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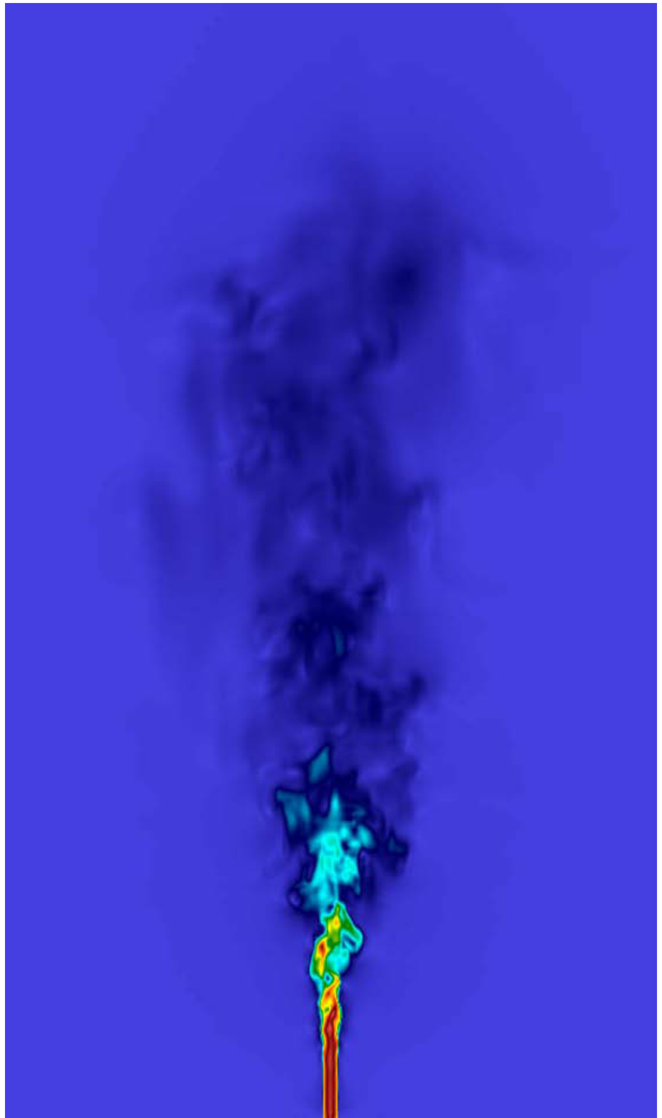
RMFM 2019 Rocky Mountain Fluid Mechanics Research Symposium



Numerical Simulations of the Supercritical Carbon Dioxide Round Turbulent Jet

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Overview

1. Introduction
2. Simulation Setup
3. Cases and Parameters
4. Ideal Gas Verification
5. sCO2 Results
6. Future Work
7. Acknowledgements
8. Questions

Supercritical Carbon Dioxide (sCO_2)

Introduction

What are supercritical fluids?

- Fluids held above critical temperature and pressure
- Liquid-like density
- Gas-like viscosity
- Sensitive density, pressure, temperature relationship
- Critical point for CO_2: T=304 K, P=7.38 MPa

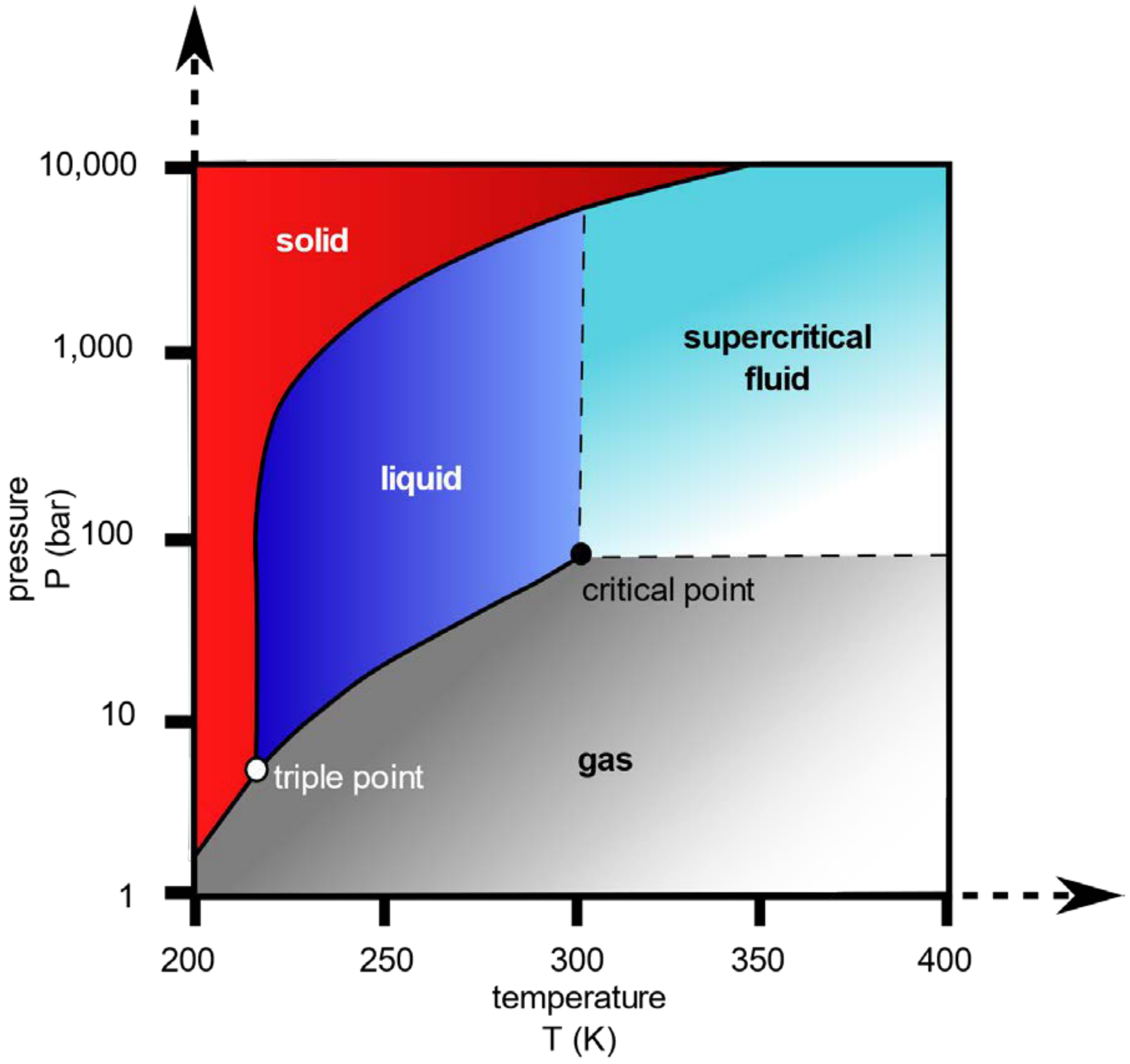

Fig. 1: Phase Diagram for Carbon Dioxide

Finney, B. & Jacobs, M. (2010). Carbon dioxide pressure-temperature phase diagram.svg. Retrieved from https://commons.wikimedia.org/wiki/File:Carbon_dioxide_pressure-temperature_phase_diagram.svg.

Supercritical fluids are important for a wide range of applications

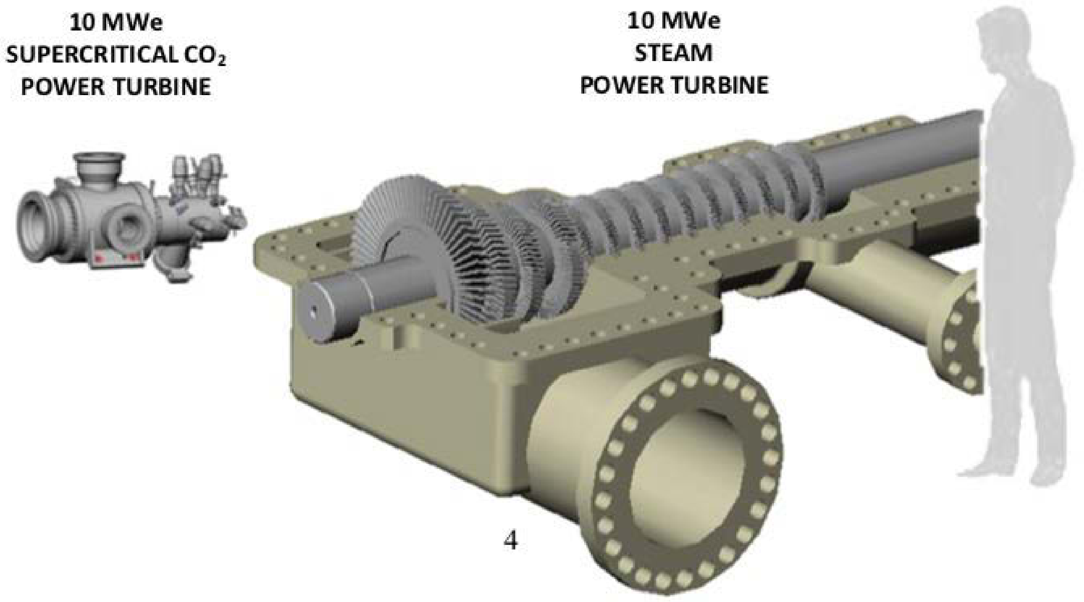

Fig. 2: 10 MWe sCO_2 power turbine compared to a 10 MWe steam turbine

- sCO_2 can be utilized in a variety of industries:
  - Closed-cycle gas turbines in advanced nuclear reactors
  - Carbon sequestration

Persichilli, M., Kacludis, A., Zdankiewicz, E., & Held, T. (2013). Supercritical CO_2 Power Cycle Developments and Commercialization: Why sCO_2 can Displace Steam. *Power-Gen India & Central Asia*. Echogen Power Systems LLC. https://www.echogen.com/documents/why-sco2-can-displace-steam.pdf.

