An Analytical Framework for Particle and Volume Data of Large-Scale Combustion Simulations

Franz Sauer[1], Hongfeng Yu[2], Kwan-Liu Ma[1]

[1]University of California, Davis
[2]University of Nebraska, Lincoln

Introduction

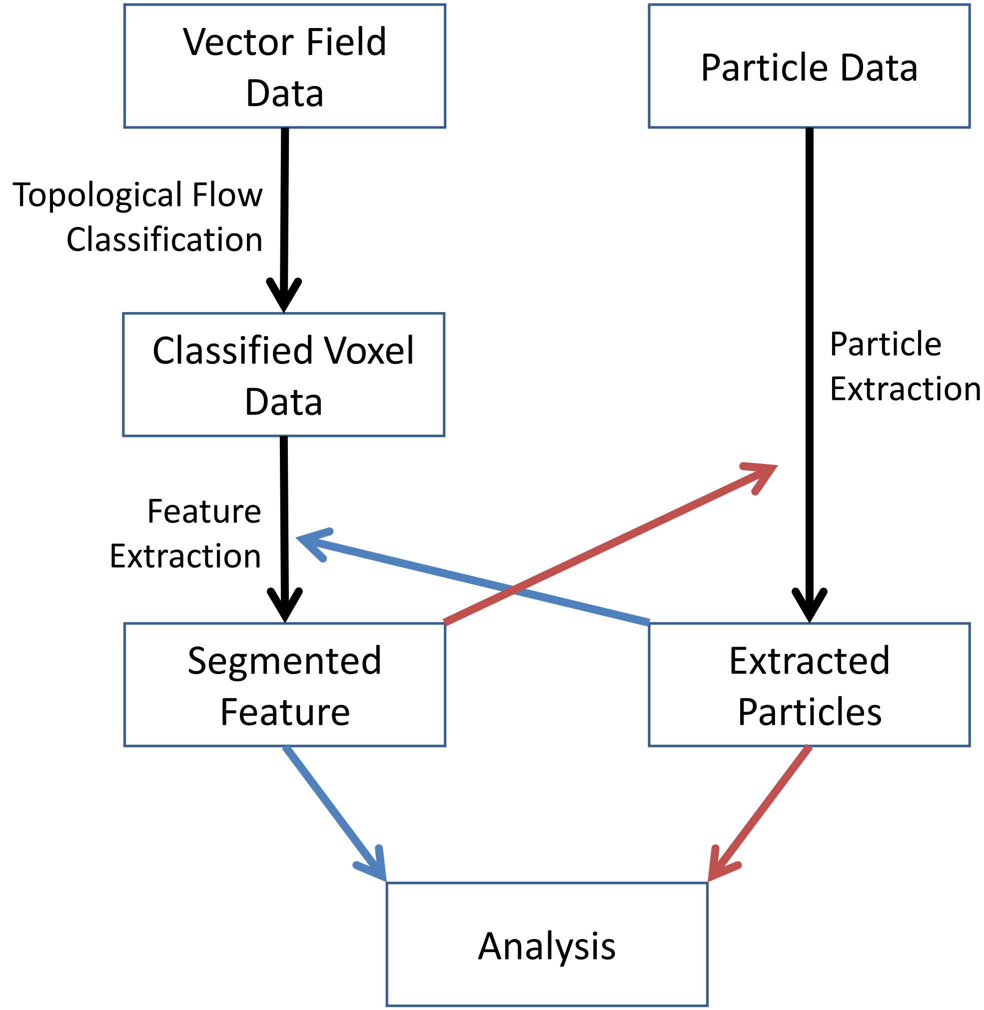
- Detailed combustion simulations
  - Essential for developing high efficiency engines
  - S3D by Sandia National Laboratories
- Two different representations of the flow
  - Eulerian specification (vector field data)
  - Lagrangian specification (particle data)
- Study data from either the Eulerian or Lagrangian viewpoints
- The ability to collate these results can be extremely useful
- Big data issues

Outline

- Framework overview
- <u>Single</u> data processing and analysis
  - Topological Feature Extraction (Eulerian)
  - Particle Query and Analysis (Lagrangian)
- <u>Joint</u> data processing and analysis
  - Feature-based particle query
  - Particle-based volume feature query
- Results
  - Performance tests
  - Example analyses
- Conclusion

Overview

- **Black** arrows represent traditional processing steps
- Red arrows represent feature-based particle query
- Blue arrows represent particle-based volume feature query



