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Institute for CLEAN AND SECURE ENERGY THE UNIVERSITY OF UTAH

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NNSA National Nuclear Security Administration

CARBON CAPTURE MULTIDISCIPLINARY SIMULATION CENTER

http://ccmsc.utah.edu

objective

- CCMSC:
  - *demonstrate positive societal impact of extreme computing*
  - *accelerate the deployment of a new technology: high efficiency (AUSC), carbon capture for pulverized coal power generation*

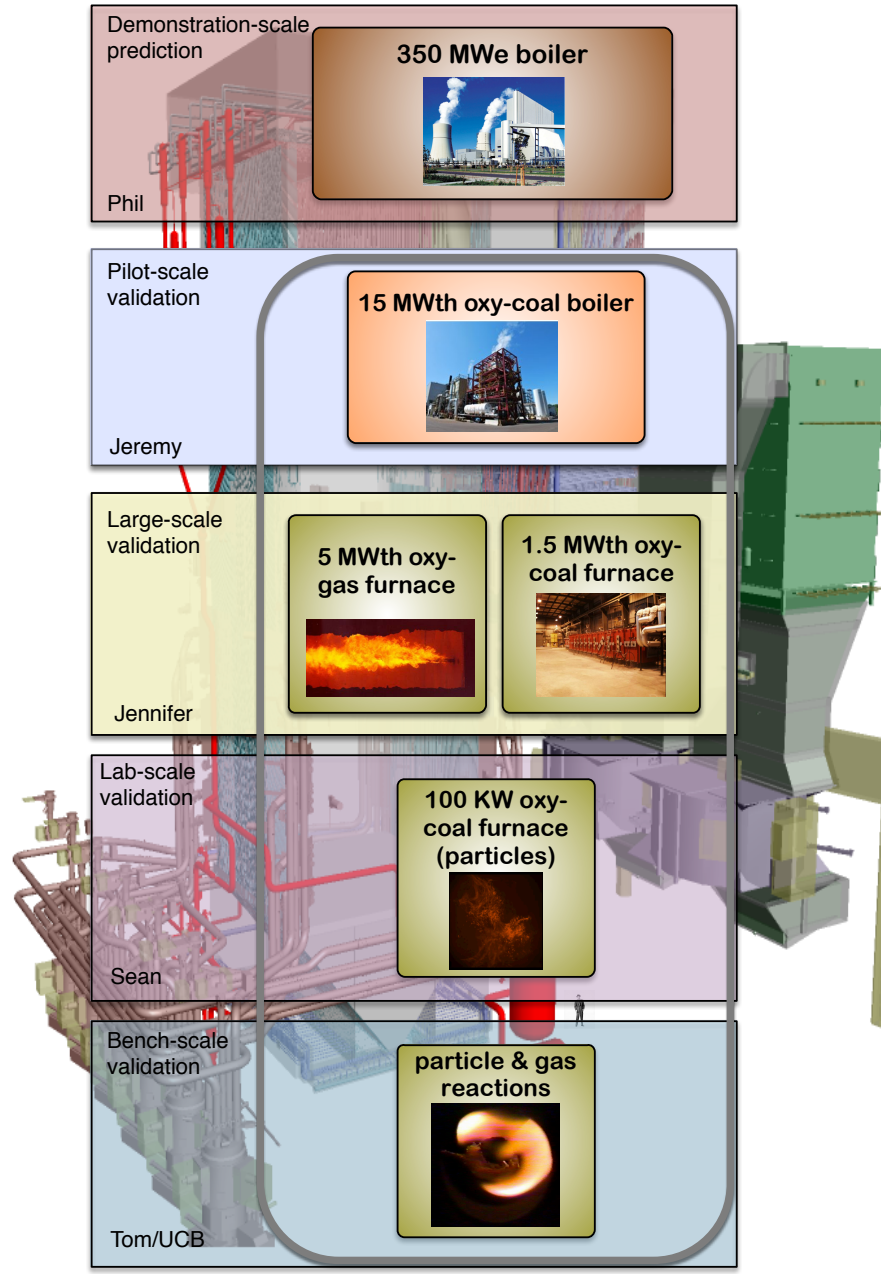
hierarchical validation

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

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

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

- strategy:
  - *industrial partners: (Alstom/GE, Thermal Engineering–Tshinghua China, Harding/consulting)*
  - *3 teams (CS,Physics,V/UQ) focused on one overarching predictive design w crosscutting components:*
    - *software engineering team*
    - *UQ hierarchy*
    - *annual re-evaluation of appropriate physics*



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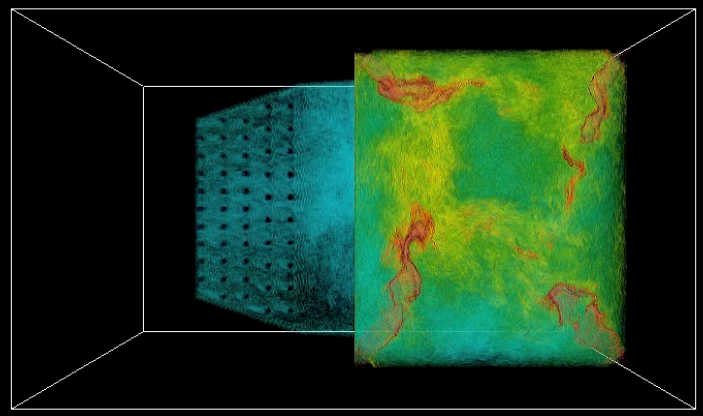
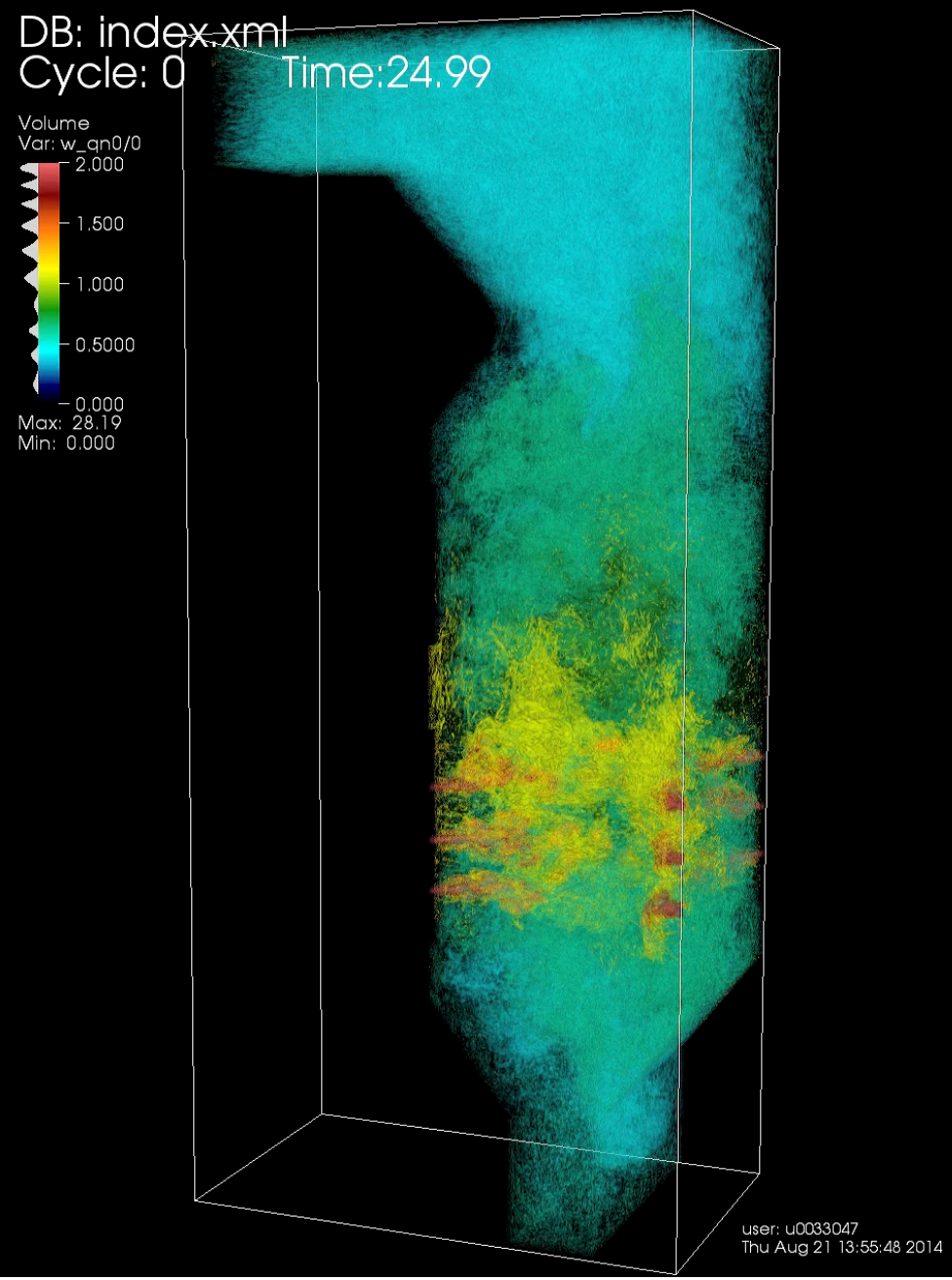
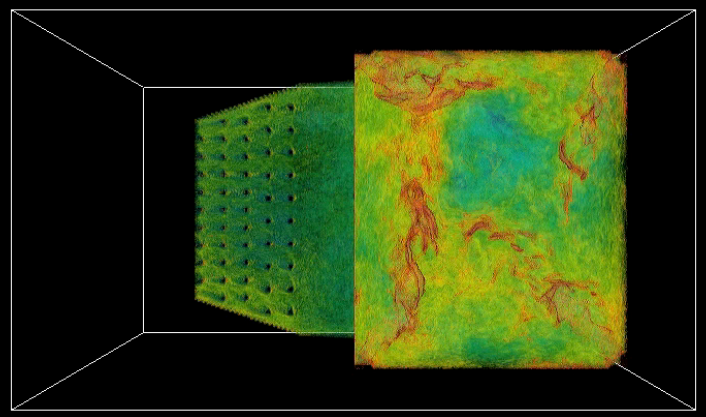
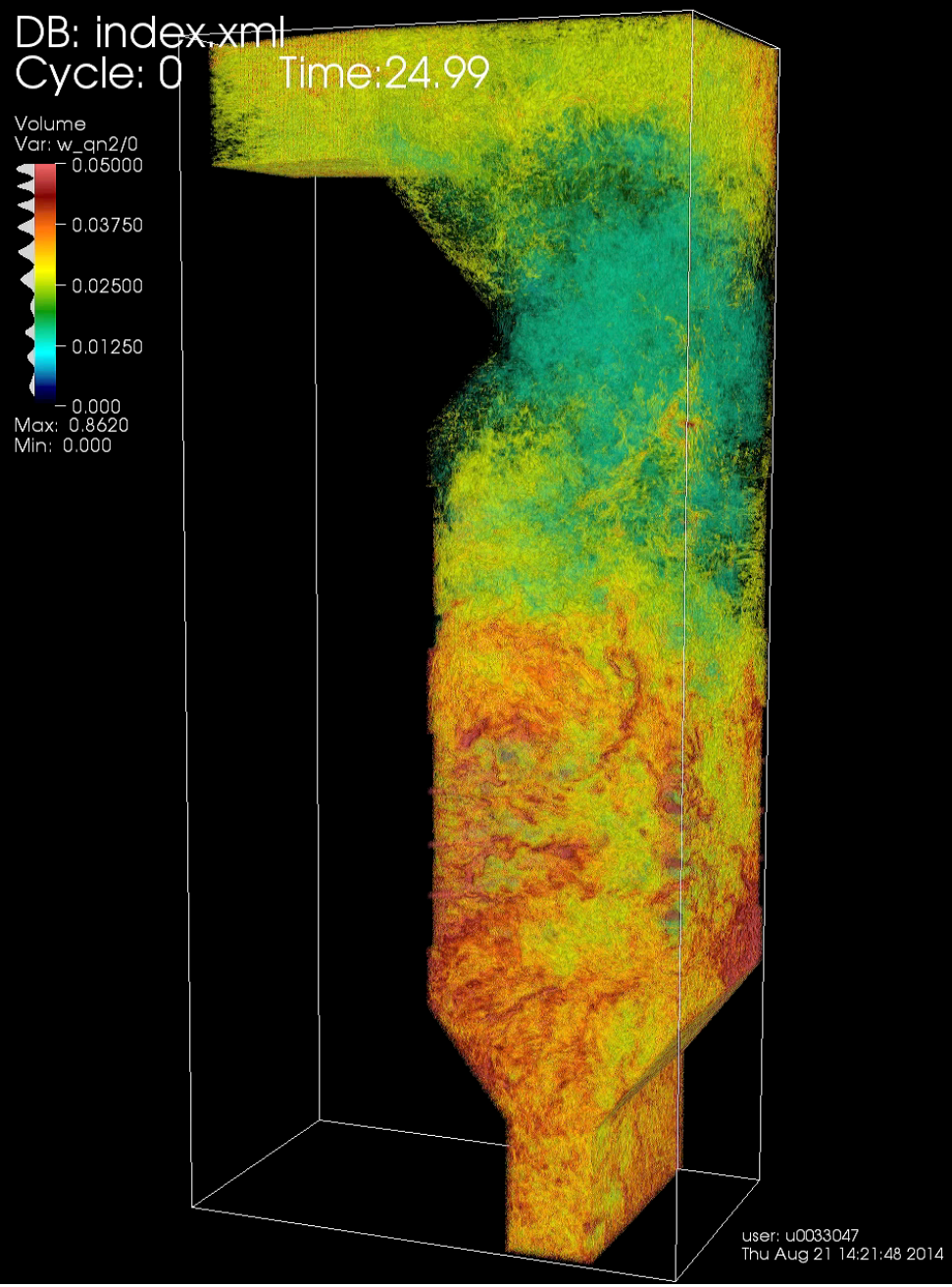




