



Leveraging the ASC Sierra Mechanics Tools for Battery Fire Prediction

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interest*

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Battery Safety Background

Use Case: Hawaii Lead Acid Batter System on Fire

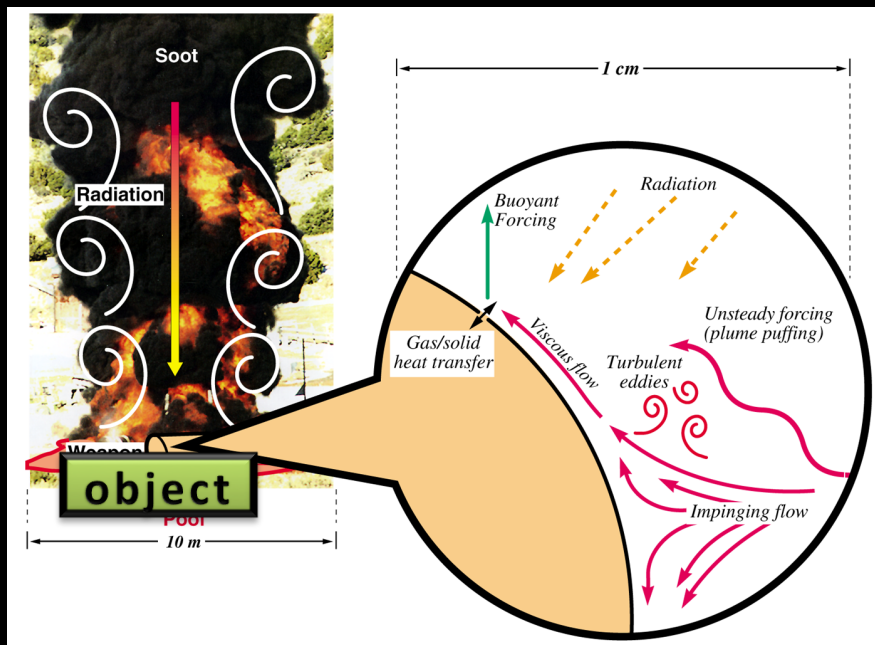
- Racks of lead acid batteries and power conditioning system inside the building
- Passive response (Hawaii is a closed water system)



- In what context could we imagine a computational capability being useful?
- Where might one find such a simulation tool?

Leveraging ASC NW Investments (Abnormal/Thermal Environment)

Goal: Leverage the Sierra-Mechanics Integrated Code simulation tool that has been designed to support the Department of Energy (DOE) Advanced Scientific Computing (ASC) program to support Science-based Stockpile Stewardship and deploy to battery fire safety analysis



Heat transfer mechanisms in a fire

Turbulent fluid mechanics (buoyant plumes)

Participating Media Radiation (PMR)

Reacting flow (hydrocarbon, particles, solids)

Conjugate Heat Transfer (CHT)

The simulation tool *predicts* the thermal environment and object response

Leveraging ASC NW Investments (Abnormal/Thermal Environment)



Object-in-hydrocarbon fire in cross flow
(volume rendered temperature field)

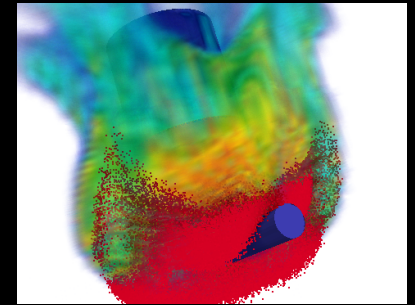
Leveraging ASC NW Investments (Abnormal/Thermal Environment)



Object-in-hydrocarbon fire
(volume rendered temperature field)

