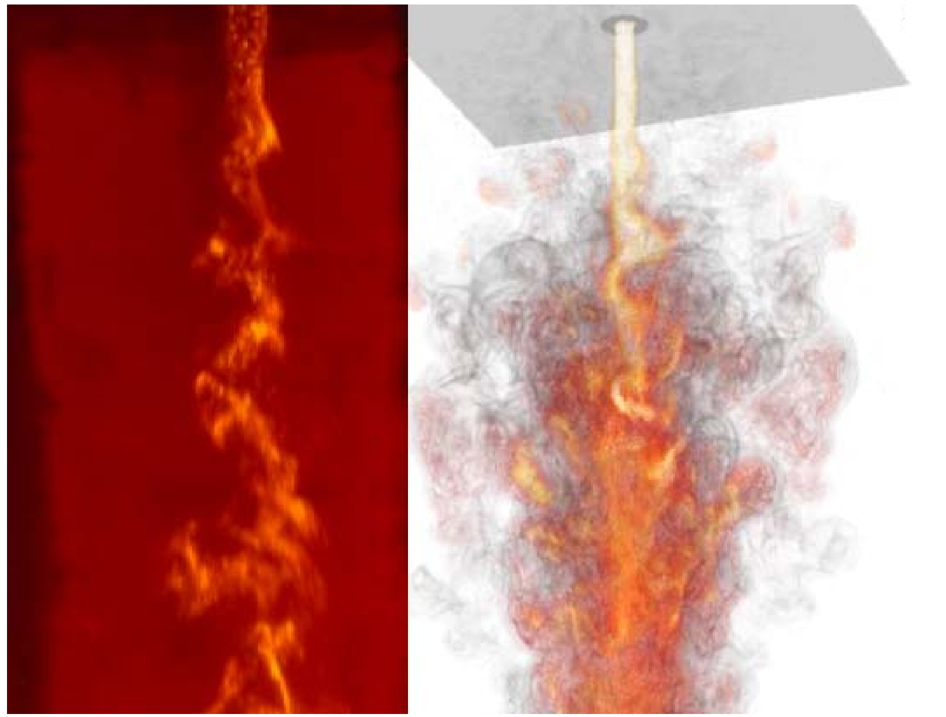
Simulation of Coal Gasification Using Large Eddy Simulation & Direct Quadrature Method of Moments



Charles M. Reid, Jeremy N. Thornock, Philip J. Smith

Institute for Clean and Secure Energy
Chemical Engineering Department, University of Utah

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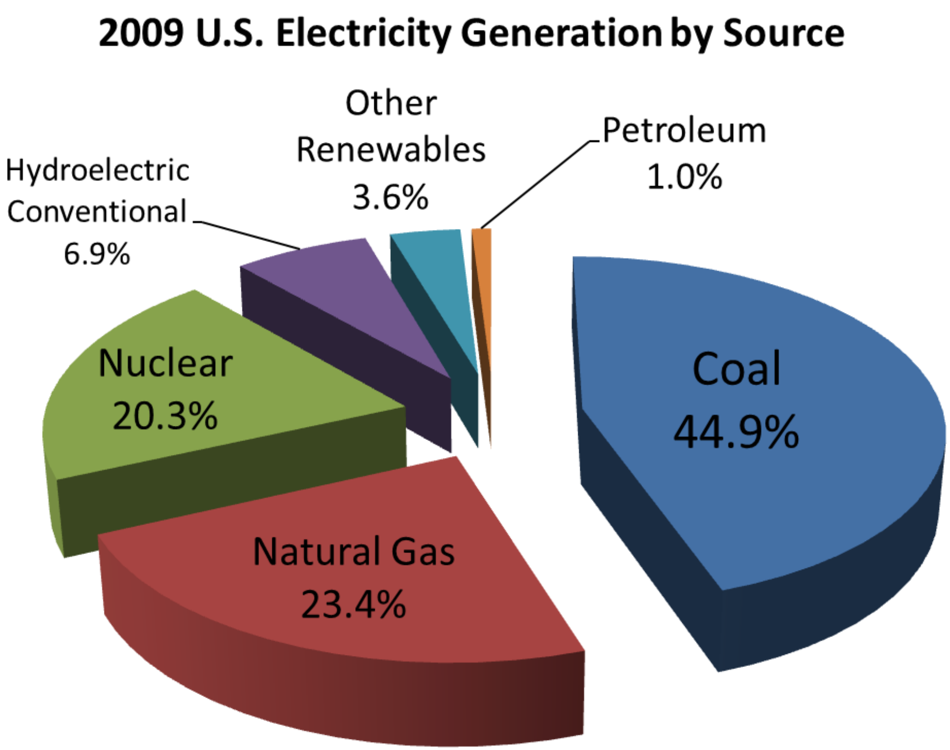
Motivation



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Motivation

- U.S. has biggest coal reserves <u>in the world</u>
- 28% of the world's coal!
- Energy has big implications:
  - Environmental
  - Economic
  - Geopolitical
  - Social & Health

Motivation

- Increasing environmental scrutiny
- Greenhouse gases
- Industry has a need for:
  - Retrofit of existing plants
  - Evaluation of new technology

Simulation

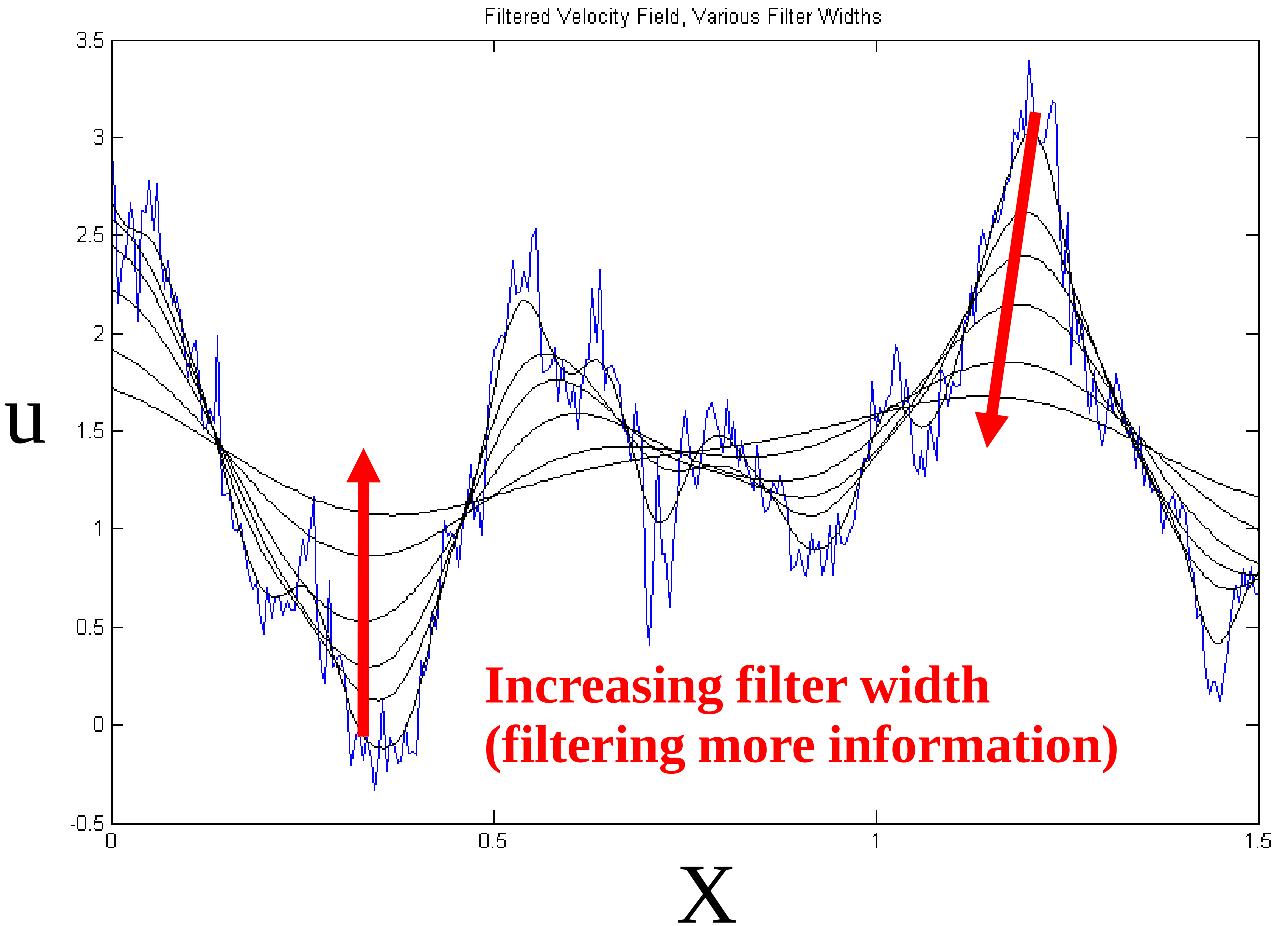
- Simulation - has potential to join experiments and theory as a research methodology
- Large-scale simulation tools can tackle difficult multi-physics problems with wide range of length and time scales

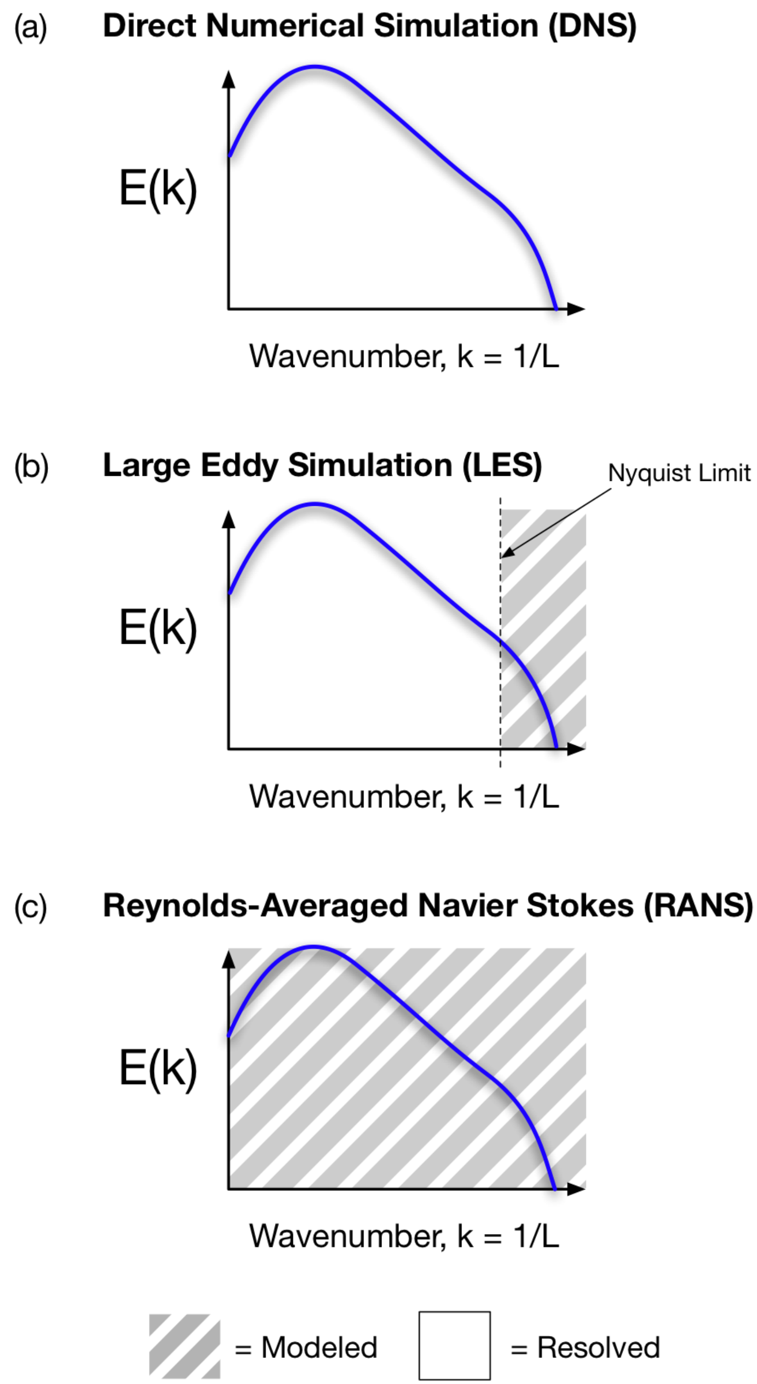
Outline/Overview

- Large eddy simulation (LES)
- Solid-Phase Models
  - Direct quadrature method of moments (DQMOM)
- Application to coal gasification
- Results & Discussion
- Conclusions