concentration of small particles





concentration of large particles

CCMSC

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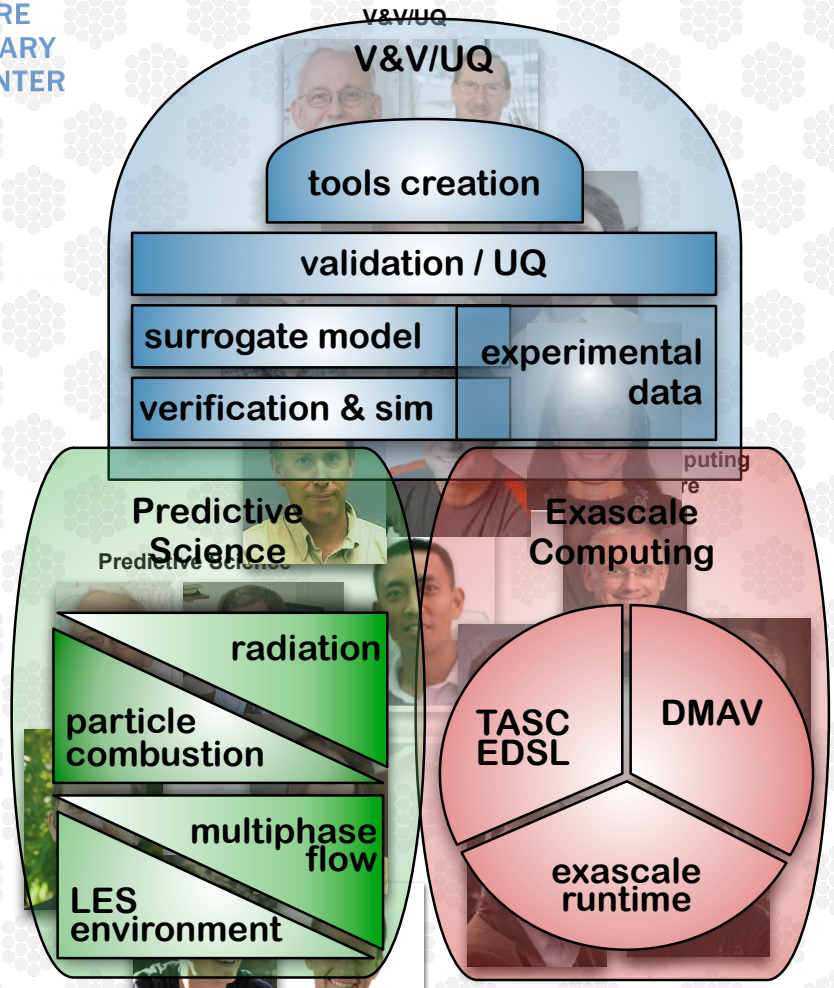
Executive Committee

Education and Outreach

year one accomplishments



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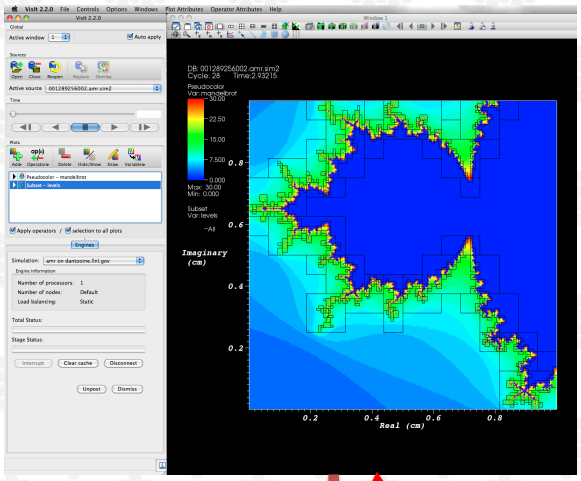
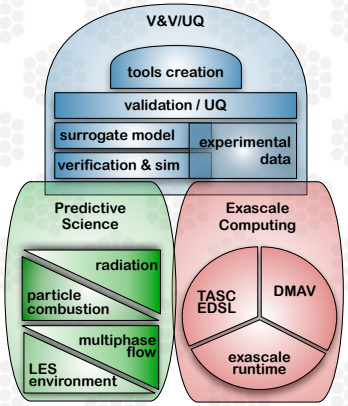
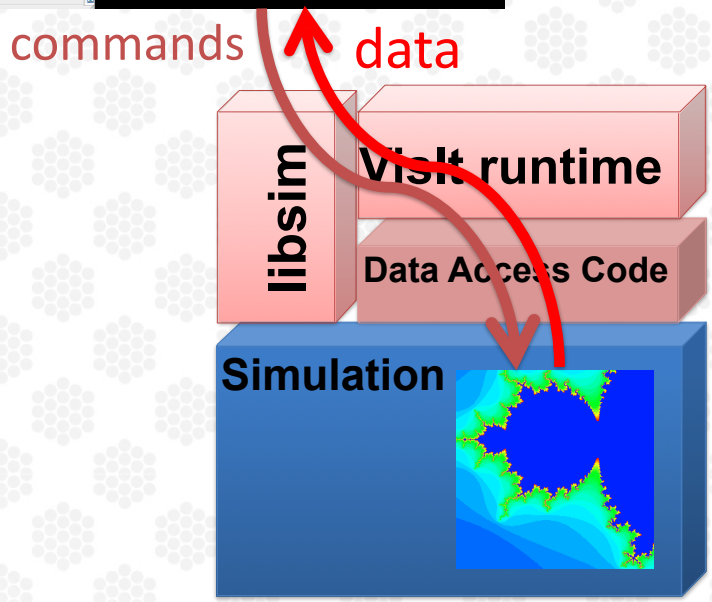
CS: VisIt-Uintah in-situ (*In–Progress*)

- Additions to Uintah to access VisIt's libsim library that simulations use for in-situ visualization.
  - *Call functions from Uintah that lets VisIt connect.*
  - *Add data access functions to Uintah that expose it's arrays as data that VisIt can process (i.e. database reader).*
  - *Link Uintah with VisIt's libsim.*

- Run the simulation and connect with VisIt.
  - *Libsim dynamically loads VisIt runtime into Uintah's address space.*
  - *Perform any of VisIt's operations on Uintah's run time simulation data.*
  - *Advance the simulation and the VisIt plots automatically update.*







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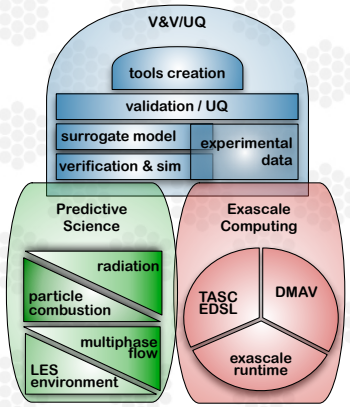
CS: Performant, expressive abstractions for present & future architectures



- C++ template metaprogramming to achieve one inlined grid loop, no temporaries.
- Compile-time consistency checking (field-operator and field-field compatibility).
- Deploys on Xeon Phi, CPU and GPU (CUDA).

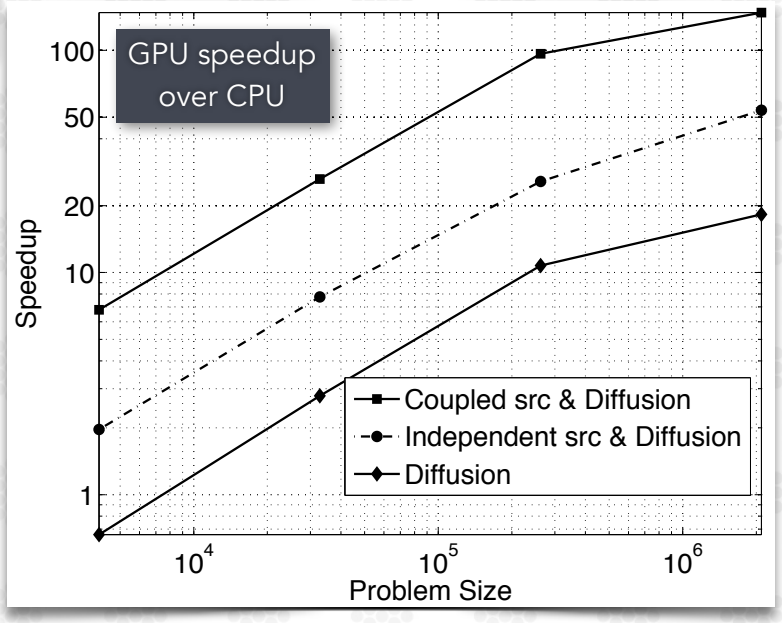
$$\phi = \nabla \cdot (\lambda \nabla T)$$

```
phi <<= divX( interpX(lambda) * gradX(temperature) )
      + divY( interpY(lambda) * gradY(temperature) )
      + divZ( interpZ(lambda) * gradZ(temperature) );
```

$$\frac{\partial \phi_i}{\partial t} = -\nabla \cdot \mathbf{J}_i + s_i$$

$$\mathbf{J}_i = -\Gamma \nabla \phi_i$$

$$s_i = f(\phi_i) \quad \text{or} \quad s_i = f(\phi_j)$$



Now being used in 5 PDE-solver projects within and without Uintah

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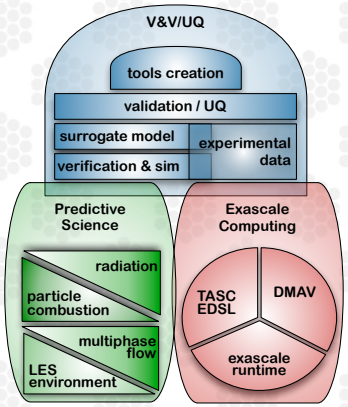
CS: Kokkos – Allocation Tracking