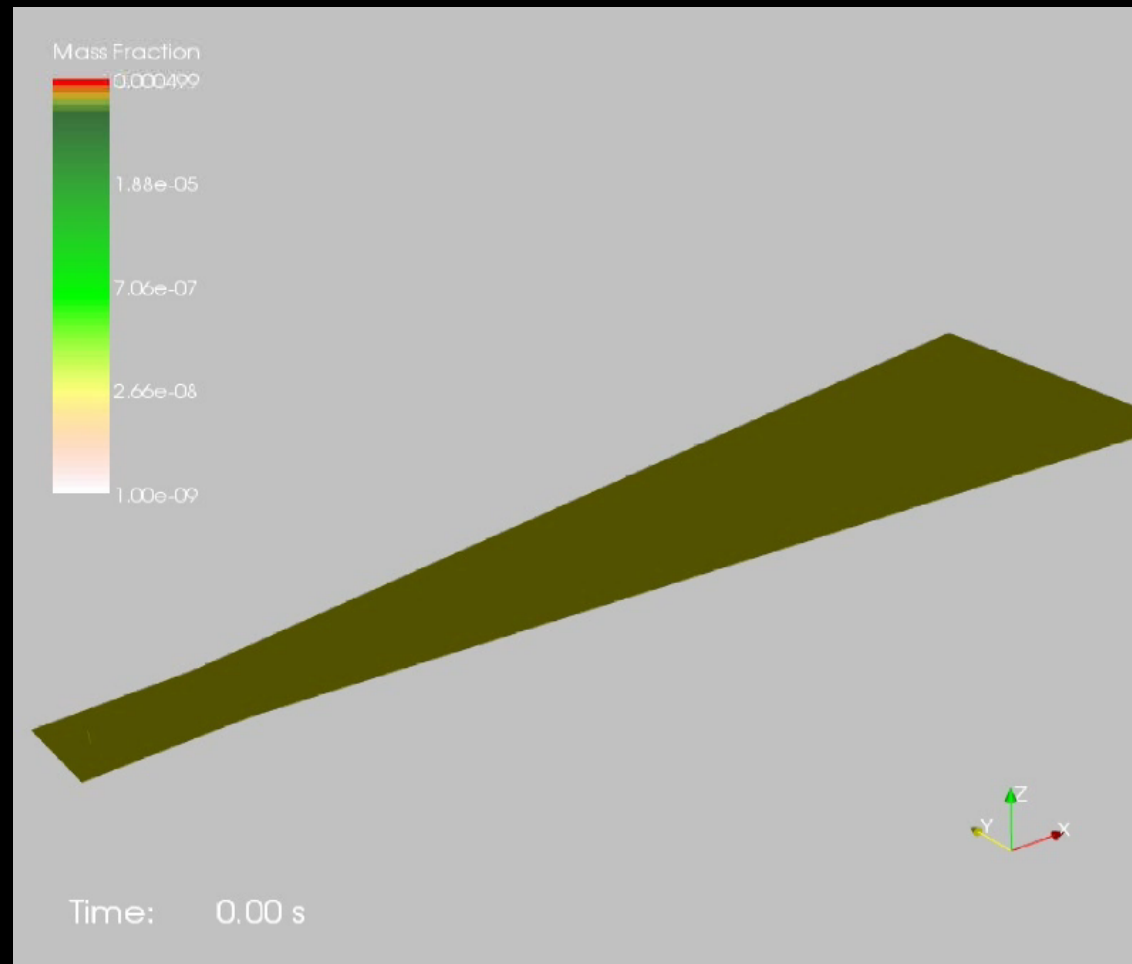


Sodium reacting flow with particle insertion



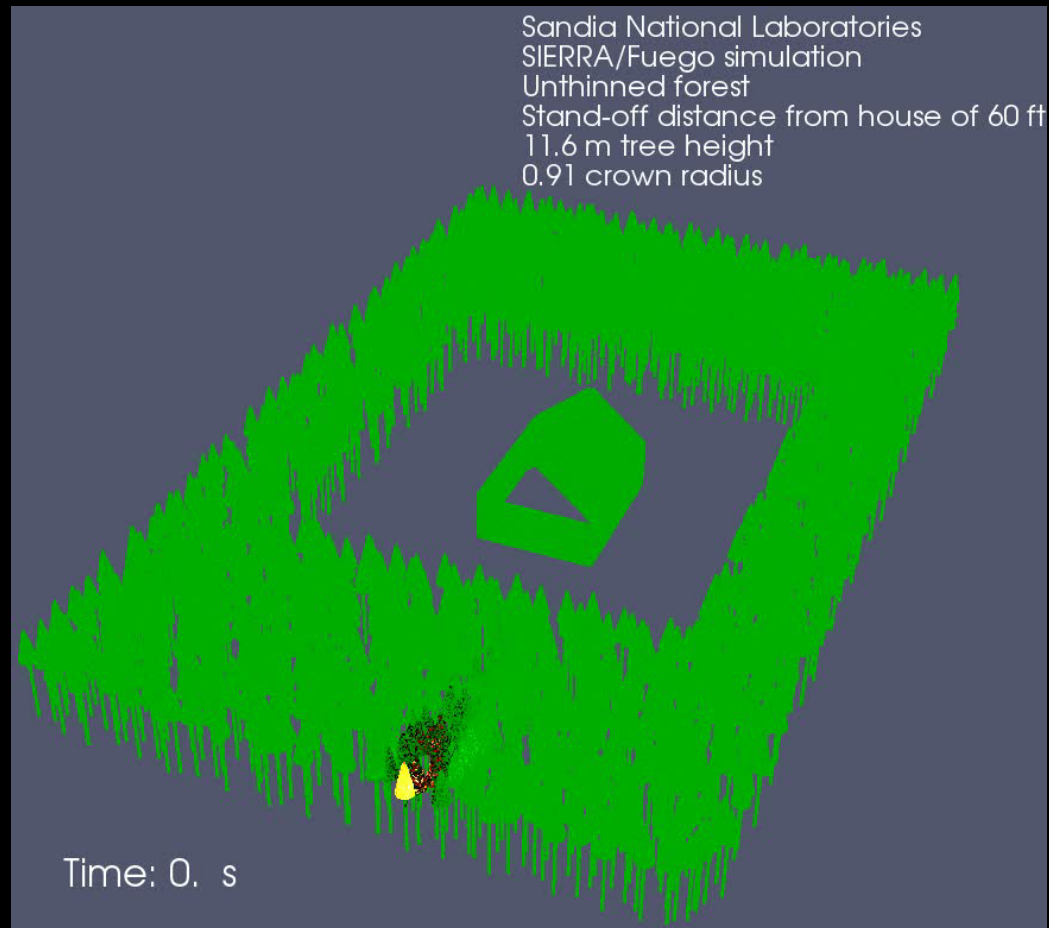
Downward AL propellant fire burn
(volume rendered temperature with particles)

Leveraging ASC NW Investments (Abnormal/Thermal Environment)



Contaminant transport (plumes) prediction over long distances

Leveraging ASC NW Investments (wild fire support for Angel Fire, NM)



Effect of thinned barrier around house on fire spread to the house

Multiphysics Coupling

(the equations and couplings)...