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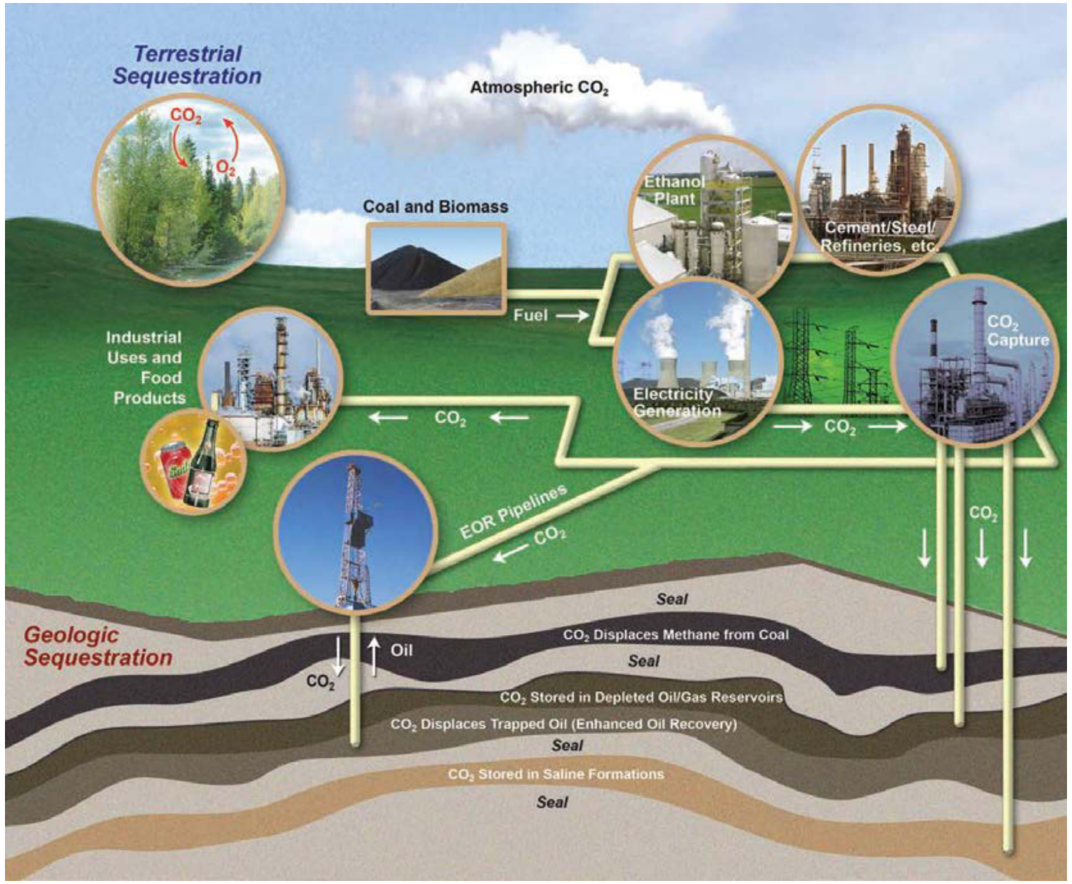


Fig. 3: Examples of Geologic Carbon Sequestration

- sCO_2 can be utilized in a variety of industries:
  - Closed-cycle gas turbines in advanced nuclear reactors
  - Carbon sequestration

The Trustees of Indiana University. 2019. *Geological Sequestration*. Retrieved from https://igws.indiana.edu/Sequestration

Current Landscape

- sCO_2 promising fluid in many fields, yet many fundamental physical aspects still unknown
- Experimental challenges with critical parameters
- Current jet research oriented toward application-specific quantities of interest.

Project Scope

Goal: simulate flow field of turbulent sCO_2 jet in order to gain better understanding of underlying physics.

- Our hypothesis is that supercritical flows for canonical round turbulent jets exhibit different physical mechanisms than those of ideal gas.
- Understanding base mechanisms of supercritical flows can add to theory related to quantities of interest across all applications
- Specifically interested in investigating velocity profiles and Reynolds stresses compared to those of ideal gas case.

Numerical Simulations

Jet Setup

PeleC

- Built on AMReX and funded by the Exascale Computing Project (ECP) through the Department of Energy (DOE), PeleC is an adaptive-mesh compressible hydrodynamics code for reacting flows
  - Models turbulence-chemistry interactions motivated by conditions in internal combustion engines
  - Can additionally handle embedded boundary conditions, non-ideal EoS, and allows for implementation of adaptive mesh refinement (AMR)
- Utilizes 2nd order finite volume formulation using the Piecewise Parabolic Method (PPM) in space and a standard RK2 time integrator to approximate solutions to the compressible Euler equations.
- To learn more visit: https://github.com/AMReX-Combustion/PeleC

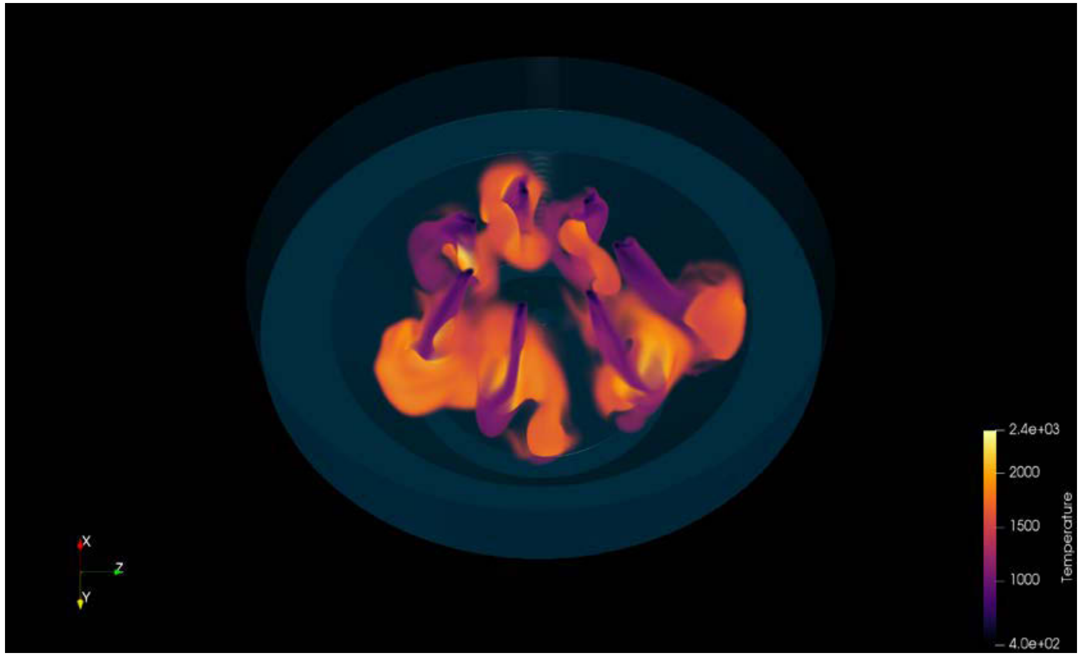


Fig 4: Injection of natural gas in a piston-bowl geometry performed using PeleC

. PELEC. Computer software. *https://www.osti.gov//servlets/purl/1374142*. Vers. 00. USDOE Office of Science (SC), Advanced Scientific Computing Research (ASCR) (SC-21). 17 May. 2017. Web.

