

# One-Dimensional Turbulence (ODT)-generated Manifolds for Large Eddy Simulation (LES) of Two-Phase Flows

SAND2009-4875C

Charles Reid

Intern, Combustion Research Facility (CRF)  
Ph.D. candidate, University of Utah (ChemE)

Mentor: Alan Kerstein

Intern Symposium Presentation  
Sandia National Labs  
Summer 2009



# Overview

- This Summer at Sandia
  - Internship and research done this summer
- Background Information
  - One-Dimensional Turbulence (ODT)
  - Large Eddy Simulation (LES)
- Intended use
  - Coal combustion
  - Manifold creation for LES using ODT



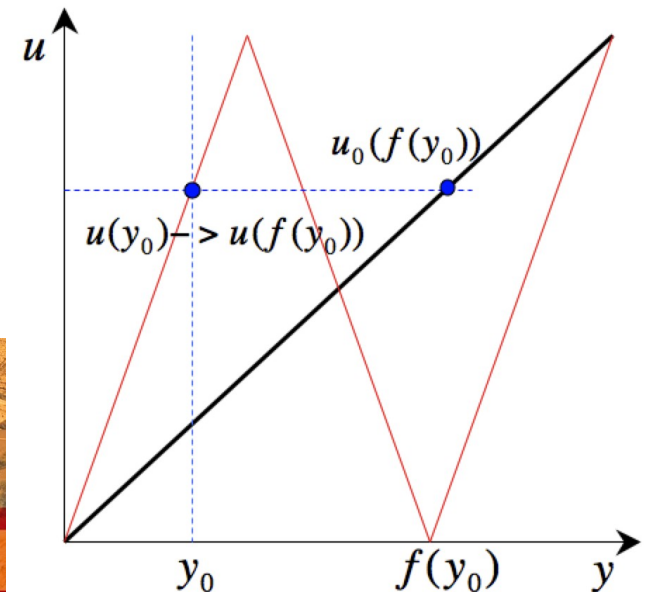
# This Summer at Sandia

- Mentor: Alan Kerstein
- One-dimensional turbulence code
  - Need for collaboratory tools
  - Doxygen, Subversion (svn)
- ODT lecture series
  - Need for more collaboratory tools
  - SmartBoard - Idea-sharing



# Background Information: One-Dimensional Turbulence

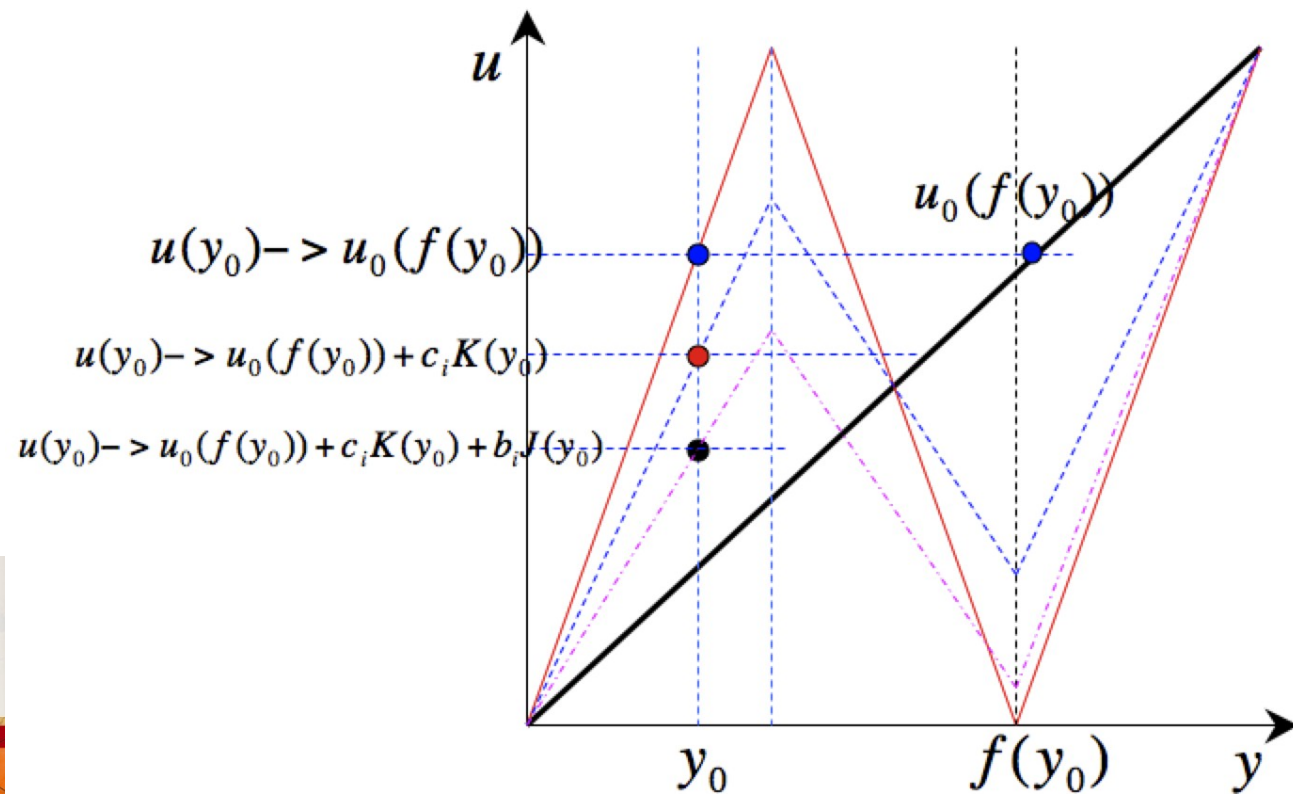
- Reduce 3 dimensions to 1 dimension: a line
- Convection term is stochastic, represents eddies
- Triplet map rearrangement:
  - Pick an eddy length scale (figure: tick marks)
  - Compress it by 1/3 and make 3 copies of it
  - Reverse the middle copy to remove discontinuities





