FLASH Code Validation
LANL Shock-Cylinder Experiment

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Target Applications

- Compact accreting stars (white dwarf, neutron star)
- Reactive hydrodynamics (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

Past Validation of Computational Modules

- Access to experiments: collaborations with LANL (shock-tube) and LLNL (high-energy density laser) experiments.
- Initial program: alpha-group collaboration on RTI (Labs & AWE)

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A comparative study of the turbulent Rayleigh–Taylor instability using high-resolution three-dimensional numerical simulations: The Alpha-Group collaboration

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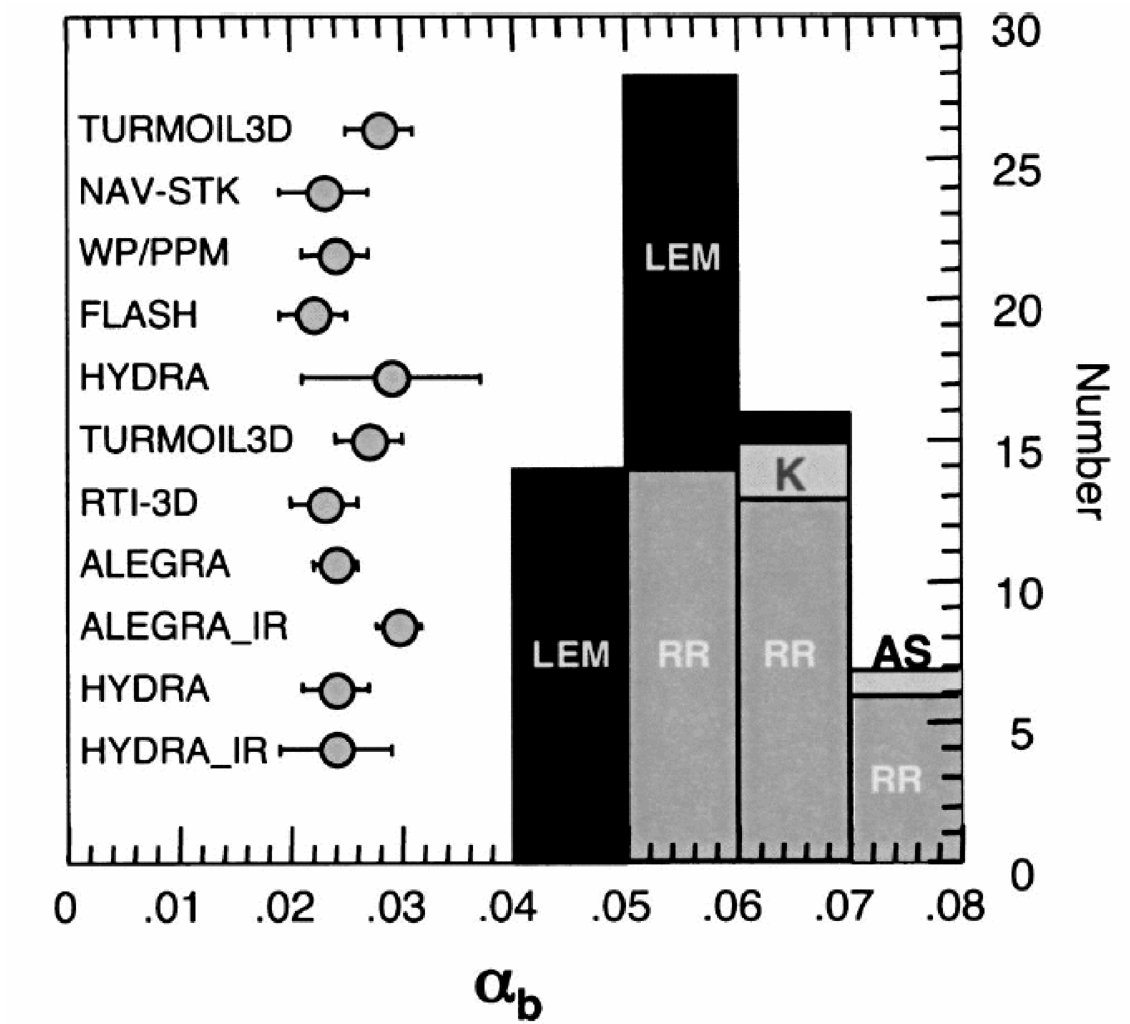
Past Validation of Computational Modules

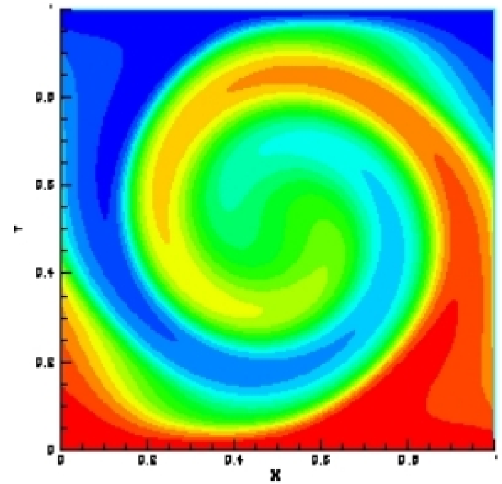
- Initial program: alpha-group collaboration on RTI (Labs & AWE)