Equations of State (EoS)

Gamma Law for Ideal Gas

$$P = (\gamma - 1)\rho\epsilon \, .$$

Used for Jet verification with air

Soave-Redlich-Kwong for Non-Ideal Gas

$$p = \frac{RT}{V_m - b} - \frac{a\,\alpha}{V_m\,(V_m + b)}$$

$$a = \frac{0.42747\,R^2\,T_c^2}{P_c}$$

$$b = \frac{0.08664\,R\,T_c}{P_c}$$

$$\alpha = \left(1 + \left(0.48508 + 1.55171\,\omega - 0.15613\,\omega^2\right)\left(1 - T_r^{0.5}\right)\right)^2$$

$$T_r = \frac{T}{T_c}$$

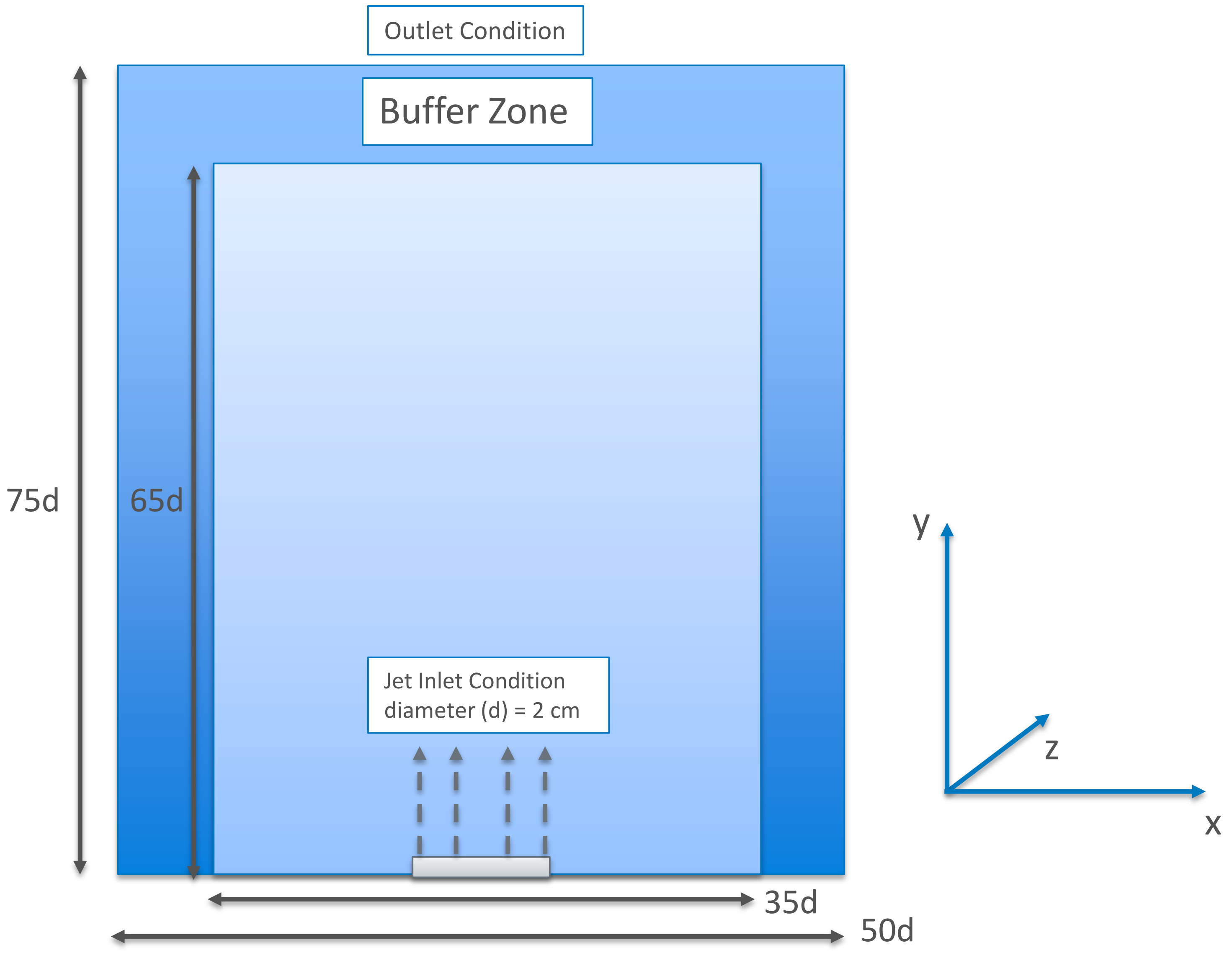
where ω is the acentric factor for the species.

More accurately handles drastic density and specific heat changes across critical point

Gallagher, B. (2012). “Equation of State Unit”. Retrieved from http://flash.uchicago.edu/~jbgallag/2012/flash4_ug/node22.html#SECTION06310000000000000000.
Soave, Giorgio (1972). "Equilibrium constants from a modified Redlich-Kwong equation of state". *Chemical Engineering Science*. 27(6): 1197–1203. doi:10.1016/0009-2509(72)80096-4 .

Schematic

- 3D Simulation
- Slice at z=0 for visualizations
- Buffer zone implemented with adaptive mesh refinement (AMR)
- Ambient temperature and pressure set to match inlet condition



Boundary Conditions

Inflow

- diameter = 2 cm
- input velocity scaled to predetermined mean velocity + noise scaled by r.m.s. profiles calculated via direct numerical simulation (DNS)

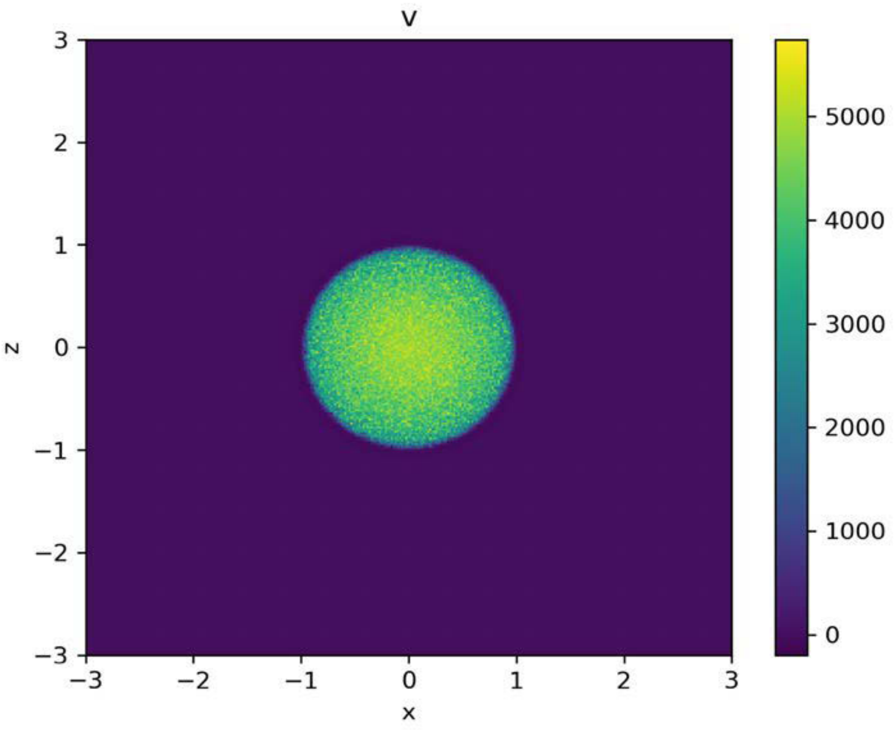
$$v = \langle v_{\text{DNS}} \rangle + \left(v'_{\text{DNS}} + \beta v'_{\text{DNS}} r_1 \sin\theta_1\right) \cdot r_2 \sin\theta_2$$
$$u = u'_{\text{DNS}} + \beta u'_{\text{DNS}} r_3 \sin\theta_3$$
$$w = w'_{\text{DNS}} + \beta w'_{\text{DNS}} r_4 \sin\theta_4$$

$$r_i = \sqrt{-2.0 \log(X_i)}$$
$$\theta_j = 2\pi X_j$$

X_n is a random number between 0 and 1

Outflow

- Impose zero gradient at boundary
- Do not implement AMR at boundary



Ideal Gas and Supercritical Fluid

Cases

Cases

We maintain a single phase fluid by staying far away from the critical point

Air

$P_{jet} = P_{ambient}$ = .101325 MPa
$T_{jet} = T_{ambient}$ = 300 K
V_{jet} = 5,000 cm/s
$\rho_{jet} \approx .001176$ g/cm^3
Re ≈ 60,000
M ≈ .144