Large Eddy Simulation

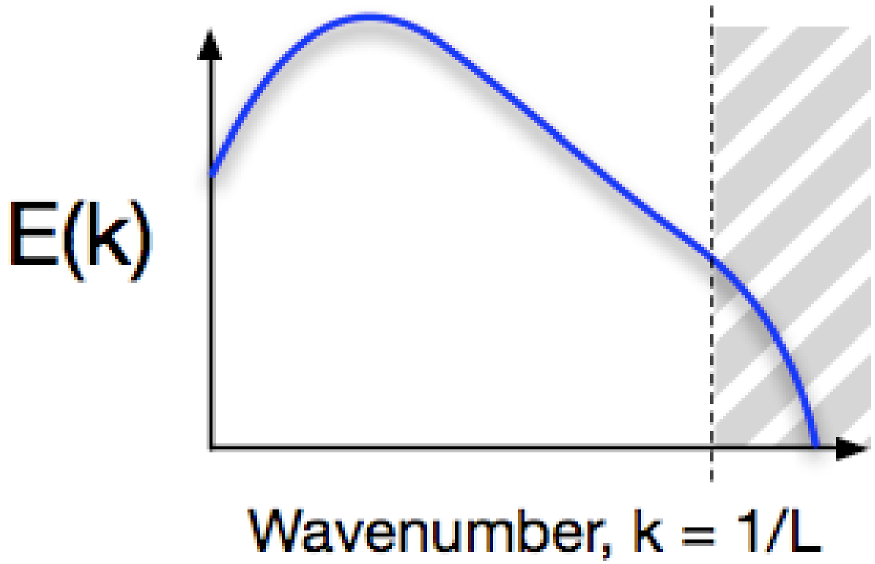
- Low-pass filtering: spatial averaging




(a) Direct Numerical Simulation (DNS)
E(k)
Wavenumber, k = 1/L
(b) Large Eddy Simulation (LES)
Nyquist Limit
E(k)
Wavenumber, k = 1/L
(c) Reynolds-Averaged Navier Stokes (RANS)
E(k)
Wavenumber, k = 1/L
= Modeled
= Resolved

Large Eddy Simulation

Scalar/Particle Energy Spectrum

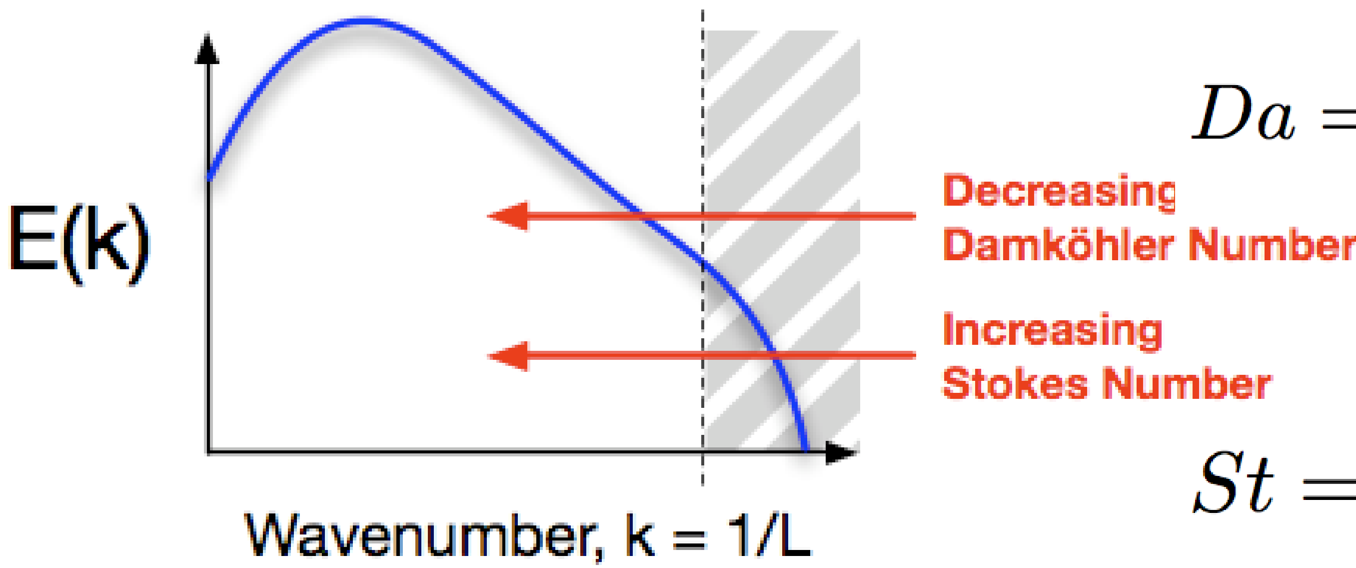


$$Da = \frac{\tau_{mixing}}{\tau_{reaction}}$$

$$St = \frac{\tau_{particle}}{\tau_{fluid}}$$

Large Eddy Simulation

Scalar/Particle Energy Spectrum



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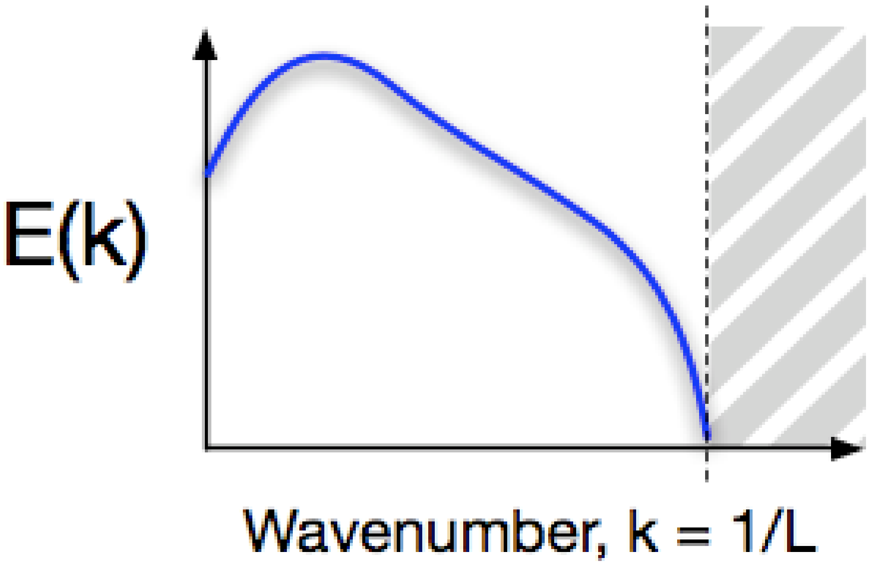
Large Eddy Simulation

Scalar/Particle Energy Spectrum



Damköhler Nyquist Limit:

$$\Delta \lesssim Da^{-\frac{1}{2}} Sc^{-\frac{3}{4}} \eta$$

Stokes Nyquist Limit:

$$\begin{cases} \text{if } \tau_{\text{eddy crossover}} < \tau_{\text{eddy lifetime}} & \Delta \lesssim \left(\frac{\tau_p \nu}{St}\right)^{1/2} \\ \text{else} & \Delta \lesssim \frac{\tau_p^2 g}{St} \end{cases}$$

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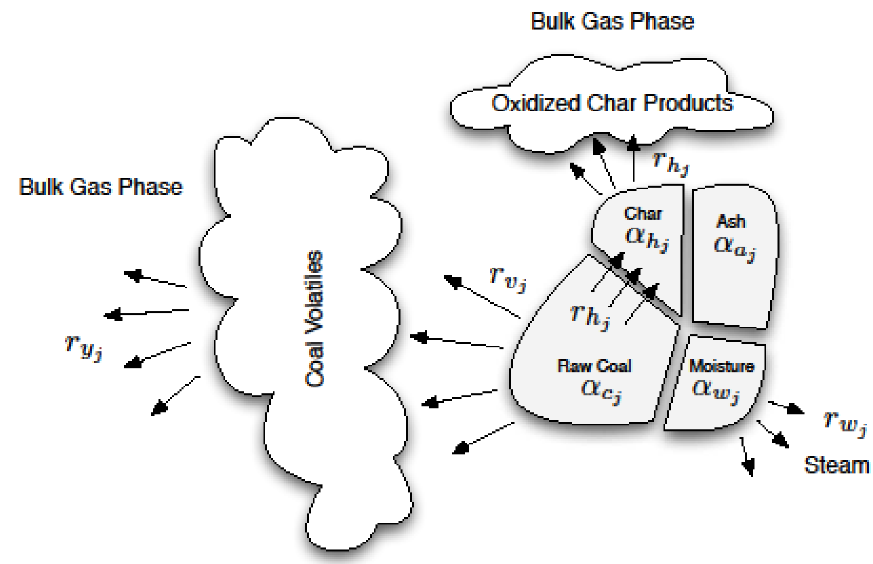
Solid Phase Models

- Characterization of particles:
- Internal coordinates = particle independent variables

(Denoted ξ)

- Lagrangian models
- Eulerian models



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Solid Phase Models

- Lagrangian: ODEs

$$\frac{d\boldsymbol{x}}{dt} = S_{\boldsymbol{x}} \qquad \frac{d\boldsymbol{\xi}}{dt} = S_{\boldsymbol{\xi}}$$

