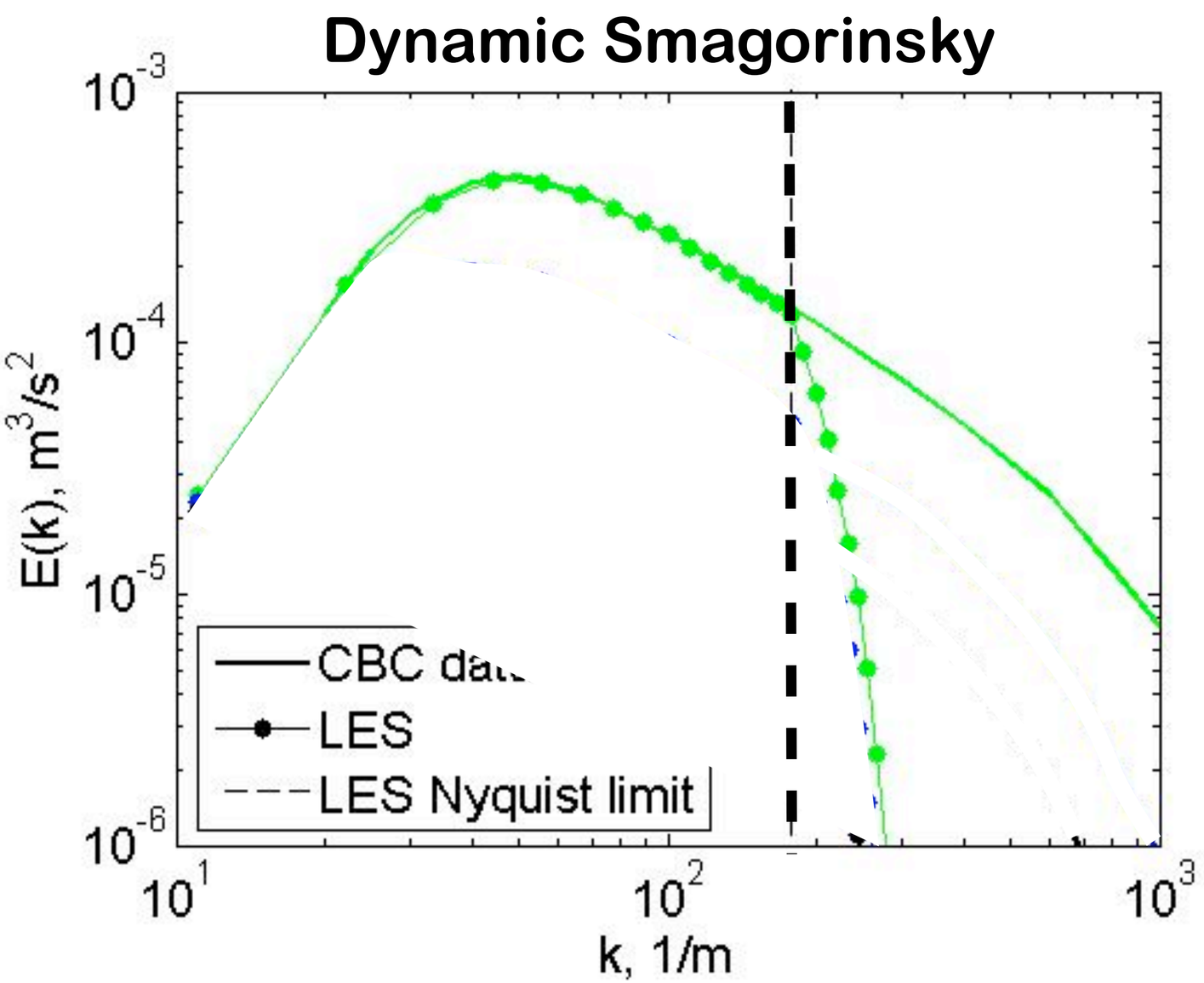
Turbulent Energy Spectrum



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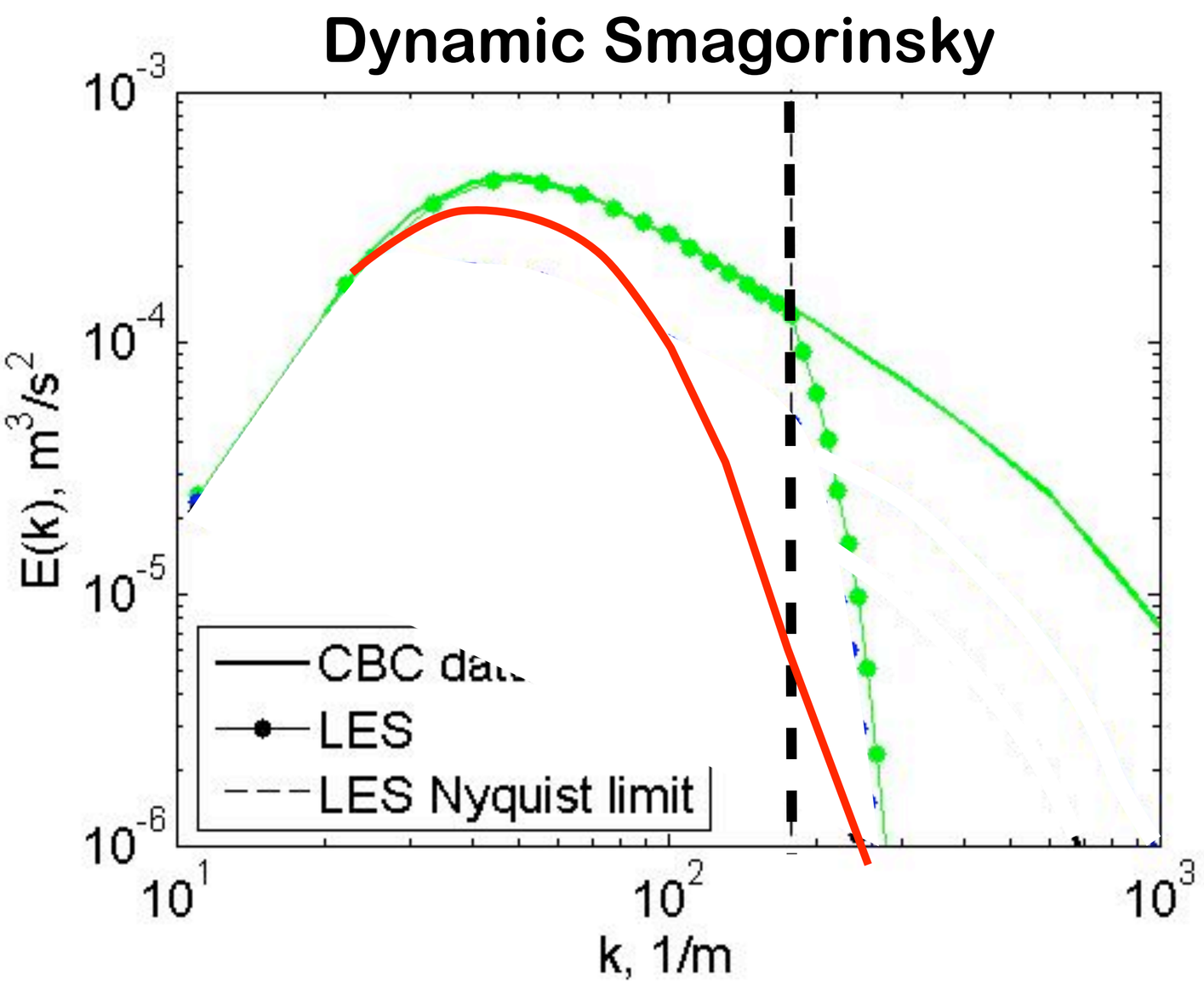

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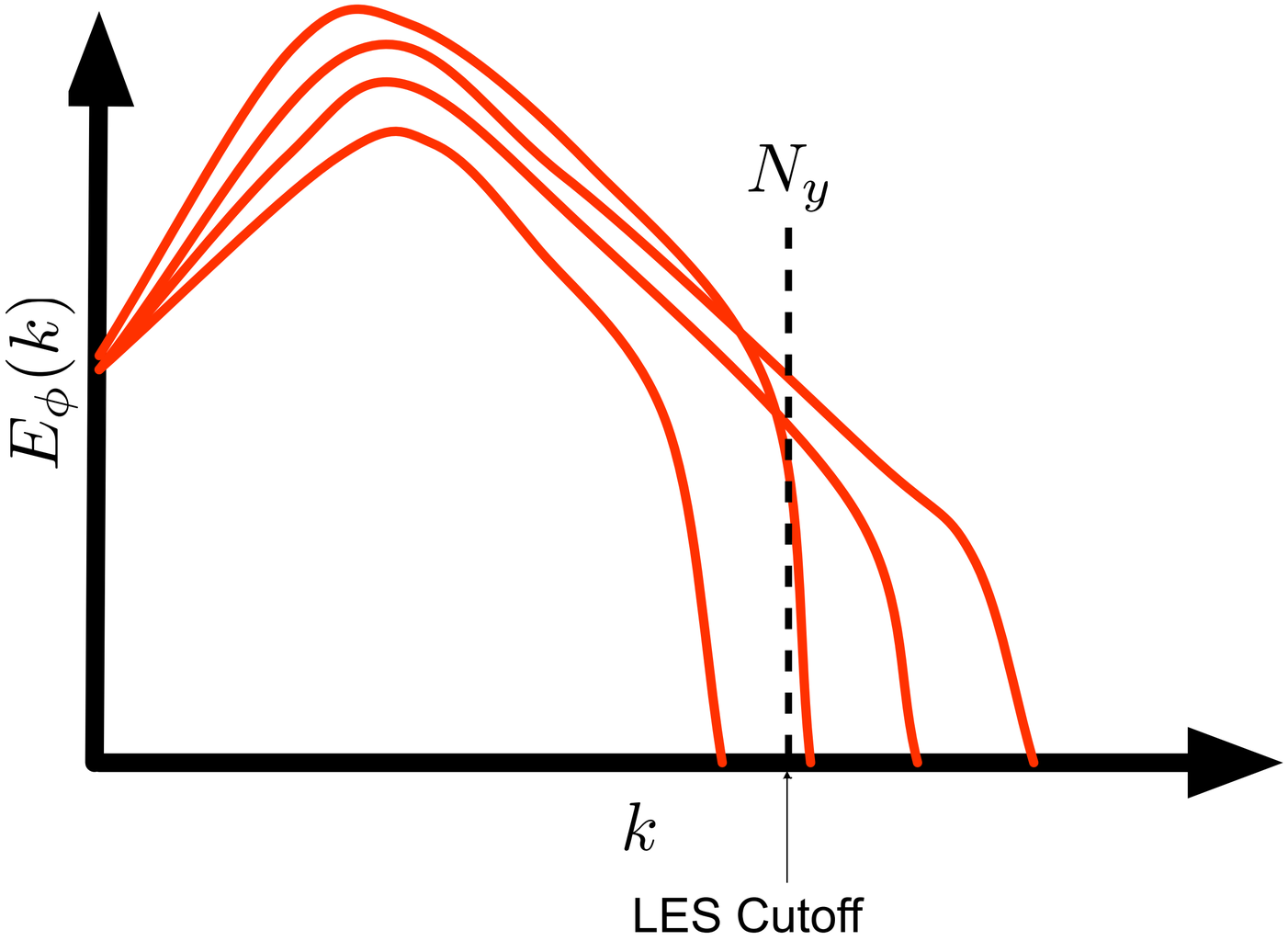
Turbulent Scalar Spectrum



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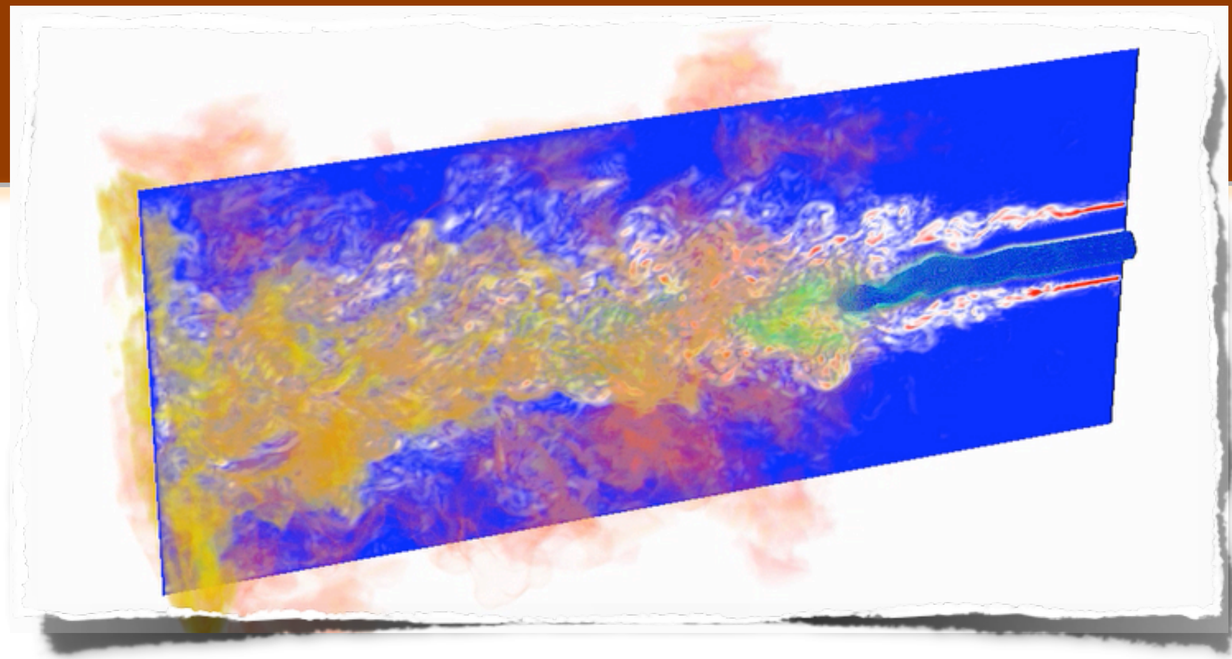

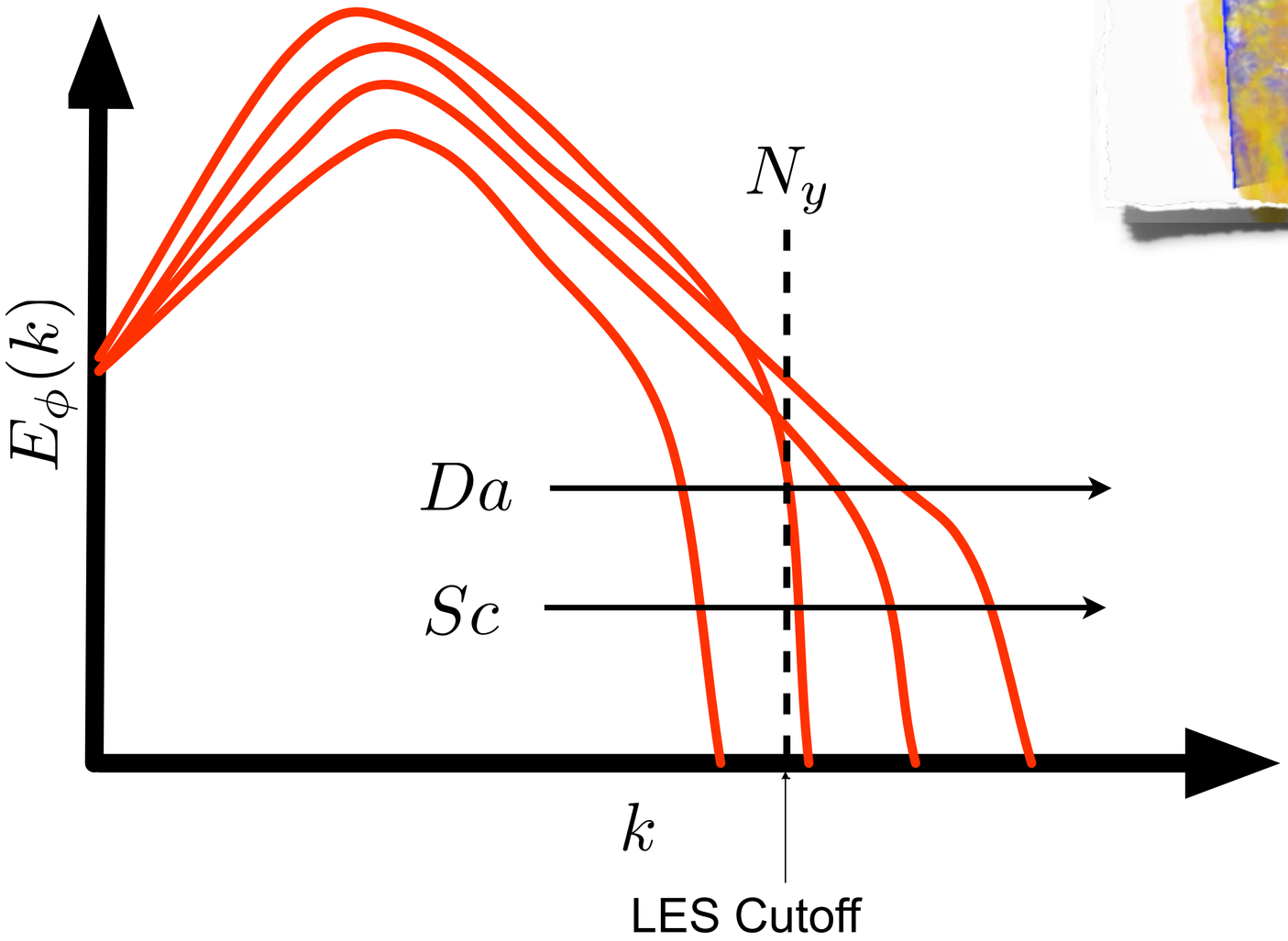

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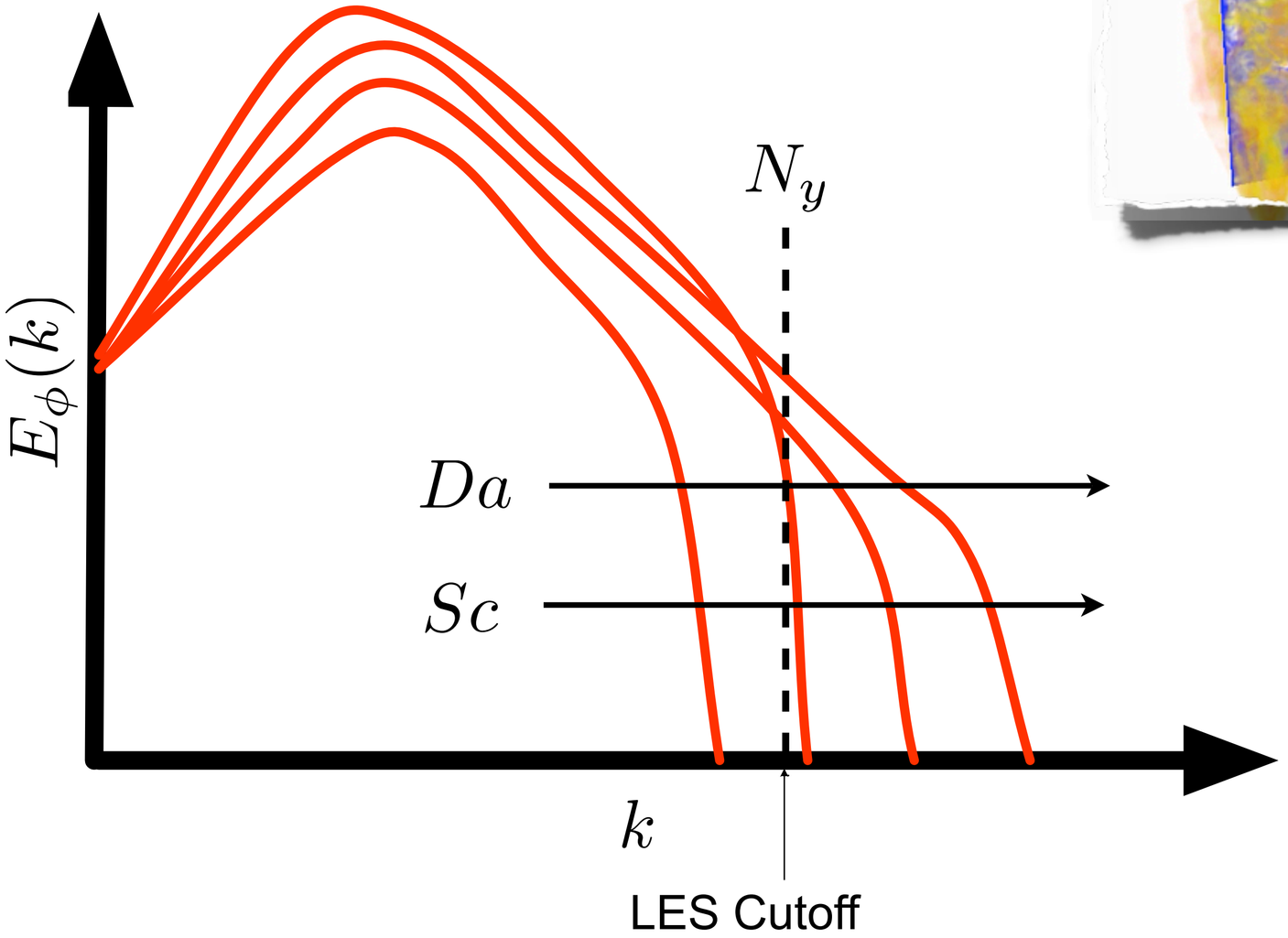
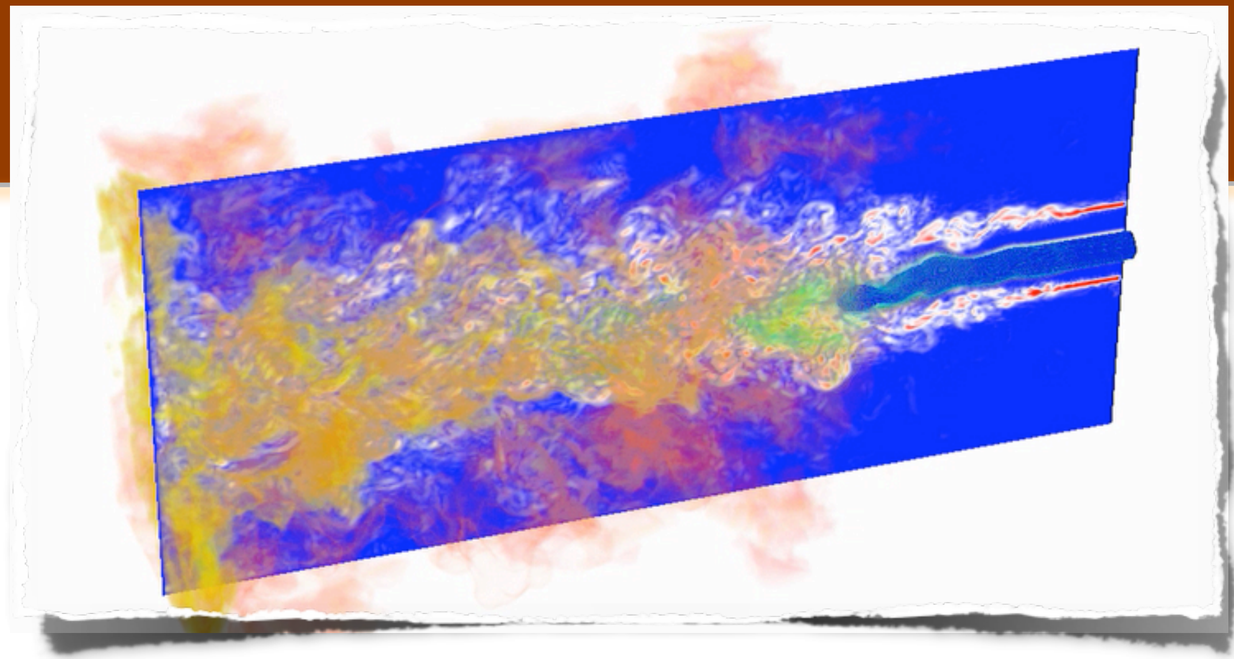
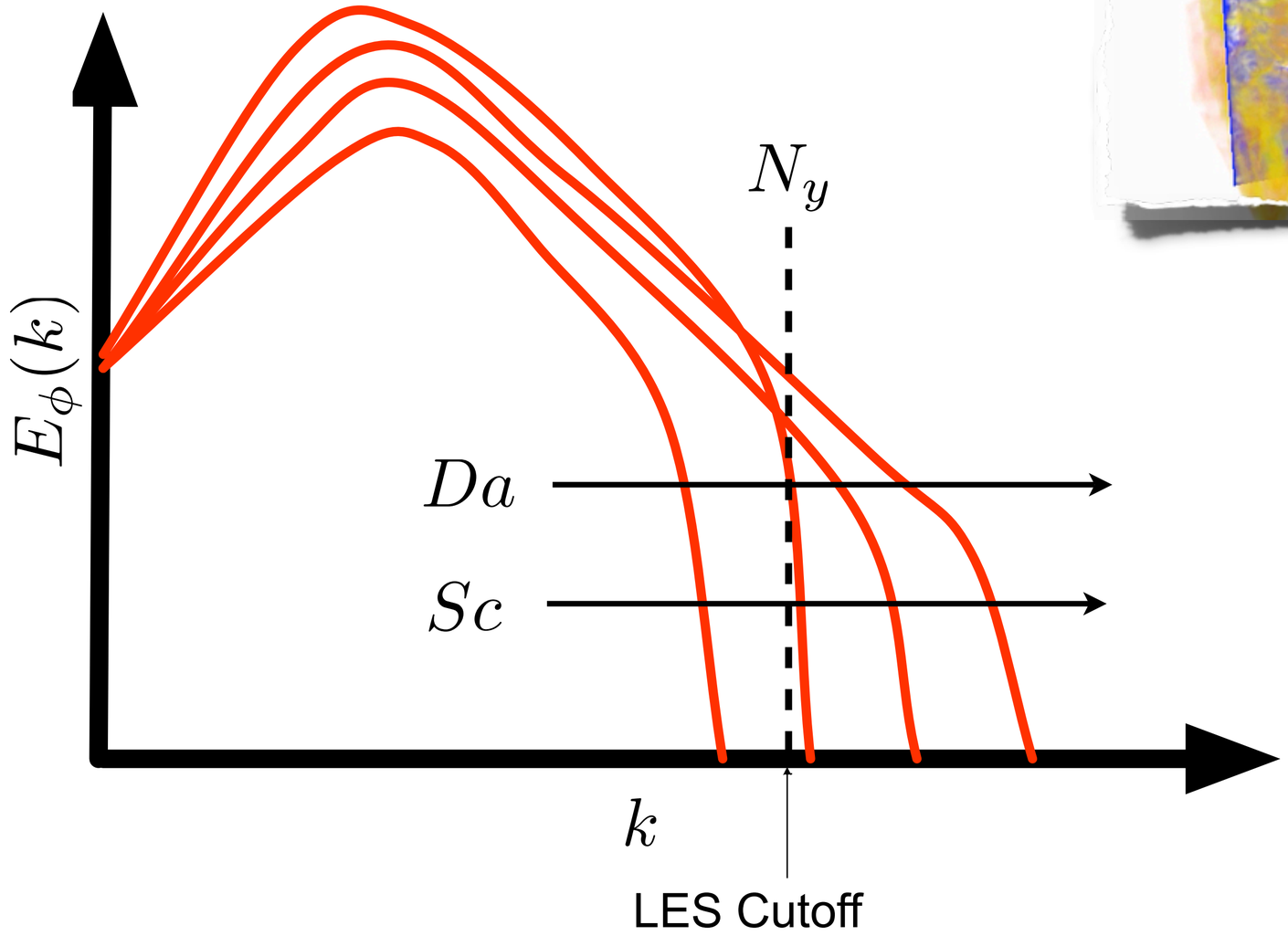
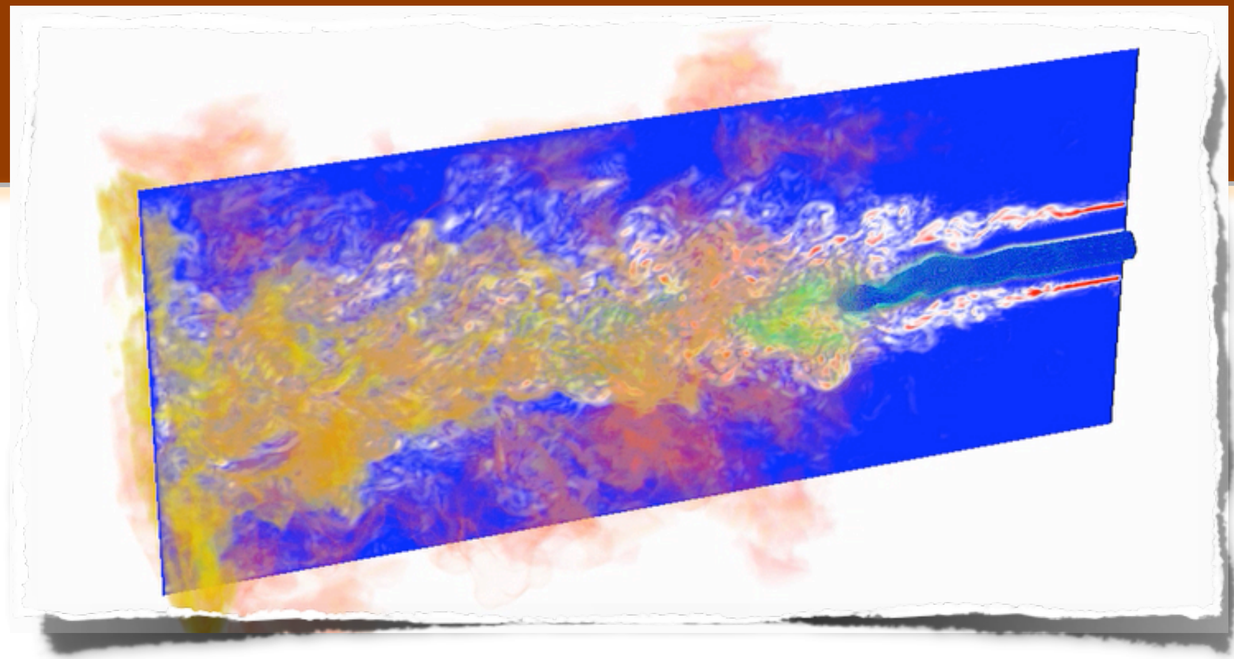




- if low wave-number process: LES offers direct resolution on the mesh! (ie, coal)