- Initial # of cells (x ,y, z): 80, 120, 80
- AMR max level: 3
- Refine when: $\text{vorticity}_{ERR} > 100$

sCO_2

$P_{jet} = P_{ambient}$ = 10.1325 MPa
$T_{jet} = T_{ambient}$ = 600 K
V_{jet} = 10,000 cm/s
$\rho_{jet} \approx .08937$ g/cm^3
Re ≈ 600,000
M ≈ .262

- Initial # of cells (x ,y, z): 80, 120, 80
- AMR max level: 3
- Refine when $\text{vorticity}_{ERR} > 100$

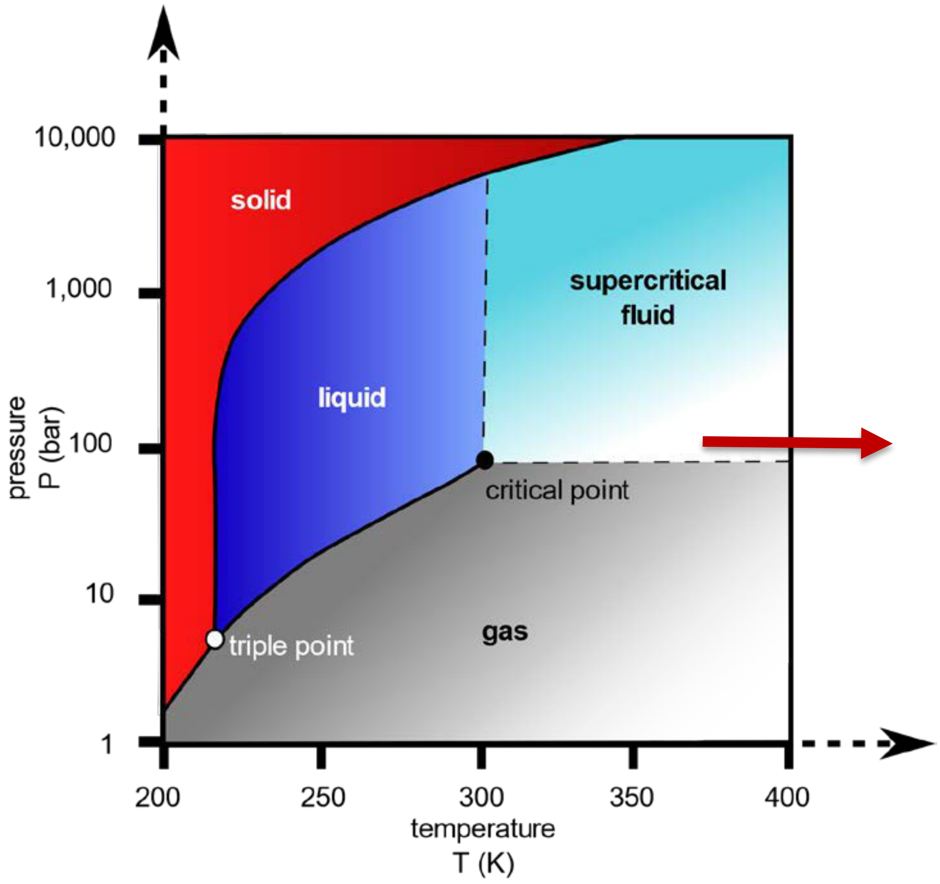


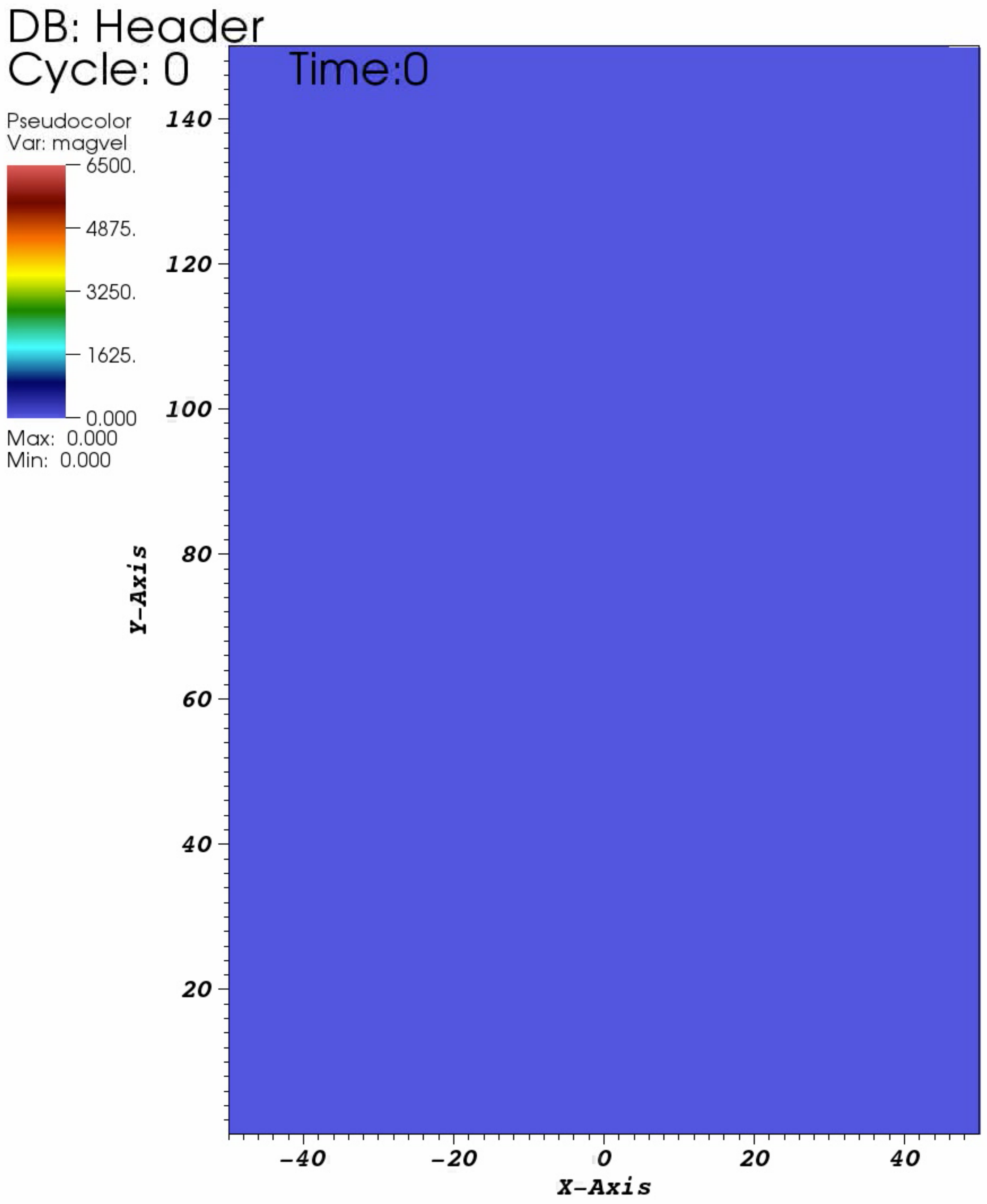
Fig. 5 : Phase Diagram for Carbon Dioxide

Finney, B. & Jacobs, M. (2010). Carbon dioxide pressure-temperature phase diagram.svg. Retrieved from https://commons.wikimedia.org/wiki/File:Carbon_dioxide_pressure-temperature_phase_diagram.svg.

