The Center for Astrophysical Thermonuclear Flashes

Validation of the FLASH Code: Two- and Three-Dimensional Simulations of Shock-Cylinder Interactions

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An Advanced Simulation & Computing (ASC)
Academic Strategic Alliances Program (ASAP) Center
at The University of Chicago

Acknowledgements

- LANL: Chris Tomkins, Mark Marr-Lyon, Bob Benjamin
- ANL: Mike Papka, Randy Hudson
  Brad Gallagher
- Vikram Dwarkadas, Tomek Plewa, Todd Dupont

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What is the FLASH Code?

- Community code for Astrophysics - Can solve a broad range of (astro)physics problems
- Designed for compressible reactive flows
- Block-structured, spatial adaptive mesh refinement (PARAMESH)
- Parallel (MPI), including I/O
- Has a modern CS-influenced architecture
- Portable: runs on many massively-parallel systems, linux boxes to ASCI machines
- Scales and performs well - Gordon Bell prize
- Is available on the web: http://flash.uchicago.edu

Verification and Validation of FLASH

V & V at the Flash Center

- Automated test suite: standard problems run nightly on several platforms, web page to display, access results
- Verification of algorithms on problems with exact solutions; typically for components of the code base
- V&V paper: "*On Validating An Astrophysical Simulation Code*", Calder, et al., ApJS 143, Nov. 2002. Validation for Rayleigh – Taylor and three-layer Richtmeyer-Meshkov problems.

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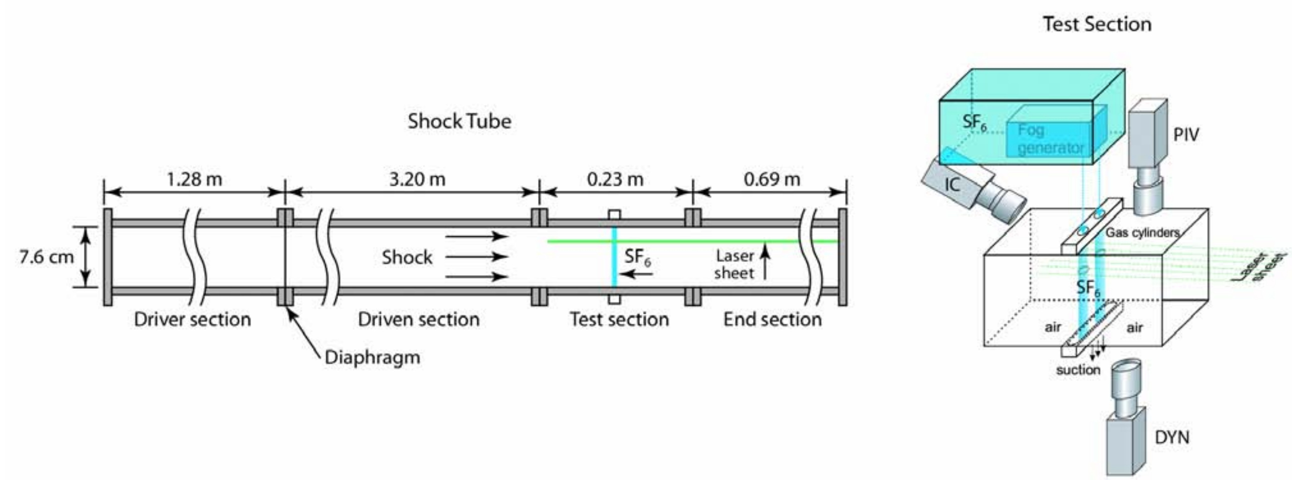
Los Alamos Shock-Cylinder Experiment



- A "cylinder" of Sulfur Hexaflouride (SF_6) falls through the air-filled test section; $M_{SF6} \sim 5\ M_{air}$
- A Mach 1.2 shock traverses the cylinder and continues down the tunnel
- Indirect SF_6 visualization, by visible-light scattering water/glycol "fog"
- Direct SF_6 visualization, by Rayleigh-scattering off SF_6 molecules
- Particle Image Velocimetry (PIV) with fog
- One image per experiment; time sequence can be constructed because of repeatability

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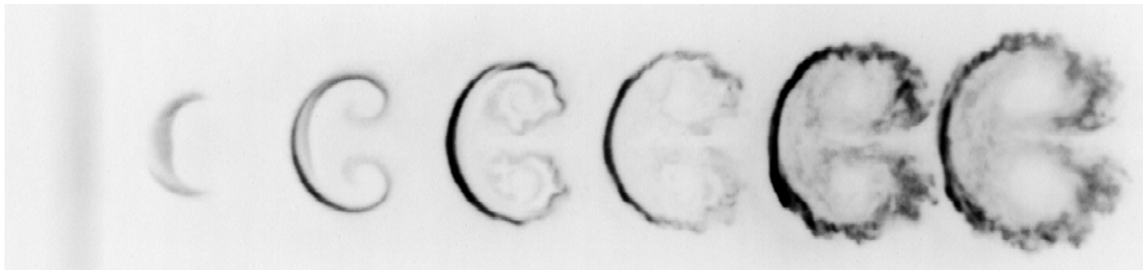
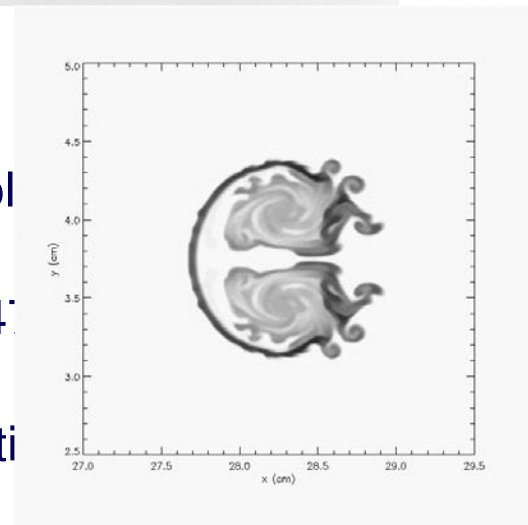
Flowfield Development

Two phases of flowfield development:

1. Shock-interaction phase:
   - Misalignment of pressure and density gradients results in baroclinic vorticity deposition at the interface as the shock traverses the cylinder
   - Compressible, wave dominated
   - Fast, < 50 μs
   - *Highly sensitive to conditions before the shock arrives*
2. Instability phase:
   - A counter-rotating vortex pair forms, and instabilities (Kelvin-Helmholtz) develop on the interface
   - Weakly compressible, dominated by viscosity, instabilities, vortex dynamics
   - Slow, ~800 μs
   - *Highly sensitive to conditions established in phase 1*

Flowfield Development





- Experimental time series, water/glycol
  SF_6 mole fraction.
- Images correspond to 50, 190, 330, 47
  after shock impact
- Composite image does not preserve ti
  relationship

Earlier Results

Some things we looked at:

- Sensitivity to simulation parameters:
  - Resolution (numerical viscosity)
  - Adaptive Mesh Refinement (AMR)
  - Courant number
  - Mesh refinement criteria
- Velocity fields
- Double cylinder configuration
- Speculative 3D calculation

… others we could have:

- Shock strength
- Equation of state

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Earlier Results

Issues/Obstacles:

Sensitivity to initial conditions:

- "Raw" RS experimental image of the initial SF_6 distribution vs. axisymmetric fit
- Initial maximum mole fraction, X_{SF6}

There is no viscosity model. Only resolution dependent numerical viscosity is present.

Validation metric. Visual comparison of experimental and computed morphology (eyeball norm)

New Results

Recent work focuses on:

- Initial conditions
- Better metrics
- Three-dimensional effects

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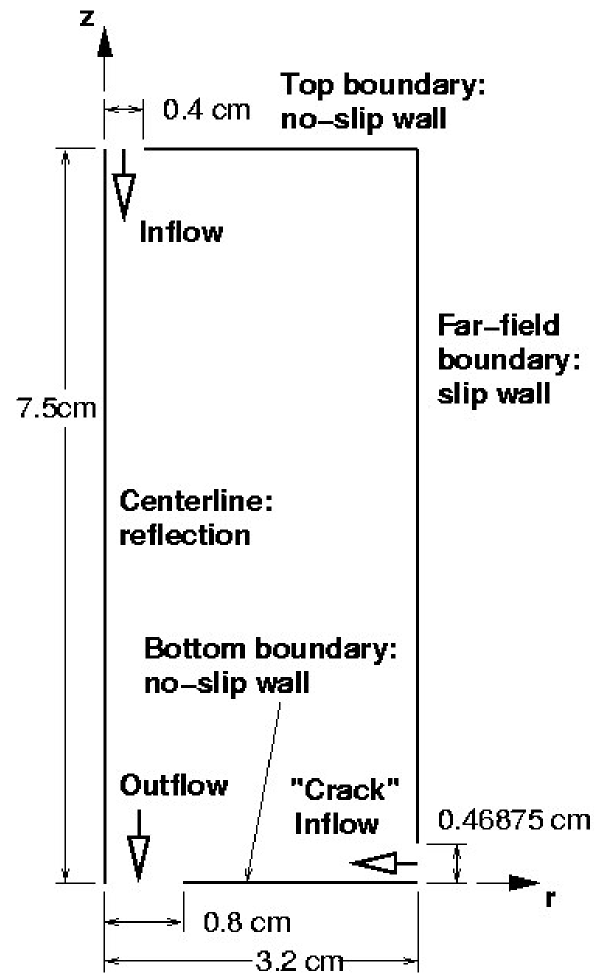
Simulations of Initial Conditions

Axisymmetric code (Todd Dupont):

- Motivation: Determine X_{SF6}
- Motivation: Initialize three-dimensional flowfield
- Solve (single) species and momentum equations and elliptic equation for pressure
- Convection, gravity, constant viscosity, constant binary diffusion, variable density, isothermal
- Run until steady state is achieved



Simulations of Initial Conditions

Axisymmetric code input parameters:

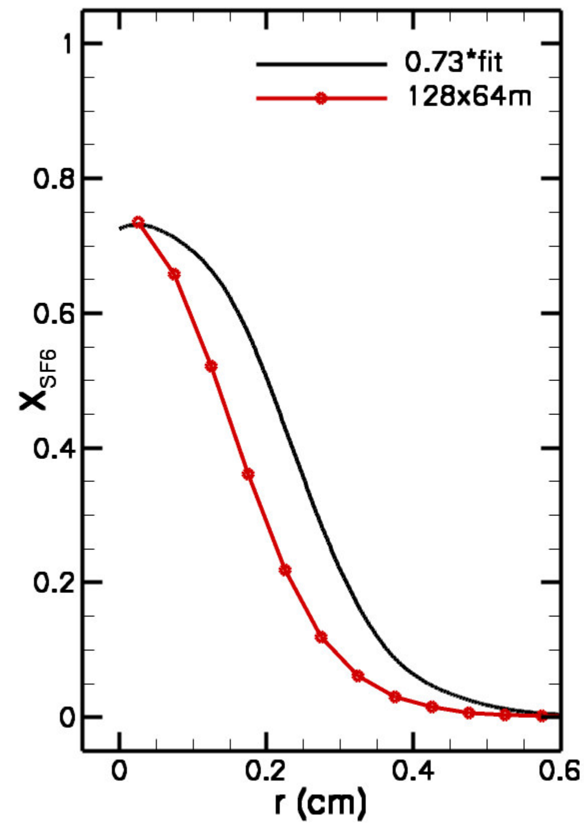
- Inlet velocity (parabolic profile)
  LANL estimate: 10 cm/s
- Inlet mass fraction of SF_6
  LANL estimate: 1.0
- Simulation Parameters - Dimensions of domain, resolution, relative sizes and flow rates

Code output:

- SF_6 mole fraction profile
  Fit to experimental image
- X_{SF6} in the image plane
  LANL estimate: 0.8