- Eulerian: NDF transport equation

$$\frac{\partial f\left(\boldsymbol{\xi};\boldsymbol{x},t\right)}{\partial t} + \frac{\partial}{\partial x_i}\left(\langle u_i|\boldsymbol{\xi}\rangle f\left(\boldsymbol{\xi};\boldsymbol{x},t\right)\right) + \sum_{j=1}^{N_\xi}\frac{\partial}{\partial \xi_j}\left(\langle G_j|\boldsymbol{\xi}\rangle f\left(\boldsymbol{\xi};\boldsymbol{x},t\right)\right) = h\left(\boldsymbol{\xi};\boldsymbol{x},t\right)$$

$$u_i = \frac{dx_i}{dt} \qquad G_j = \frac{d\xi_j}{dt}$$

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Solid Phase Models

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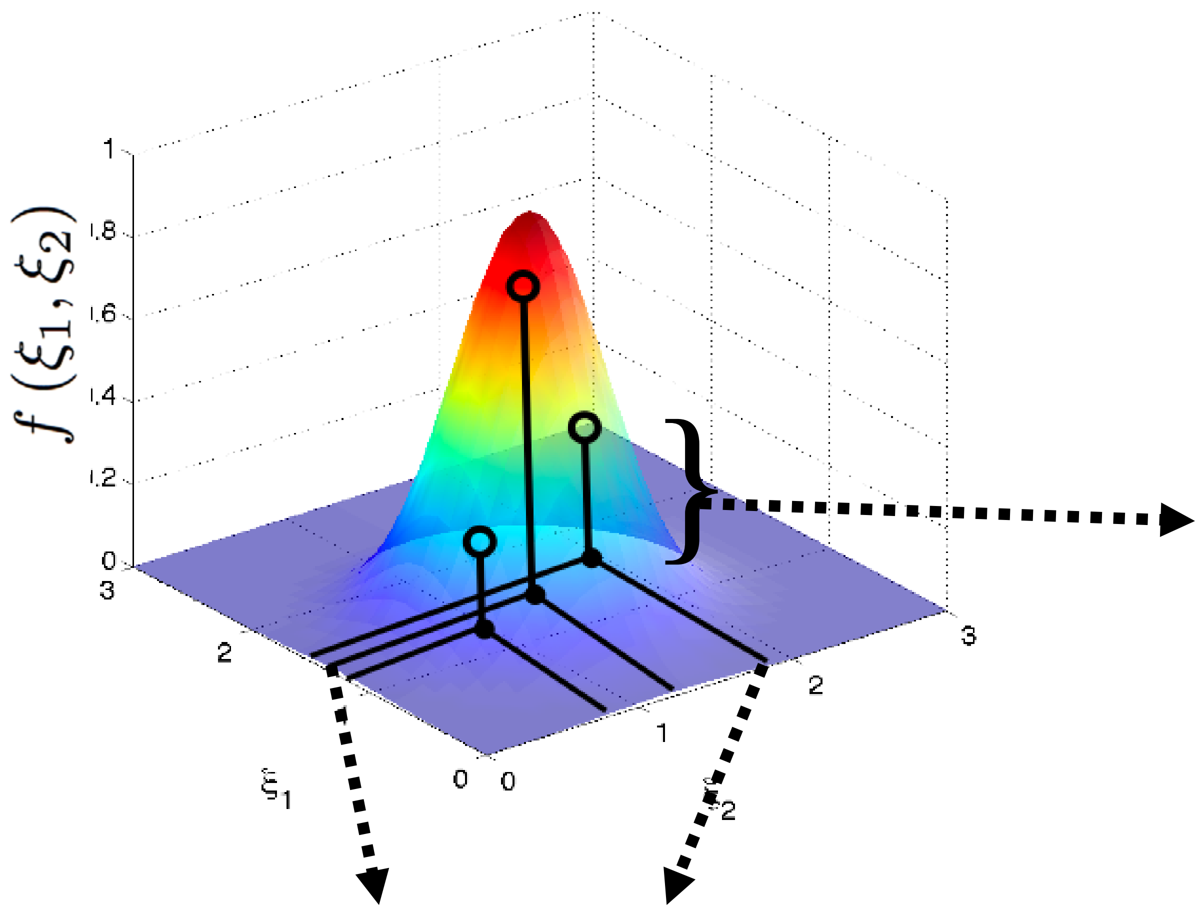
$$u_i = \frac{dx_i}{dt} \qquad G_j = \frac{d\xi_j}{dt}$$

Moment Methods

- Moment definition: $$m_k = \int_{-\infty}^{+\infty} \xi^k f(\xi)\, d\xi$$
- Multi-fluid method
  - Solids = "fluid" phase
  - Zeroth, first moments
  - What about adding another "fluid" phase?
- Multi-environment models

Direct Quadrature Method of Moments (DQMOM)



Weights
(i.e. how many particles are in that environment)

Abscissas (i.e. what values of ξ the particles have)

Direct Quadrature Method of Moments (DQMOM)

- Weight/weighted abscissa transport equations

$$\frac{\partial w_\alpha}{\partial t} + \frac{\partial}{\partial x_i}\left(\langle u_i|\boldsymbol{\xi}\rangle\, w_\alpha\right) = a_\alpha$$

$$\frac{\partial s_{j,\alpha}}{\partial t} + \frac{\partial}{\partial x_i}\left(\langle u_i|\boldsymbol{\xi}\rangle\, s_{j,\alpha}\right) = b_{j,\alpha}$$

- Source terms come from solution to linear system

$$\mathbf{Ax=B}$$

- Linear system comes from moment transform of NDF transport equation

DQMOM Implementation

- Numerical issues solving Ax=B
  - Abscissas overlapping
  - Linearly dependent moments
  - Small weights
  - Large values of $G_j = \frac{d\xi_j}{dt}$
- For > 2 environments, A always ill-conditioned (condition number ~10^{16})
- Contamination of one cell means contamination of all cells
- LU solvers, QR solvers, SVD solvers, Lapack solvers, Numerical Recipes solvers...........

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Optimized Moments Approach

- Professor Rodney Fox, "Optimal Moment Sets for Multivariate DQMOM", Ind. Chem. Eng. 2009.
- Replace abscissas in moment transform terms with optimal abscissas (star script)
- Because moment transform is linear, linear transform matrix ($\mathbf{M}^{\star}$) can be factored out on bot

$$
\begin{aligned}
\mathbf{A}\mathbf{x} &= \mathbf{B} \\
\mathbf{A}\left(\mathbf{A}^{\star}\right)^{-1}\mathbf{A}^{\star}\mathbf{x} &= \mathbf{B} \\
\mathbf{M}^{\star}\mathbf{A}^{\star}\mathbf{x} &= \mathbf{M}^{\star}\mathbf{B}^{\star} \\
\mathbf{A}^{\star}\mathbf{x} &= \mathbf{B}^{\star}.
\end{aligned}
$$

Implementation of DQMOM in Large Eddy Simulation

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Arches LES Code

- Finite volume
- 2nd Order Runge-Kutta, Strong Stability-Preserving
- Dynamic local similarity SGS model
- DOM Radiation calculation
- Object-Oriented C++
- Part of the Uintah Computational Framework (UCF)

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Uintah Framework

- Component-based
- Structured grid
- Load balancing
- Taskgraph to schedule tasks and manage resources/data
- Provides parallelization to thousands of processors

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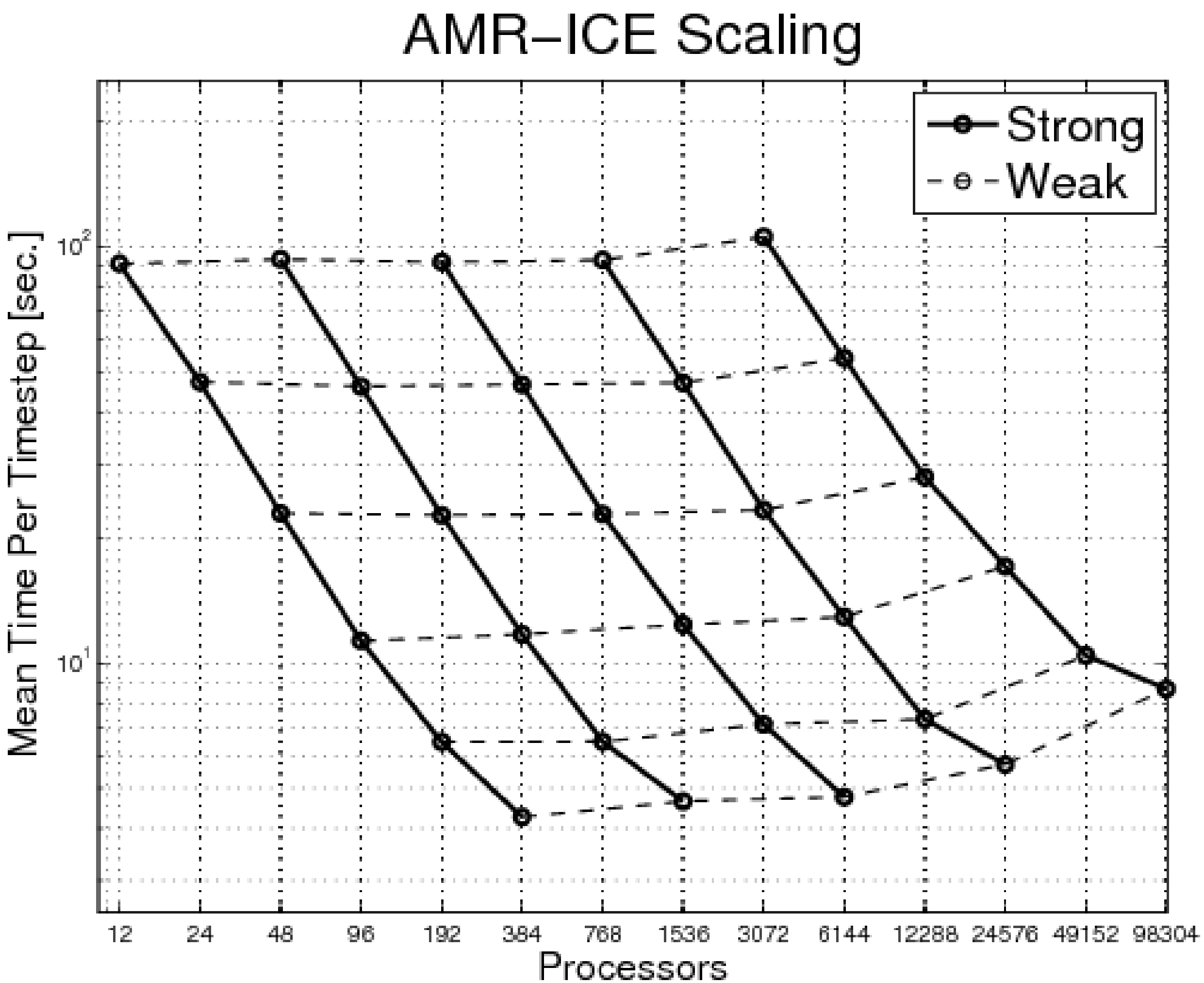
Uintah Framework



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Coal Models

- Equilibrium chemistry
- Kobayashi 2-step devolatilization

$$\text{(raw coal)} \xrightarrow{k_1} Y_1\,\text{(volatiles)} + (1 - Y_1)\,\text{(char)}$$

$$\text{(raw coal)} \xrightarrow{k_2} Y_2\,\text{(volatiles)} + (1 - Y_2)\,\text{(char)}$$

$$\begin{aligned} A_1 &= 3.7 \times 10^5\, s^{-1} \\ A_2 &= 1.46 \times 10^{13}\, s^{-1} \\ E_1 &= -17,600\, {}^{kcal}/_{kmol} \\ E_2 &= -60,000\, {}^{kcal}/_{kmol} \end{aligned}$$

Ubhayakar (1976)

- Particle heat transfer: radiation, convection
  - DOM, 2 ordinates
  - Nusselt # convection model