Checking the simulation with a familiar fluid

Ideal Gas

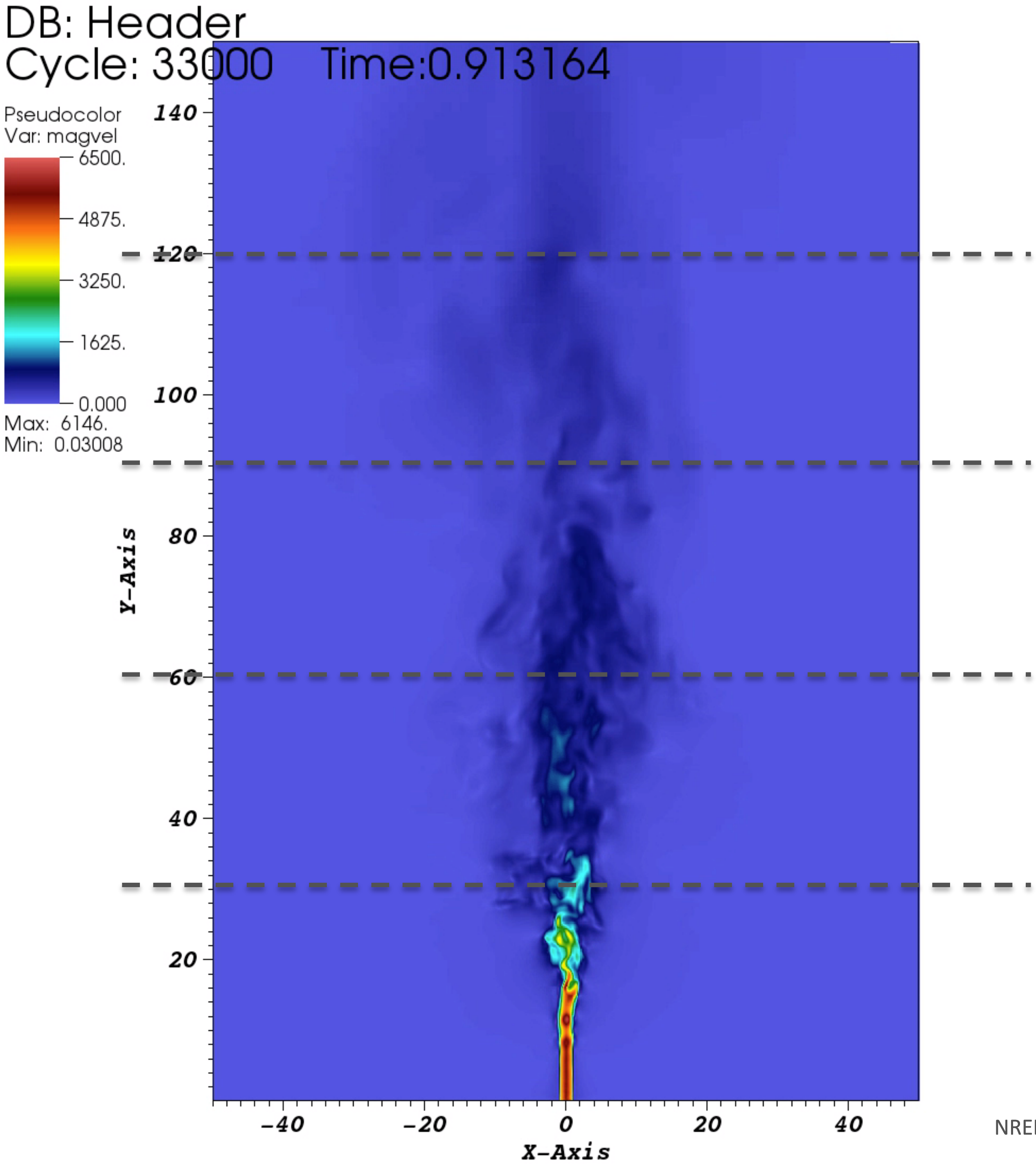
Air Jet



Note: Current simulations do not include a subgrid scale model; future ones will.

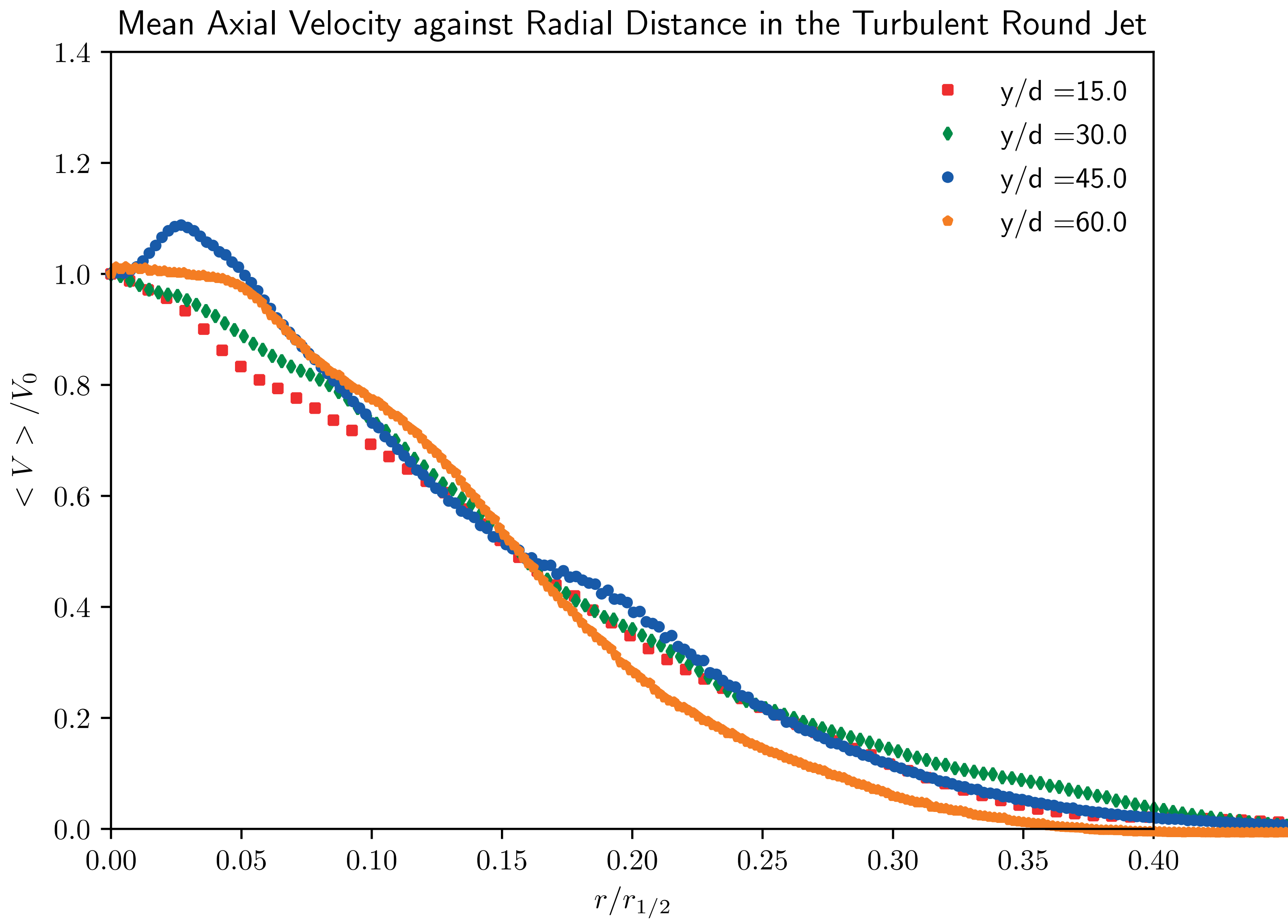
Air Jet

- Plots saved every 500 time steps
- Slices made every 30 cm in y direction from y = 30 to 120
- Means calculated with last 10 plot files



Air Jet:
Velocity Profiles

- Profiles begin to collapse into one curve in self-similar region expected by theory