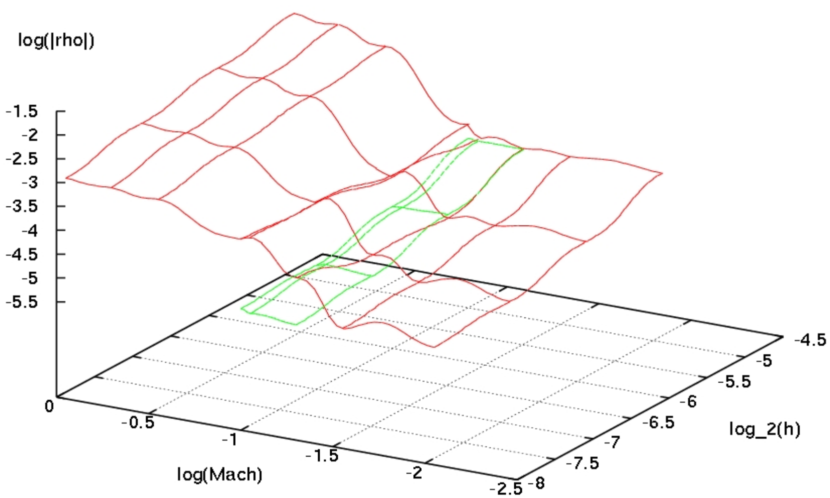


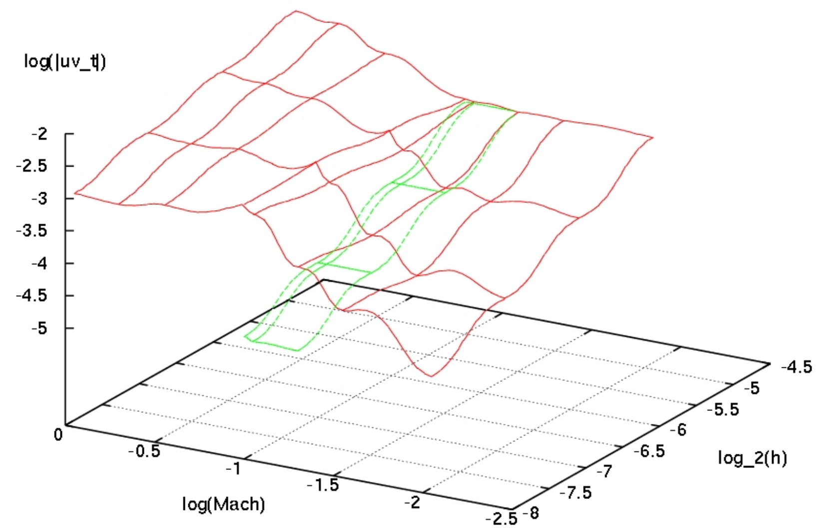
Verification of Low Mach Number Flow Solver

- Motivation
  gravity waves, nova pre-TNR, WD pre-ignition

- Low speed projection method (Colella and Pao,1999)
  - Based on projection method for incompressible flows
  - Valid for subsonic or weakly compressible flow
  - Velocity field decomposition
    Incompressible part: explicit solver
    Acoustic part: implicit solver

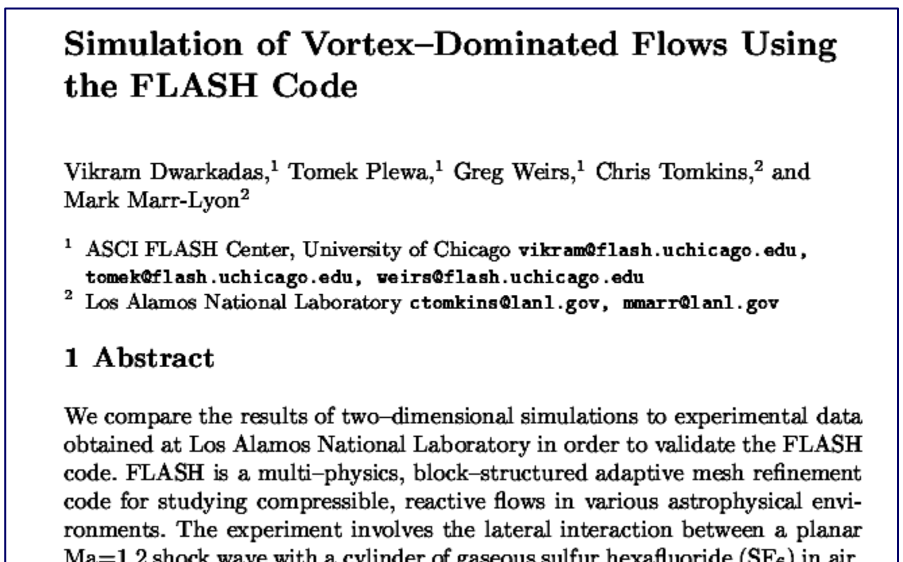






Current Validation of Computational Modules

- Access to experiments: collaborations with LANL (shock-tube) and LLNL (high-energy density laser) experiments
- Current program: shock-tube shock-cylinder experiment (LANL)
- Presentations at the AMR Chicago workshop and HEDLA (posters), and La Jolla V&V workshop and IWPCTM9 (talks); working towards the refereed journal publication