Fluid/Thermal

Fluids:

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \frac{\partial}{\partial x_j} \bar{\rho} \tilde{h} \tilde{u}_j = - \frac{\partial}{\partial x_j} (\bar{q}_j + \tau_{hu_j}) - \frac{\partial \bar{q}_i^r}{\partial x_i} + \frac{\partial P}{\partial t} + \tilde{u}_j \frac{\partial P}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j}$$

Thermal:

$$\rho C_P \frac{\partial T}{\partial t} + \frac{\partial}{\partial x_j} q_j = S_T$$

Coupling:

$$q_j^s n_j^s = q_j^f n_j^f$$

PMR/Thermal

RTE:

$$s_j \frac{\partial}{\partial x_j} I(\vec{r}, s) + (\bar{\mu}_a + \bar{\mu}_s) I(\vec{r}, s) = \bar{\mu}_a I_b + \mu_s \frac{G}{4\pi}$$

Thermal:

$$\rho C_P \frac{\partial T}{\partial t} + \frac{\partial}{\partial x_j} q_j = S_T$$

Coupling:

$$q_j^s n_j^s = q_j^R n_j^R$$

Fluid/PMR

Fluids:

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \frac{\partial}{\partial x_j} \bar{\rho} \tilde{h} \tilde{u}_j = - \frac{\partial}{\partial x_j} (\bar{q}_j + \tau_{hu_j}) - \frac{\partial \bar{q}_i^r}{\partial x_i} + \frac{\partial P}{\partial t} + \tilde{u}_j \frac{\partial P}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j}$$

RTE:

$$s_j \frac{\partial}{\partial x_j} I(\vec{r}, s) + (\bar{\mu}_a + \bar{\mu}_s) I(\vec{r}, s) = \bar{\mu}_a I_b + \mu_s \frac{G}{4\pi}$$

Coupling:

$$\frac{\partial \bar{q}_i^r}{\partial x_i} = \mu_a [4I_b - G(\vec{r})]$$

Particle coupling is handled through
Particle Source in Cell
technique (explicit
Lagrangian, implicit Eulerian)

Multiphysics Coupling (put together)

Surface-based coupling

$$lhs_{h_{ije}} + = \sum_{j=1}^N \left(\int_{\Gamma_h^e} \lambda \psi_i^e \psi_j^e d\Gamma \right) \quad I(\vec{r}) = \frac{1}{\pi} \left[\tau \sigma T^{env4} + \varepsilon \sigma T^4 + (1 - \varepsilon - \tau) H(\vec{r}) \right]$$

$q_w = \lambda(h - h_w)$ ← Thermal
 ↑ Dirichlet condition

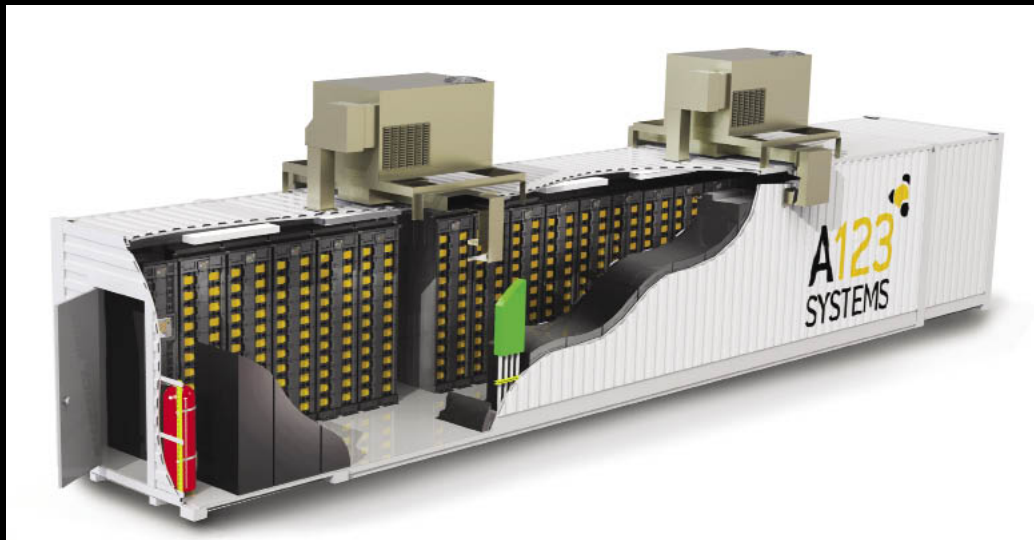
$$q_n = -(K \nabla T) \cdot \hat{n} = q_b = h(T - T^\infty) + \varepsilon(\sigma T^4 - H)$$

Fuego
 Syrinx

$$lhs_{T_{ije}} + = \sum_{j=1}^N \left(\int_{\Gamma_h^e} (h + 4\varepsilon \sigma T_j^{*3}) \psi_i^e \psi_j^e d\Gamma \right)$$