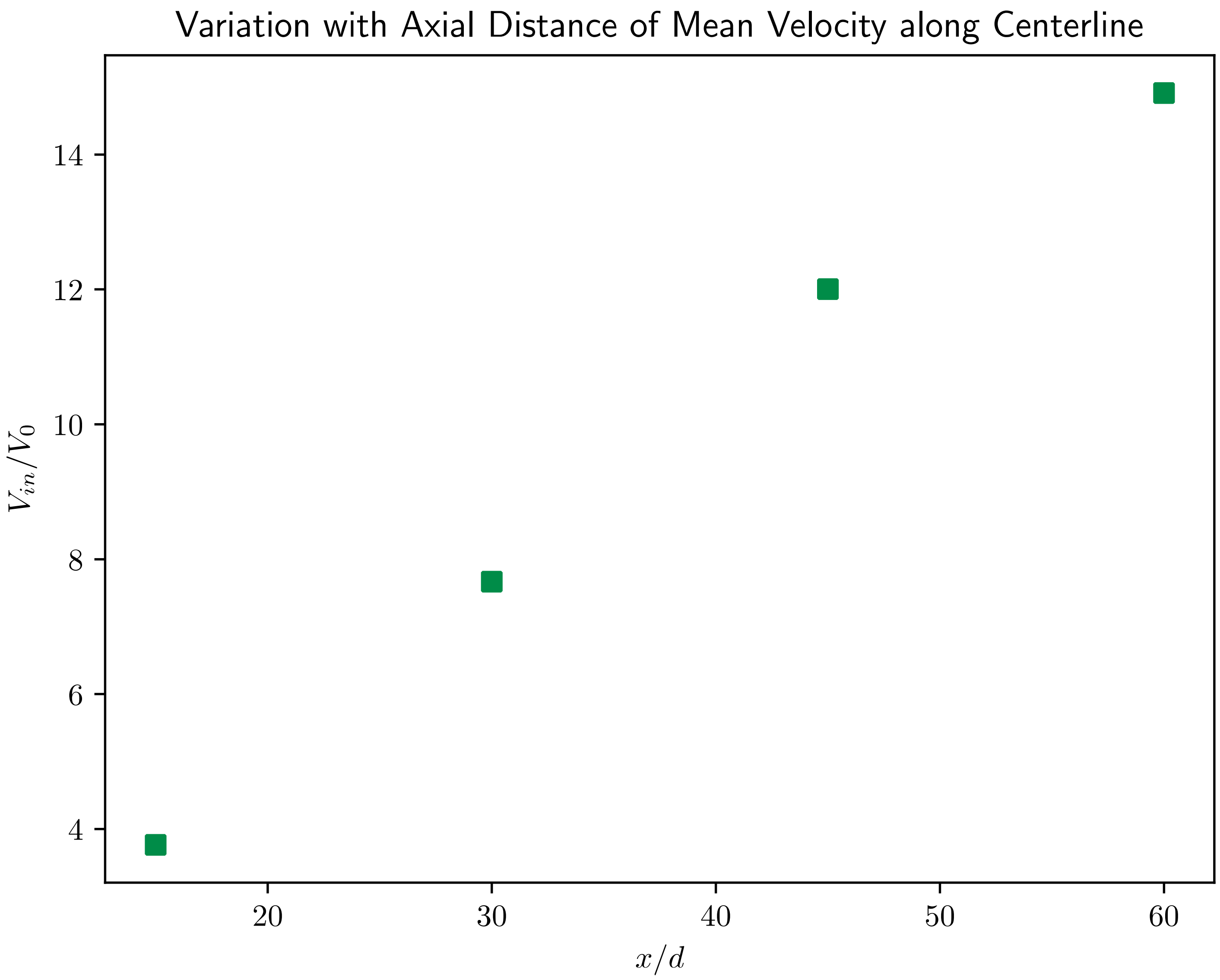


Note: Simulation has not yet reached statistically stationary steady state

Air Jet: Centerline Scaling

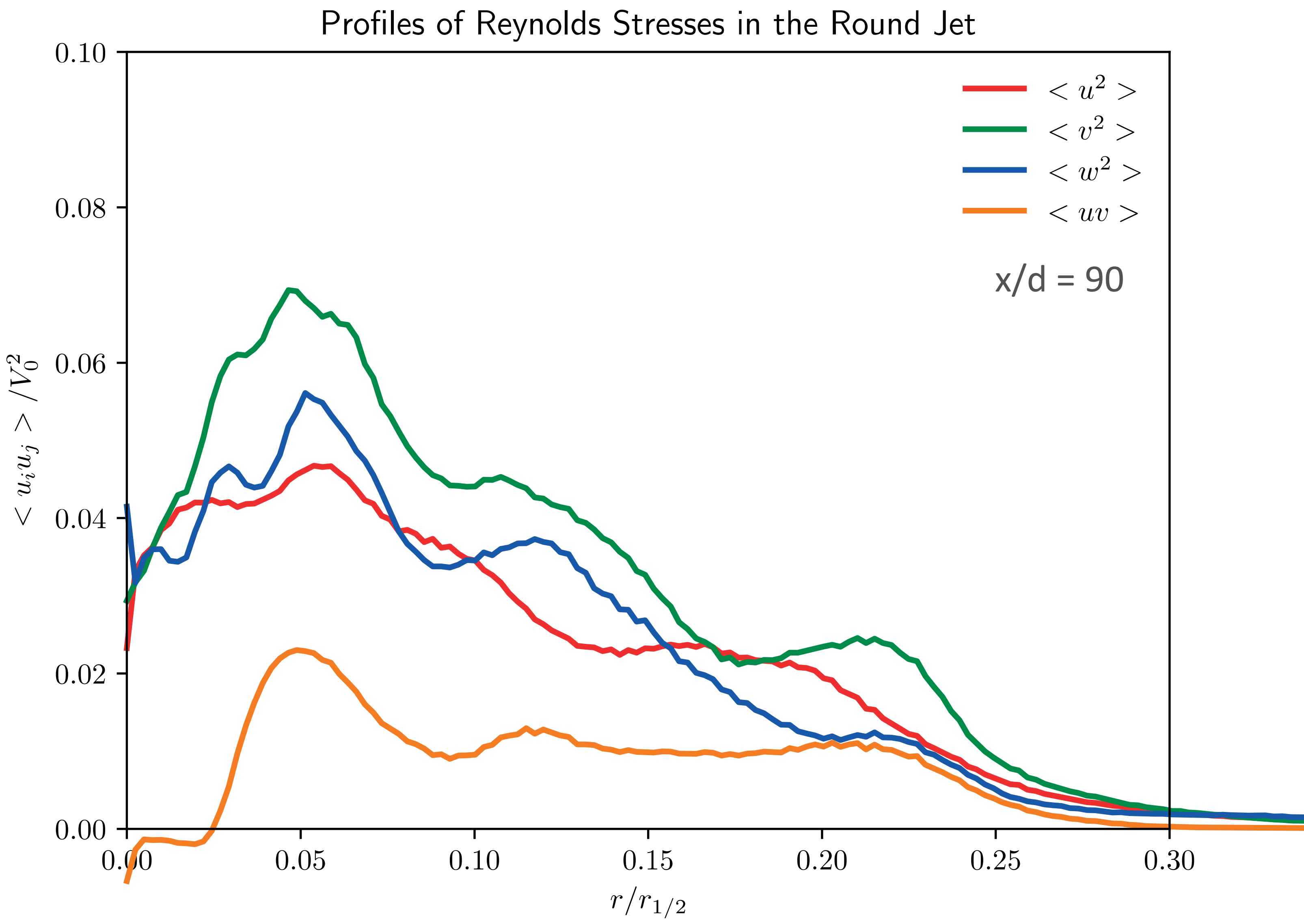
- Close to linear relationship expected by theory: $V_0 \sim x^{-1}$

Note: Simulation has not yet reached statistically stationary steady state



Air Jet:
Reynolds Stresses

- Approaching profiles of Reynolds stresses expected from experimental results



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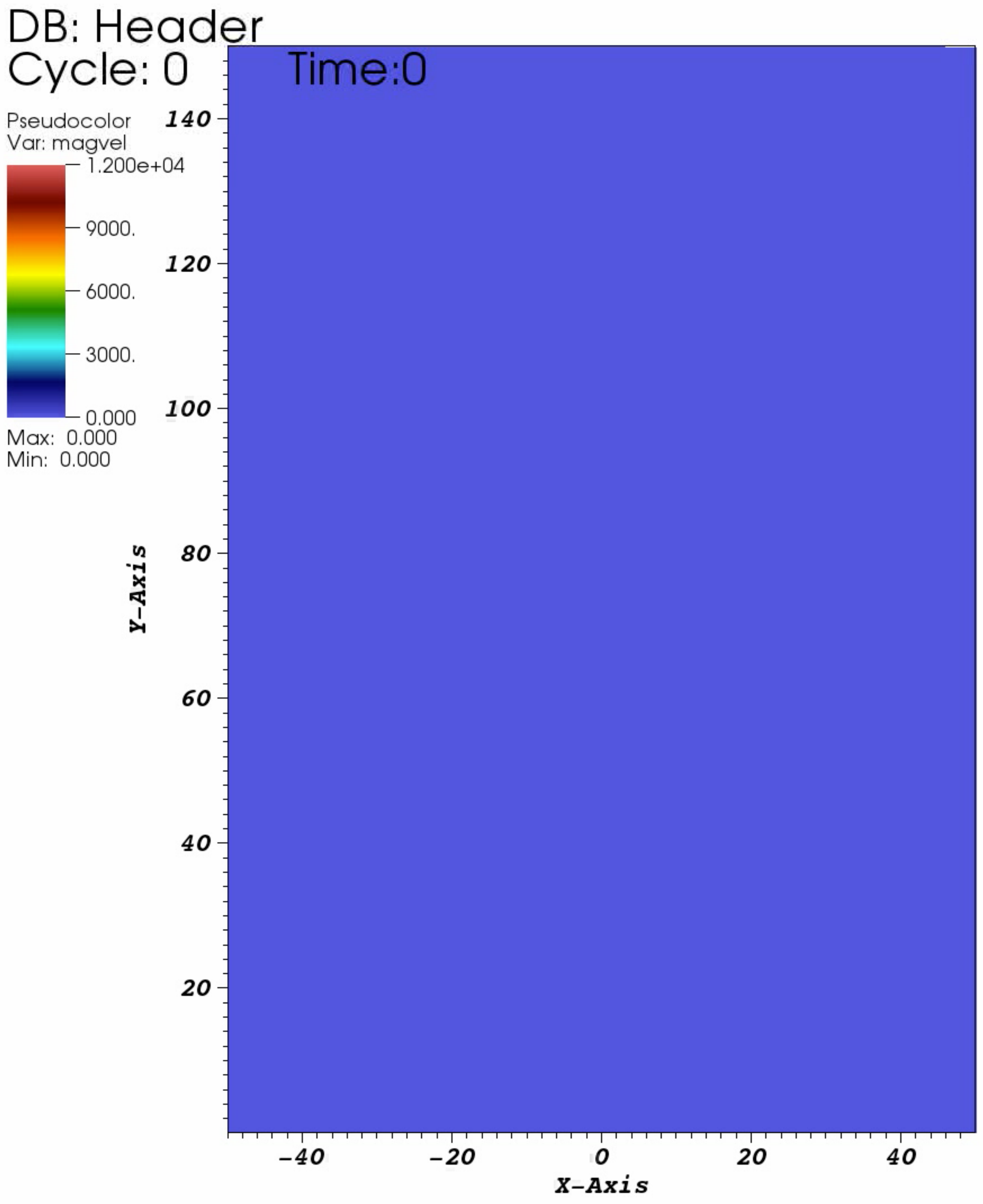
The Supercritical Round Turbulent Jet