Simulation of Vortex–Dominated Flows Using the FLASH Code

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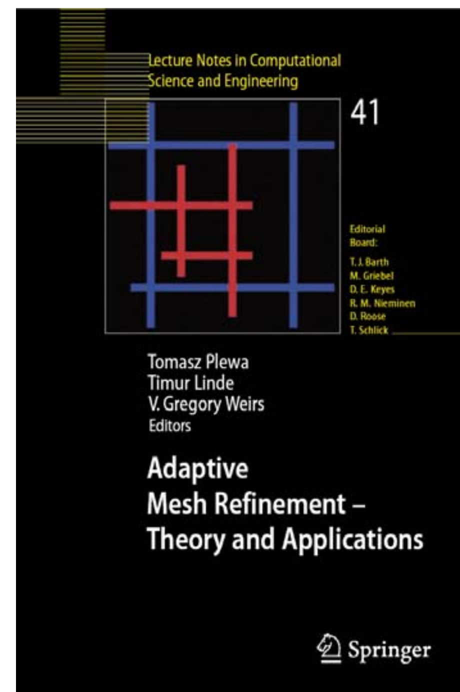
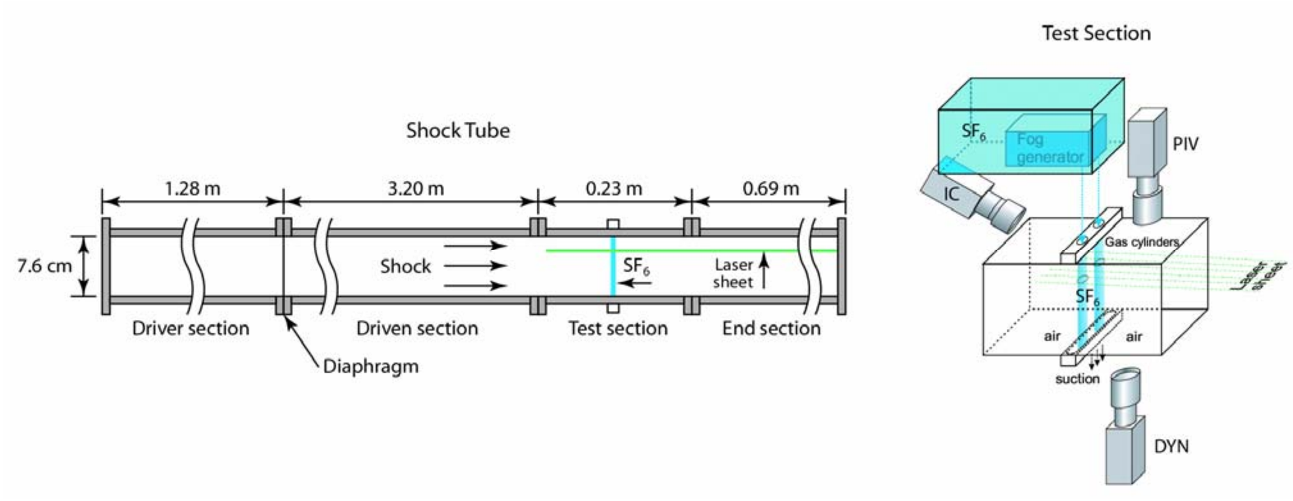
1 Abstract

We compare the results of two–dimensional simulations to experimental data obtained at Los Alamos National Laboratory in order to validate the FLASH code. FLASH is a multi–physics, block–structured adaptive mesh refinement code for studying compressible, reactive flows in various astrophysical environments. The experiment involves the lateral interaction between a planar Ma=1.2 shock wave with a cylinder of gaseous sulfur hexafluoride (SF_6) in air.



Case Study: LANL Shock-Cylinder Experiment



- A column of sulfur hexafluoride (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

Flowfield Development

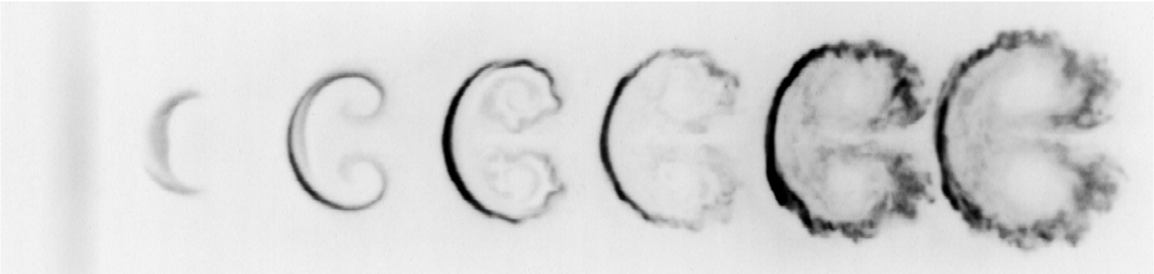
Phase I: shock-interaction

- 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

Phase II: instability growth

- A counter-rotating vortex pair forms, and secondary 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 I*

Flowfield Development



- Experimental time series, water/glycol fog visualization of SF_6 mole fraction.
- Images correspond to 50, 190, 330, 470, 610, and 750 μs after shock impact
- Composite image does not preserve time-distance relationship