Turbulent Scalar Spectrum





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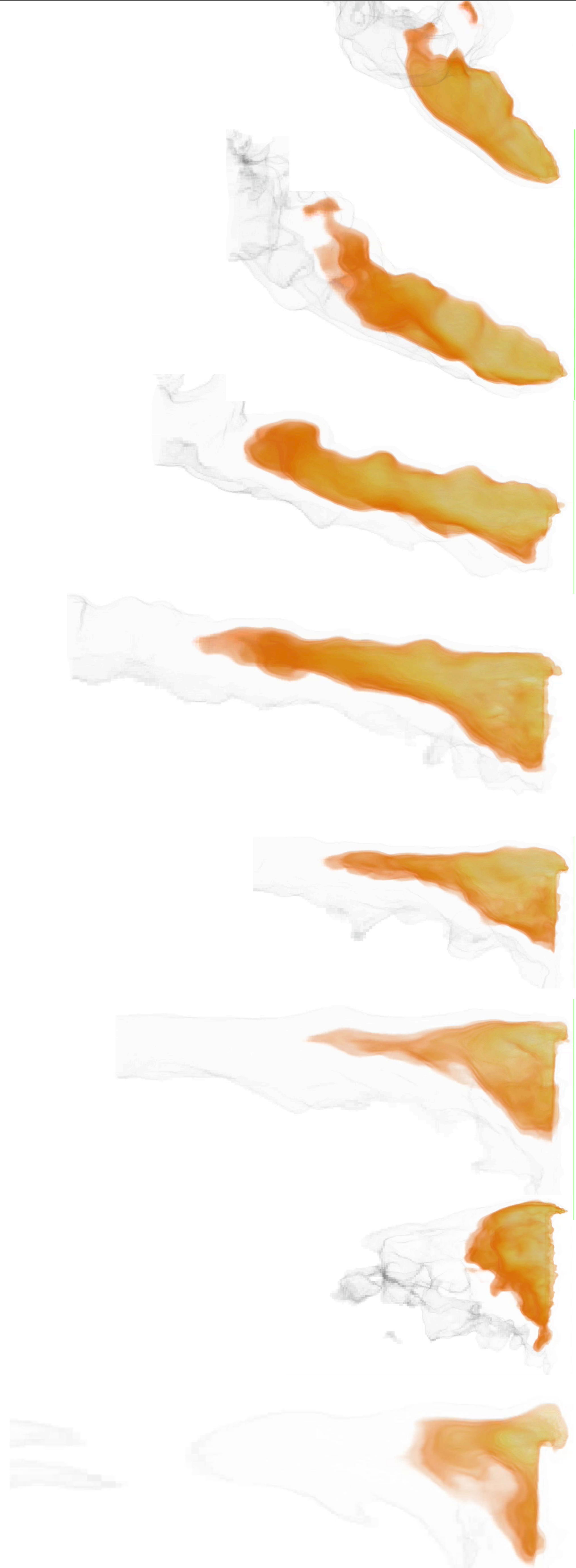
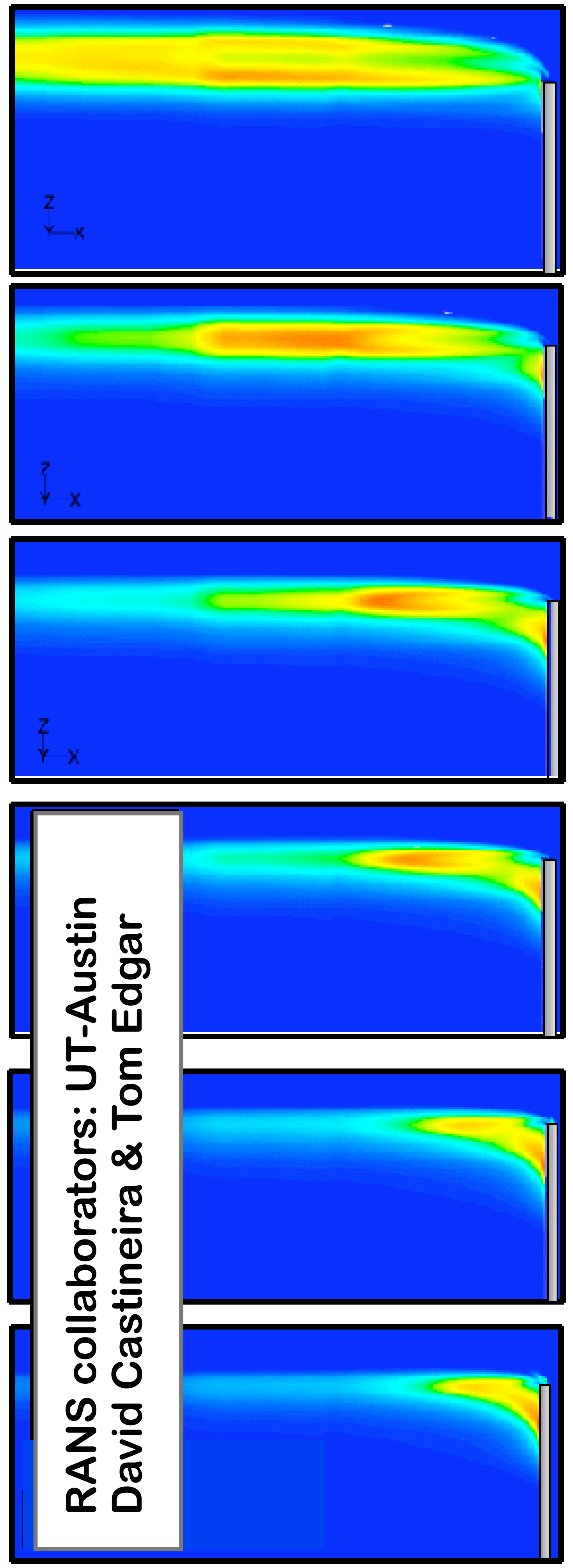
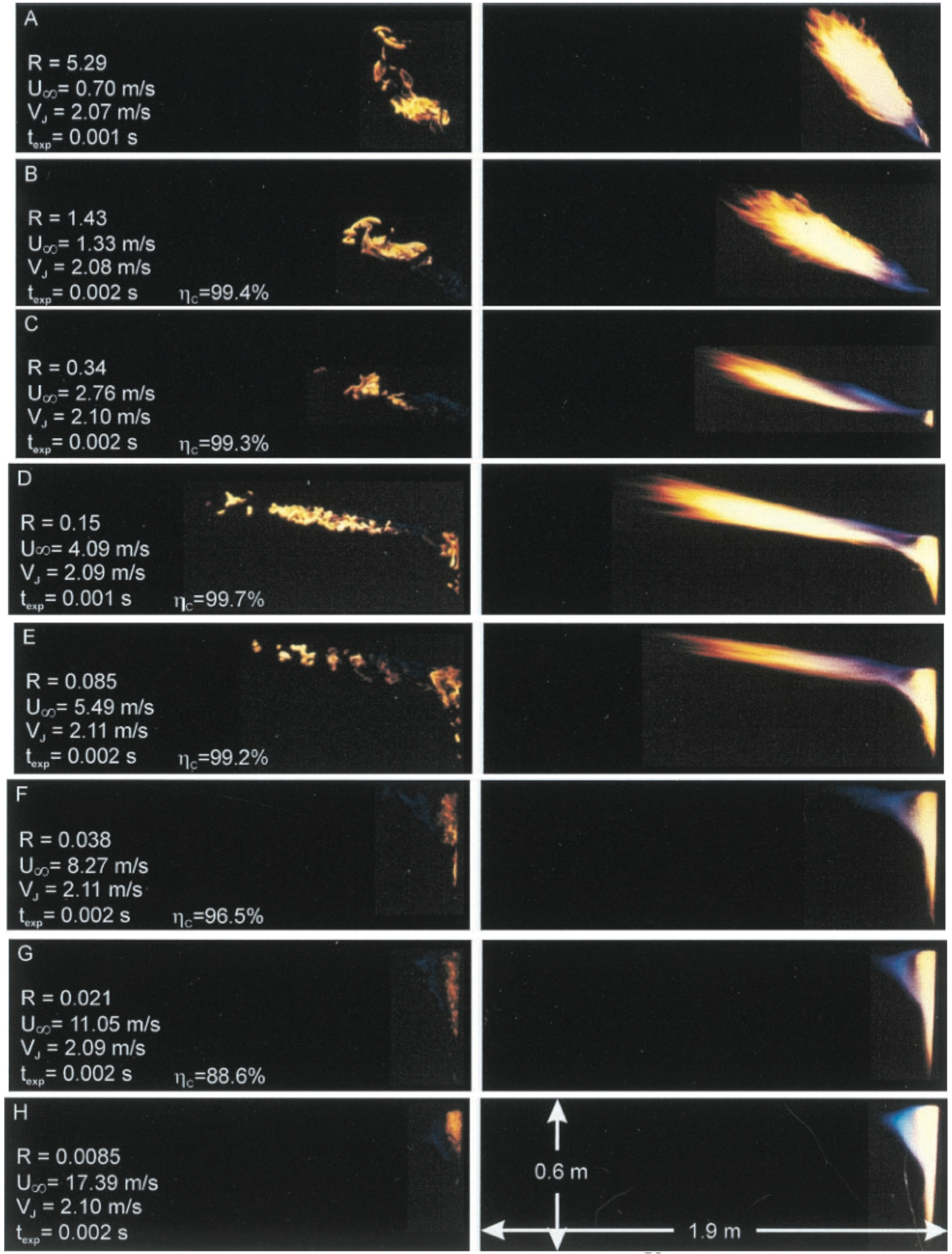
- if high wave-number process: need multiscale models that accurately feed the resolved scale



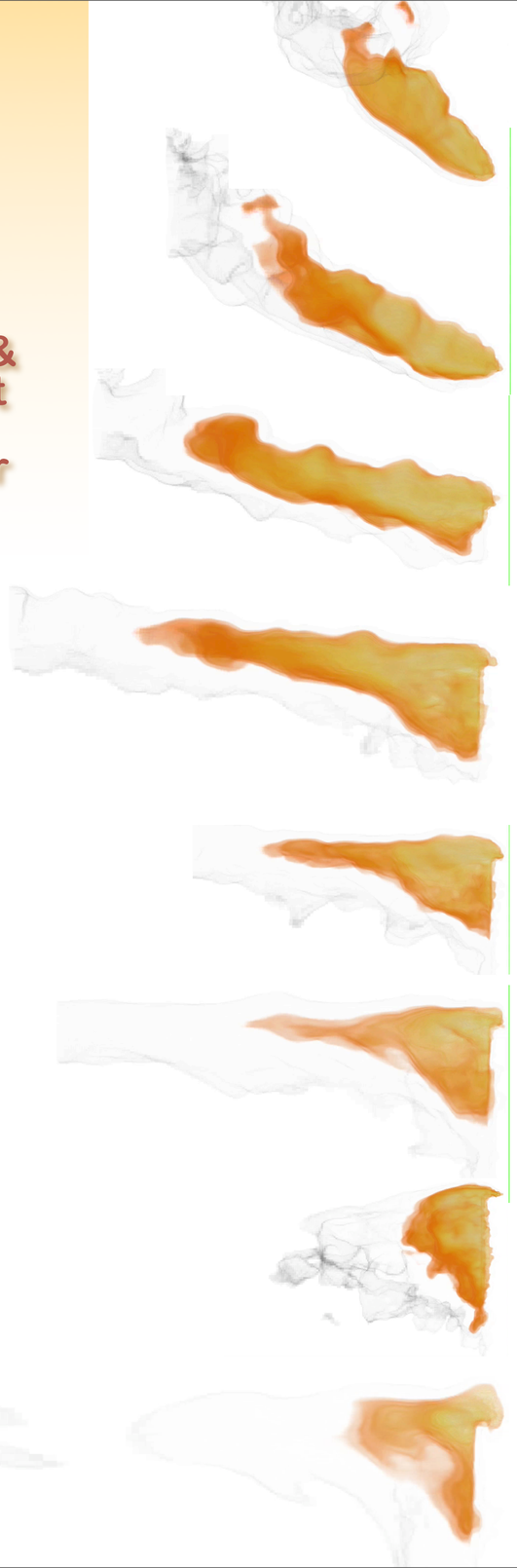


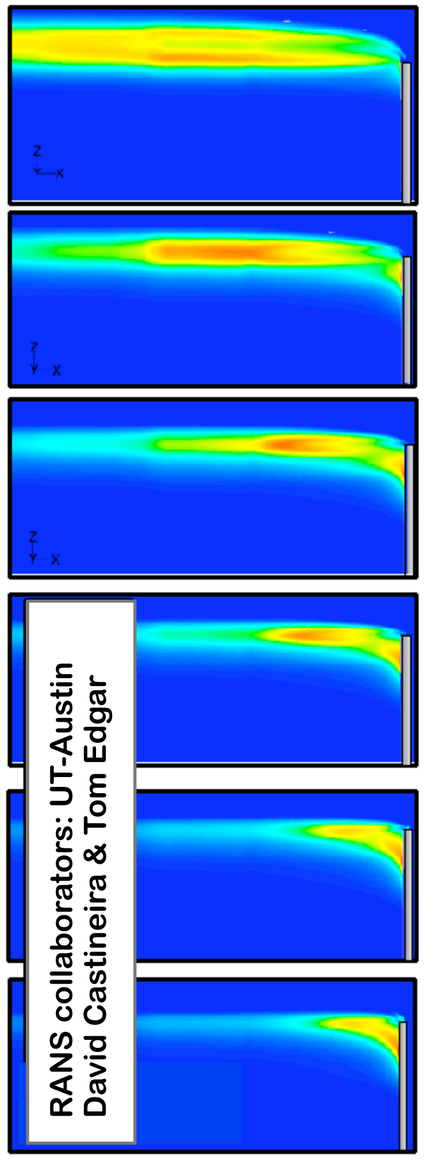
RANS collaborators: UT-Austin
David Castineira & Tom Edgar

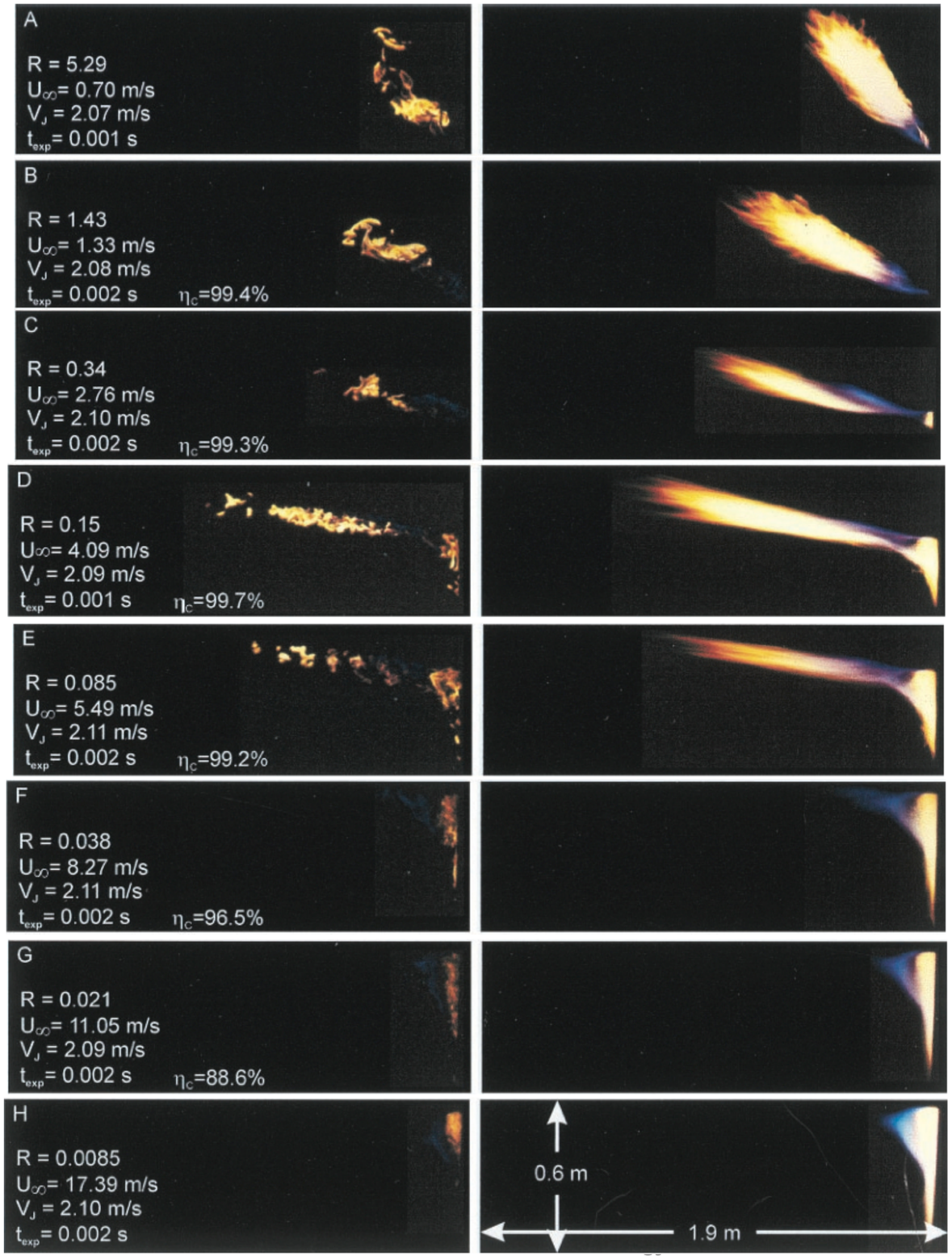


A
R = 5.29
U_∞= 0.70 m/s
V_J = 2.07 m/s
t_{exp}= 0.001 s
B
R = 1.43
U_∞= 1.33 m/s
V_J = 2.08 m/s
t_{exp}= 0.002 s
η_c=99.4%
C
R = 0.34
U_∞= 2.76 m/s
V_J = 2.10 m/s
t_{exp}= 0.002 s
η_c=99.3%
D
R = 0.15
U_∞= 4.09 m/s
V_J = 2.09 m/s
t_{exp}= 0.001 s
η_c=99.7%
E
R = 0.085
U_∞= 5.49 m/s
V_J = 2.11 m/s
t_{exp}= 0.002 s
η_c=99.2%
F
R = 0.038
U_∞= 8.27 m/s
V_J = 2.11 m/s
t_{exp}= 0.002 s
η_c=96.5%
G
R = 0.021
U_∞= 11.05 m/s
V_J = 2.09 m/s
t_{exp}= 0.002 s
η_c=88.6%
H
R = 0.0085
U_∞= 17.39 m/s
V_J = 2.10 m/s
t_{exp}= 0.002 s
0.6 m
1.9 m

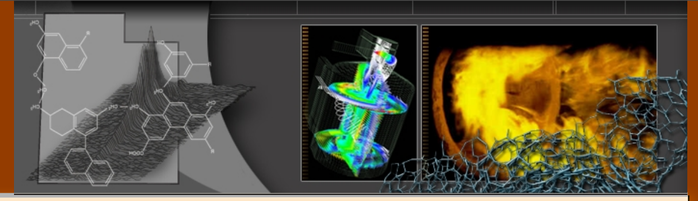
flare shape & size (buoyant force) - low wave number processes







oxy-coal predictivity



hierarchical validation and uncertainty quantification

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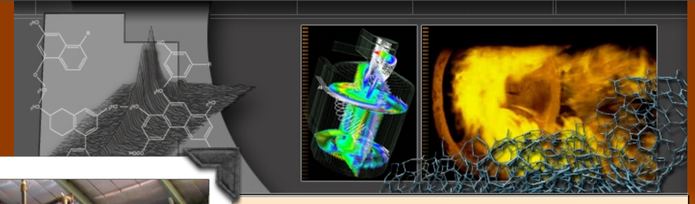
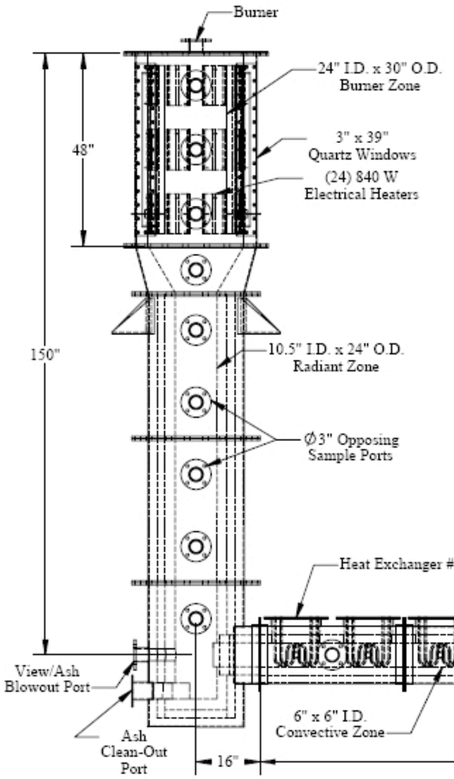


Why LES?



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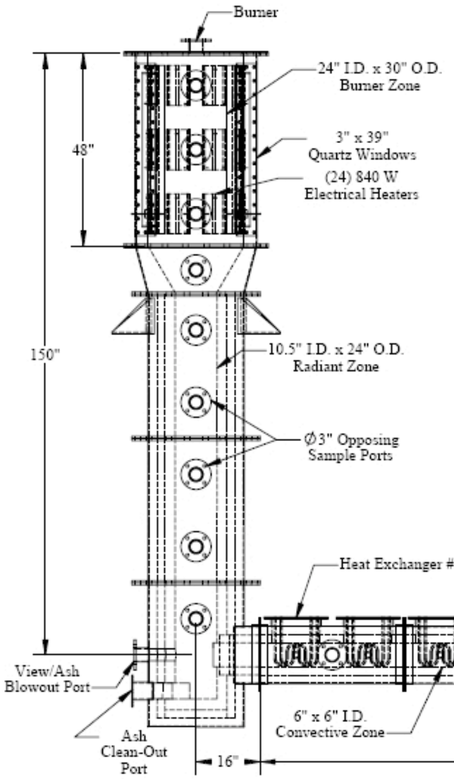
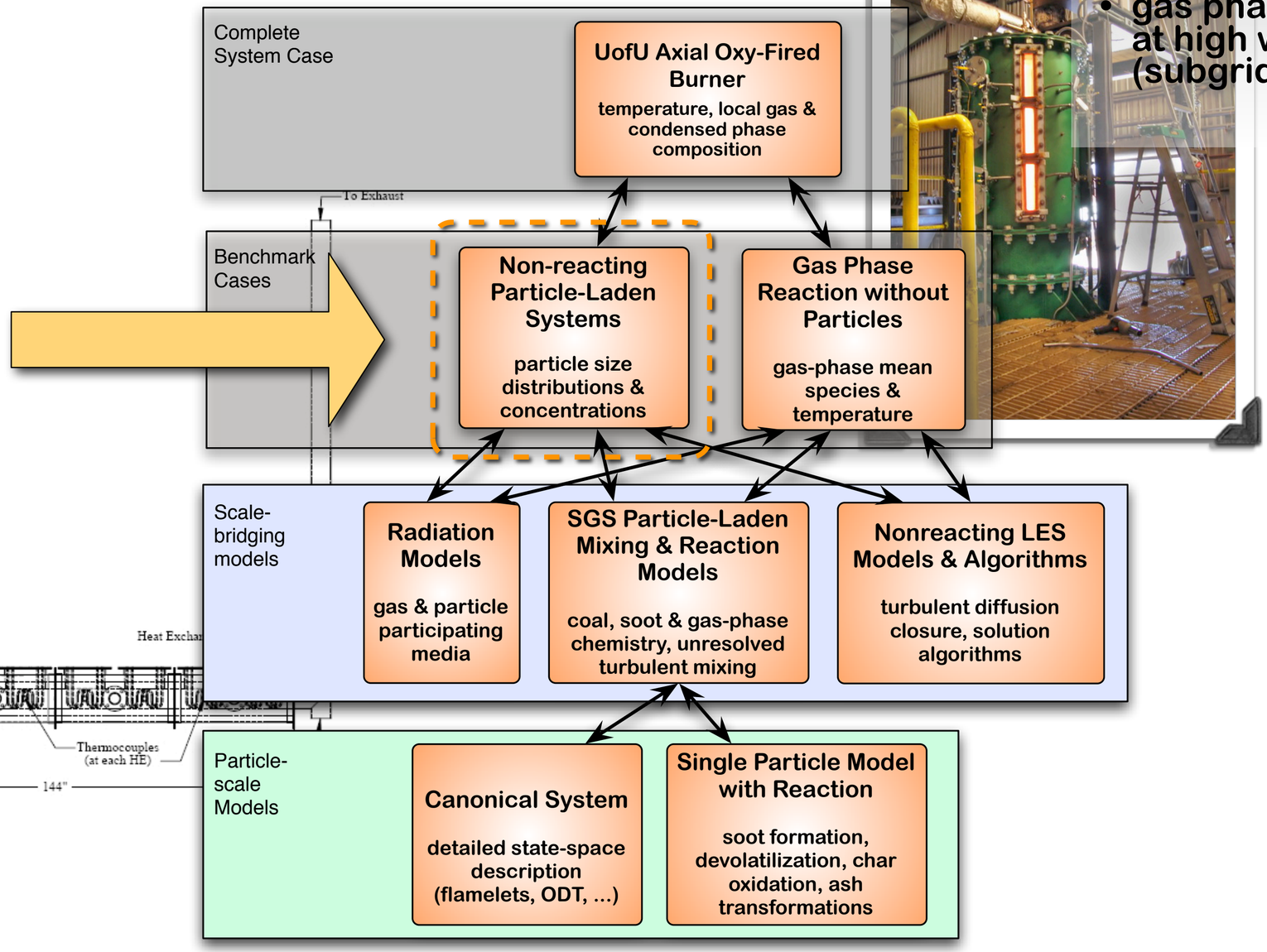
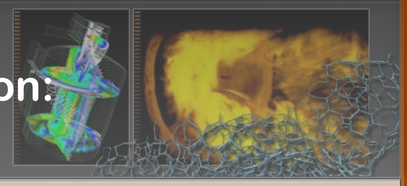




observation:



- particles transport and react at low wave numbers
- gas phase reactions occur at high wave numbers (subgrid-scale modeling)

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oxy-coal predictivity

hierarchical validation and uncertainty quantification

⇨particle dynamics: particle clustering

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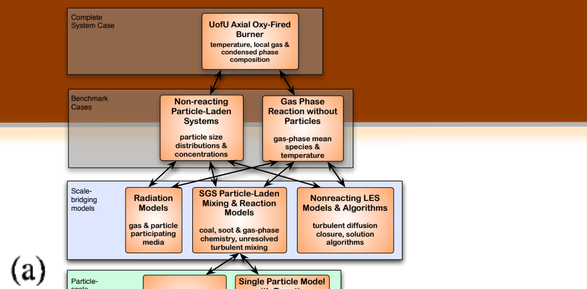

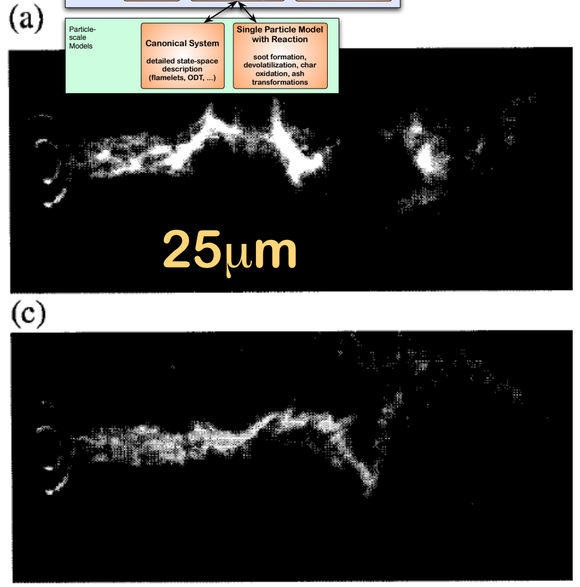

Budilarto & Sinclair-Curtis

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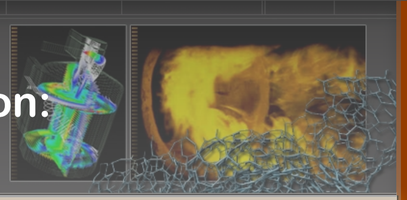

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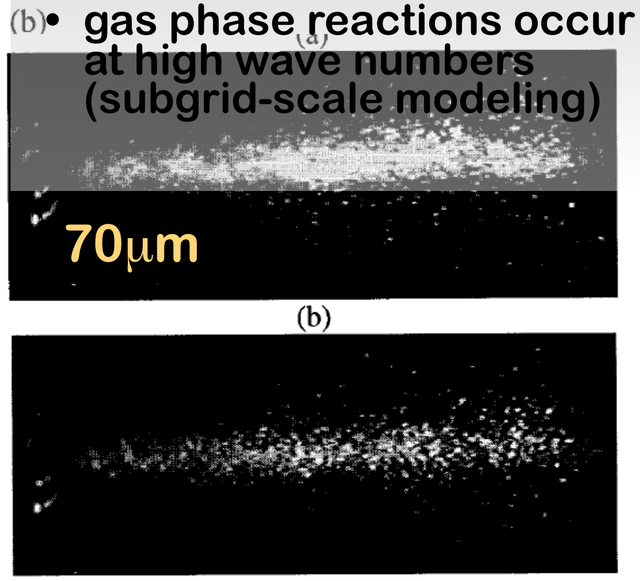

- eddy interactions

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oxy-coal predictivity

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⇨particle dynamics: particle clustering

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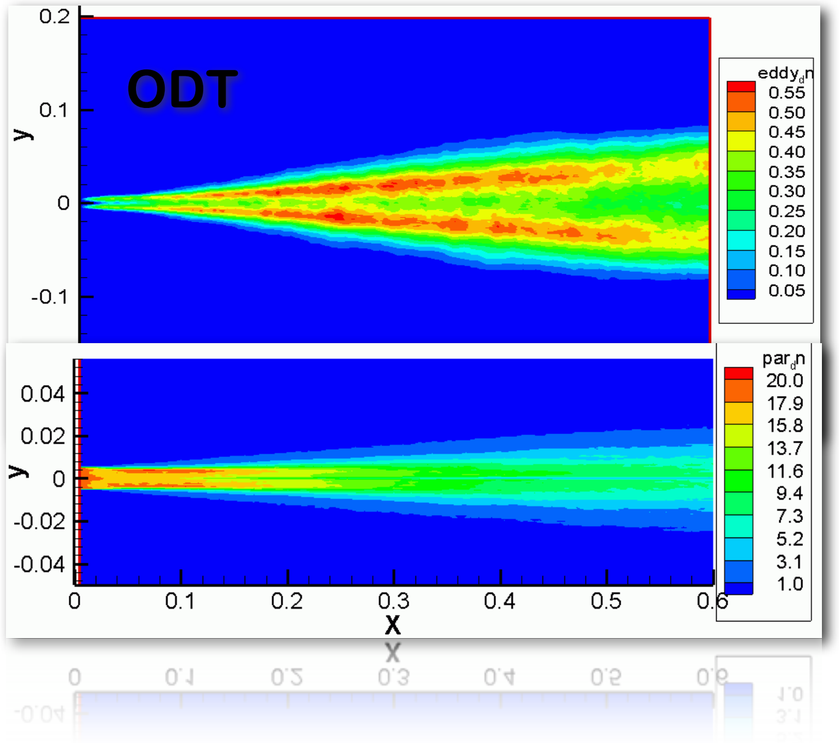
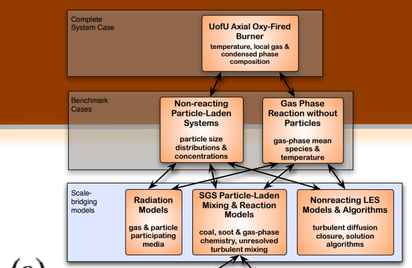
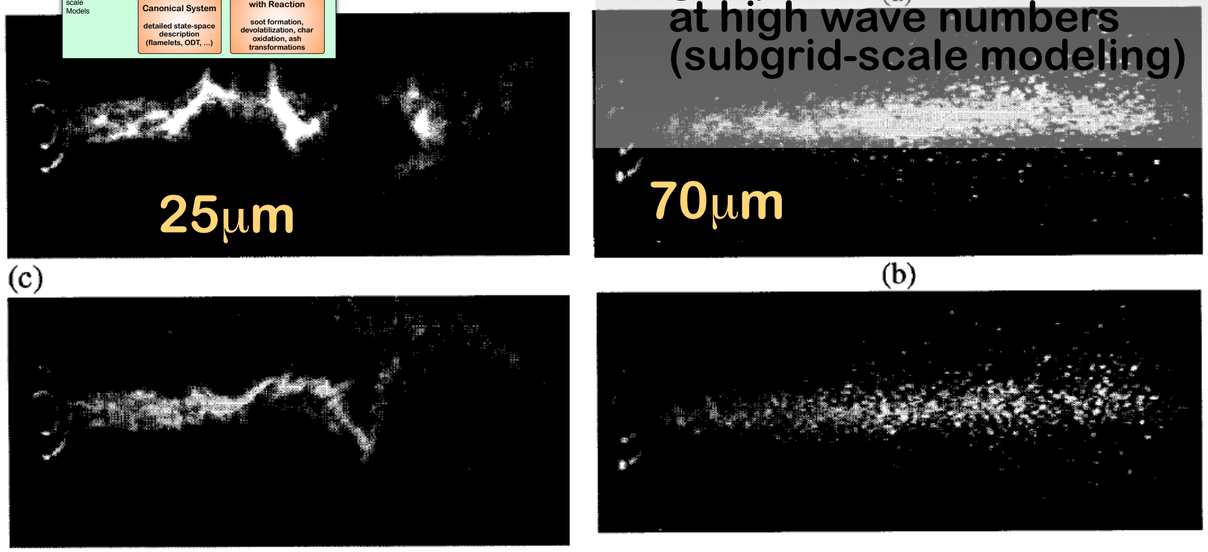
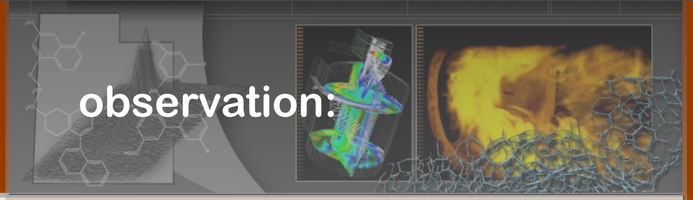






Budilarto & Sinclair-Curtis



- particles transport and react at low wave numbers
- gas phase reactions occur at high wave numbers (subgrid-scale modeling)
- eddy interactions