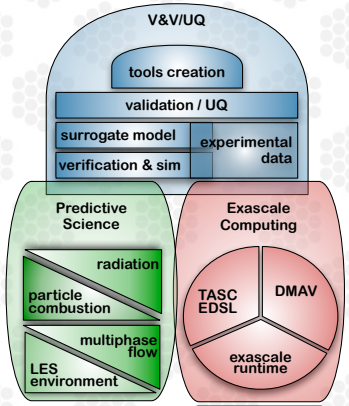


- Kokkos memory tracking HAD several limitations preventing Uintah integration
  - *Single master thread allocated/deallocated all memory*
  - *Tracking data structure not thread safe*
  - *O(log(n)) to find reference count and reference count not thread safe*
  - *O(n) to insert or delete an allocation record (sorted vector)*
  - *Poor support for memory not allocated by Kokkos*
  - *Unable to use texture cache with CUDA memory not allocated by Kokkos*

- Revised allocation tracking (code review Feb 6)
  - *Any host thread can allocate or deallocate memory*
  - *Lock-free data structure to manage allocation records*
  - *O(1) to find reference count and atomic reference count*
  - *O(1) to delete an allocation record; amortized O(1) to insert, O(n) worst case*
  - *Improved support for memory not allocated by Kokkos*
  - *Much easier to incrementally refactor code*
  - *Can use texture cache with CUDA memory not allocated by Kokkos*

- These changes remove design incompatibilities that prevents Uintah integration
- We will now investigate use of Kokkos in Uintah as an alternative to DSLs

CS: Uintah & VisIt Release Efforts



- Release Version 1.6.0 (1/30/2015)
  - *Wasatch/Nebo DSL now part of ARCHES component*
  - *Available/tested on multiple OS distributions: Debian, Ubuntu, Fedora, CentOS, OpenSuse, MacOSX*
  - *Installation (15 pgs) and User (300+ pgs) Manuals*
  - *Runs and scales on all major DOE & NSF platforms - Mira , Titan , Stampede Vulcan*

- Coordination with VisIt 2.9.0 release
  - *Uintah's data archive format database reader is now included in VisIt's build_visit script*

- Uintah is now part of the standard parallel binary builds of VisIt.
  - *VisIt with Uintah is being fully supported at DOE and other HPC sites.*
  - *Uintah users no longer build separate components to use VisIt.*
  - *Transfers build and support issues to the VisIt team.*
  - *Fully supports builds on multiple Linux systems e.g Debian Jessie, Fedora 21, Opensuse13.2,CentOS 7,Ubuntu 14.10*
  - *Includes new flexibility with Uintah's data archive format database reader.*

Physics: particles

Gas-Phase Transport

Mass Balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V_{\mathrm{cv}}} \rho \,\mathrm{d}V + \oint_{S_{\mathrm{cv}}} \rho \boldsymbol{u}\cdot\hat{\boldsymbol{n}}_{\mathrm{out}}\,\mathrm{d}S = 0$$

Momentum Balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V_{\mathrm{cv}}} \rho \boldsymbol{u} \,\mathrm{d}V + \oint_{S_{\mathrm{cv}}} (\rho \boldsymbol{u}\boldsymbol{u} - \boldsymbol{\tau})\cdot\hat{\boldsymbol{n}}_{\mathrm{out}}\,\mathrm{d}S = \int_{V_{\mathrm{cv}}} (\rho \boldsymbol{g} - \nabla p)\,\mathrm{d}V$$

Species Balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V_{\mathrm{cv}}} \rho f \,\mathrm{d}V + \oint_{S_{\mathrm{cv}}} (\rho \boldsymbol{u} f - D\nabla f)\cdot\hat{\boldsymbol{n}}_{\mathrm{out}}\,\mathrm{d}S = 0$$

Enthalpy Balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V_{\mathrm{cv}}} \rho h \,\mathrm{d}V + \oint_{S_{\mathrm{cv}}} (\rho \boldsymbol{u} h - k\nabla t + q_{\mathrm{rad}})\cdot\hat{\boldsymbol{n}}_{\mathrm{out}}\,\mathrm{d}S = 0$$

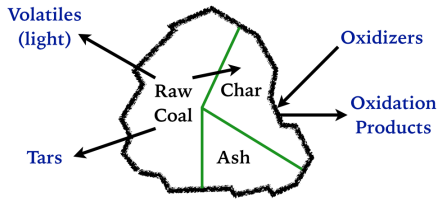
Coal

$$\eta \equiv \frac{m_{\mathrm{coal}}}{m_{\mathrm{primary}} + m_{\mathrm{secondary}} + m_{\mathrm{coal}}}$$

$$f_{\mathrm{p}} \equiv \frac{m_{\mathrm{primary}}}{m_{\mathrm{primary}} + m_{\mathrm{secondary}} + m_{\mathrm{coal}}}$$

$$f \equiv \frac{m_{\mathrm{primary}}}{m_{\mathrm{primary}} + m_{\mathrm{secondary}}}$$

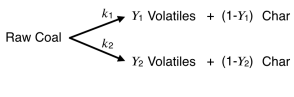
$$f_{\mathrm{p}} = (1-\eta) f$$



Radiation Transport

Discrete Ordinates

RMC Ray Tracing



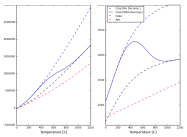
Heat Capacity

$$C_{\mathrm{p,coal}} = x_{\mathrm{rc}} C_{\mathrm{p,rc}} + x_{\mathrm{ch}} C_{\mathrm{p,ch}} + x_{\mathrm{ash}} C_{\mathrm{p,ash}}$$

$$C_{\mathrm{p,ash}} = 754 + 0.586(T - 273.15) \quad \left[\tfrac{\mathrm{J}}{\mathrm{kg\,K}}\right],$$

$$C_{\mathrm{p},i} = \frac{R}{M_{\mathrm{W},i}}\left[g_1\left(\frac{380}{T}\right) + 2g_1\left(\frac{1800}{T}\right)\right] \quad \left[\tfrac{\mathrm{J}}{\mathrm{kg\,K}}\right]$$

$$\text{where} \quad g_1(z) \equiv \frac{z^2\exp(z)}{[\exp(z)-1]^2} \quad (i \text{ is rc or ch})$$



Dispersed-Phase Transport

Lagrangian

Position, Velocity, Diameter, Enthalpy, Constituents

$$\frac{\mathrm{d}\boldsymbol{x}_p}{\mathrm{d}t} = \boldsymbol{v}_p \qquad \frac{\mathrm{d}\boldsymbol{x}_p}{\mathrm{d}t} = \boldsymbol{v}_p$$

$$\frac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} = \boldsymbol{a}_p \qquad \frac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} = \boldsymbol{a}_p$$

$$\frac{\mathrm{d}d_p}{\mathrm{d}t} = G_p \qquad \frac{\mathrm{d}\boldsymbol{\psi}_p}{\mathrm{d}t} = \boldsymbol{G}_{\psi,p}$$

$$\frac{\mathrm{d}h_p}{\mathrm{d}t} = q_p$$

$$\frac{\mathrm{d}m_{i,p}}{\mathrm{d}t} = n_{i,p}$$

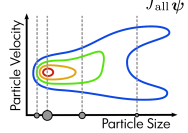
$$\vdots$$

runtime

Histograms, PDFs & NDFs:

$$\mathcal{N}(\boldsymbol{v},\boldsymbol{\psi};\boldsymbol{x},t) = m_0\, f_{V,\Psi}(\boldsymbol{v},\boldsymbol{\psi};\boldsymbol{x},t),$$

$$\text{where} \quad m_0(\boldsymbol{x},t) \equiv \int_{\text{all }\boldsymbol{\psi}}\int_{\text{all }\boldsymbol{v}} \mathcal{N}(\boldsymbol{v},\boldsymbol{\psi};\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{v}$$



Eulerian

Population Balance:

$$\frac{\partial \mathcal{N}}{\partial t} + \nabla_x(\boldsymbol{v}\mathcal{N}) + \nabla_v(\boldsymbol{a}\mathcal{N}) + \nabla_\psi(\boldsymbol{G}_\psi\mathcal{N}) = B - D + \mathbb{C}$$

$$\mu_{\boldsymbol{k}_v,\boldsymbol{k}_\psi}(\boldsymbol{x},t) \equiv \iint v_1^{k_{v,1}}\cdots\psi_1^{k_{\psi,1}}\cdots\mathcal{N}(\boldsymbol{v},\boldsymbol{\psi};\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{\psi}$$

Moment Transport:

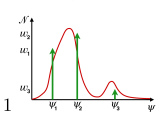
$$\frac{\partial}{\partial t}\left(\mu_{\boldsymbol{k}_v,\boldsymbol{k}_\psi}\right) + \nabla_x\left(\mu_{\boldsymbol{k}_v,\boldsymbol{k}_\psi}\right) - \overline{\boldsymbol{a}}_{\boldsymbol{k}_{v-1},\boldsymbol{k}_\psi} - \overline{\boldsymbol{G}}_{\psi,\boldsymbol{k}_v,\boldsymbol{k}_{\psi-1}} = \overline{B}_{\boldsymbol{k}_v,\boldsymbol{k}_\psi} - \overline{D}_{\boldsymbol{k}_v,\boldsymbol{k}_\psi} + \overline{\mathbb{C}}_{\boldsymbol{k}_v,\boldsymbol{k}_\psi}$$

Quadrature Methods:
(avoiding ad hoc closures)

$$\mu_k = \sum_{i=1}^{N_{\mathrm{env}}} w_i \psi_i^k$$

...exact for:

$$k = 0, 1, \ldots, 2N_{\mathrm{env}} - 1$$



$$\int g(\psi)\mathcal{N}\,\mathrm{d}\psi \approx \sum_{i=1}^{N_{\mathrm{env}}} w_i g(\psi_i)$$

- Higher-order moment closure (3-15),
- Cross moments for coupling of properties,
- Easier for non-diffusive problems.

Devolatilization

Single Reaction:

$$S_{\mathrm{rc}} = -r, \quad S_{\mathrm{vol}} = Yr \quad S_{\mathrm{ch}} = (1-Y)r$$

$$r = A\exp\left(\frac{-E_a}{RT}\right) m_{\mathrm{rc}}$$

Two Competing Reactions:

$$S_{\mathrm{rc}} = -(r_1 + r_2), \quad S_{\mathrm{vol}} = Y_1 r_1 + Y_2 r_2, \quad S_{\mathrm{ch}} = (1-Y_1)r_1 + (1-Y_2)r_2$$

$$r_n = A_n \exp\left(\frac{-E_{a,n}}{RT}\right) m_{\mathrm{rc}}$$

Yamamoto:

$$S_{\mathrm{rc}} = -r, \quad S_{\mathrm{vol}} = Yr, \quad S_{\mathrm{ch}} = (1-Y)r$$

$$r = FA\exp\left(\frac{-E_a}{RT}\right) m_{\mathrm{rc}}$$

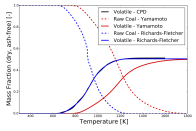
$$F = \exp\left(\sum_{i=0}^{5} c_i G^i\right), \quad \text{where} \quad G \equiv \frac{m_{\mathrm{rc},0} - m_{\mathrm{rc}}}{m_{\mathrm{rc},0}}$$

Richards-Fletcher:

$$S_{\mathrm{rc}} = -(r_1 + r_2), \quad S_{\mathrm{vol}} = Y_1 r_1 + Y_2 r_2, \quad S_{\mathrm{ch}} = (1-Y_1)r_1 + (1-Y_2)r_2$$

$$r_n = F_n A_{\mathrm{a},n} \exp\left(\frac{-E_{\mathrm{a},n}}{RT}\right) m_{\mathrm{rc}}$$

$$F_n = \exp\left(\sum_{i=0}^{5} c_{n,i} G^i\right), \quad \text{where} \quad G \equiv \frac{m_{\mathrm{rc},0} - m_{\mathrm{rc}}}{m_{\mathrm{rc},0}}$$