Past Focus

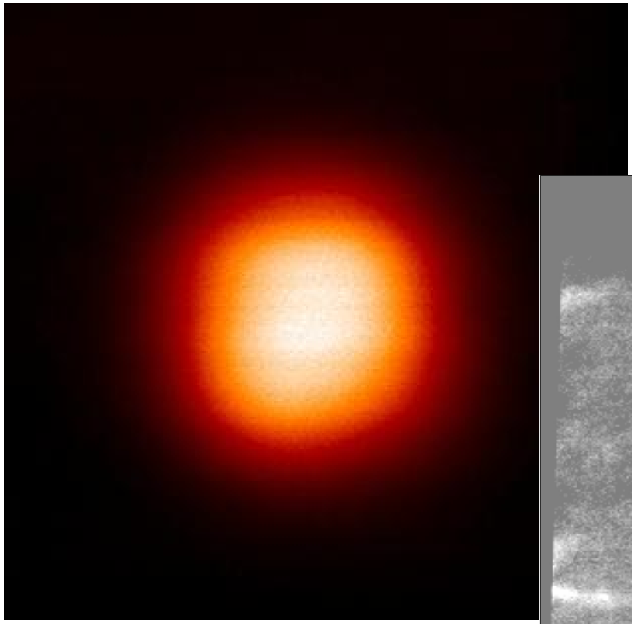
Aspects considered in depth:

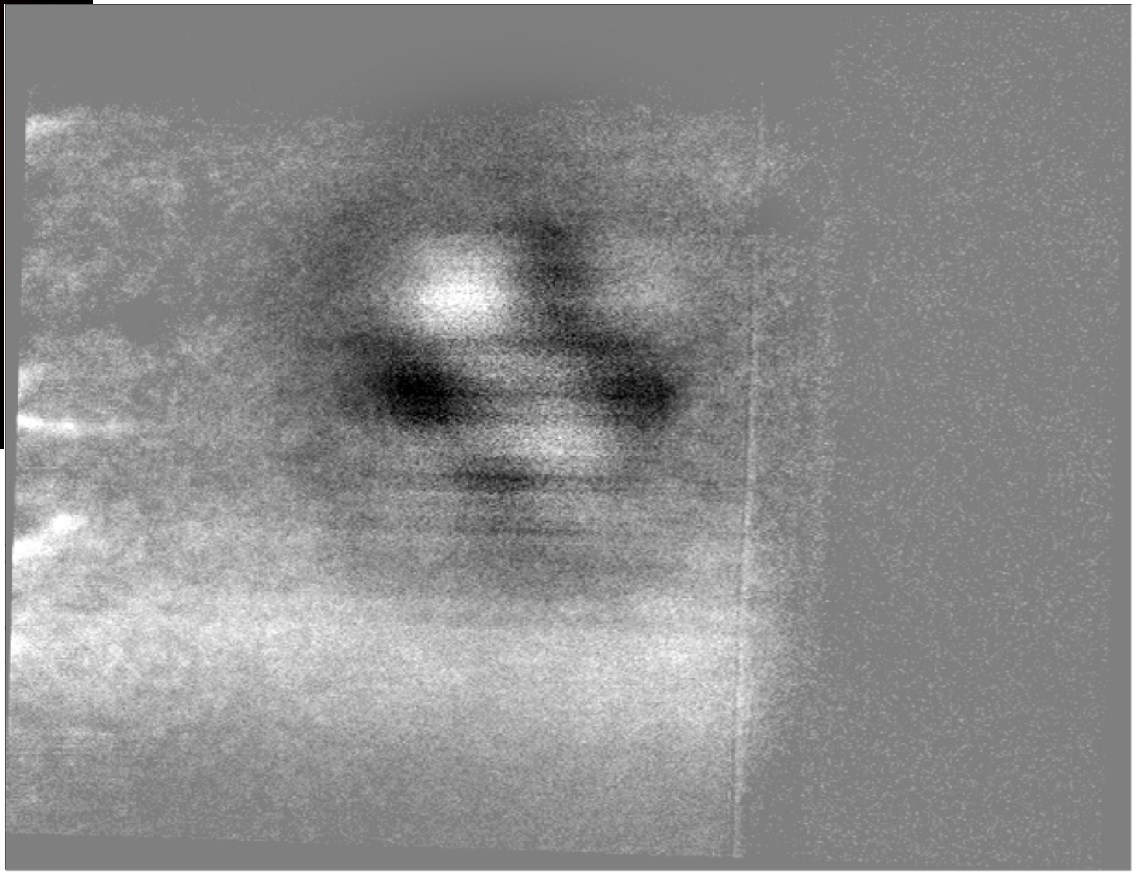
- Initial conditions
- Sensitivity to simulation parameters:
  - Resolution (numerical viscosity)
  - Adaptive Mesh Refinement (AMR)
  - Courant number
  - Mesh refinement criteria
- Velocity fields
- Double cylinder configuration
- Speculative 3-D calculation

Other possible aspects:

- Shock strength
- Equation of state

Initial Conditions: Cylinder Cross-section



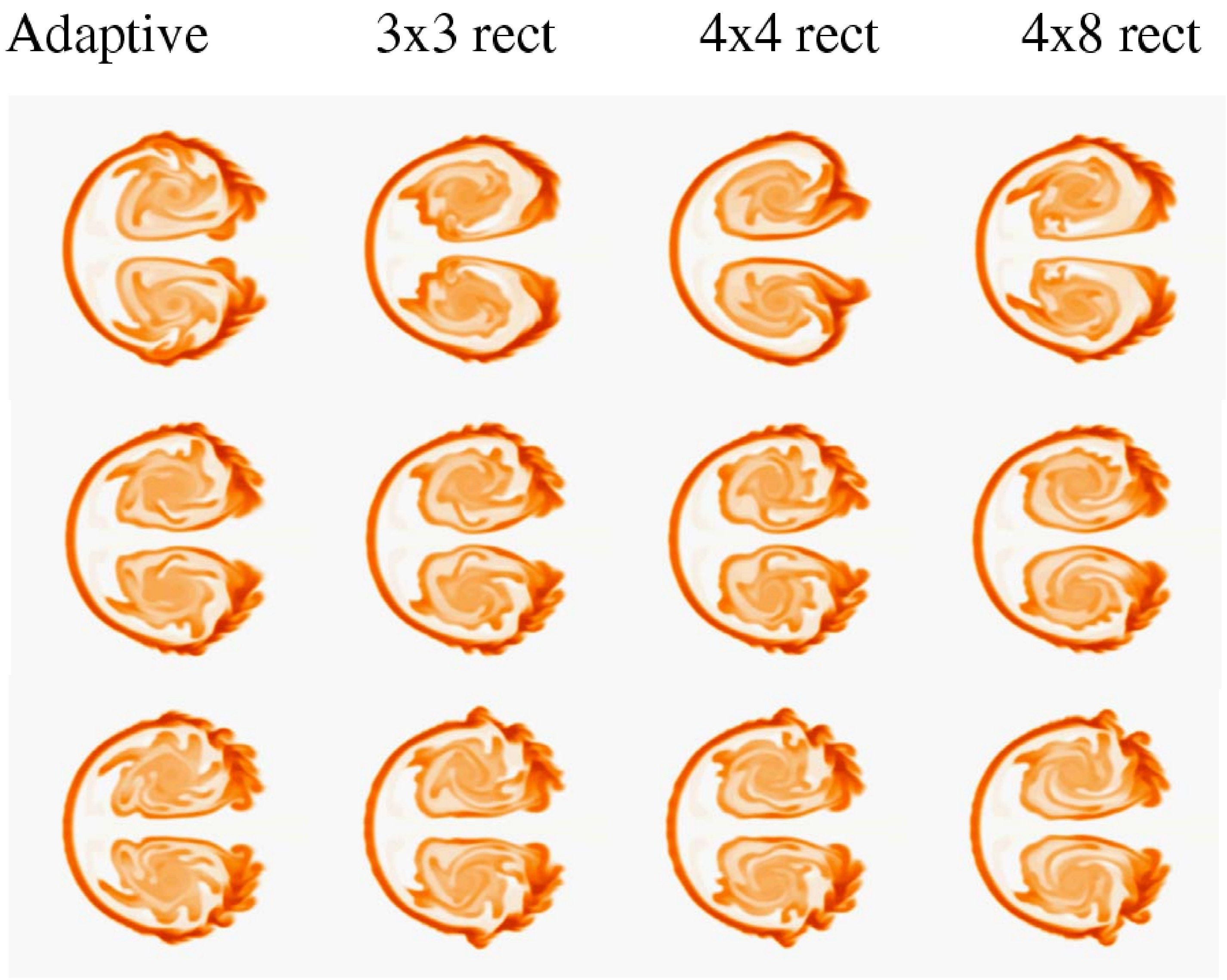


CFL dependency

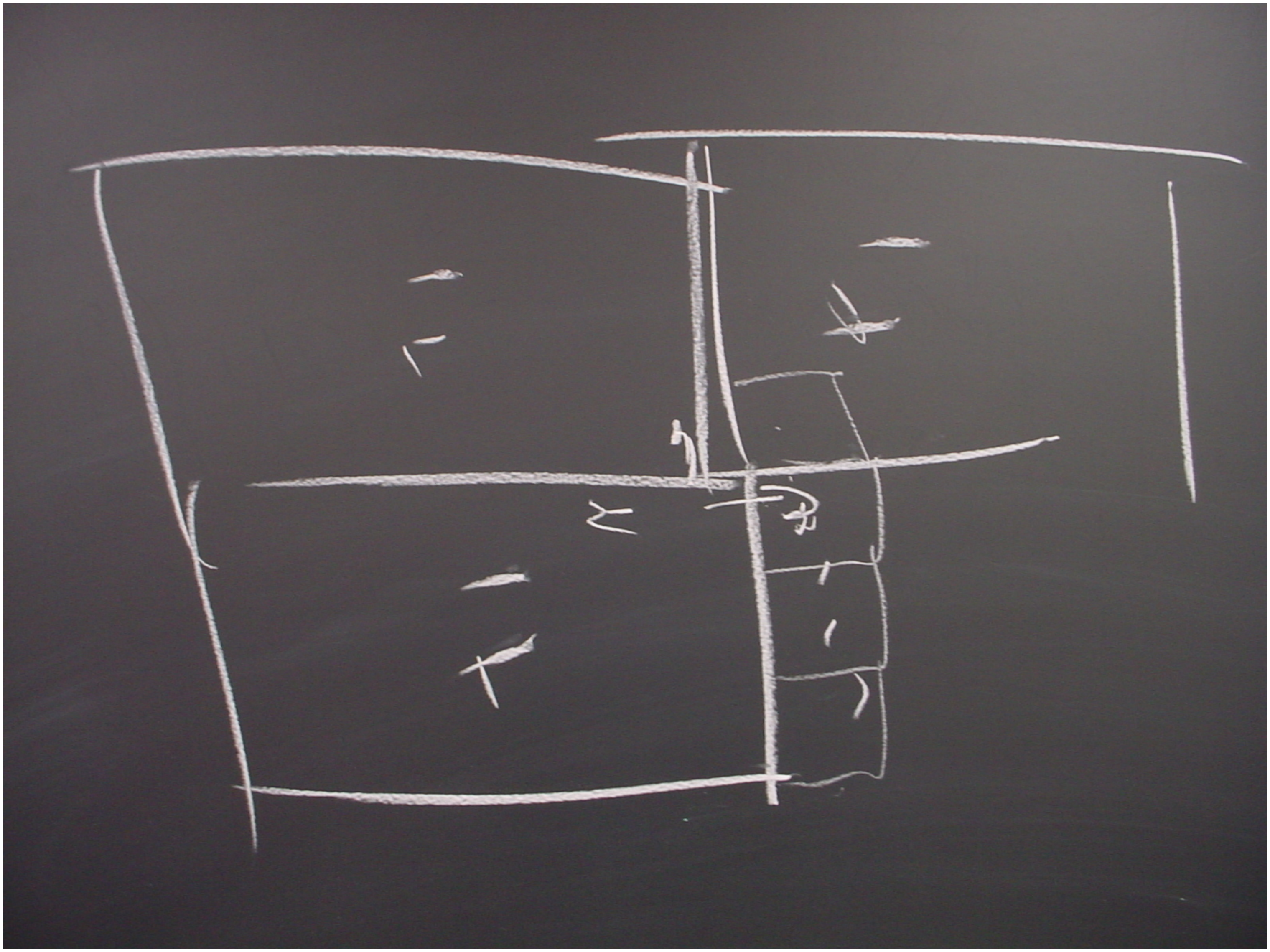