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oxy-coal predictivity

hierarchical validation and uncertainty quantification

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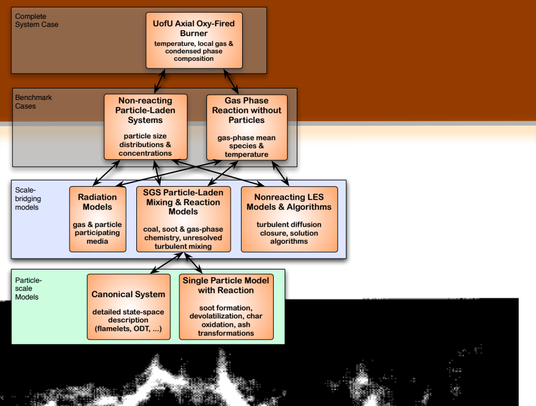
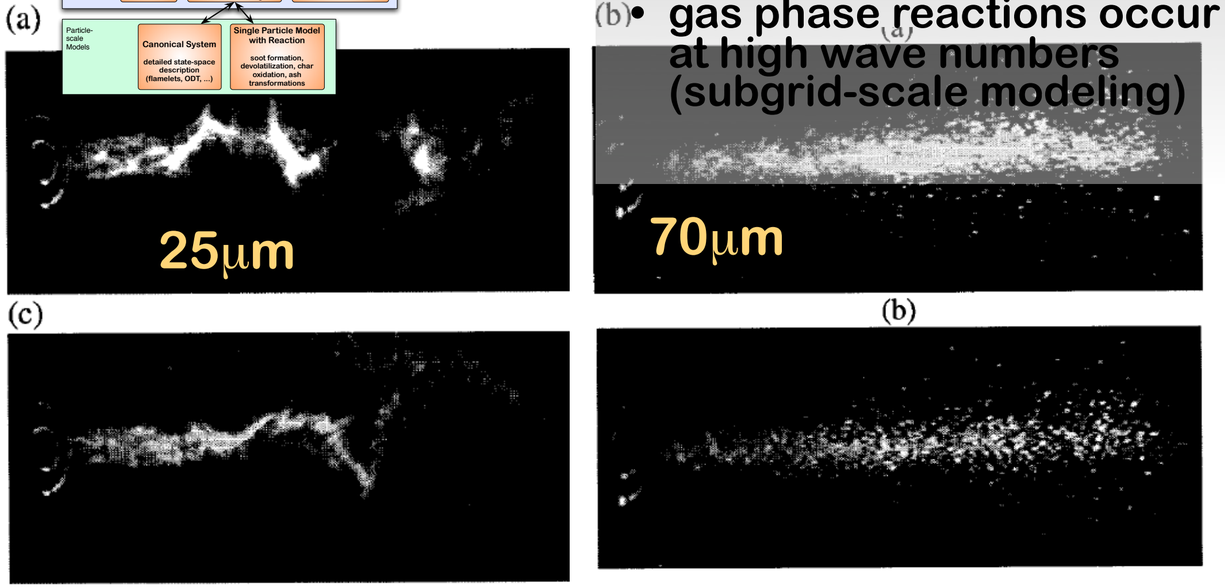
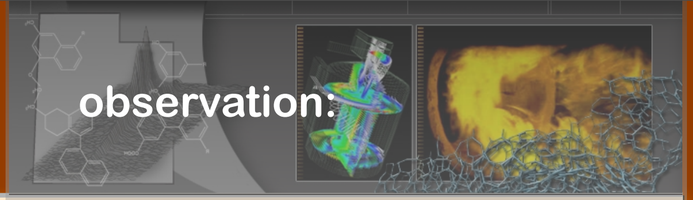




Budilarto & Sinclair-Curtis

observation:



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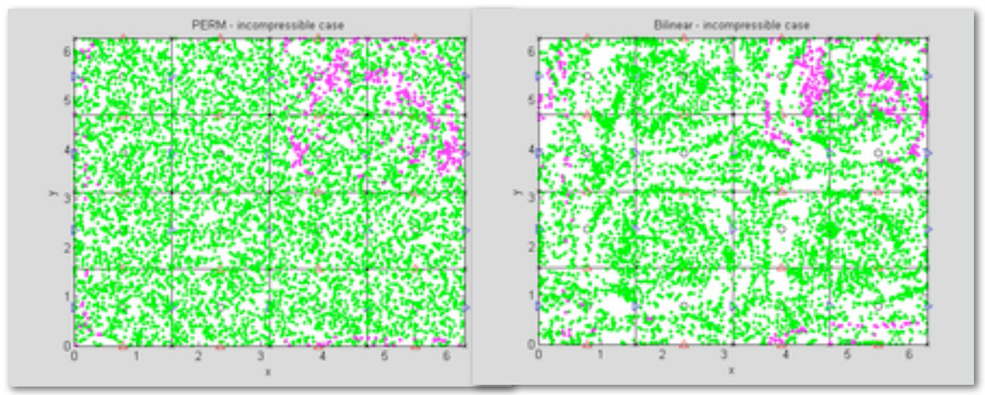

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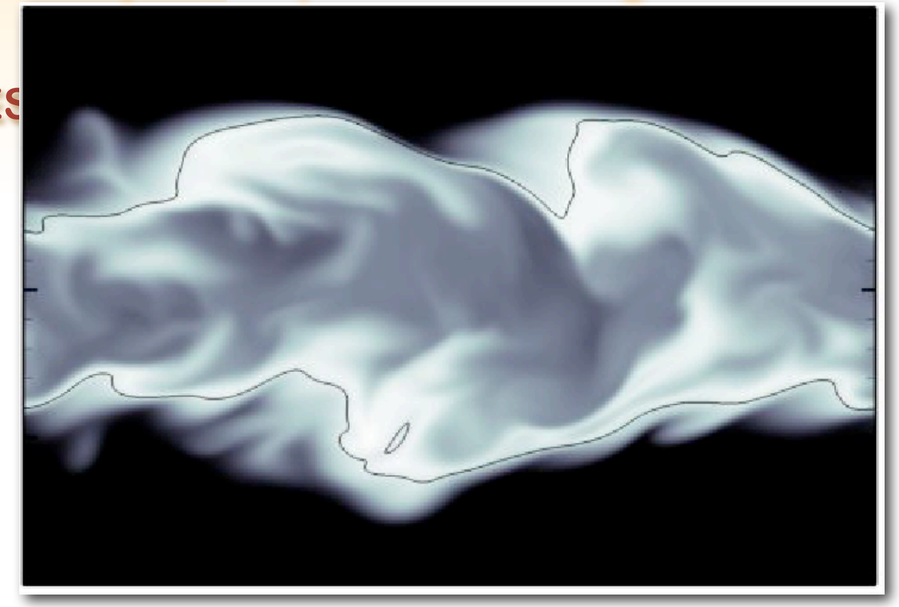

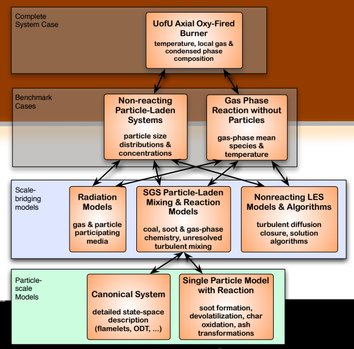

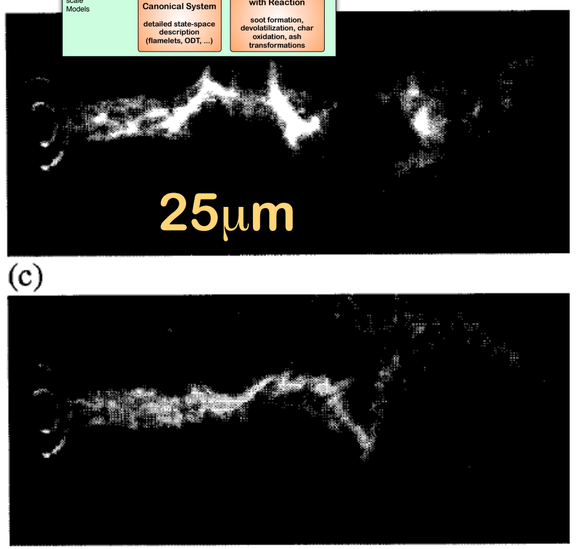

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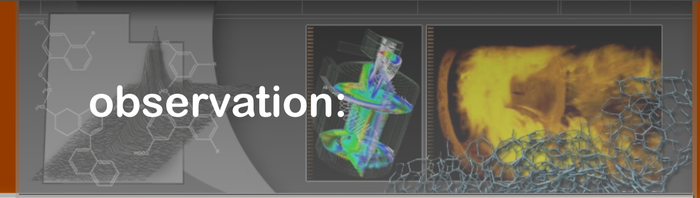

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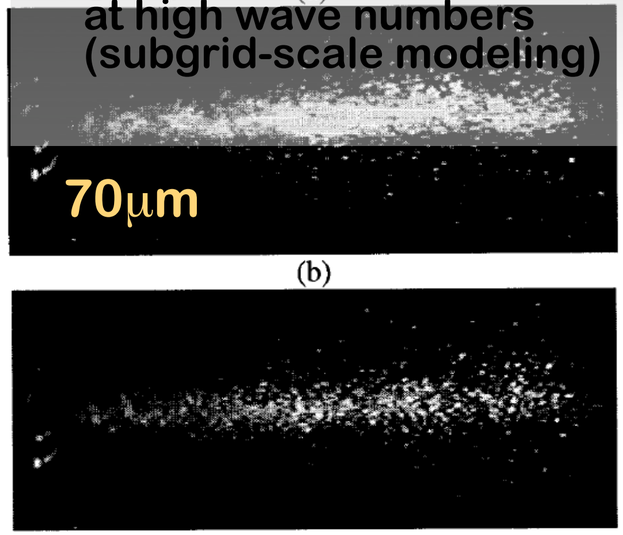
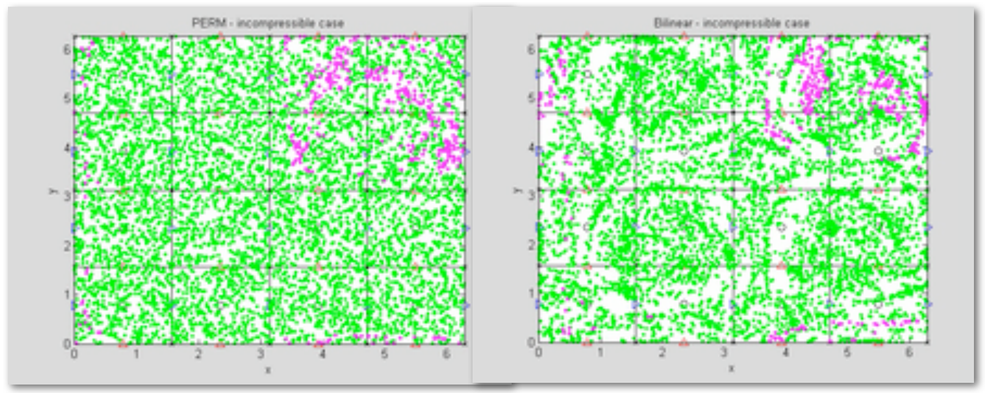


- eddy interactions
- changing density
- differential diffusion



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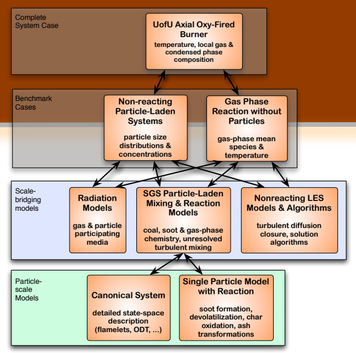

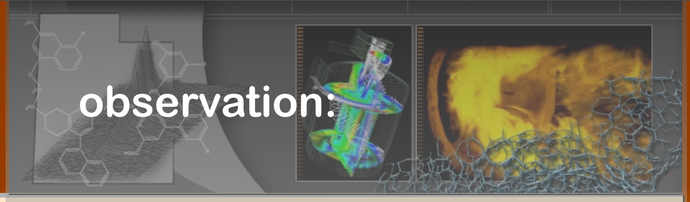

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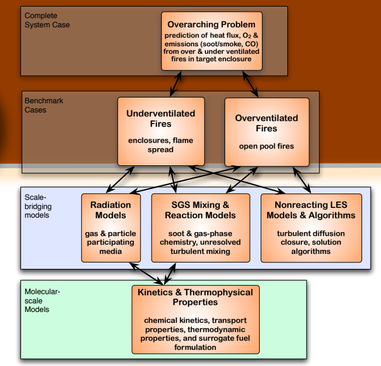
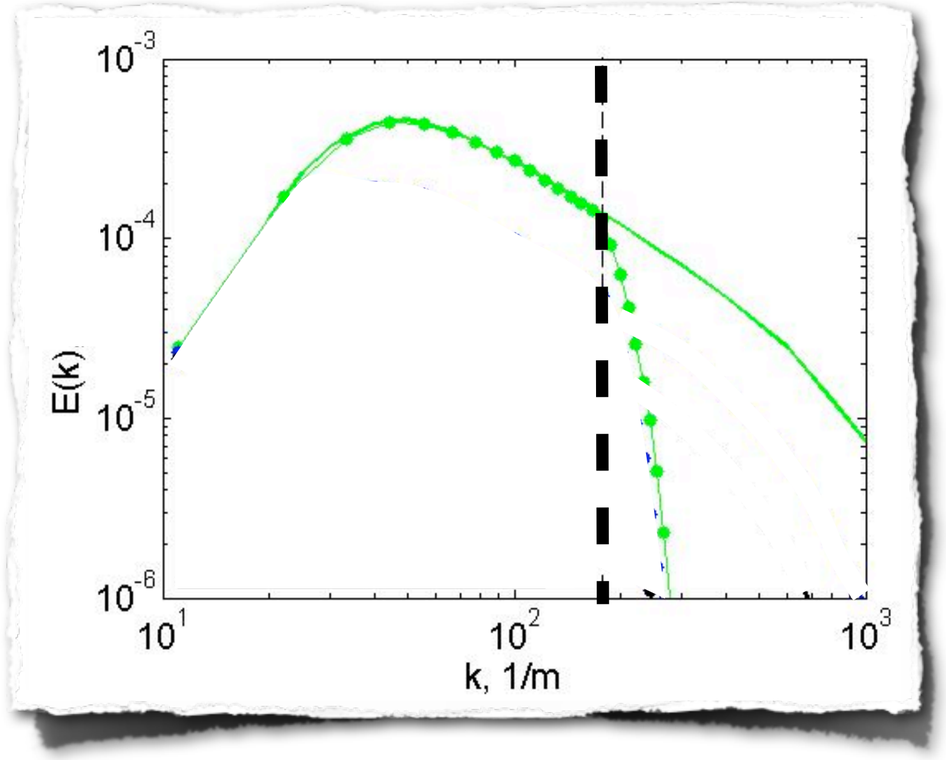
Manifold Models:
Reaction & Mixing Models (high wave number)





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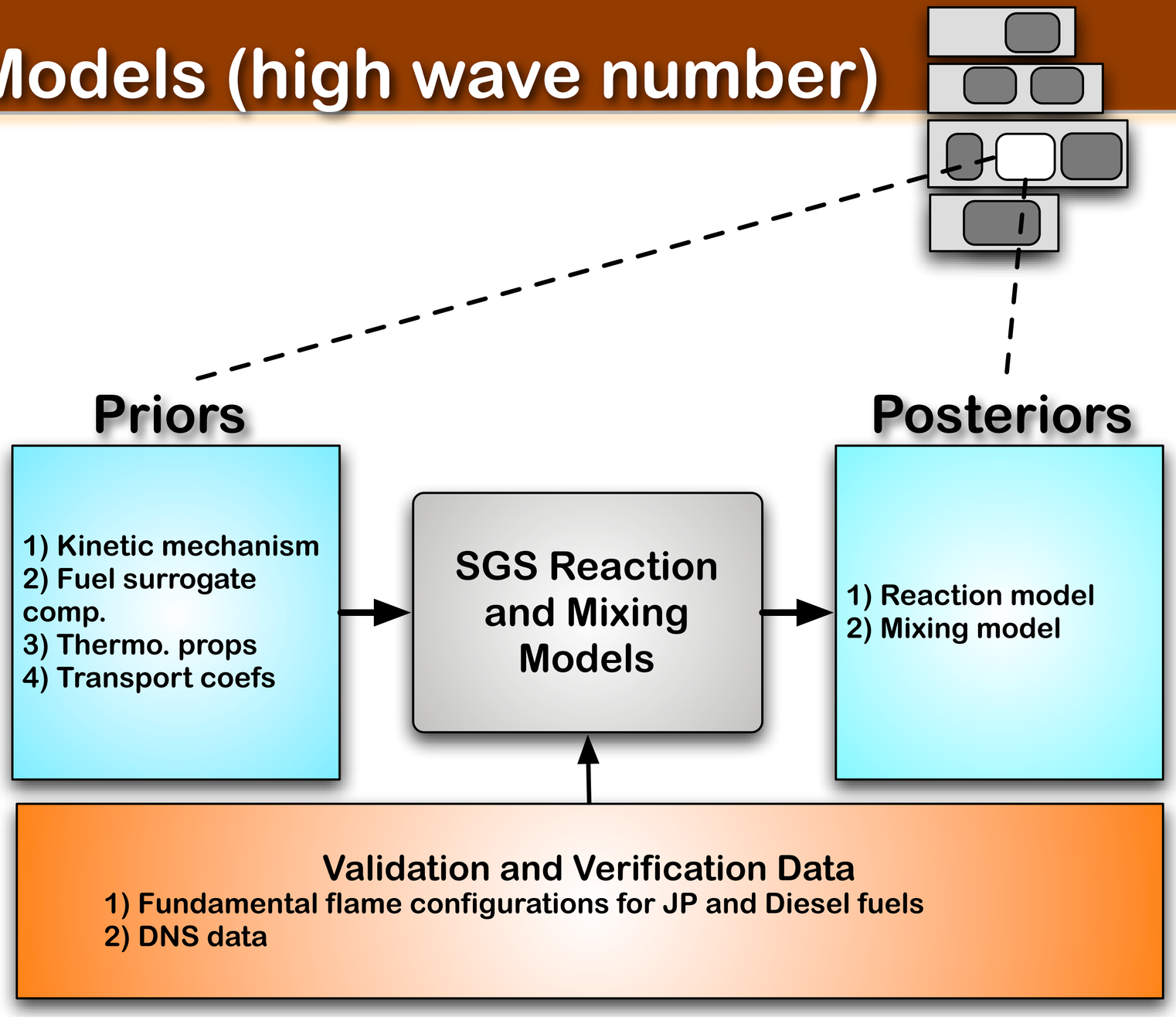
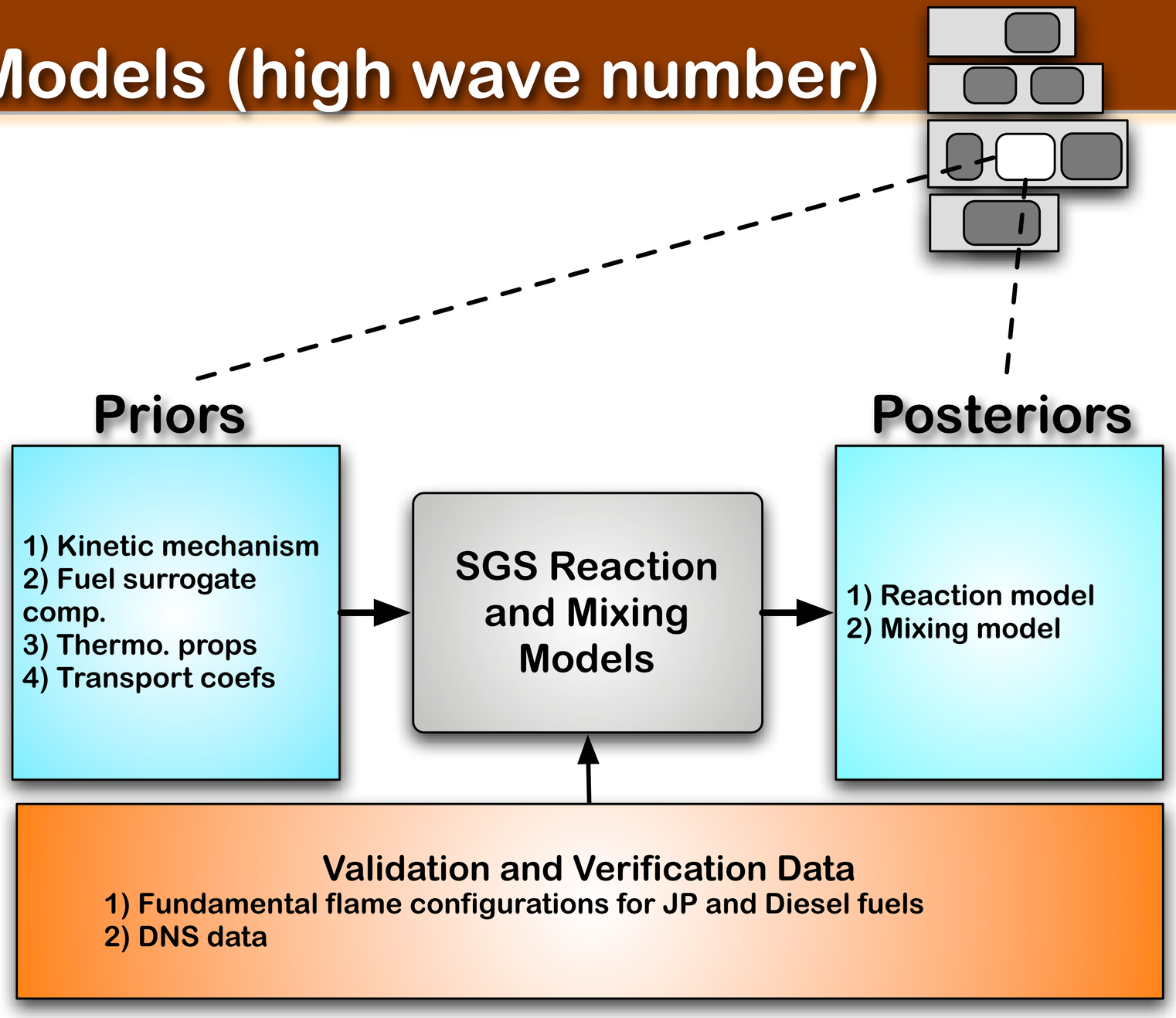


Manifold Models:
Reaction & Mixing Models (high wave number)

Reduction Methods Motivated by Simplified Chemical Kinetics

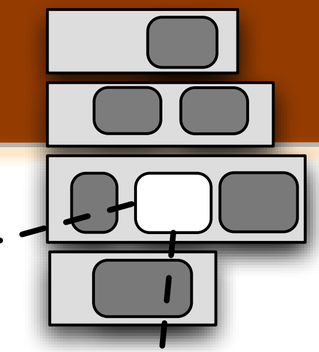
- Infinitely fast chemistry
- Equilibrium
- Global reactions
- Quasi-steady state and partial equilibrium



Manifold Models:
Reaction & Mixing Models (high wave number)

Mathematically Motivated Reduction Schemes

- Computational Singular Perturbation (CSP)
- Intrinsic Lower Dimensional Manifold (ILDM)
- Rate Controlled Constrained Equilibrium (RCCE)



Priors

1) Kinetic mechanism
2) Fuel surrogate comp.
3) Thermo. props
4) Transport coefs

SGS Reaction and Mixing Models

Posteriors

1) Reaction model
2) Mixing model

Validation and Verification Data

1) Fundamental flame configurations for JP and Diesel fuels
2) DNS data

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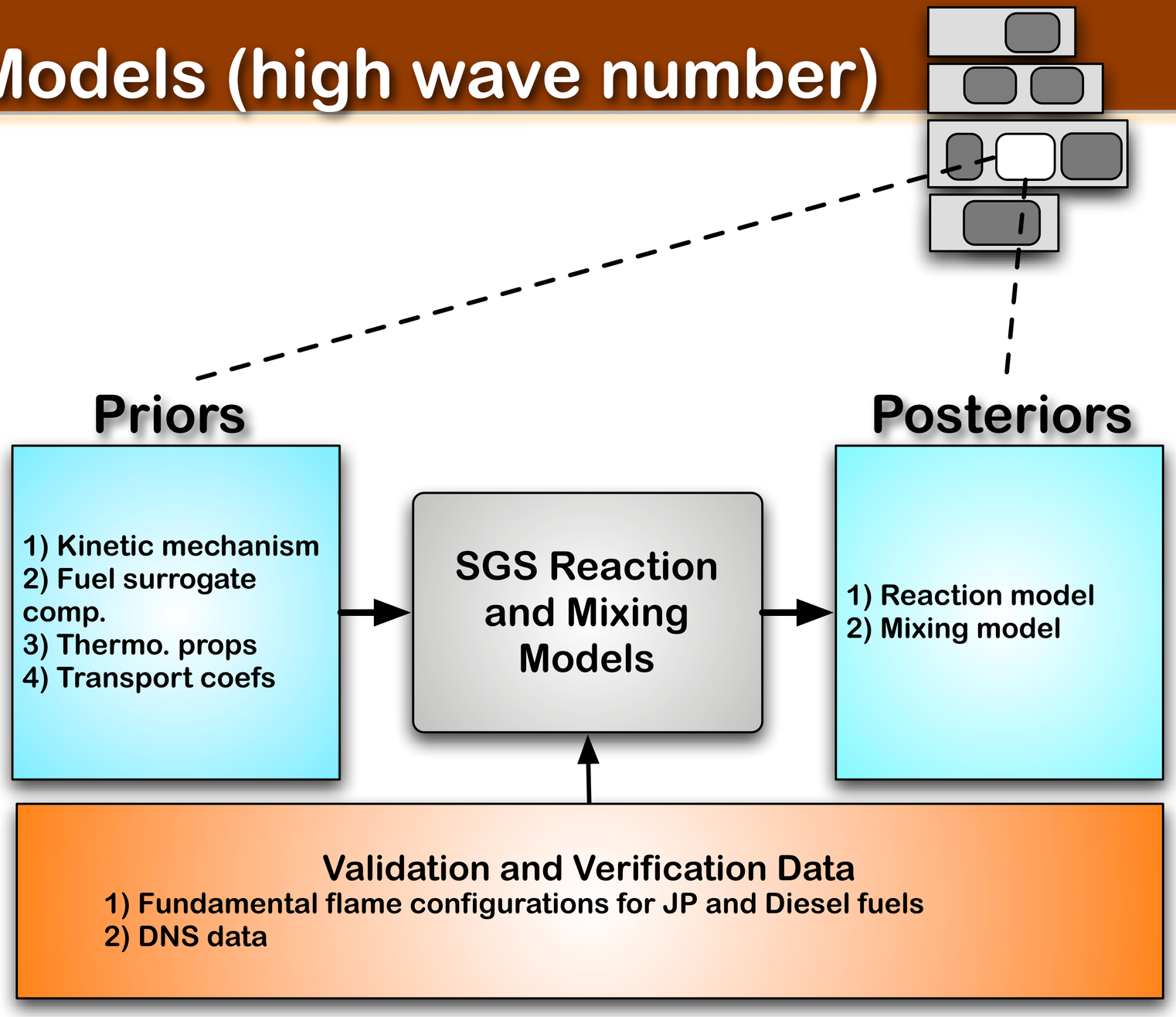
Manifold Models:
Reaction & Mixing Models (high wave number)

Techniques that Utilize the Concept of a Manifold

- Flame Prolongation of ILDM (FPI)
- Flamelet Generated Manifolds (FGM)
- Phase Space ILDM (PS-ILDM)



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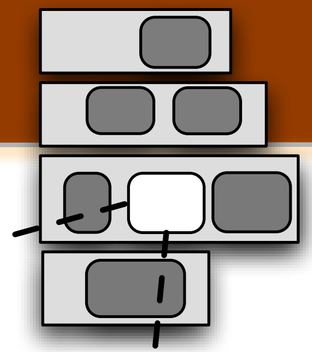

Our Approach: Generalized Manifolds

- SGS manifold span unresolved scales
- Canonical flames to generate SGS data (flamelets, ODT)
- PCA to identify SGS manifold mapping parameters (with quantifiable uncertainty)
- Solve transport for PCA parameters

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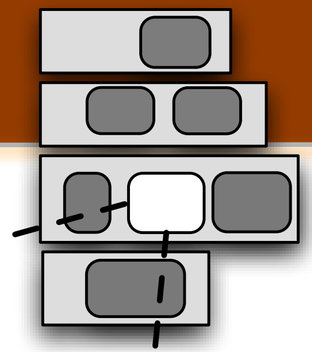

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$$\phi(\rho, T, Y_1, Y_2, \ldots Y_s) \approx \phi(\eta_1, \eta_2, \ldots \eta_n) = \phi(\eta)$$

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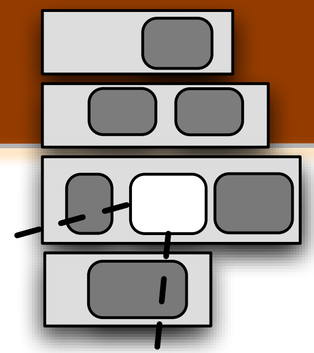

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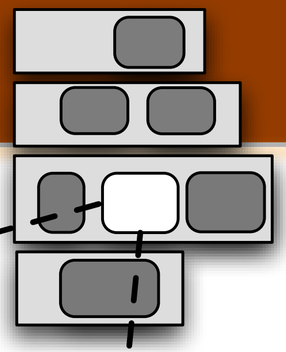

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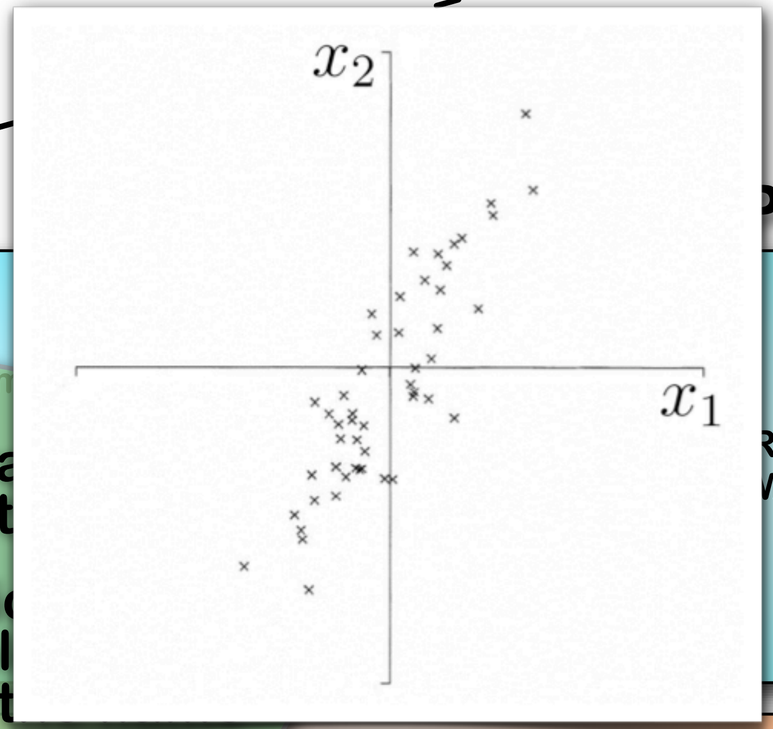

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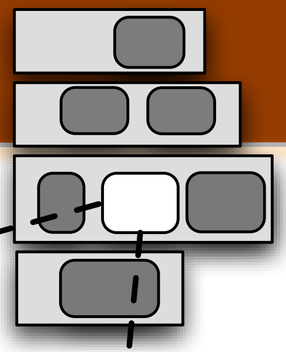

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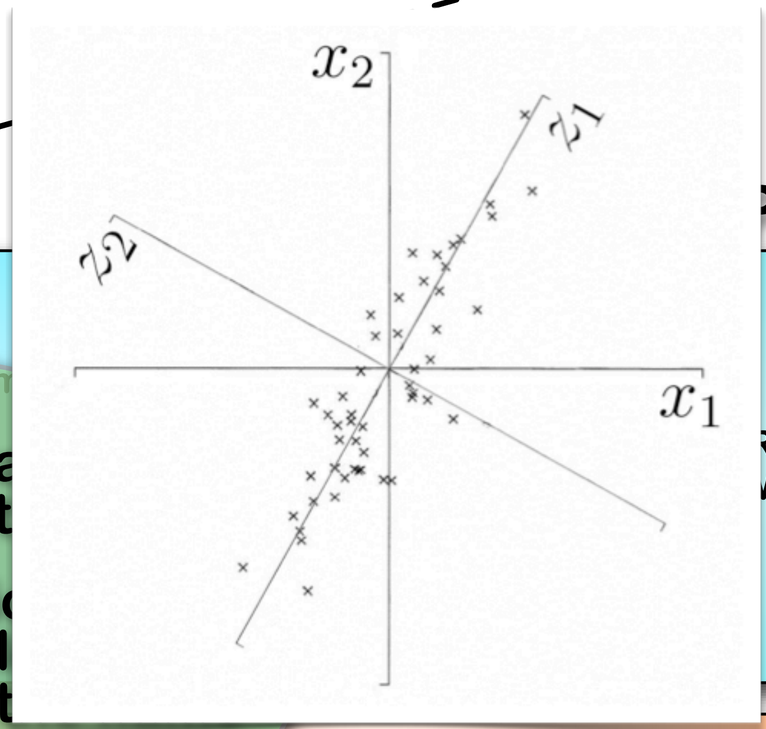

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Manifold Models: Reaction & Mixing Models (high-pressure combustion)