Char Oxidation

$$r_{\mathrm{ch.\,ox.}} = A\exp\left(\frac{-E_a}{RT_p}\right) p_{\mathrm{O_2},s}^n$$

$$y_{\mathrm{O_2},s} = \gamma + (y_{\mathrm{O_2},\infty} - \gamma)\exp\left(\frac{-r_{\mathrm{ch.\,ox.}}\, d_p}{2CD_{\mathrm{O_2}}}\right),$$

$$\text{where} \quad \gamma = OF - 1, \quad OF = \tfrac{1}{2}(1+\psi),$$

$$\psi = \frac{r_0}{1+r_0}, \quad r_0 = A_0\exp\left(\frac{-E_{a,0}}{RT_p}\right) p_{\mathrm{O_2},s}^{n_0}$$

Transport Moments / Transport Weights & Abscissas

Single Property

QMOM
...with exact moment-inversion algorithm

Multiple Properties

CQMOM
...with approx. moment-inversion algorithm

DQMOM
...with linear solve difficult to avoid a singular system

Drag

$$\frac{\boldsymbol{F}_p}{m_p} = \left(\Theta_v \frac{f_{\mathrm{drag}}}{\tau_p}(\boldsymbol{u} - \boldsymbol{v}_p) + \frac{\boldsymbol{g}(\rho_p - \rho_{\mathrm{fl}})}{\rho_p}\right)$$

$$\tau_p \equiv \frac{\rho_p d_p^2}{18\mu_{\mathrm{fl}}} \qquad Re_p \equiv \frac{\rho_{\mathrm{fl}} d_p |\boldsymbol{u} - \boldsymbol{v}_p|}{\mu_{\mathrm{fl}}}$$

$$f_{\mathrm{drag}} = \begin{cases} 1 + 0.15 Re_p^{0.687}, & \text{when } Re_p < 994 \\ 0.0183 Re_p, & \text{otherwise} \end{cases}$$

Heat Flux

$$\boldsymbol{q}_{\mathrm{rad}} = K_{\mathrm{abs},p}(\boldsymbol{I} - \sigma T_p^4)$$

$$q_{\mathrm{conv}} = \Theta_T A h (T_{\mathrm{fl}} - T_p)$$

$$h = \frac{k\,Nu}{d_p}$$

$$Nu = 2.0 + (0.4 Re_p^{1/2} + 0.06 Re_p^{2/3}) Pr^{0.4}$$

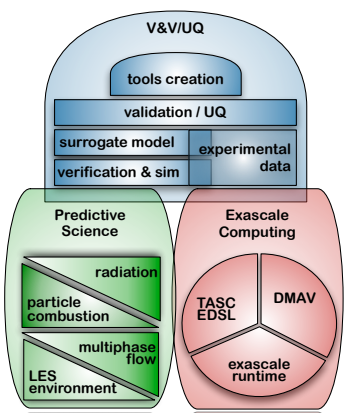
$$q_{\mathrm{rxn}} = \Delta h_{\mathrm{rxn}} r_{\mathrm{ch.\,ox.}}$$

Blowing

$$\Theta_T \equiv \frac{h^\bullet}{h}, \quad \Theta_v \equiv \frac{f_{\mathrm{drag}}^\bullet}{f_{\mathrm{drag}}}$$

$$\Theta = \frac{\phi}{\exp(\phi) - 1}$$

$$\phi_T = \frac{n_p C_{\mathrm{p}}}{h}, \quad \phi_v = \frac{n_p}{\frac{1}{2}\rho_{\mathrm{fl}} f_{\mathrm{drag}} |\boldsymbol{u} - \boldsymbol{v}_p|}$$



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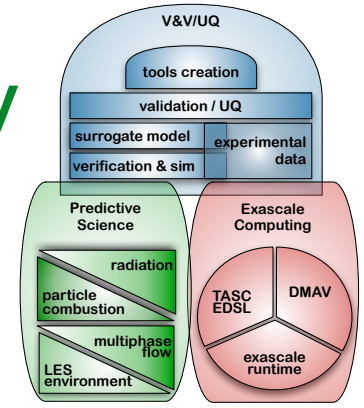
Predictive Science - Multi-Phase Flow
CCMSC: Fall TST
Sean Smith, AbouAbbas, John "Mike" Parra-Alvarez

- Avoid equations in presentations, ...but sometimes unavoidable.

- Notation and variable definitions

Physics: Devolatilization Model Form Uncertainty



- Model Form Uncertainty by design
  - *form and physics apropos to multi-physics simulation*
  - *same uncertain parameter across hierarchy*

- model form 1: CPD
  - *'gold standard' but complex*
  - *13 uncertain parameters + 5 coal specific parameters*
  - *limited to low temperature data (< 1200K)*

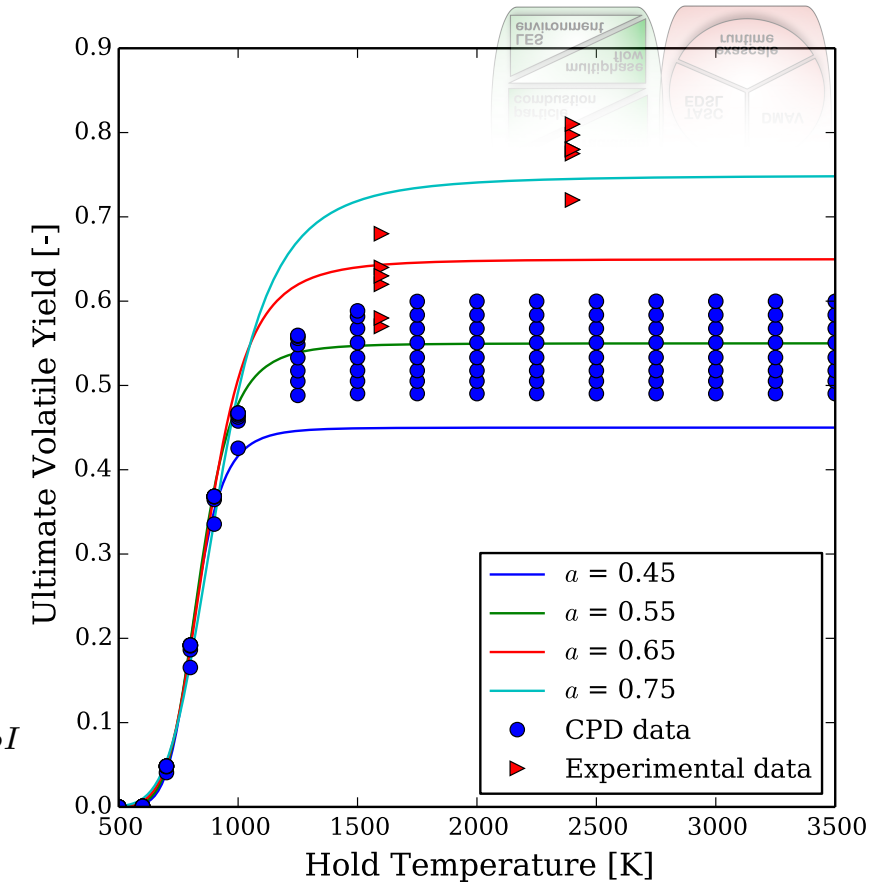
- model form 2': FOWY
  - *1 free parameter (a) per coal type*

$$\frac{\mathrm{d}V}{\mathrm{d}t} = A \exp\left(\frac{-(E_0 + \sigma_a Z)}{T_P}\right)(V_f - V)$$

- utilize V/UQ with consistency constraint
  - *year 1: use CPD and 1 high T expt. data set*
  - *satisfying 30 quantities of interest (QoI)*
  - *DOE with 5 final temperatures and 3 heating rates*
  - *year 2 & beyond: add all available experimental data*

$$(1-\gamma)l_i \leq M_i(\mathbf{x}) - d_i \leq (1-\gamma)u_i \qquad \text{for } i = 1, ..., N_{QoI}$$

$$\beta_p \geq x_p \geq \alpha_p \qquad \text{for } i = 1, ..., n$$



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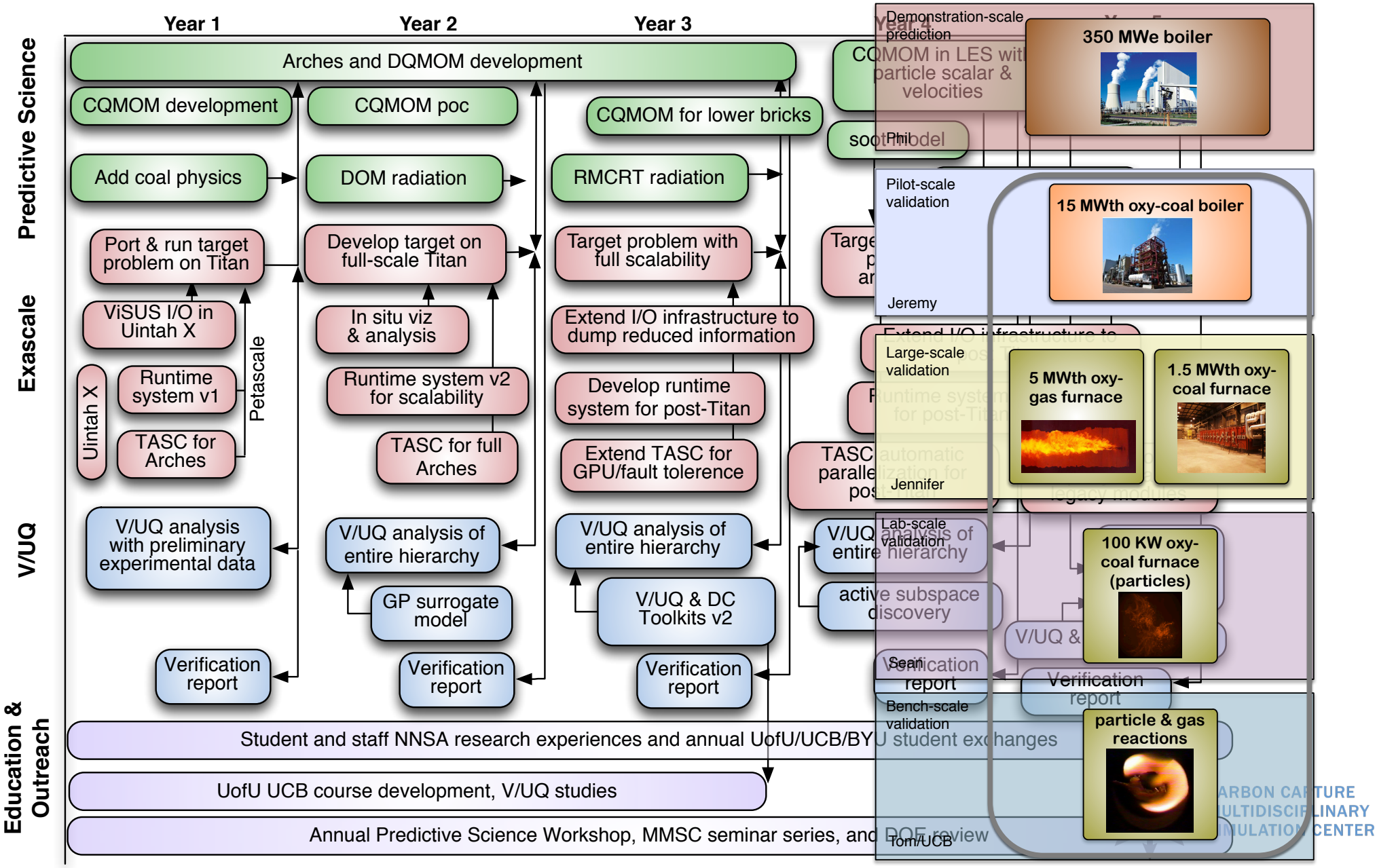
Year 1
Year 2
Year 3
Predictive Science
Exascale
V/UQ
Education & Outreach
Arches and DQMOM development
CQMOM development
CQMOM poc
CQMOM for lower bricks
Add coal physics
DOM radiation
RMCRT radiation
Port & run target problem on Titan
Develop target on full-scale Titan
Target problem with full scalability
ViSUS I/O in Uintah X
In situ viz & analysis
Extend I/O infrastructure to dump reduced information
Uintah X
Runtime system v1
Petascale
Runtime system v2 for scalability
Develop runtime system for post-Titan
TASC for Arches
TASC for full Arches
Extend TASC for GPU/fault tolerence
V/UQ analysis with preliminary experimental data
V/UQ analysis of entire hierarchy
V/UQ analysis of entire hierarchy
GP surrogate model
V/UQ & DC Toolkits v2
Verification report
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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
Demonstration-scale prediction
350 MWe boiler
Phil
Pilot-scale validation
15 MWth oxy-coal boiler
Jeremy
Large-scale validation
5 MWth oxy-gas furnace
1.5 MWth oxy-coal furnace
Jennifer
Lab-scale validation
100 KW oxy-coal furnace (particles)
Sean
Bench-scale validation
particle & gas reactions
Tom/UCB

physical attributes:

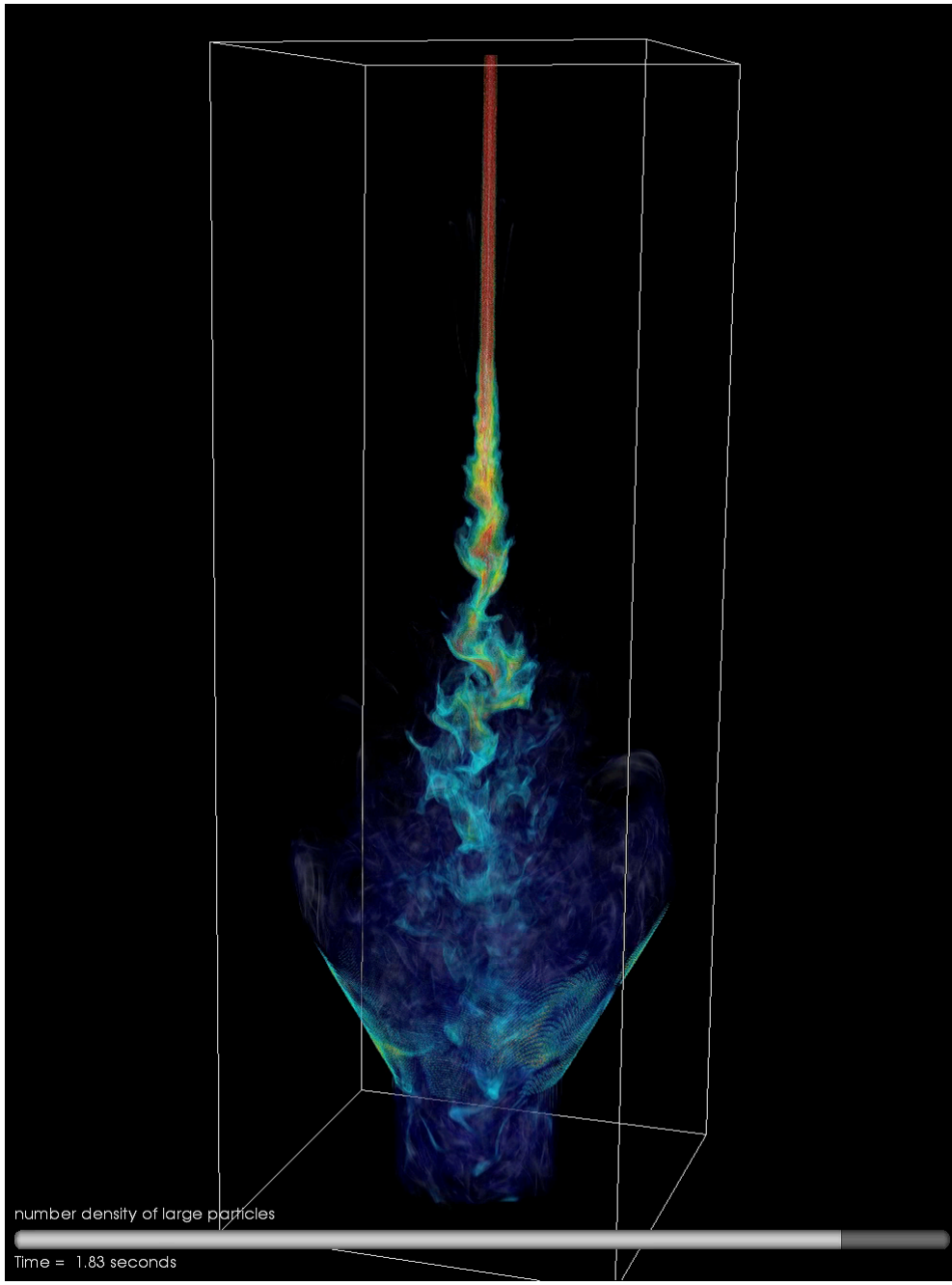
- 0.6x0.6x1.7m (1/220 BSF) (1/15,800 prediction)
- Primary inlet:
  -coal feed rate = 1.058e-3 kg/s,
  -carrier gas = 1.79e-3 kg/s, 0.838 CO_2 + 0.162 O_2
- Secondary inlet:
  -gas = 2.079 kg/s, pure O_2
- Purge (radiometer-CO_2) inlet:
  -gas = 2.856e-4 kg/s pure CO_2
- SUFCO coal (UT) particle sizes = 20 (65%),50 (25%),100 (10%) microns
- 100 KWt

model attributes:

- radiation: S_8 (once every 30 time steps)
- DQMOM with 7 internal coordinates (3 quadrature nodes)
- The FOWY devolatilization model
- Murphy-Shaddix (2005) char oxidation model

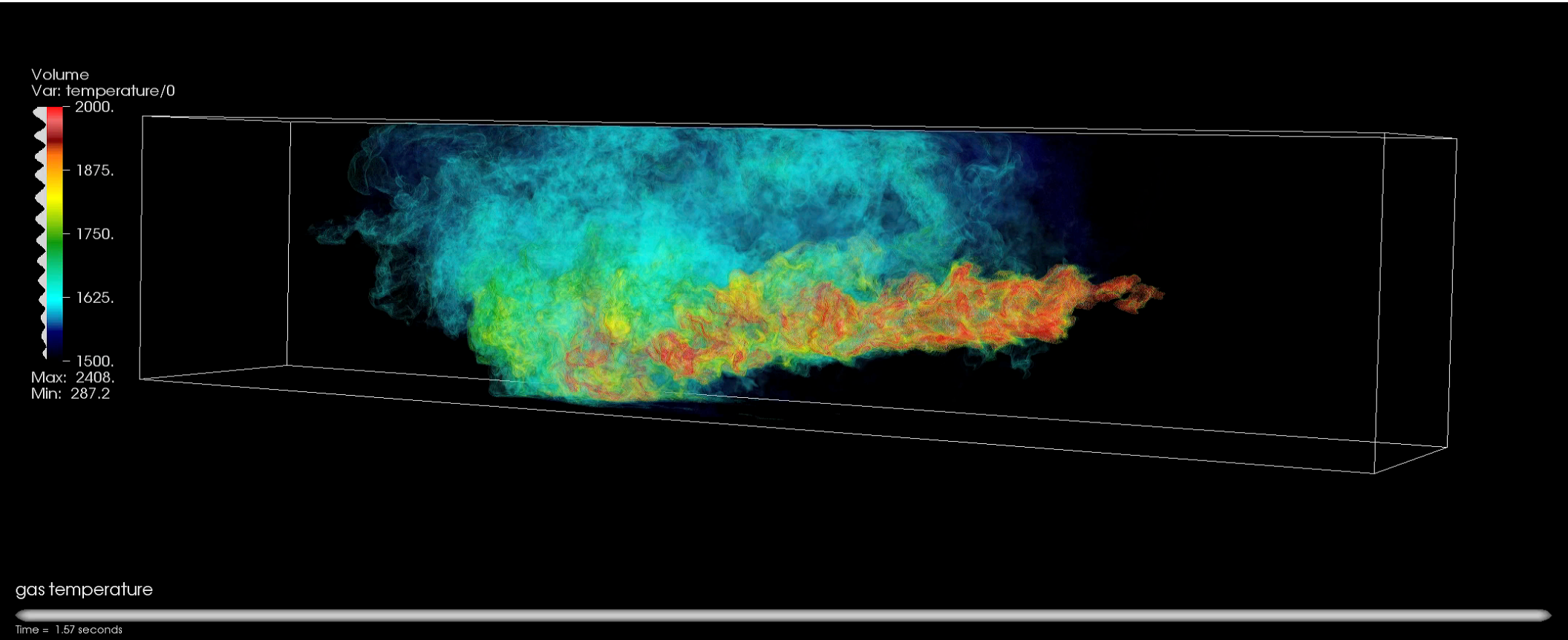
numerical attributes:

- $(2mm)^3$ resolution producing 65 million cells
- ~85 microsecond time steps
- 35% volume wasted on intrusions
- 20^3 cells/patch
- Vulcan: cases failed to run on 9 different occasions due to bad nodes or writing errors, with 25 successful 12 hour runs (26.5% failure). (these running errors only seen on psmall partition of vulcan)

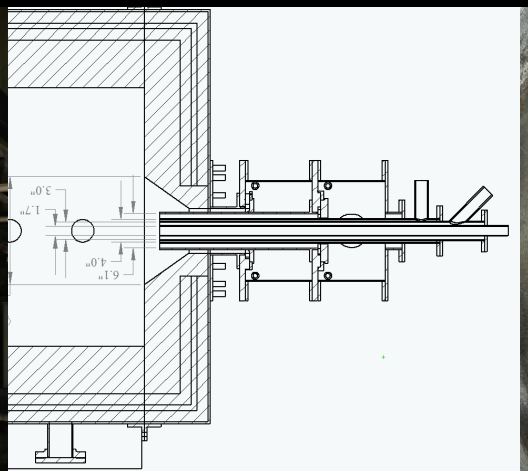


CARBON CAPTURE
MULTIDISCIPLINARY
SIMULATION CENTER

OFC


Volume
Var: temperature/0
2000.
1875.
1750.
1625.
1500.
Max: 2408.
Min: 287.2
gas temperature
Time = 1.57 seconds

CARBON CAPTURE
MULTIDISCIPLINARY
SIMULATION CENTER
L1500



physical attributes:

- simulation 4 boxes:
  - 1.36m, 1.44m, 3.36m
  - 9.44m, 2.88m, 3.36m
  - 0.90m, 3.60m, 3.36m
  - 1.36m, 5.76m, 3.36m
- s80 inlets, the corner coal injectors, and O_2/RFG streams
- various injection angles
- 3 platens, 20 u-tubes, 38 tube bundles
- 15 MWt (German lignite)

model attributes:

- radiation: S_8 (once every 15 time steps)
- DQMOM with 7 internal coordinates (particle size distribution changed)
- The FOWY devolatilization model
- Murphy-Shaddix (2005) char oxidation model
- Wall heat transfer computed with thickness and thermal conductivity (UQ)

numerical attributes:

- $1cm^3$ resolution producing 137million cells
- 20^3 cells/patch (17^3 cells/patch)
- 16,384 cores (Titan & Vulcan)
- target machine Vulcan & Titan (memory issues)

V/UQ:

- we have performed more V/UQ analysis on this cases
- paper presented at recent Industrial Combustion (AFRC) mtg.
- currently working on refined V/UQ pass