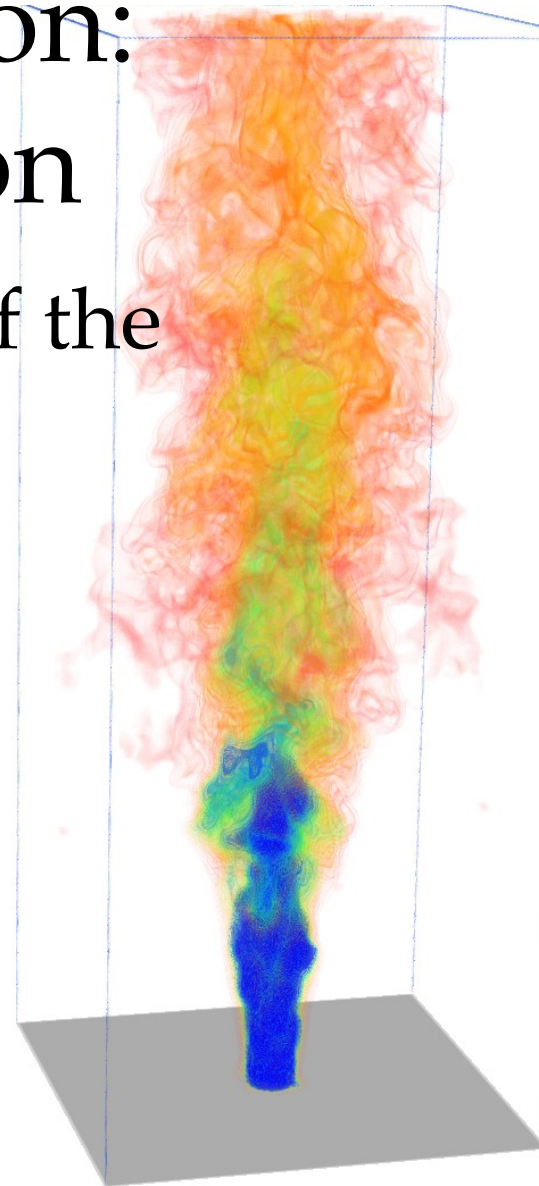
# Background Information: One-Dimensional Turbulence

- Triplet maps represent the turbulent convection (the "eddy")
- Conservation of mass and momentum are satisfied



# Background Information: Large Eddy Simulation

- LES captures large-scale structures of the turbulent flow
- Large scales are resolved
- Small scales are modeled
- Chemical reactions & particles:  
All happen at unresolved scales!
- LES creates need for subgrid models