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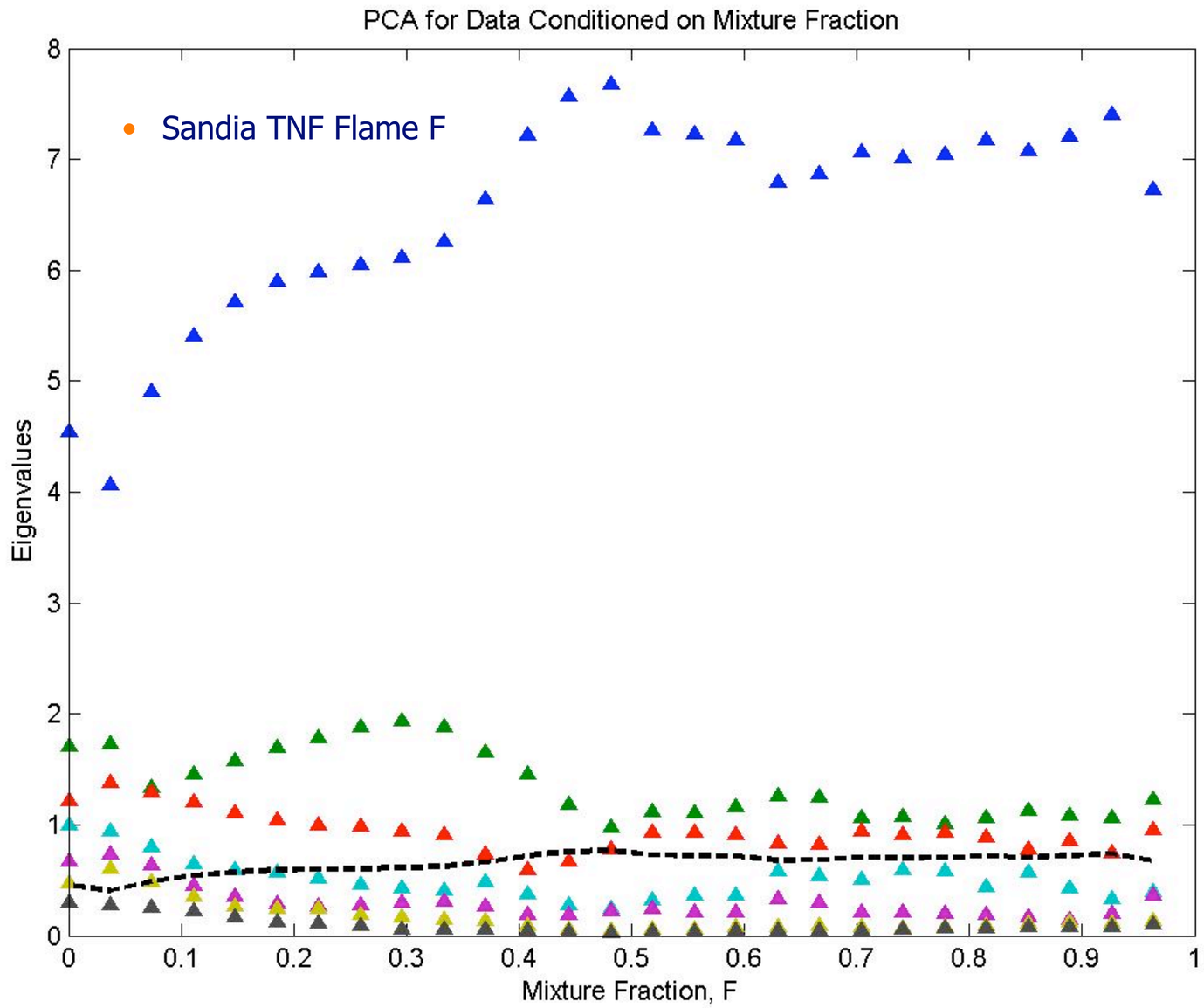

$$\phi(\rho, T, Y_1, \ldots$$

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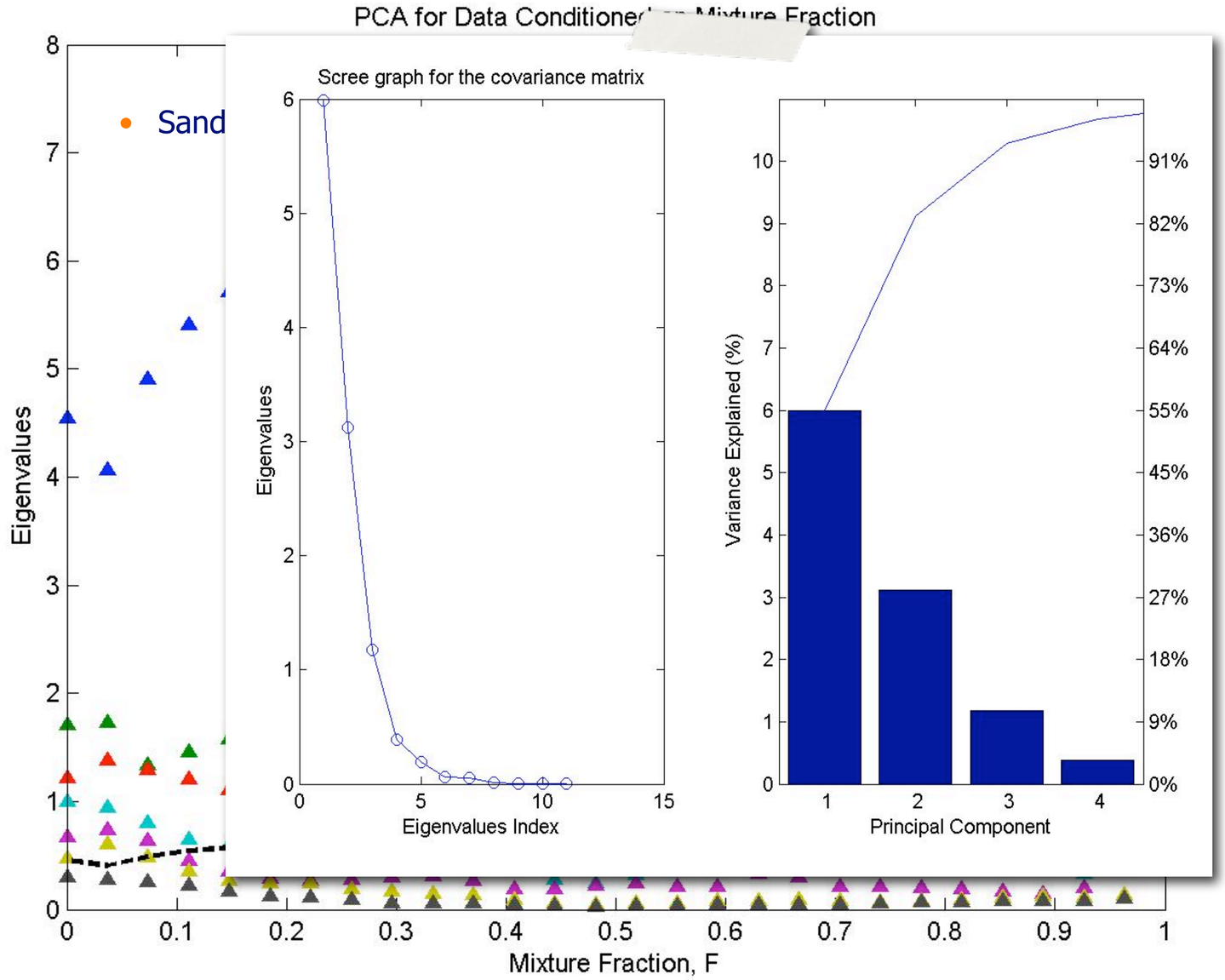

$$\phi(\rho, T, Y_1, \ldots) = f(\ldots)$$

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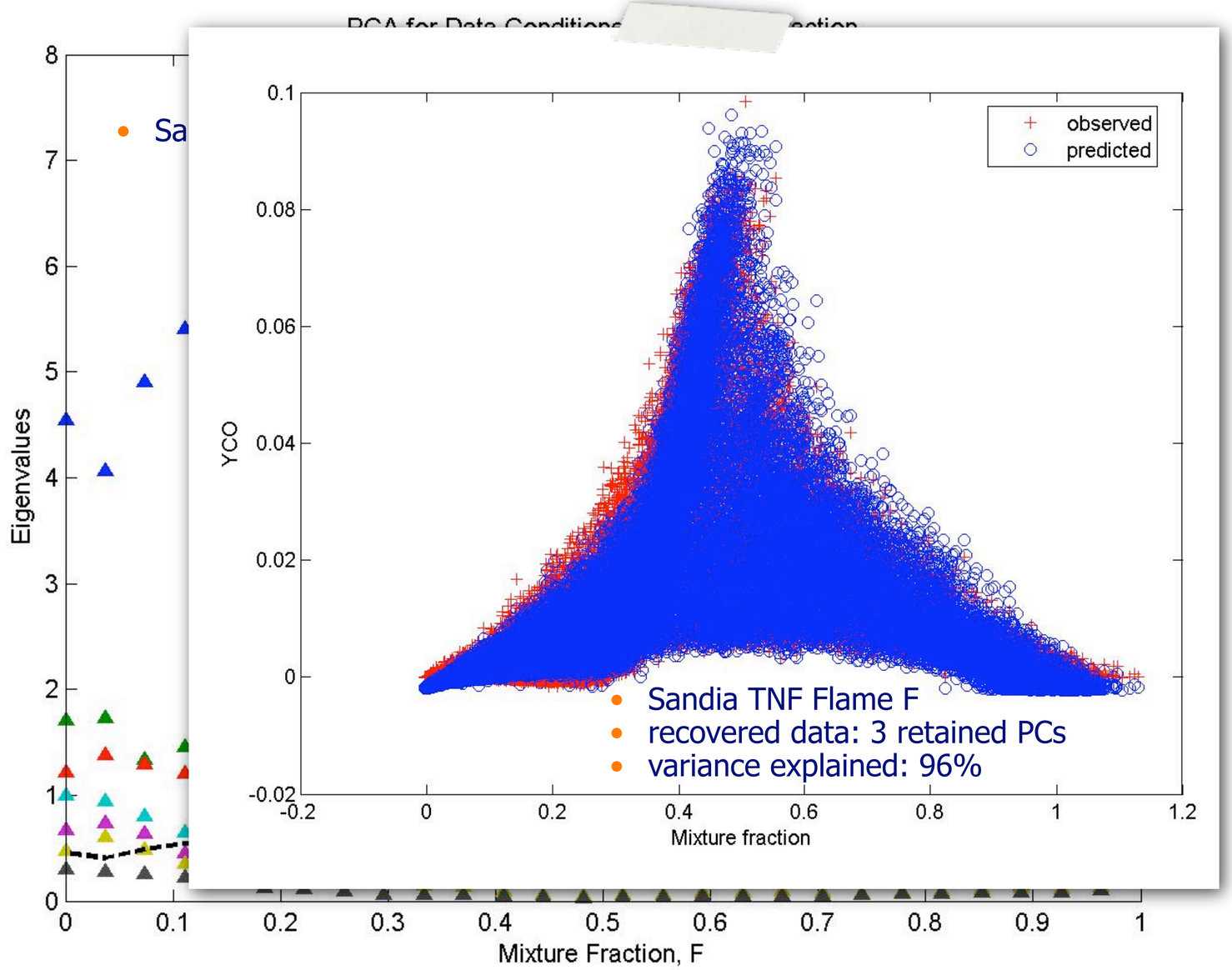

$$\phi(\rho, T, Y_1, \ldots) = f(\eta_1, \eta_2, \ldots \eta_n) \quad (1)$$

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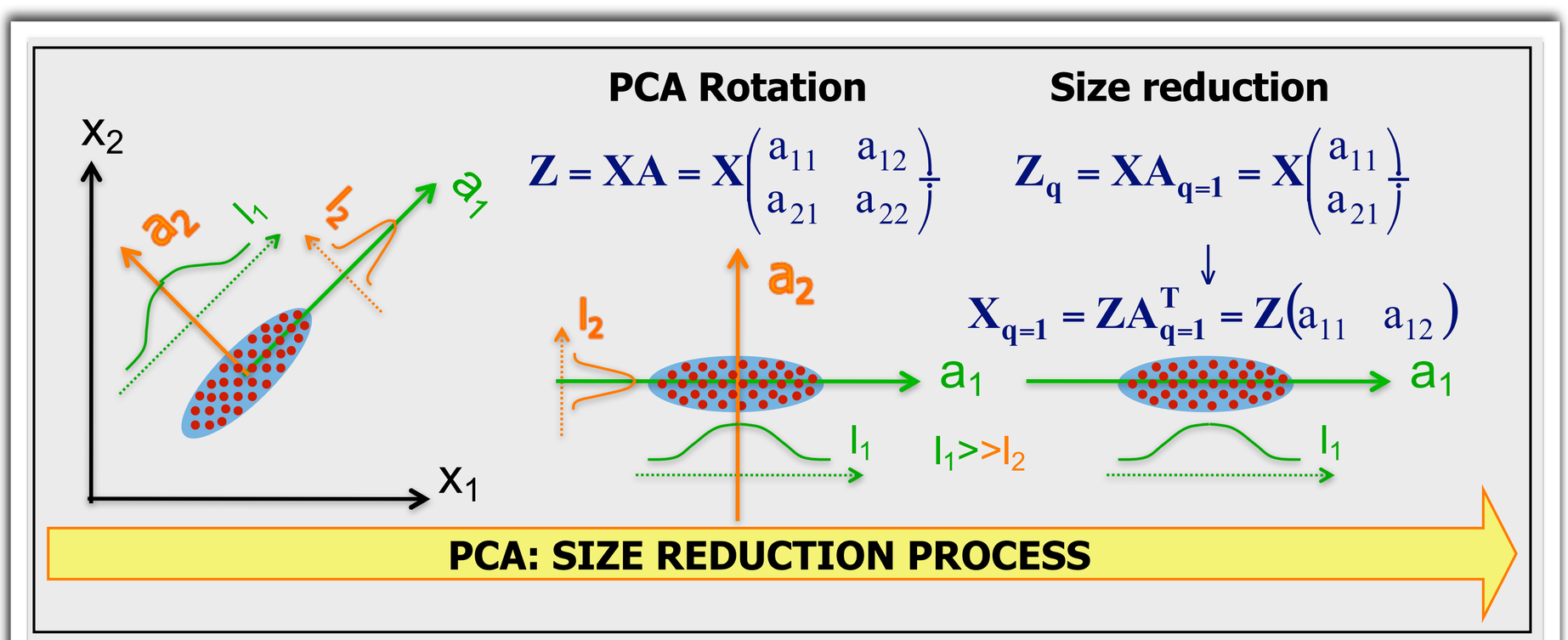
Principal Compoent Analysis (PCA)

- **Size reduction** via **PCA:**
  - **PCs defined by the linear transformation**

$$\mathbf{Z = XA} \quad \text{®} \quad \mathbf{X = ZA^T} \quad \text{being} \quad \mathbf{A^{-1} = A^T}$$

  - **X can be approximated by a subset $\mathbf{A_q}$ (q<<p), of A**

$$\mathbf{X \approx X_q = ZA_q'}$$



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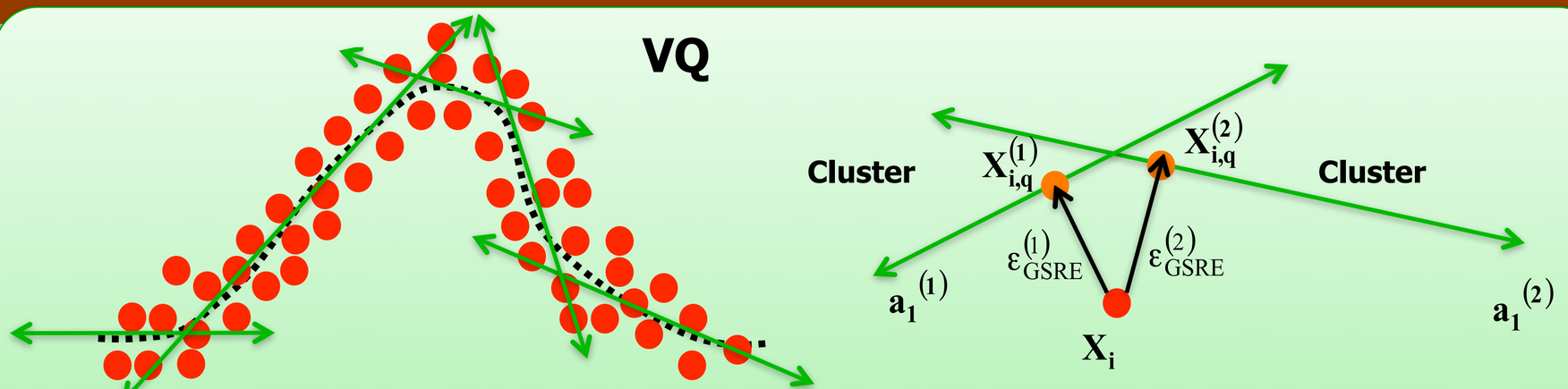

USING THE VQ ALGORITHM, PARTITION IS NOT INDEPENDENT OF THE FOLLOWING PROJECTION ONTO THE LOW-DIMENSIONAL SUBSPACE

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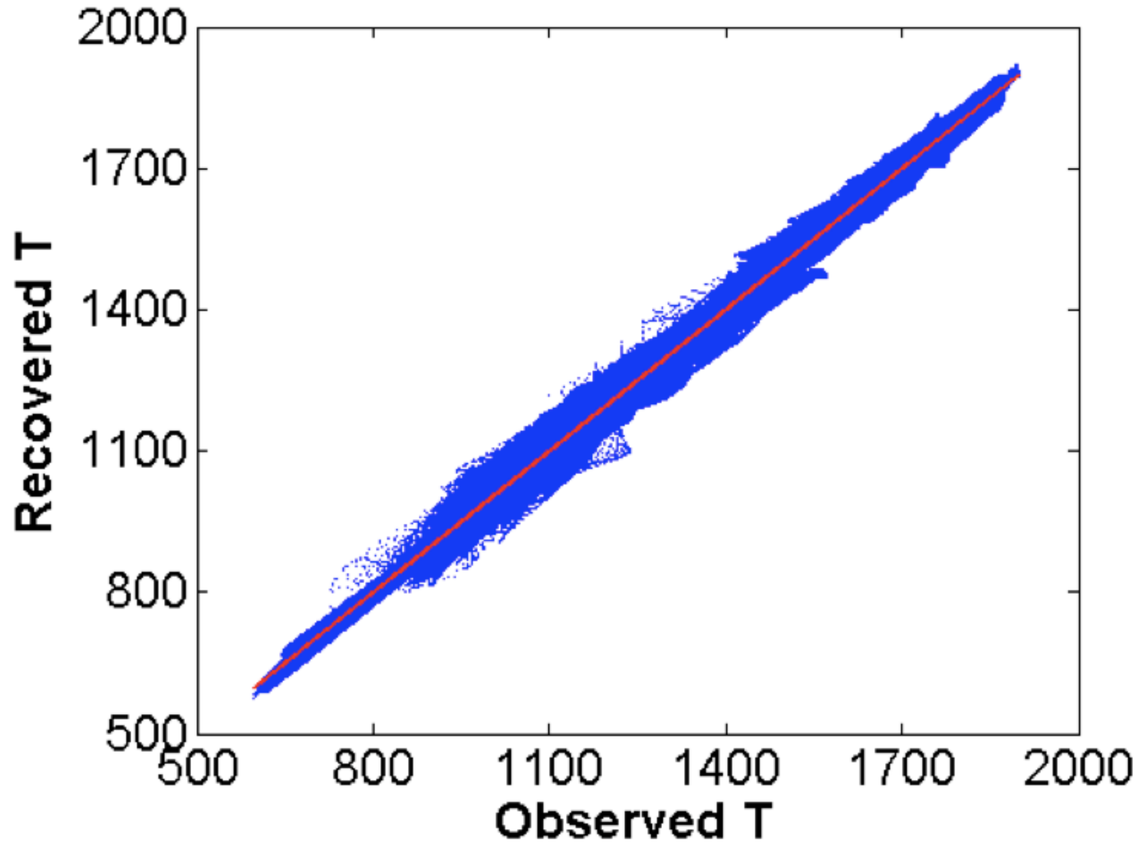
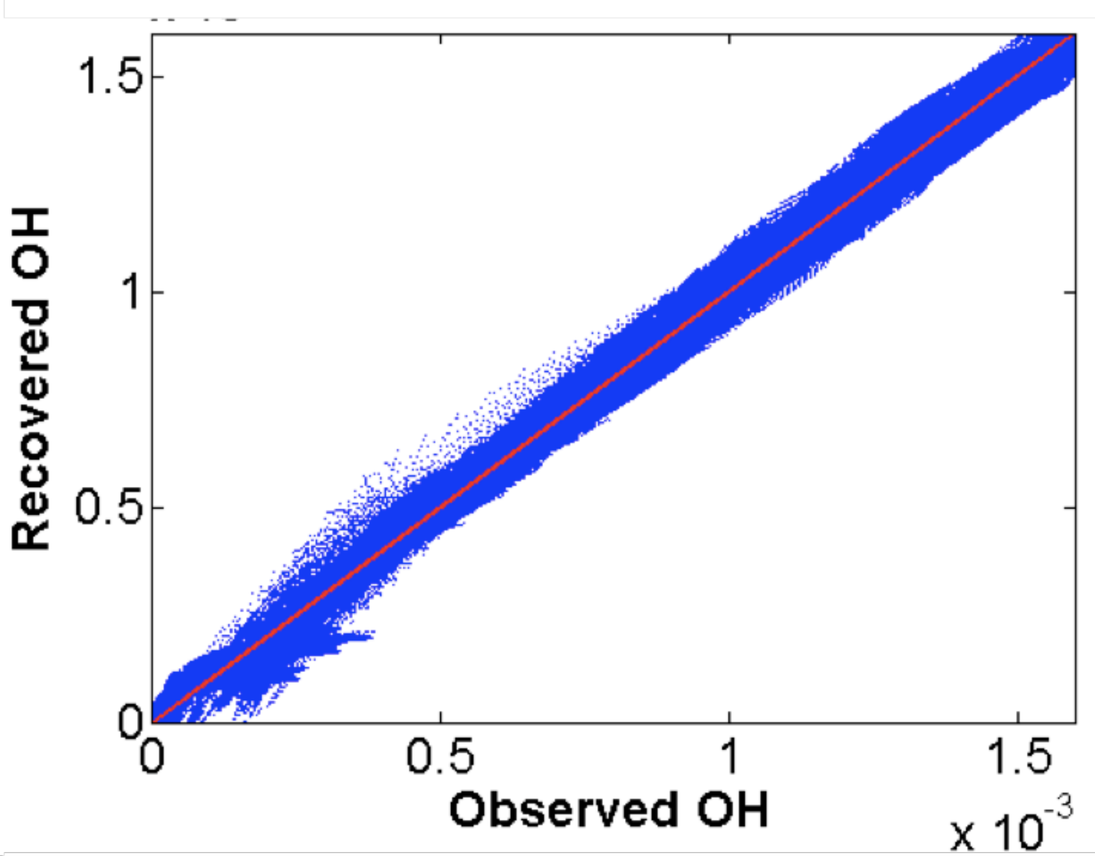
VQPCA Results of DNS flame with significant extinction

q=4 and k=8, $\varepsilon_{GSRE,n}$= 0.04





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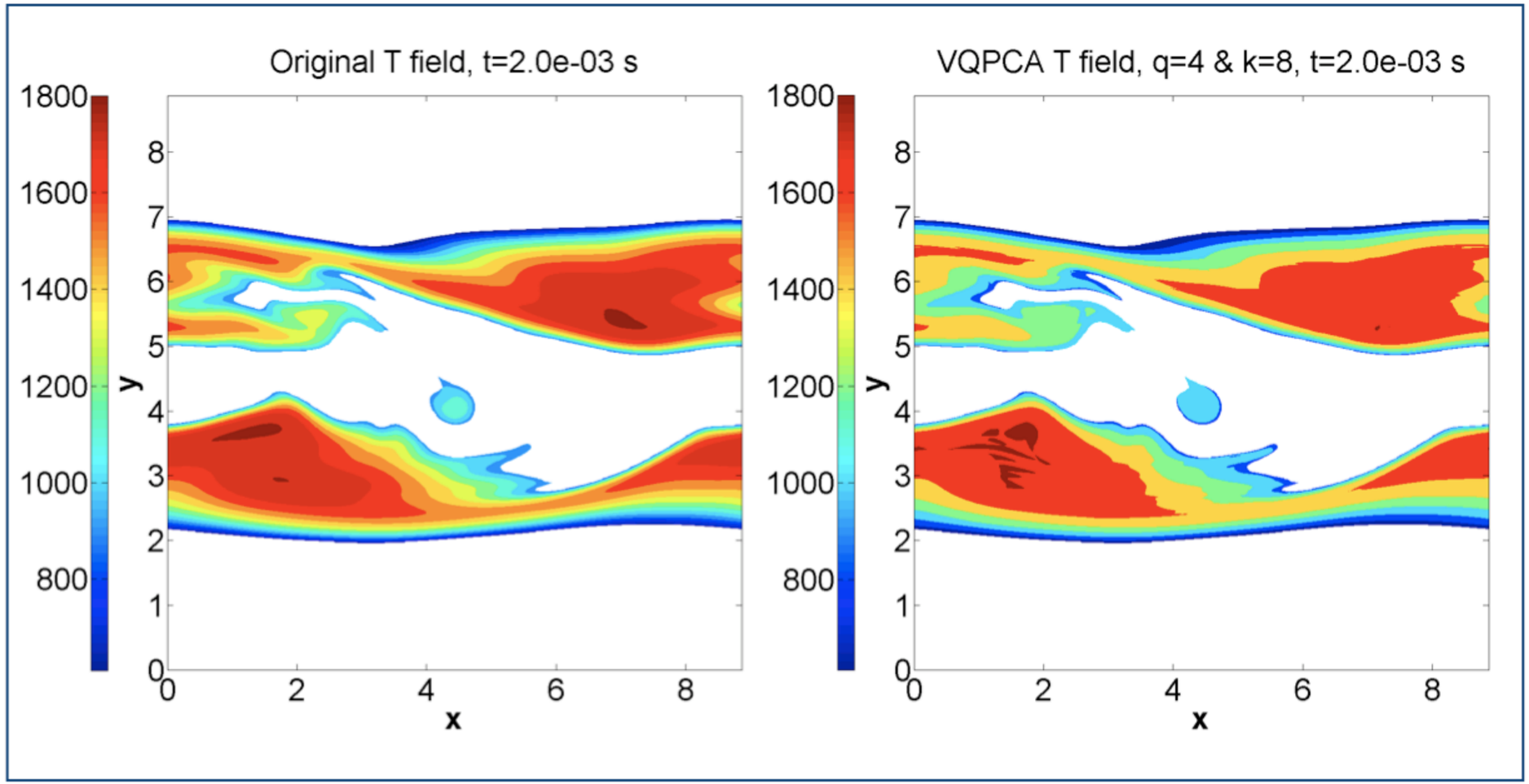

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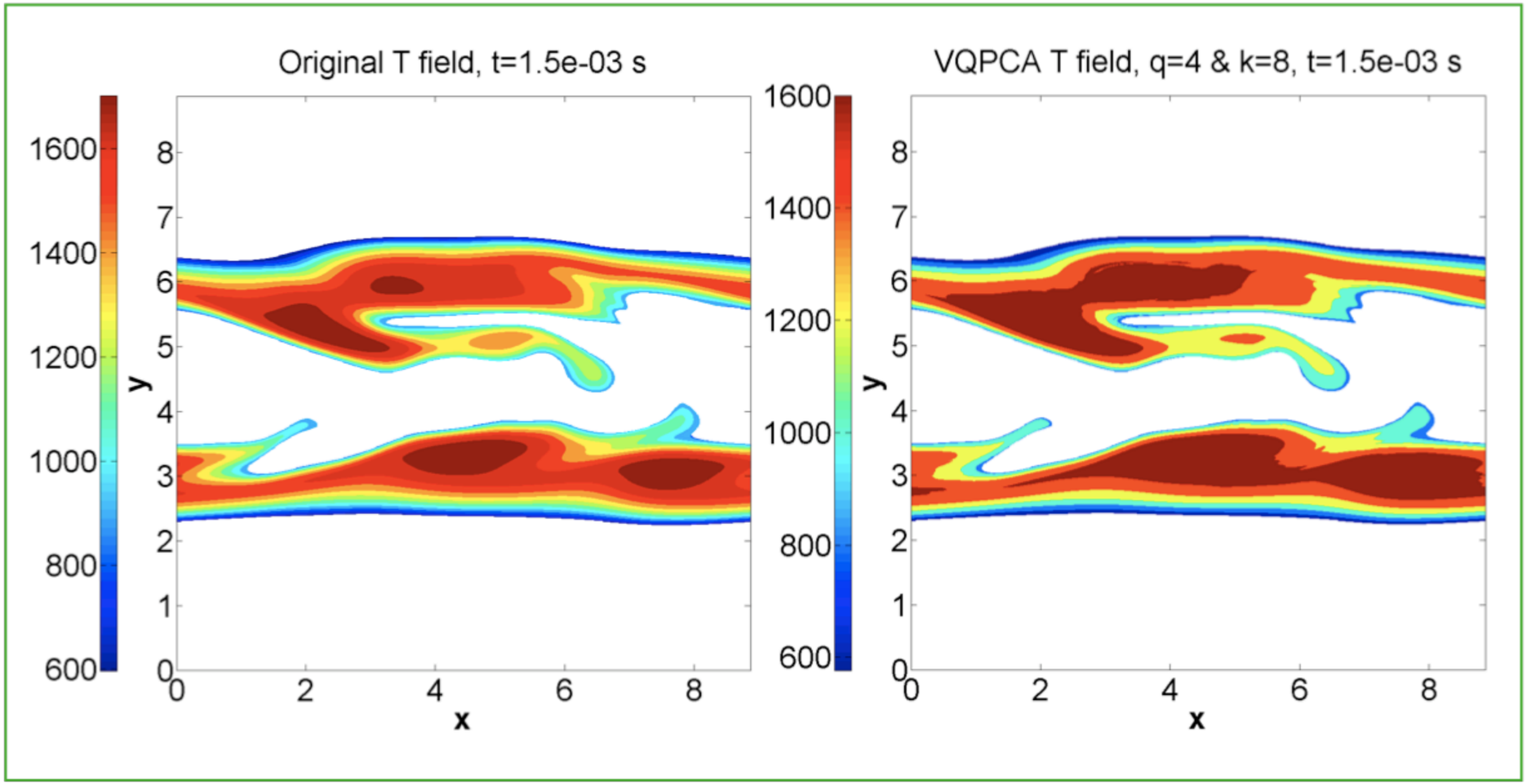

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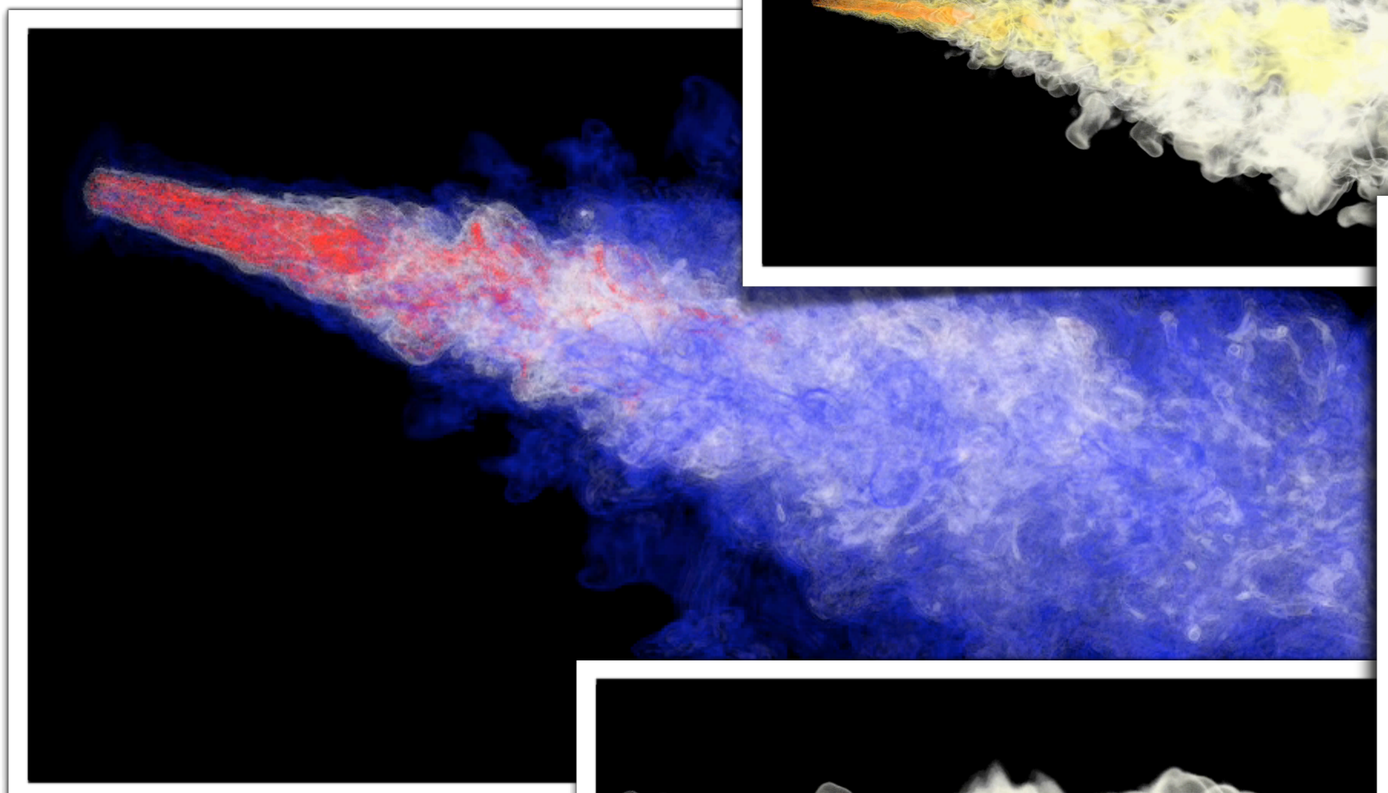
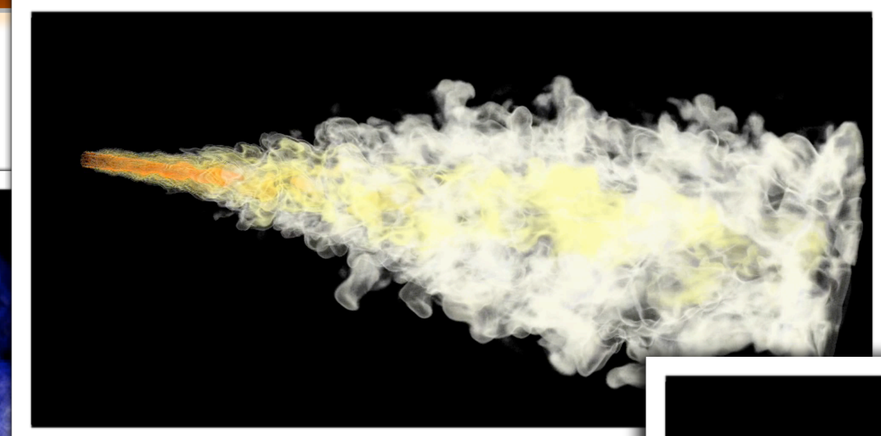
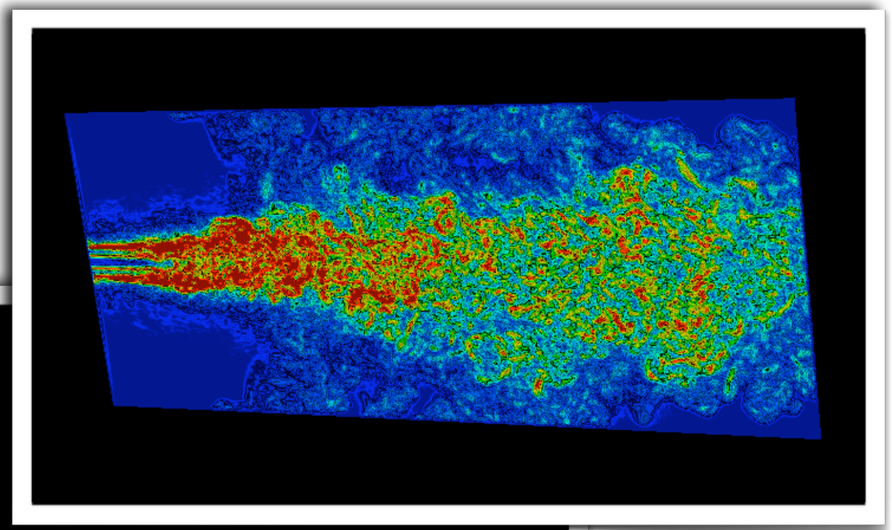
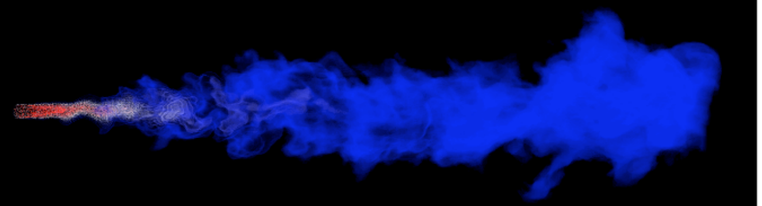
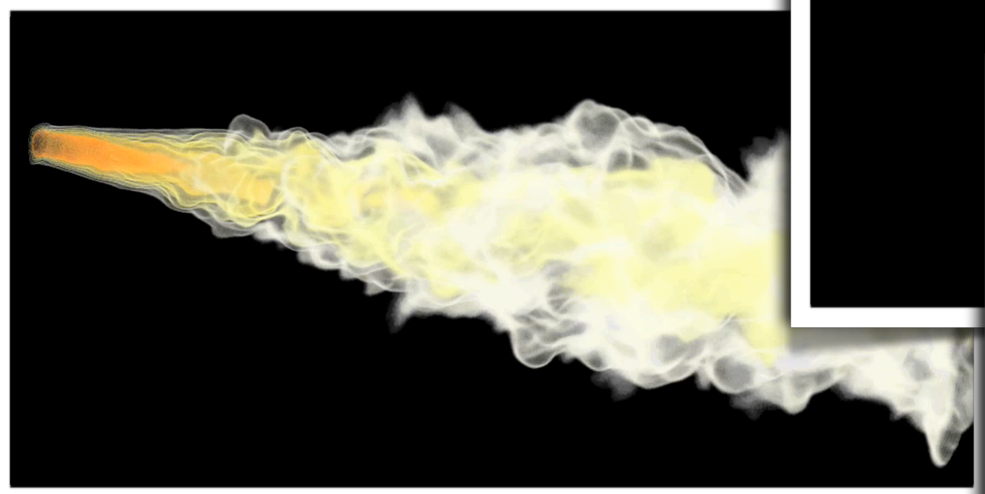
Oxy-Coal Near Burner Simulation:
can LES predict net heat flux from a new oxy-coal retrofit?