Complex Geometries

power conditioning system
racks of batteries

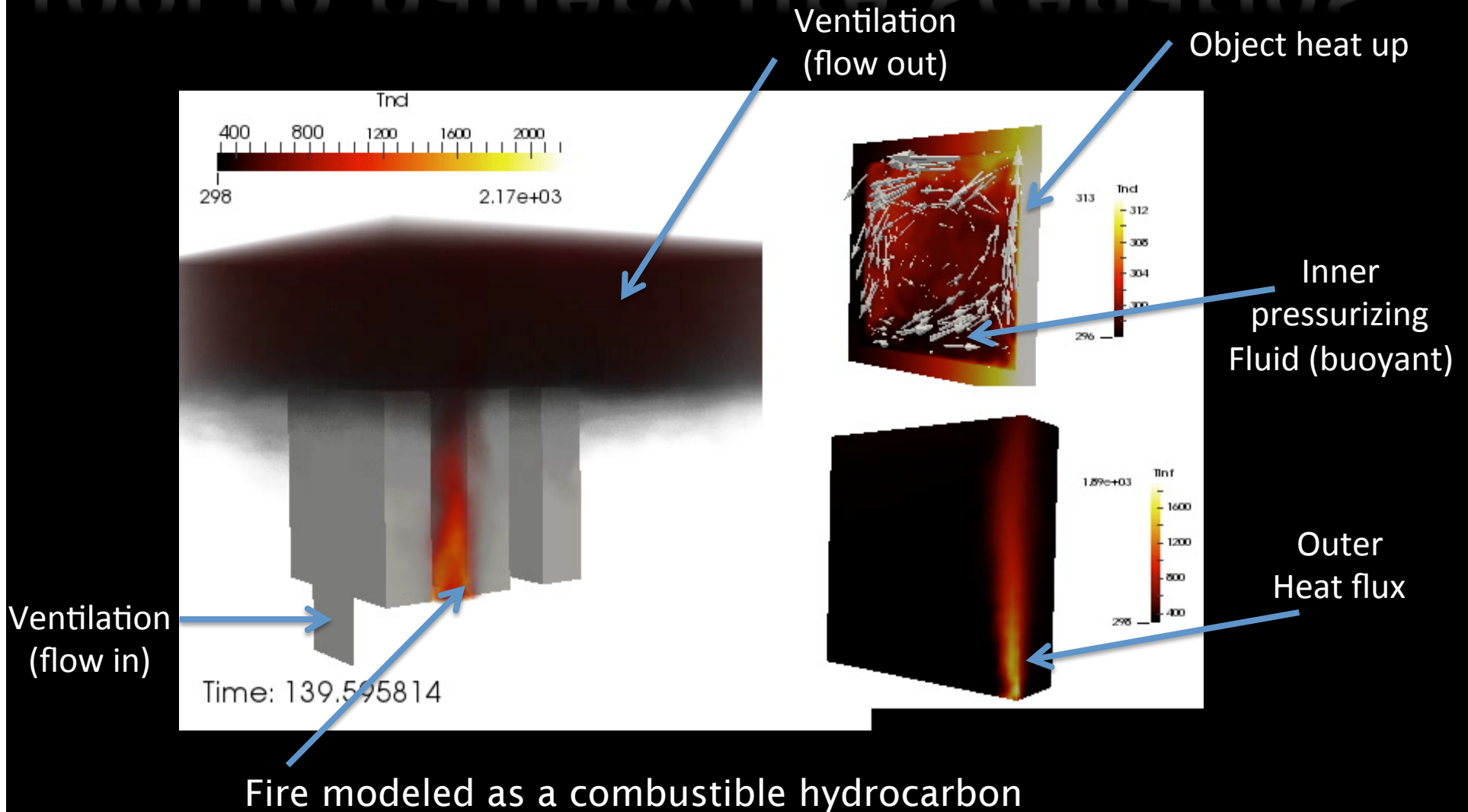


Plug-and-play Lithium Ion trailer

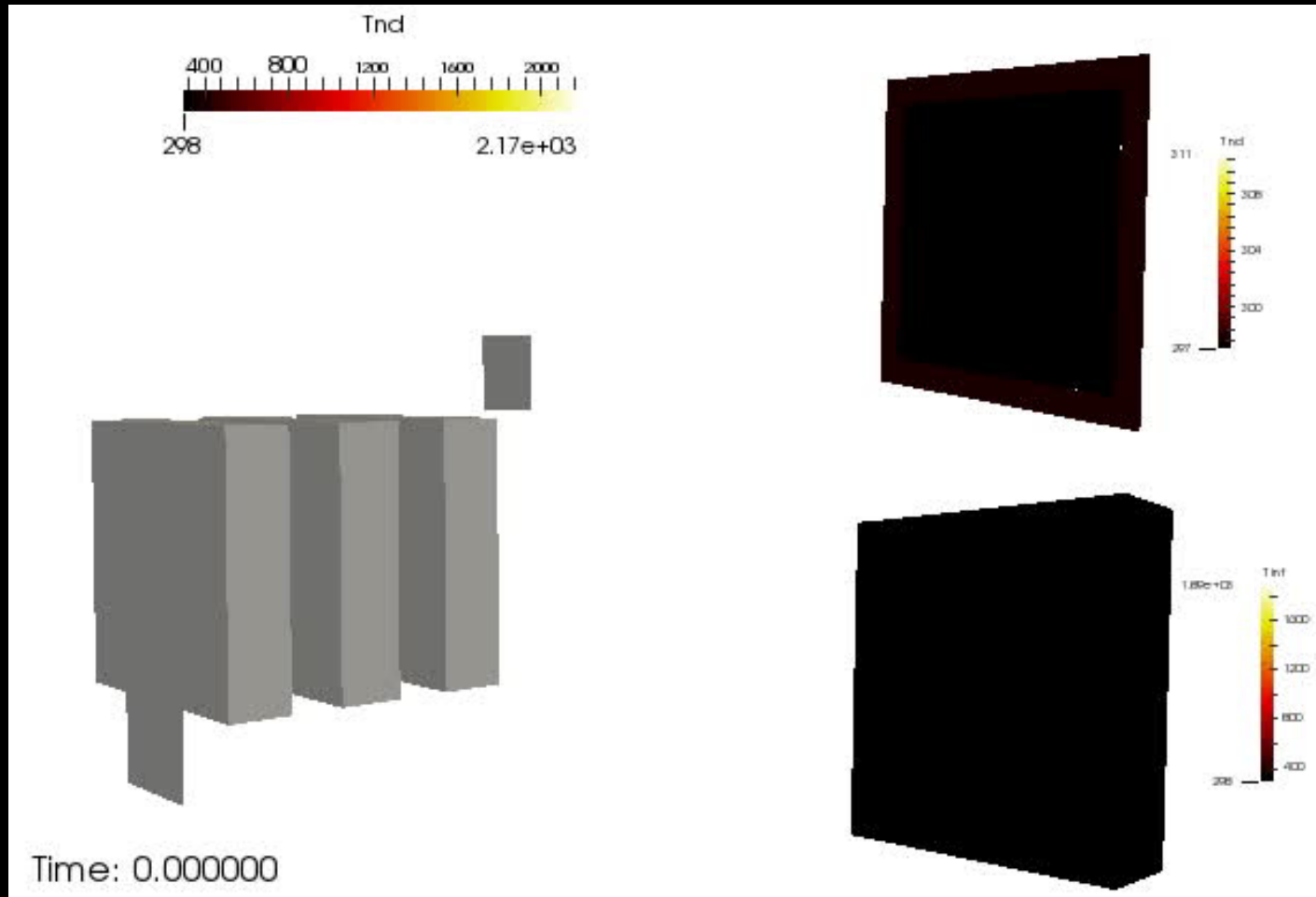


Lead acid Alaska facility
