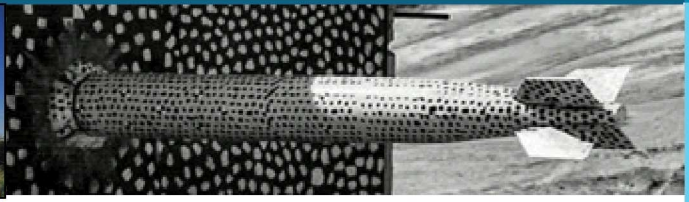
Oct 14-15 Fall 2019
Technical Meeting
Albuquerque, NM, USA



Western States Section Combustion Institute

SAND2019-12429C

# Modeling High Heat Flux Combustion of Coniferous Trees Using Chemically Reacting Lagrangian Particles



Hector Mendoza; hmendo@sandia.gov; (505)845-0431
Structural and Thermal Analysis Department

Alex Brown: Fire Sciences and Technology Department
Allen Ricks: Technical Analysis Departmant

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

# Outline of Presentation

1. Introduction and overview of experimental Work
2. Numerical model overview
3. Simulation approach
   - Computational domain and boundary conditions
   - Calibration of flux profile for simulations
   - Creating representative computational trees
4. Resulting model and simulations
   - Preliminary model, based on first data set
   - Understanding proper tree representation using mass loss and other key metrics on first data set
   - Using model from first data set to understand unexpected behavior of second data set
5. Summarizing remarks

# Introduction and Motivation



Conventional burning => 25-200 $kW/m^2$

Different physical events can occur where pulsed, high heat flux burn may occur:

- Lightning strikes
- Metal fires

Pulsed high heat flux scenarios are unique in that:

- Ignition phenomena might be different from more conventional burning
  - Comparatively fast ignition
  - Flaming may or may not be sustained
  - Significant scale effects may exist
- Reaction kinetics may not be linear through the regime change
- Transition to more conventional burning might occur

Sandia has unique capability to impose pulsed, high heat fluxes on test materials

- Led to unique testing that produced unique dataset to test modeling capabilities…

# Overview of Experimental Work

Facility: High heat flux tests performed at SNL Solar Tower

- Field of 214 heliostat mirrors
- Can concentrate heat fluxes > 3,000 $kW/m^2$
  - Total power > 6.2 $MW_{th}$
- Relevant fluxes at meter-scale spot

Testing: Testing was performed over two phases

- Phase 0: Single tree tested
  - Single fluence condition
- Phase 1: Four trees tested
  - Multiple fluence conditions
  - **Only one tree with *Fluence Condition #1* is discussed here**

Focus of this study:

- A unique high heat flux data set has been obtained from SNL tests, therefore =>
  - A reacting flow, CFD model was developed/calibrated using Phase 0 data to simulate high heat flux scenarios.
  - Calibrated model was used to provide insight on Phase 1 experiments

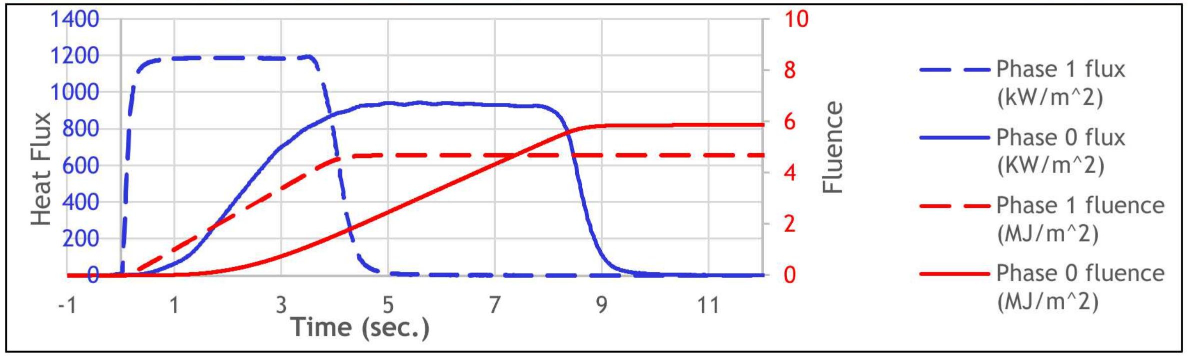
# Phase 0 and Phase 1 Test Videos

**Phase 0:** "**ramped**" increase on the incident flux

- Peak Flux: 1200 kW/m$^2$
- Fluence: 5.7 MJ/m$^2$
- Sustained Ignition observed near 4 seconds


**Phase 0:** "**step**" increase on the incident flux

- Peak Flux: 900 kW/m$^2$
- Fluence: 4.7 MJ/m$^2$
- Some ignition observed, but not prolonged



Goal is to use test data to produce a calibrated model

# Modeling Overview



SIERRA/Fuego V 4.44 was used as the main tool:

- A low Mach number reacting flow CFD Eulerian code
- Massively parallelized
- Handles various sub-grid turbulence models including:
  - RANS (Reynolds Averaged Navier Stokes),
  - LES (Large Eddy Simulation), and
  - **TFNS** (Temporally Filtered Navier Stokes)
- Includes models for pyrolysis, combustion, radiation, and participating media.
  - Multi-step reaction model (Di Blasi) for biomass pyrolysis [1]
  - Eddy Dissipation Concept (EDC) model is incorporated for reacting flow to capture combustion
  - Soot formation from EDC included as participating media in radiation solve
- Chemically reacting Lagrangian particle capability
  - Loosely coupled to Eulerian mesh
    - Species, mass, energy, and momentum source terms
  - Different particle arrangements can represent different forms of combustible matter
  - Particles released when decomposition exceeds critical threshold

[1] C. Di Blasi, "Modeling Chemical and Physical Processes of Wood and Biomass Pyrolysis.," *Progress in Energy and Combustion Science, V*ol. 34, No. 1, pp. 47-90, 2008.