Results

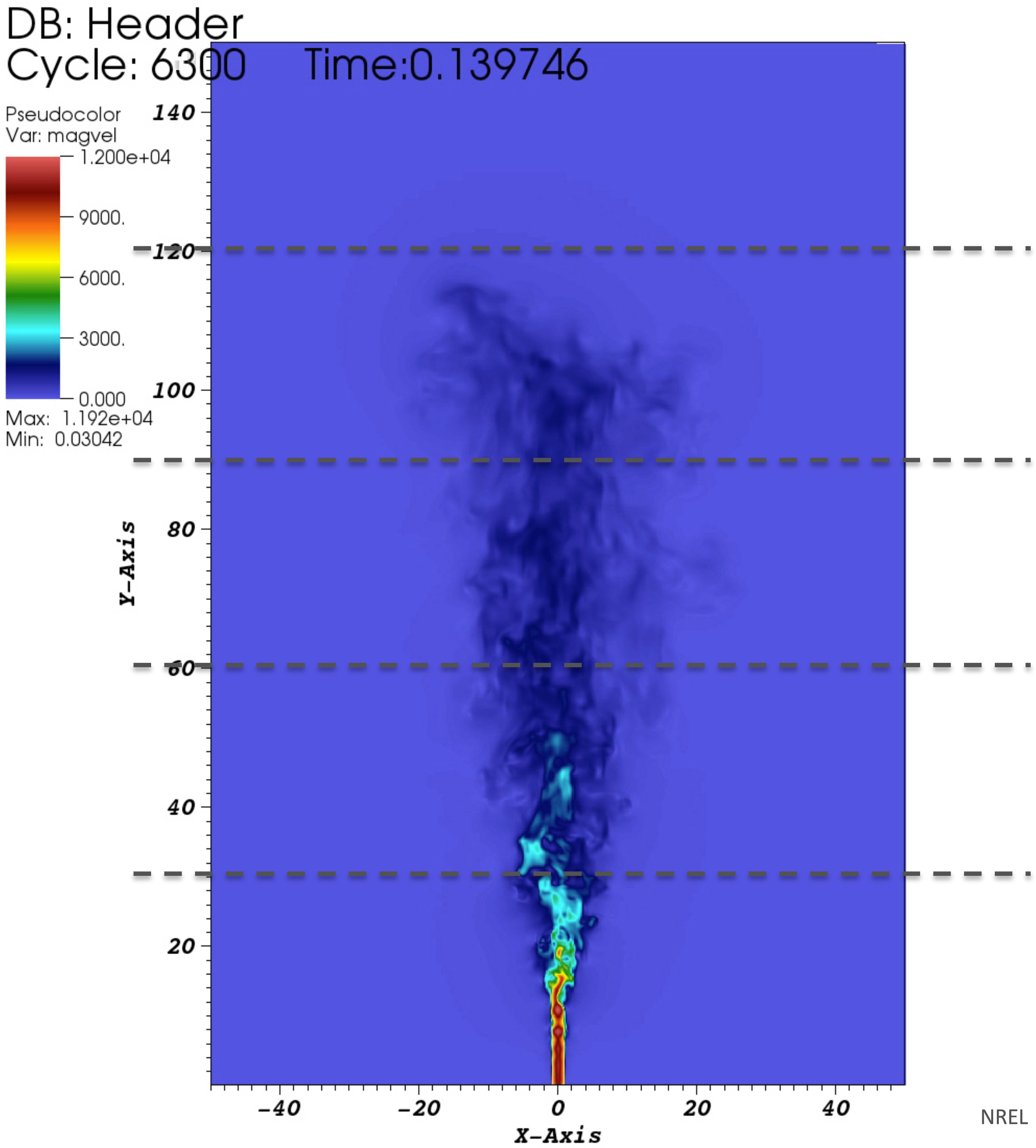
sCO_2 Jet



Note: Current simulations do not include a subgrid scale model; future ones will.

sCO_2 Jet

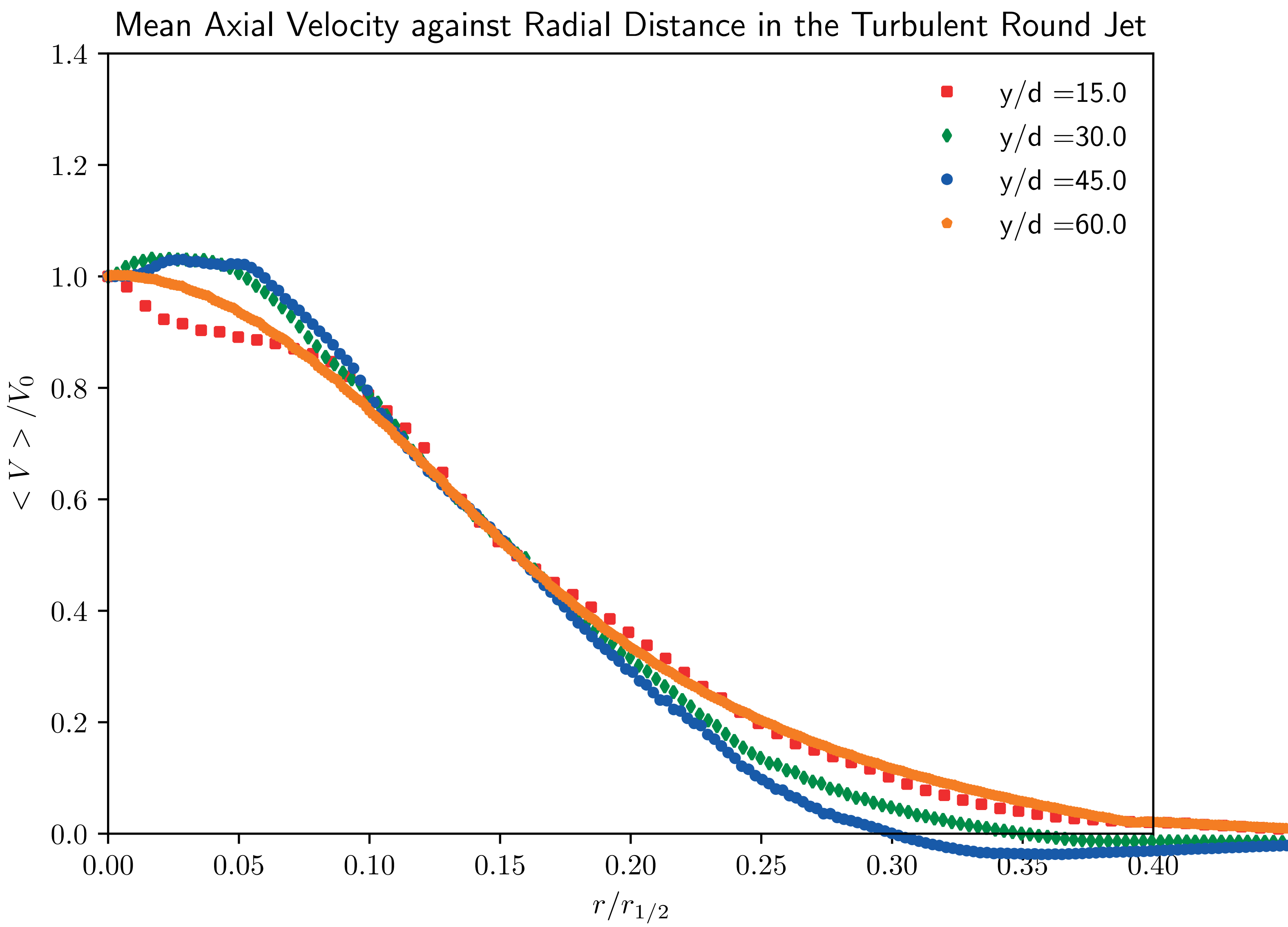
- Plots saved every 300 time steps
- Slices made every 30 cm in y direction from y = 30 to 120
- Means calculated with last 10 plot files



sCO_2 Jet: Velocity Profiles

- Profiles begin to collapse into one curve in self-similar region expected by theory.