Coal Models

- Fast equilibrium Eulerian particle velocity model (Balachandar 2008)

$$\frac{(u_{particle} - u_{gas})}{u_k} \approx (1-\beta)\left(\frac{\tau_{particle}}{\tau_k}\right)^{1/2}$$

$$\beta = \frac{3}{\frac{2\rho_p}{\rho_f} + 1}$$

$\beta = 3$ Buoyant particles (bubbles)

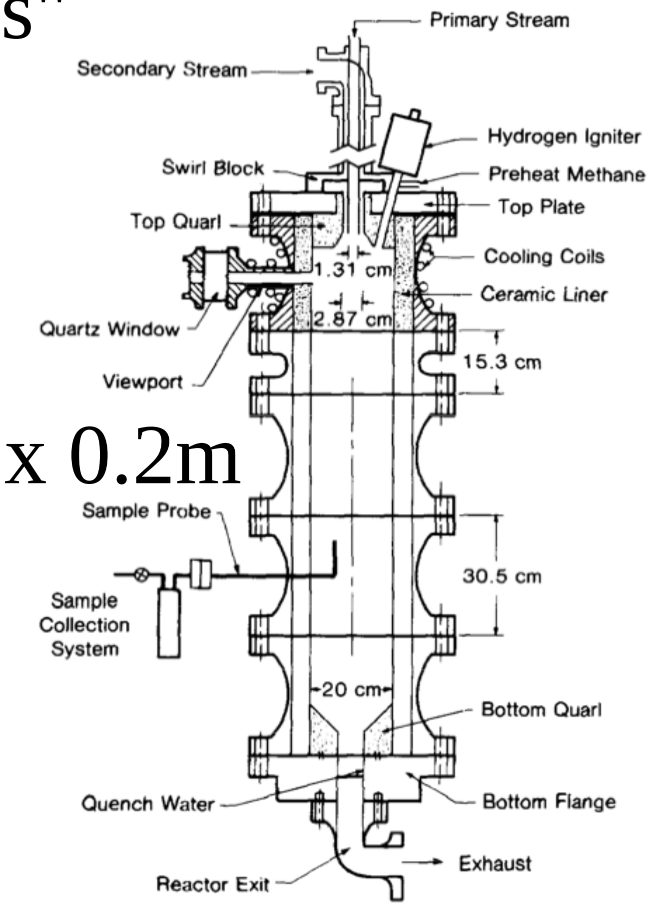
$\beta = 0$ Heavy particles

- Soelburg et al. 1984, "Entrained Flow Gasification of Coal 1: Evaluation of Mixing and Reaction Processes"

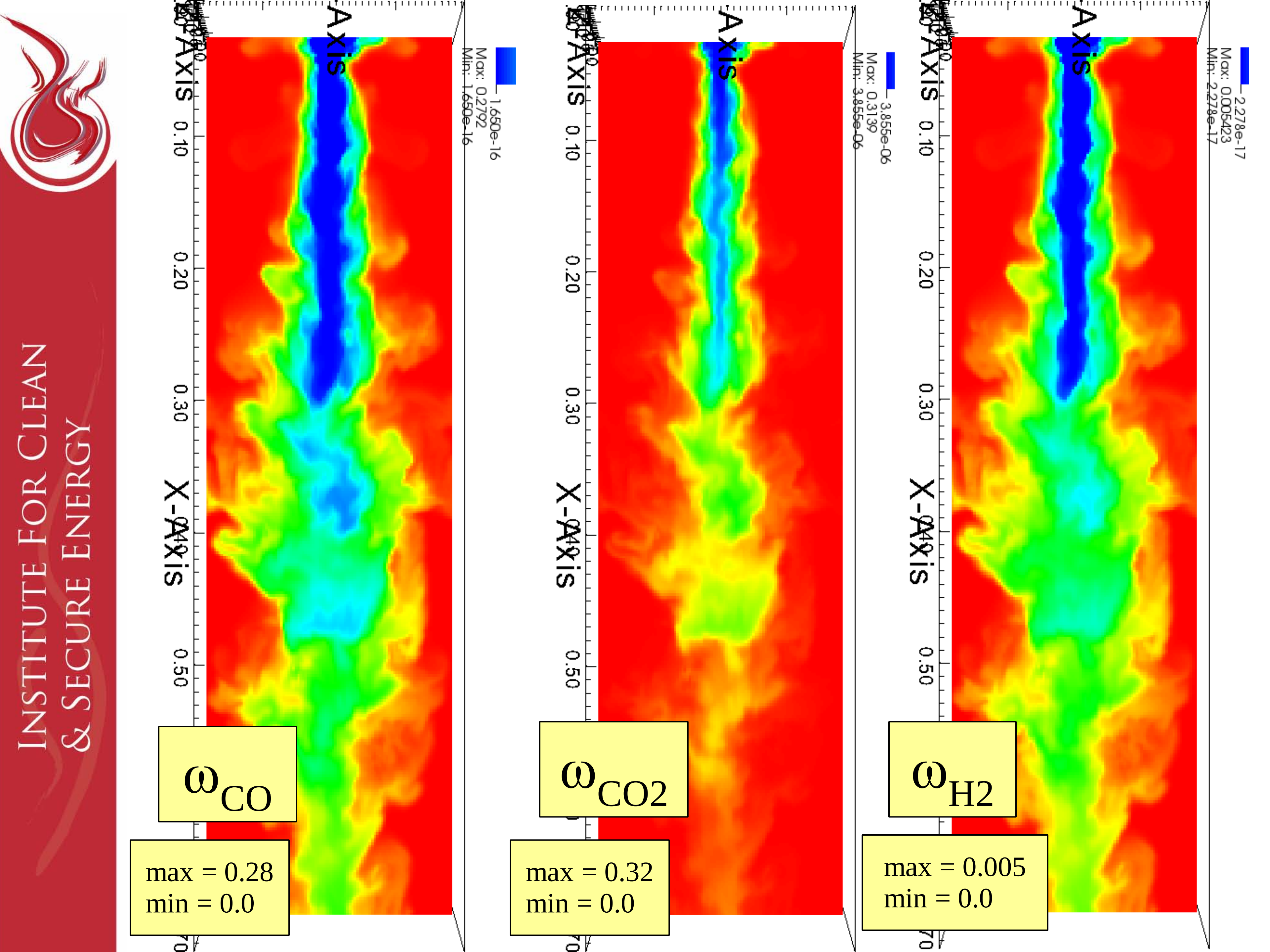
- Simulation: No walls

- Domain: 0.7m x 0.2m x 0.2m

- 350 x 100 x 100 (resolution of 2 mm)



DQMOM + LES
Coal Gasification Results



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X-Axis
Y-Axis
0.10
0.20
0.30
0.50
Max: 0.2792
Min: 1.650e-16
Max: 0.3139
Min: 3.855e-06
Max: 0.005423
Min: 2.278e-17
ω_{CO}
max = 0.28
min = 0.0
ω_{CO2}
max = 0.32
min = 0.0
ω_{H2}
max = 0.005
min = 0.0

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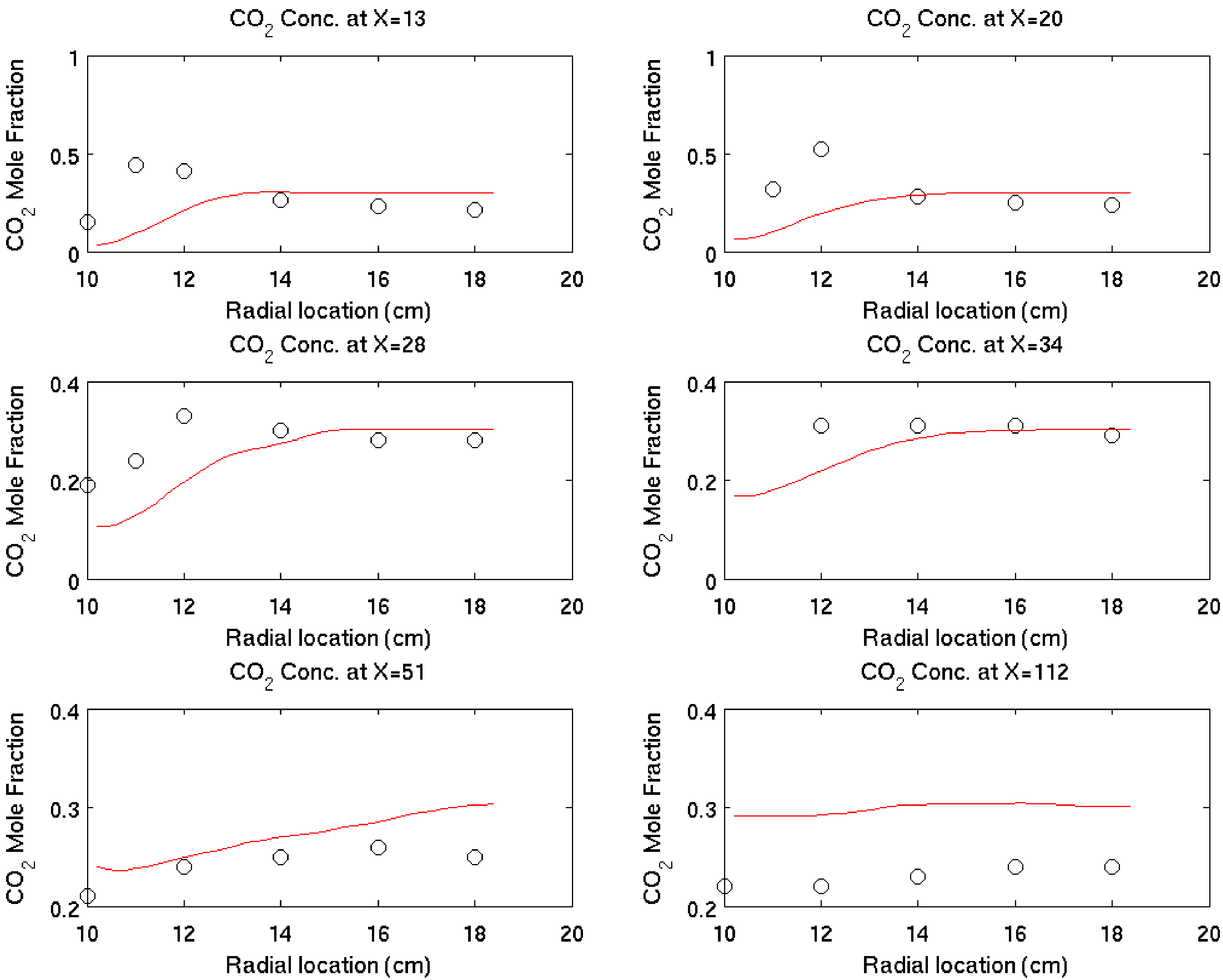

