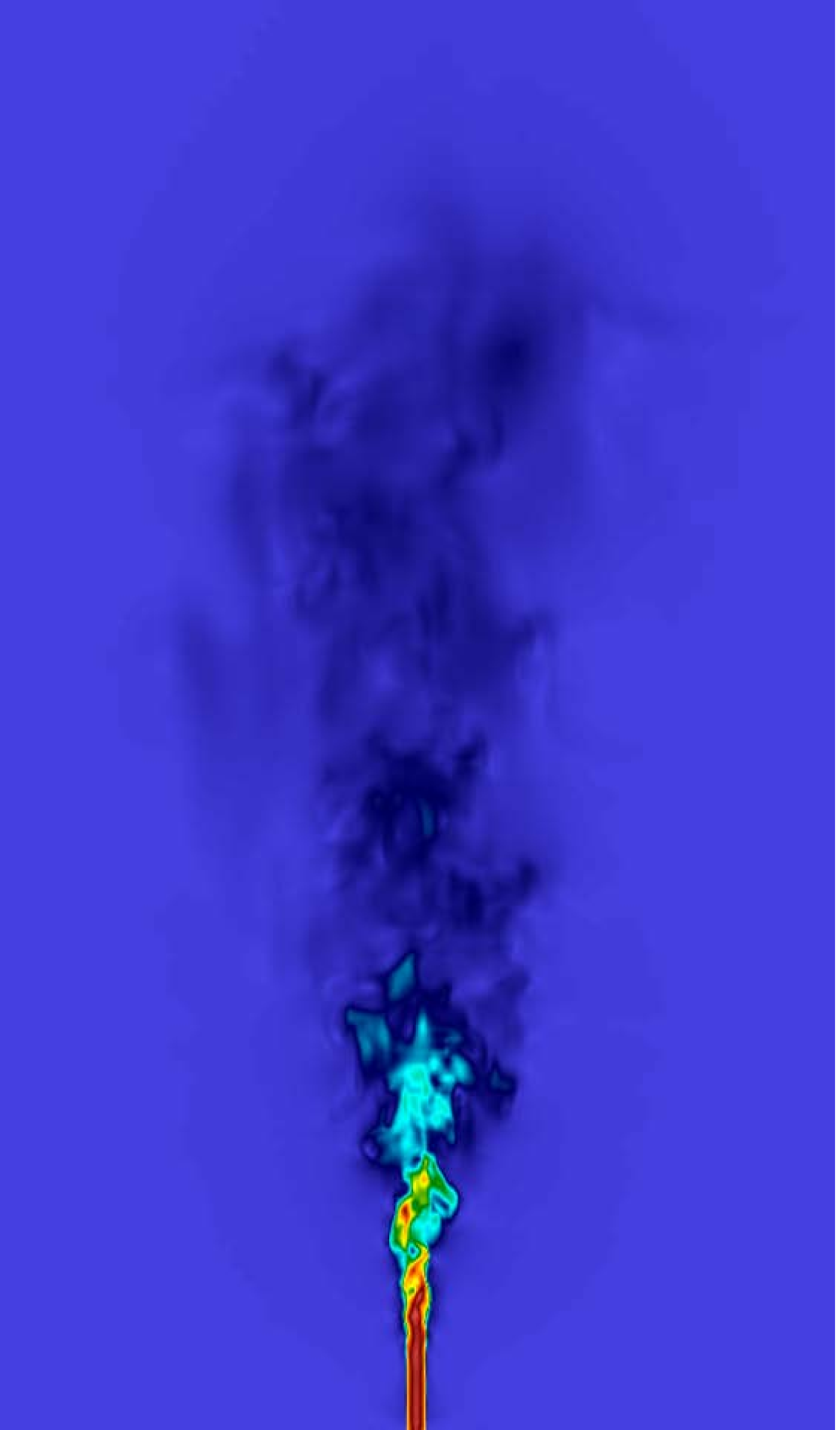
SIAM CSE21 – Thursday, March 4



Adaptive Mesh Refinement Large Eddy Simulation of the Supercritical Carbon Dioxide Round Turbulent Jet

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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

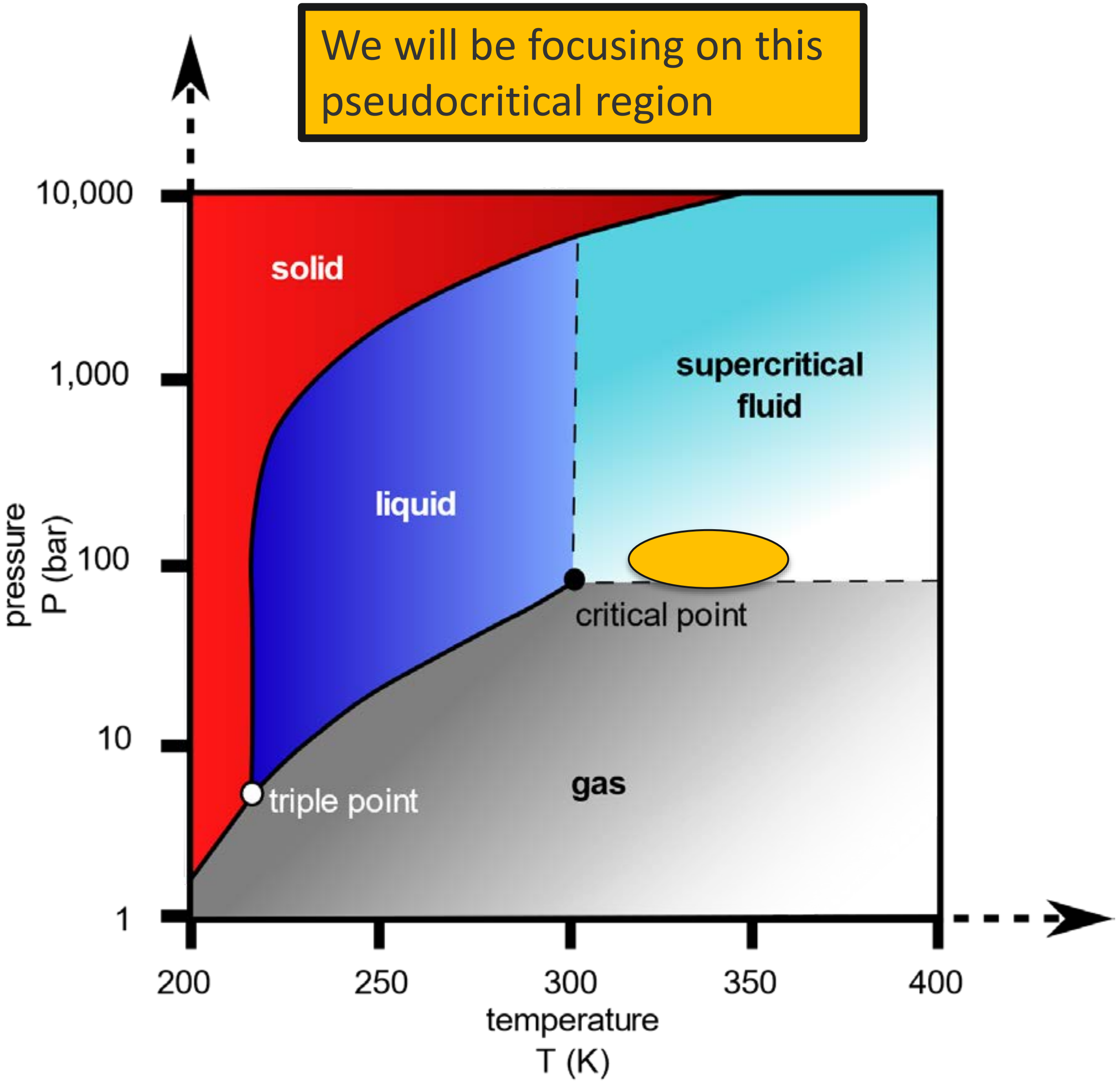

Fig. 1: Phase Diagram for Carbon Dioxide

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

- sCO_2 can be utilized in a variety of industries:
    - Closed-cycle gas turbines
    - Carbon sequestration
- sCO_2 promising fluid in many fields, yet many fundamental physical aspects still unknown
- Experimental challenges with pseudocritical parameters
- Current jet research oriented toward application-specific quantities of interest.