Inlet Y_{SF6} = 1.0

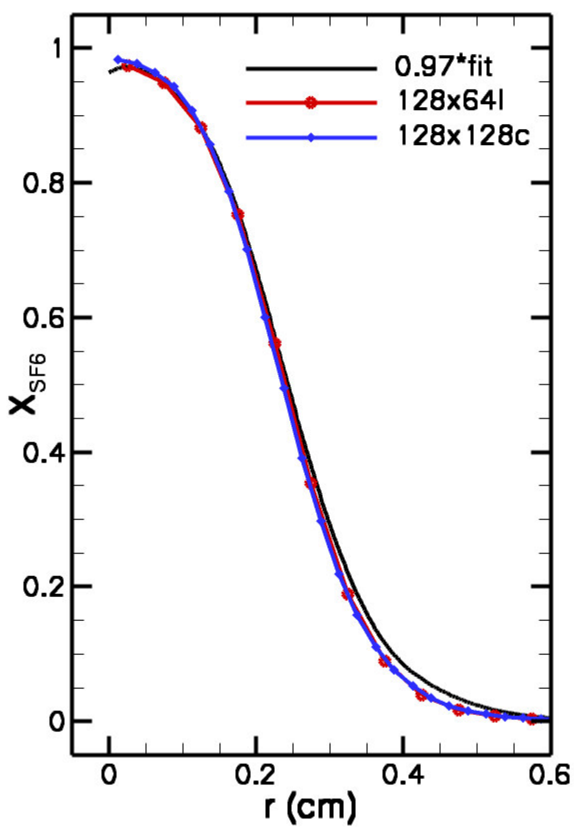
Inlet v_z = 10.0 cm/s

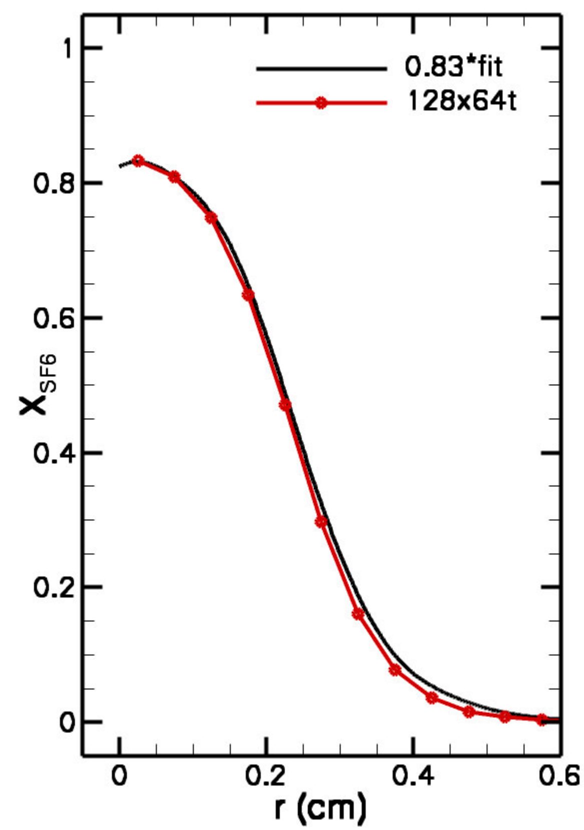


Simulations of Initial Conditions

Inlet Y_{SF6} = 1.0
Inlet v_z = 25.0 cm/s

Inlet Y_{SF6} = 0.9685
Inlet v_z = 23.43 cm/s





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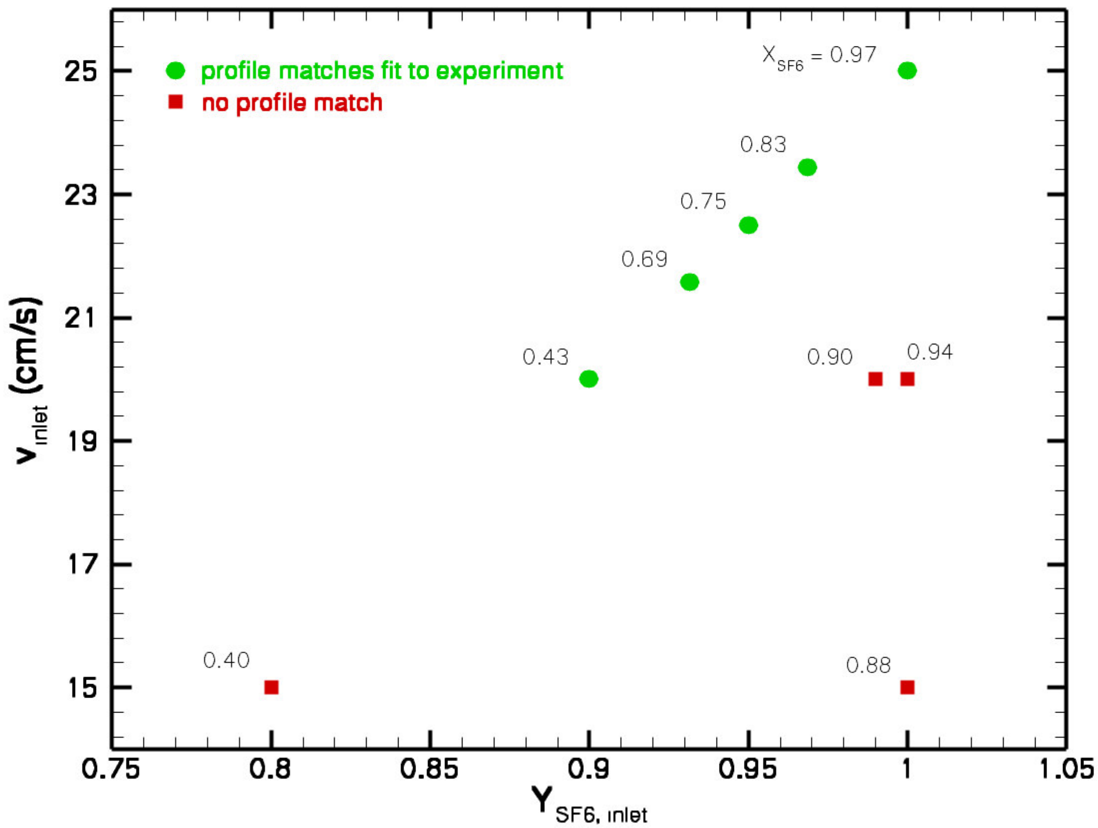
Simulations of Initial Conditions



- Initial conditions in the experimental image plane are highly sensitive to inlet conditions

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Looking for Better Metrics

While visual comparisons were ok to start with, we need a better basis for comparison to experimental data. A new metric should be:

- Quantitative
- Well-defined
- Physically meaningful

Circulation and self-induced vortex velocity both measure the vorticity deposited during the shock interaction

- Insensitive to small scale structure
- Insensitive to numerical (and physical) viscosity

These provide:

1. A way to probe the initial composition gradients (X_{SF6})
2. A necessary first step in correlating the vorticity deposited and the growth of secondary instabilities

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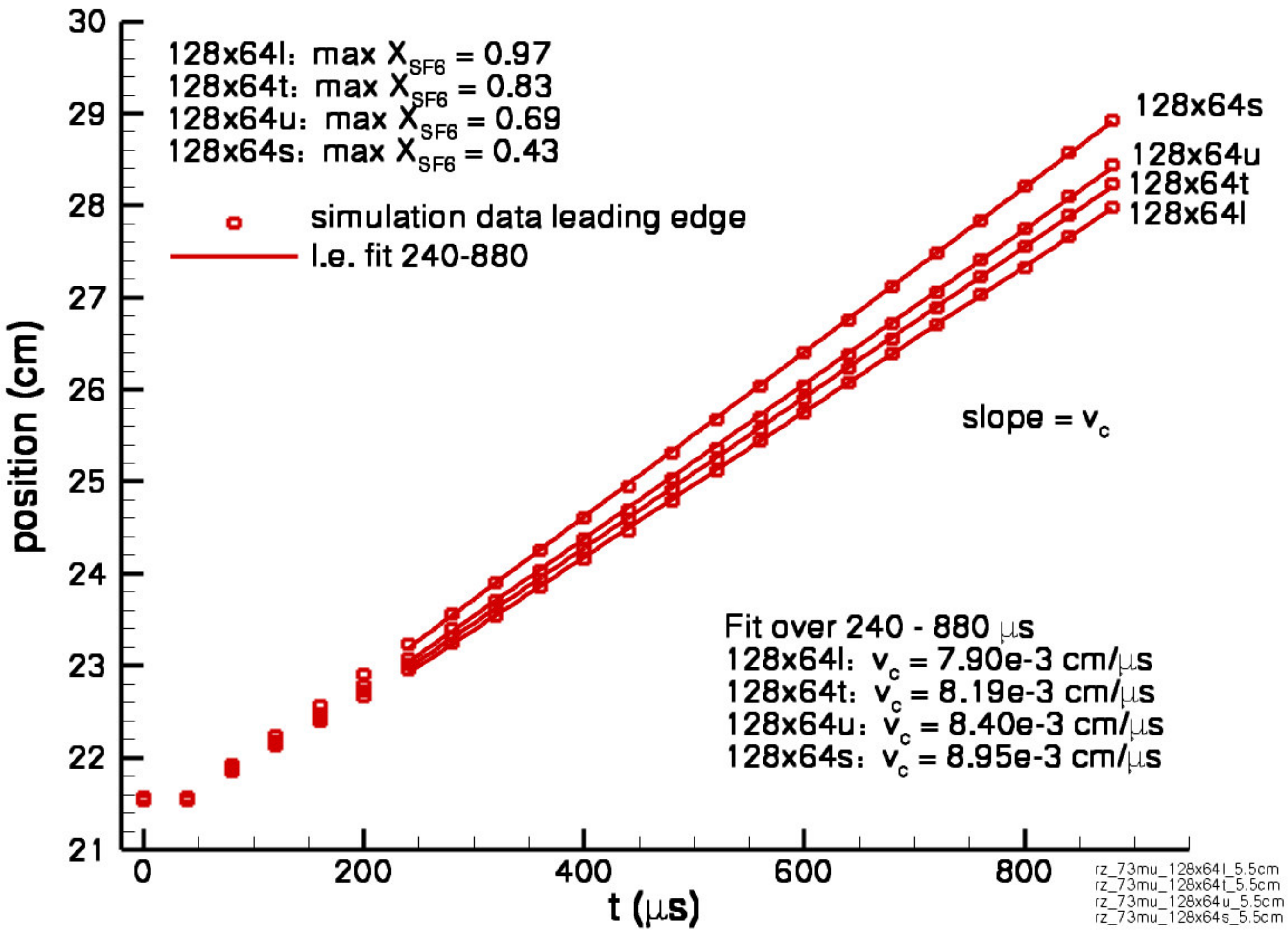
Convective Velocity



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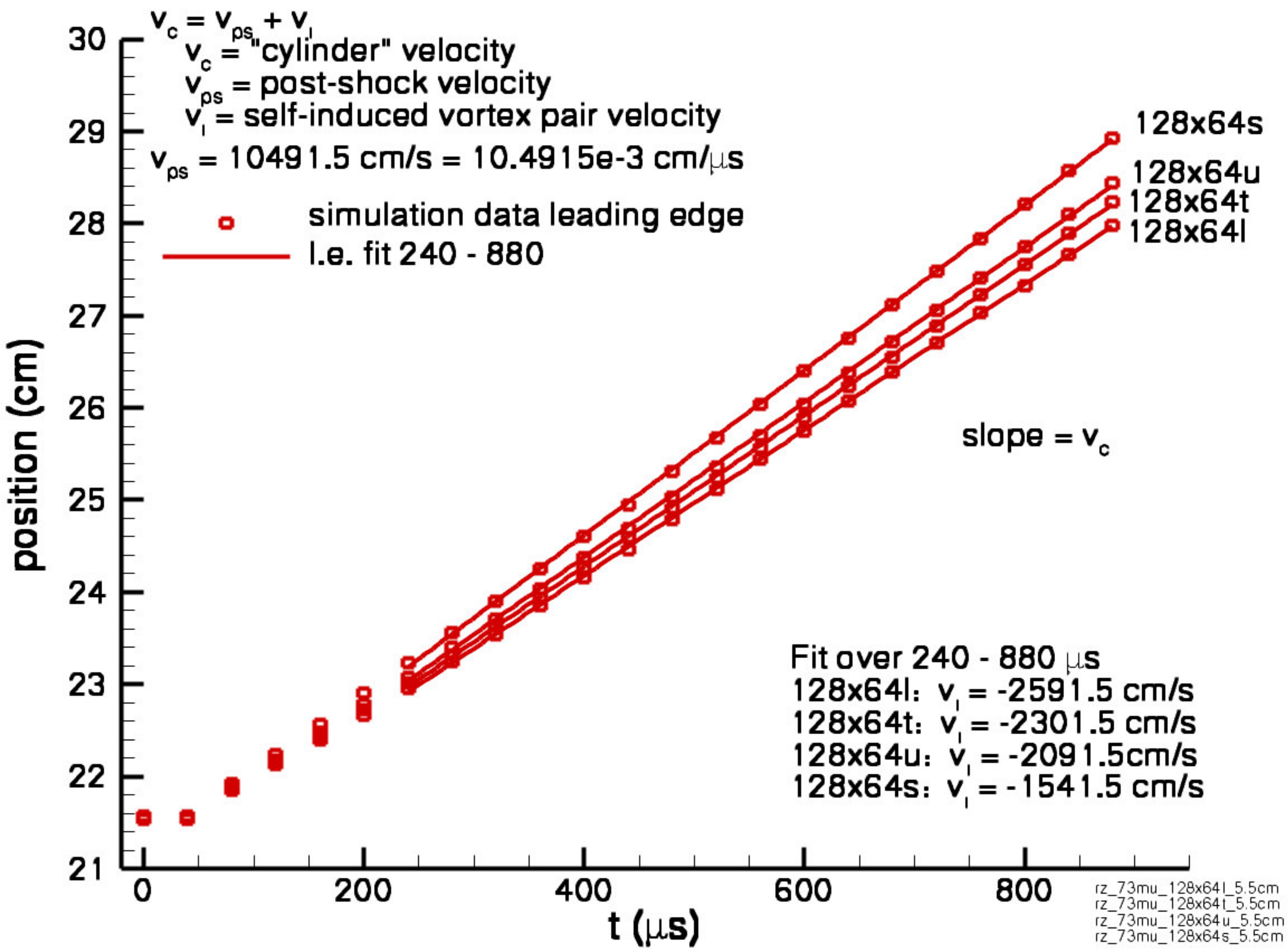
Self-Induced Velocity