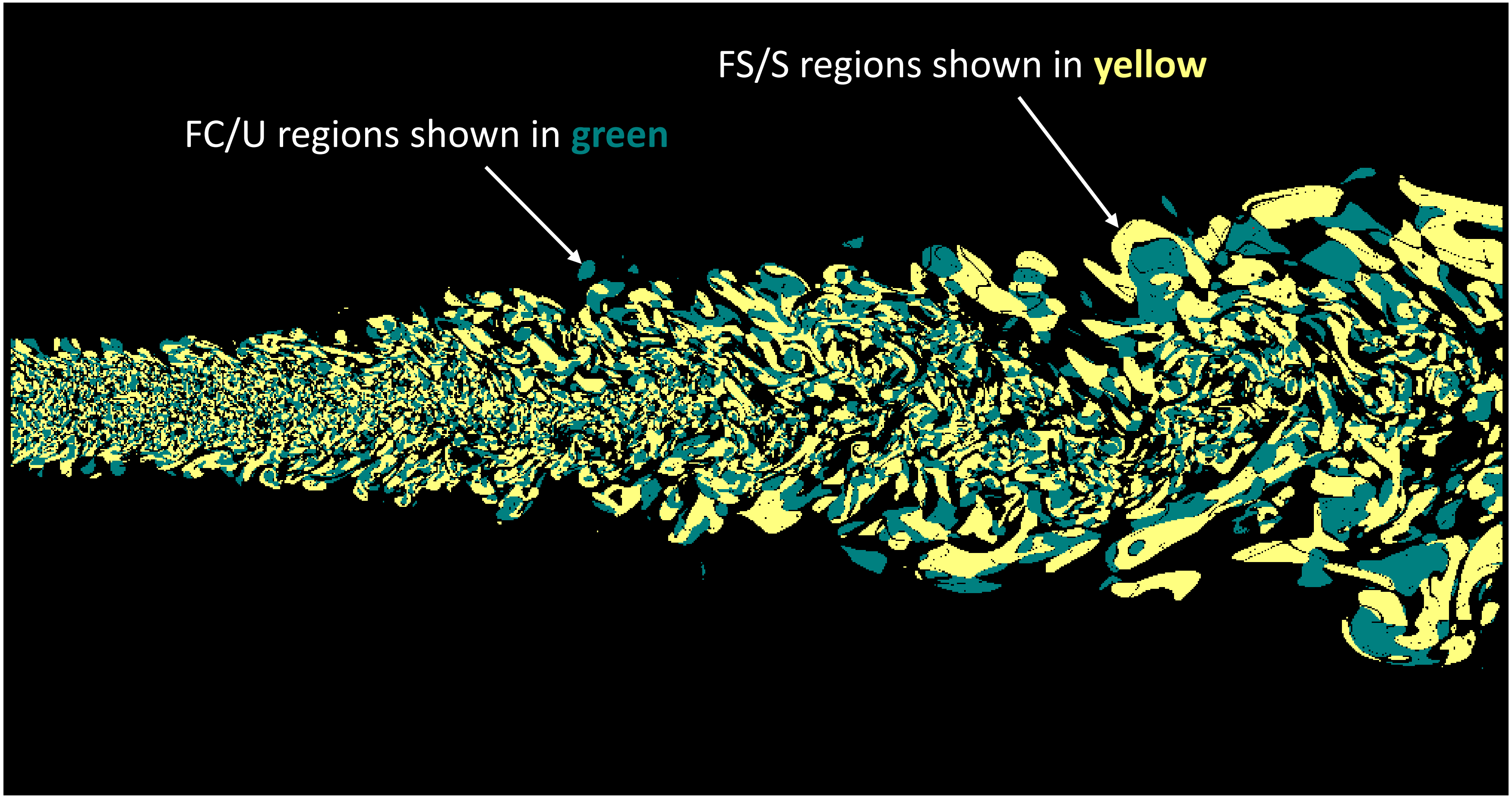
Topological Flow Classification

- Use a method proposed by Chong et al.[1]
  - Compute a local rate-of-deformation tensor
  - Categorize into one of 27 fundamental types
- Only a few dominated patterns present in simulation flows

Classification	Topological Description
2	Node / node / node, unstable (NNN/U)
11	Node / saddle / saddle, stable (NSS/S)
12	Node / saddle / saddle, unstable (NSS/U)
18	***Focus / stretching, stable (FS/S)***
19	Focus / stretching, unstable (FS/U)
20	Focusing / compressing, stable (FC/S)
21	***Focusing / compressing, unstable (FC/U)***

[1]M. S. Chong, A. E. Perry, and B. J. Cantwell. *A General Classification of Three Dimensional Flow Fields*. Physics of Fluids, vol. 2, pp. 765-777, 1990.

Topological Flow Classification



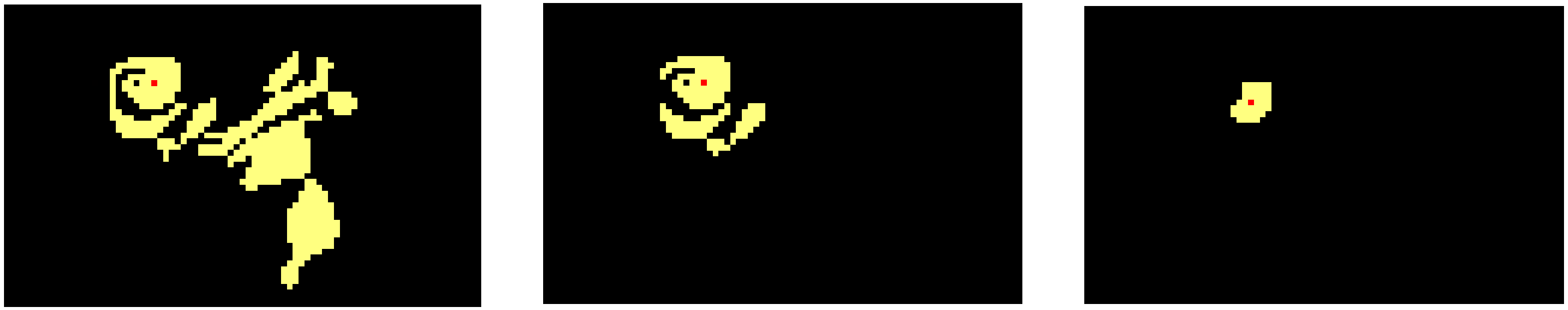
Topological Feature Extraction

- High turbulence leads to features that are heavily interwoven
- Growing regions based on connectivity will span the entire dataset
- Need a way to “pinch off” features of interest
- Use a modified version of standard region growing techniques
  - Measure a voxel’s “connectivity strength”
  - User defined threshold

Topological Feature Extraction

Modified region growing

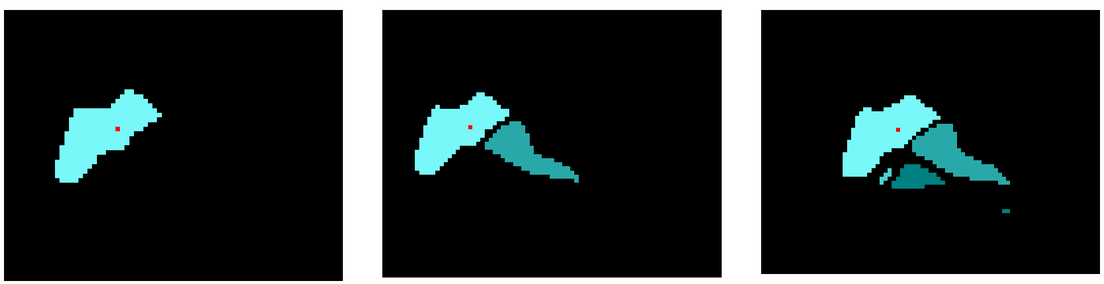
1. Users select a feature of interest by placing a seed point
2. Neighboring voxels of like topotype are added to a queue
3. Iterate through the queue
    a) Check "connectivity strength" by counting like neighbors
    b) Add to region if the count exceeds threshold
    c) Add like neighbors to queue
4. Growing finishes when queue is empty