# Simulation Approach: Computational Domain and Boundary Conditions

Computational tree in the middle of a cubic domain

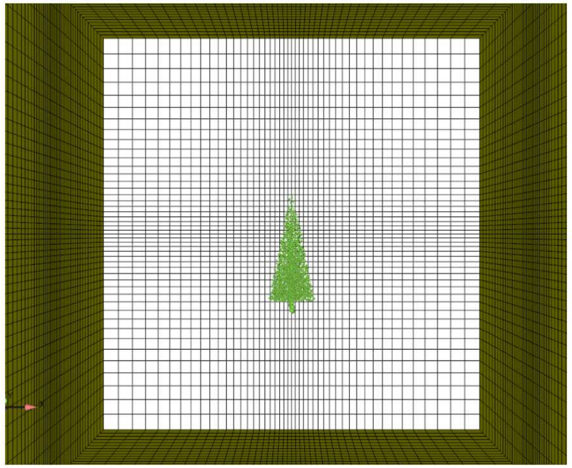
- Dual bias scheme used to produce fine resolution mesh around tree
- 98,000 elements, element sizes in rage of 5cm – 20cm

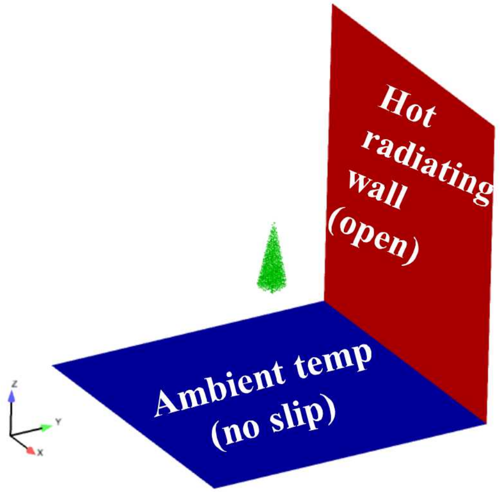
Fluid BCs

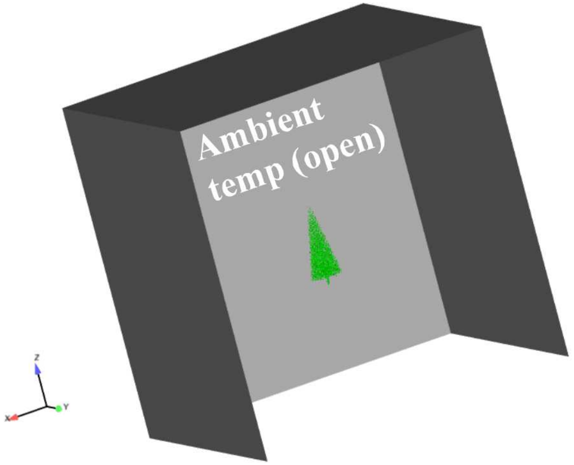
- Ambient temp, no-slip wall boundary used on surface below tree
- Ambient temp, open boundary for remaining surfaces

Radiation BCs

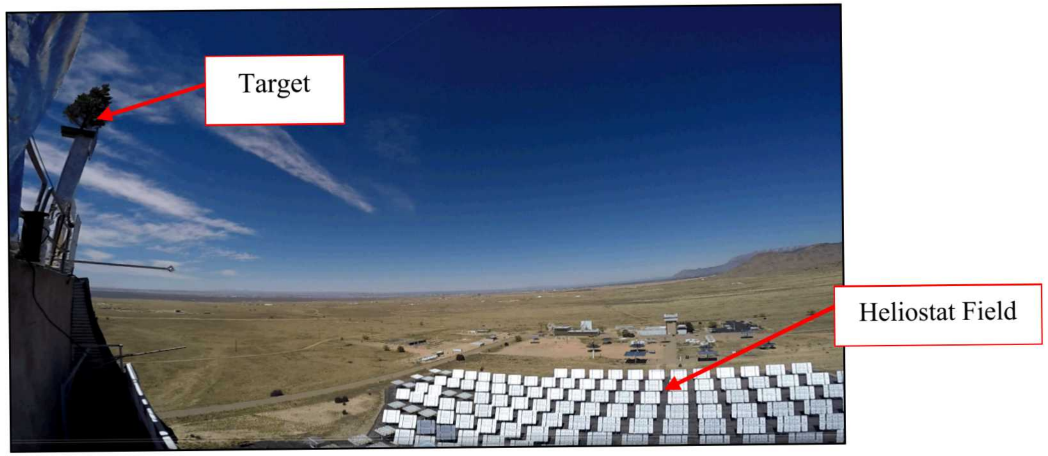
- Hot wall used to impose an incident radiative flux on tree
  - Temp of hot wall needs to be calibrated to obtain desired flux (calibration explained on next slide)
- Remaining walls => non-emitting/absorbing

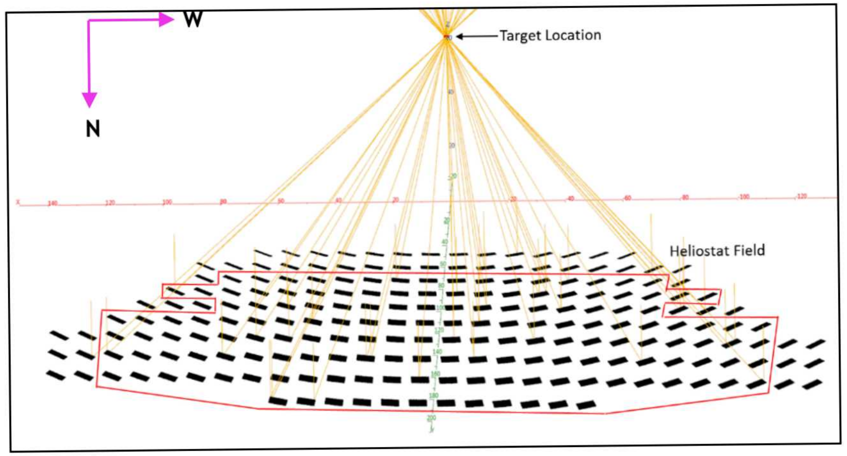




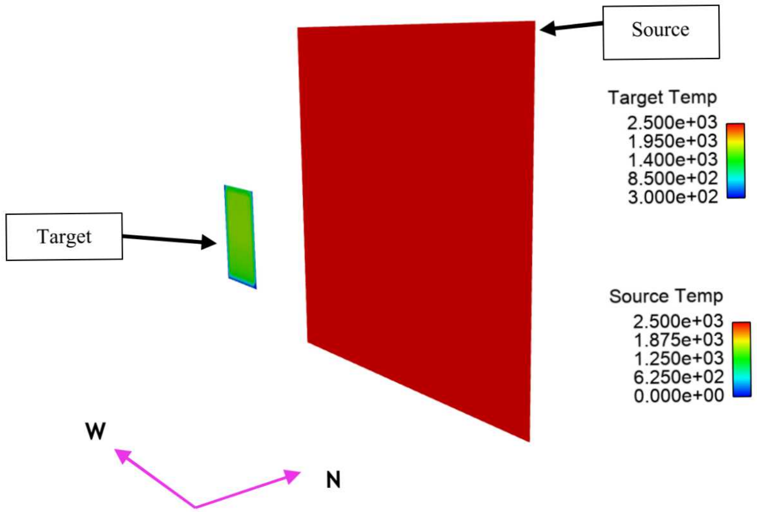



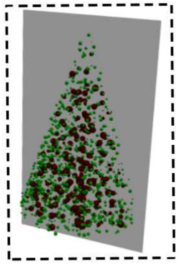
# Simulation Approach: Flux Profile Calibration