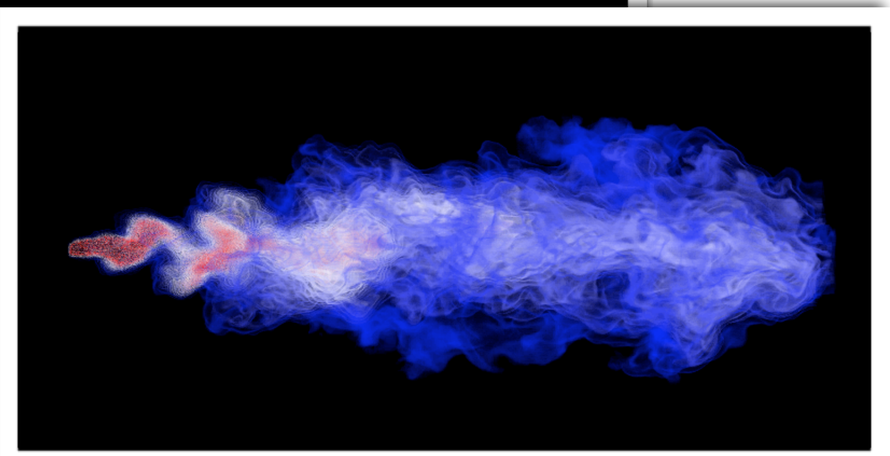












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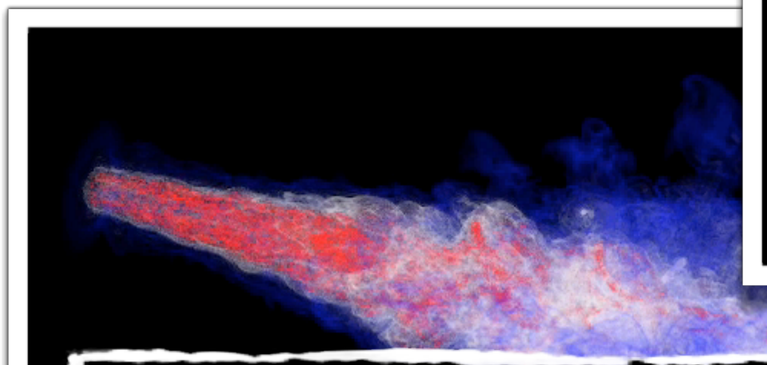
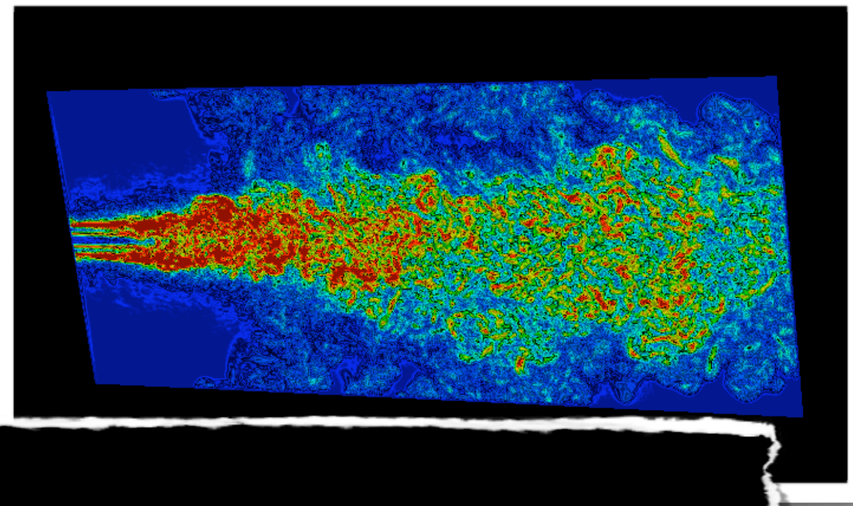
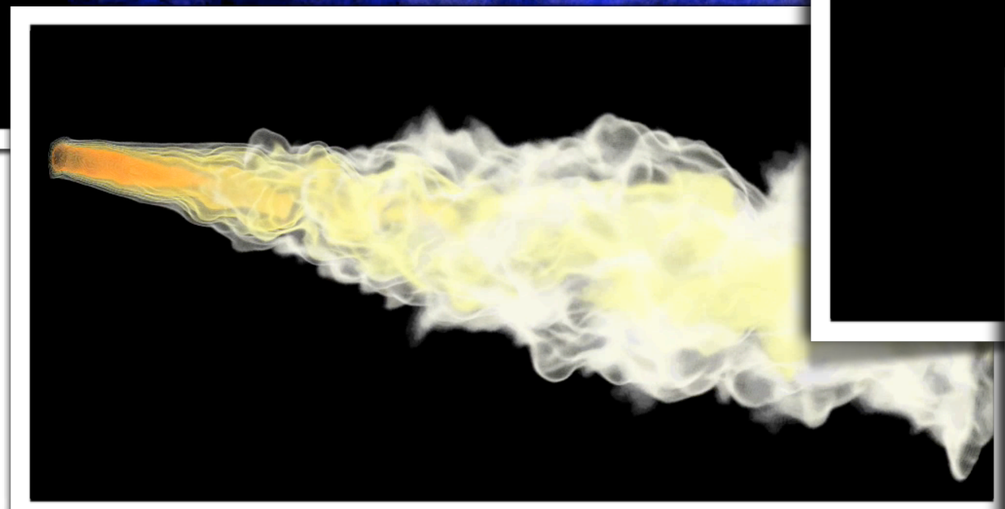
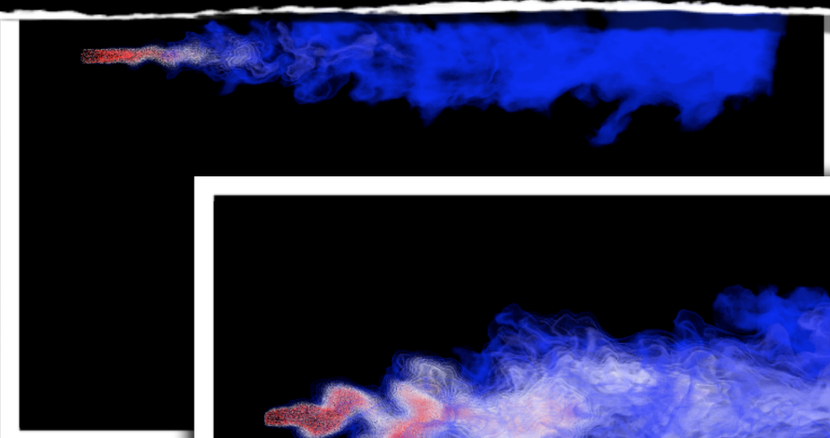
Oxy-Coal Near Burner Simulation:
can LES predict net heat flux from a new oxy-coal retrofit?

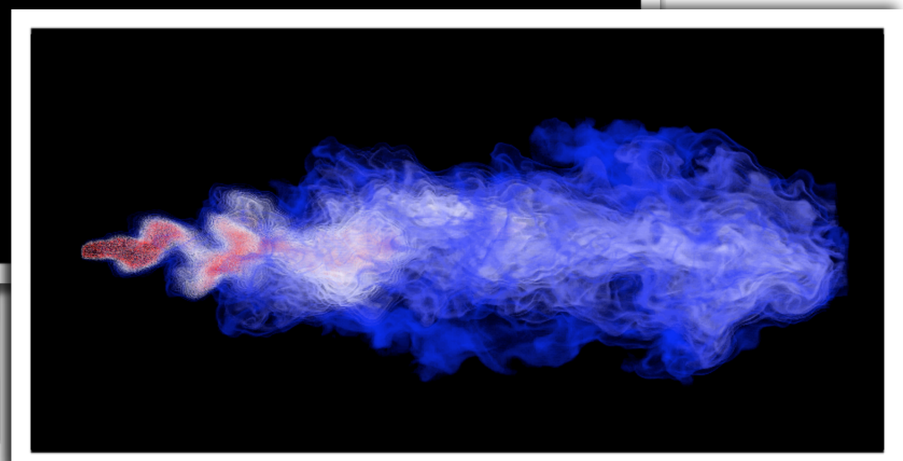




Simulation Prediction Uncertainty
= f(numerical error , modeling error , b.c. uncertainty, experimental/calibration error)







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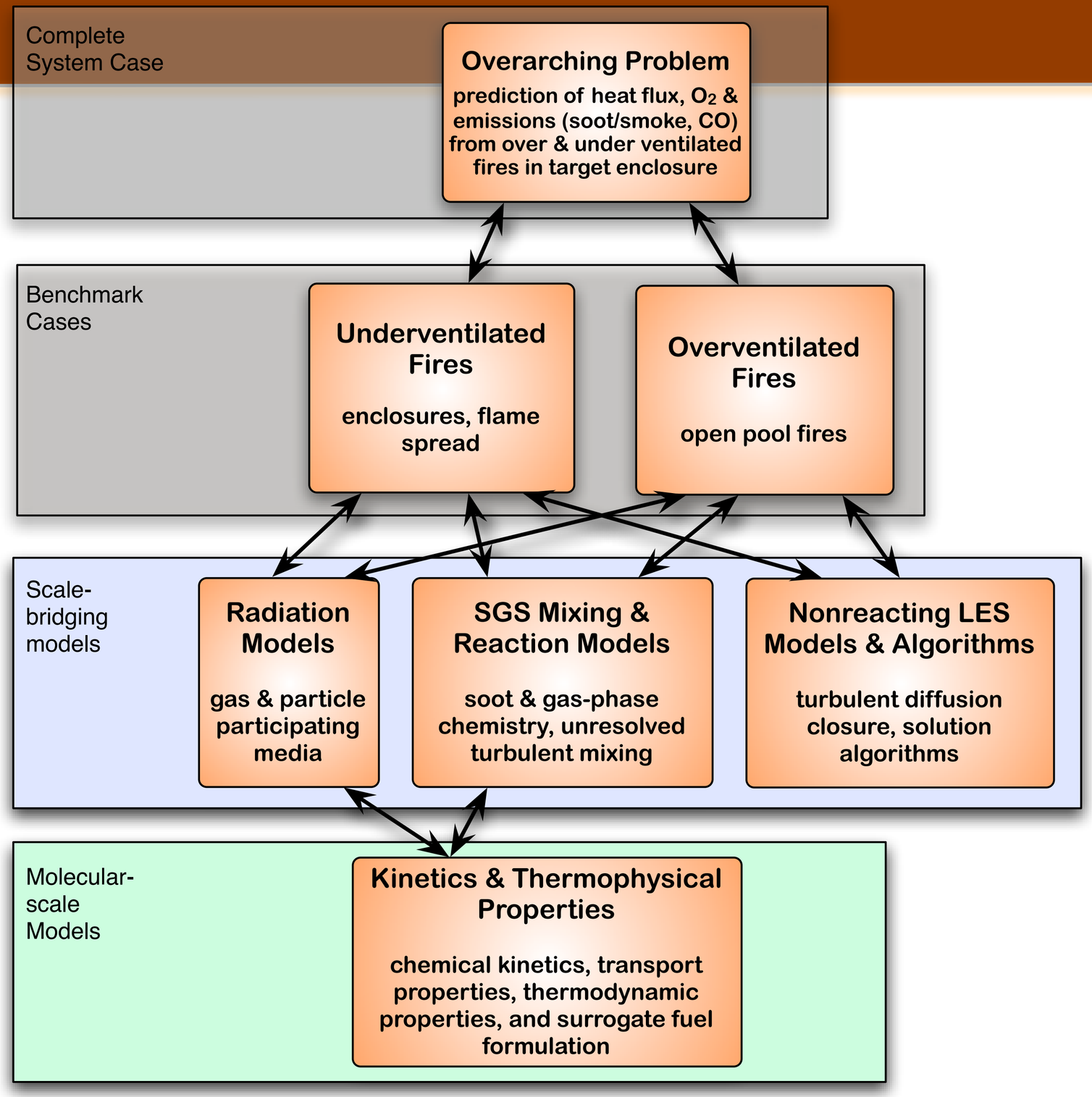
V&V


Complete System Case
Overarching Problem
prediction of heat flux, O_2 & emissions (soot/smoke, CO) from over & under ventilated fires in target enclosure
Benchmark Cases
Underventilated Fires
enclosures, flame spread
Overventilated Fires
open pool fires
Scale-bridging models
Radiation Models
gas & particle participating media
SGS Mixing & Reaction Models
soot & gas-phase chemistry, unresolved turbulent mixing
Nonreacting LES Models & Algorithms
turbulent diffusion closure, solution algorithms
Molecular-scale Models
Kinetics & Thermophysical Properties
chemical kinetics, transport properties, thermodynamic properties, and surrogate fuel formulation

V&V

Complete System Case

Overarching Problem

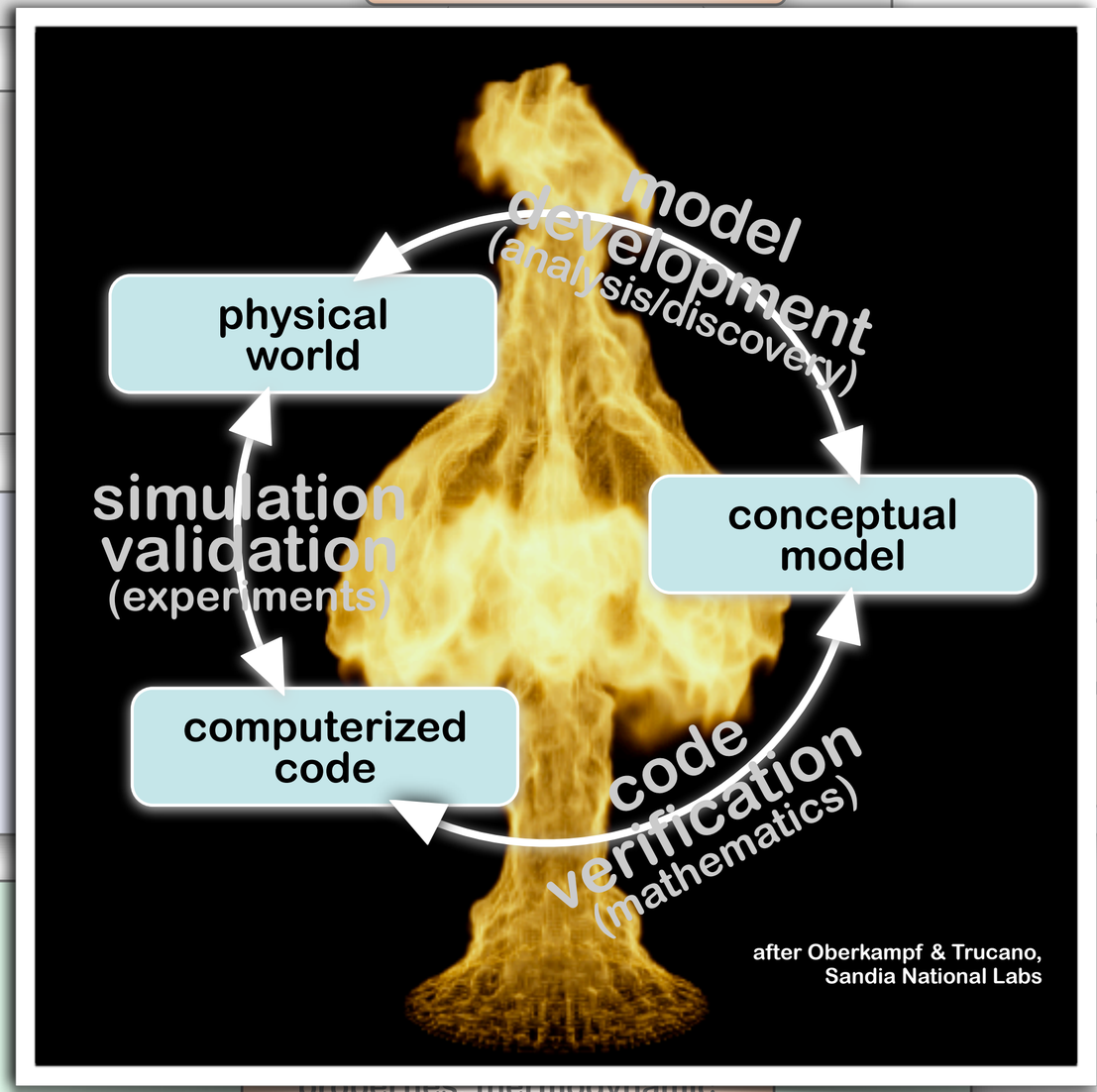
prediction of heat flux, O_2 & emissions (soot/smoke, CO) from over & under ventilated fires in target enclosure

Benchmark Cases

Scale-bridging models

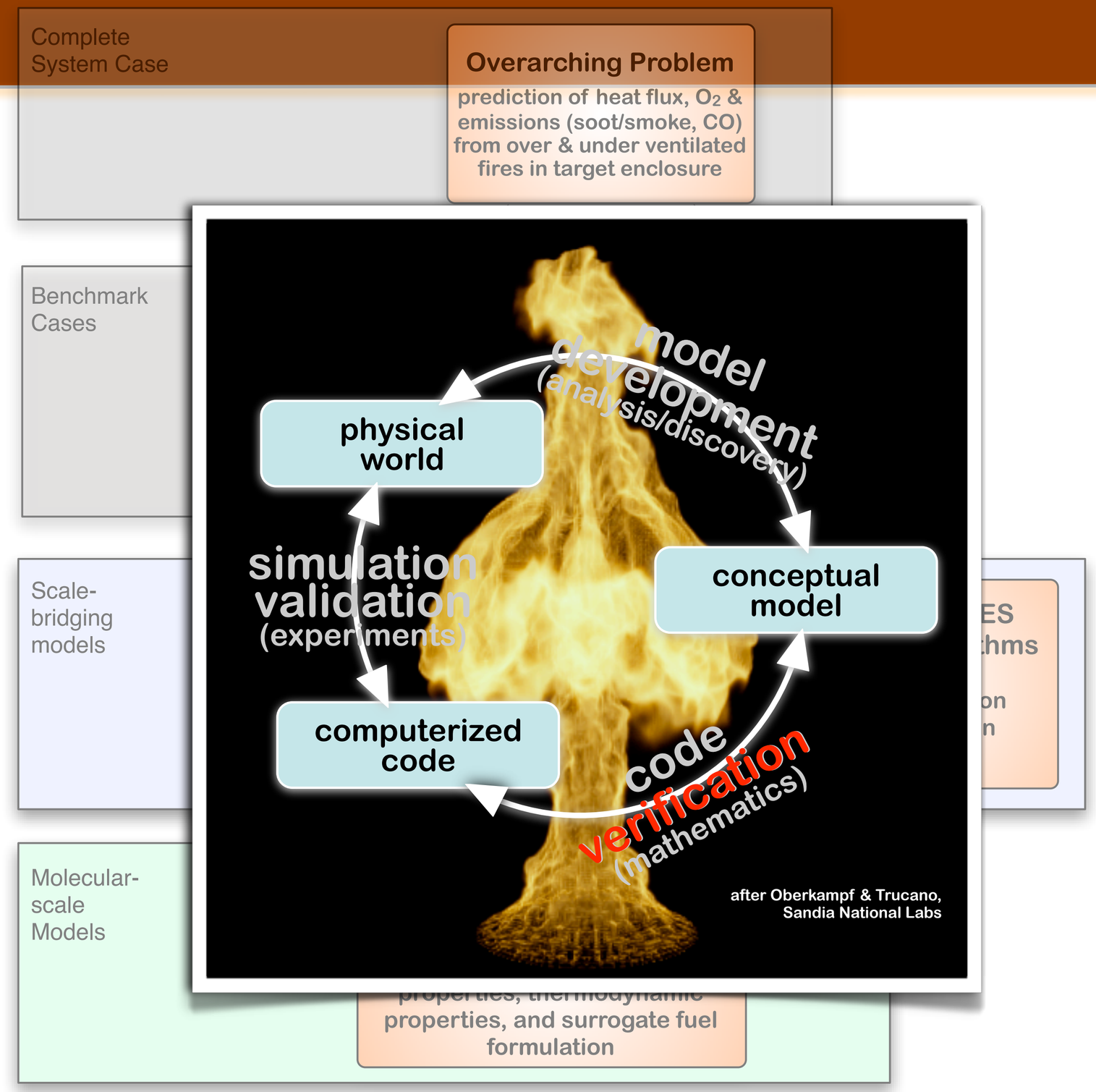
Molecular-scale Models

properties, thermodynamic properties, and surrogate fuel formulation



V&V

- **Verification:** The process of determining the degree to which a model implementation accurately represents the mathematical description of the conceptual model from the perspective of the intended uses of the model.



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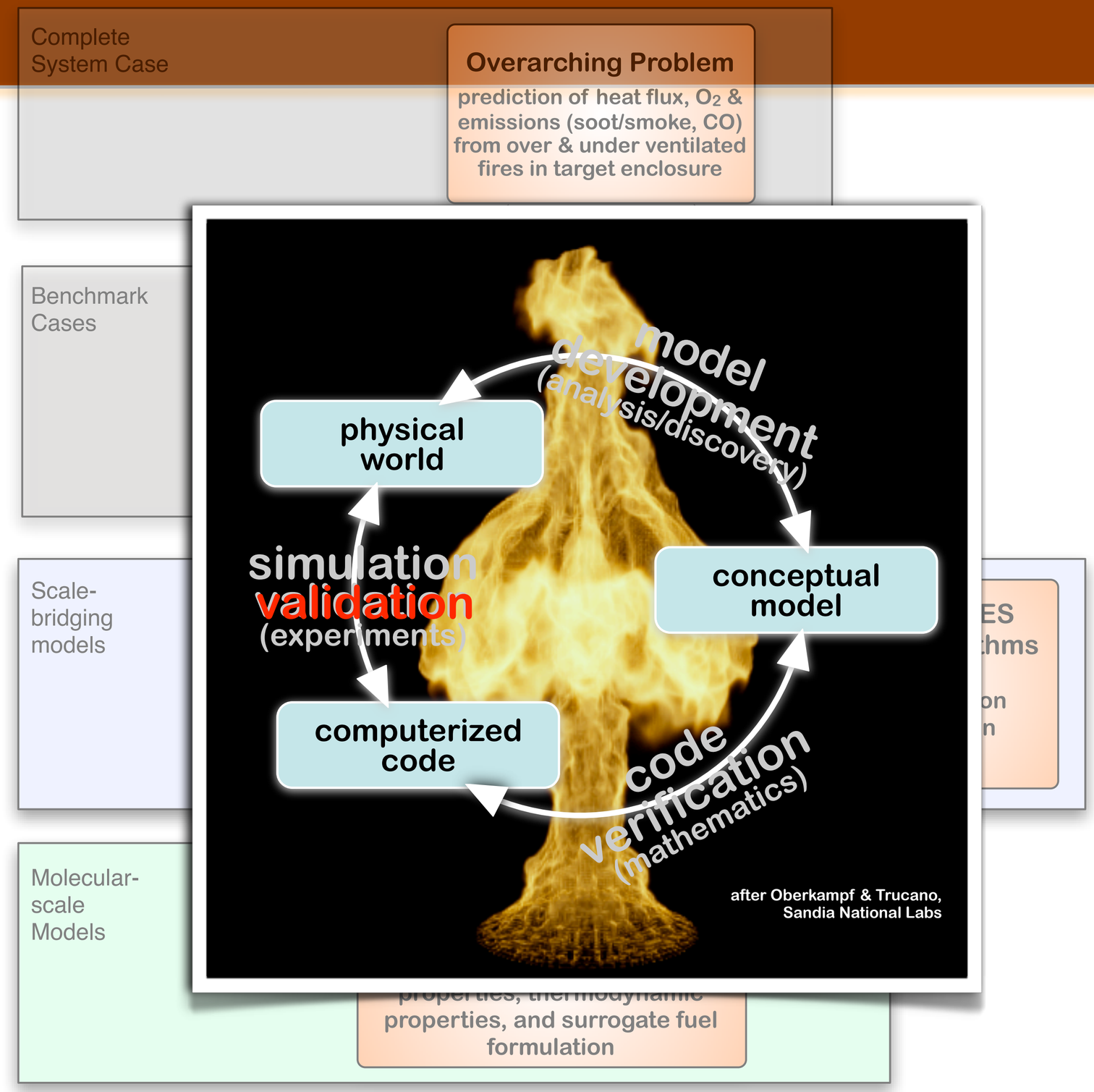
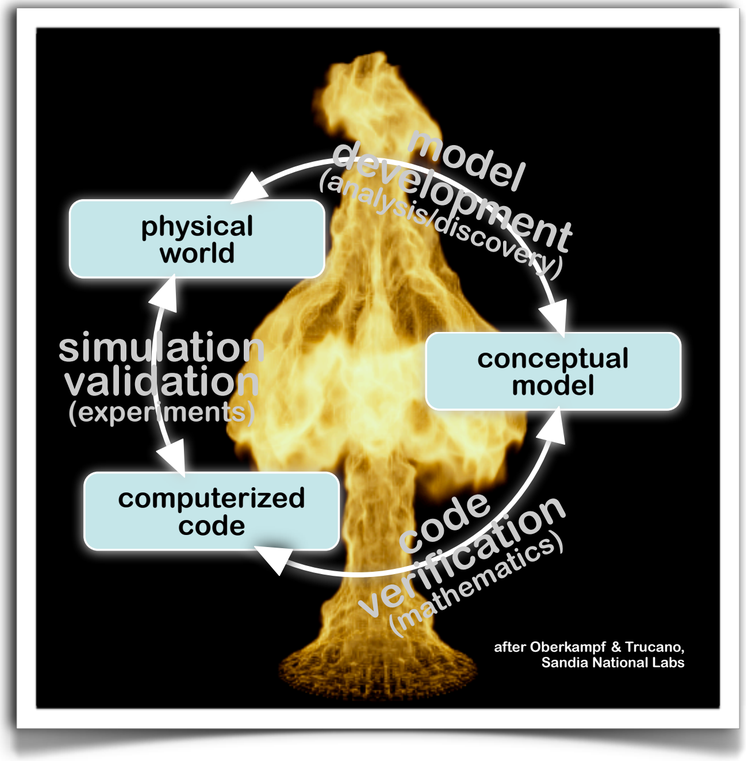
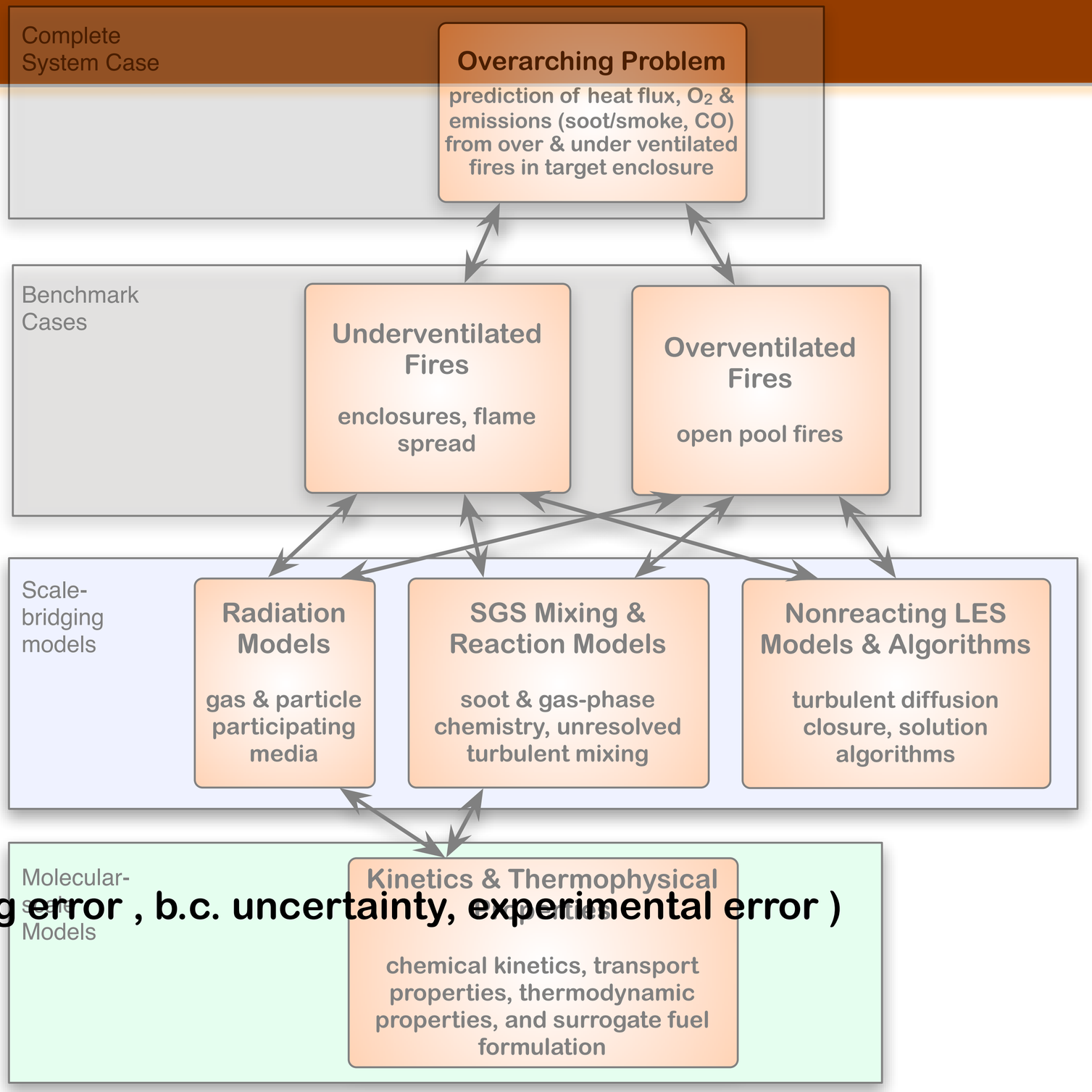
V&V

- **Verification:** The process of determining the degree to which a model implementation accurately represents the mathematical description of the conceptual model from the perspective of the intended uses of the model.
- **Validation:** The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.