designed to replace back-
up diesel

Applying Sierra simulation tool to battery fire scenarios

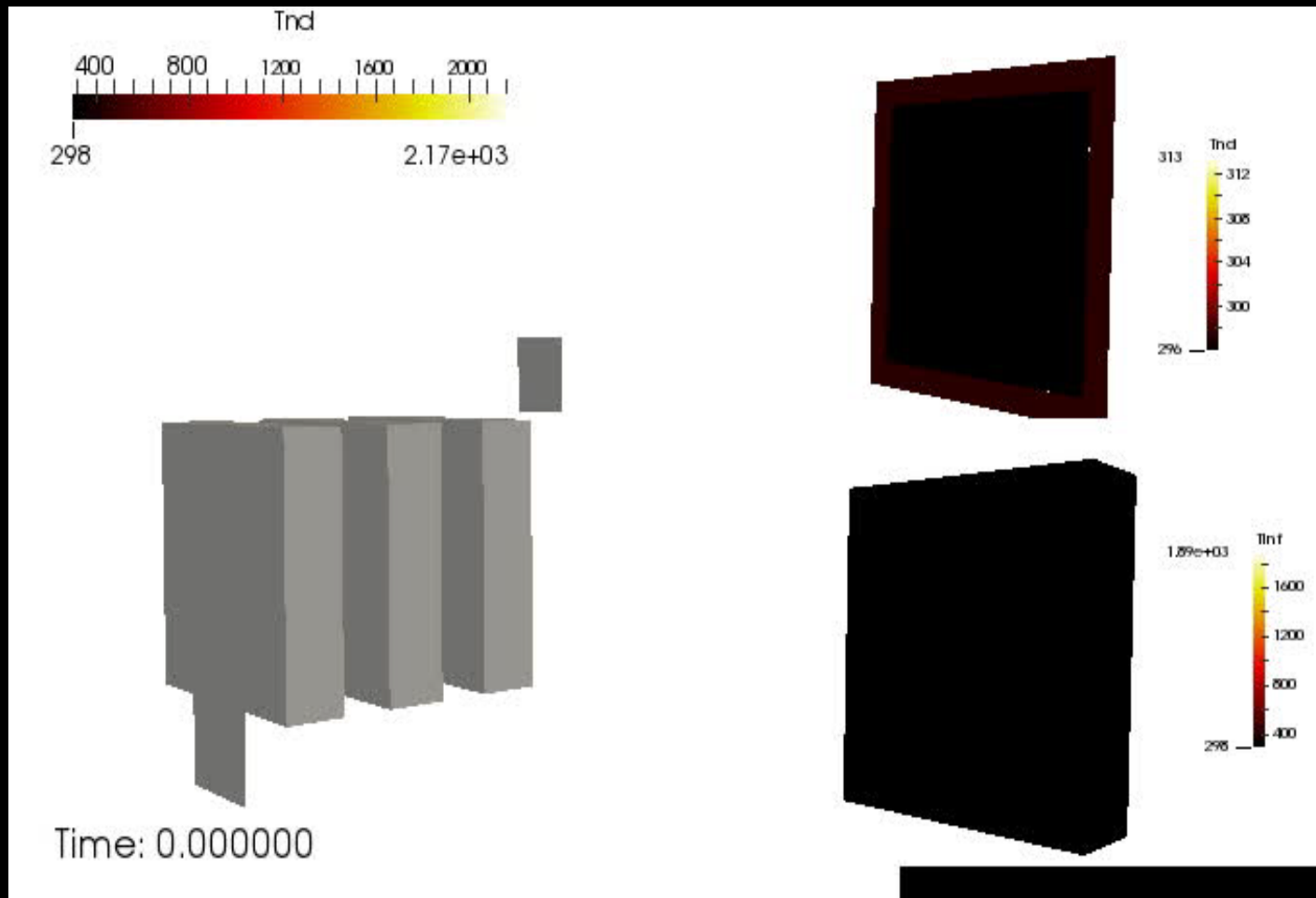


Ventilation effect on fire plume dynamics (1/3)