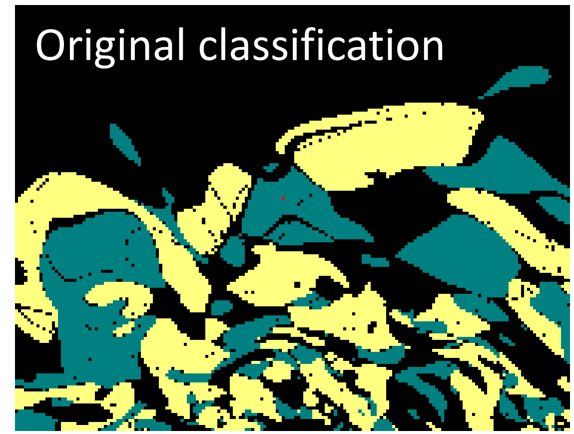
Increasing Threshold →

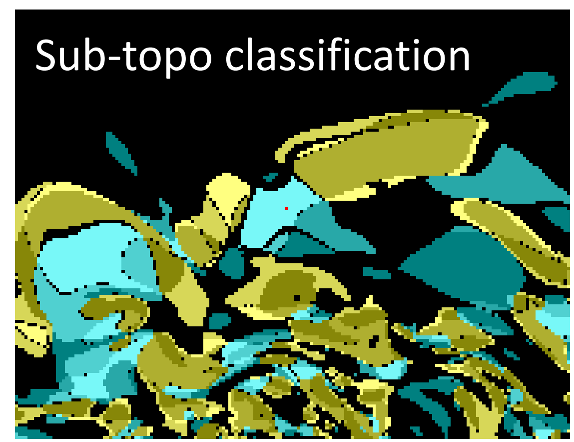
Topological Feature Extraction

- Alternate extraction method using sub-classifications
- Divide classifications into 4 sub-types
- Grow each sub-region separately
  - Count number of bordering voxels
  - Connect according to a threshold
- Adds an extra level of control



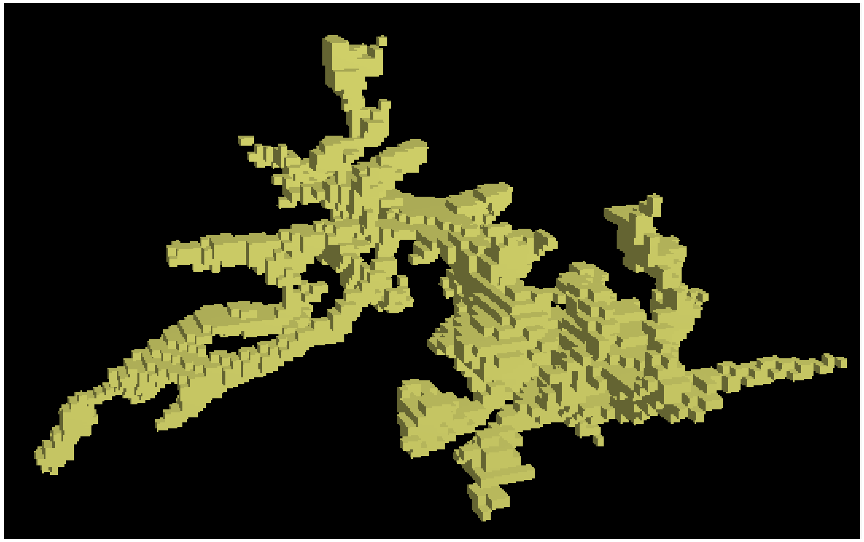
Increasing Threshold →





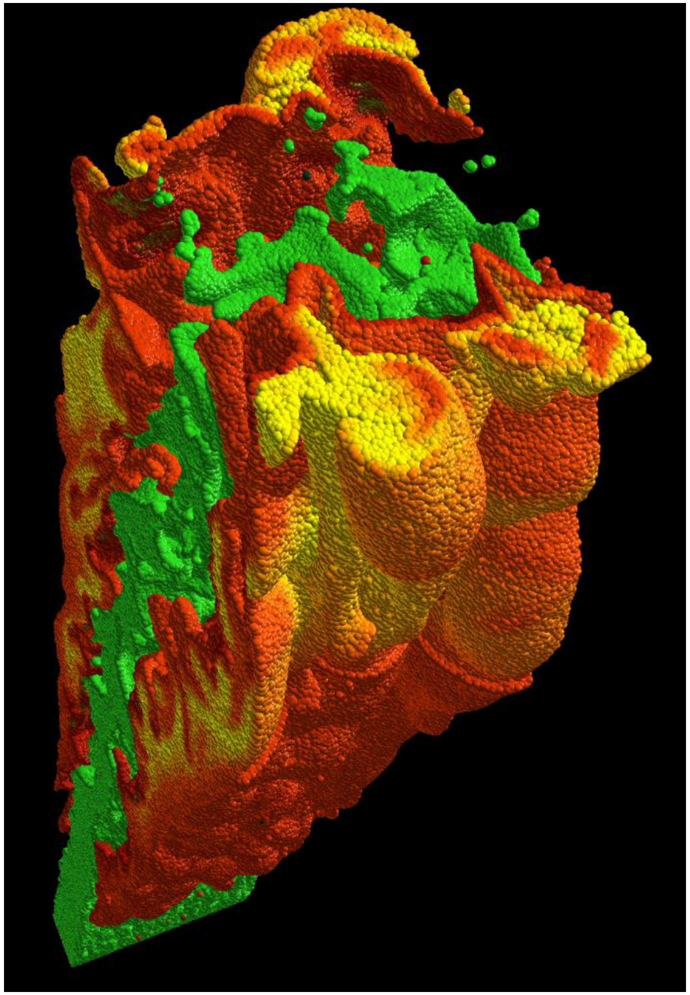
Topological Feature Extraction

- Parallelize via master-worker paradigm
  - Master process views an entire slice
  - 3D domain is split among worker processes
- Grow a 2D region in serial on master node
- Treat each voxel as a seed point and distribute to worker nodes for growing
- Growing must continue across boundaries
  - Send message to neighboring node
  - Add necessary voxels to its queue