V&V



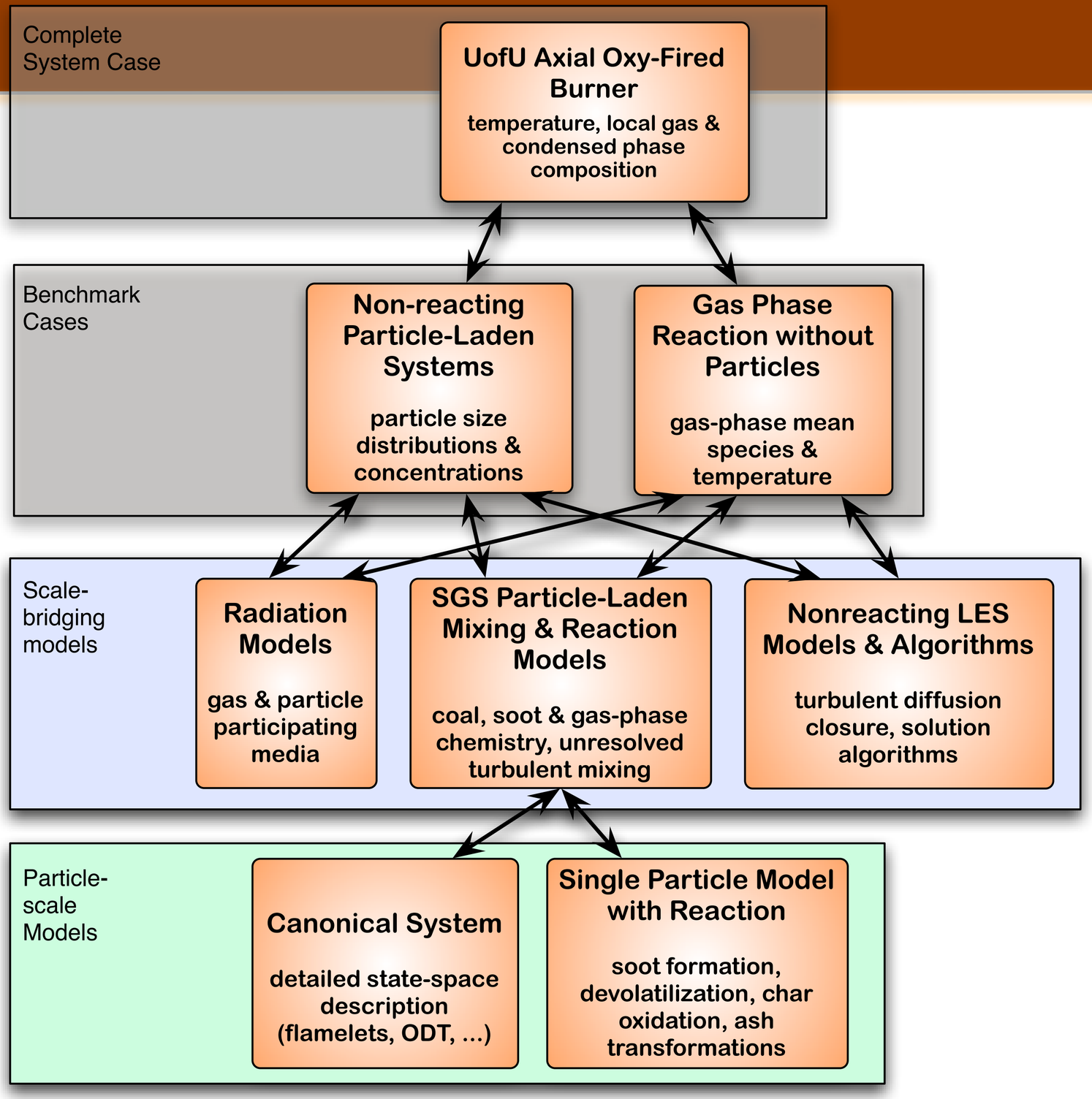


Simulation Output Uncertainty

= f (verification error , modeling error , b.c. uncertainty, experimental error)

= lots of computer time

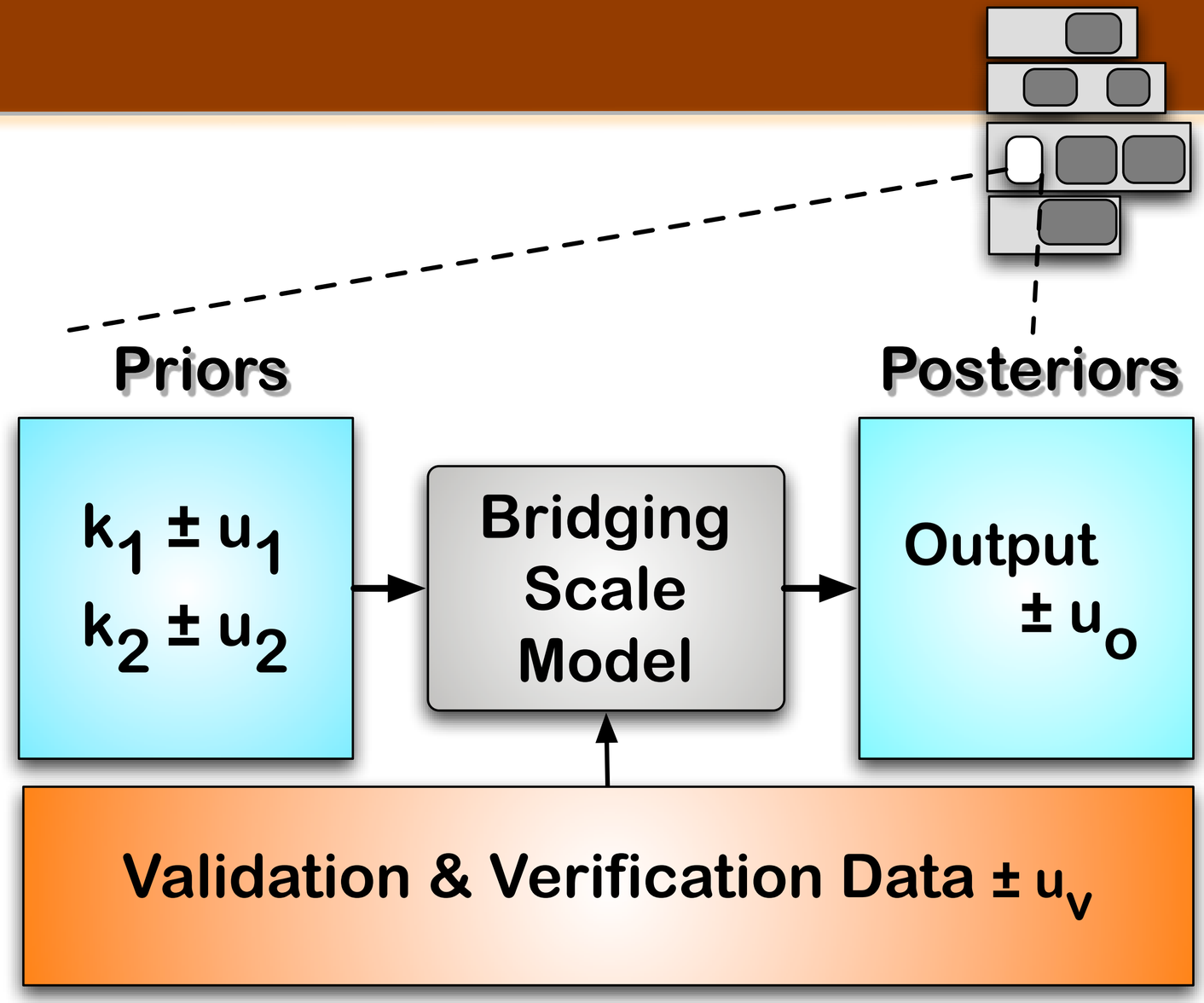
Data Consistency



Data Consistency

Simulation Output Uncertainty

- propogation of
  - modeling error
  - b.c. uncertainty
- constrained by
  - experiment error
  - numerical error



Data Consistency

Simulation Output Uncertainty

- propogation of
  - modeling error
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optimization objective

subject to:

all parameters are within prior bounds

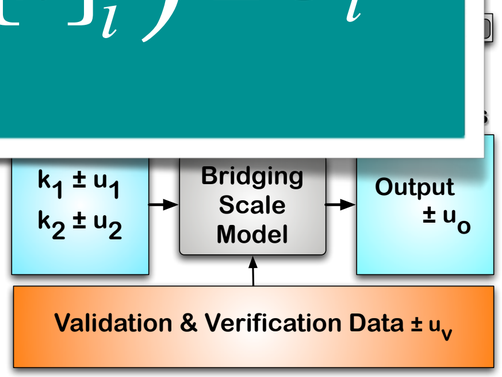
$$k_{1,\min} \le k_1 \le k_{1,\max}$$

$$k_{2,\min} \le k_2 \le k_{2,\max}$$

$$\cdots$$

all model predictions are within experiment bounds

$$L_i \le M_i\left(\{k\}_i\right) \le U_i$$



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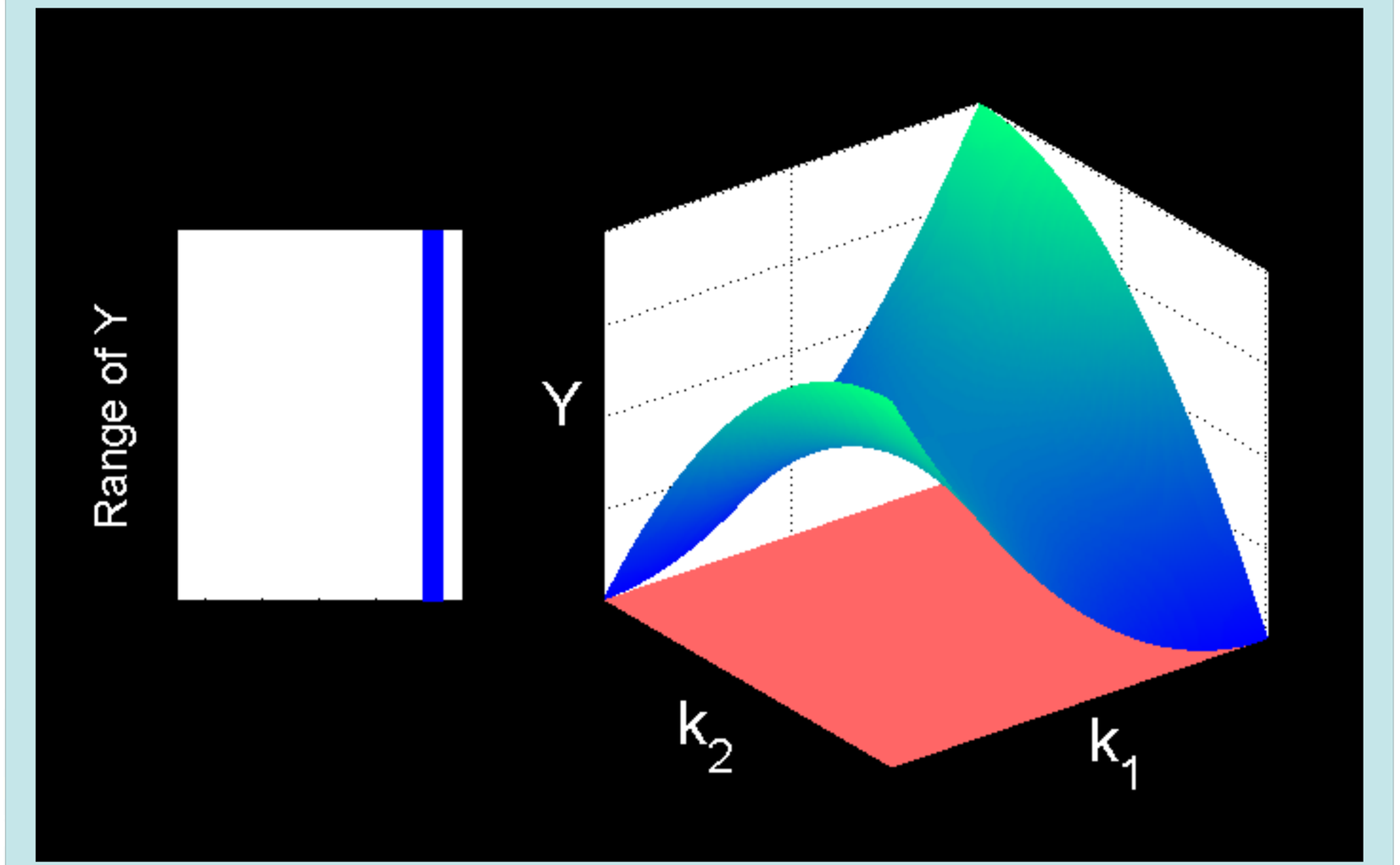
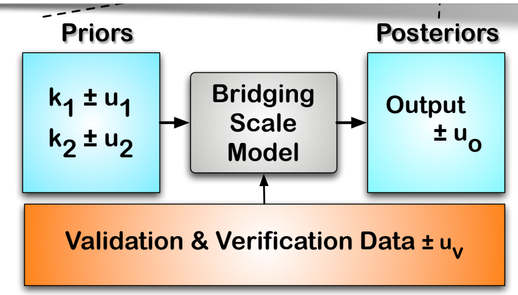


op
ob

subject to:

$$\left.\begin{array}{l} \\ \\ \\ \cdots \\ \text{all model predictions are within experiment bounds} \\ L_i \le M_i\left(\{k\}_i\right) \le U_i \end{array}\right\}$$



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Data Consistency

Simulation Output Uncertainty

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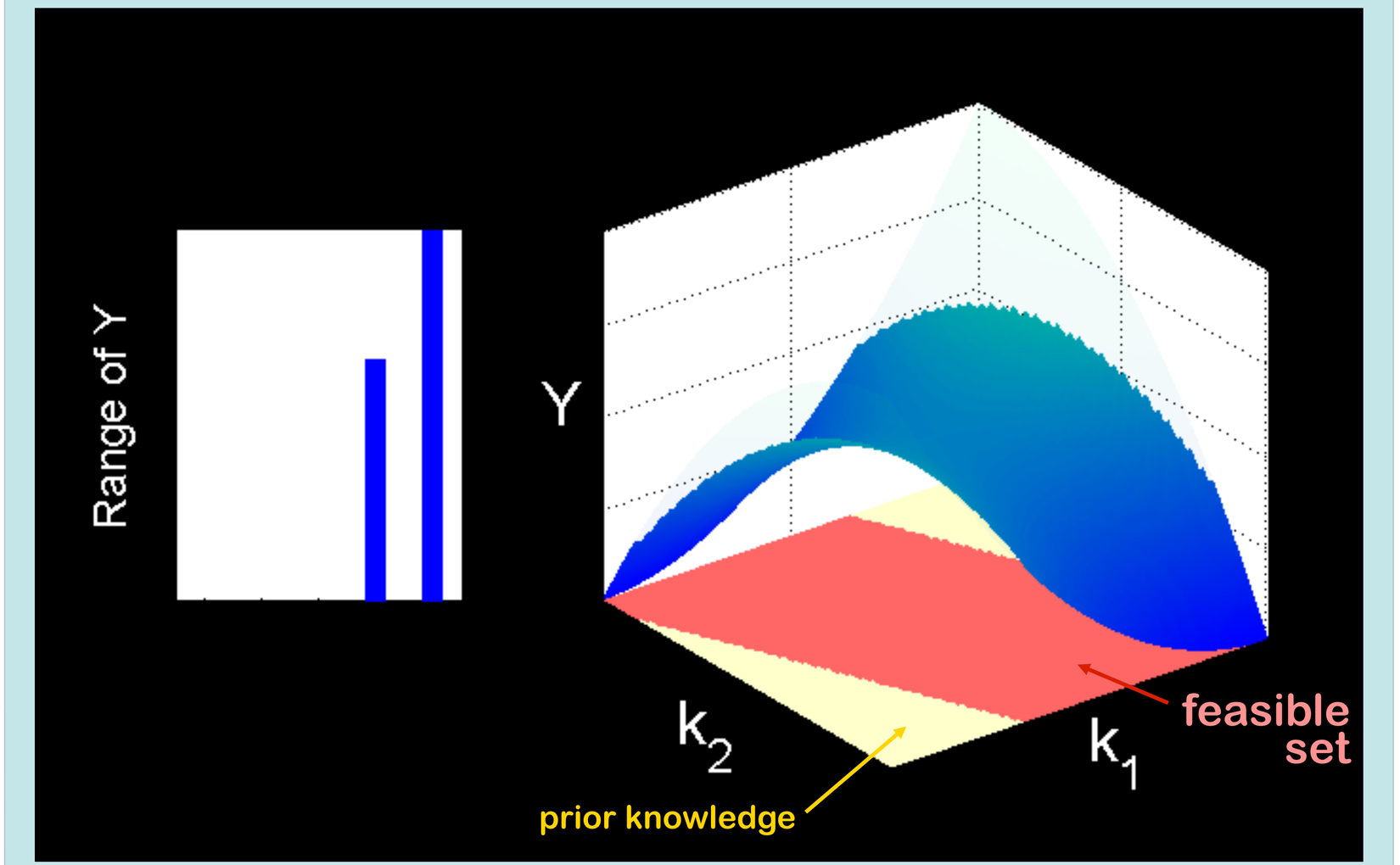

op
ob

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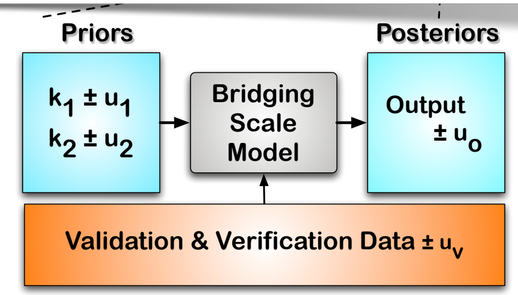

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Data Consistency

Simulation Output Uncertainty

- **propogation of**
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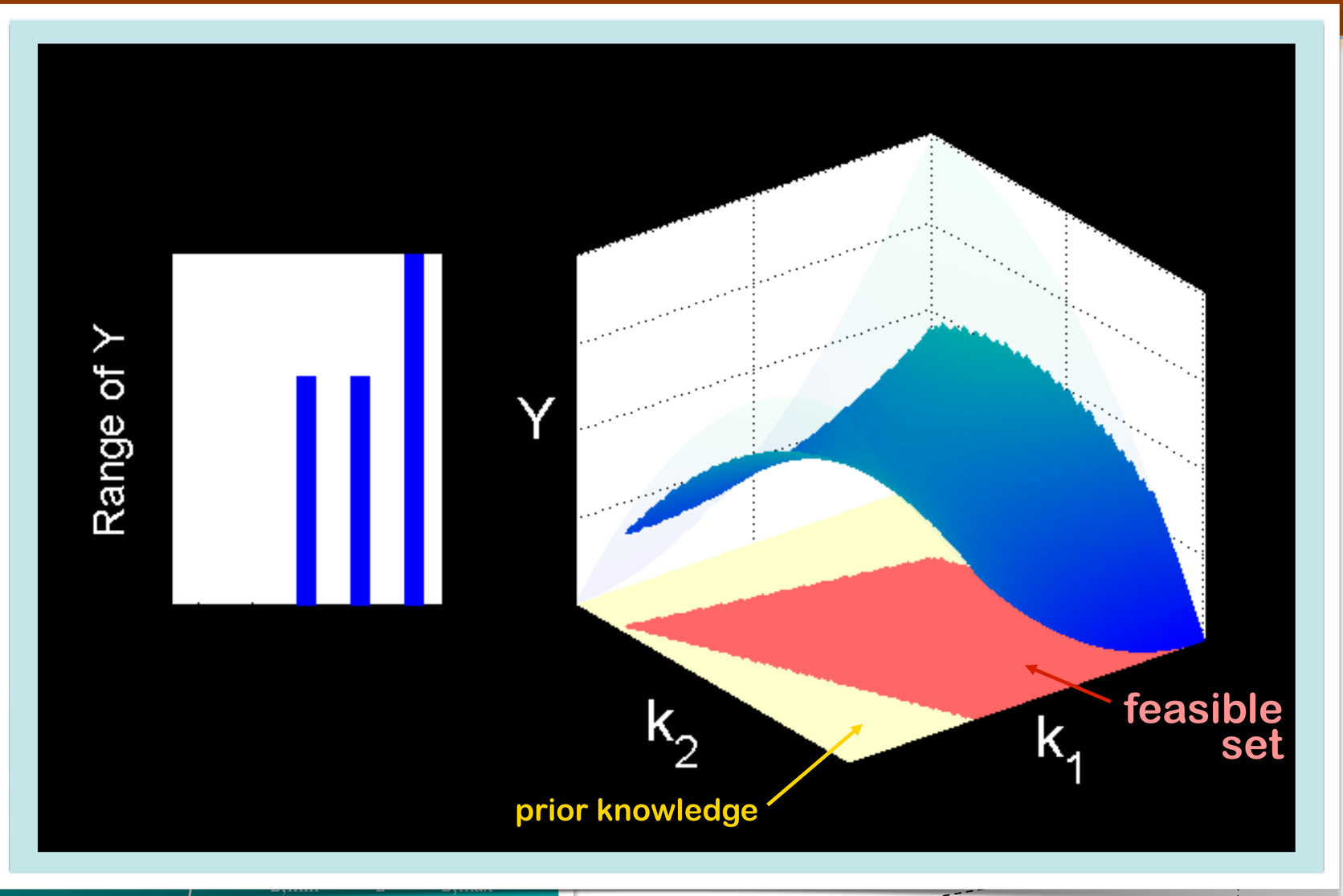


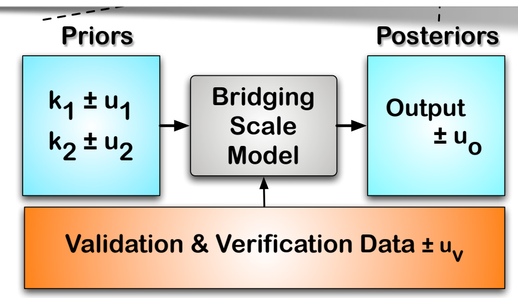
op
ob

subject to:

$$\vdots$$

all model predictions are within experiment bounds

$$L_i \leq M_i\left(\{k\}_i\right) \leq U_i$$



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Data Consistency

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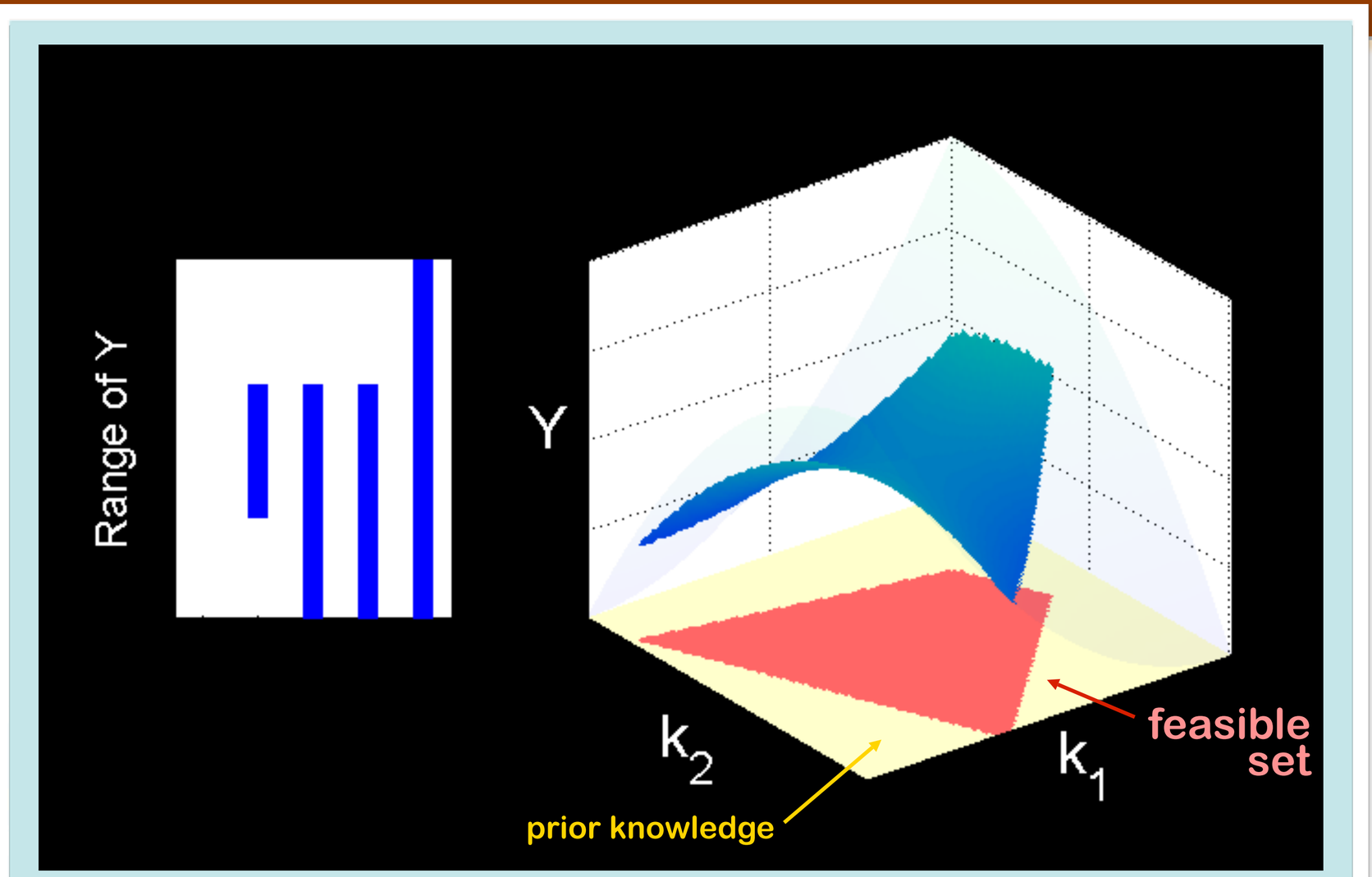

op
ob

subject to:

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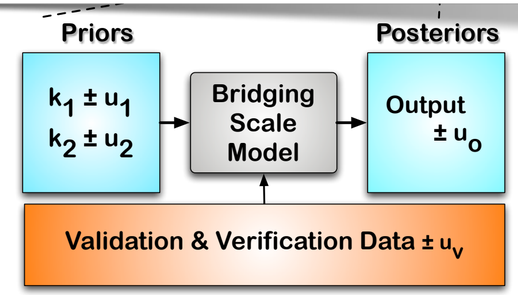

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Data Consistency

Simulation Output Uncertainty

- **propogation of**
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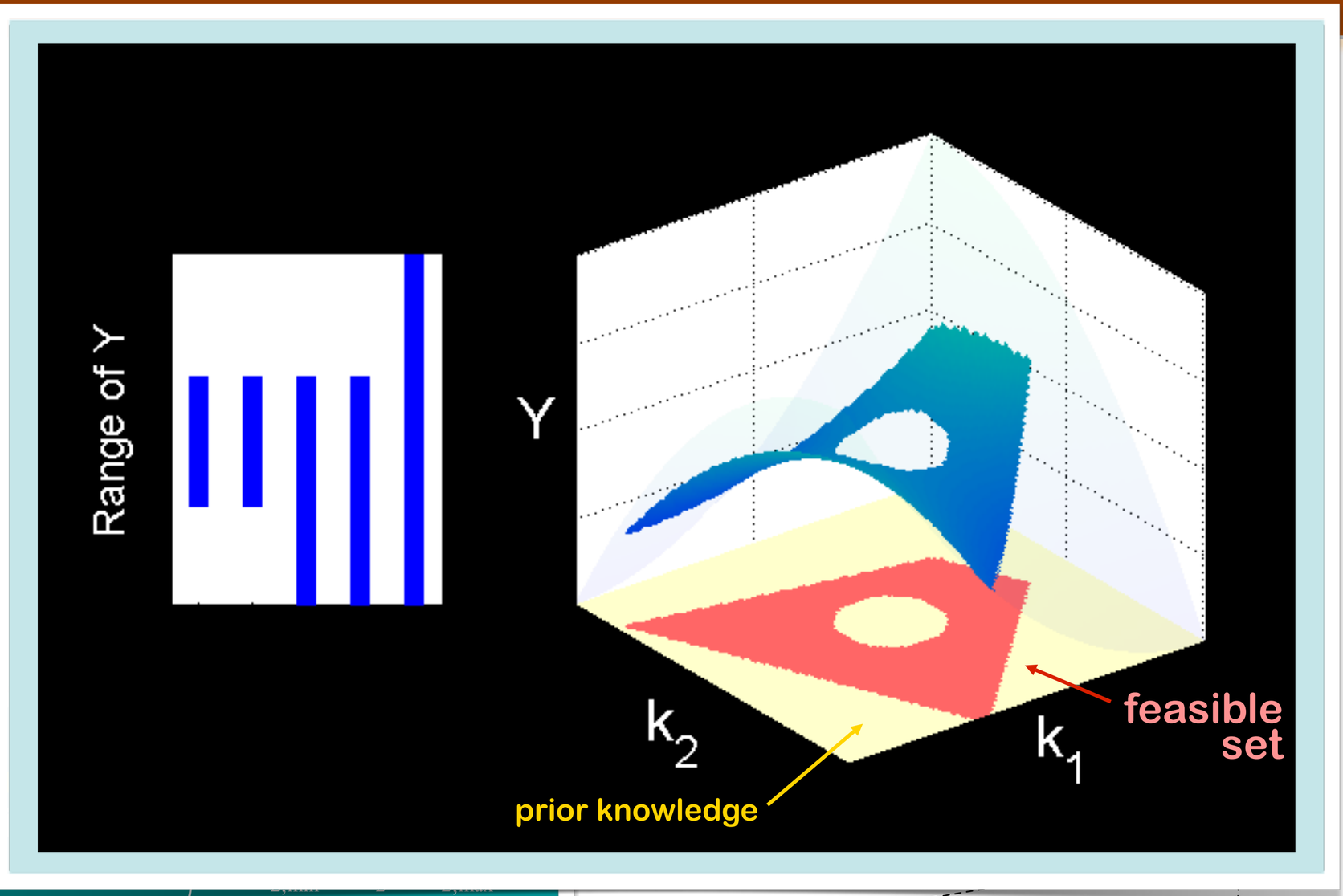
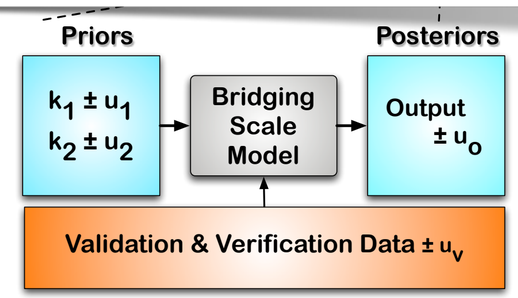


op
ob

subject to:

all model predictions are within experiment bounds

$$L_i \le M_i\left(\{k\}_i\right) \le U_i$$



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Data Consistency

Simulation Output Uncertainty

- propogation of
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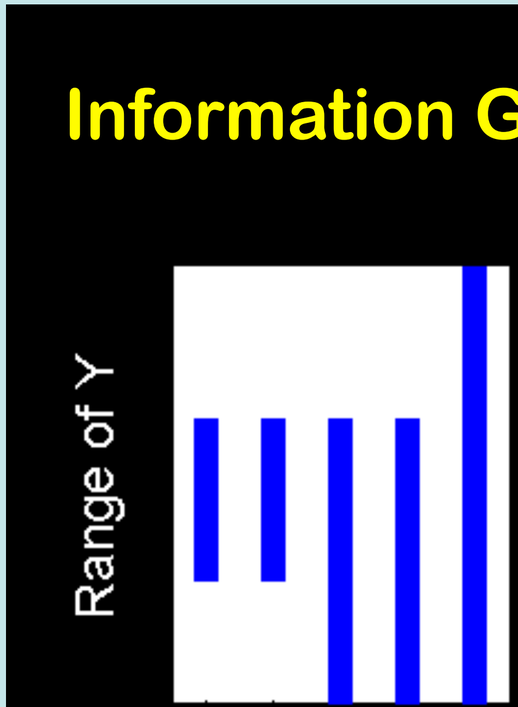
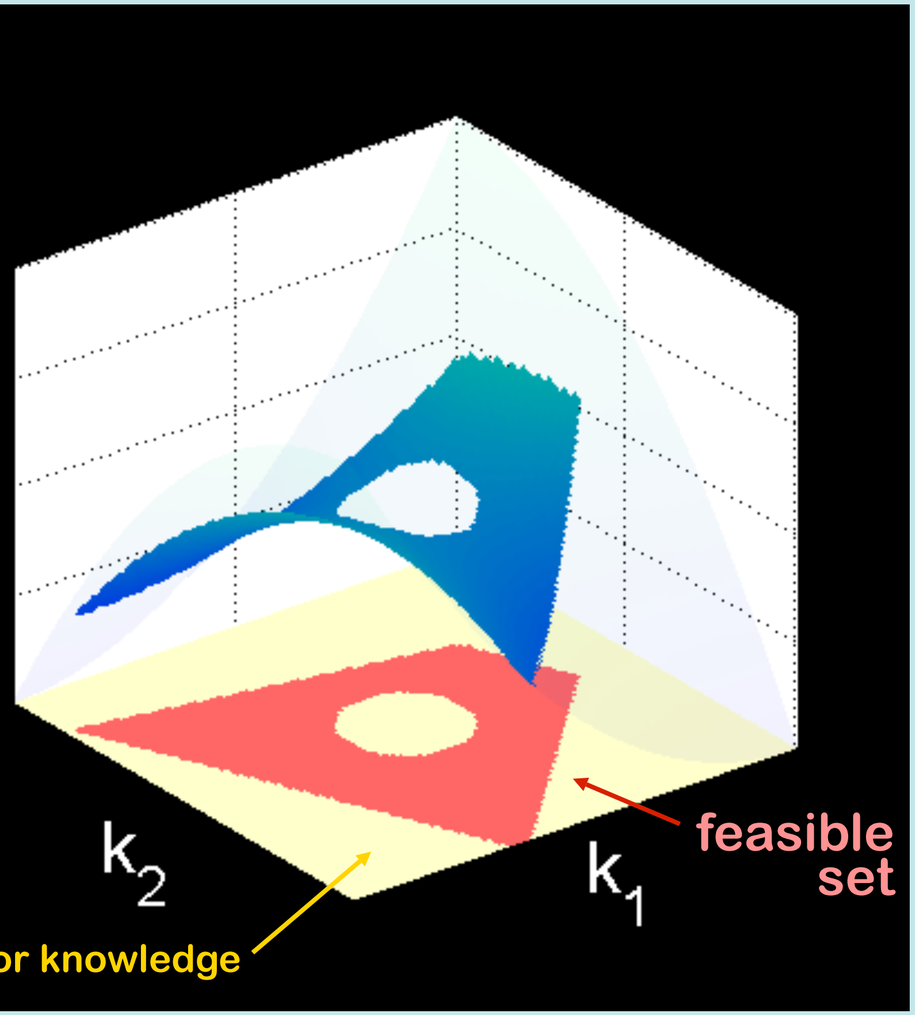
- constrained by
  - experiment error
  - numerical error