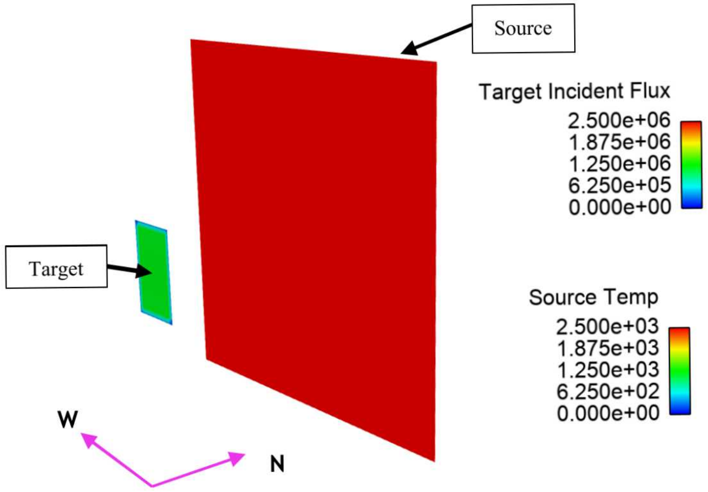



- Flux calibration performed on a panel with outer tree dimensions
- Radiative heat flux imposed on target panel by a hot wall (source)



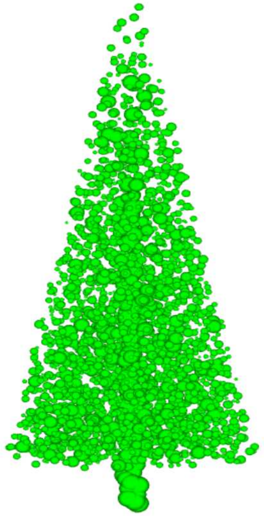


# With computational domain defined, how do we represent trees?

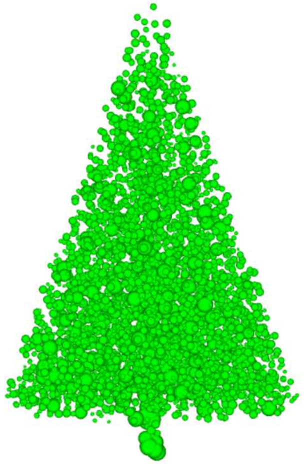
# Tree Representation using Chemically Reacting Lagrangian Particles



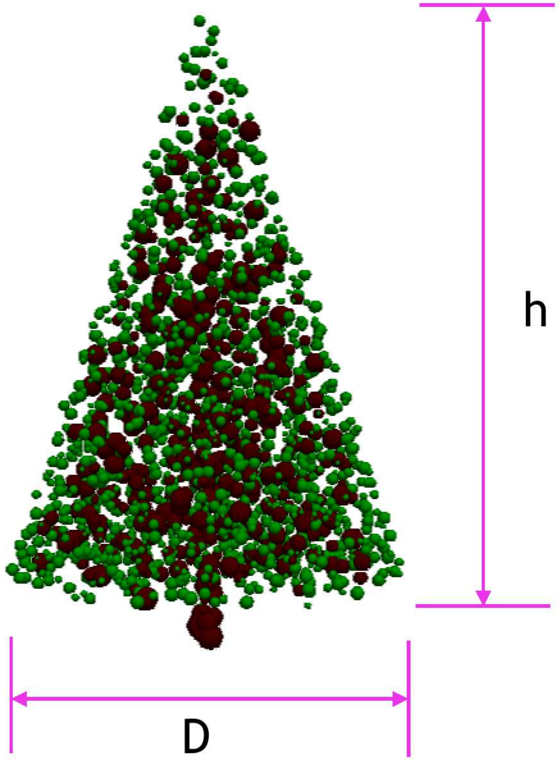
Phase 0
D=0.61 m
h=1.47 m



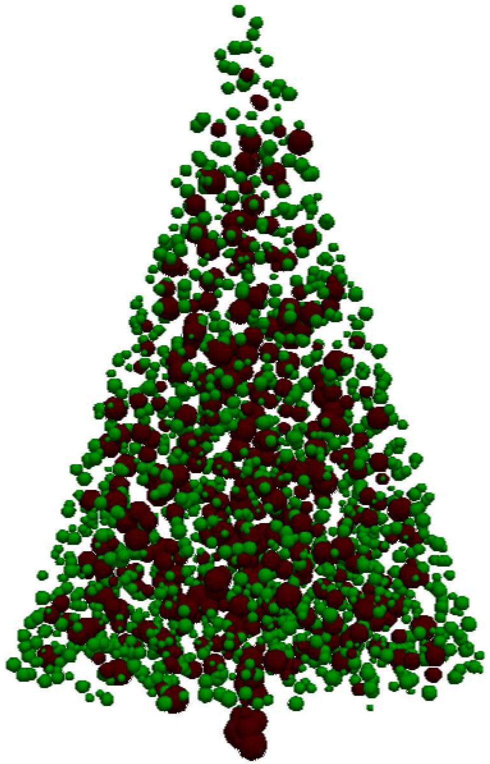
Phase 1
D=0.86 m
h=1.24 m



- Needles are represented by a larger amount of smaller Lagrangian particles
- Twigs and trunk are represented by a smaller amount of larger Lagrangian particles



# Tree and Environment Composition



## Composition of particles

- Twigs
  - Cellulose/dry-fuel
  - $H_2O$
- Needles
  - Cellulose/dry-fuel
  - $H_2O$