Particle Query and Analysis

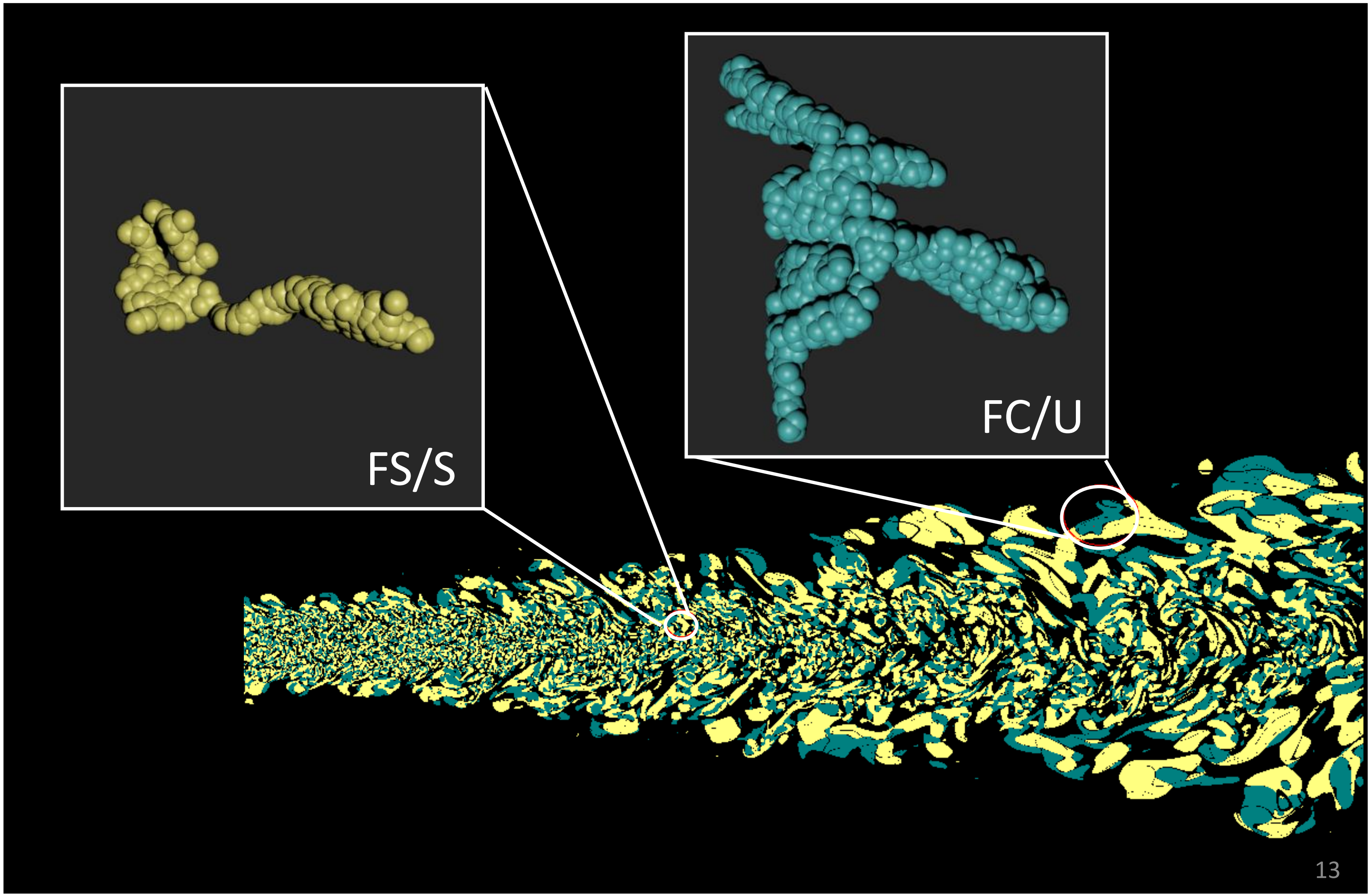
- Extract subsets of particles based on its properties (temperature, mixture fraction, etc.)
- Embarrassingly parallel
  - Each worker node can extract independently
  - Requires a single pass
- Visualized as point-sprites
  - Each node renders its subset of particles separately
  - Combined on master node by checking depth buffers



Feature-Based Particle Query

- Study the properties of features using particle data
- Identify and extract particles encapsulated by a feature of interest
- Extend the particle query to accept voxel data
    - 3D bitmask represents the feature
    - Minimize communication cost
- Map the spatial location of the particle to voxel space
- Check against bitmask

Feature-Based Particle Query



Particle-based Volume Feature Query

- Study flow classifications based on particle data
- Map each extracted particle to voxel space
- Generate a 3D bitmask describing the location of particles
    - Direct comparison to volume data
    - Use as a set of seed points for region growing
- Trajectory assisted feature tracking
    - Assemble particle data into trajectories
    - Use as a correspondence between features at different timesteps