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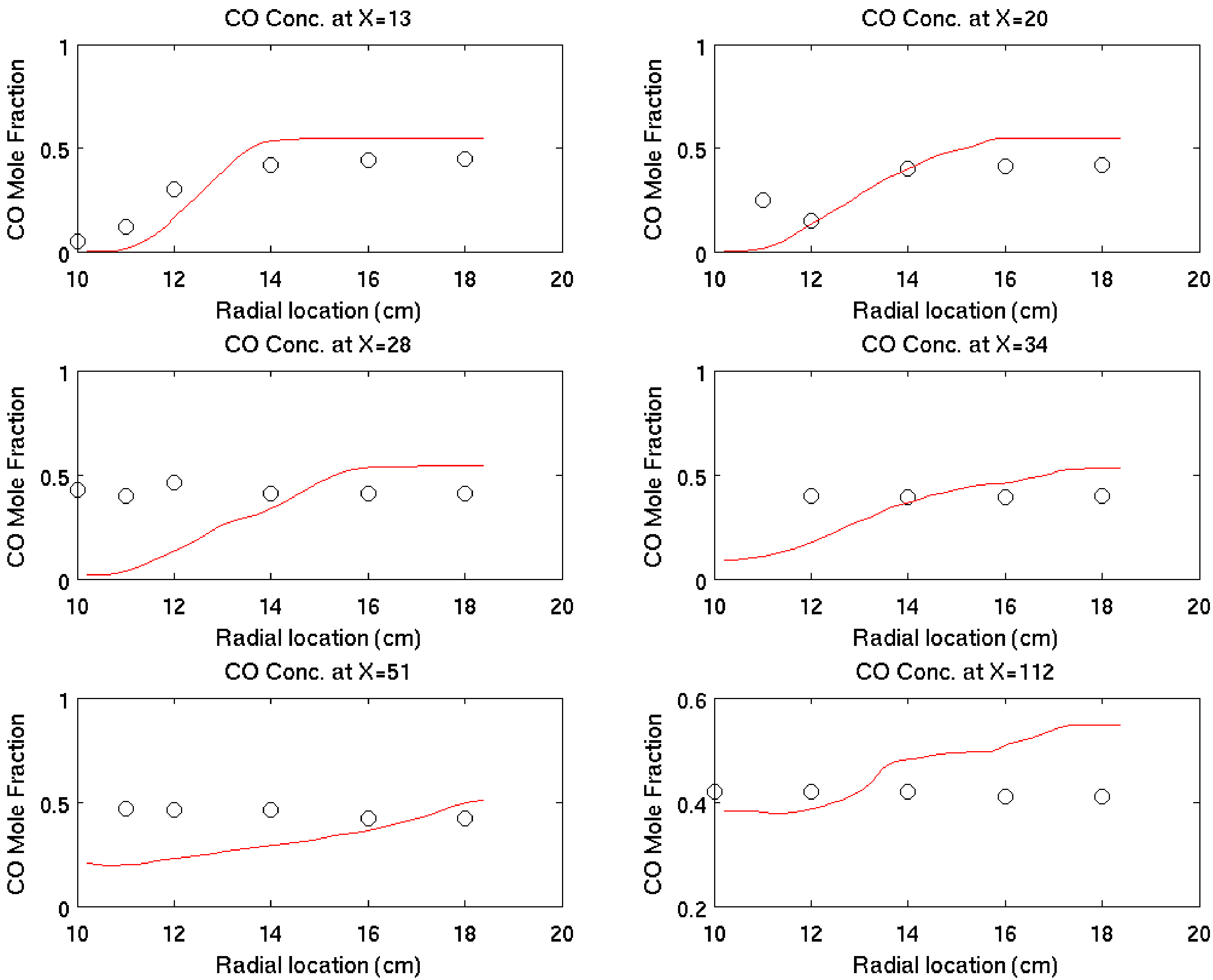

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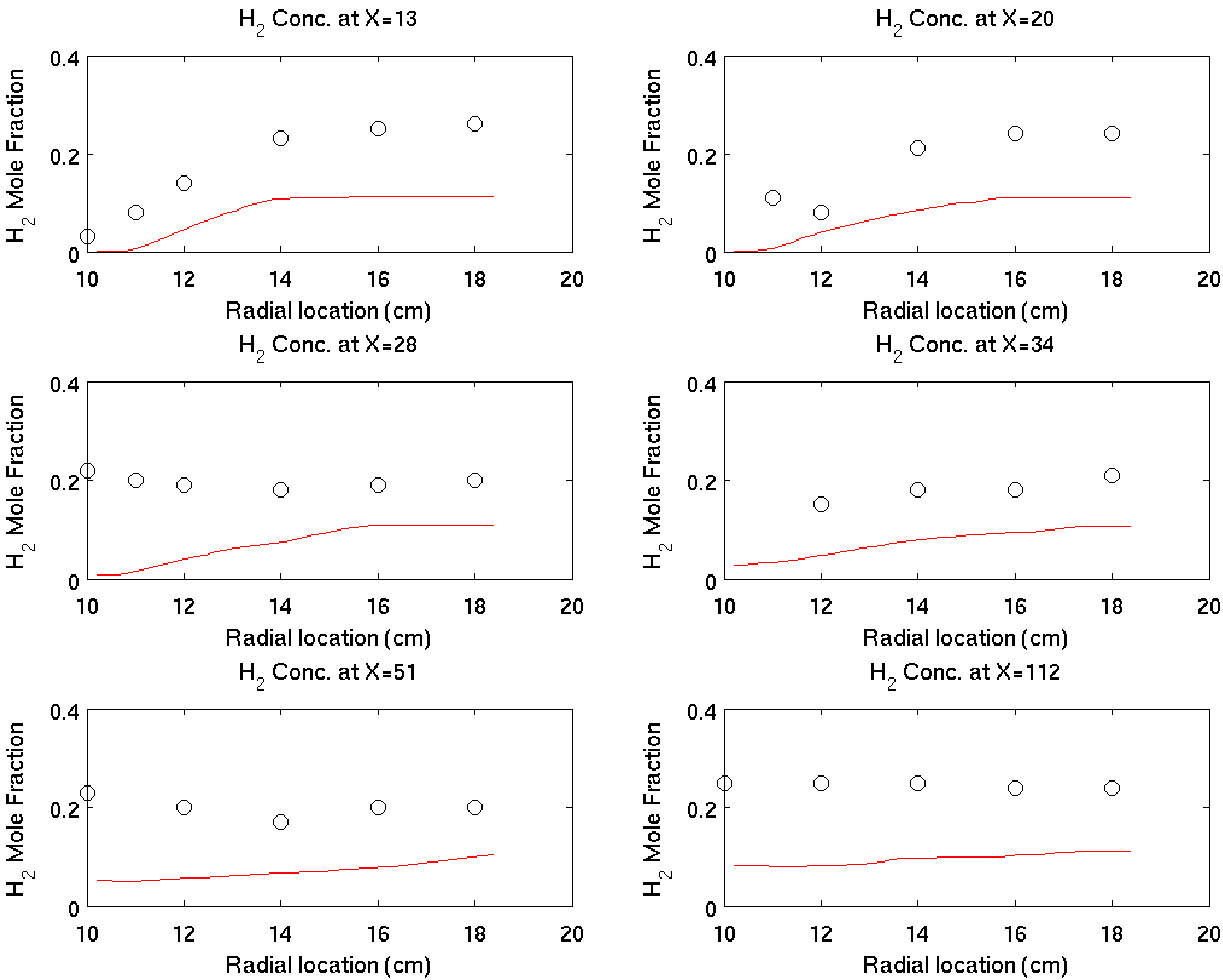