CFL=0.8

CFL=0.4

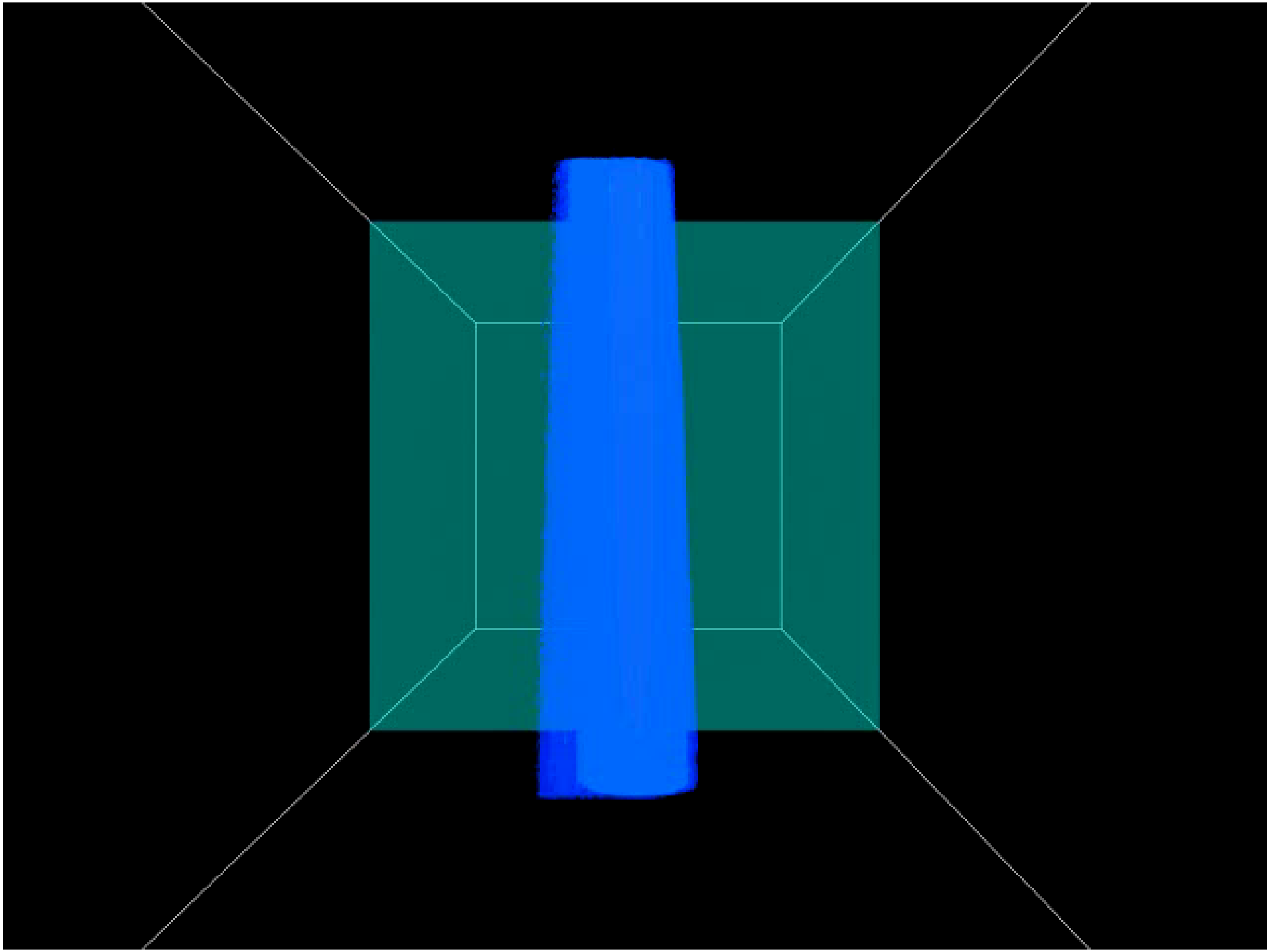
CFL=0.2



FLASH Code is the AMR code



3-D Shock-Cylinder Interaction (speculative)