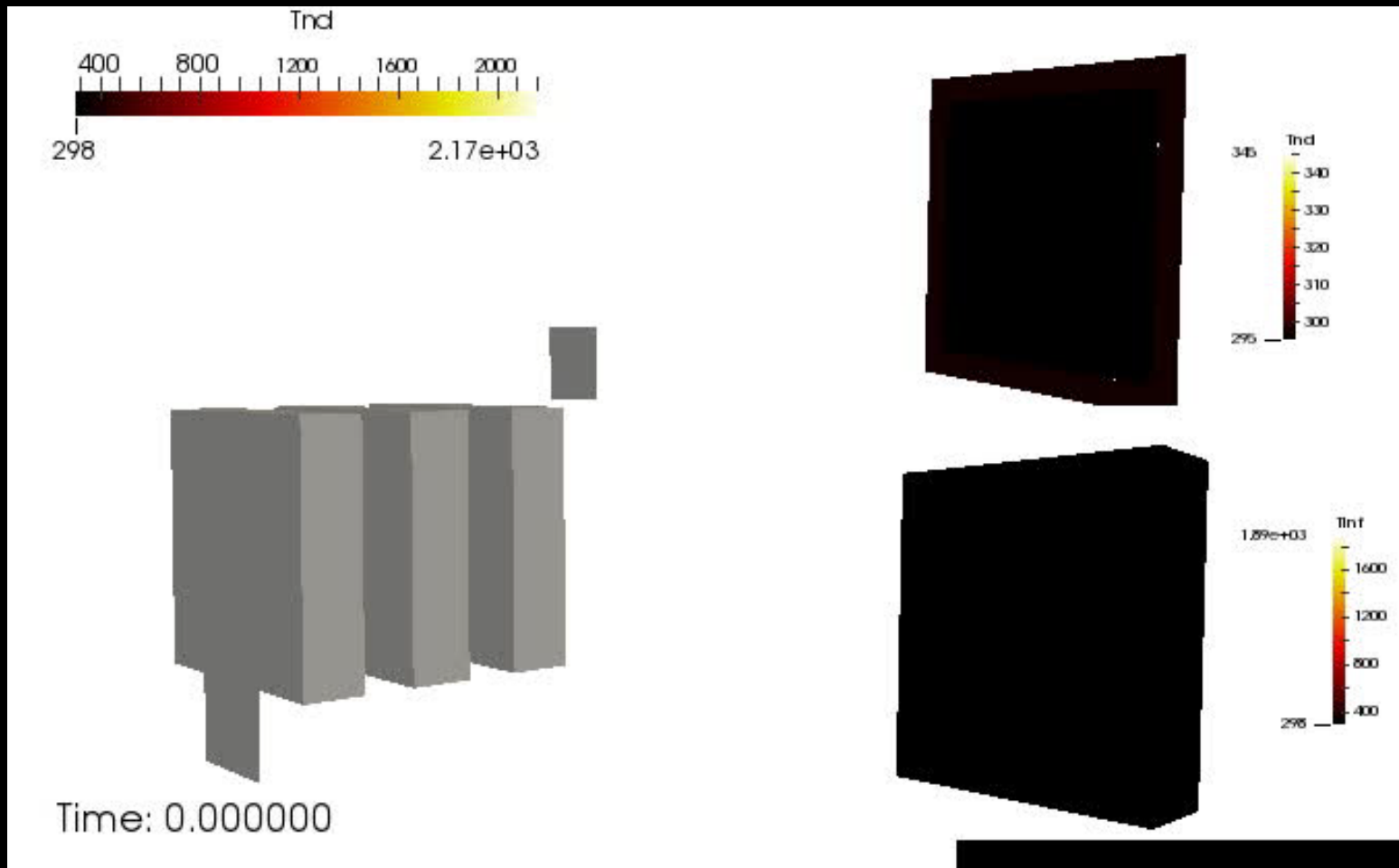
No Ventilation

Ventilation effect on fire plume dynamics (2/3)