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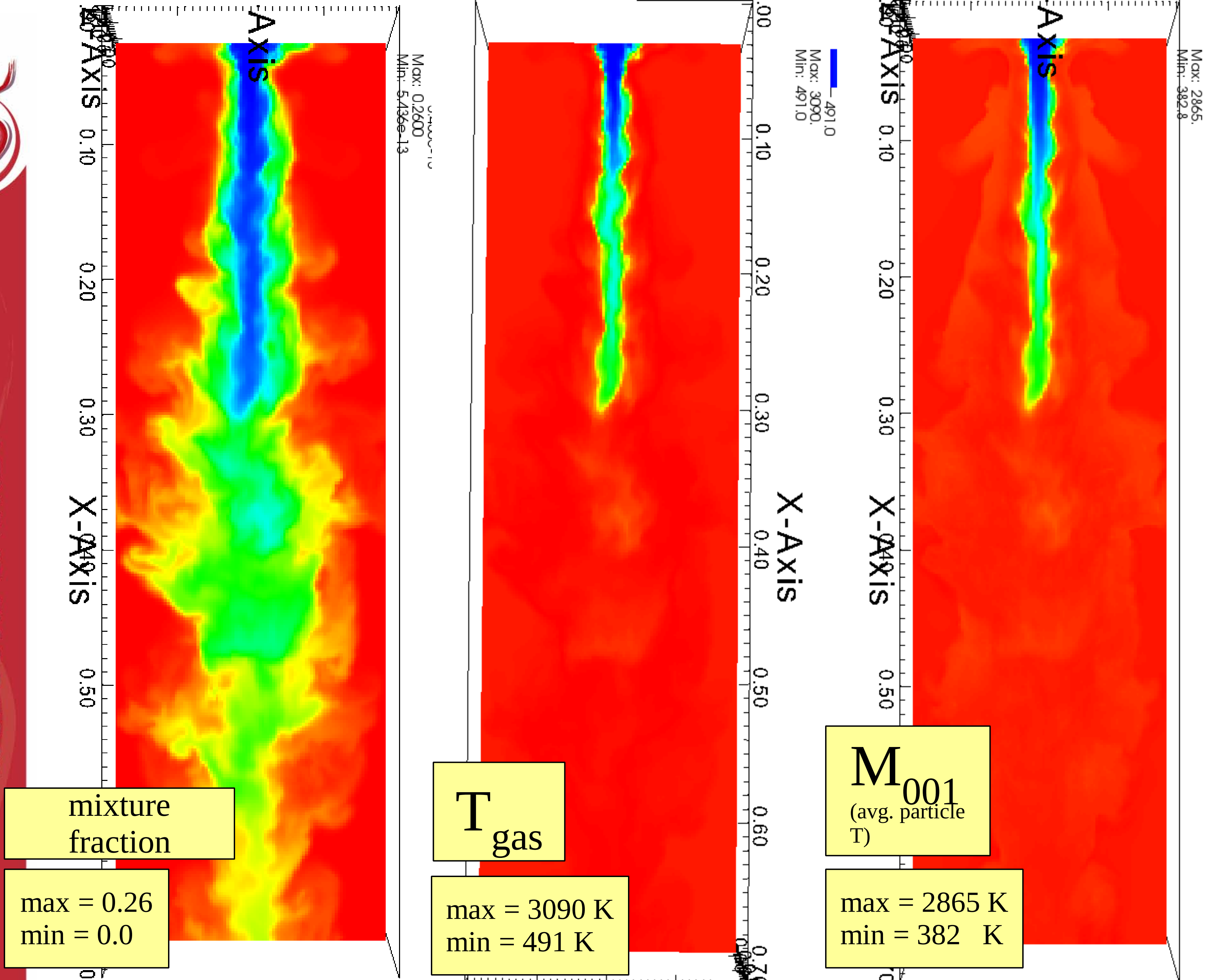
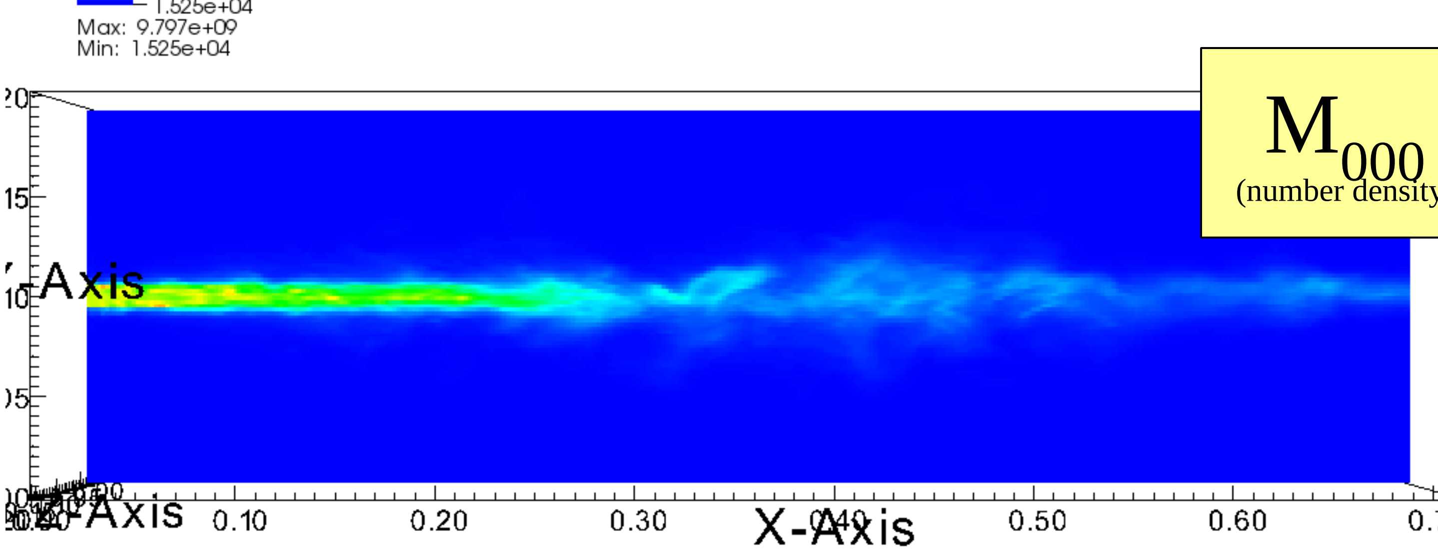
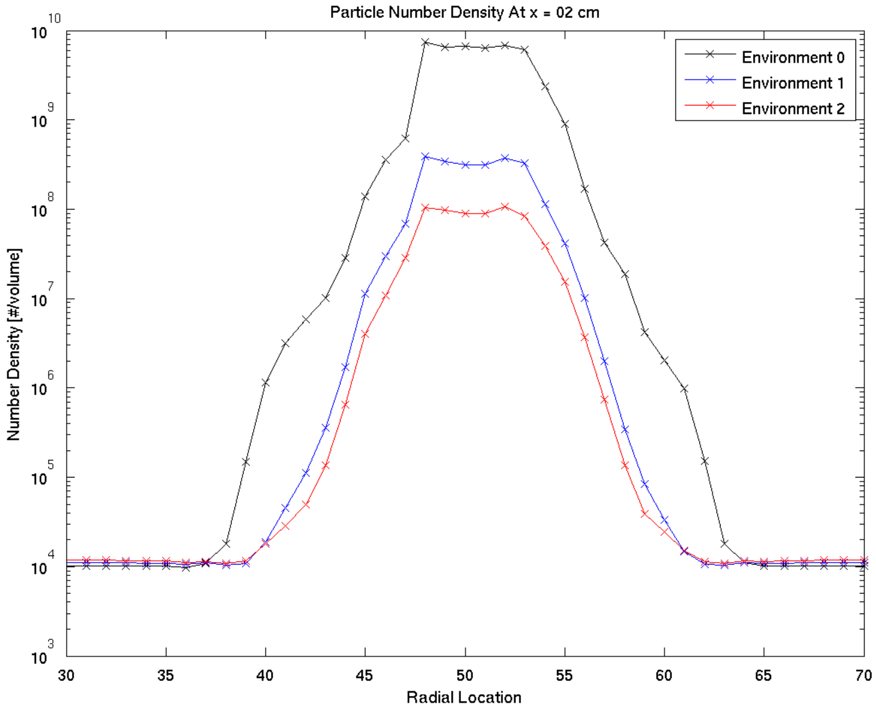
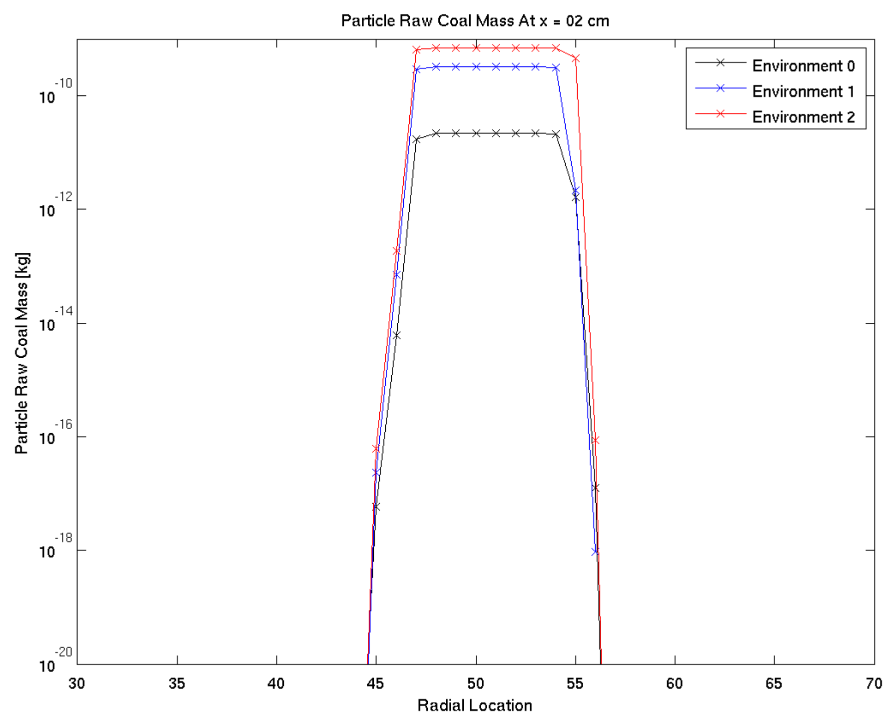
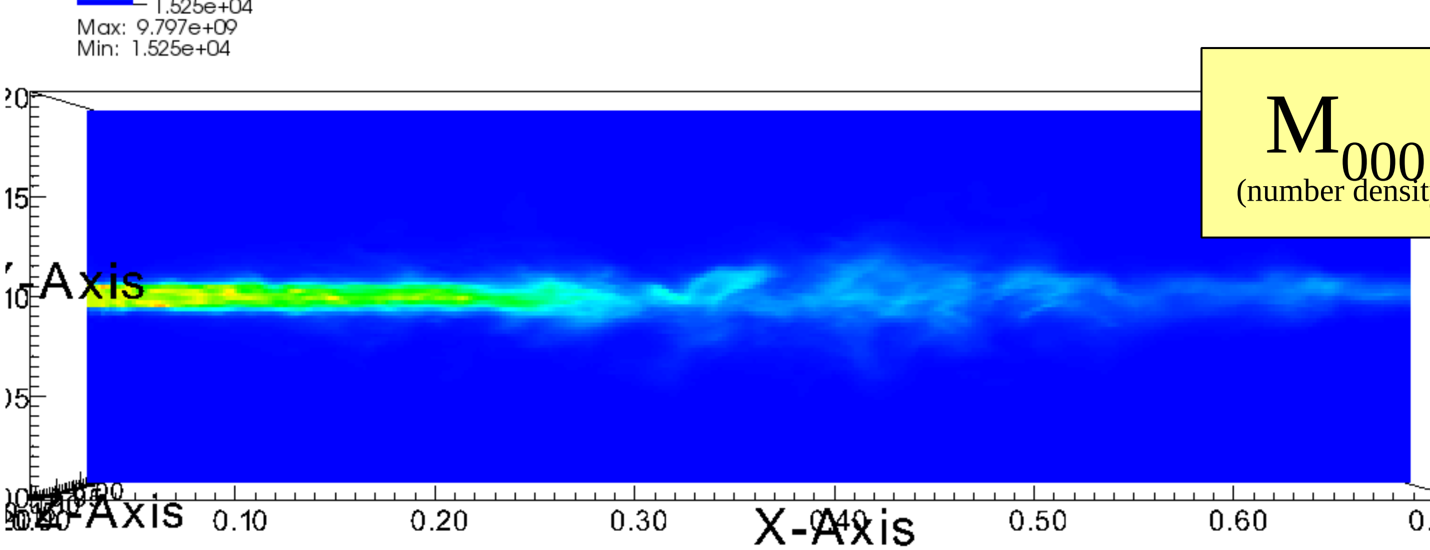




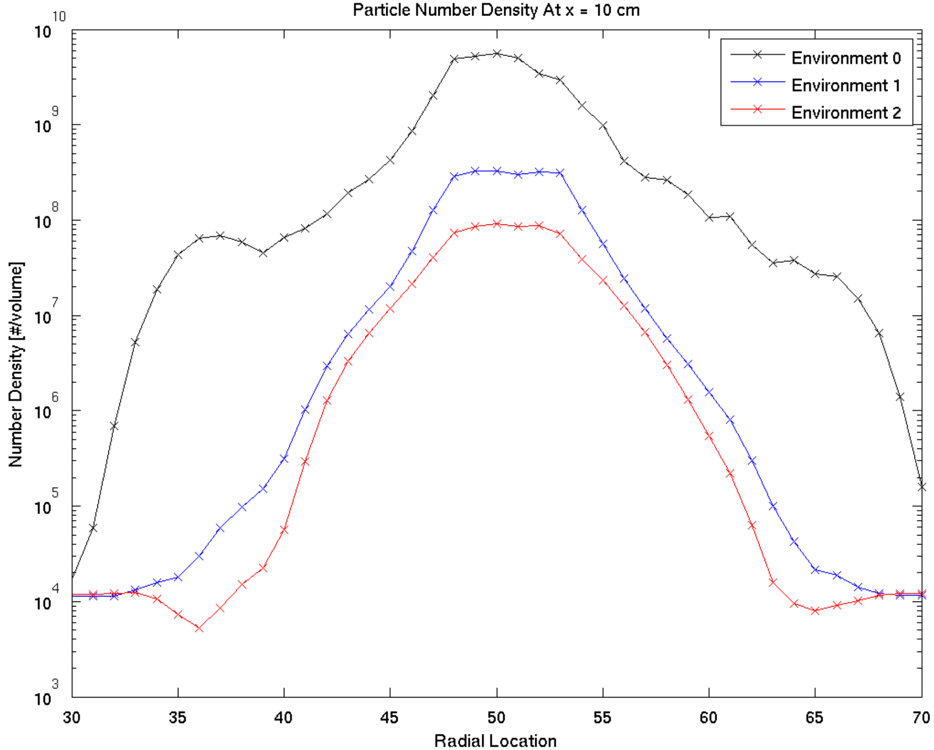
M_{000}
(number density)