## Properties of interest for recreation of tree

- Mass of simulation trees are matched to actual trees
- Dimensions of trees are matched by height and diameter
- Percent of cone volume filled by particles
- Surface-area-of-particles / Volume-of-cone ratio is maintained at ~33 $m^{-1}$

## Air composition

- 23.14% $O_2$ and 76.86% $N_2$ by mass

# Resulting Simulations

# Calibrated Model, Based on Phase 0

Flux/fluence profiles replicated from tests

Representative fuel source for combustion reactions

- Octane

EDC Combustion model

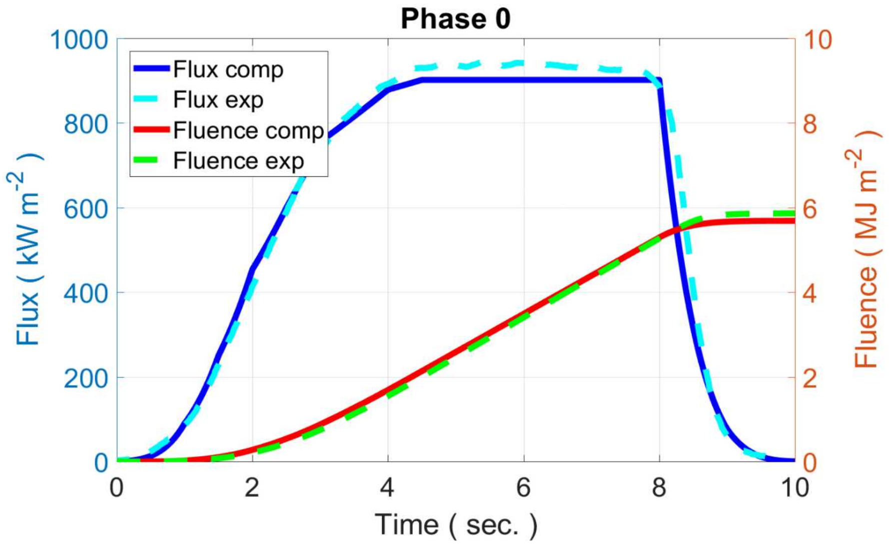
- Extinguishing (γχ=0) occurs at ~48 sec., similar to test.

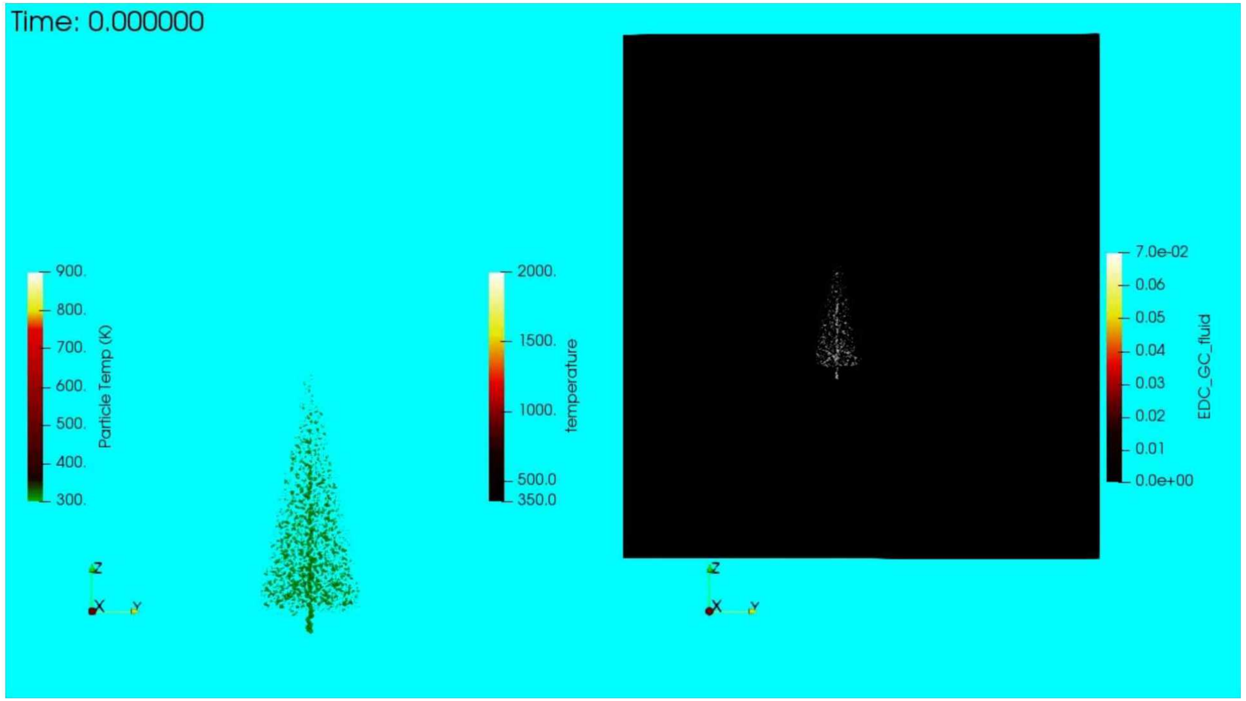
Resultant model was calibrated by adjusting particle composition:

- Needles: 75% fuel / 25% $H_2O$
- Branches: 70% fuel / 30% $H_2O$

Resultant model had composition dryer than suggested by literature[2]:

- Not unexpected: Drag model is off, and conduction between particles is not considered.
- 5% difference between needles and branches still respected, however.




[2] C. Philpot, "The Moisture Content of Ponderosa Pine and Whiteleaf Manzanita Foliage in the Central Sierra Nevada," U.S. Deparetment of Agriculture - Forest Service, Berkeley, California, 1963.

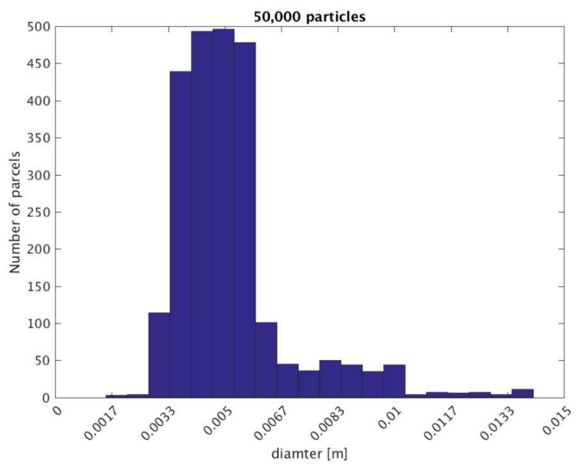
Initial model developed with 55k particles, but what defines an appropriate tree representation?