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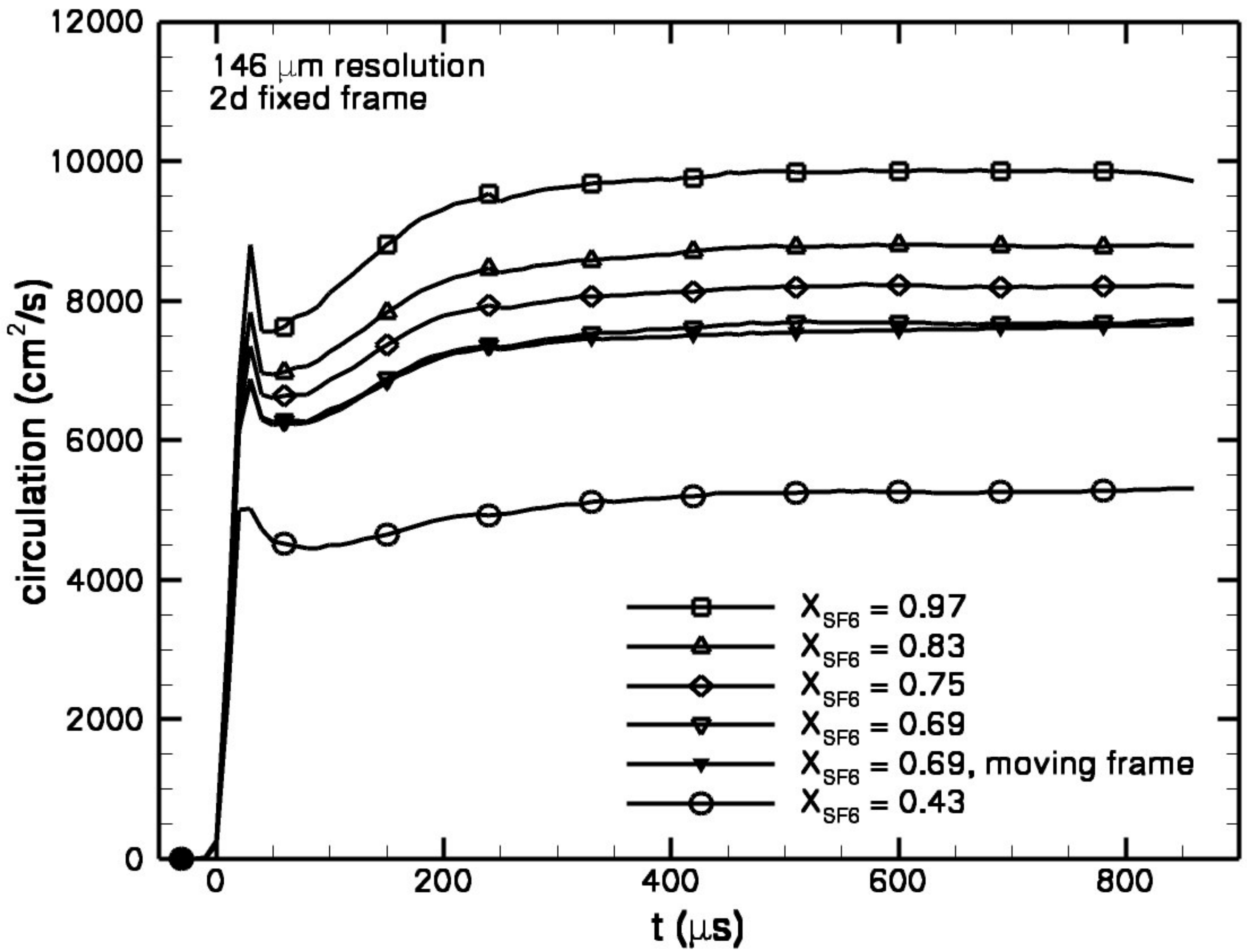
Circulation

- Circulation is the integral of vorticity:

$$\Gamma = \iint \overline{\varpi} \cdot dA$$

- We consider only the z-component of vorticity
- We integrate over the lower-y half of the domain (lower half in the spanwise dimension)

Circulation: Effect of Initial SF_6 Mole Fraction



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3D Simulations

Are three-dimensional effects important?

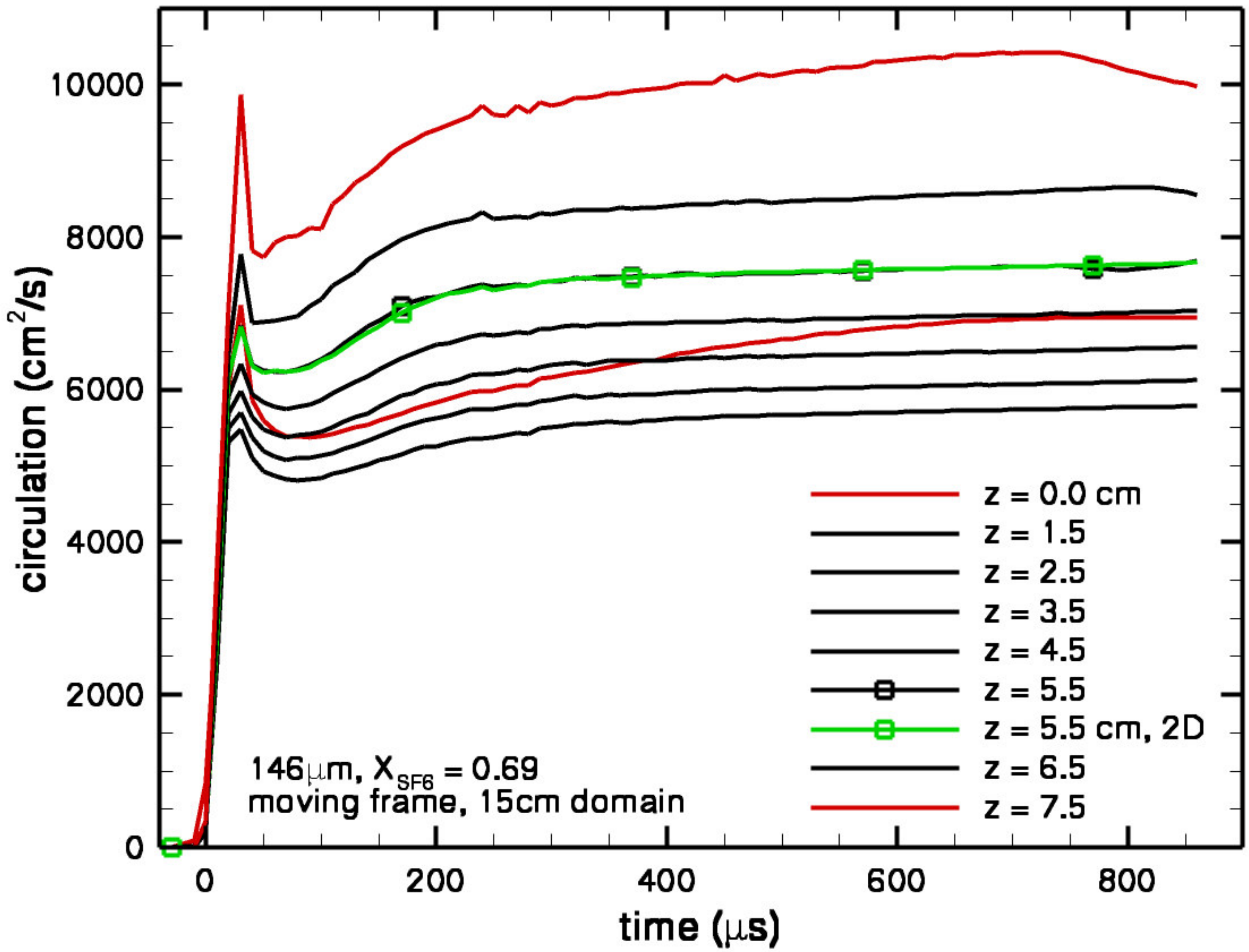
- SF_6 and air diffuse as the SF_6 flows through the tunnel, leading to vertically varying composition, and thus density, gradients
- Instability growth and small scale structure are generally three-dimensional

We are just beginning to analyze 3D simulations.

- Run 1: 146 μm, X_{SF6} = 0.97 in image plane, fixed frame
- Run 2: 146 μm, X_{SF6} = 0.83 in image plane, fixed frame
- Run 3: 146 μm, X_{SF6} = 0.69 in image plane, moving frame

We have left the validation program proper – no experimental data (yet)

3D Simulation: Circulation



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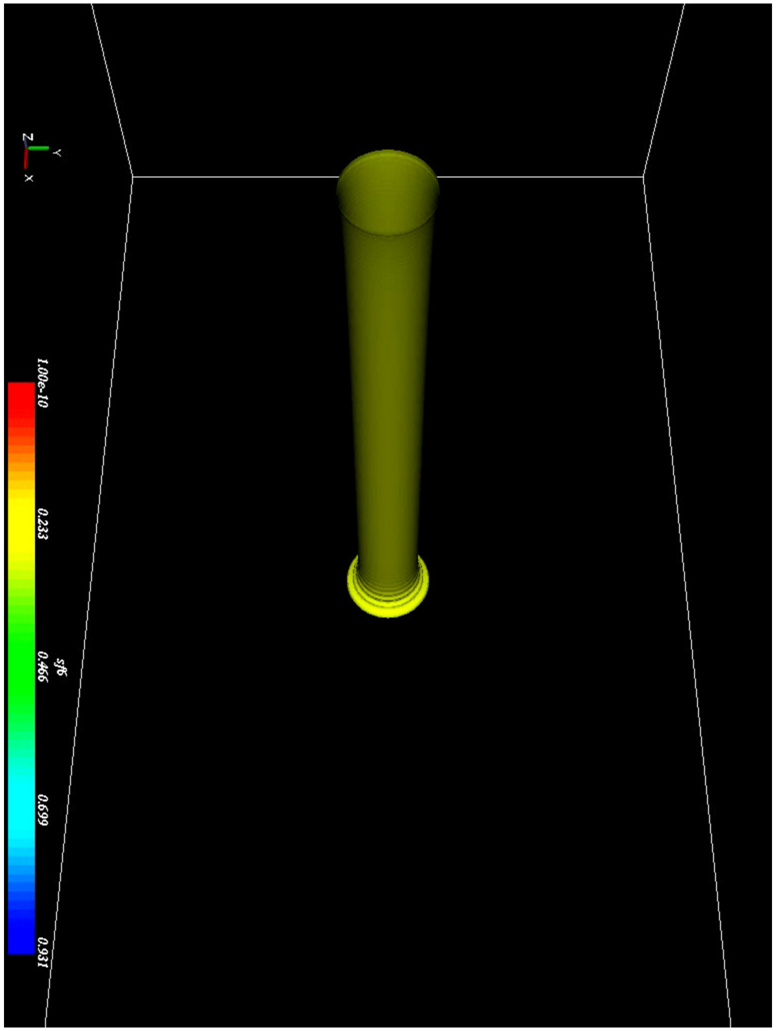
3D Simulation: Flow Visualization



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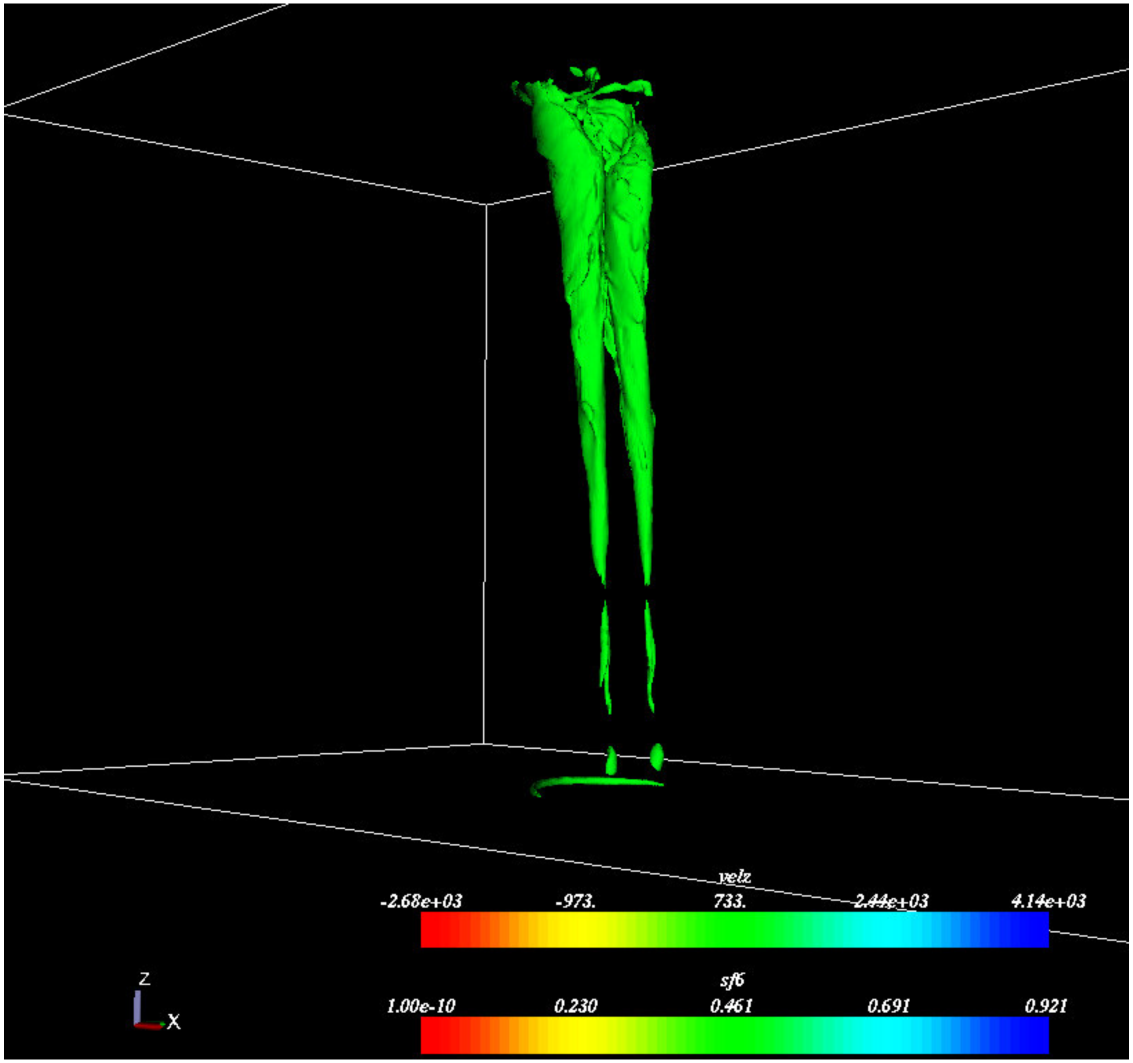
3D Simulation: Flow Visualization