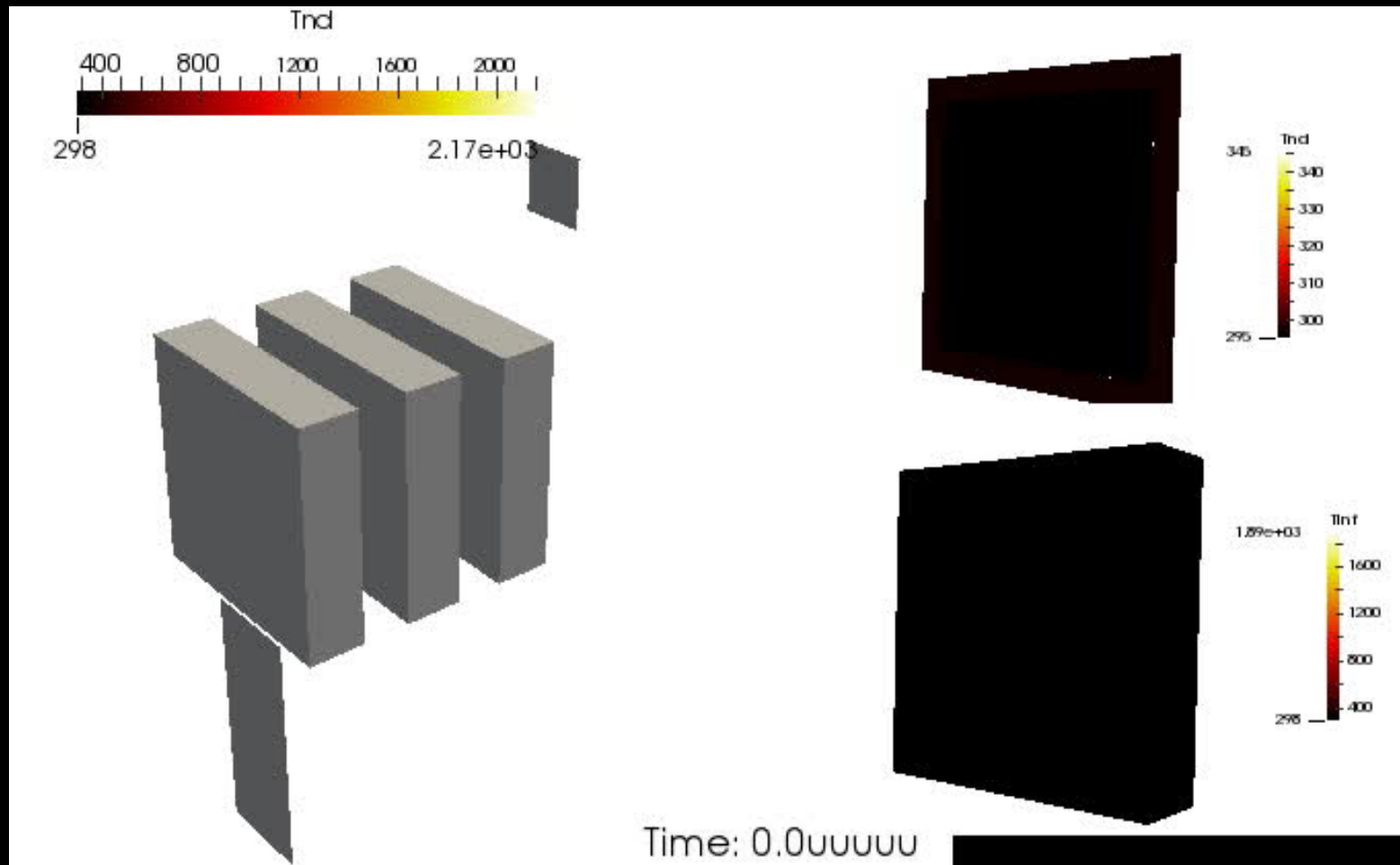
Ventilation is 1 m/s

Ventilation effect on fire plume dynamics (3/3)