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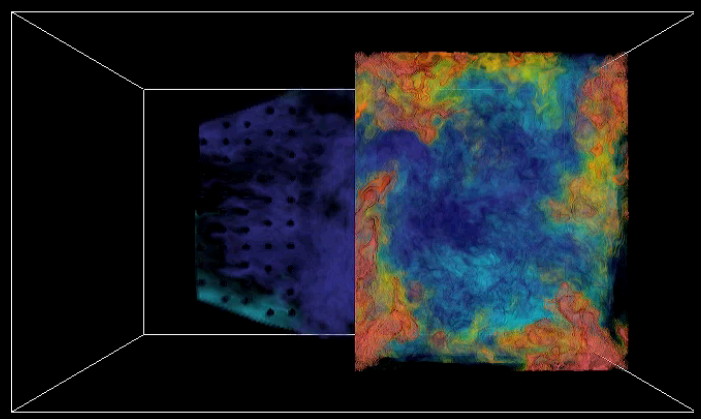
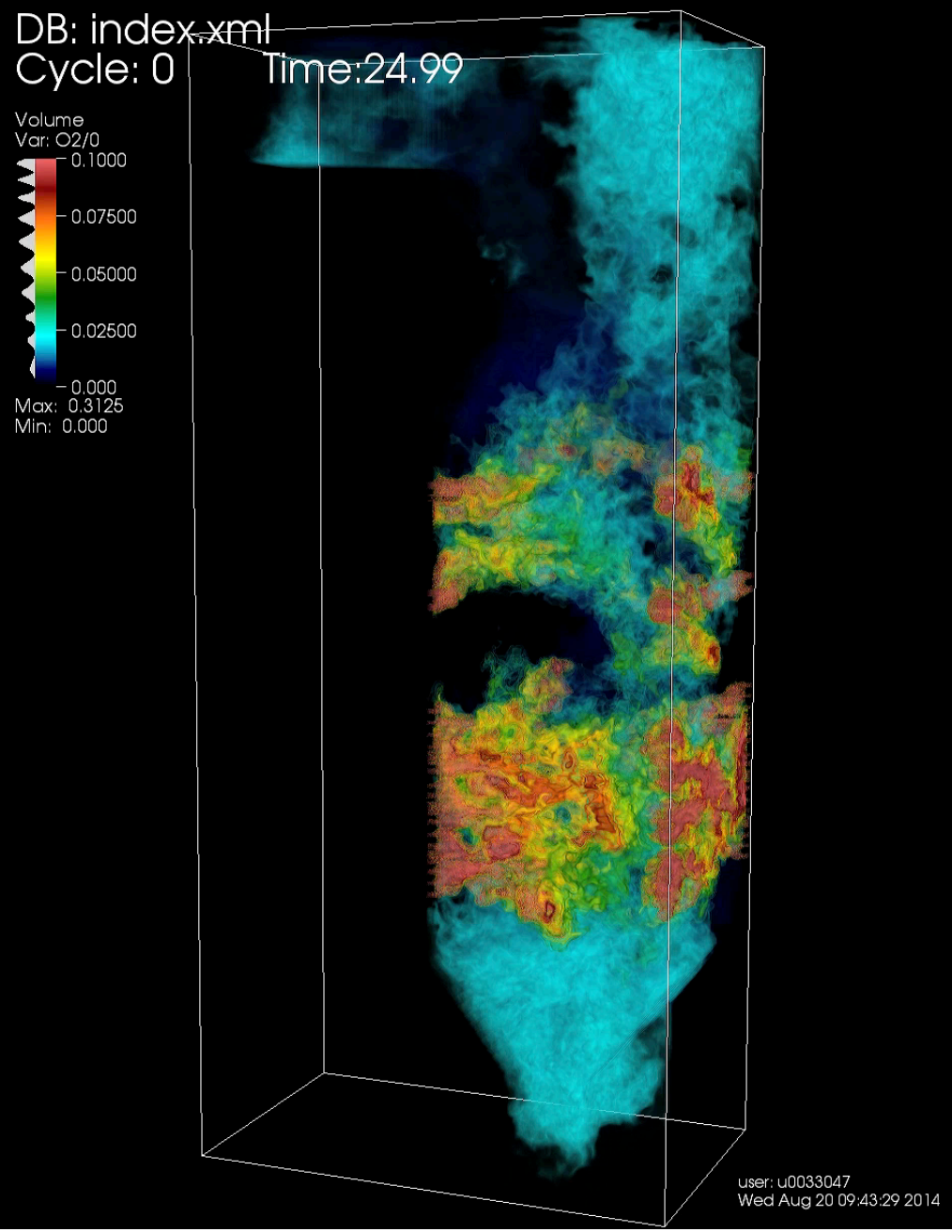
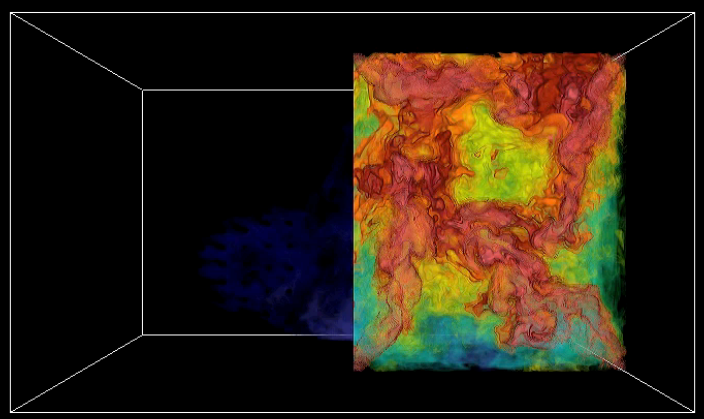
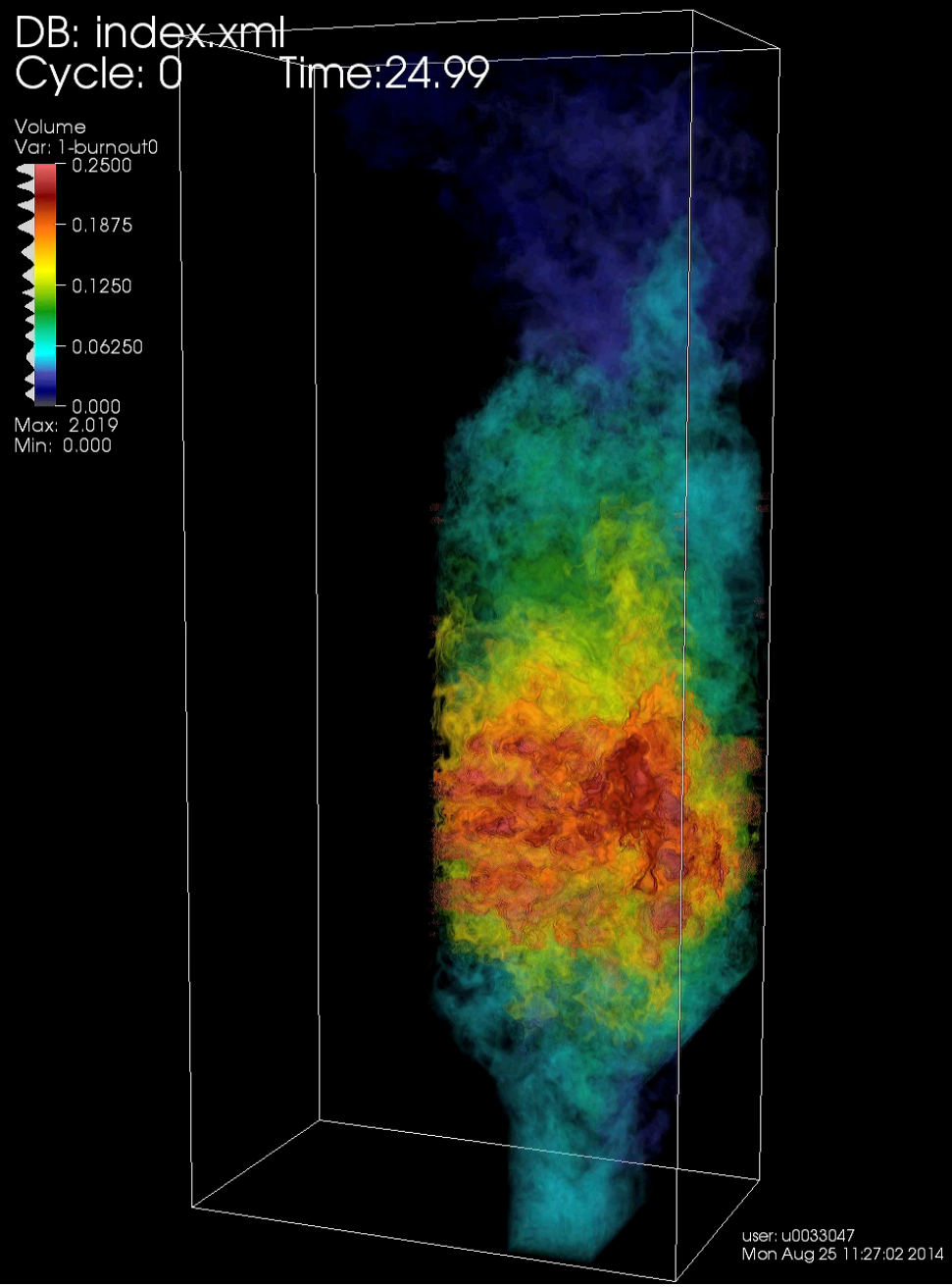
BSF