$X_{SF6} = 0.69$

$t = 750\ \mu s$

Note vertical tubes of positive z-velocity, associated with the two primary vortex cores

Spreading as the top wall is approached indicates acceleration

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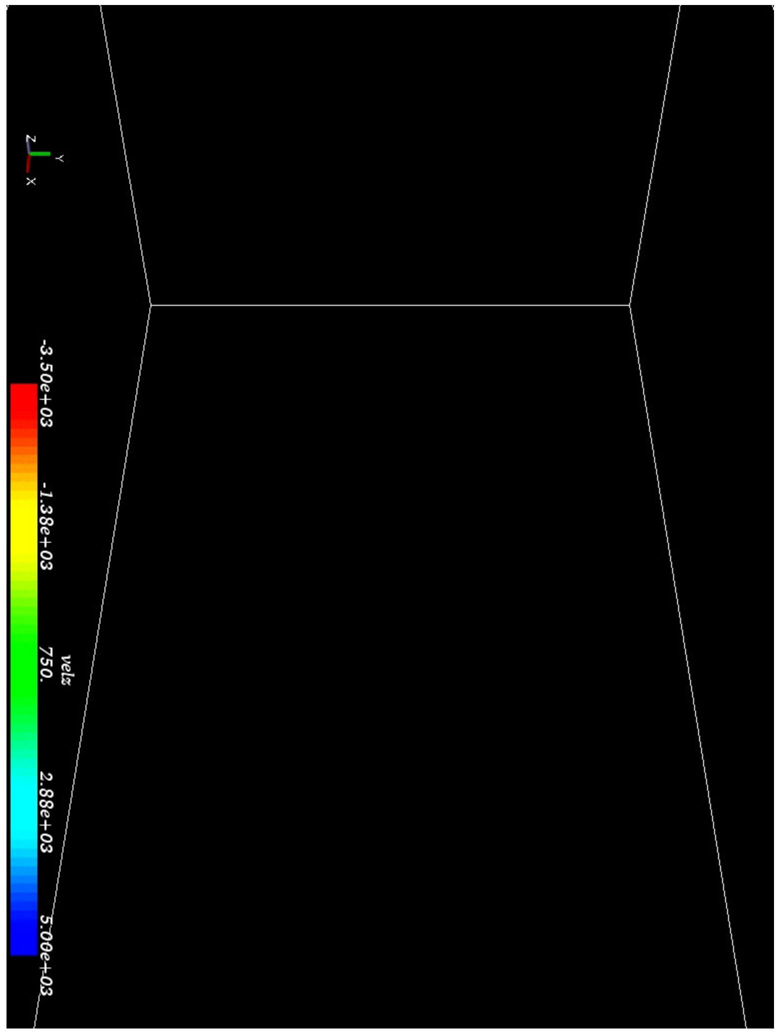
3D Simulation: Flow Visualization



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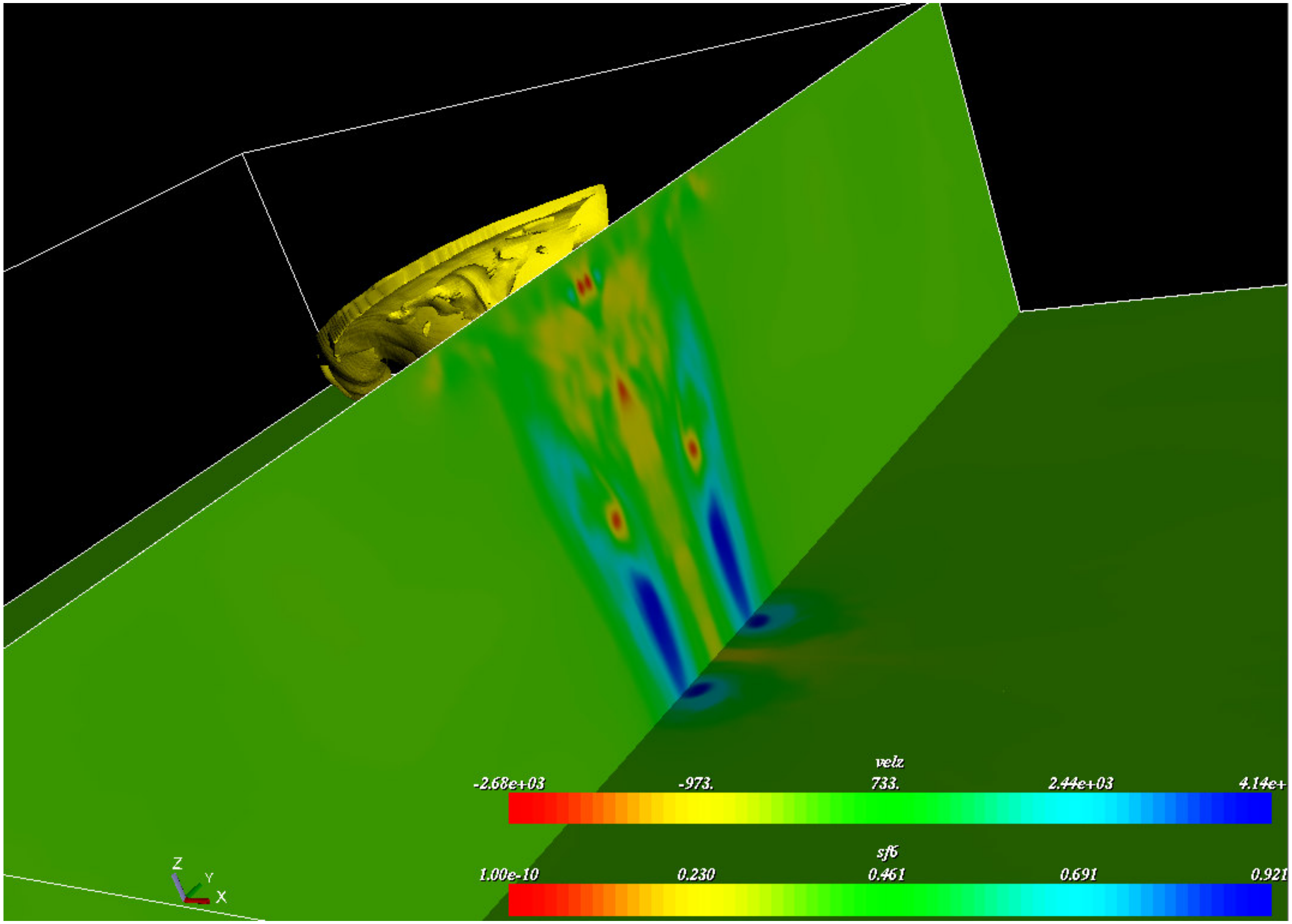
3D Simulation: Flow Visualization



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Summary

- Early validation for the shock-cylinder interaction was qualitative and focused on the influence of simulation parameters
- Work in progress:
  - Examines a range of initial conditions
  - Seeks quantitative, physically meaningful metrics
  - Examines 3D effects

What is the FLASH Code?

Target Applications:

- Compact accreting stars (white dwarf, neutron star)
- Reactive flows (DNS or subgrid model)
- Initial conditions close to hydrostatic equilibrium (self-gravity)
- Complex EOS (dense nuclear matter)

Example: Type Ia Supernova

- Massive white dwarf
- Subgrid model for nuclear flame
- Self-gravity
- Degenerate EOS

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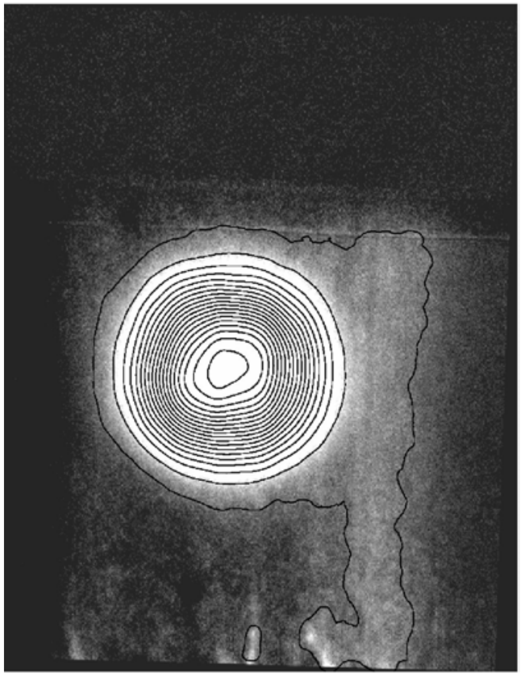
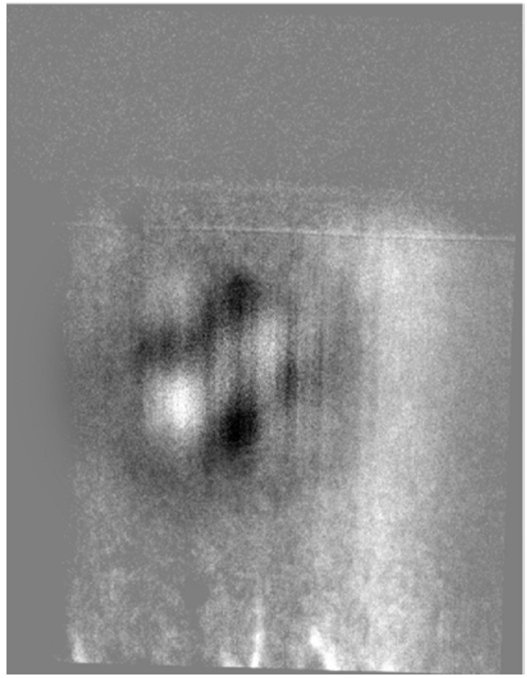
Raw Experimental Images





- Raw image (left) – actually, an average of several images. Pixel values are measured intensity (Rayleigh scattering,) and range from 0 to 165. (We added the contours.)
- Residual after subtracting smooth, axisymmetric fit. Pixel values range from -10 to +10.

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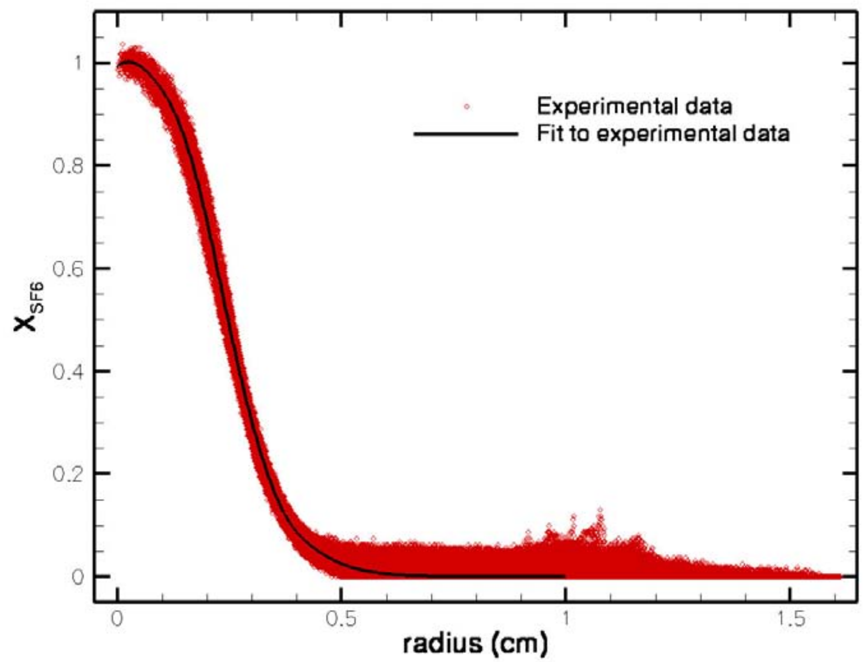
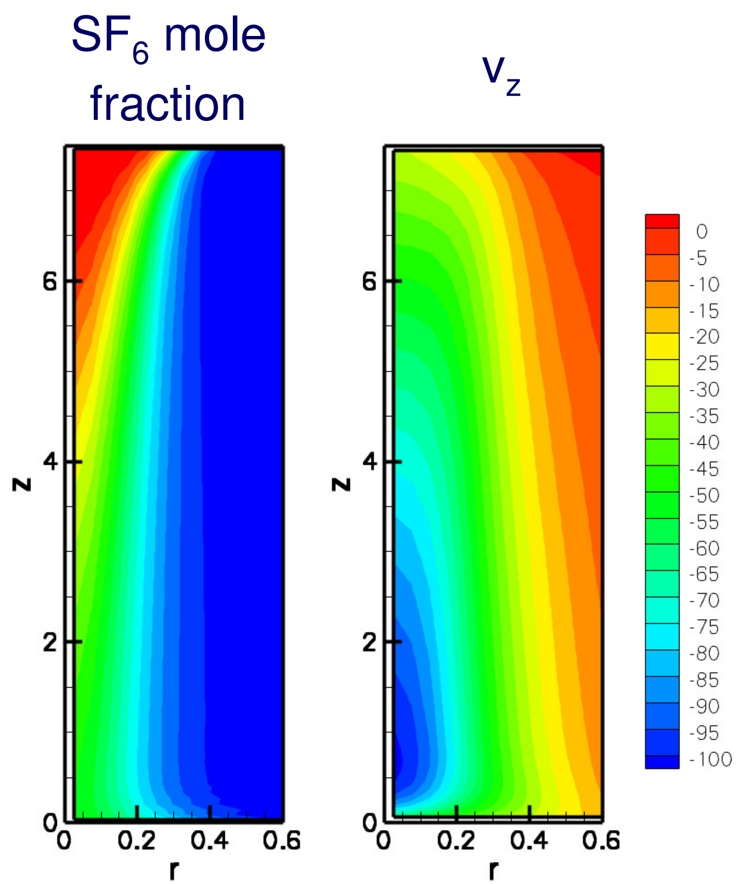
Axisymmetric Fit to Experimental Image