Information Gain:



$$I = 1 - \frac{\text{Posterior Range}}{\text{Prior Range}}$$



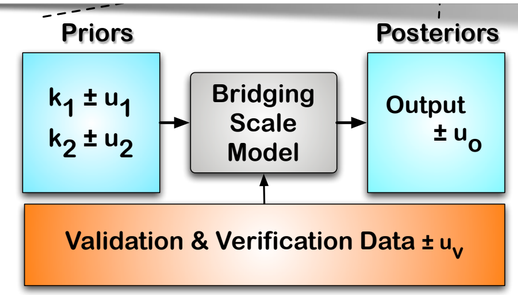
op
ob

subject to:

$$\vdots$$

all model predictions are within experiment bounds

$$L_i \le M_i\left(\{k\}_i\right) \le U_i$$



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Data Consistency

Simulation Output Uncertainty

- propogation of
  - modeling error
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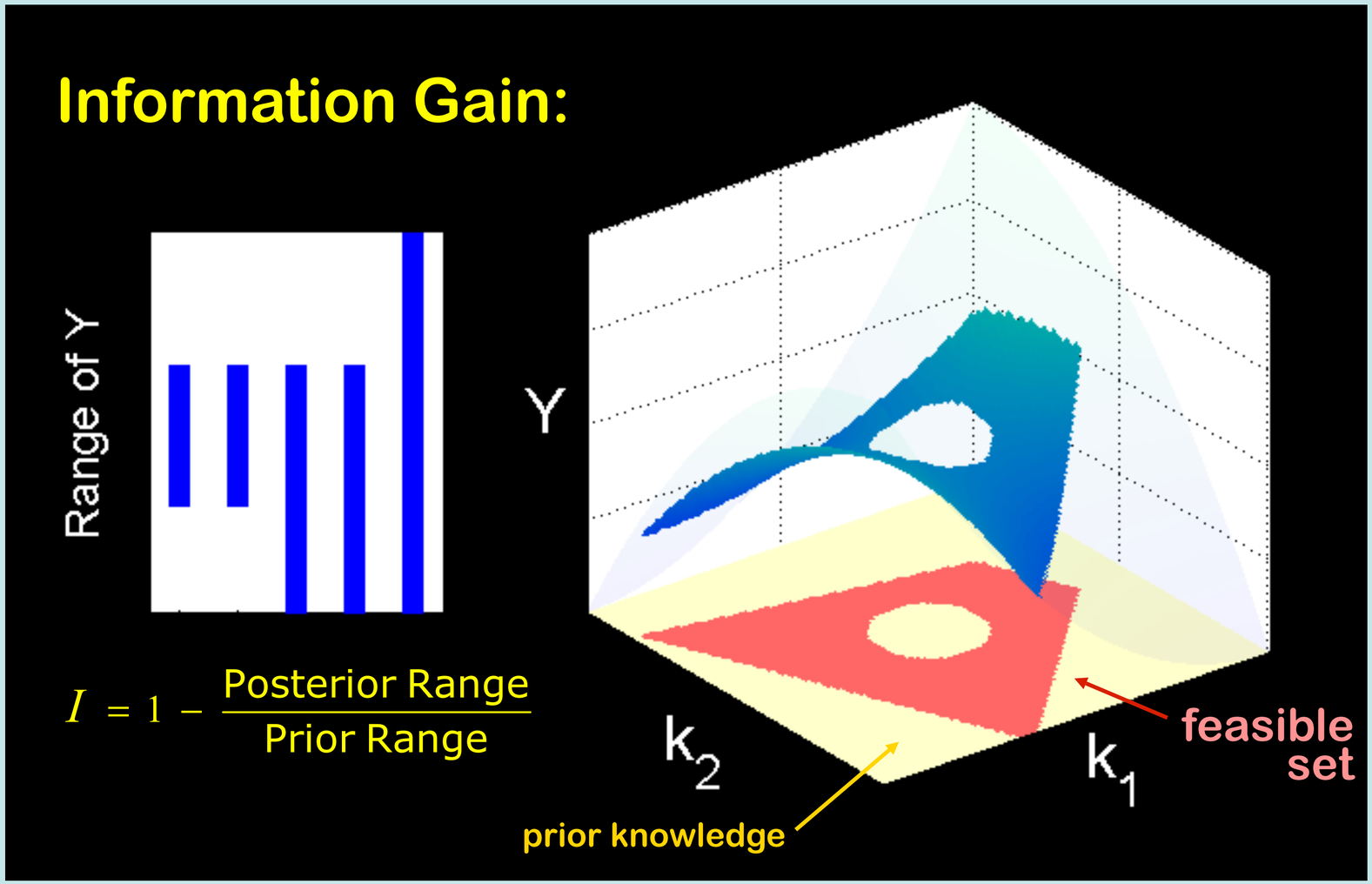
- constrained by
  - experiment error
  - numerical error

require consistency between simulation data and experimental data

Information Gain:



op
ob

subject to:

...

all model predictions are within experiment bounds

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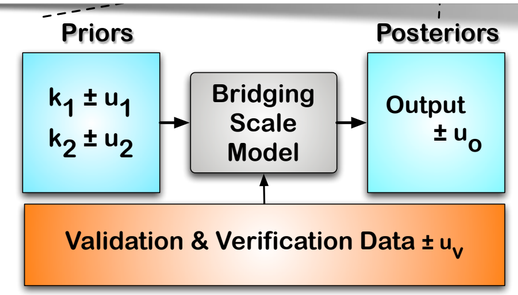

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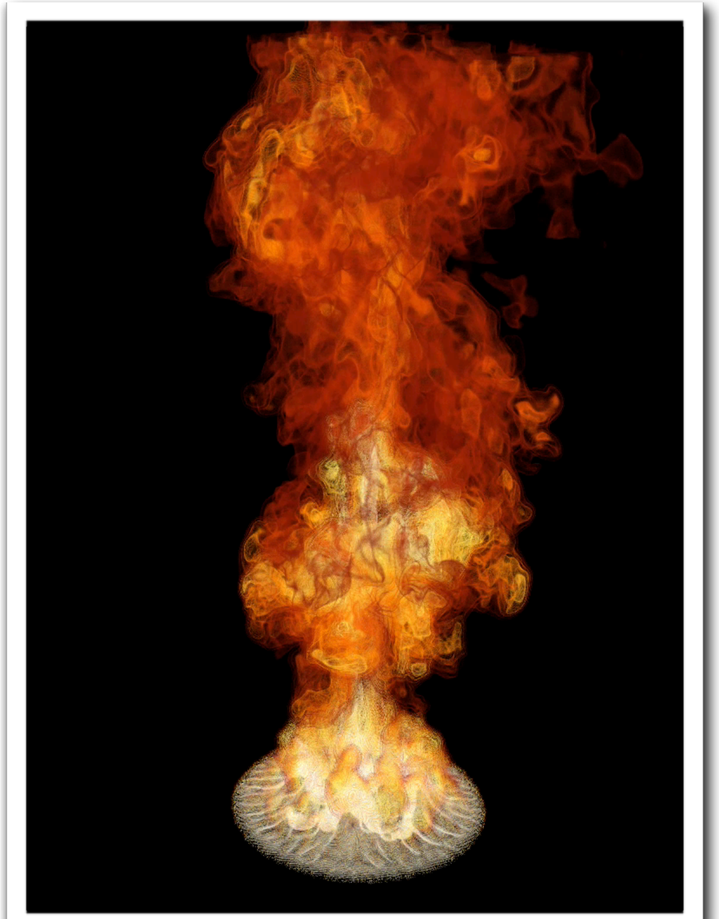
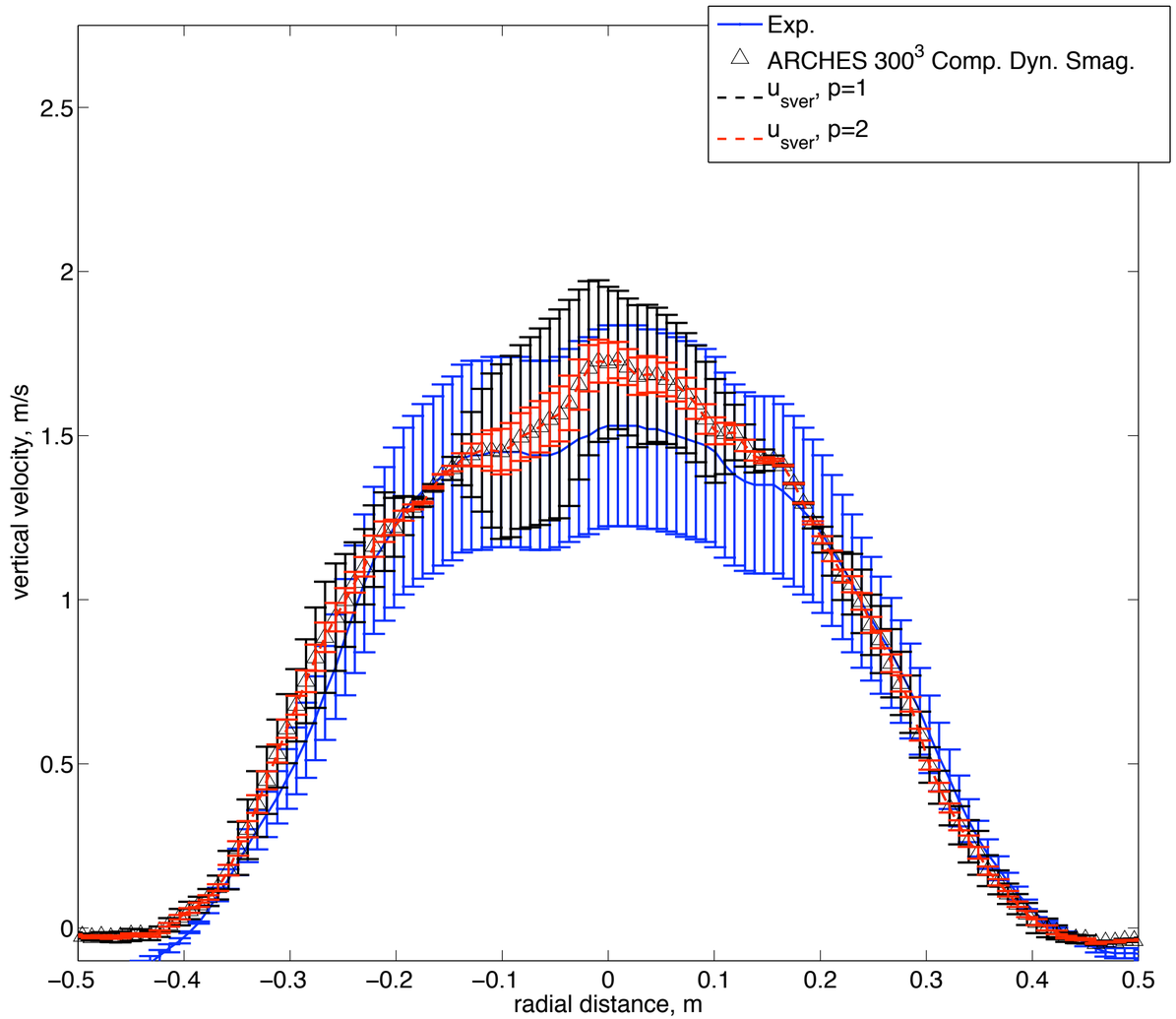
Error Budget



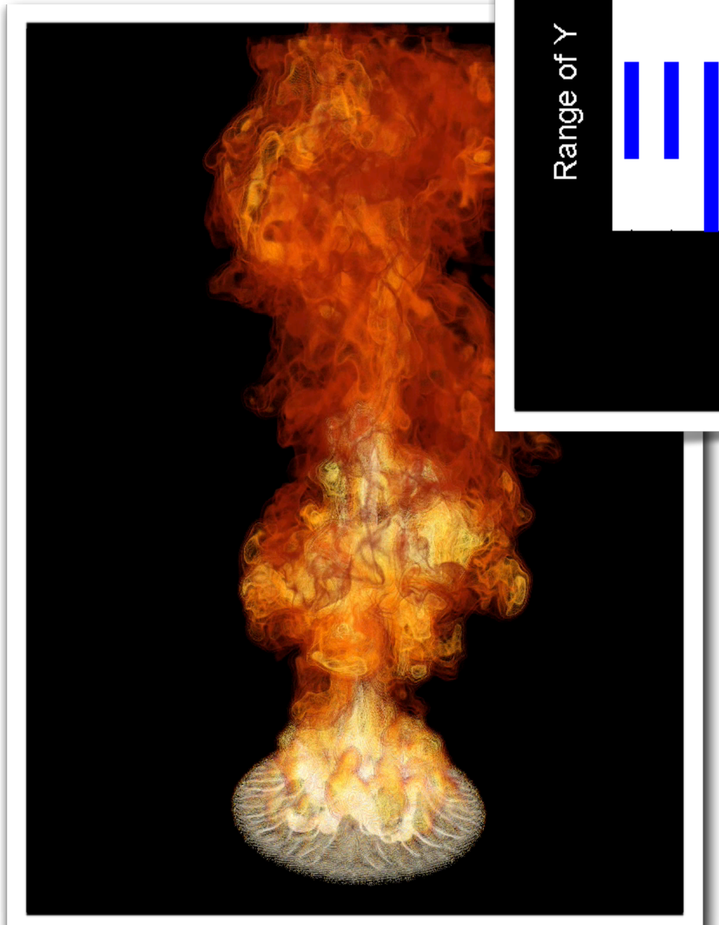


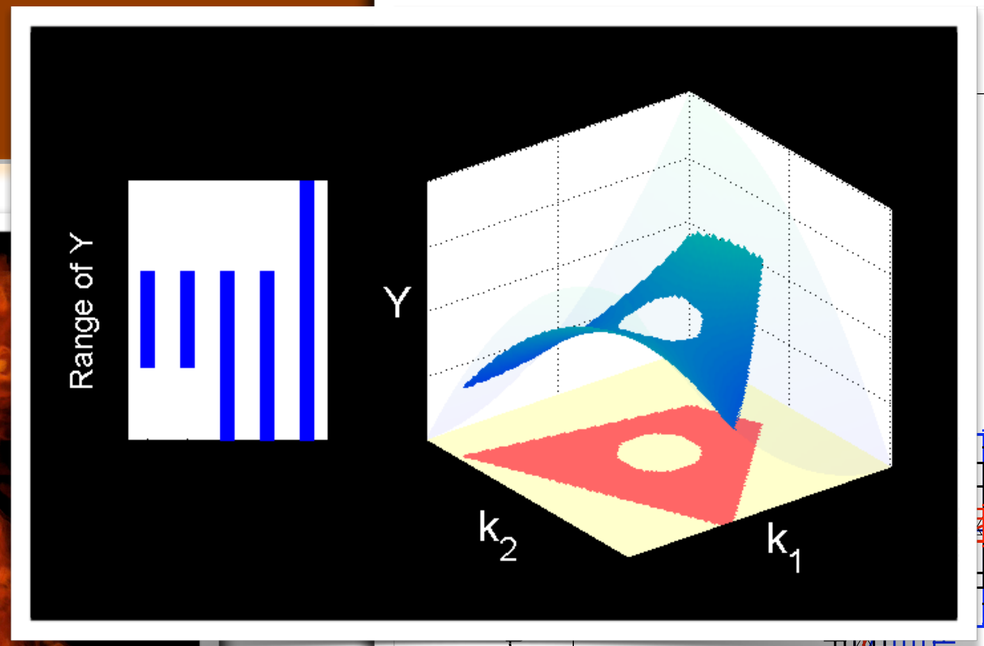
Simulation Output Uncertainty

= f (verification error , modeling error , b.c. uncertainty, experimental error)

= lots of computer time

Error Budget





Simulation Output Uncertainty

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validation hierarchy

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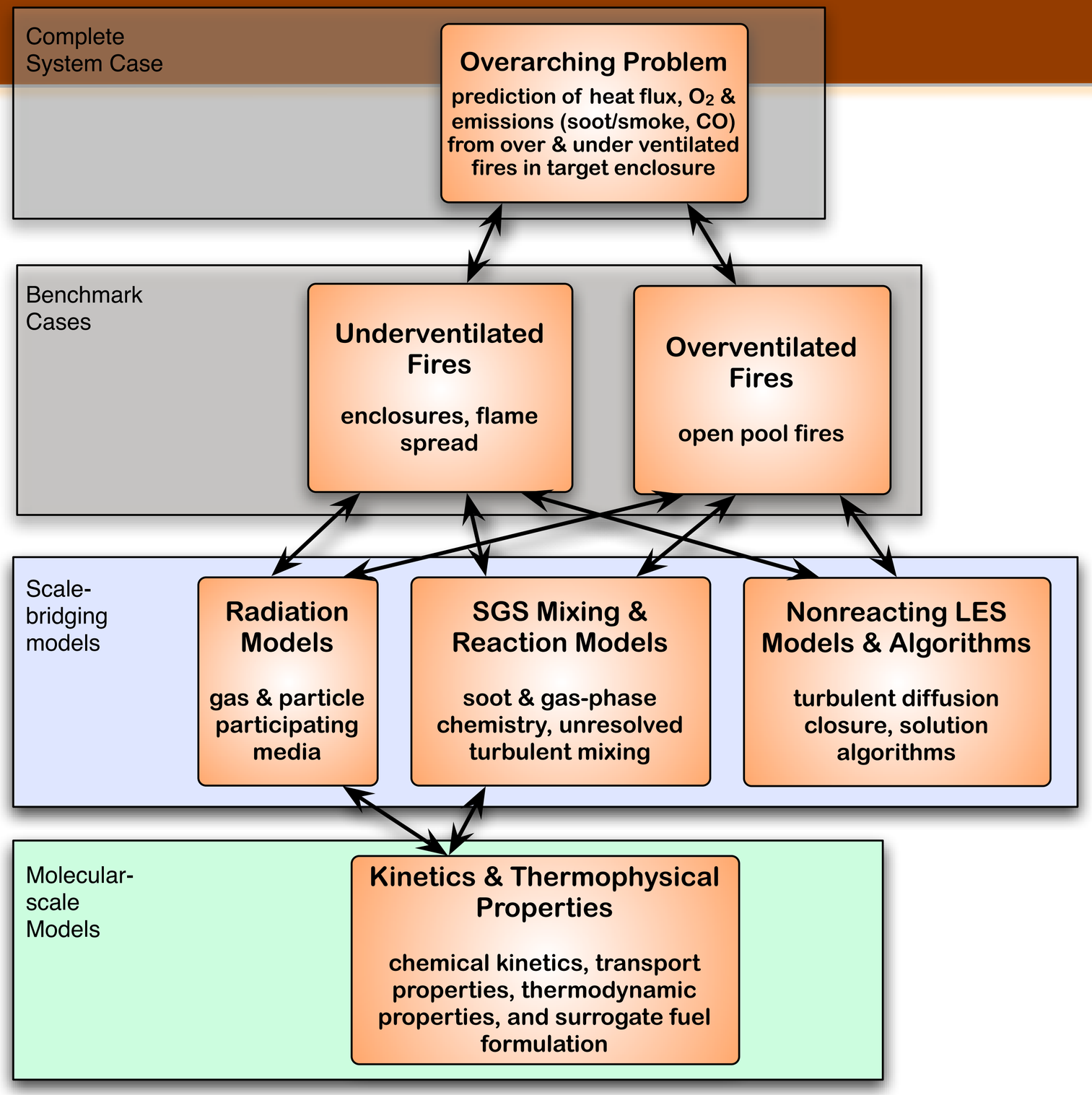

validation hierarchy

- **driven by overarching problem (intended use of simulation)**

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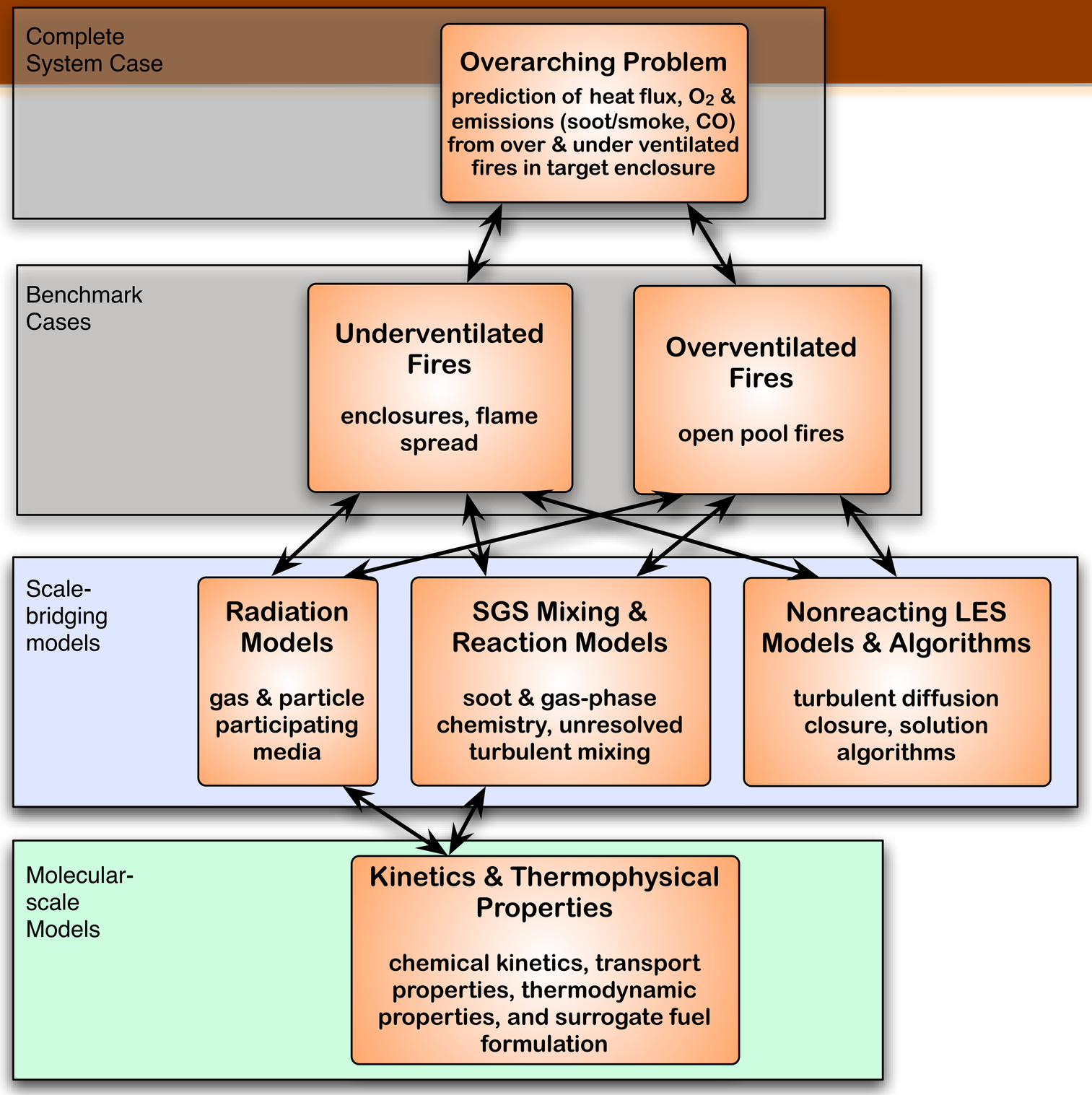

validation hierarchy

- **driven by overarching problem (intended use of simulation)**
- **hierarchical coupling**

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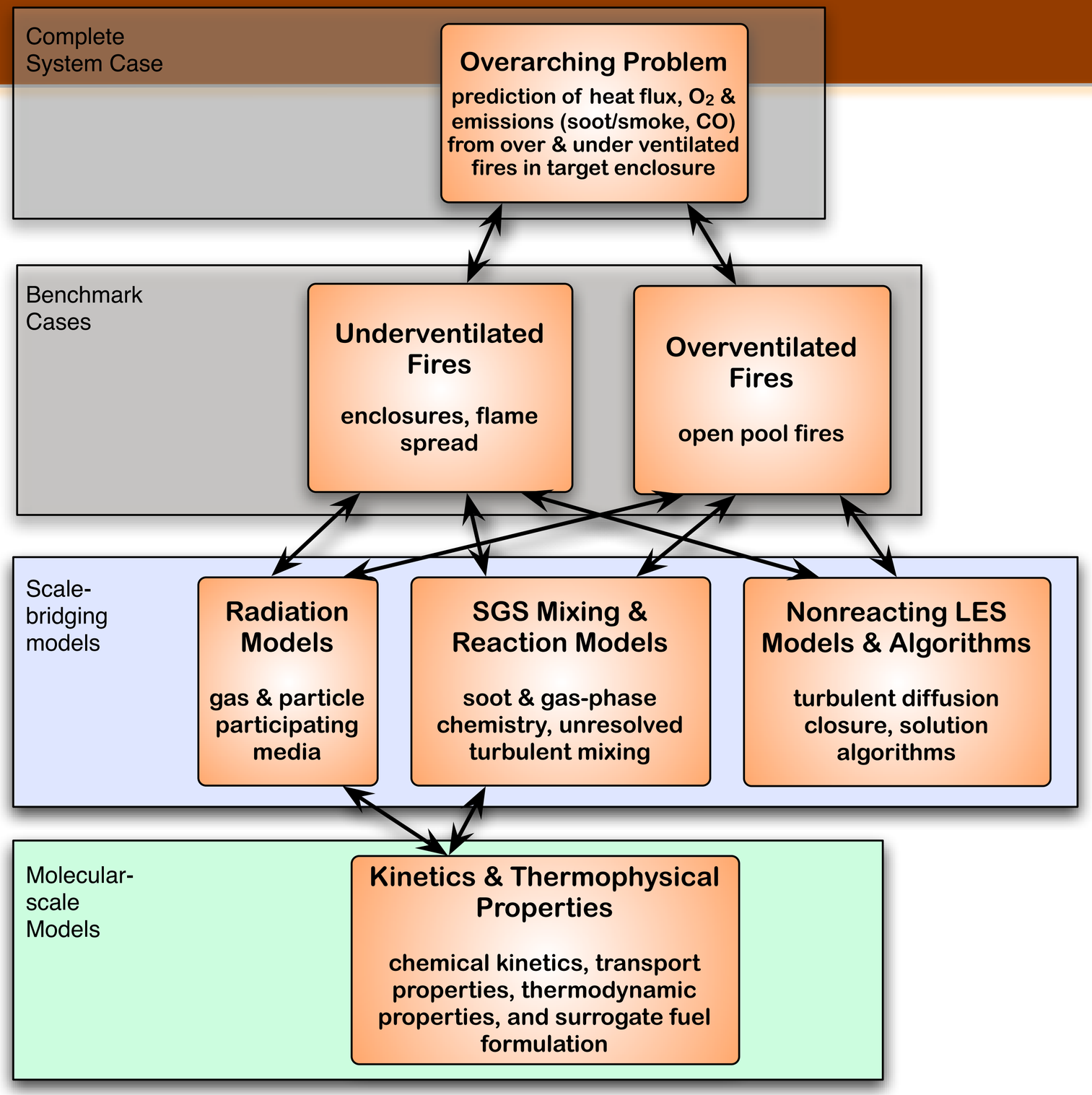
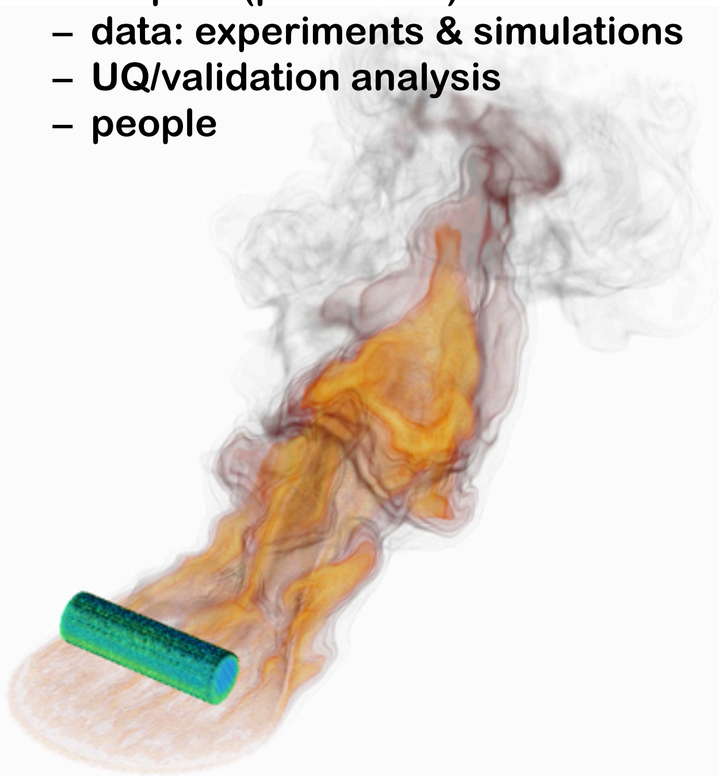


validation hierarchy

- driven by overarching problem (intended use of simulation)
- hierarchical coupling
- definition of each brick:
  - inputs (priors: new & inherited)
  - outputs (posteriors)
  - data: experiments & simulations
  - UQ/validation analysis
  - people



validation hierarchy

- driven by overarching problem (intended use of simulation)
- hierarchical coupling
- definition of each brick:
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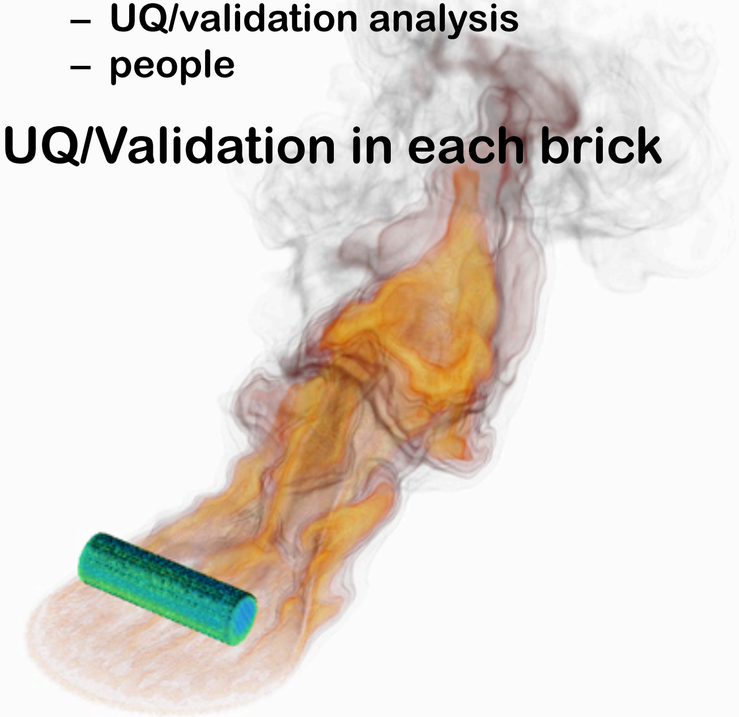
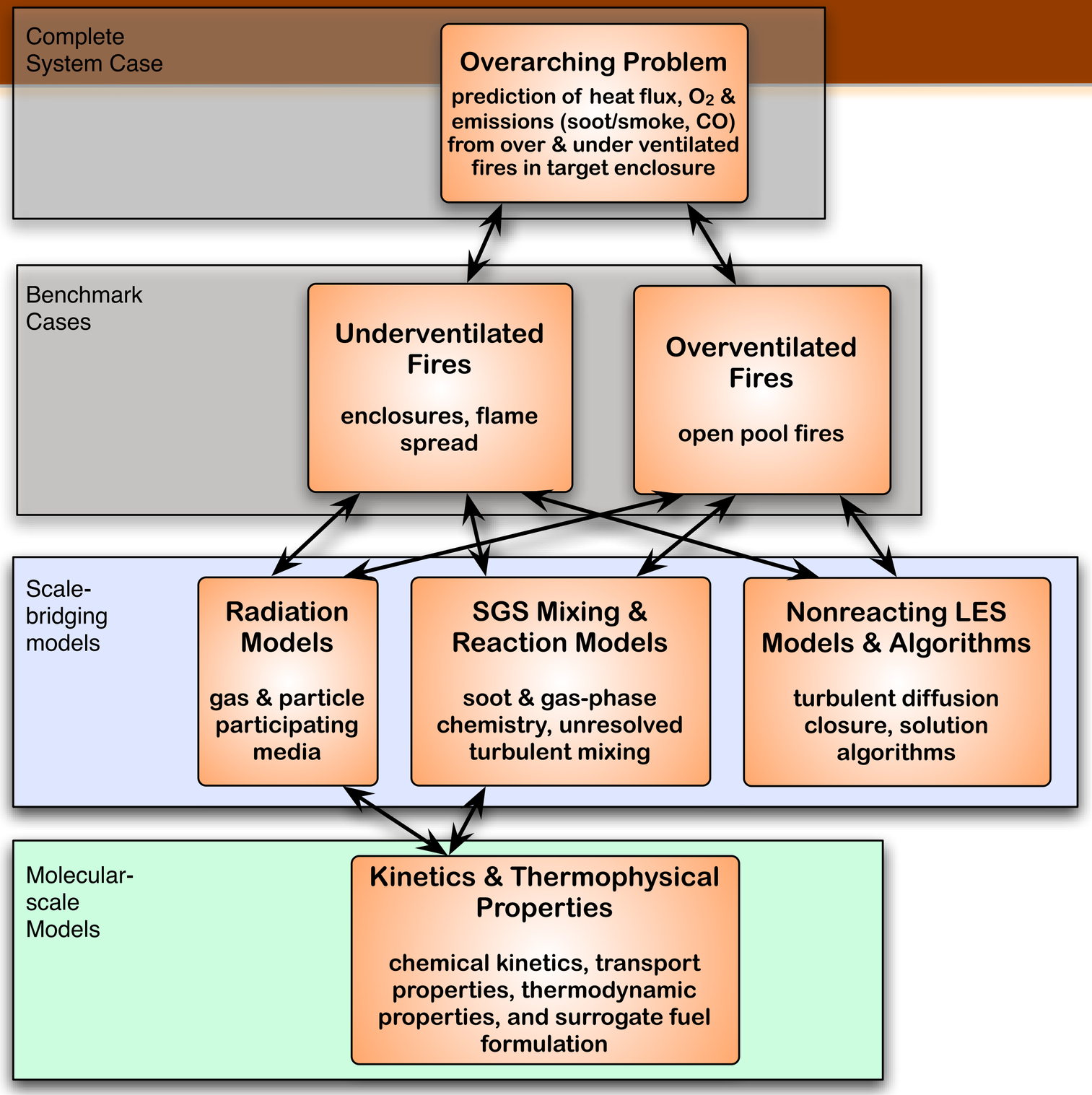
  - data: experiments & simulations
  - UQ/validation analysis
  - people
- UQ/Validation in each brick