# Background Information: Large Eddy Simulation

- If your LES code tracks a variable  $Z$ , it throws away small scale information
- The subgrid portion (the part that's thrown away) is  $Z'$
- The resulting "filtered" variable is  $\bar{Z}$

$$Z = \bar{Z} + Z'$$

- You are spatially-averaging, instead of time-averaging





# Intended Use: Coal Combustion

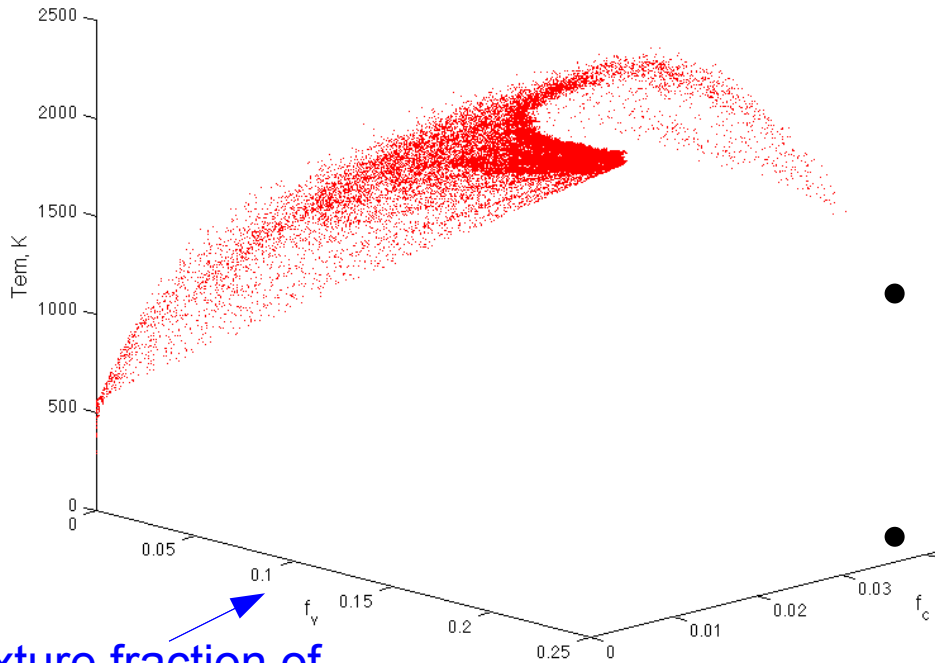
- The ultimate goal is to simulate coal combustion and gasification
- Subgrid models for:
  - Reacting coal particle chemistry
  - Coal particle velocity
  - Combusting volatile gases
  - Soot particles
- Complex multiphysics problem





# Manifold Methods for Reaction Manifolds

- Thermochemical state as function of reduced set of independent variables
- Dimensionality reduction
- In LES, this is called the "reaction model"



mixture fraction of  
volatile coal gas

mixture fraction of  
char fraction in coal particles

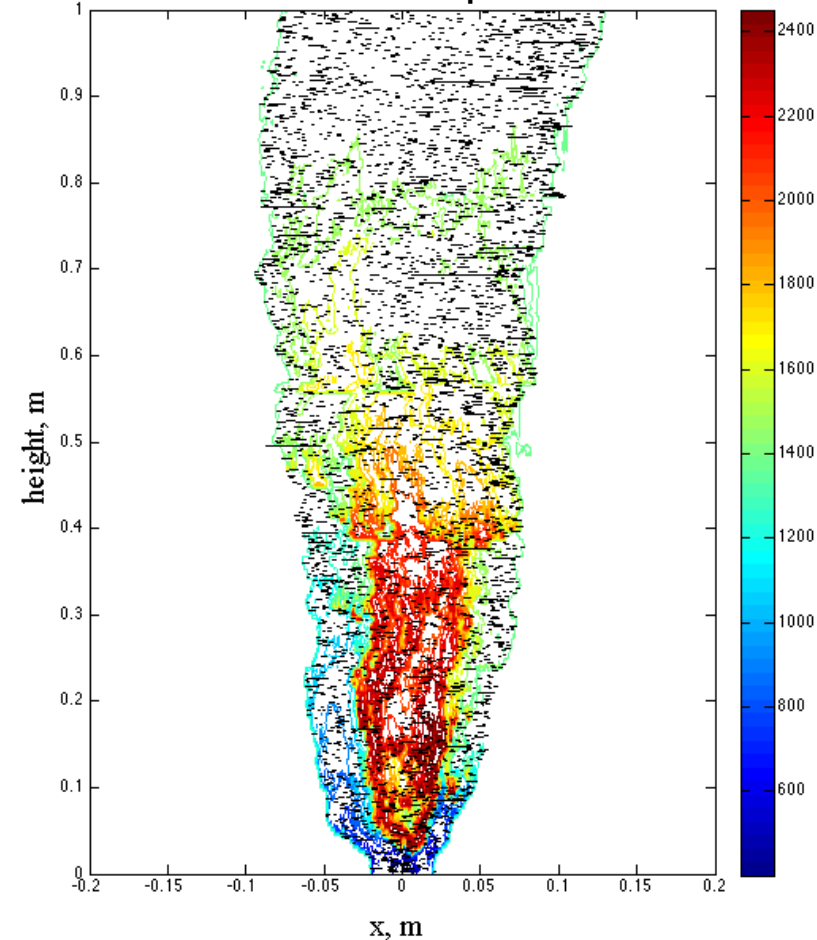
Intern Symposium Presentation  
Sandia National Labs  
Summer 2009