Initial Observations

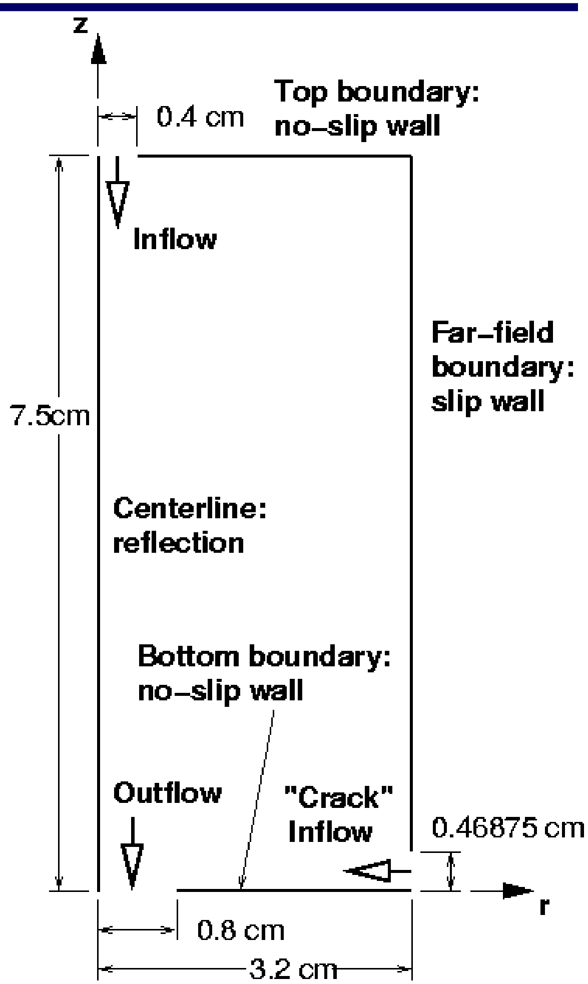
- Close interaction with experimentalists, understanding of experimental parameters
- Exercising the code in less violent regime has a potential of exposing higher-order numerical errors
- Lack of tools aiding data analysis in validation