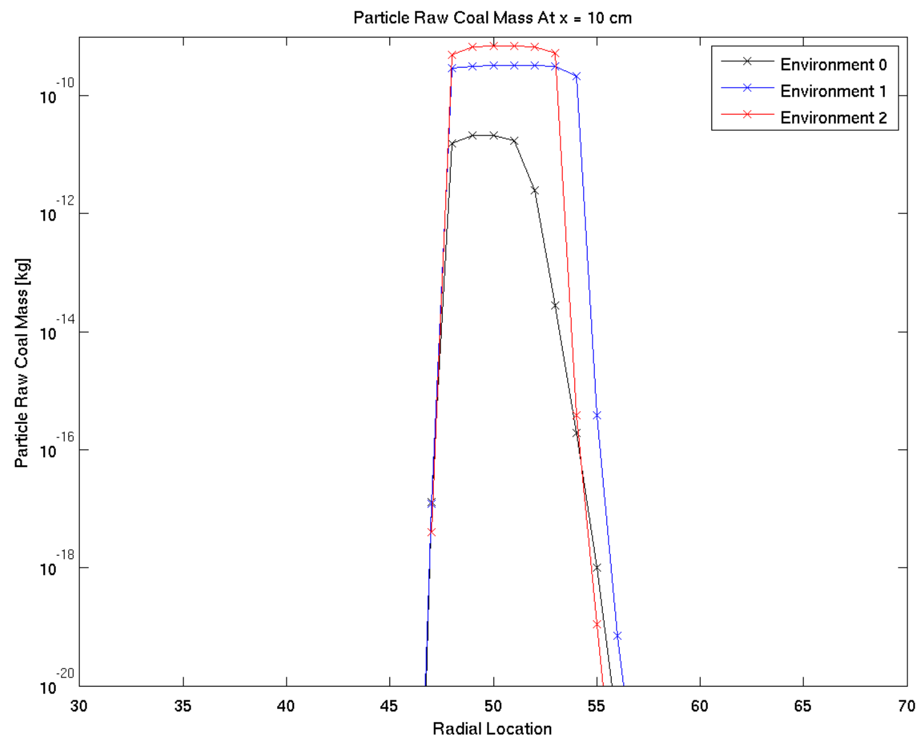






M_{000}
(number density)





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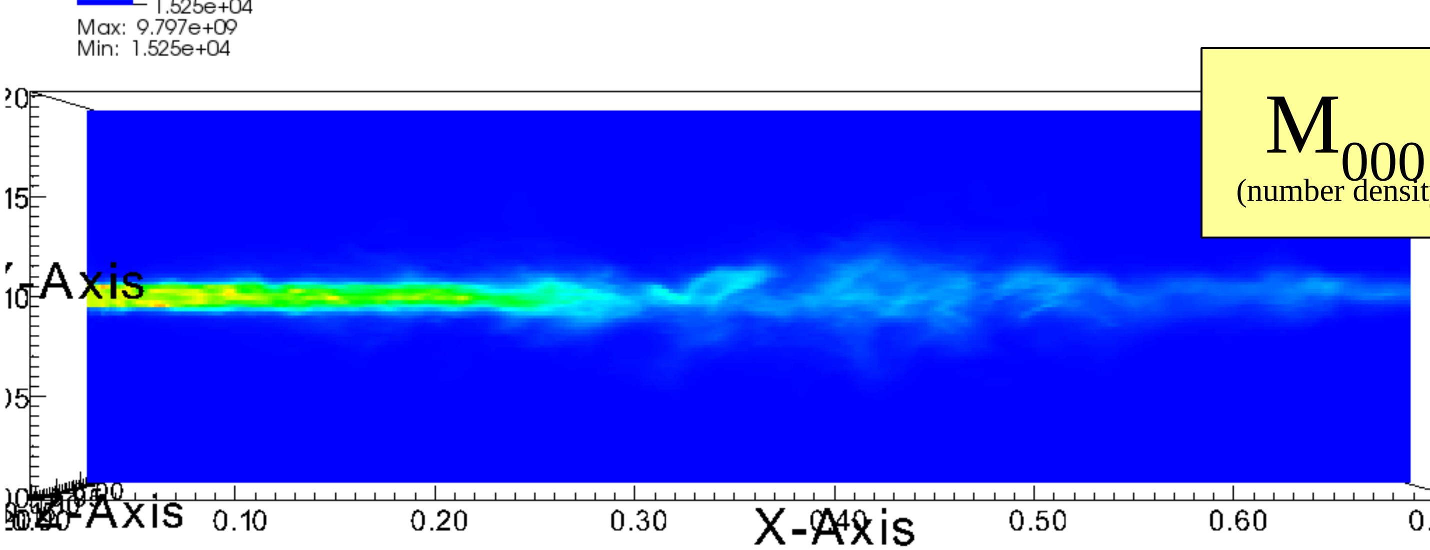
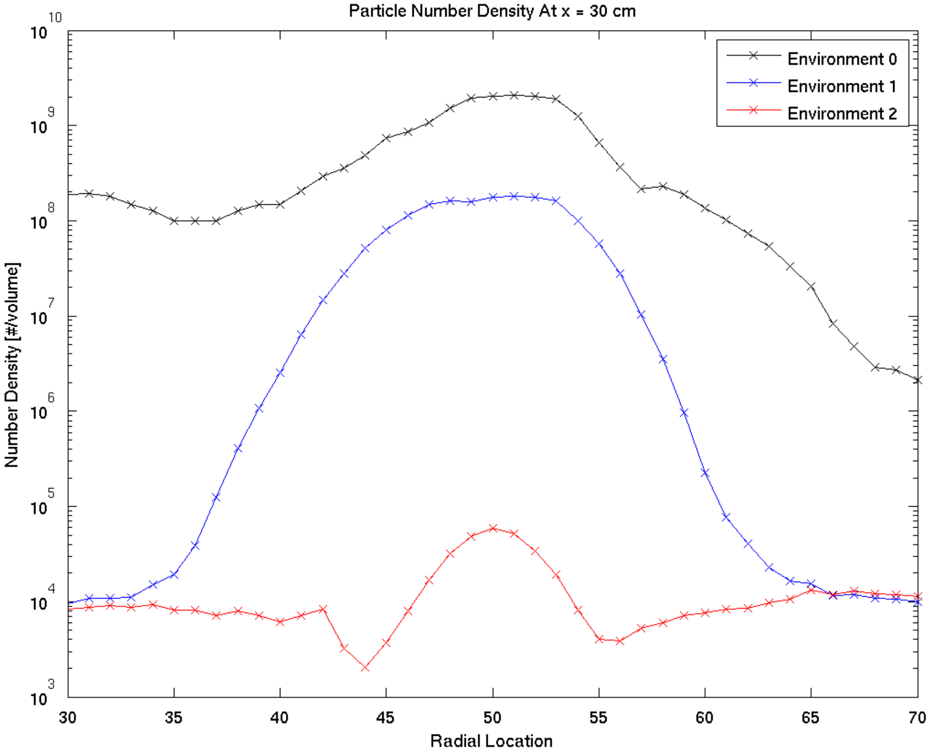
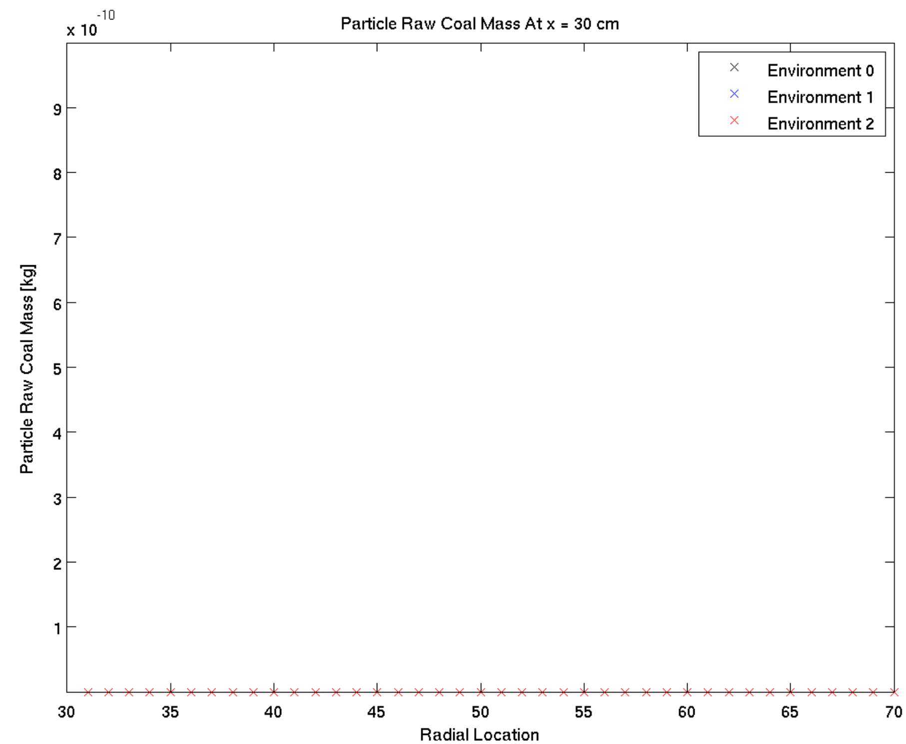
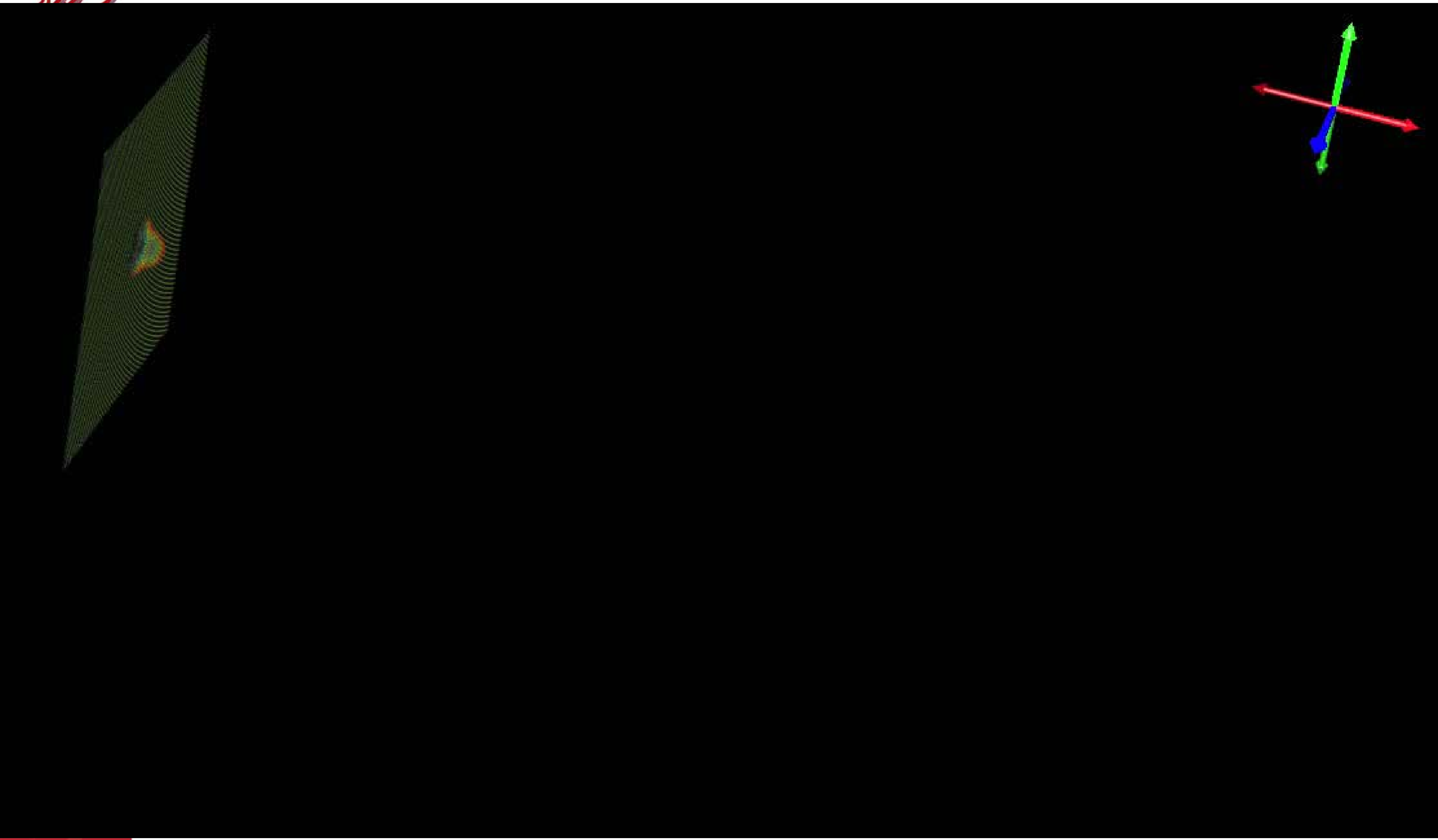