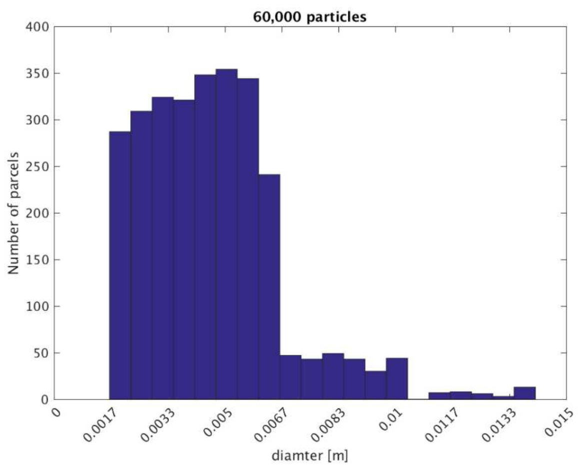
# Study on Total Particles Used to Represent Tree

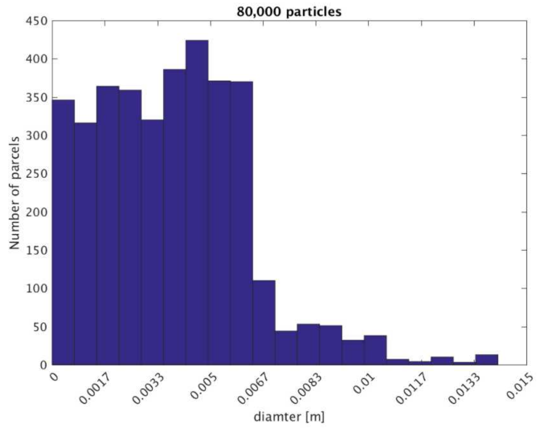
Sobel Sequence determines random, uniform distribution of particles within conical volume

Size distribution study

- Studied mass loss under Phase 0 flux/fluence conditions using different number of particles to represent tree
- Key parameters were preserved: (1) Initial mass, (2) surface area, and (3) tree dimensions were maintained constant
  - Particle size distribution was modified to maintain total SA as number of particles was increased.



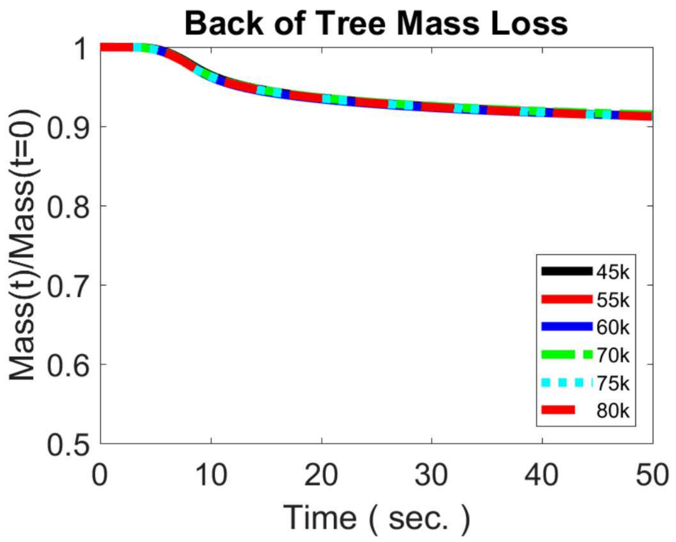



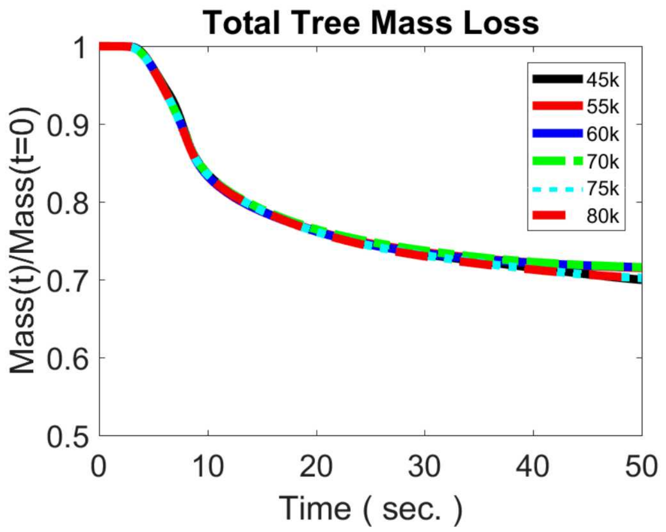
# Tree Mass Loss with Various Representations

As long as key parameters were preserved, results were comparable using different number of particles:

- ~28% total mass loss
- ~9% lost on back portion



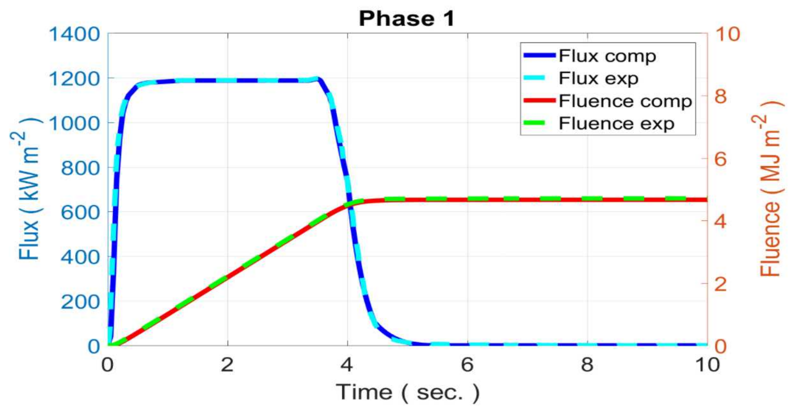

| Tree Composition | Extinguishing time (sec) |
|---|---|
| 45k | ~50 |
| 55k | ~48 |
| 60k | ~48 |
| 70k | ~49 |
| 75k | ~49 |
| 80k | ~50 |