- Eventually a formula consisting of several Gaussians was developed
- Almost all of our previously published work was initialized with this fit.
- The maximum initial mole fraction of SF_6, X_{SF6}, must be assumed



Gravity Balances Diffusion

- If the inlet velocity is too low, the profile is too narrow (closer to the centerline than the experimental data): gravitational acceleration of SF_6 leads to necking
- If the velocity is too high, the profile is too steep: diffusion does not have enough time to act
- The inlet mass fraction affects the gravitational acceleration and the output X_{SF6}



Inlet v_z = 15.0 cm/s

Inlet Y_{SF6} = 1.0

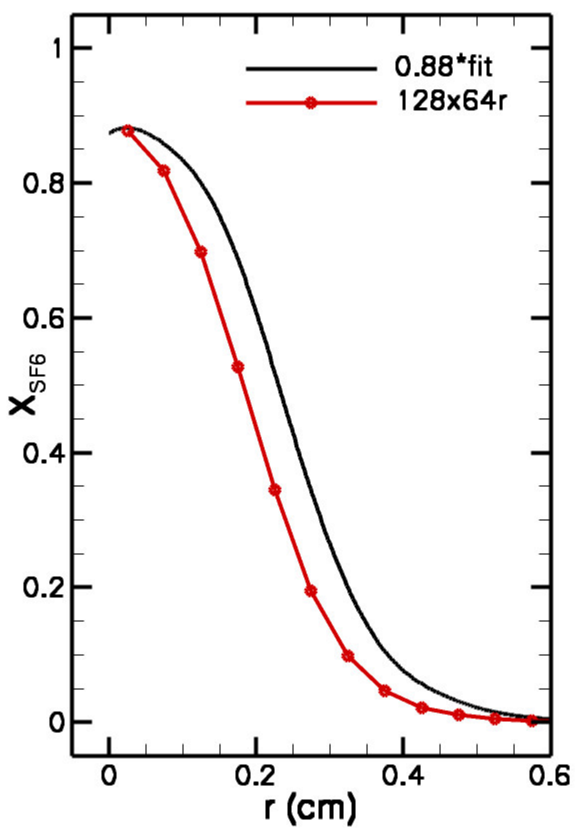
Simulations of Initial Conditions

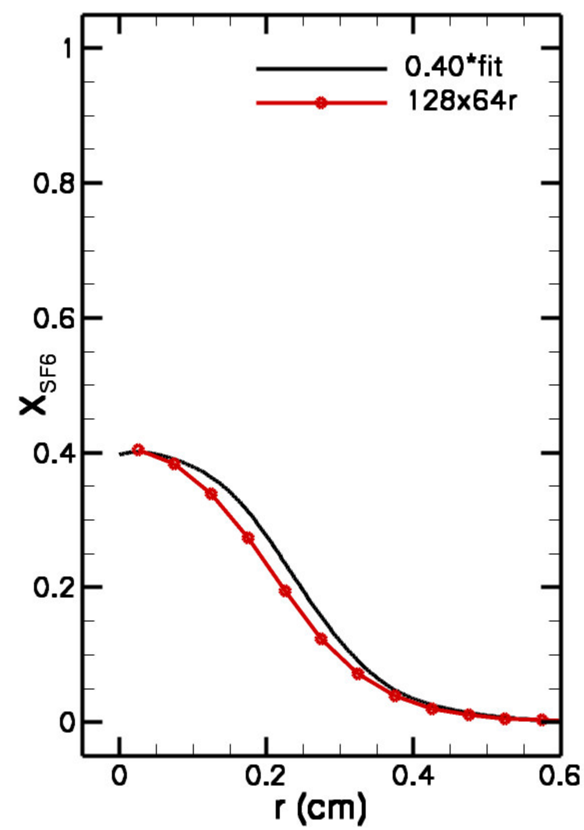
Inlet Y_{SF6} = 1.0

Inlet v_z = 15.0 cm/s

Inlet Y_{SF6} = 0.8

Inlet v_z = 15.0 cm/s





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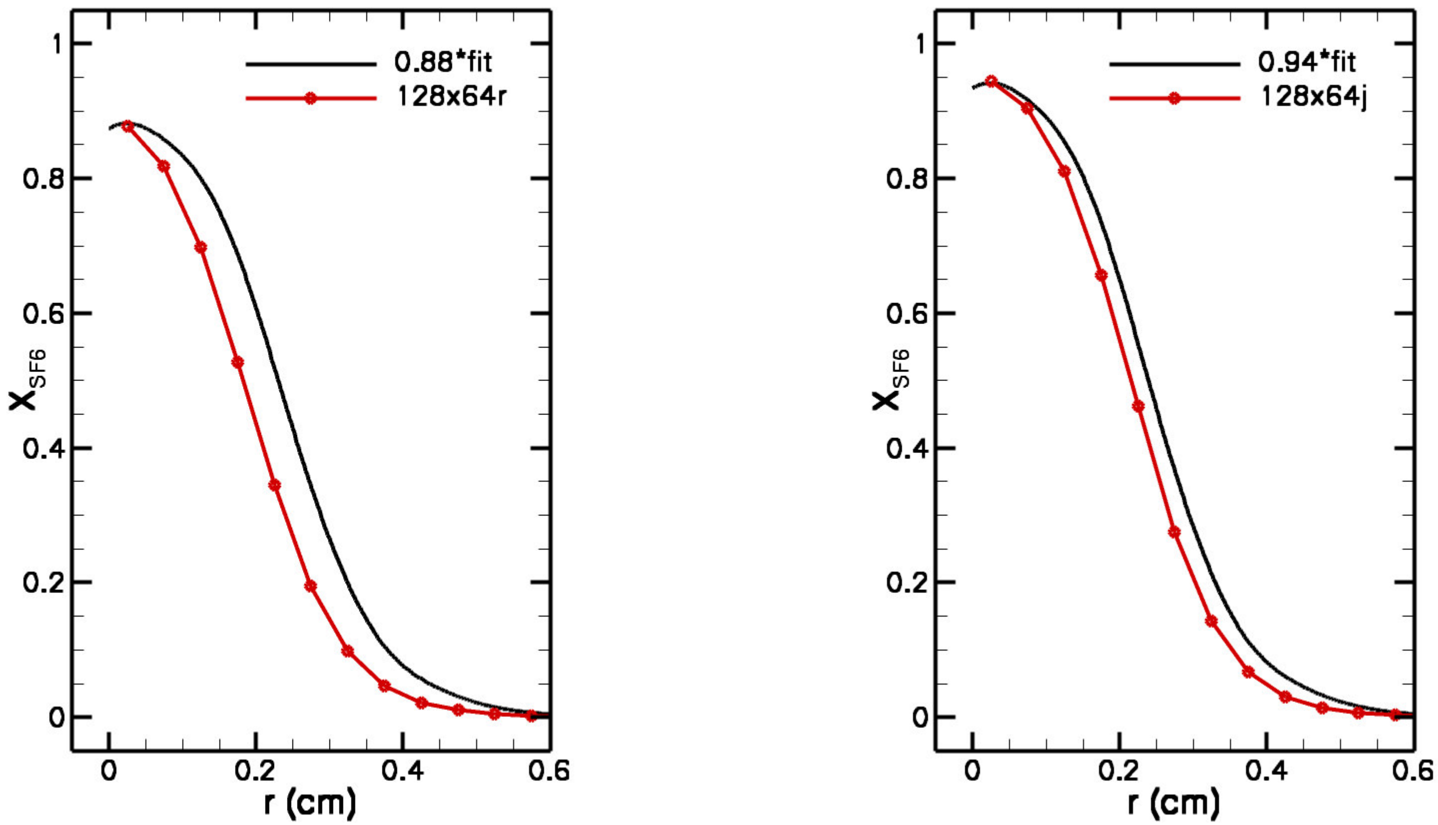
Simulations of Initial Conditions

Inlet Y_{SF6} = 1.0
Inlet v_z = 15.0 cm/s

Inlet Y_{SF6} = 1.0
Inlet v_z = 20.0 cm/s



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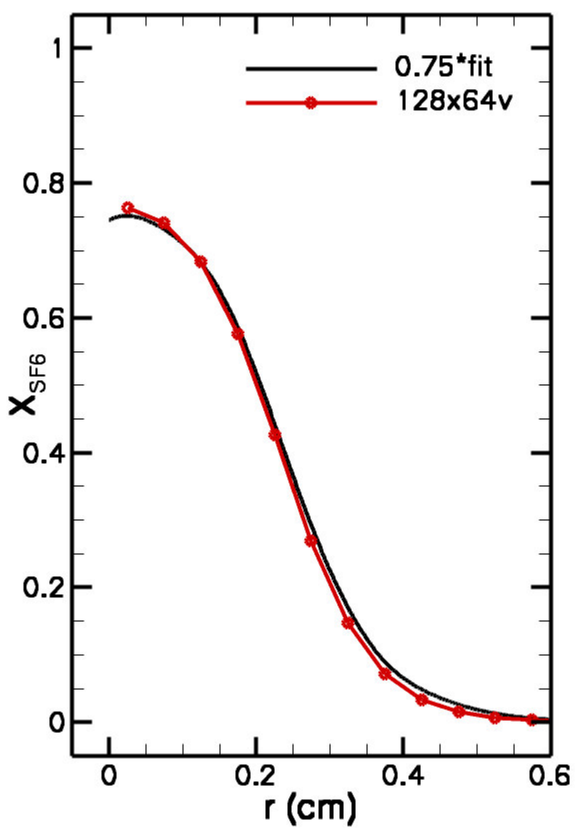
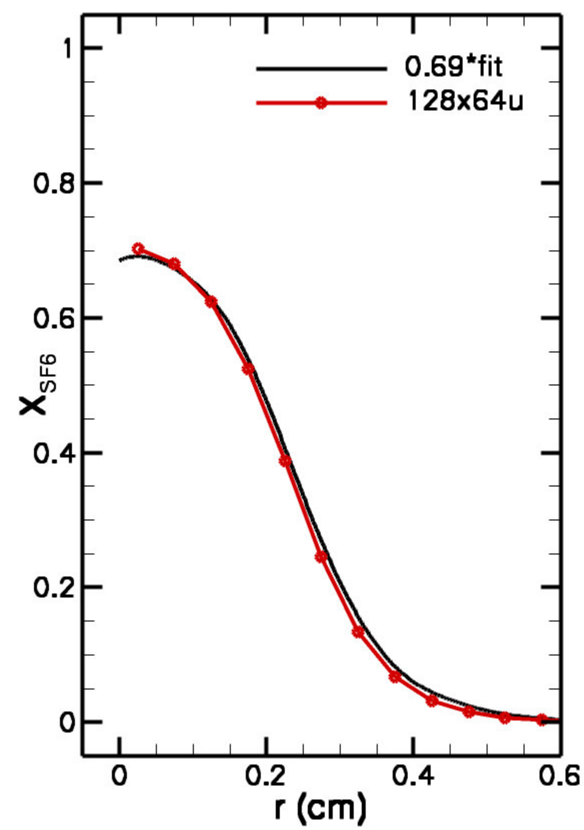
Simulations of Initial Conditions