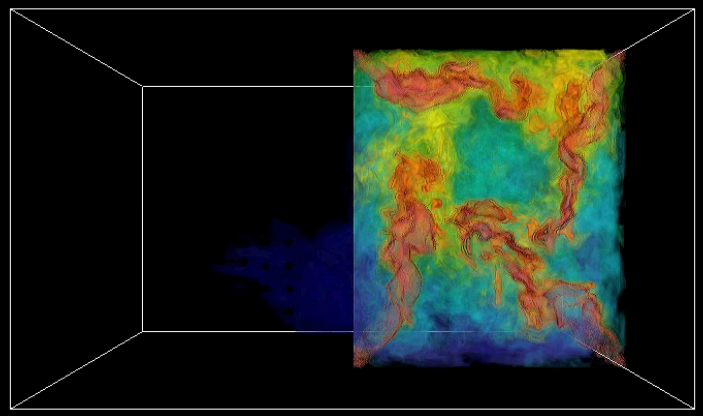


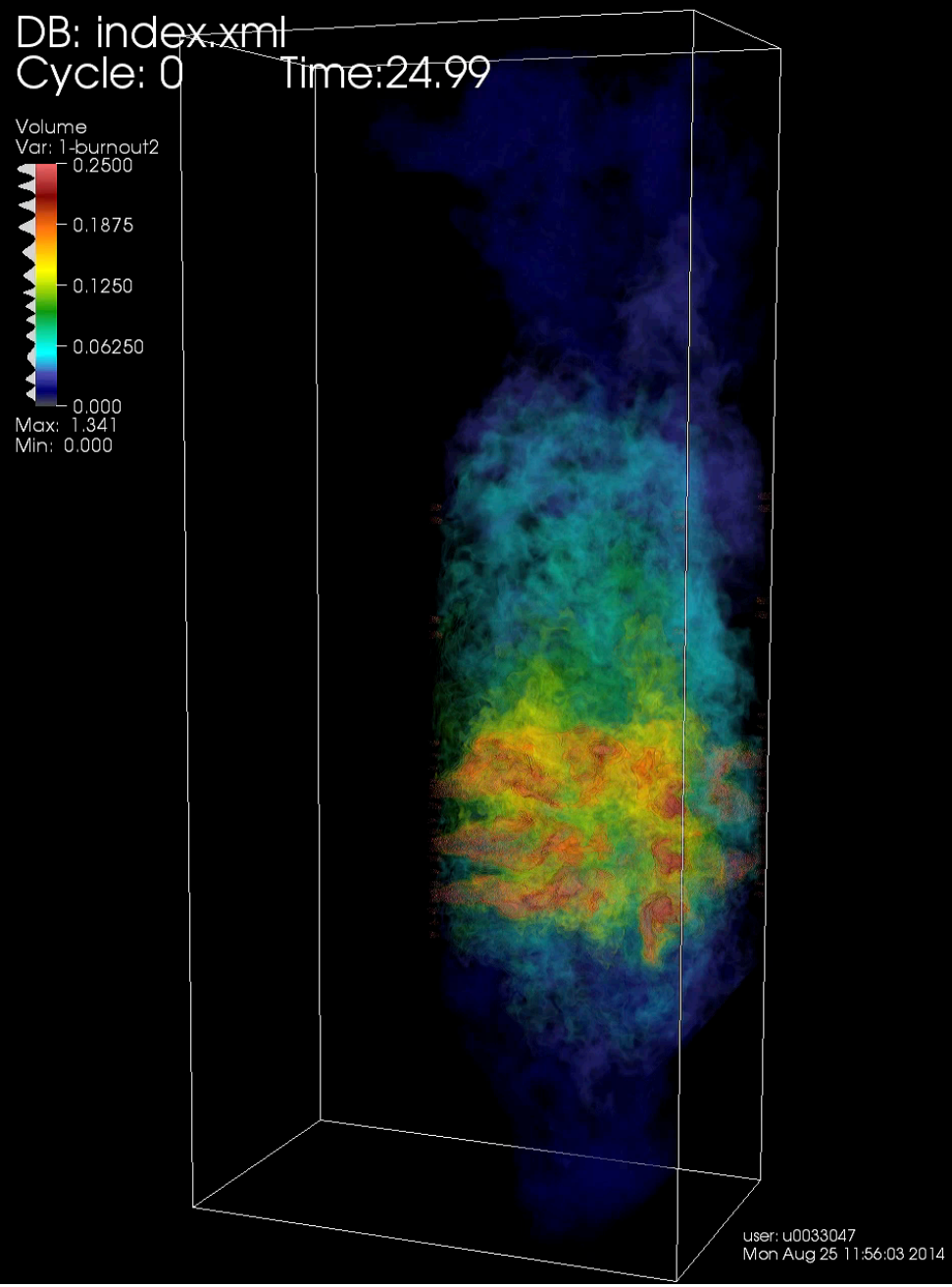
O_2 concentration





burnout of small particles





burnout of large particles

- AUSC:
  - *760C steam temperature*
  - *>12% reduction in fuel consumption carbon dioxide emissions over 600C USC units*
  - *materials - expensive*

- what will change from USC:
  - *superheater and reheater tube banks will use materials like 740H and 230 nickel.*
  - *furnace enclosure material in the upper enclosure is creep strength enhanced ferritic steel requiring field PWHT of the tube to tube joints and possibly the membrane panel seams.*
  - *steam piping is 740H nickel or better.*

- boiler arrangement / design is evolving
  - *price of nickel is so high that position of steam turbine must be a consideration*
  - *Siemens AG has proposed an horizontal boiler*

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overarching problem

ALSTOM

SIEMENS

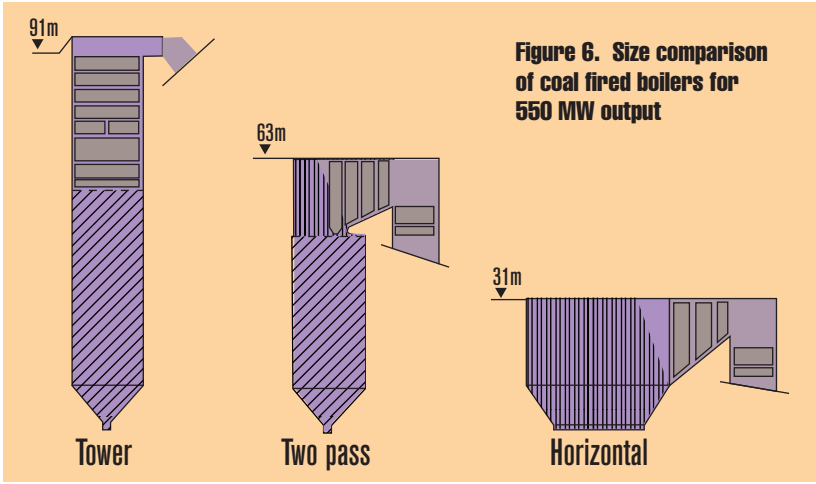
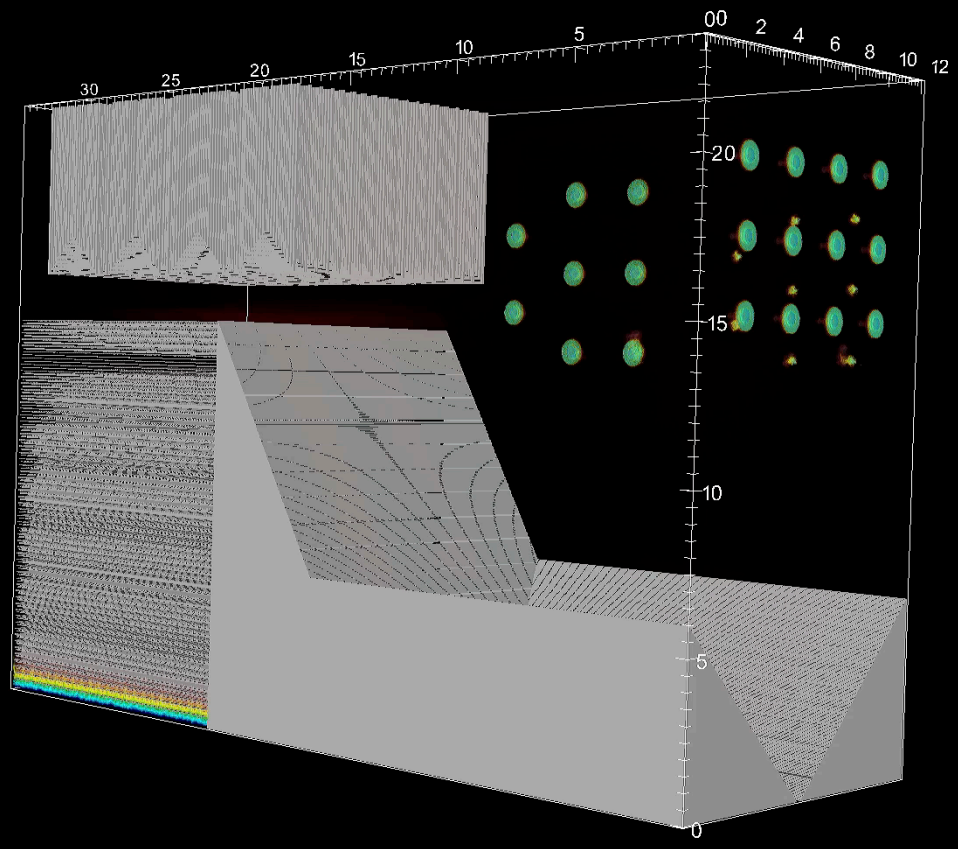


Figure 6. Size comparison of coal fired boilers for 550 MW output



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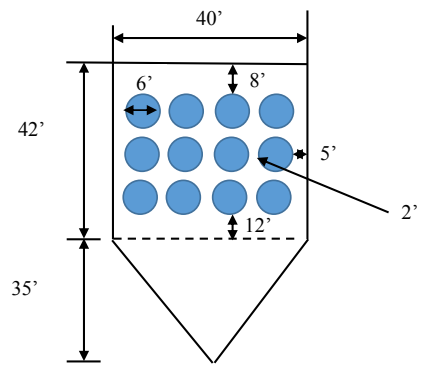
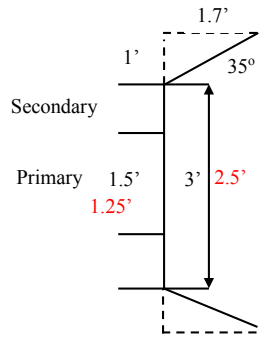
overarching problem

1st year target boiler design prediction

FRONT WALL

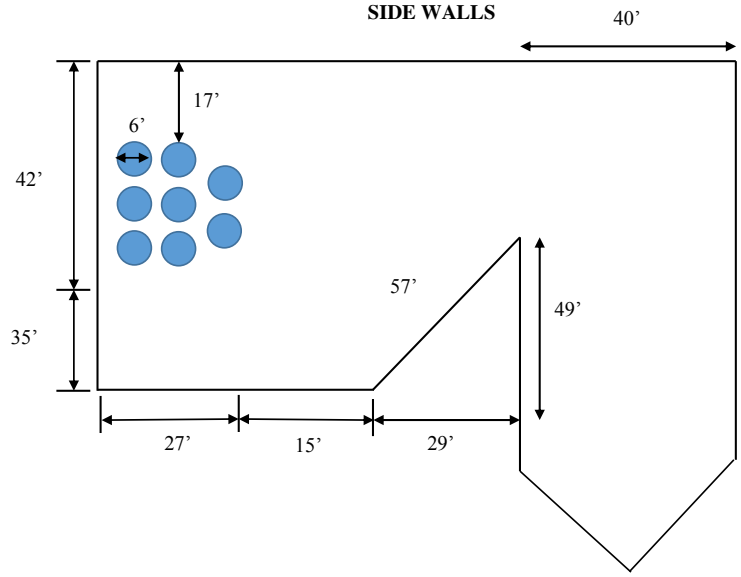


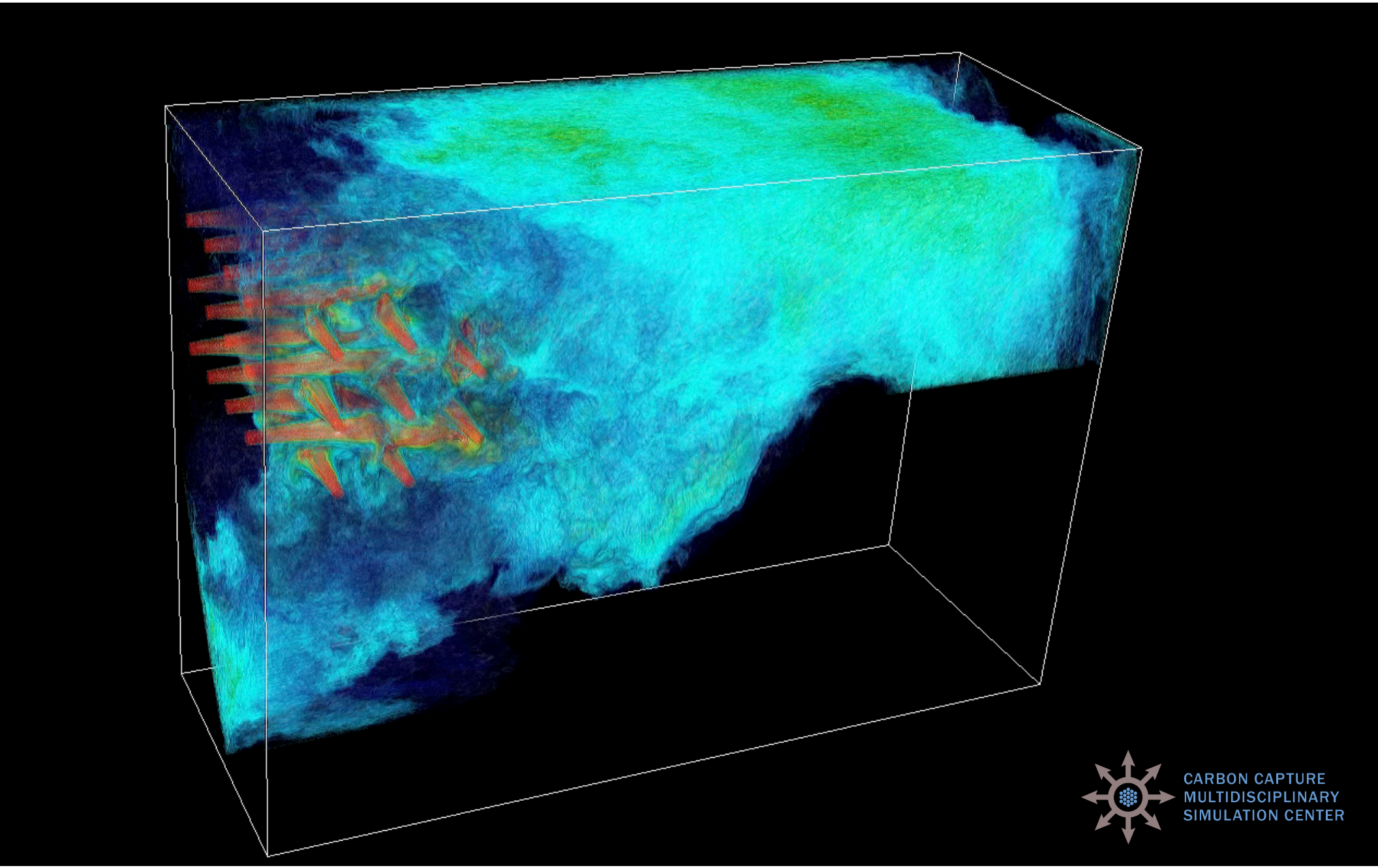
BURNER



Note: Red numbers are for side wall burners.