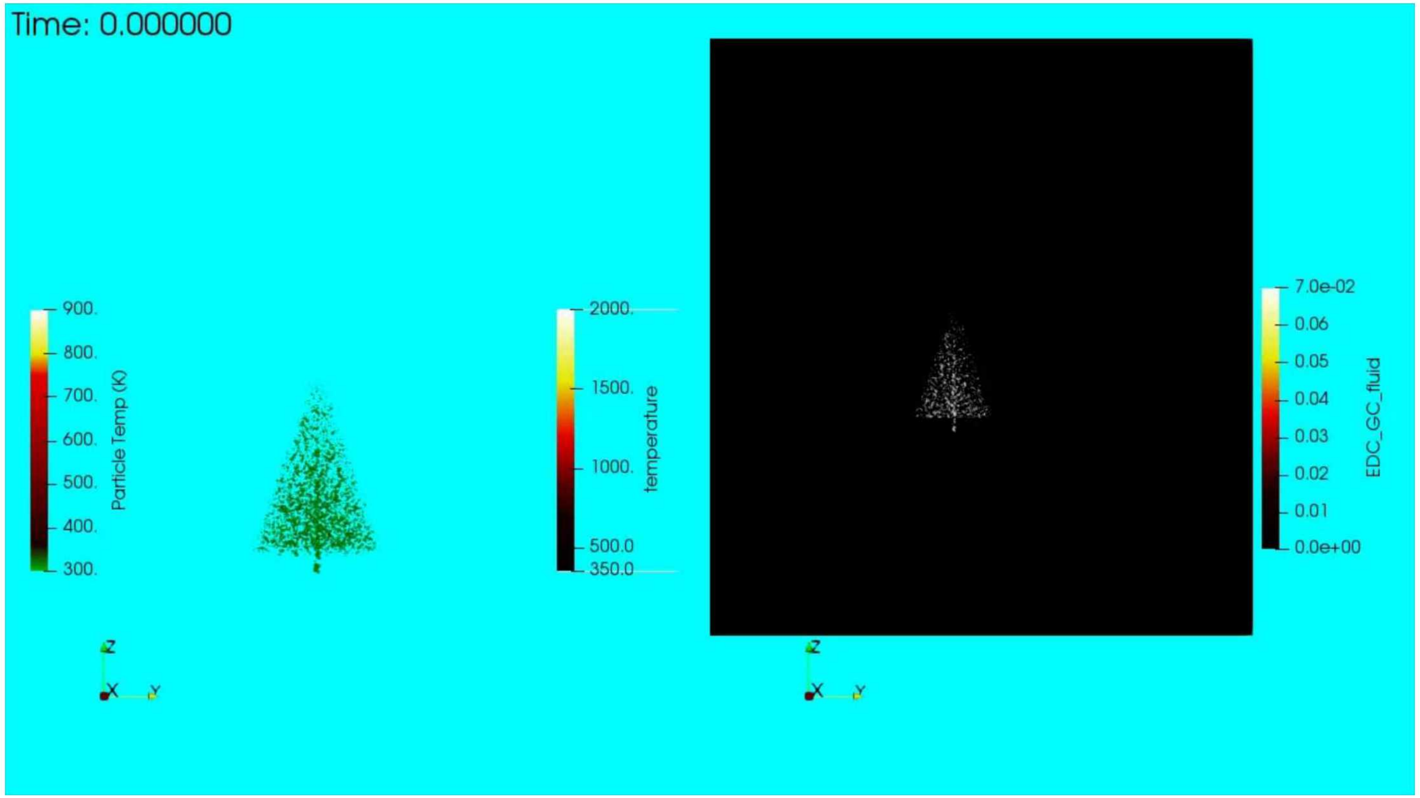



60k particles was chosen as baseline

# Applying Model to Phase 1 Conditions…

# Test Videos of *Phase I, Tree I* and Preliminary Simulation




Test behavior was unexpected!

- Preliminary model predicted ignition (20 sec duration), but ignition was only briefly observed in test
- Based on Phase 0 test results, prolonged ignition would have been expected, but it was not observed
  - Therefore => Use simulation tools to understand potential factors influencing discrepancies

# Post-test Analysis on Phase 1, Tree 1 Test

## Test Observations

- Tree ignited, but only for a brief period of time
- Large **cloud** observed blowing towards direction of heat source

## Hypothesis

- Moisture content of trees could have contributed to various effects:
  1. Moisture content could have been higher in Phase 1 tree
     - Lowers likelihood of ignition due to latent heat of $H_2O$ within tree
  2. Trees with higher moisture concentrations could produce larger **vapor cloud,** as observed:
     a) Cloud could cause significant attenuation of radiant heat flux experienced by tree
     b) Cloud could cool combustible matter, thereby reducing temperatures near incident flux
- Wind direction and speed could have also negatively impacted tests
  - Strong winds in direction of heat source can blow vapor/soot towards source, further attenuating incident radiation