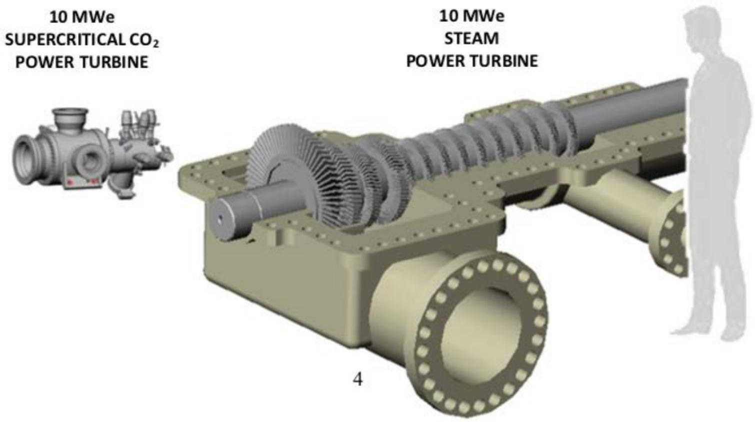

Fig. 2a: 10 MWe sCO_2 power turbine compared to a 10 MWe steam turbine

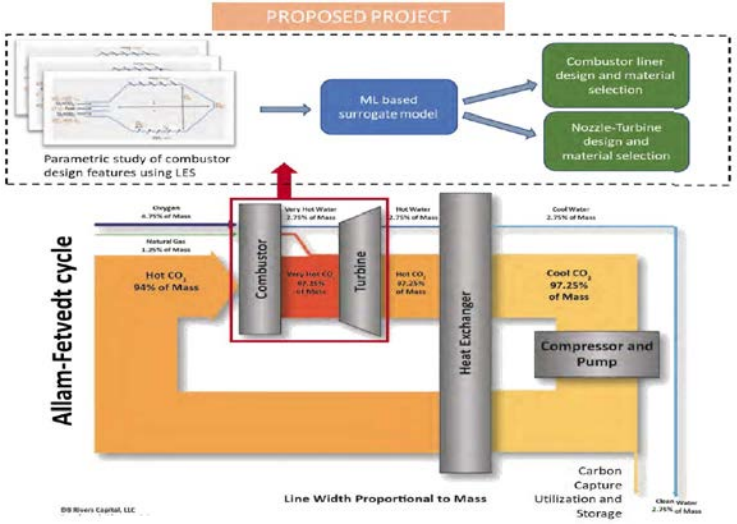

Fig. 2b: Overview of project with 8Rivers Capital: https://hpc4mtls.llnl.gov/projects.html

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.

Supercritical fluids are important for a wide range of applications

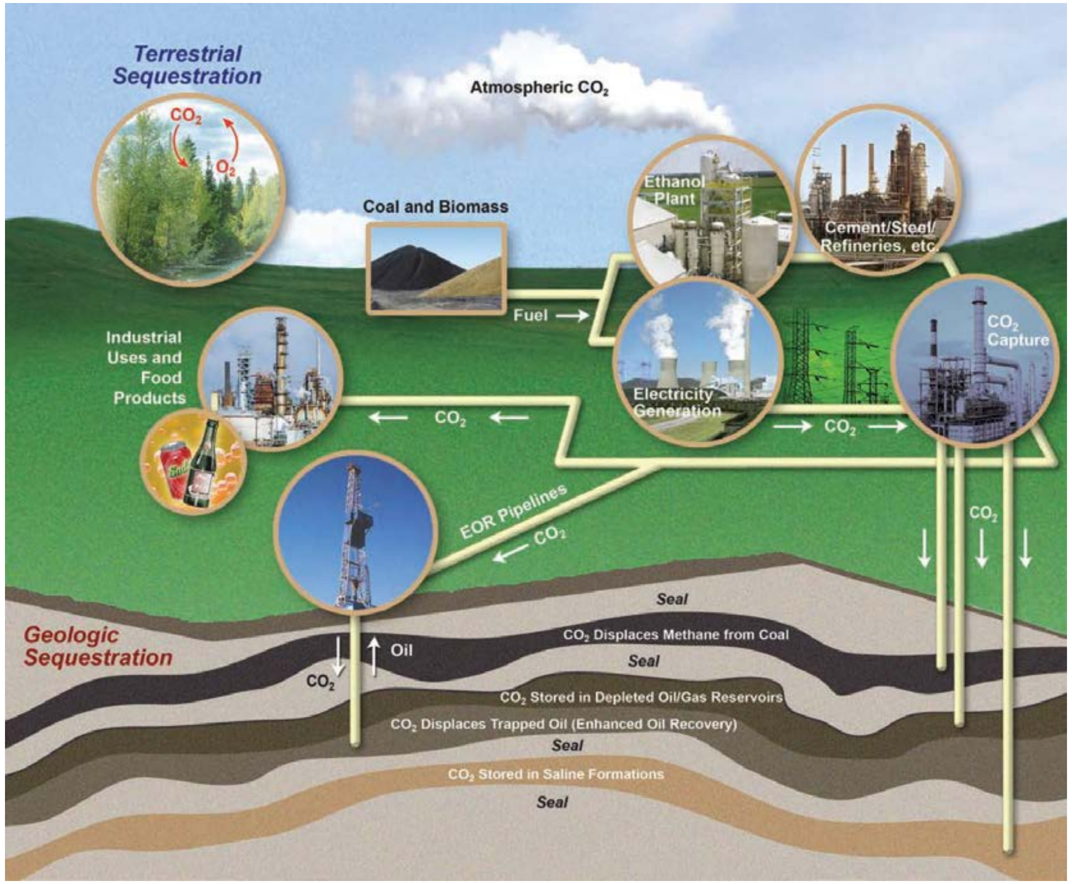

Fig. 3: Examples of Geologic Carbon Sequestration

- sCO_2 can be utilized in a variety of industries:
  - Closed-cycle gas turbines in advanced nuclear reactors
  - Carbon sequestration
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The Trustees of Indiana University. 2019. *Geological Sequestration*. Retrieved from https://igws.indiana.edu/Sequestration

Supercritical fluids are important for a wide range of applications

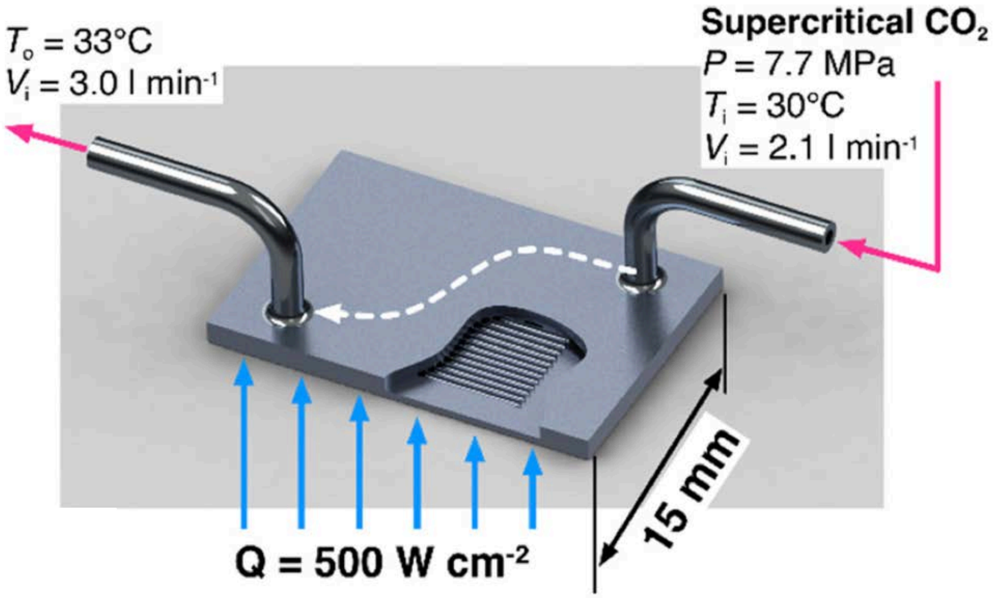

Fig. 4: Another promising application of sCO_2 is in high flux thermal management.