SIDE WALLS

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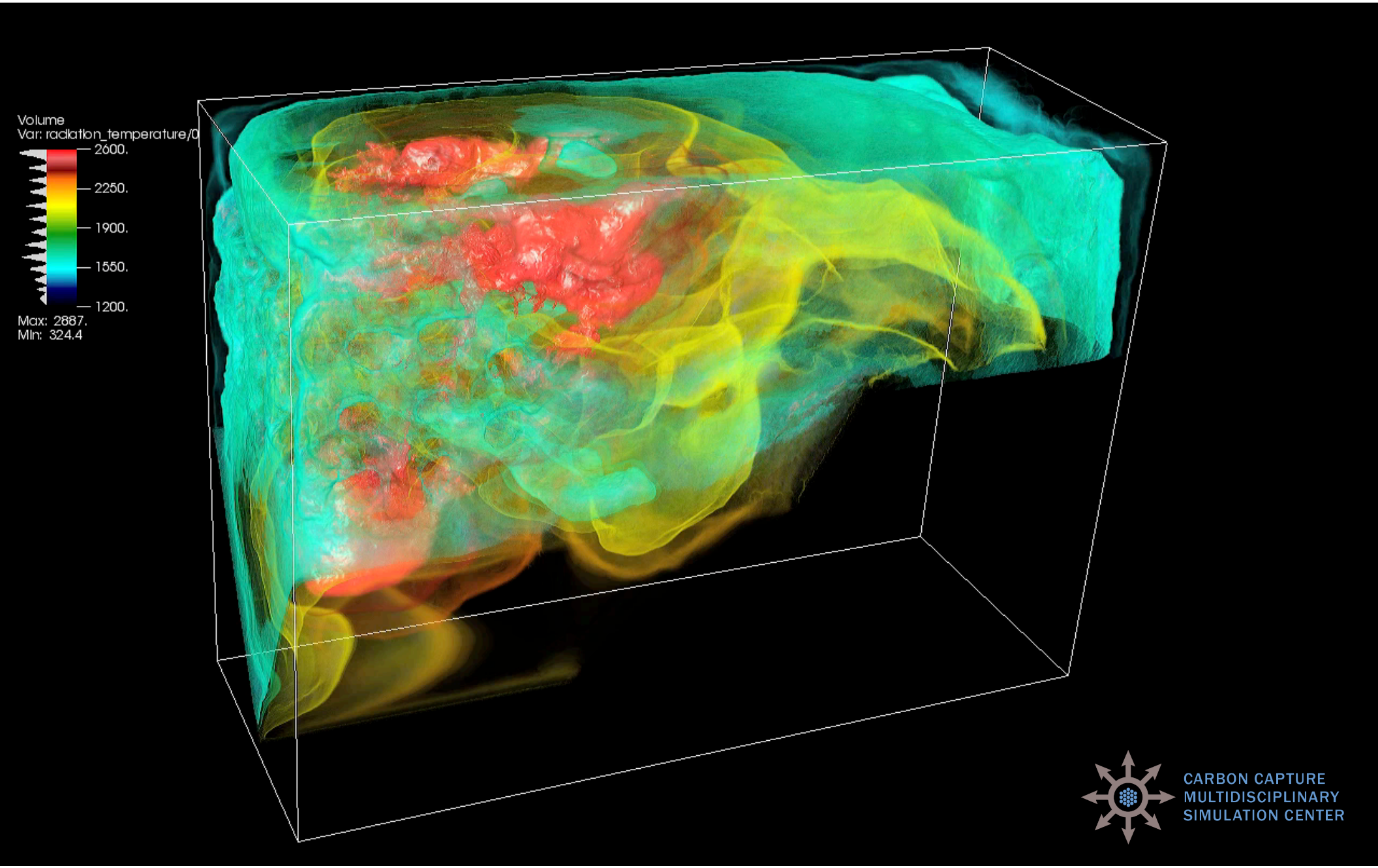
Volume
Var: radiation_temperature/0
2600.
2250.
1900.
1550.
1200.
Max: 2887.
Min: 324.4
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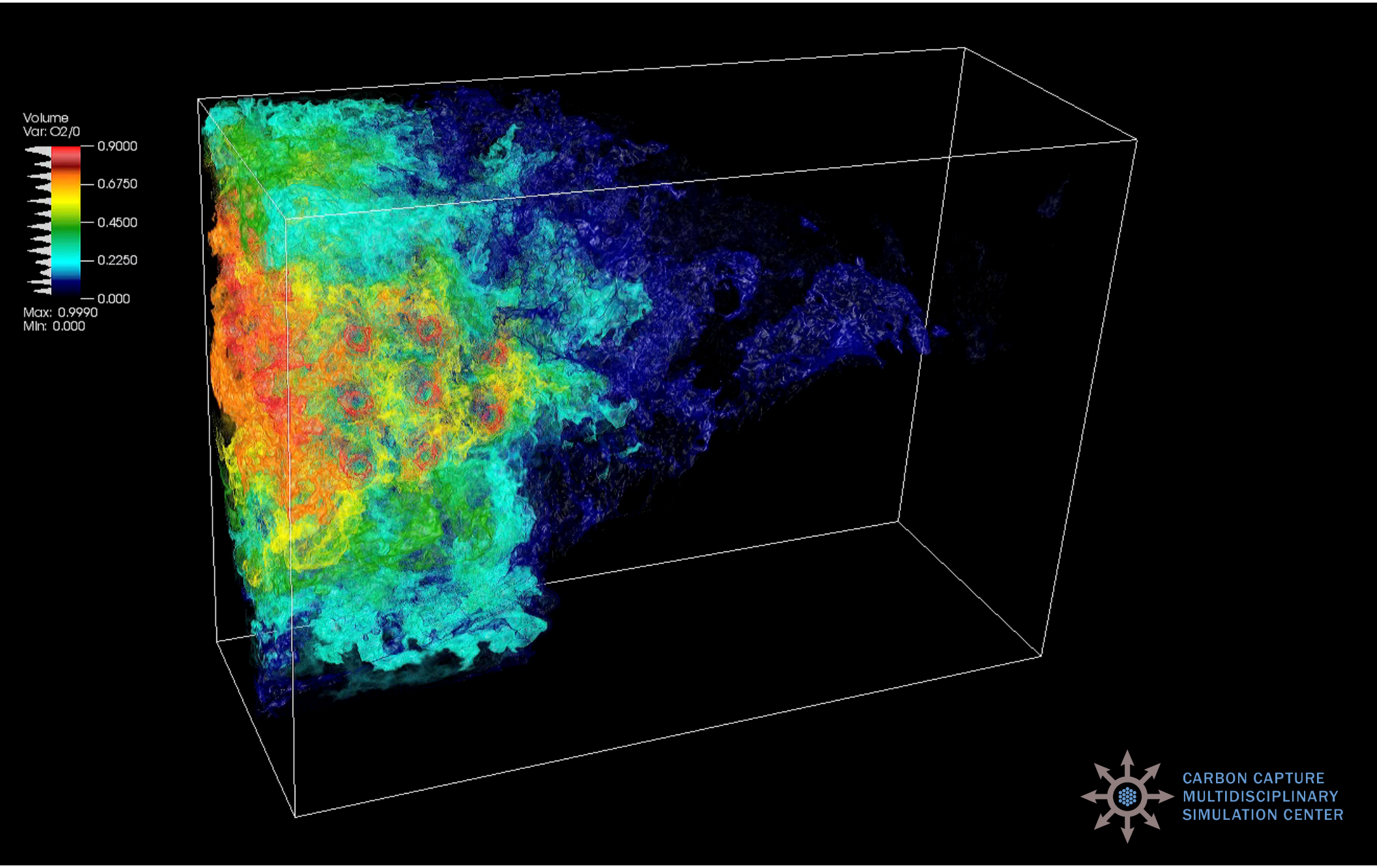
Volume
Var: O2/0
0.9000
0.6750
0.4500
0.2250
0.000
Max: 0.9990
Min: 0.000
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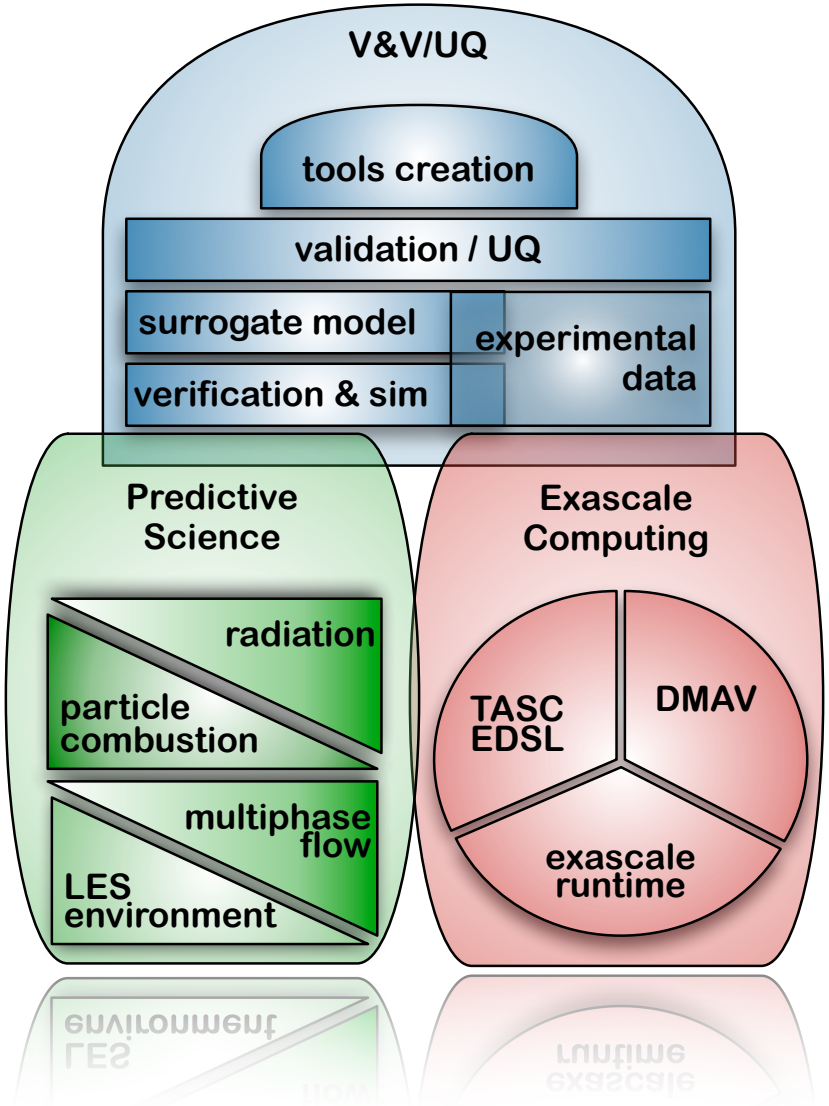
Demonstrate that extreme computing can accelerate deployment of a low-cost, low-carbon energy solution for power generation: AUSC oxy-coal !



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