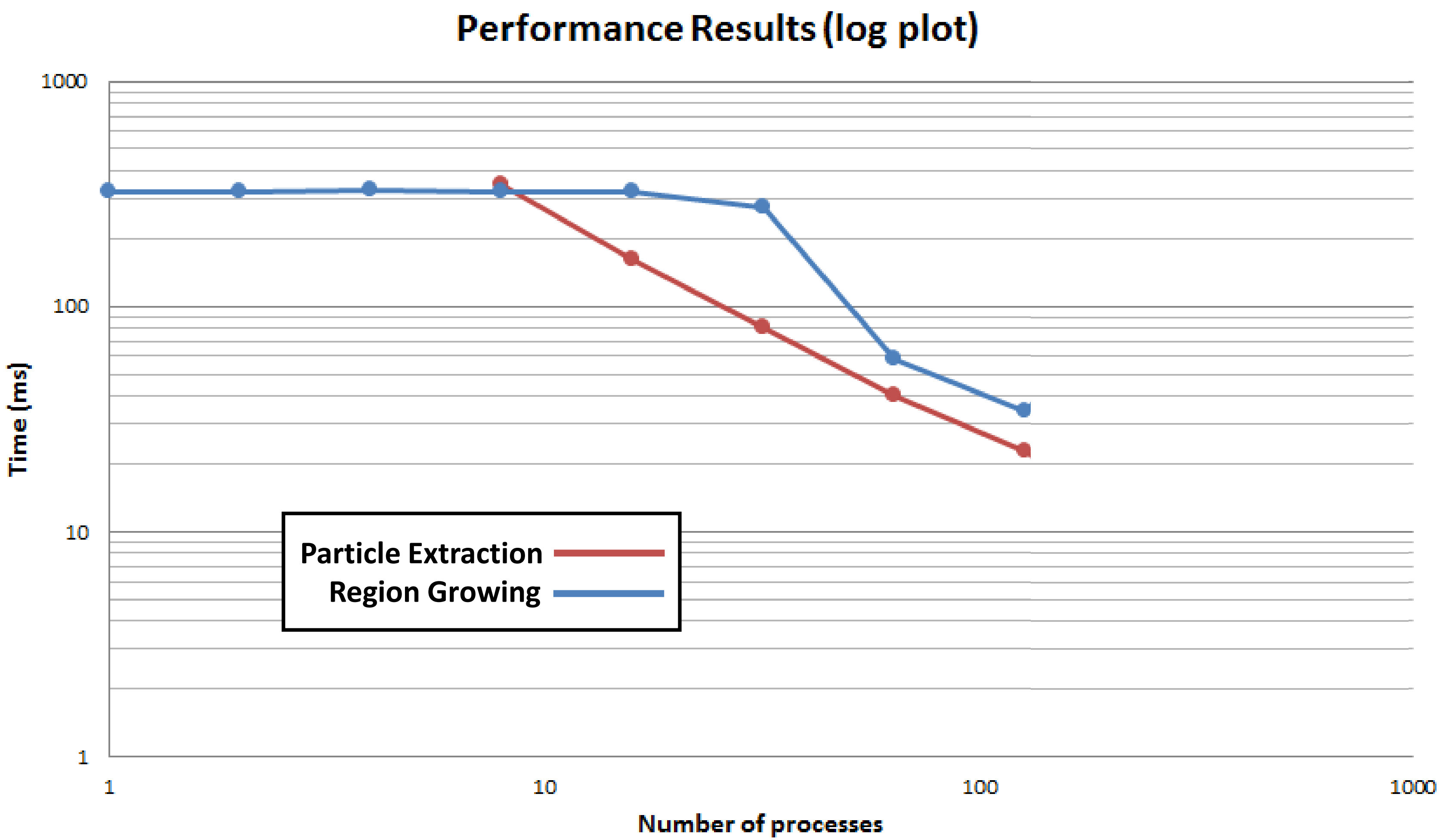
Results

- Real simulation data of a turbulent lifted ethylene jet
  - Vector field data (2025 x 1600 x 400 grid)
  - Particle data (~40 million particles)
- National Energy Research Scientific Computing Center (NERSC)
  - Hopper - 6,384 node Cray XE6 system
  - Each node consists of two AMD ‘MagnyCours’ 2.1-GHz processors