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Fronk, B. & Rattner, A. . (2016). High-Flux Thermal Management with Supercritical Fluids. *Journal of Heat Transfer*. pp. 124501-1-4. 138. 138(12). https://doi-org.proxy.lib.fsu.edu/10.1115/1.4034053
National Academies of Sciences, Engineering, and Medicine. 2020. *Advanced Technologies for Gas Turbines*. Washington, DC: The National Academies Press. https://doi.org/10.17226/25630.

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

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 learn more visit: https://github.com/AMReX-Combustion/PeleC

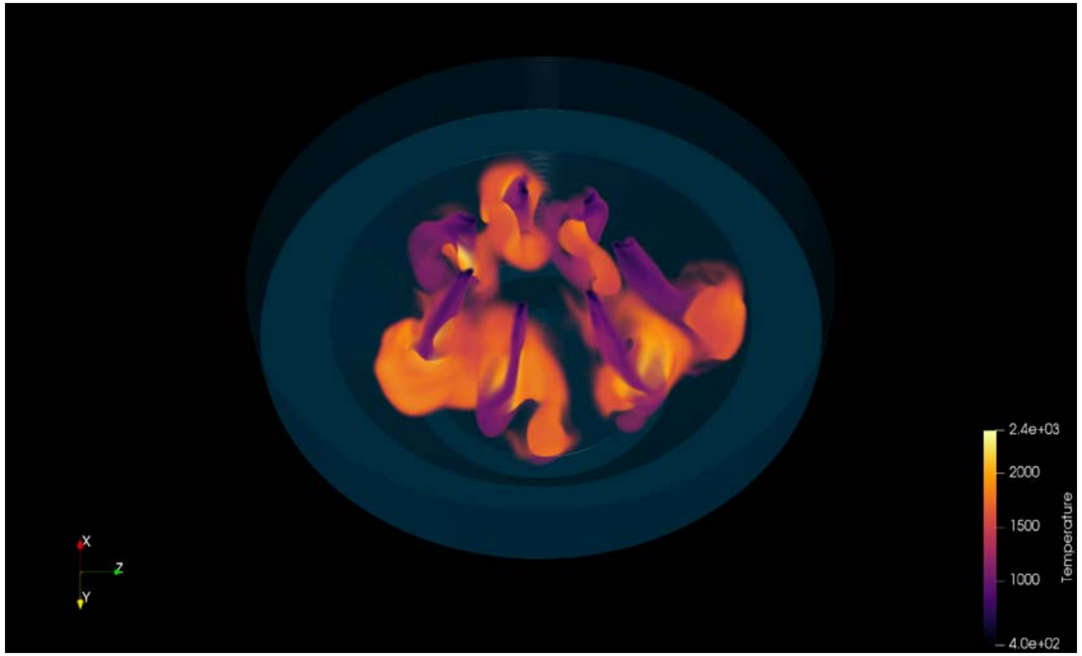


Fig 5: Injection of natural gas in a piston-bowl geometry performed using PeleC

. 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.

Needed to more accurately handle 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.
Rasmussen, E., Shashank, Y., & Martin, M. (2021). “How equation of state selection impacts accuracy near the critical point: Forced convection supercritical CO2 flow over a cylinder.” *The Journal of Supercritical Fluids.* 105141. 171. https://doi.org/10.1016/j.supflu.2020.105141
Martin, M., Rasmussen, E. & Shashank, Y. (2019). “Nonlinear Heat Transfer from Particles in Supercritical Carbon Dioxide Near the Critical Point.” *Journal of Thermal Science and Engineering Applications.* 034501 (5 pages). 12(3). https://doi.org/10.1115/1.4045222

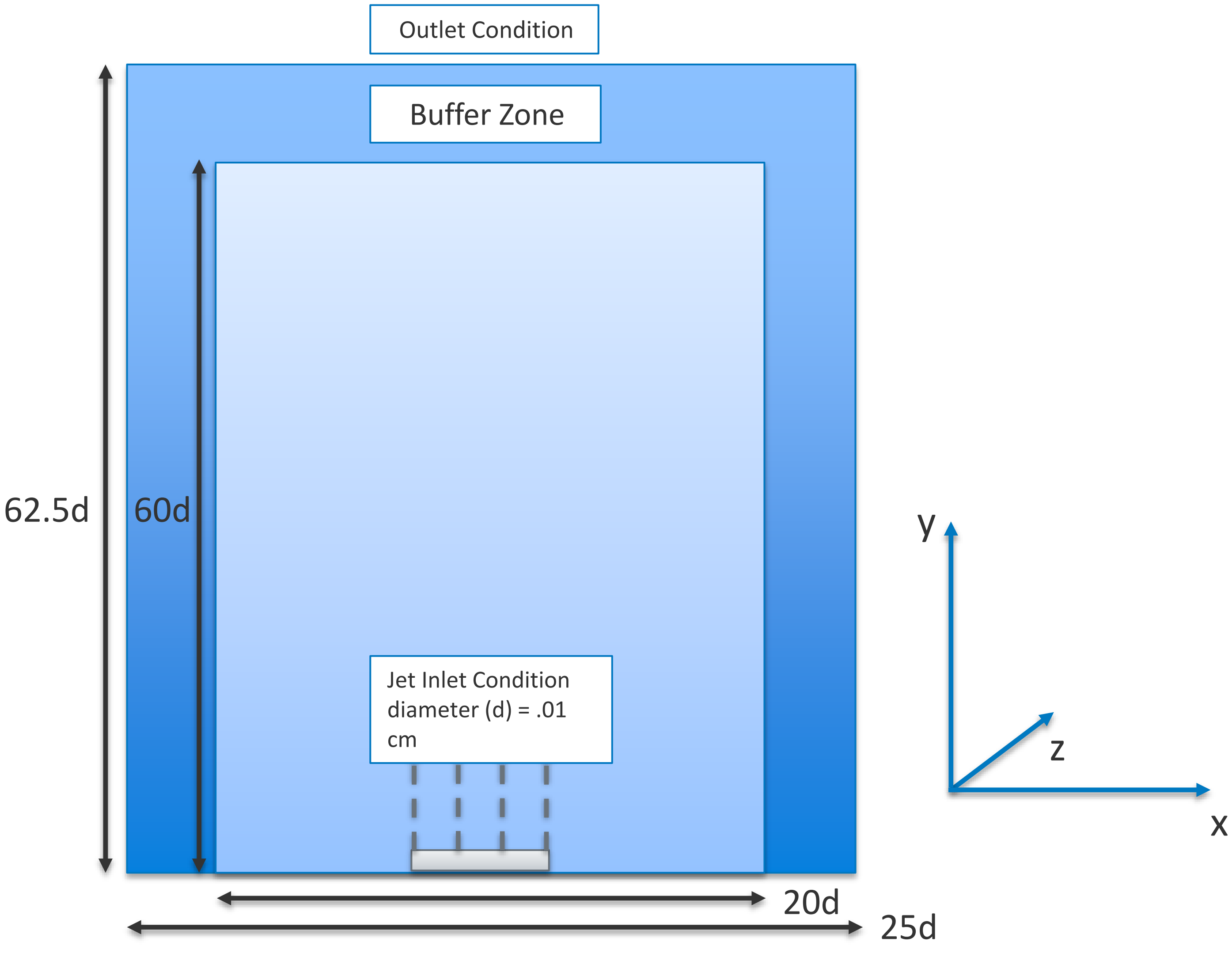
Large Eddy Simulation (LES) modeling

- Dynamic Smagorinsky Model for compressible flow
  - Filter type: 3 point box filter approximation
  - Filter-Grid ratio: 2