Inlet Y_{SF6} = 0.95
Inlet v_z = 22.50 cm/s

Inlet Y_{SF6} = 0.9315
Inlet v_z = 21.85 cm/s





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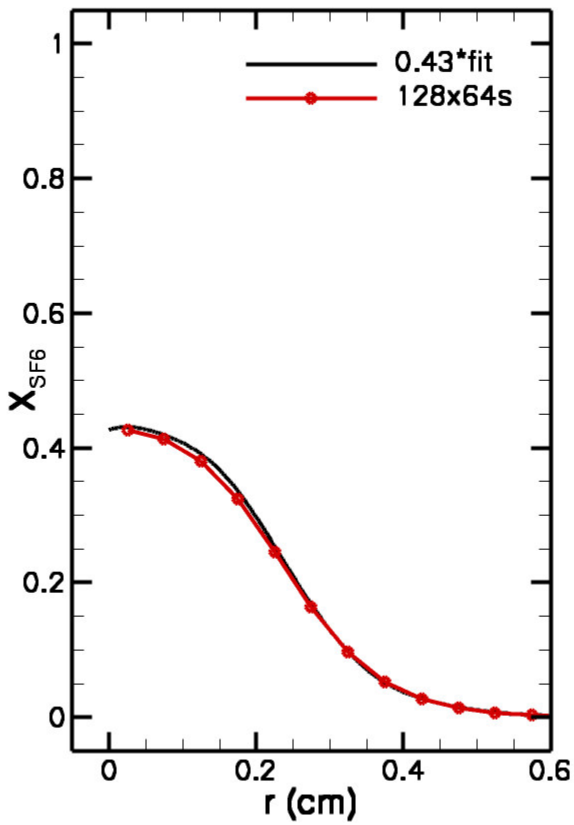
Simulations of Initial Conditions

Inlet $Y_{SF6} = 0.9$

Inlet $v_z = 20.0$ cm/s



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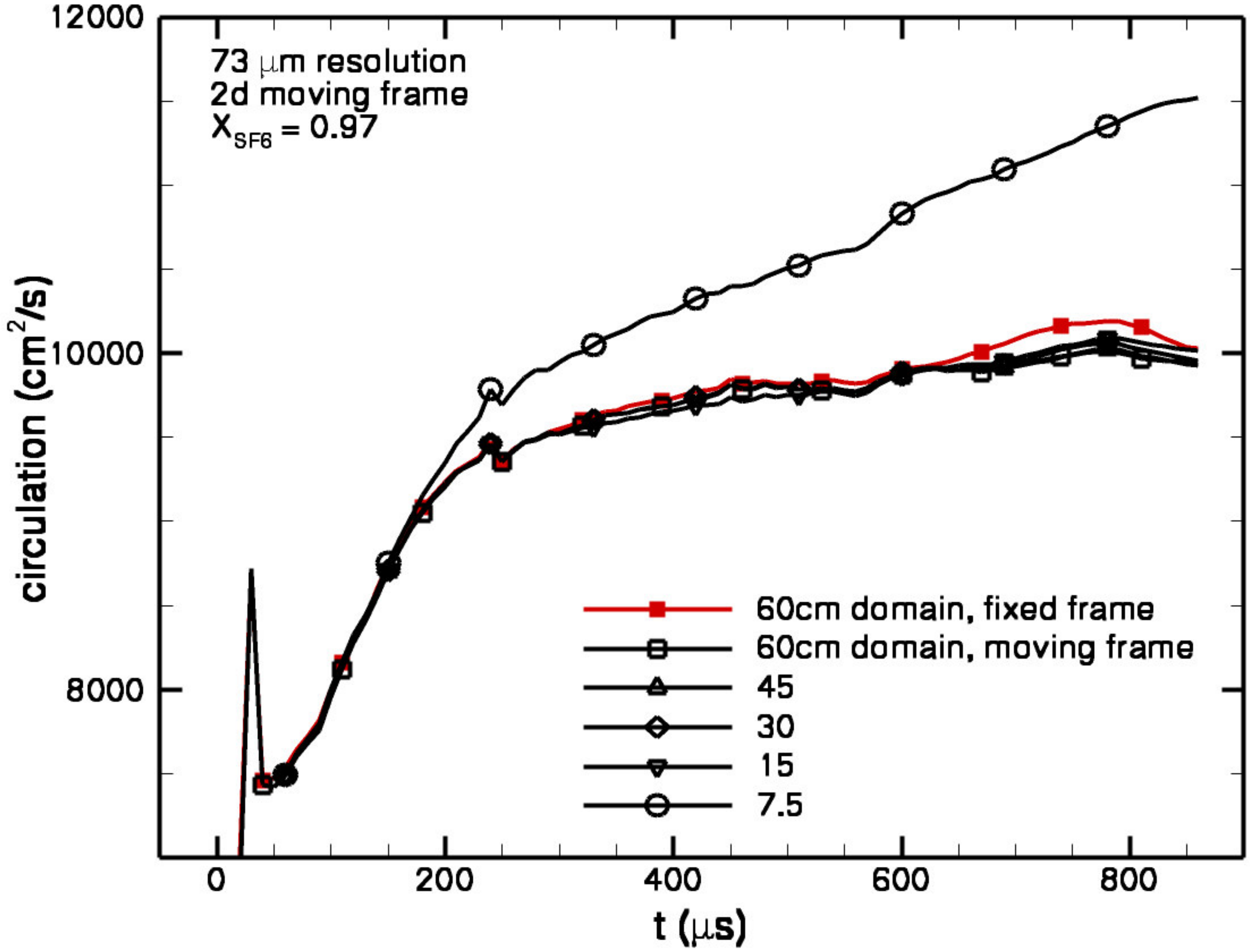
Circulation: Effect of Domain Size



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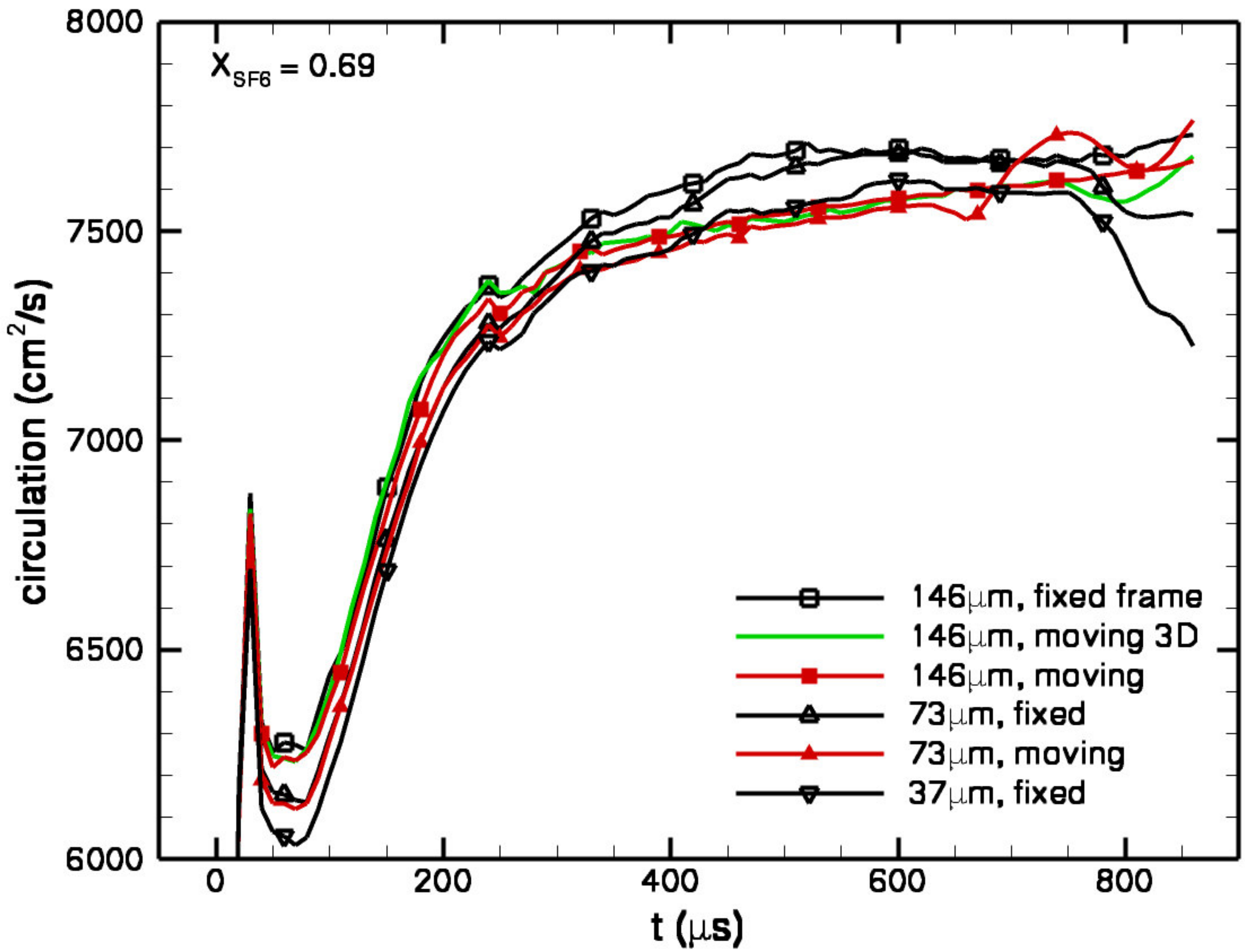
Circulation: Effects of Resolution and Ref. Frame



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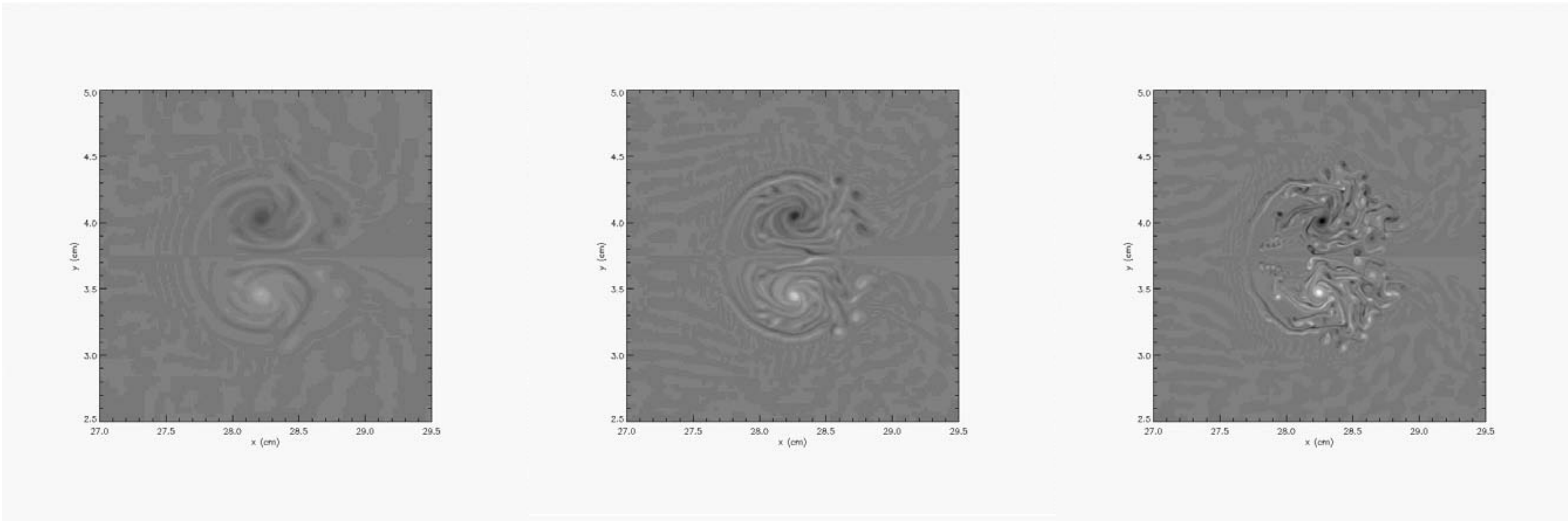
Vorticity: Effects of Resolution and Ref. Frame



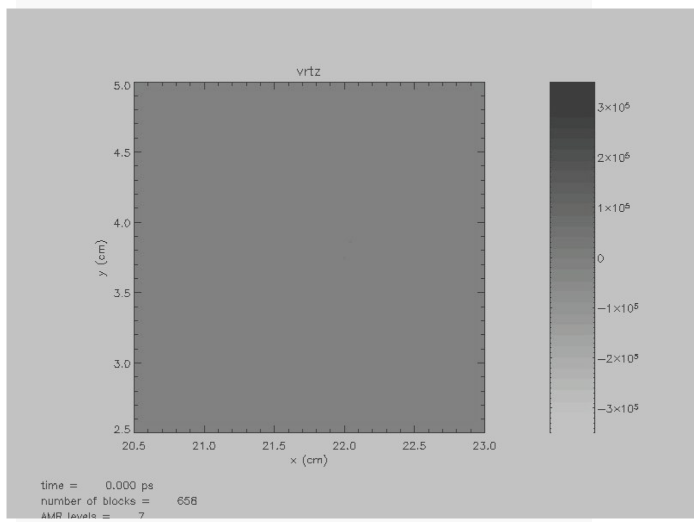
X_{SF6} = 0.69

t=750 µs

146 µm, 73 µm, 37 µm

Fixed frame (upper row)

Moving frame (lower)