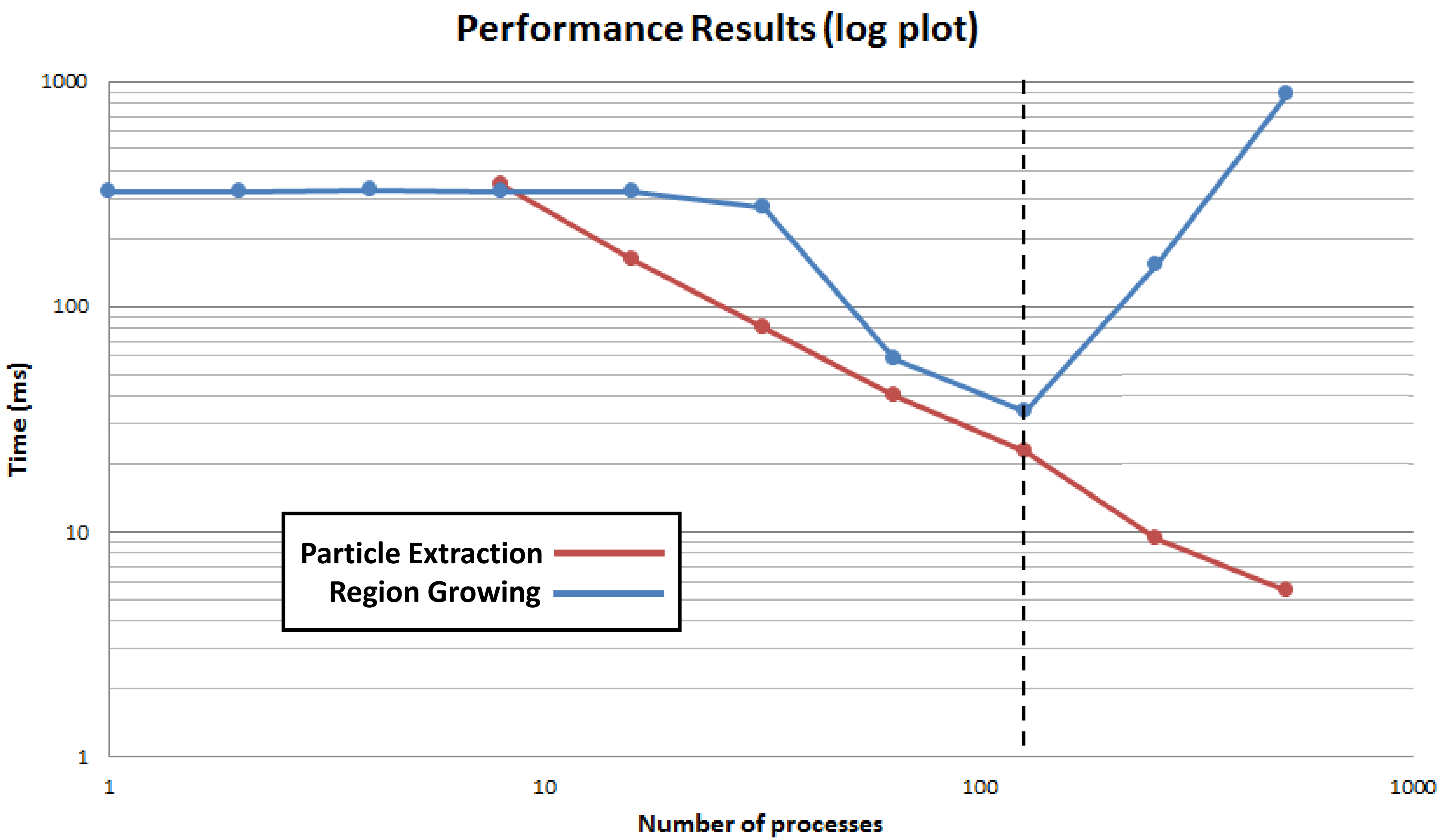
Performance Tests

- Region growing time dependent on feature size
  - Tests involve a feature at a scale of interest to scientists
  - Approximately 10,000 voxels
- Separate tests for feature and particle extraction phases
- Do not reflect I/O times (both the particle and volume data have already been distributed to all nodes)