Martín, M. Pino, U. Piomelli, and G. V. Candler (2000). “Subgrid-Scale Models for Compressible Large-Eddy Simulations.” *Theoretical and Computational Fluid Dynamics.* 13(5): 361–376
Sagaut, P. and R. Grohens (1999). “Discrete filters for large eddy simulation.” *International Journal for Numerical Methods in Fluids.* 31: 1195-1220

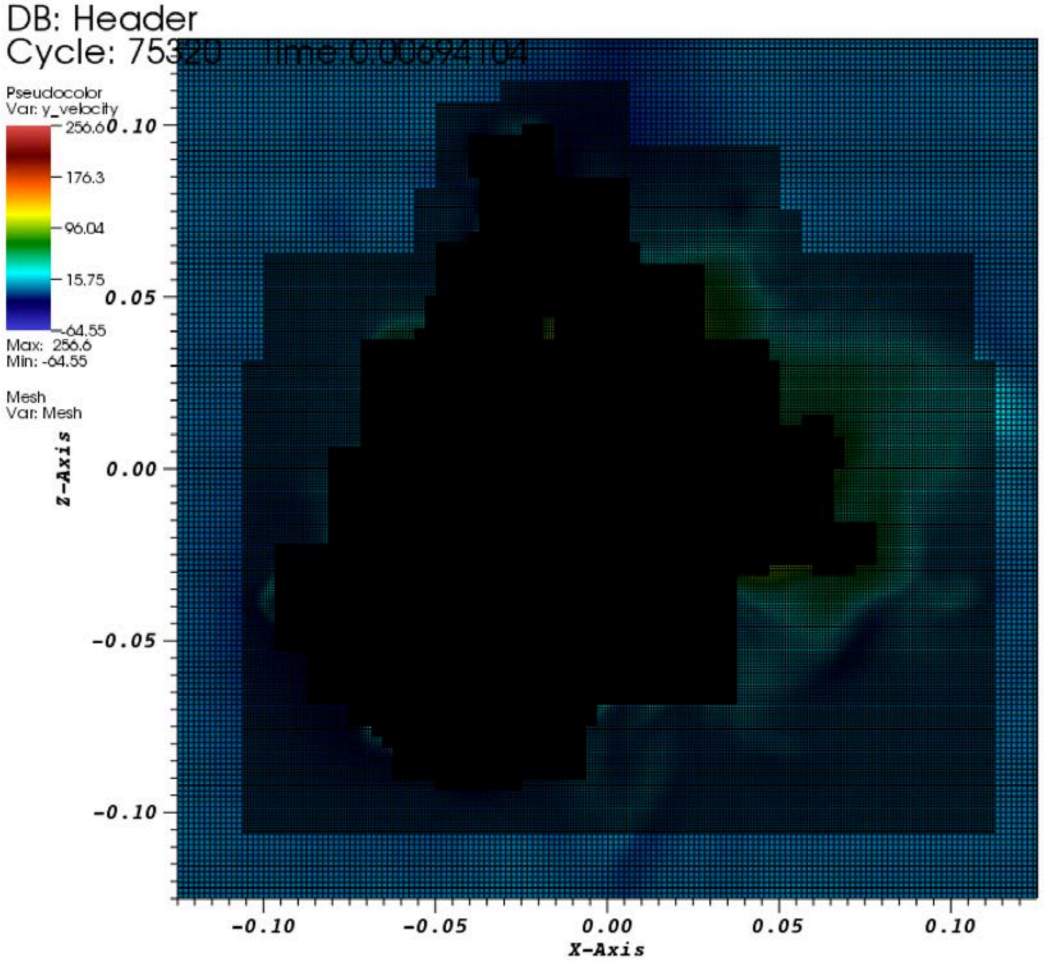
Schematic

- 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
- # of cells on coarse grid (x ,y, z): 80, 200, 80
- AMR max level: 4
- Refine when vorticity$_{ERR}$ > 5000



Performing LES in HPC environment

- Simulations utilize 576 MPI Ranks
  - 36 ranks per node across 16 nodes
  - Roughly 17k cells per MPI Rank
- Each plot file contains approximately 34 GB of data
- We use the NREL Eagle supercomputer to perform simulations
- PeleC has been shown to scale very well on this system and other HPC systems (e.g. ORNL Summit)
- Dynamic load balancing of AMR levels allows for maximum utilization of the system
- The Intel suite of compilers was used



Boundary Conditions

Inflow

- diameter = .01 cm
- input velocity scaled to predetermined mean velocity + noise scaled by r.m.s. profiles calculated via direct numerical simulation (DNS)

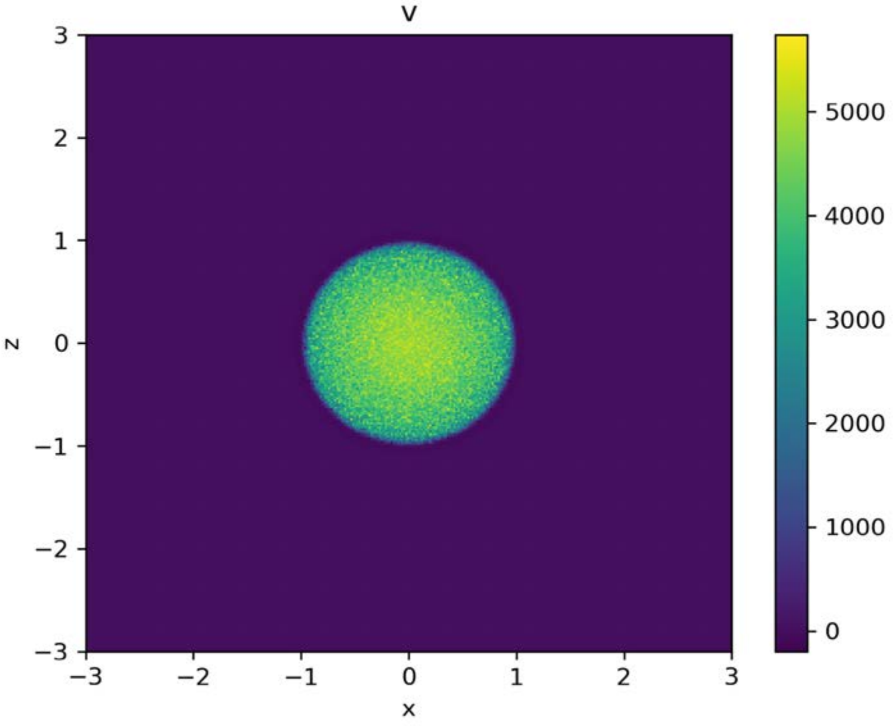
$$
\begin{aligned}
v &= \langle v_{\mathrm{DNS}} \rangle + \left(v'_{\mathrm{DNS}} + \beta v'_{\mathrm{DNS}} r_1 \sin\theta_1 \right) \cdot r_2 \sin\theta_2 \\
u &= u'_{\mathrm{DNS}} + \beta u'_{\mathrm{DNS}} r_3 \sin\theta_3 \\
w &= w'_{\mathrm{DNS}} + \beta w'_{\mathrm{DNS}} r_4 \sin\theta_4
\end{aligned}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

$$
\begin{aligned}
r_i &= \sqrt{-2.0 \log\left(X_i\right)} \\
\theta_j &= 2\pi X_j
\end{aligned}
$$

X_n is a random number between 0 and 1

Outflow

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



Exploring Injections Near the Pseudocritical Point

- We want to look at cases near the critical point to study large changes in specific heat