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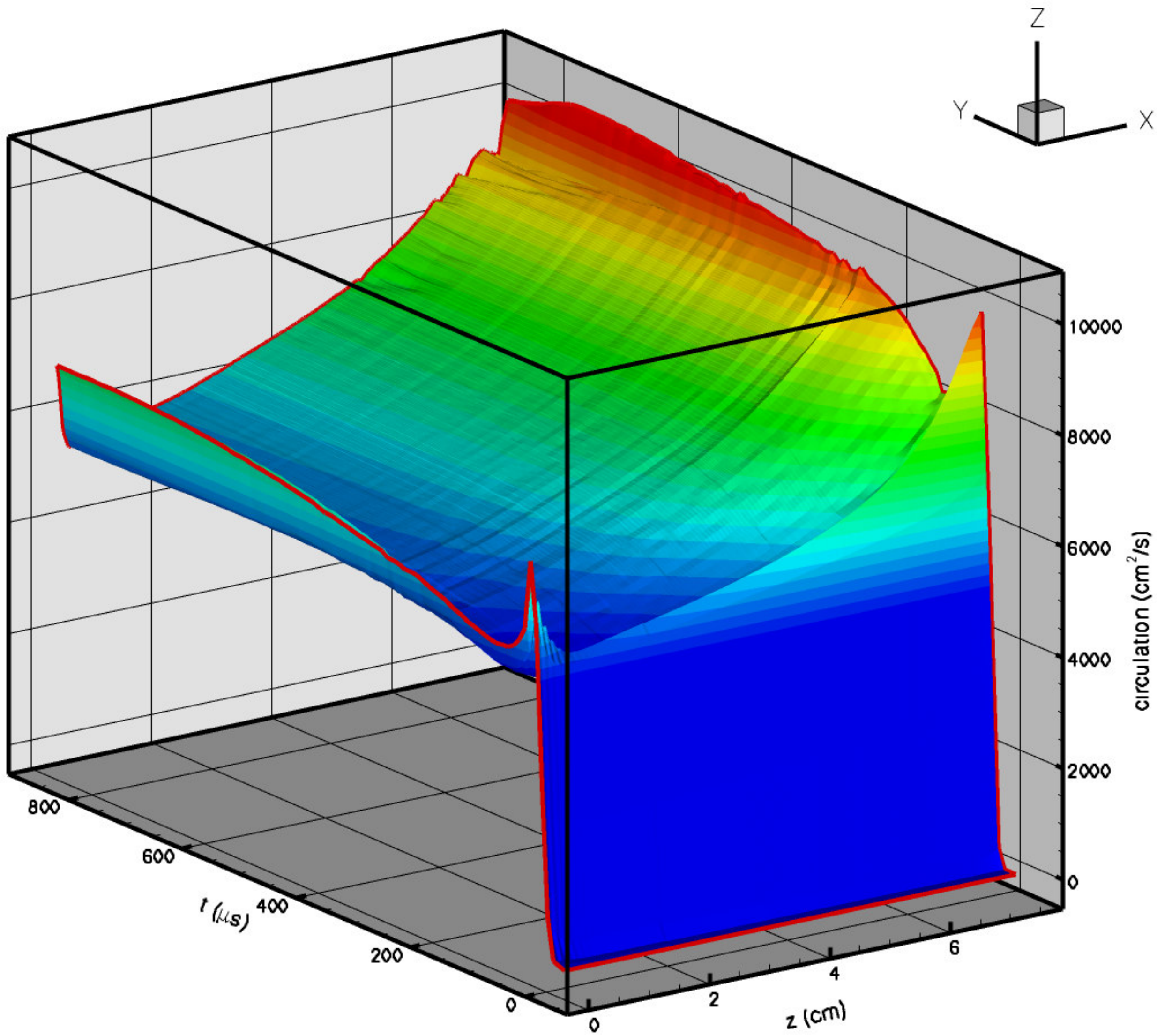
3D Simulation: Circulation



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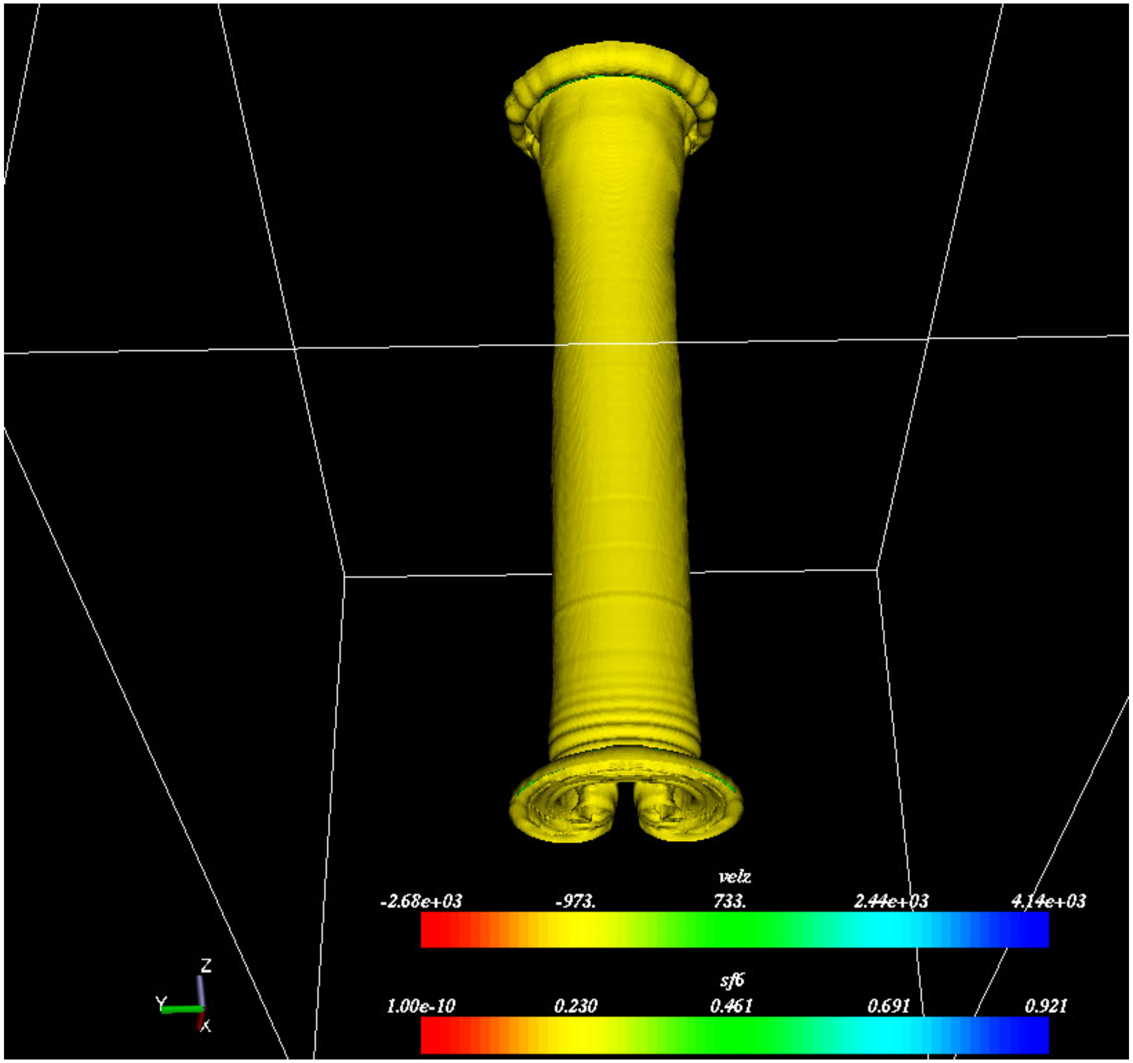
3D Simulation: Flow Visualization



$X_{SF6} = 0.69$

$t = 750\ \mu s$

Front of cylinder is smooth; instabilities are not apparent

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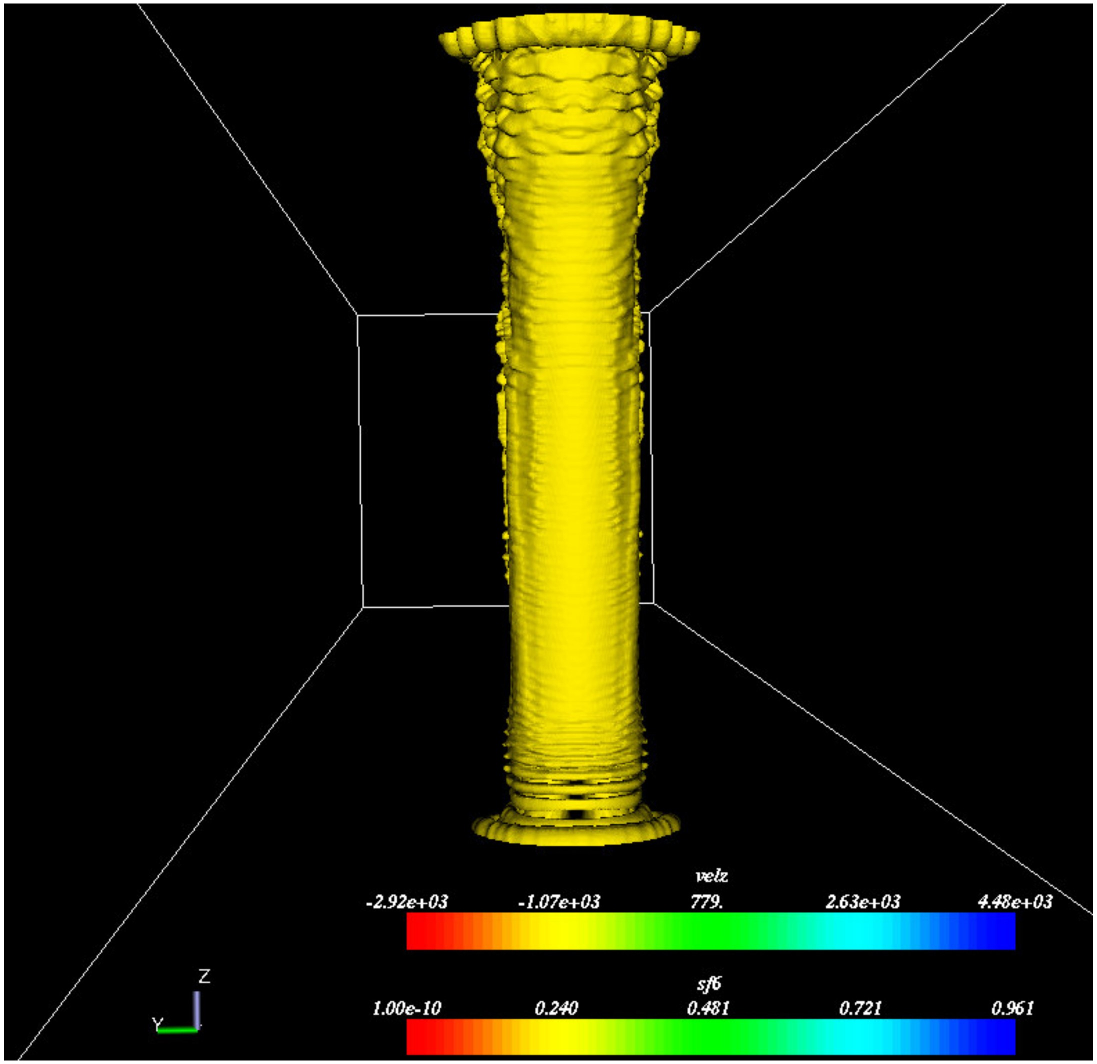
3D Simulation: Flow Visualization



$X_{SF6} = 0.97$

$t = 750\ \mu s$

Instabilities are visible even on the front of the cylinder

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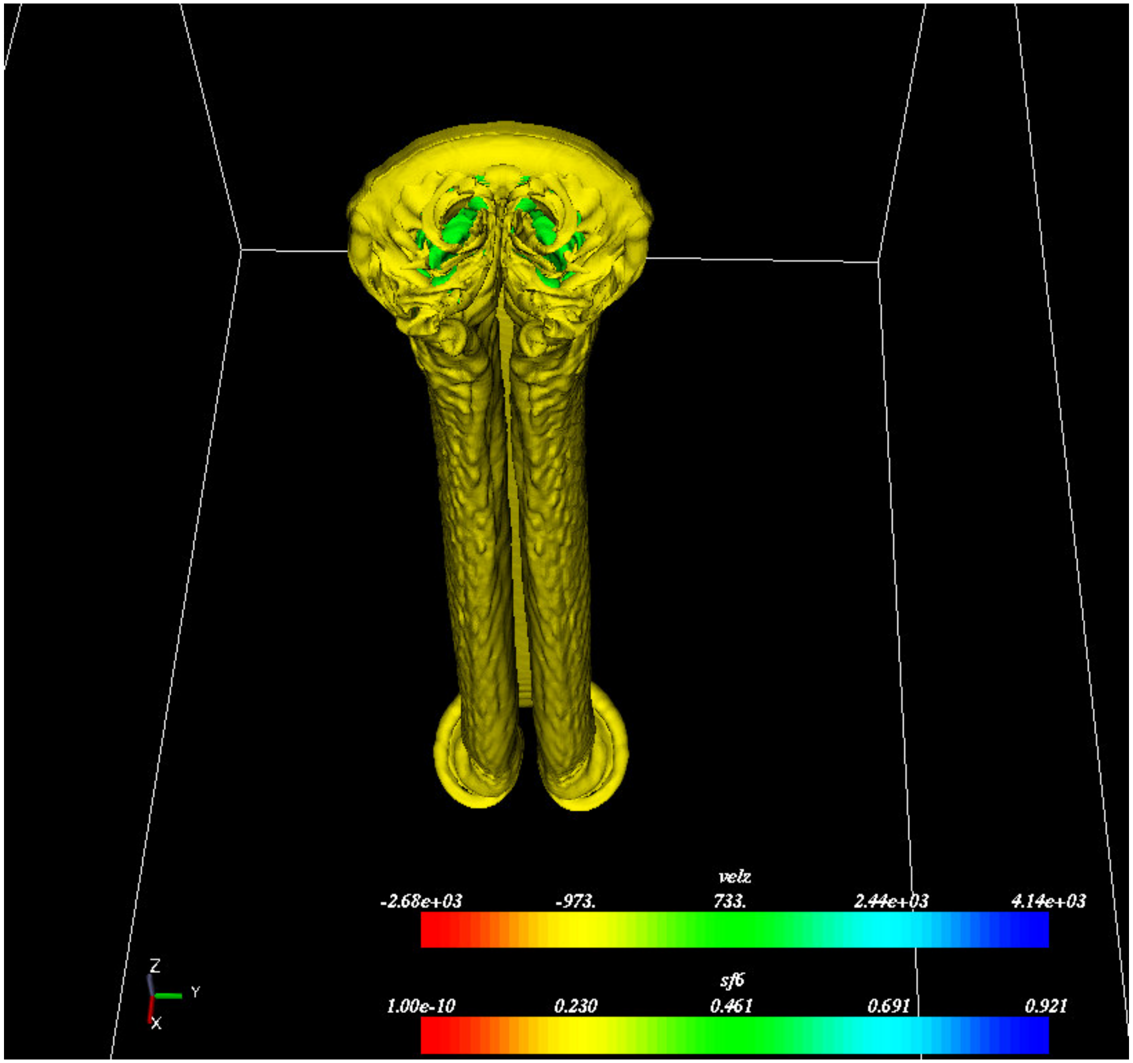
3D Simulation: Flow Visualization