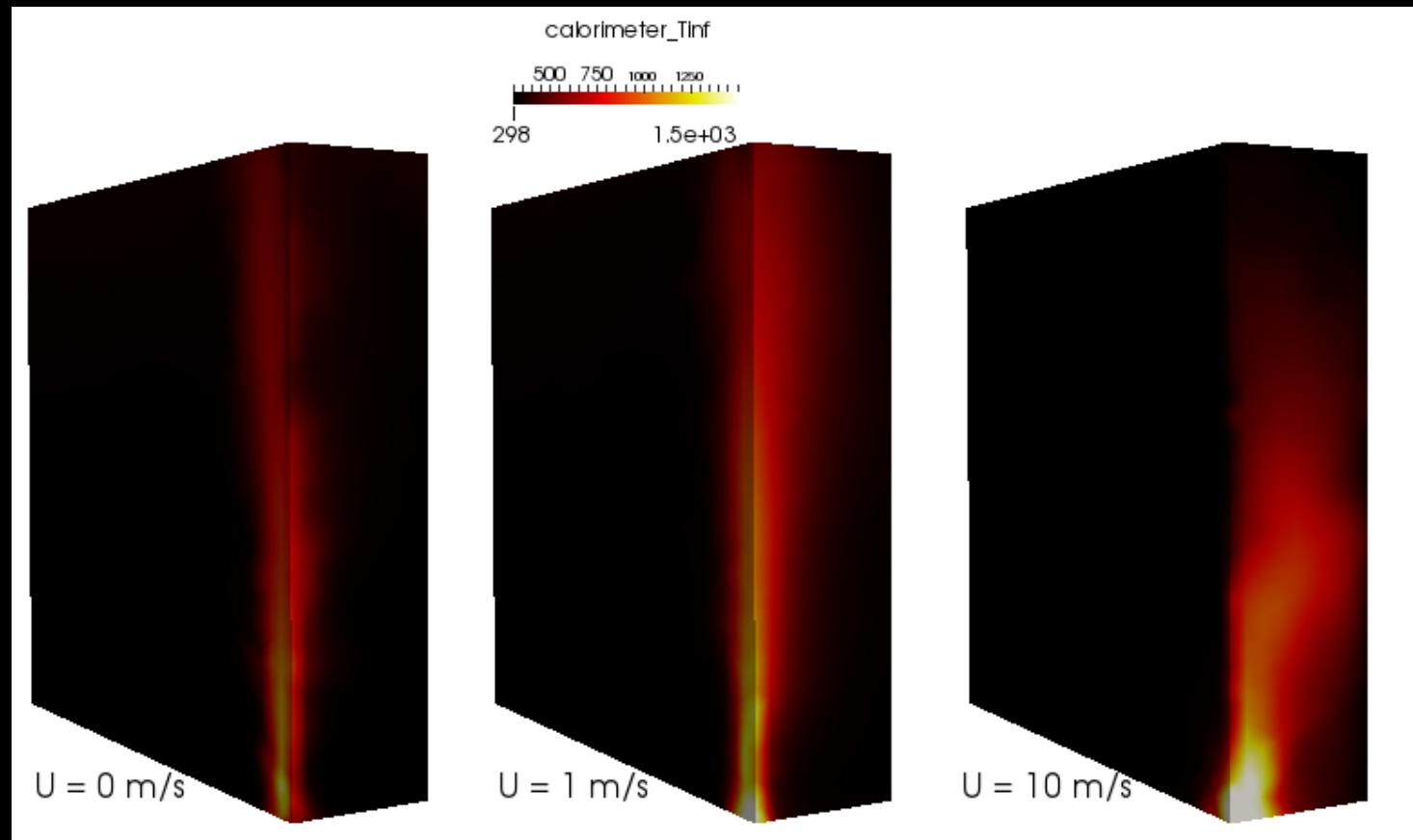
Ventilation is 10 m/s

Ventilation effect on fire plume dynamics (3/3)



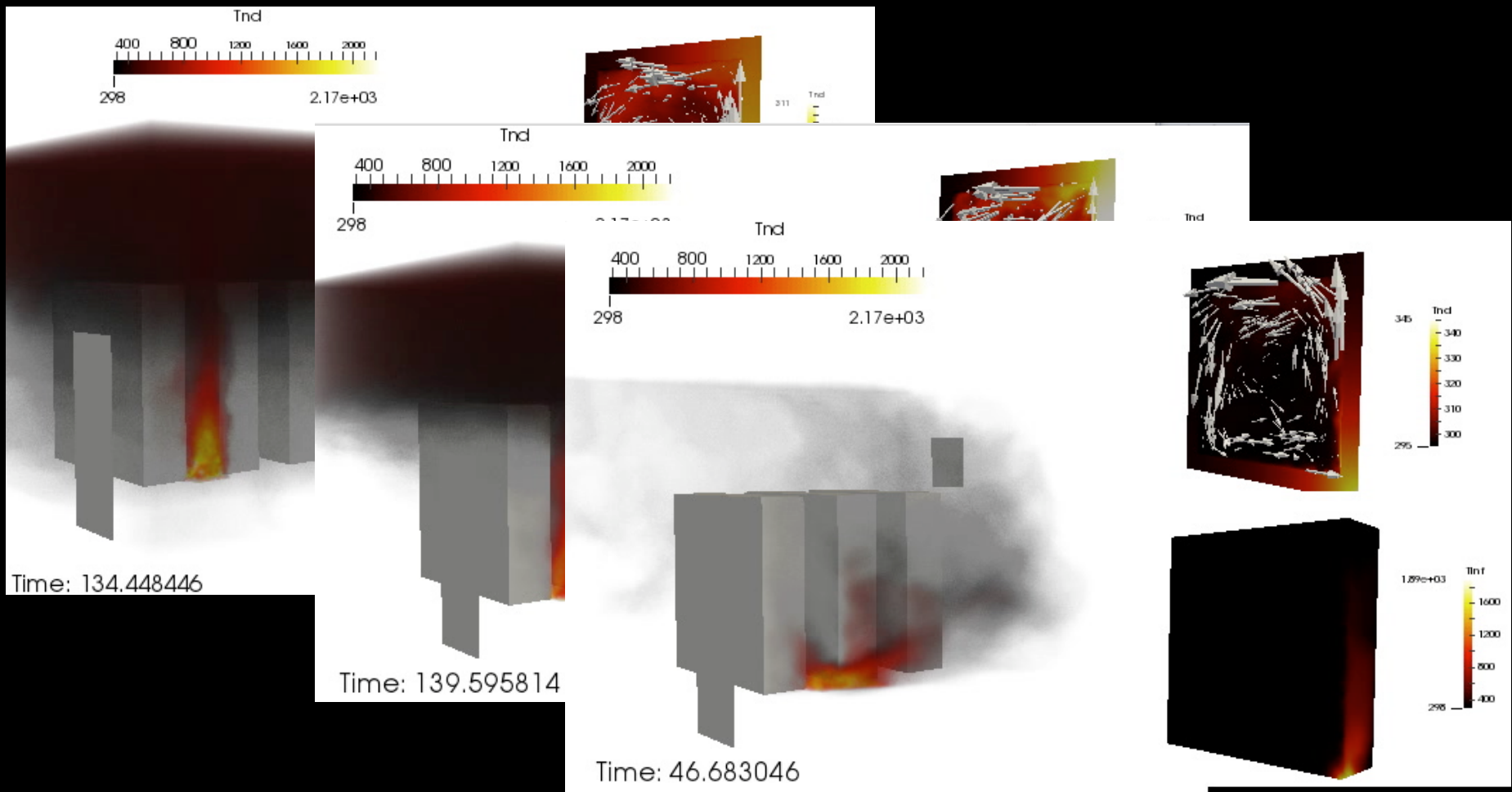
Ventilation is 10 m/s; now velocity vectors shown

UQ: Heat Flux Sensitivity to Ventilation



Reference Temperature for three ventilation configurations

UQ: Plume Dynamics



Three ventilation comparison still shot

Conclusions

Predicting object response to a fire environment requires coupling of turbulent fluid mechanics, Participating Media Radiation, Thermal conduction, pressurization and spray combustion

The Sierra low Mach module Fuego, which has a pedigree of supporting the Abnormal/Thermal environment, is a natural candidate to simulate battery fire use cases; demonstrations provided

Room ventilation has a first order effect on plume dynamics

Detailed chemistry for batteries (Li-ion) and advanced models are required