Parameters

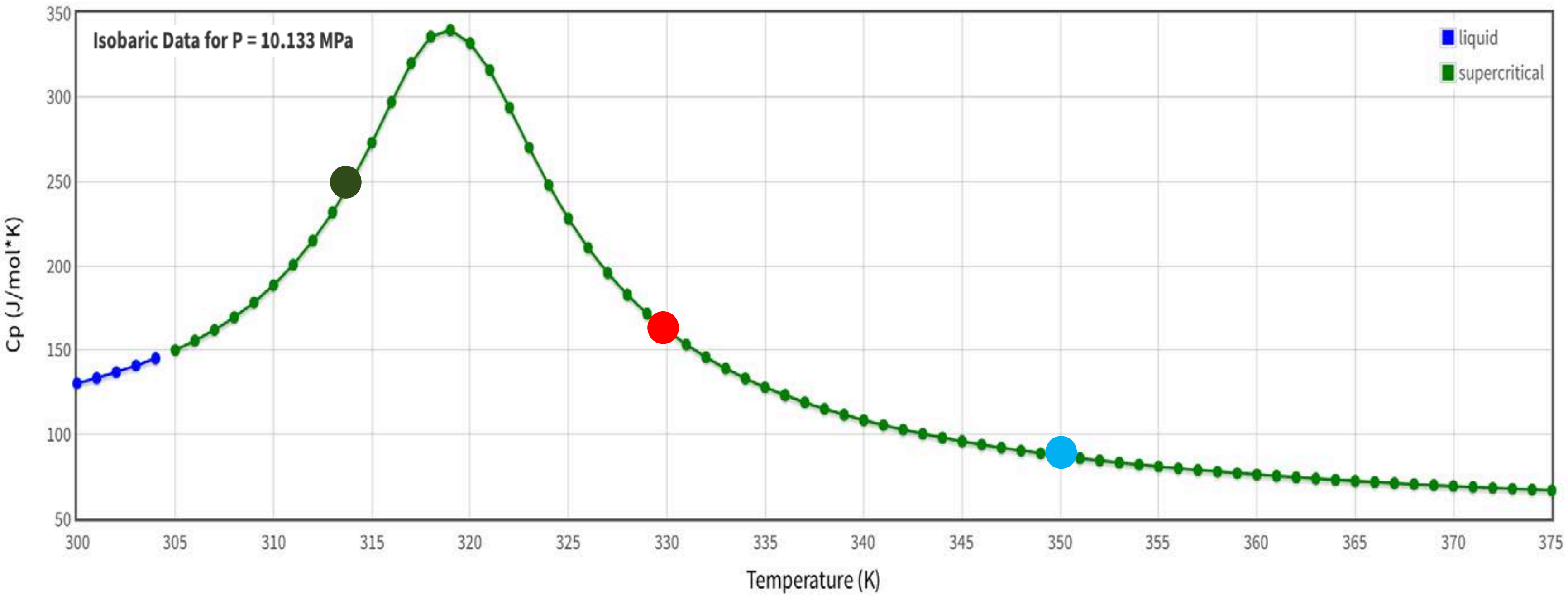
$P_{jet} = P_{ambient} = 10.1325$ MPa
$T_{jet} = 330$ K
$T_{ambient} = 330$ K / 314 K / 350 K
$V_{jet} = 1{,}800$ cm/s
$\rho_{jet} \approx .329941$ g/cm^3
Re $\approx$ 22,911
M $\approx$ .08

We focus here for brevity on Case 1.

Case 1: $T_{ambient} = T_{jet}$

Case 2: $T_{ambient} < T_{jet}$

Case 3: $T_{ambient} > T_{jet}$



National Institute of Standards and Technology. “Isobaric Properties for Carbon Dioxide.” *NIST Chemistry WebBook, SRD 69,* 2018, https://webbook.nist.gov/cgi/fluid.cgi?P=10.1325&TLow=300&THigh=375&TInc=1&Applet=on&Digits=6&ID=C124389&Action=Load&Type=IsoBar&TUnit=K&PUnit=MPa&DUnit=g%2Fml&HUnit=kJ%2Fmol&WUnit=m%2Fs&VisUnit=cP&STUnit=N%2Fm&RefState=DEF. Accessed 23 October 2019.

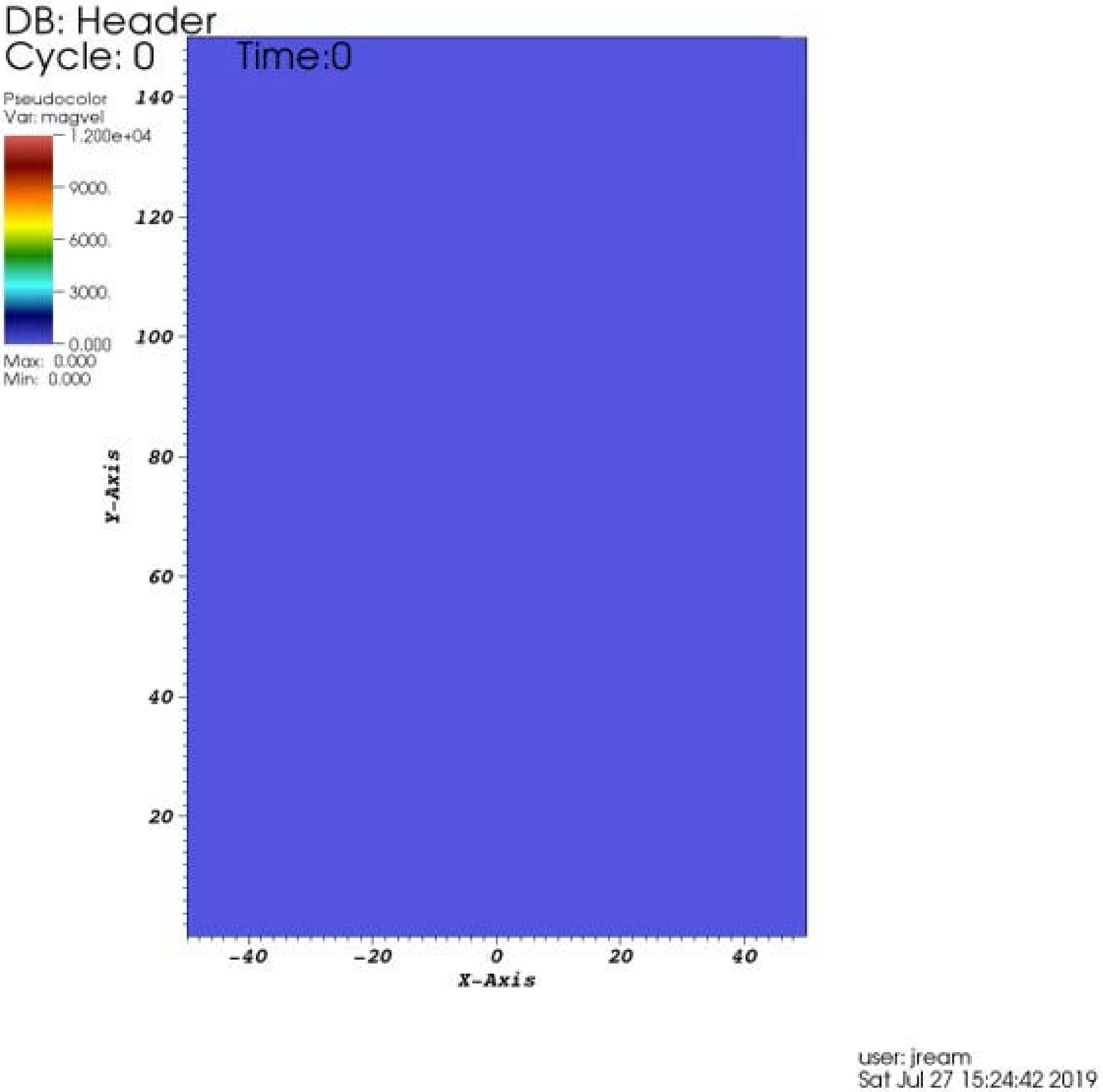
sCO_2 Jet

Parameters

$P_{jet} = P_{ambient} = 10.1325$ 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