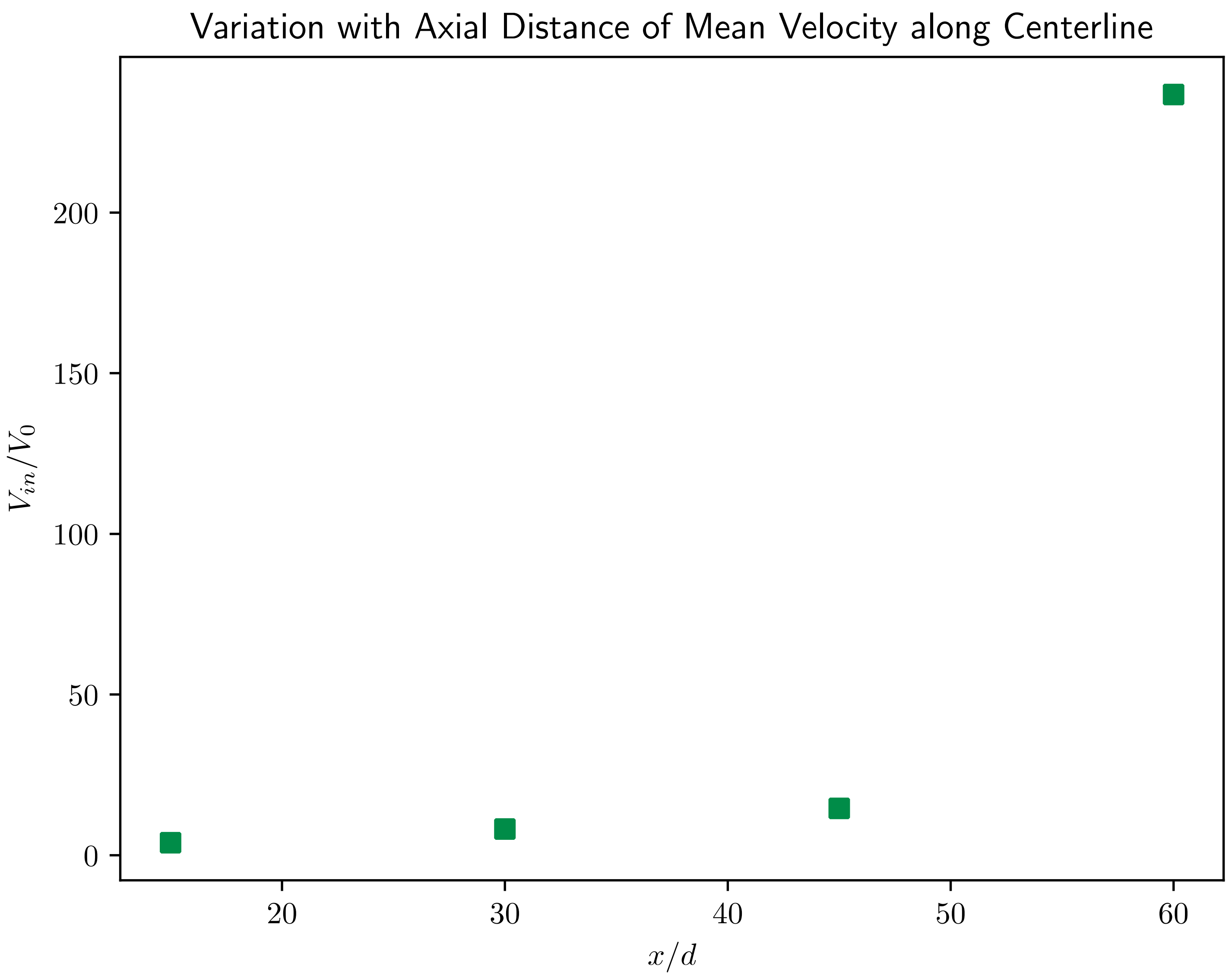
Note: Simulation has not yet reached statistically stationary steady state



sCO_2 Jet: Centerline Scaling

- Jet has only just reached x/d=60 in simulation so relationship is still undetermined.

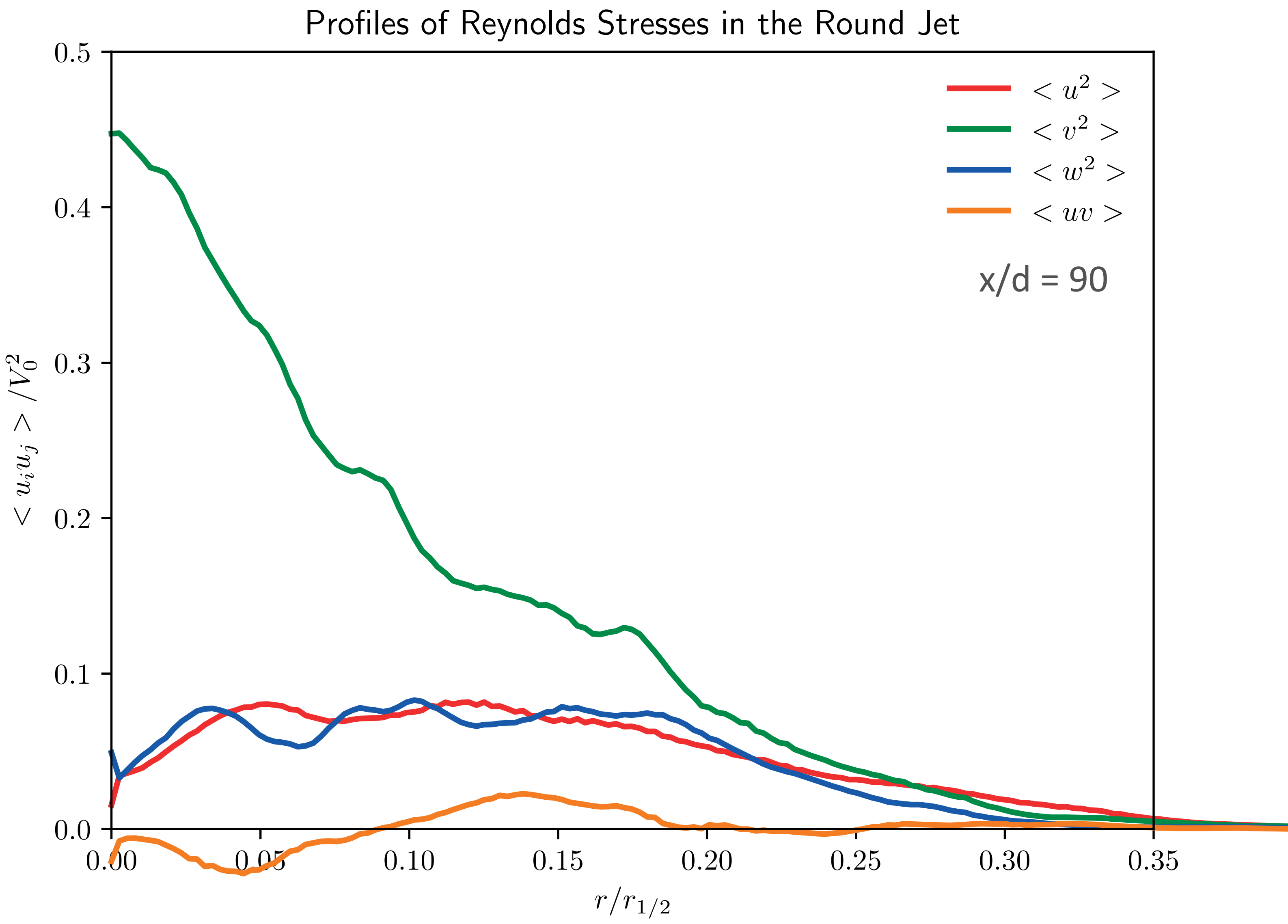
Note: Simulation has not yet reached statistically stationary steady state



sCO_2 Jet: Reynolds Stresses

- General trends for Reynolds stresses match experimental data but magnitude is very high due to current time in simulation.

Note: Simulation has not yet reached statistically stationary steady state



Where will these results take us?

Next Steps

Future Work

So far, we've simulated an ideal gas case to verify jet setup and an sCO_2 case to establish that PeleC can handle simulations at supercritical conditions. Next, we will:

- Continue sCO_2 simulations to reach a statistically stationary state in order to improve accuracy of velocity profile and Reynolds stress information
- Incorporate subgrid scale models to perform Large Eddy Simulation (LES)
- Simulate sCO_2 jet injection into ambient air to incorporate more complicated dynamics and applications

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Questions?

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