# Can we use our model to test our hypothesis?

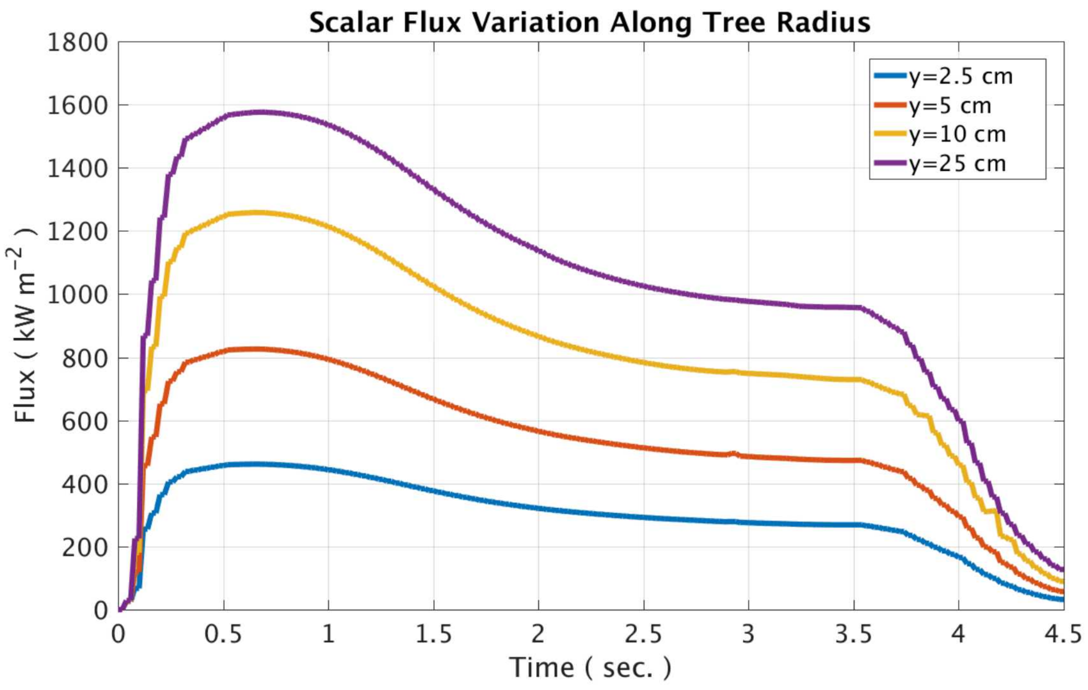
# Scalar Flux Variation Within a Tree

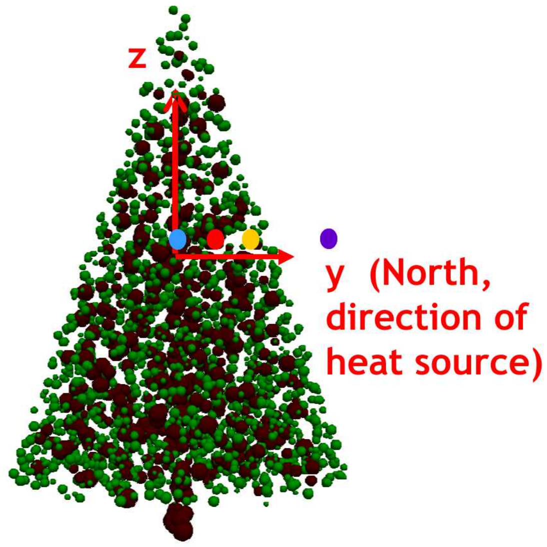


With 4-second heat flux exposure:

- Model captures scalar flux attenuation towards tree center
  - Peak incident flux is highest on radii further away from tree center in the north direction (purple line)

**Attenuating effects of macro tree components are apparent, but could the incident flux be affected by particulate or vapor?**



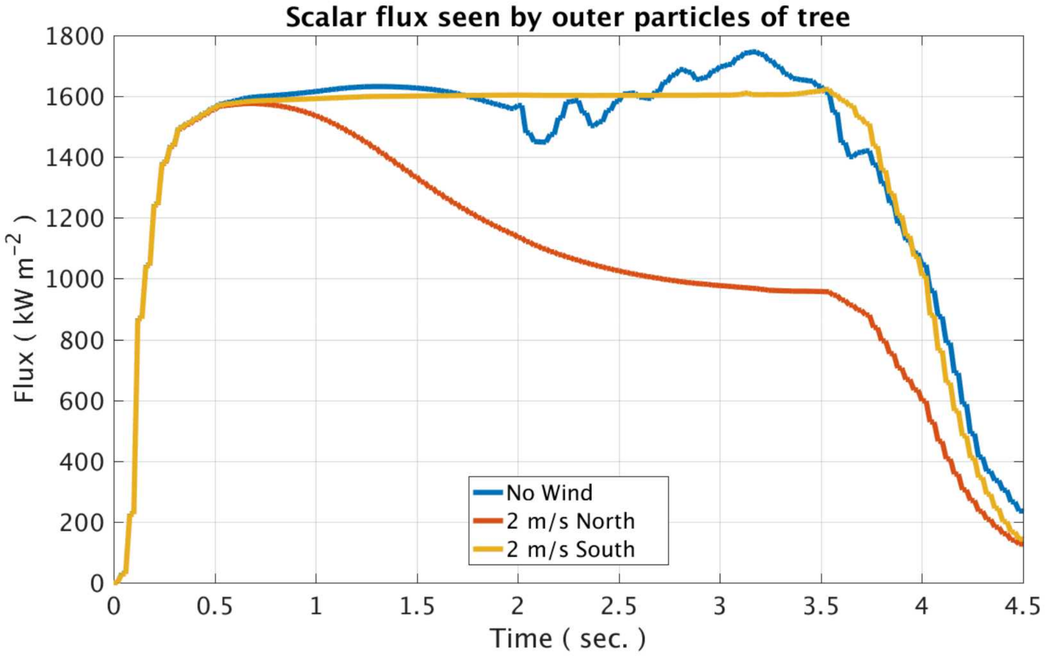
# Particulate/Wind Effects on Flux observed by tree

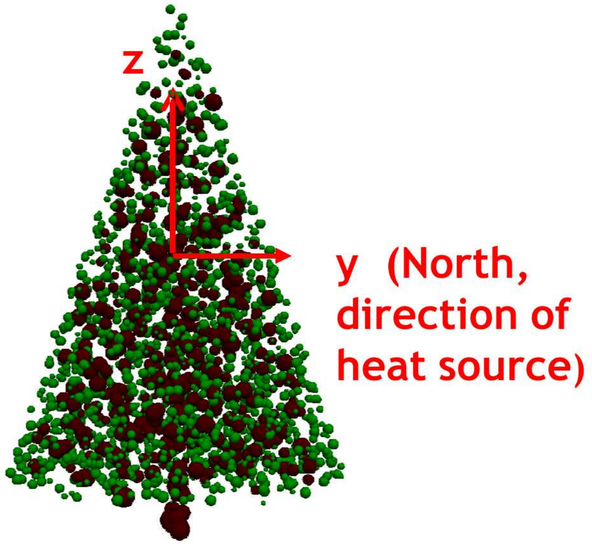
Wind blowing North (towards the heat source) results in obstruction on incident flux due to particulate

- Significant attenuation (orange line)

Wind blowing South (away from heat source) removes obstruction of particulate

- Negligible attenuation (yellow line)