# ODT and Manifolds

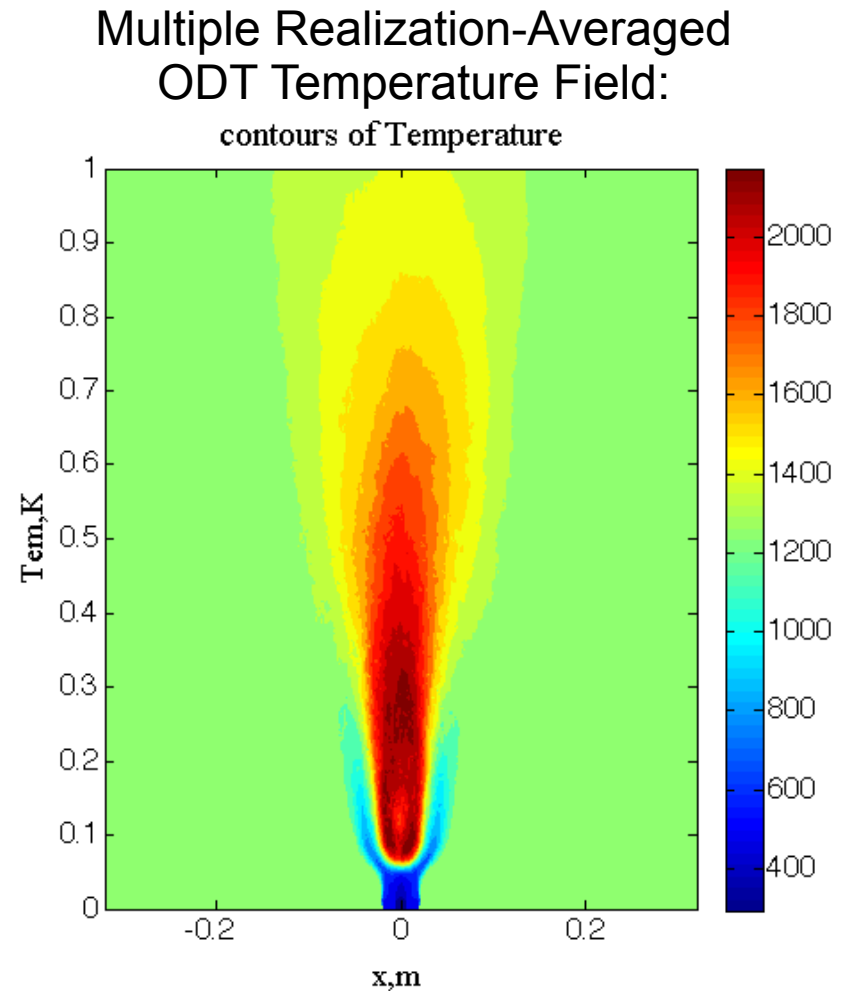
- ODT removes nonlinear convection term
- Governing equation becomes 1-D reaction diffusion equation
- ODT resolves smallest scales of flow
  - particles
  - reactions