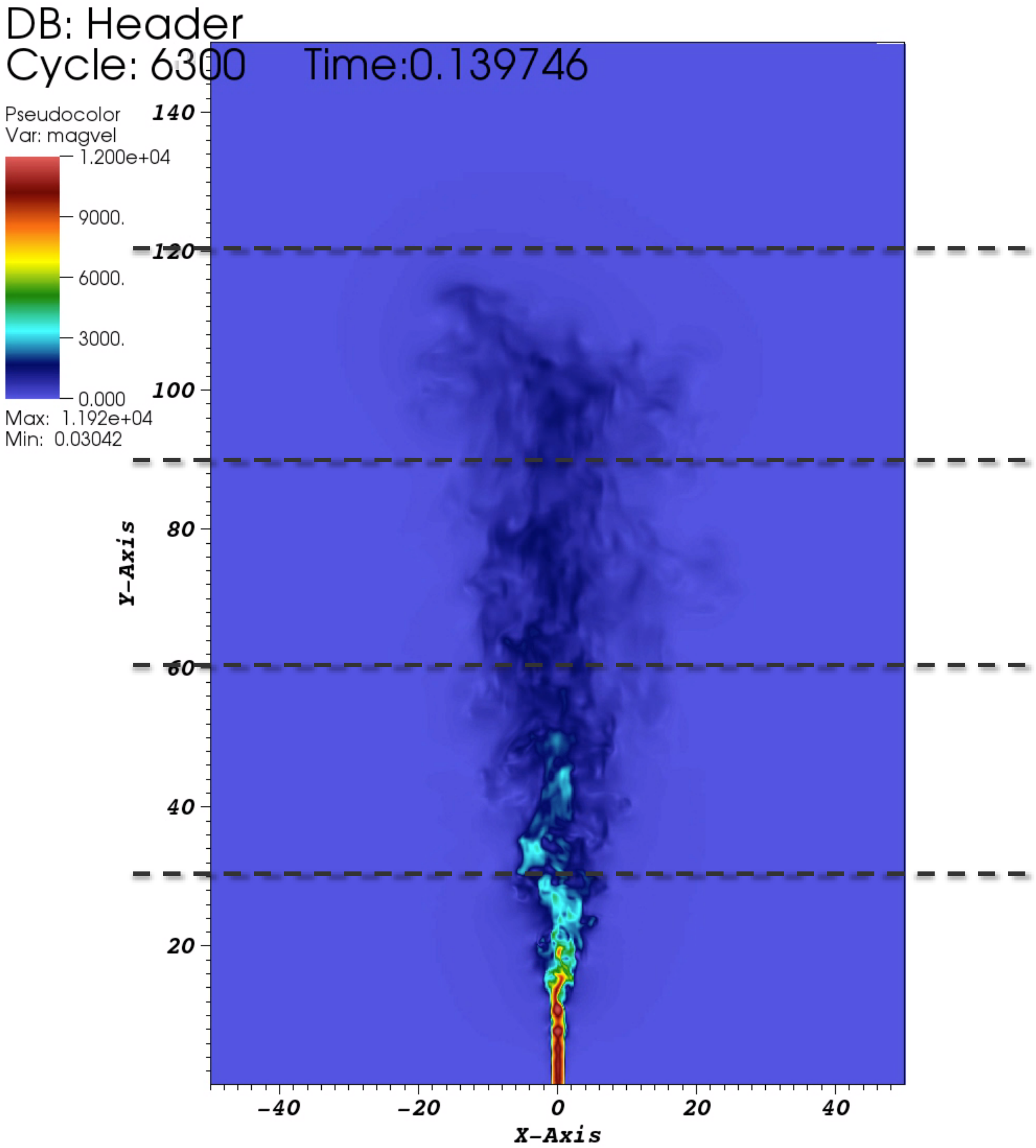
- Initial # of cells (x ,y, z): 80, 120, 80
- AMR max level: 3
- Refine when vorticity$_{ERR} > 100$

Note: Current simulations do not include a subgrid scale model; future ones will. The following is a coarse grid, capability establishing simulation.



sCO_2 Jet

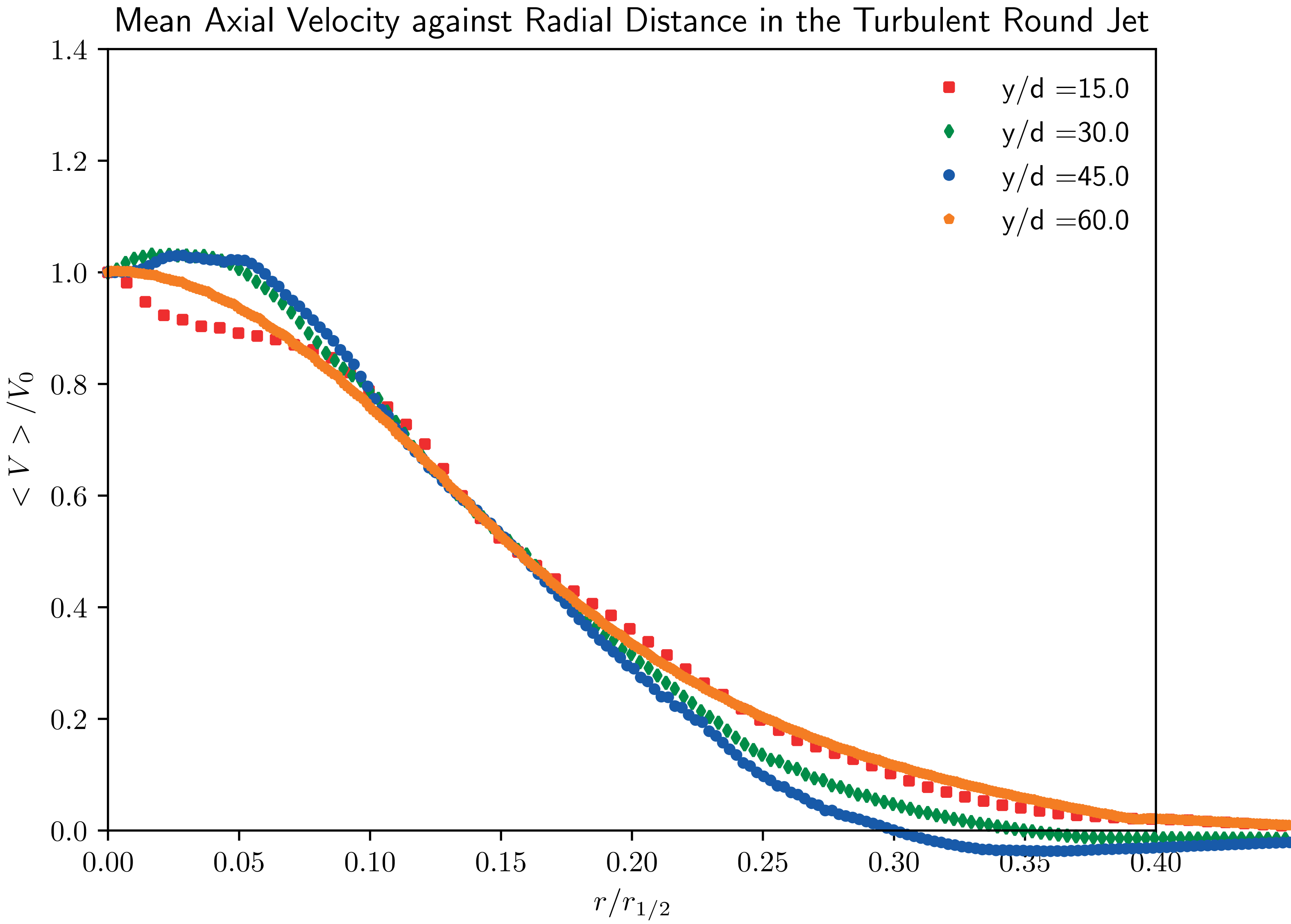
- Plots saved every 300 time steps
- Slices made every 30 cm in y direction from y = 30 to 120
- Means calculated with last 10 plot files