$X_{SF6} = 0.69$

$t = 750\ \mu s$

Mild structures are visible on the back of the cylinder

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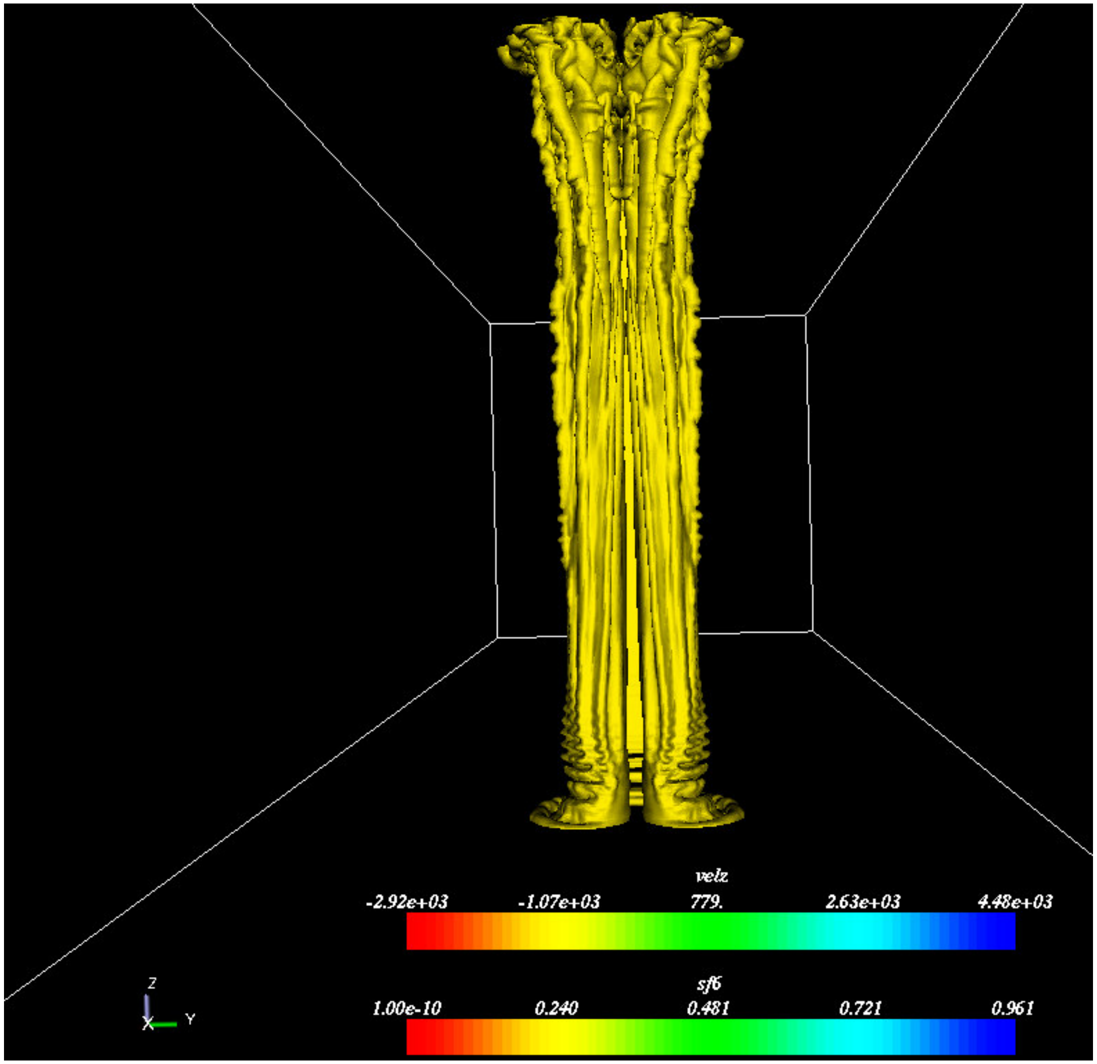
3D Simulation: Flow Visualization



X_{SF6} = 0.97

t = 750 μs

Well-developed structures are visible on the back of the cylinder

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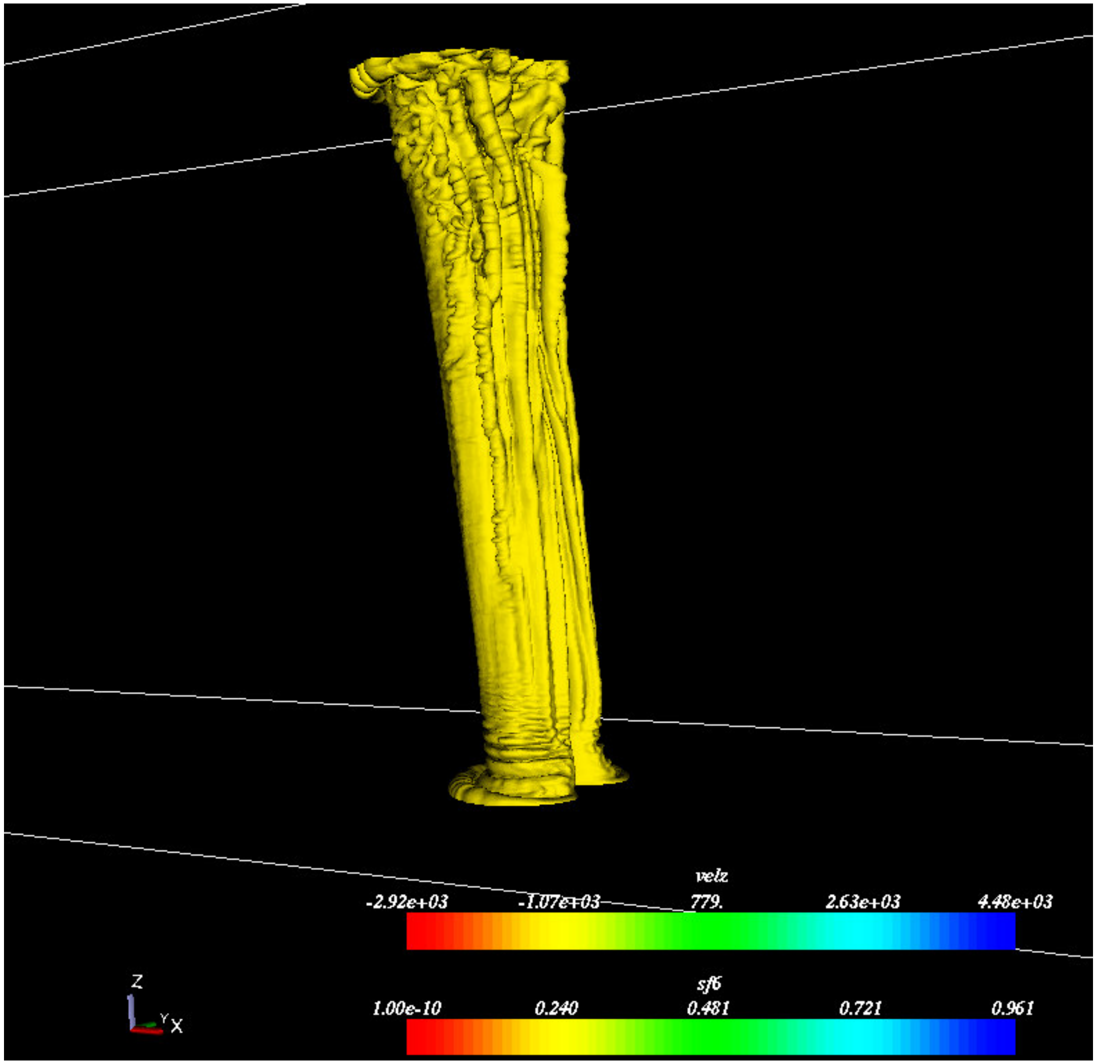
3D Simulation: Flow Visualization



$X_{SF6} = 0.97$

$t = 750\ \mu s$

More structure is visible near the top wall than the bottom

The top of the cylinder has a higher self-induced velocity, resulting in a slight tilt

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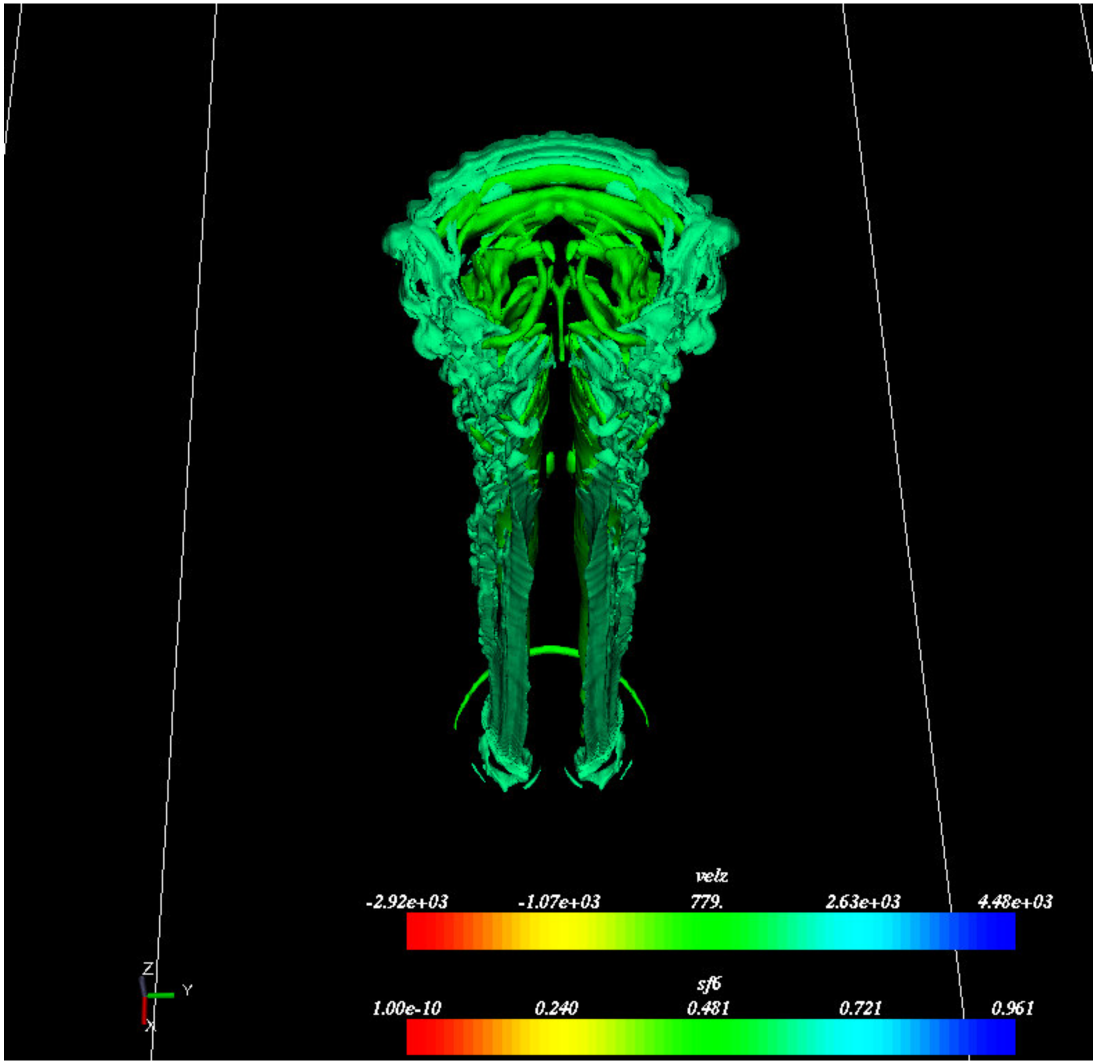
3D Simulation: Flow Visualization



$X_{SF6} = 0.97$

$t = 750\ \mu s$

Note vertical tubes of positive z-velocity, associated with the two primary vortex cores

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