Instantaneous ODT Temperature Field



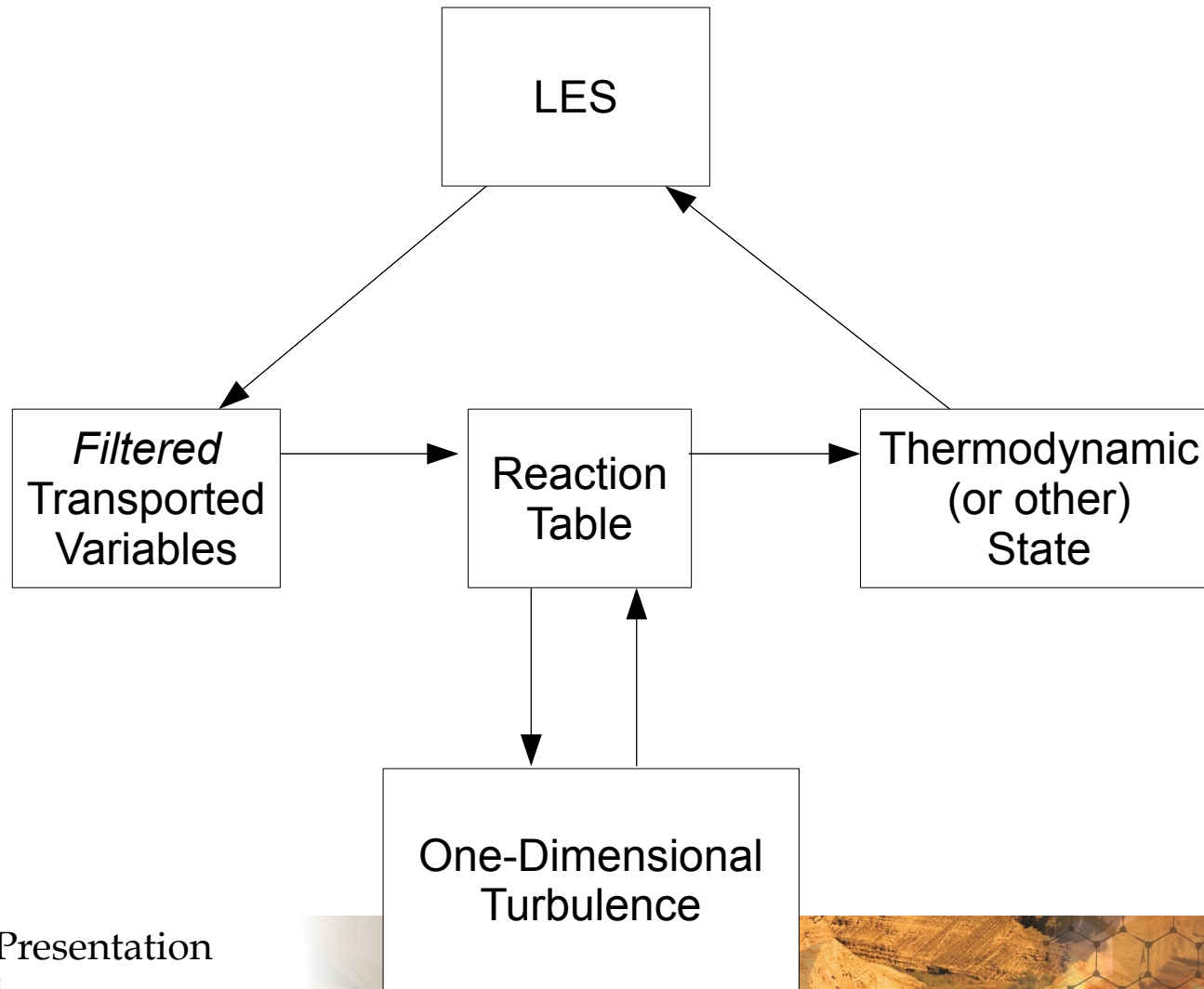
# ODT and Manifolds

- Statistics from multiple ODT realizations
- Tabulate manifolds for large eddy simulation
- Finding thermochemical state is made computationally cheap





# Overview/Summary



# Conclusions & Future Work

- One-dimensional turbulence statistics show good agreement with DNS statistics
- Use ODT to identify, generate, and tabulate manifolds
- Use manifolds to reduce computational cost
- "Make room" for better and more expensive models



# Acknowledgement

- Dr. Alan Kerstein  
Sandia mentor
- Dr. Phil Smith  
University of Utah advisor
- Sandia National Labs & its employees





# Questions

Intern Symposium Presentation  
Sandia National Labs  
Summer 2009