sCO_2 Jet: Velocity Profiles

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

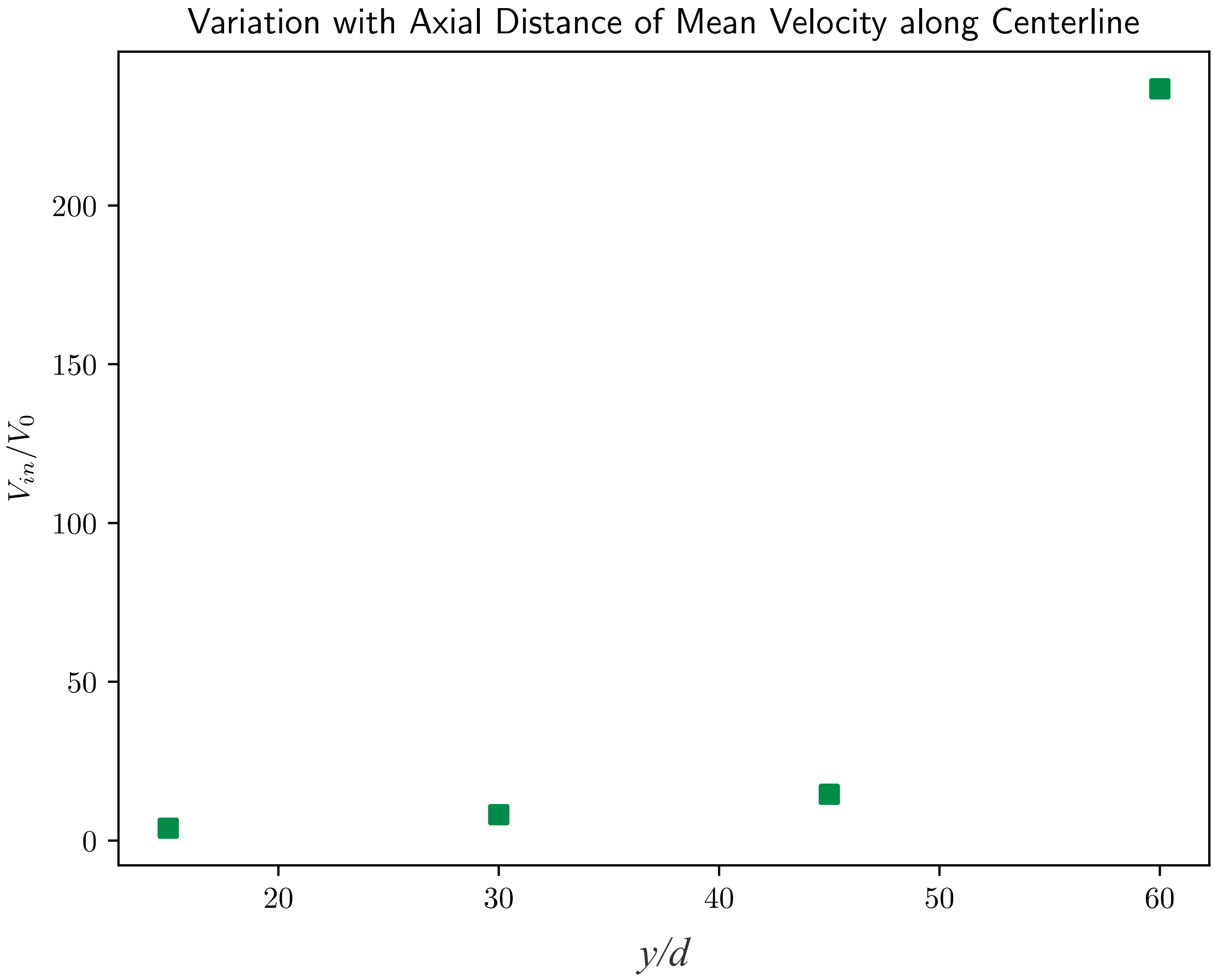
Note: Simulation has not yet reached statistically stationary steady state



sCO_2 Jet: Centerline Scaling

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

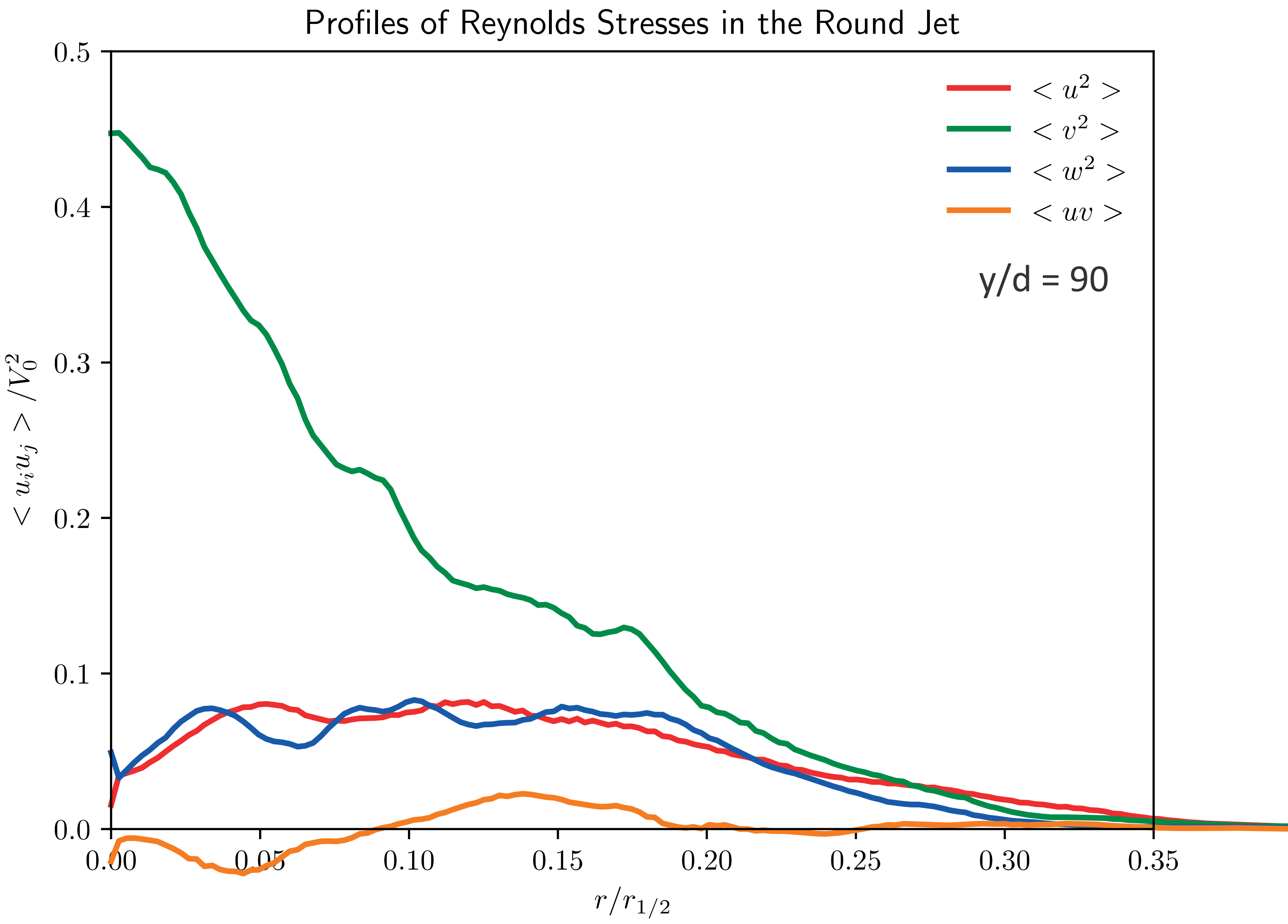
Note: Simulation has not yet reached statistically stationary steady state