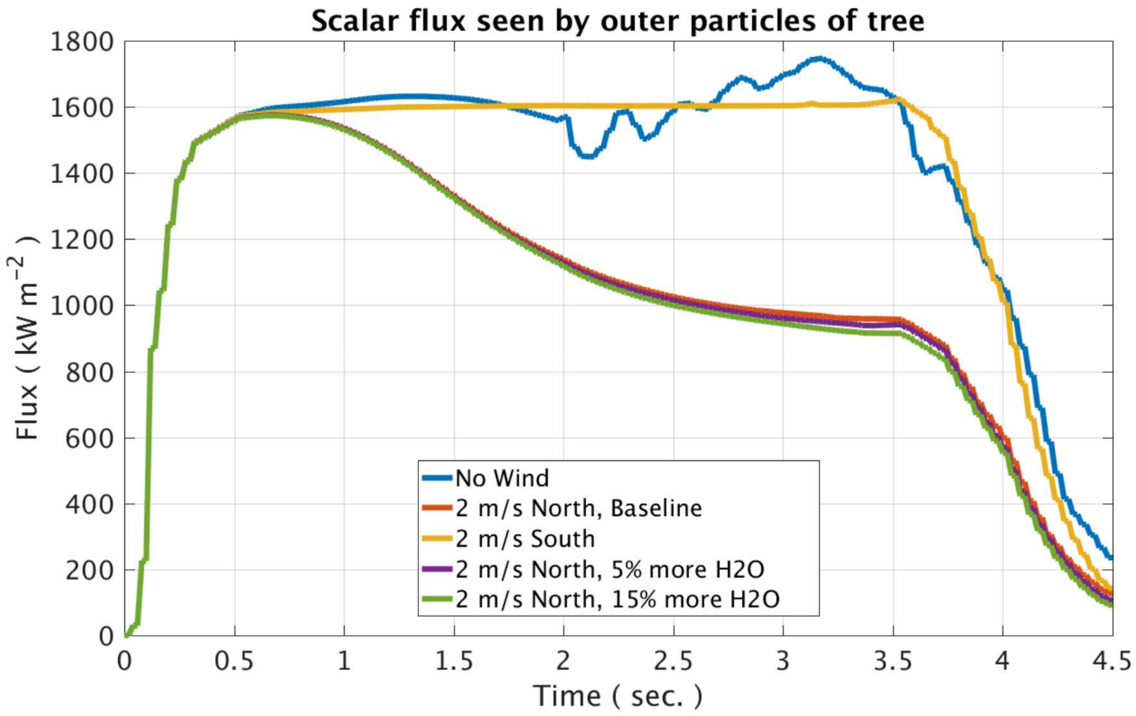


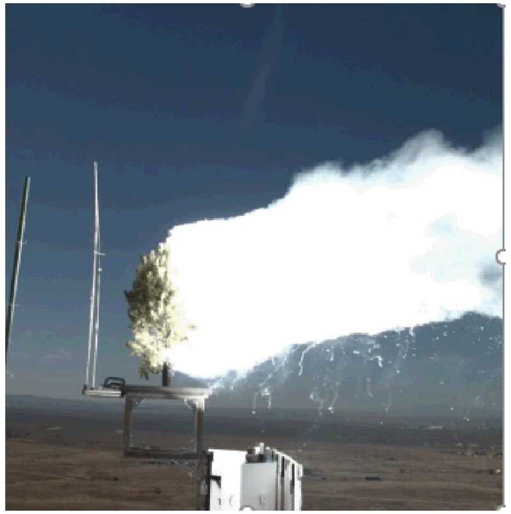
# Moisture/Wind Effects on Flux observed by tree

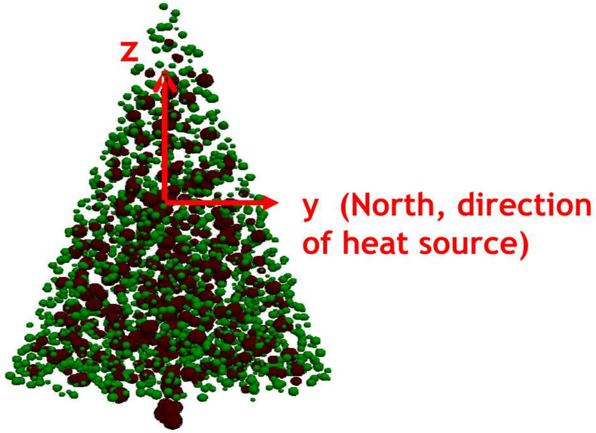
Moisture composition of tree particles had minimal effect on incident heat flux when compared to the effect of wind, but…

- Scattering effect of evaporating droplets (see image) not captured by Fuego simulation, only absorption/emission of water vapor [3] [4].
  - Potential impact captured by attenuating effect of other participating media (e.g. soot)




MH17






[3] D. Martin, "The Use of a Water Mist Curtain as a Radiation Shield," Department of Fire Safety Engineering, Lund University, Lund, Sweden, 2015.
[4] L. Dombrovsky, V. Solovjov and B. Webb, "Attenuation of Solar Radiation by a Water Mist From the Ultraviolet to the Infrared Range," Journal of Quantitative Spectroscopy & Radiative Transfer, vol. 112, pp. 1182-1190, 2010.

**Slide 24**

**MH14** Note that I could have a plot where I run a simulation with different soot production rates (can probably easily change that in EDC model)
Mendoza, Hector, 8/30/2019

**MH17** I Could, but probably won't happen today, 10/1/2019
Mendoza, Hector, 10/1/2019

# Summarizing Remarks



- The work outlines capability of using SIERRA/Fuego for modeling meter-scale ignition and burn of biomass exposed to high heat flux scenarios
- A unique approach is taken to construct computational coniferous trees using chemically reacting Lagrangian particles
- Model was calibrated with experimental data from high heat flux tests performed at SNL, and key parameters for modeling were highlighted:
  - Mass, tree dimensions, SA/V ratio, and representative boundary conditions
- Calibrated model helped provide insight to variations in outcomes between Solar Tower Phase 0 and Phase 1 test results
- There is room for improvement and some adjustments need to be made to have this type of model be a more accurate tool, **but current work shows encouraging results to continue pursuing model refinement**.
  - Recommendations:
    - Implement proper handling of scattering of water droplets
    - Conduction between neighboring particles would help capture heat conduction experienced throughout a real tree on fire: Already implemented in Fuego, but not in current models.
    - Drag model needs work (*will be discussed in other presentation of forest model…please attend ☺*)
    - One mesh size was predominantly used and compared to a refined case, but a thorough mesh convergence study is recommended

# Thank you!