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validation hierarchy

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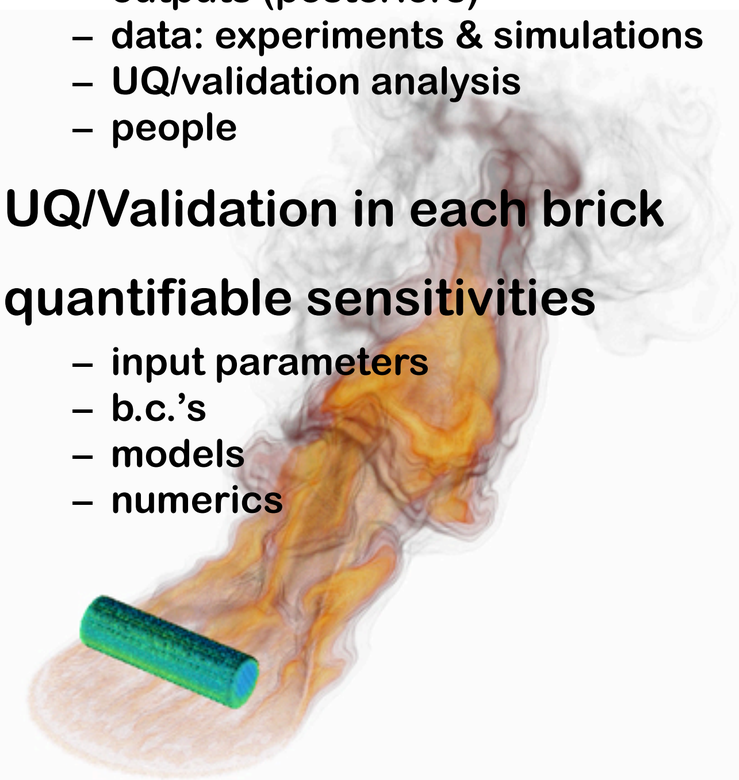
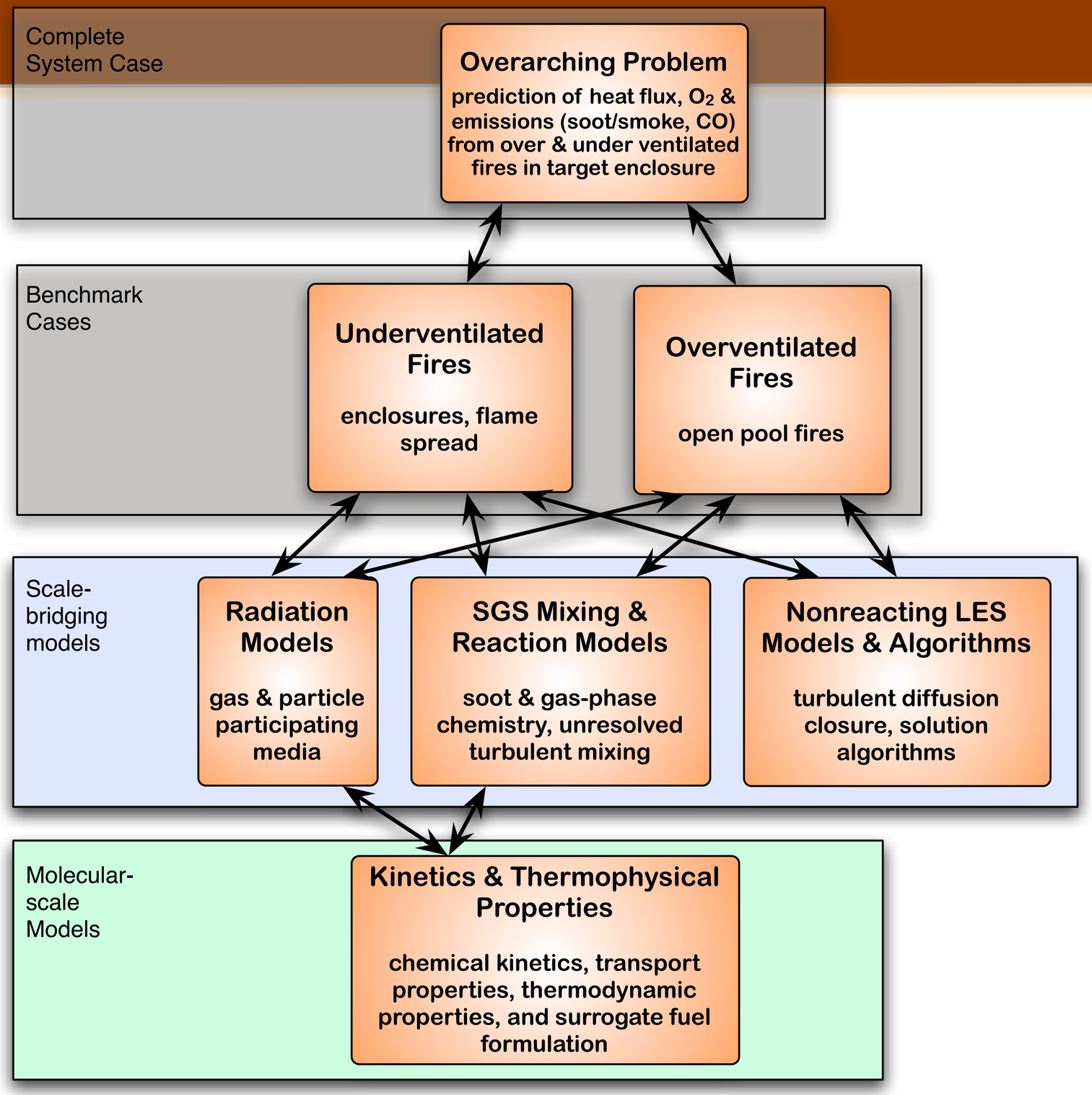
  - people
- UQ/Validation in each brick
- quantifiable sensitivities
  - input parameters
  - b.c.'s
  - models
  - numerics





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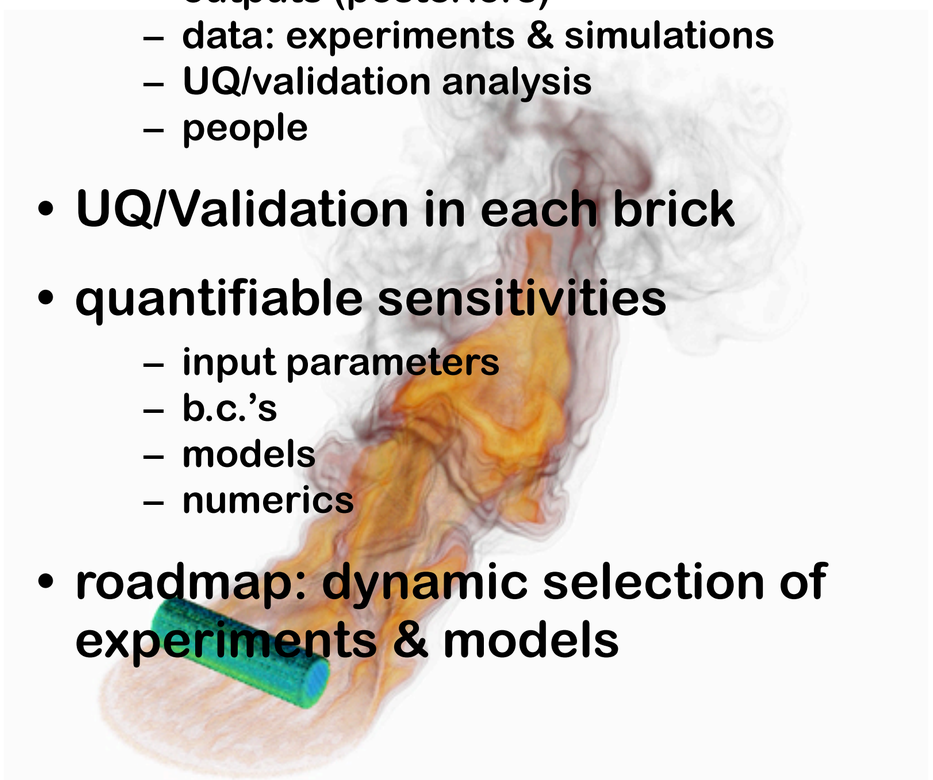
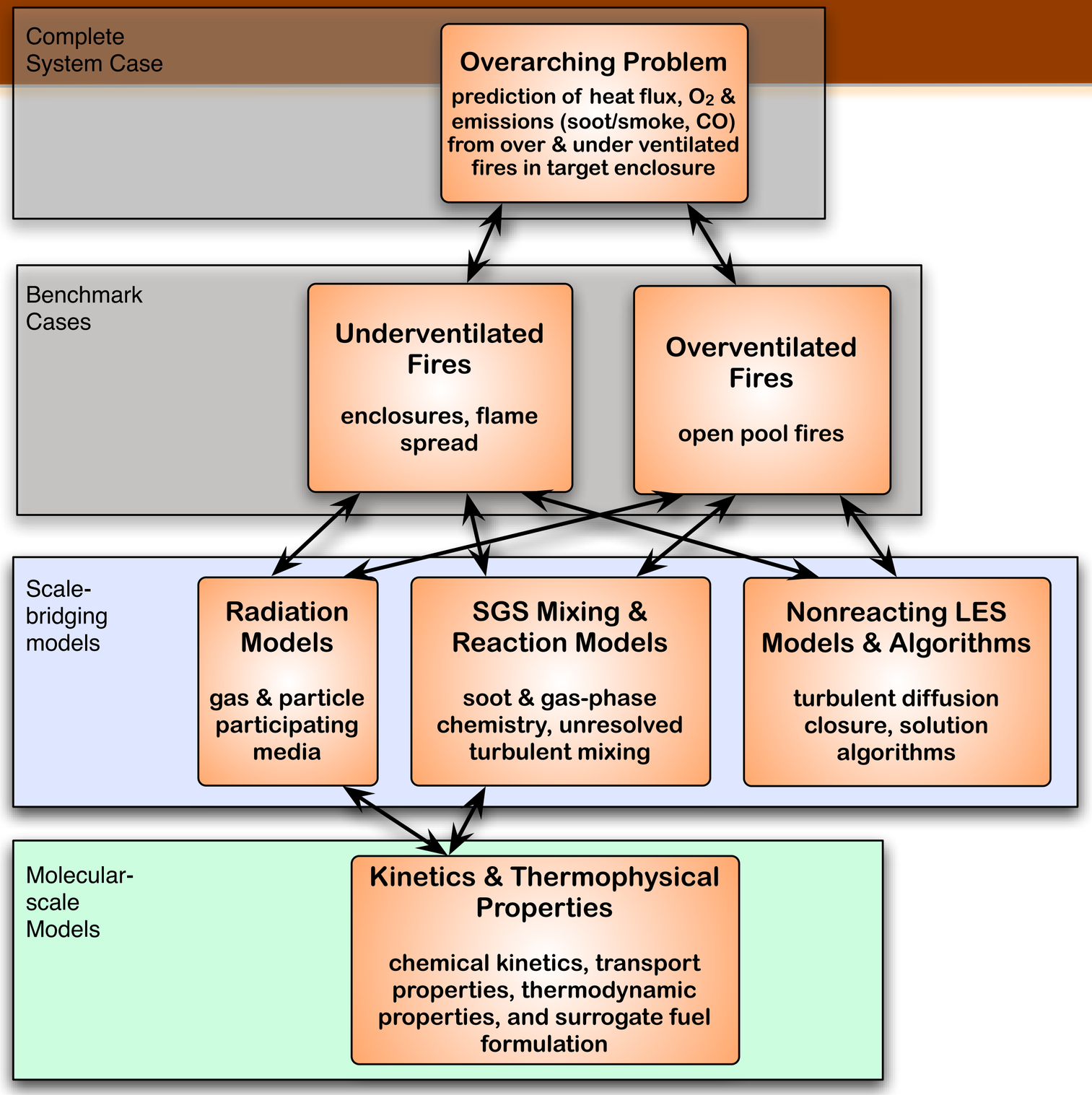
validation hierarchy

- driven by overarching problem (intended use of simulation)
- hierarchical coupling
- definition of each brick:
  - inputs (priors: new & inherited)
  - outputs (posteriors)
  - data: experiments & simulations
  - UQ/validation analysis
  - people
- UQ/Validation in each brick
- quantifiable sensitivities
  - input parameters
  - b.c.'s
  - models
  - numerics
- roadmap: dynamic selection of experiments & models





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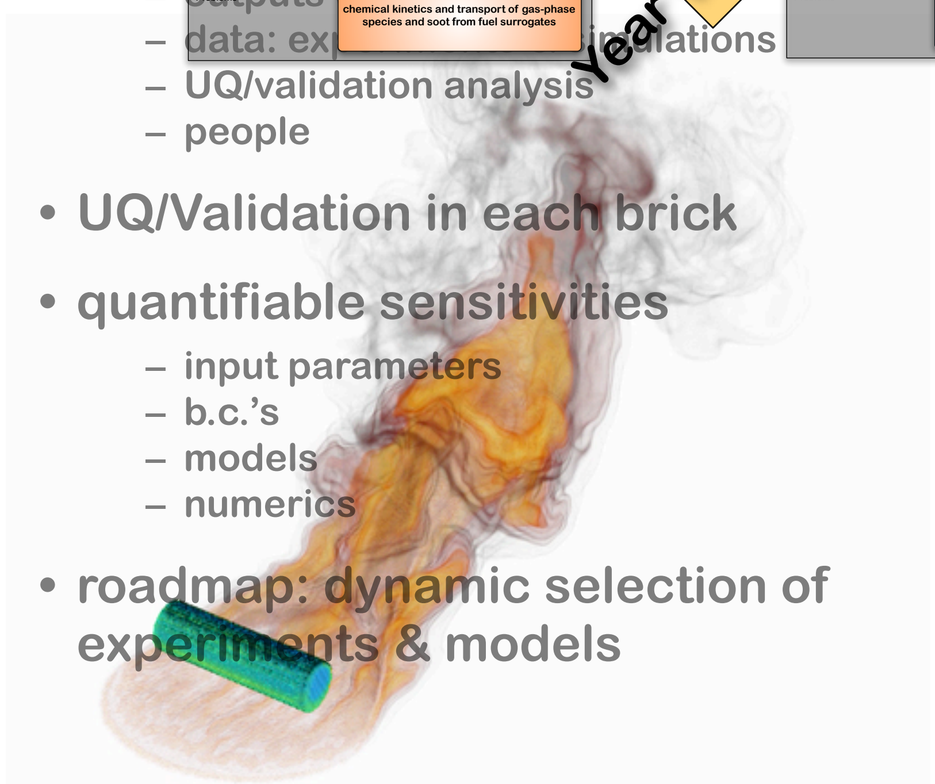
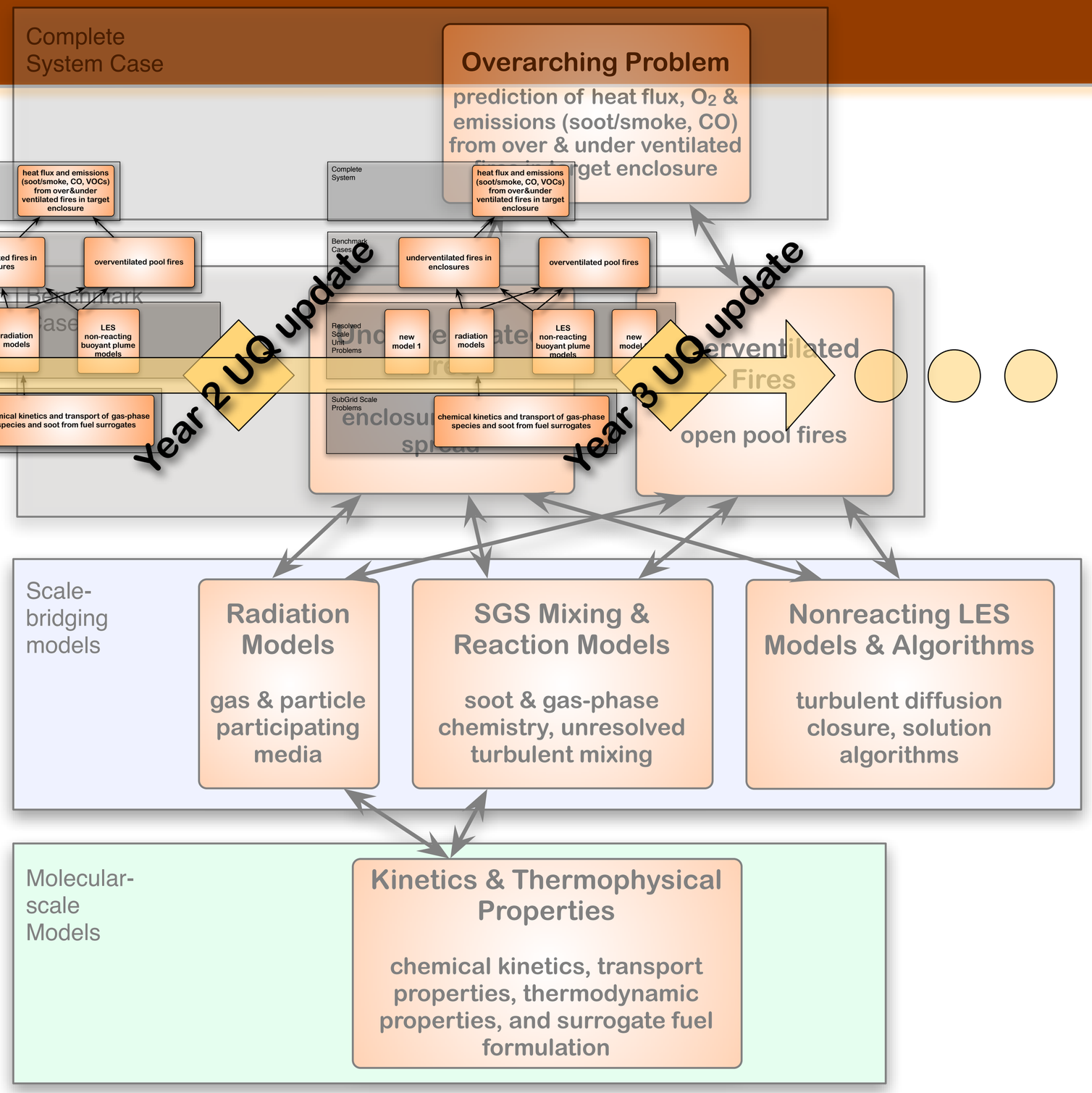
validation hierarchy

- driven by overarching problem (intended use of simulation)
- hierarchical building block approach
- definition of validation domain
  - inputs (priors: new & improved)
  - outputs
  - data: experiments & simulations
  - UQ/validation analysis
  - people
- UQ/Validation in each brick
- quantifiable sensitivities
  - input parameters
  - b.c.'s
  - models
  - numerics
- roadmap: dynamic selection of experiments & models





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validation hierarchy

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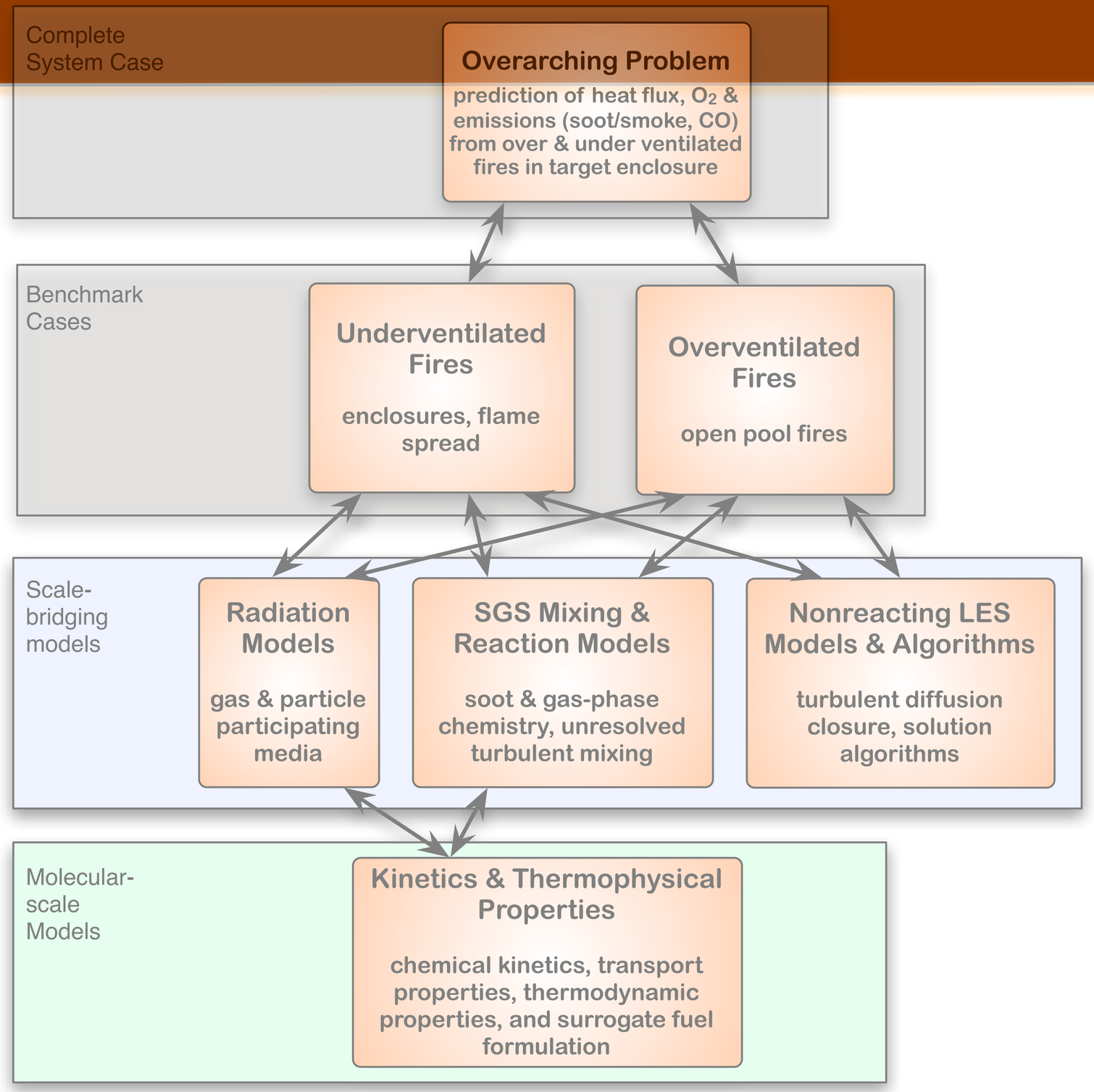
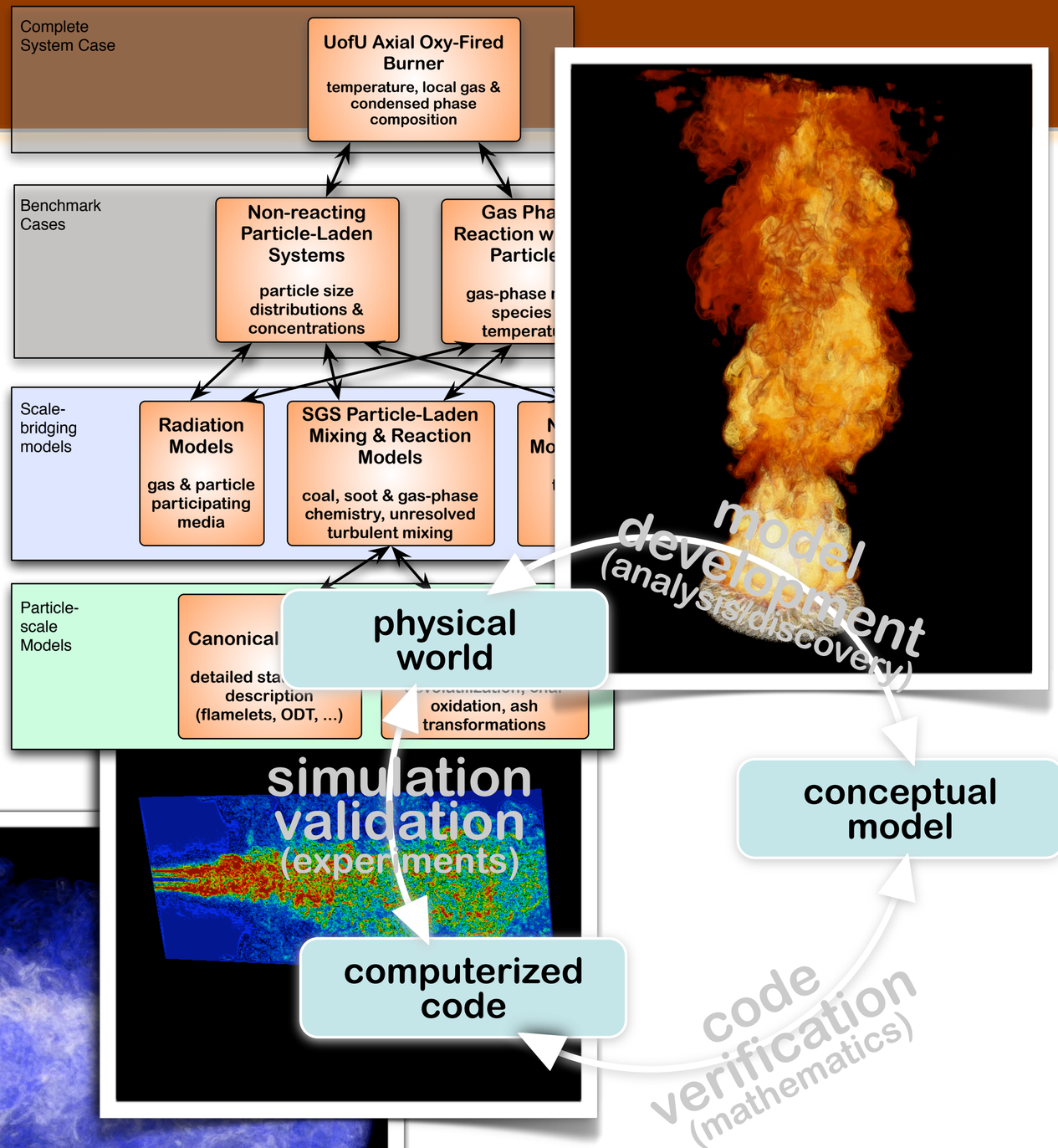
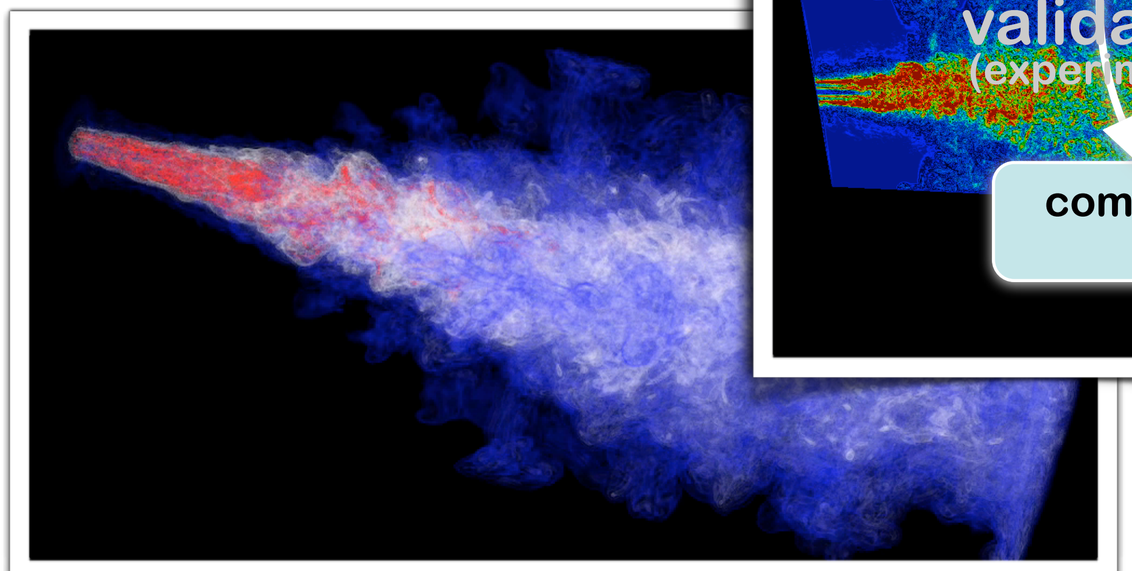


Conclusion

Leveraging Moore's Law for Chemical Reaction Engineering

- today's problems require V&V / uncertainty quantification for each prediction
- consistency requirements using all data (simulation & experimental)
- resolve more physics (i.e. LES)
- manifold methods for reduced dof models
- room for contributions





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