sCO_2 Jet: Reynolds Stresses

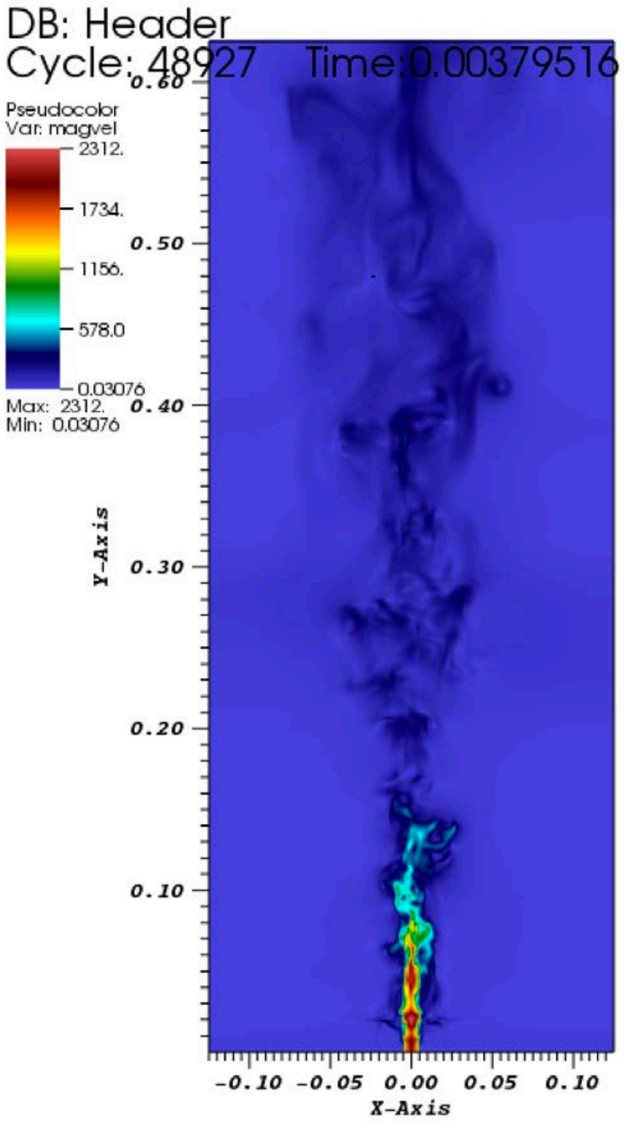
- General trends for Reynolds stresses match experimental data but magnitude is very high due to current time in simulation.

Note: Simulation has not yet reached statistically stationary steady state



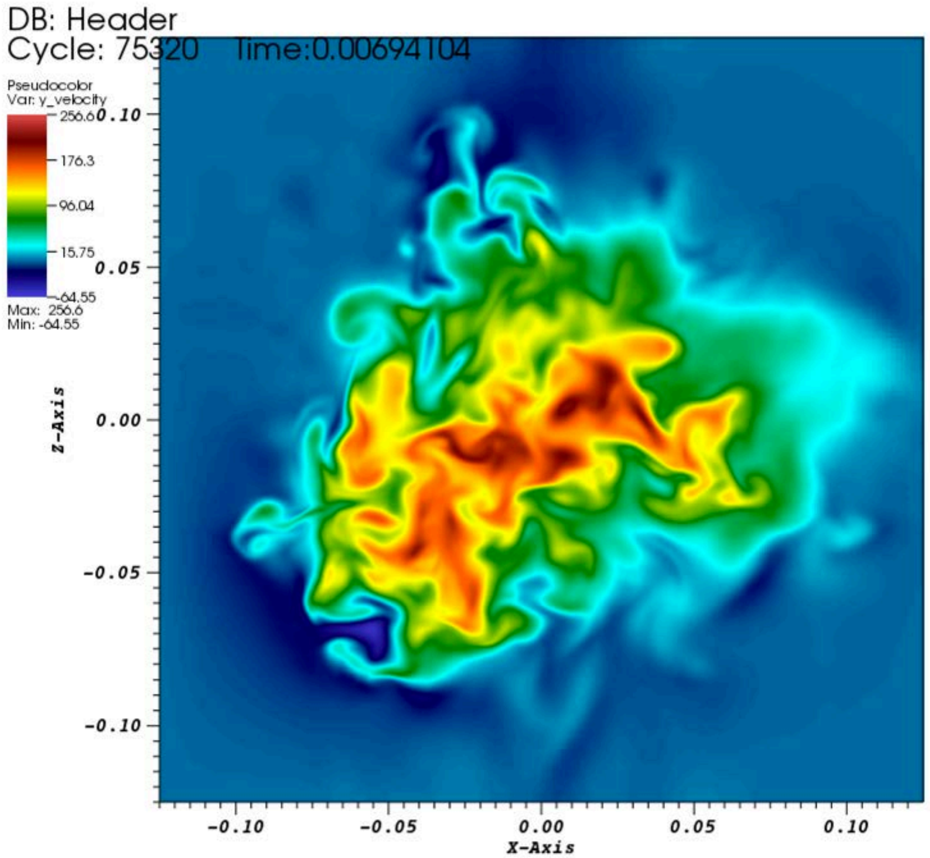
Current Status of Simulations

- All three cases have run to completion: 2 flow throughs of coarse (max 1 level) refinement and 10 subsequent flow throughs of fine (max 4 level) refinement.
- 100 plots saved per flow through
- Means calculated with last 200 plot files

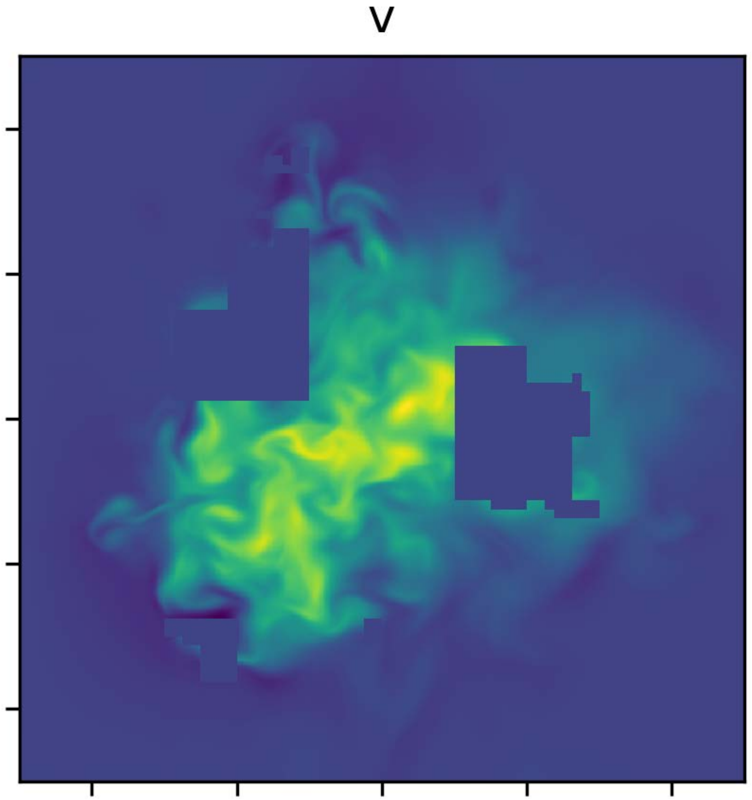


Post-Processing Large Datasets in HPC environments

At this point, all three cases have reached statistically stationary steady state, but we are now having issues with slicing large datasets in the HPC environment.



When visualizing using VisIt, data is intact



Sample output from slicing tool is not intact.

Currently, building custom post-processing tools to extract data.

Acknowledgements

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- This work was supported by the Department of Energy's Office of Science through the Exascale Computing Project (ECP), managed through Oak Ridge National Laboratory.

Questions?

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