Performance Tests



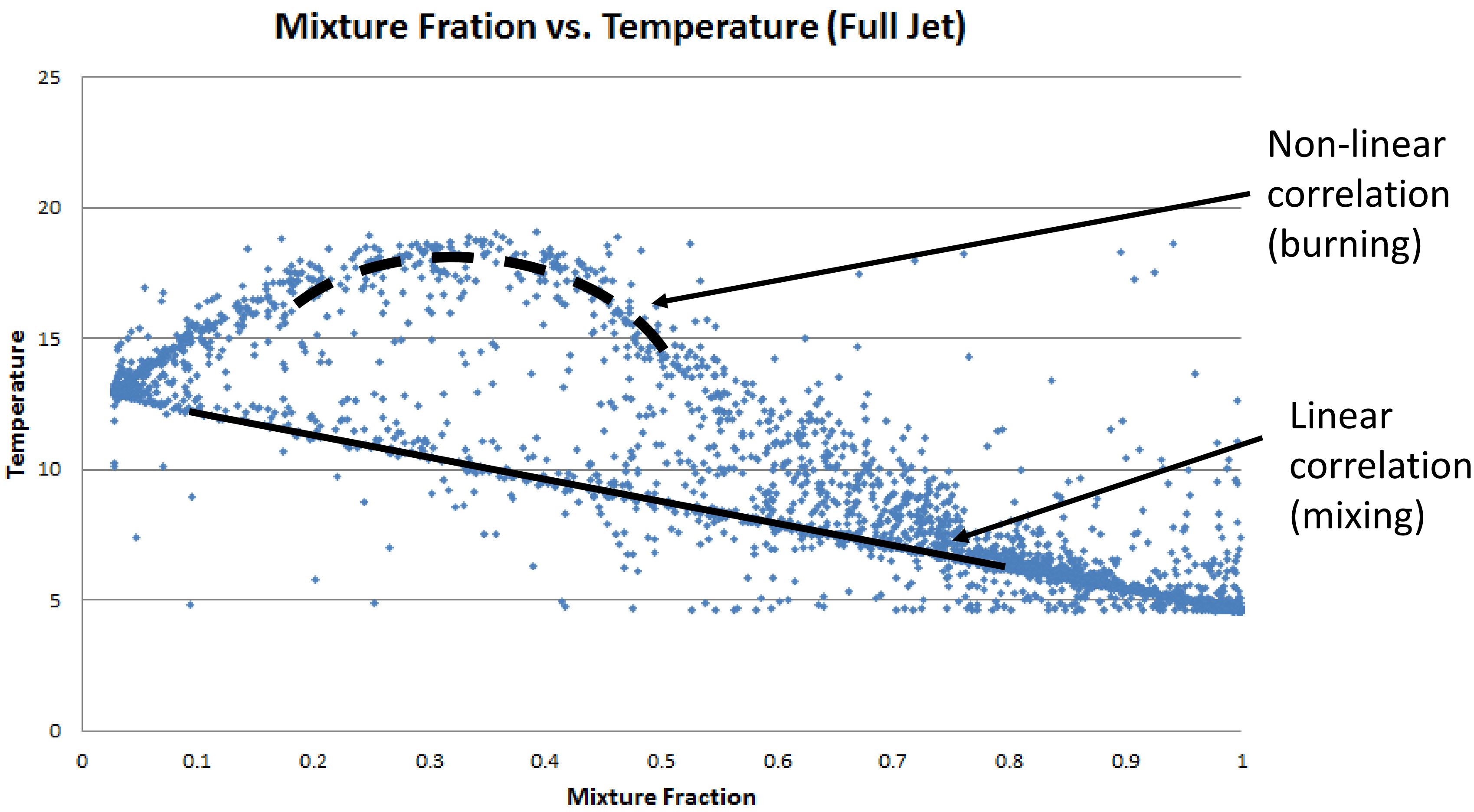
Performance Tests



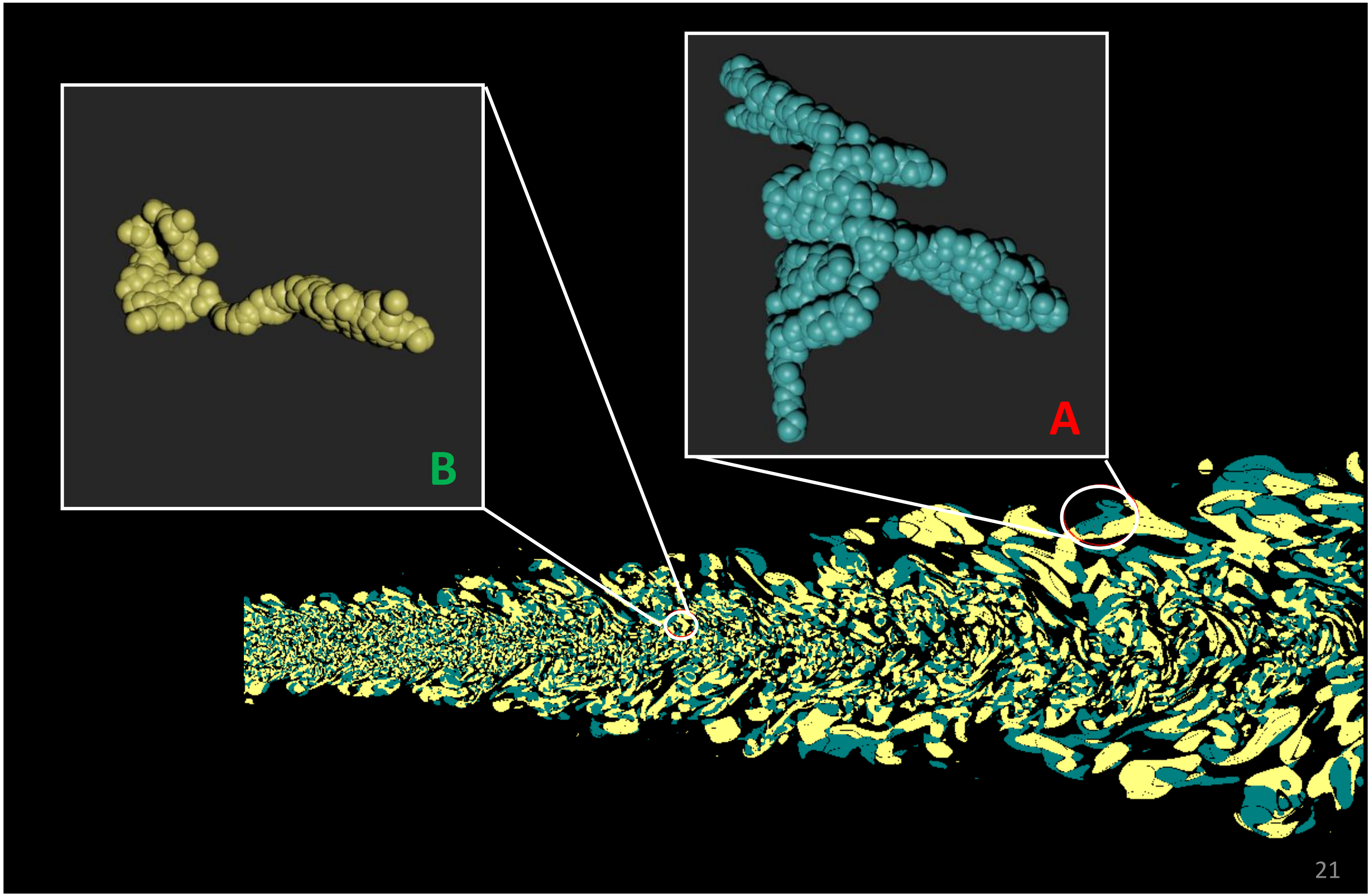
Sample Analyses

- Feature-based particle query
- Dataset represents a non-premixed jet
  - Fuel and oxidizer are injected separately
  - Mixing and burning in some portions of the jet
  - Just mixing in other portions
- Mixture fraction becomes an important variable
- Look at relationship with temperature to determine if burning occurs