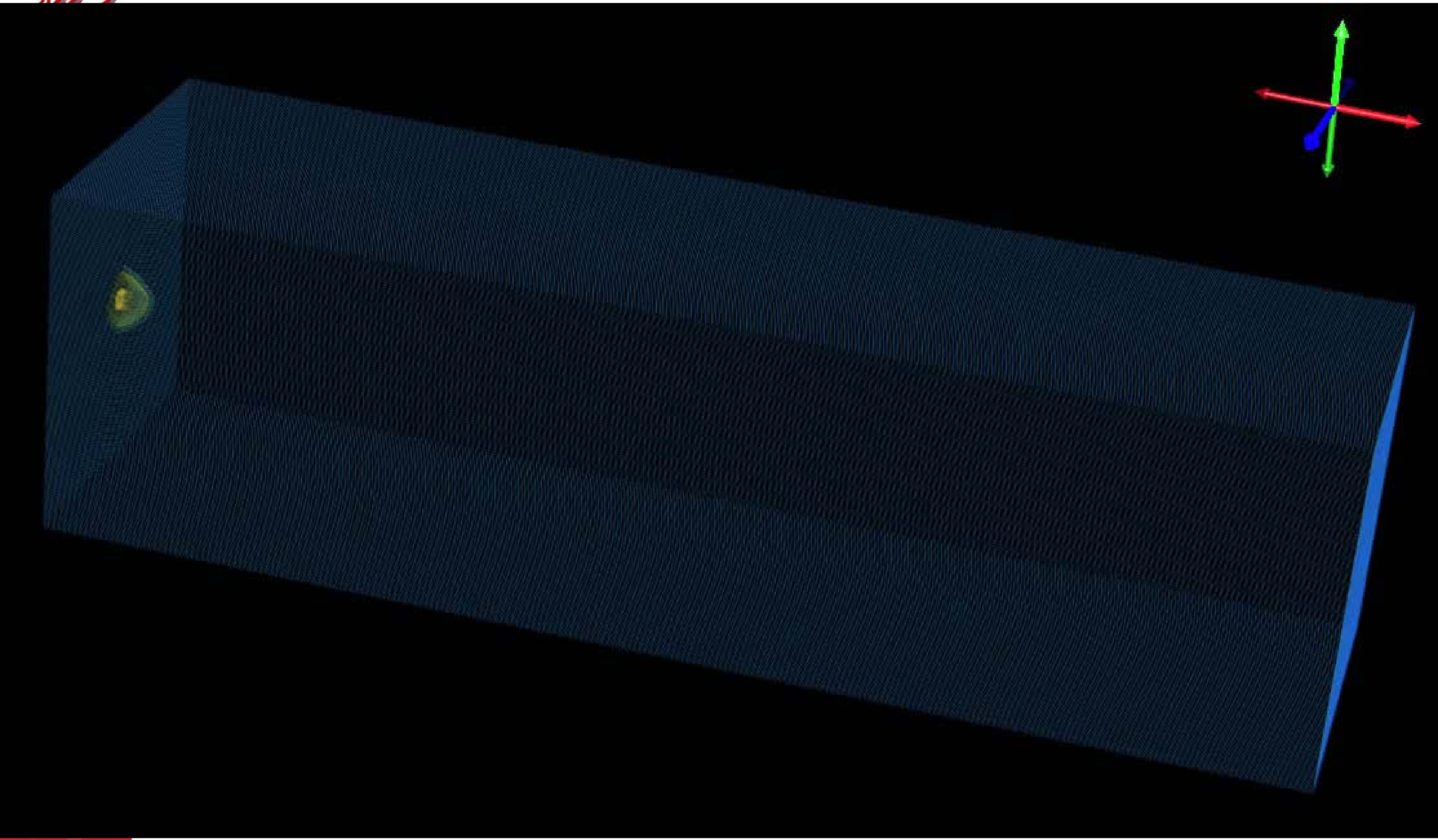




Volume-Rendering: CO Concentration



Volume-Rendering: Mean Particle Size



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Summary of Results

- Not focusing on how well the simulation reproduced the data
- Demonstrating a *procedure* for implementation of DQMOM in a massively parallel large-eddy simulation code
- What we've implemented, and why we're excited about it
- Gasification physics - lots of experience, existing numerical techniques
- 1DCOG, PCGC2/PCGC3, Glacier, Banff

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Where To Go From Here?

- Improving coal gasification physics
- Improving particle physics
- Increase number of internal coordinates
- Begin formal validation procedure

Professor Philip Smith,
University of Utah

Professor Jeremy Thornock,
University of Utah

Professor Rodney Fox,
Iowa State University

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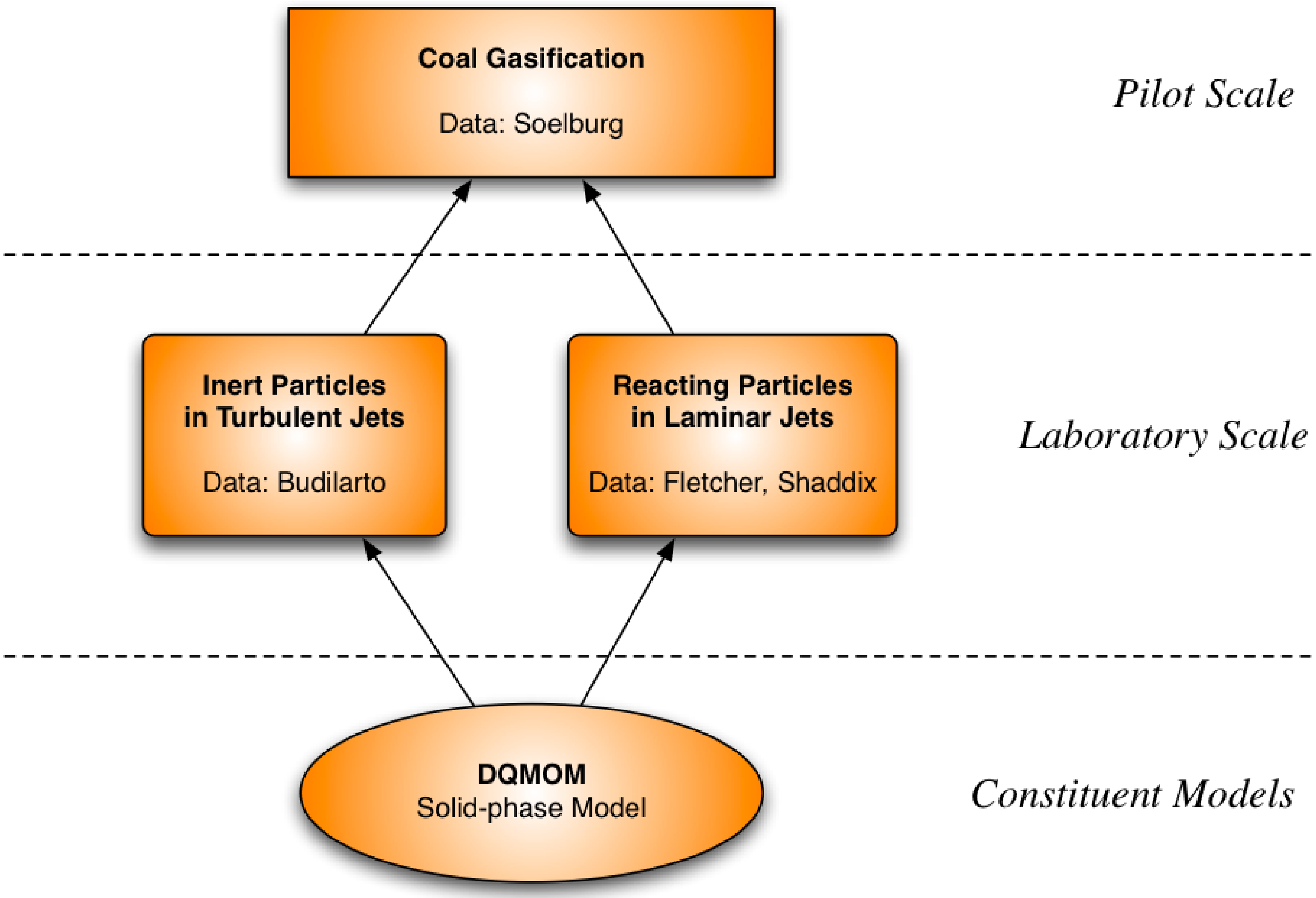
Questions?

Validation Roadmap:



Matrix Expressions

$$\mathbf{A_1} = \left(1 - \sum_{m=1}^{N_\xi} k_m\right) \prod_{n=1}^{N_\xi} \langle \xi_n \rangle_\alpha^{k_n}$$

$$\mathbf{A_{j+1}} = (k_j)\left(\langle \xi_j \rangle_\alpha^{k_j - 1}\right)\left(\prod_{n \neq j,\, n=1}^{N_\xi} \langle \xi_n \rangle_\alpha^{k_n}\right)$$

$$\mathbf{S} = -\sum_{n=1}^{N_\xi}\left[\sum_{\alpha=1}^{N} w_\alpha \left(-k_n \langle \xi_n \rangle_\alpha^{k_n - 1}\right)\left(\prod_{m \neq n, m=1}^{N_\xi} \langle \xi_m \rangle_\alpha^{k_m}\right)\left(G_n\left(\langle \xi_n \rangle_\alpha\right)\right)\right]$$

Moment Definitions

$$m_k \approx \frac{\sum_{\alpha=1}^{N} w_\alpha \left\langle \xi \right\rangle_\alpha^k}{\sum_{\alpha=1}^{N} w_\alpha}$$

$$m_{\boldsymbol{k}} \text{⌘} \frac{\sum_{\alpha=1}^{N} \left\{ w_\alpha \left(\prod_{j=1}^{N_\xi} \left\langle \xi_j \right\rangle_\alpha^{k_j} \right) \right\}}{\sum_{\alpha=1}^{N} w_\alpha}$$