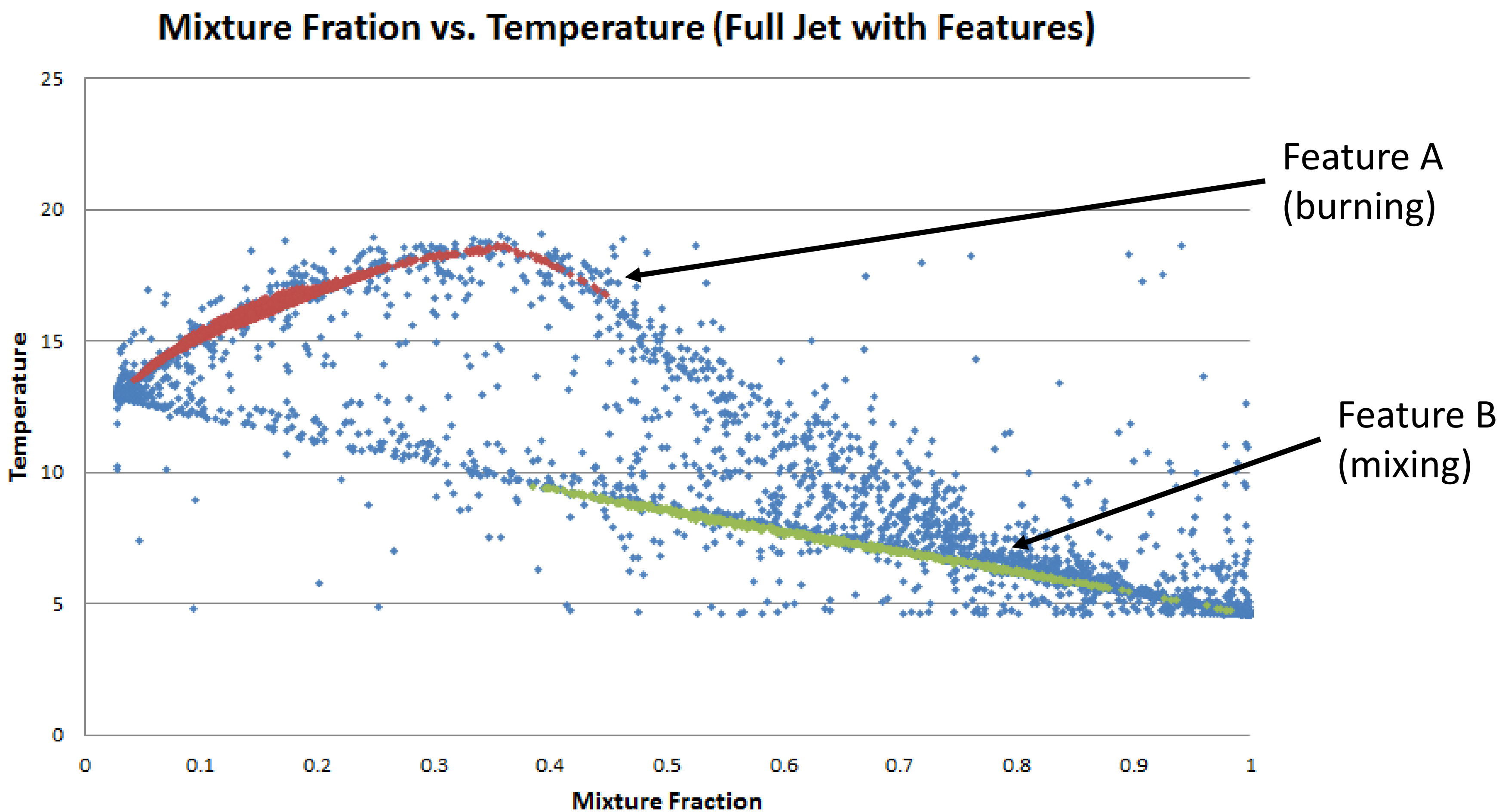
Sample Analyses



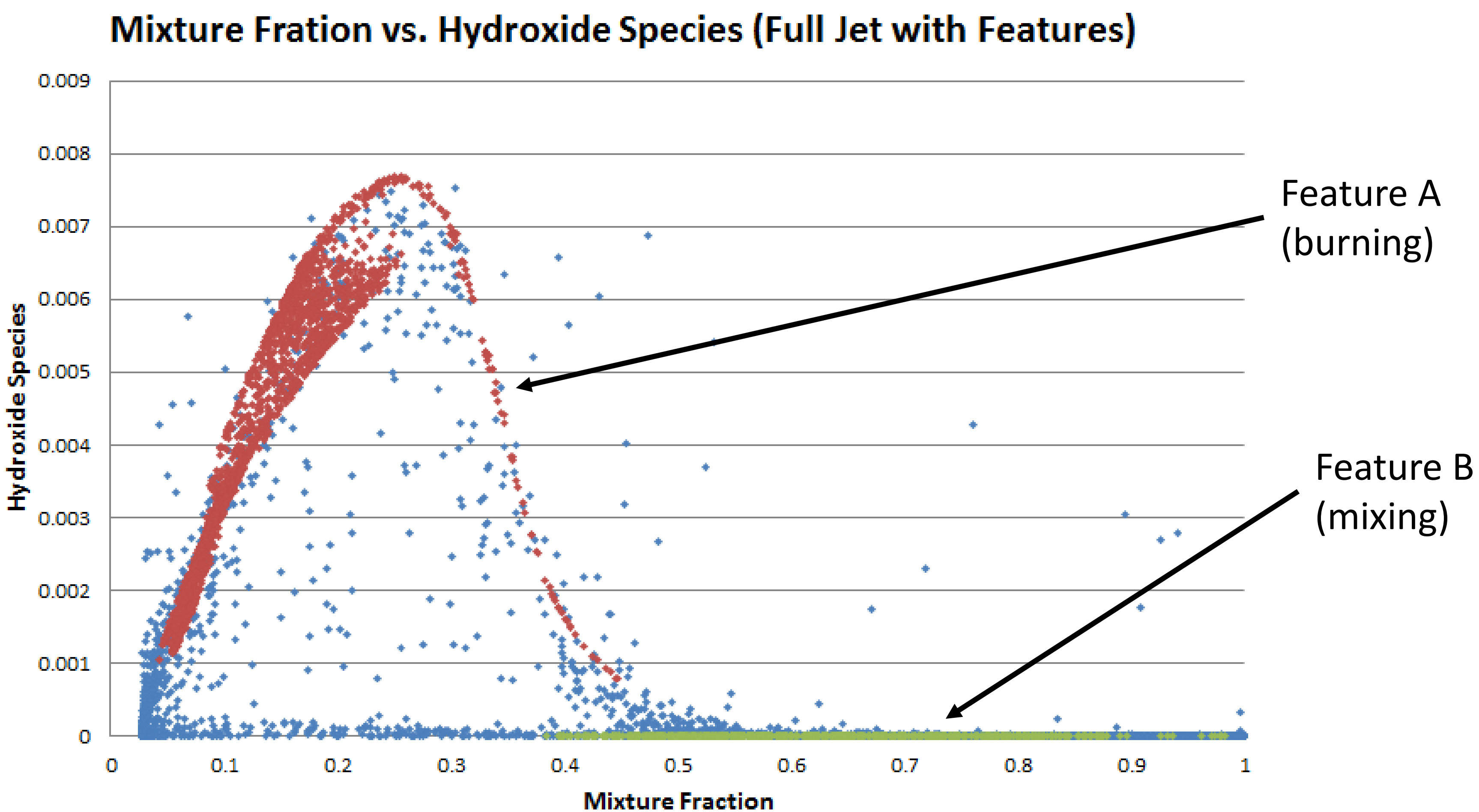
Sample Analyses



Sample Analyses



Sample Analyses



Sample Analyses

- Particle-based Volume Feature Query
- Range query on temperature
  - Extract the hottest/coldest parts of the jet
  - Look at the flow classifications
- Hot portions: 35.9% FS/S and 23.2% FC/U
- Cold portions: 32.6% FS/S and 21.6% FC/U
- Similar breakdown for mid range temperatures

Conclusion and Future Work

- Present a framework that performs parallel data analyses on particle and volume data
- Modifications to region growing to aid in extracting turbulent flow features
- Parallelization leads to large speedups
  - Particle extraction scales very well
  - Region growing portion can still be improved
- Generalize to other datasets
- Explore trajectory assisted feature tracking
- In situ analysis and visualization

Acknowledgments

- Sandia National Laboratories
- Jackie Chen and Ray Grout
- National Science Foundation through grants OCI-0905008, OCI-0850566, OCI-0749227, CCF-0811422
- Department of Energy through grants DEFC02-06ER25777, DE-CS0005334, DE-FC02-12ER26072 with program managers Lucy Nowell and Ceren Susut-Bennett

Thank You

Questions?