Current Focus

- Initial conditions
- Better metrics
- Three-dimensional effects

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

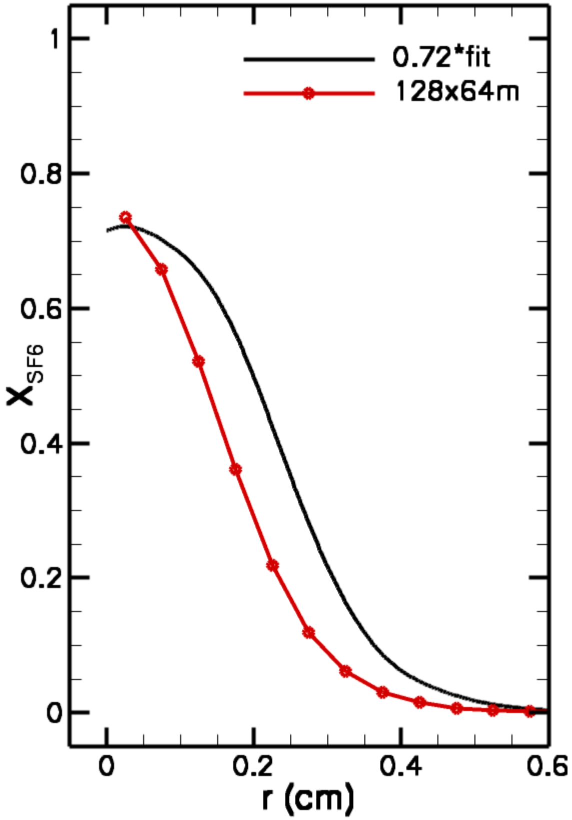


Simulations of Initial Conditions

- 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

- 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



Gravity-Diffusion Competition

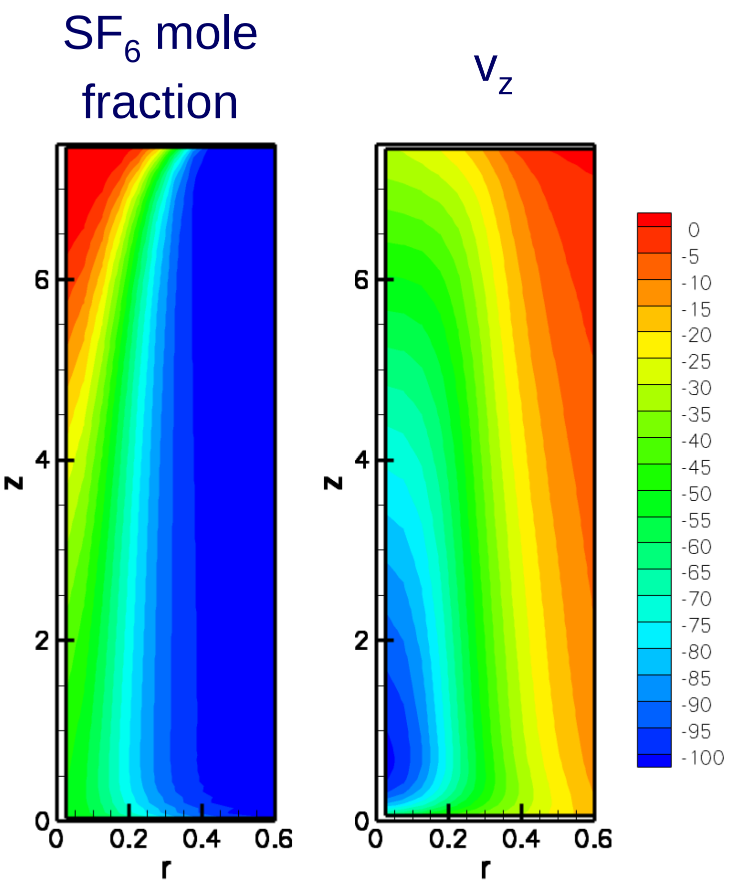
- Inlet velocity too low

  the profile is too narrow (closer to the centerline than the experimental data): gravitational acceleration of SF_6 leads to necking

- Inlet velocity 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}

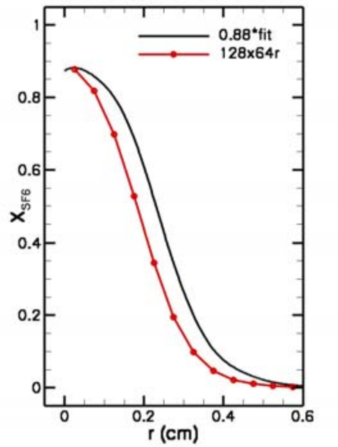


Inlet v_z = 15.0 cm/s

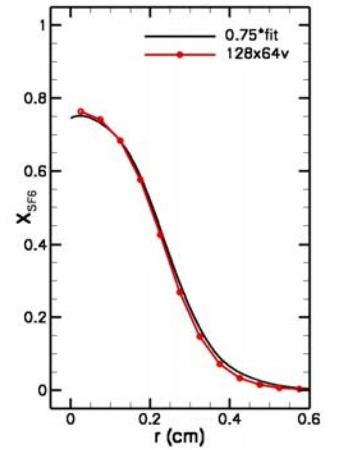
Inlet Y_{SF6} = 1.0

Simulations of Initial Conditions

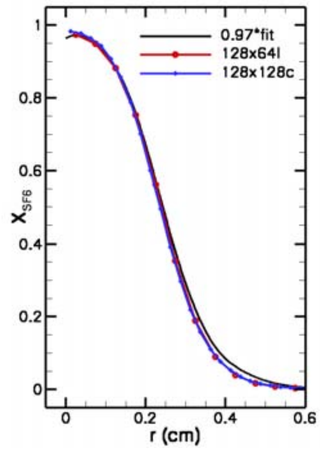
Inlet Y_{SF6} = 1.0
Inlet v_z = 15.0 cm/s



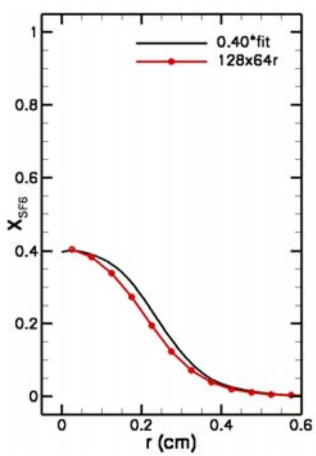
Inlet Y_{SF6} = 0.95
Inlet v_z = 22.50 cm/s



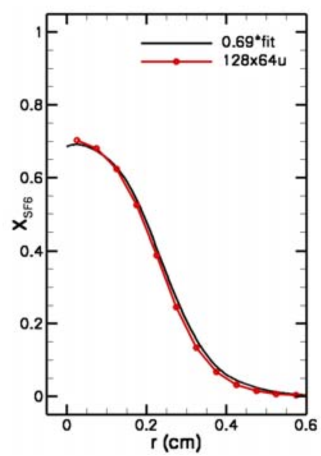
Inlet Y_{SF6} = 1.0
Inlet v_z = 25.0 cm/s



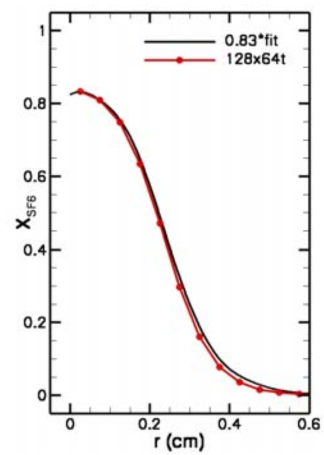
Inlet Y_{SF6} = 0.8
Inlet v_z = 15.0 cm/s



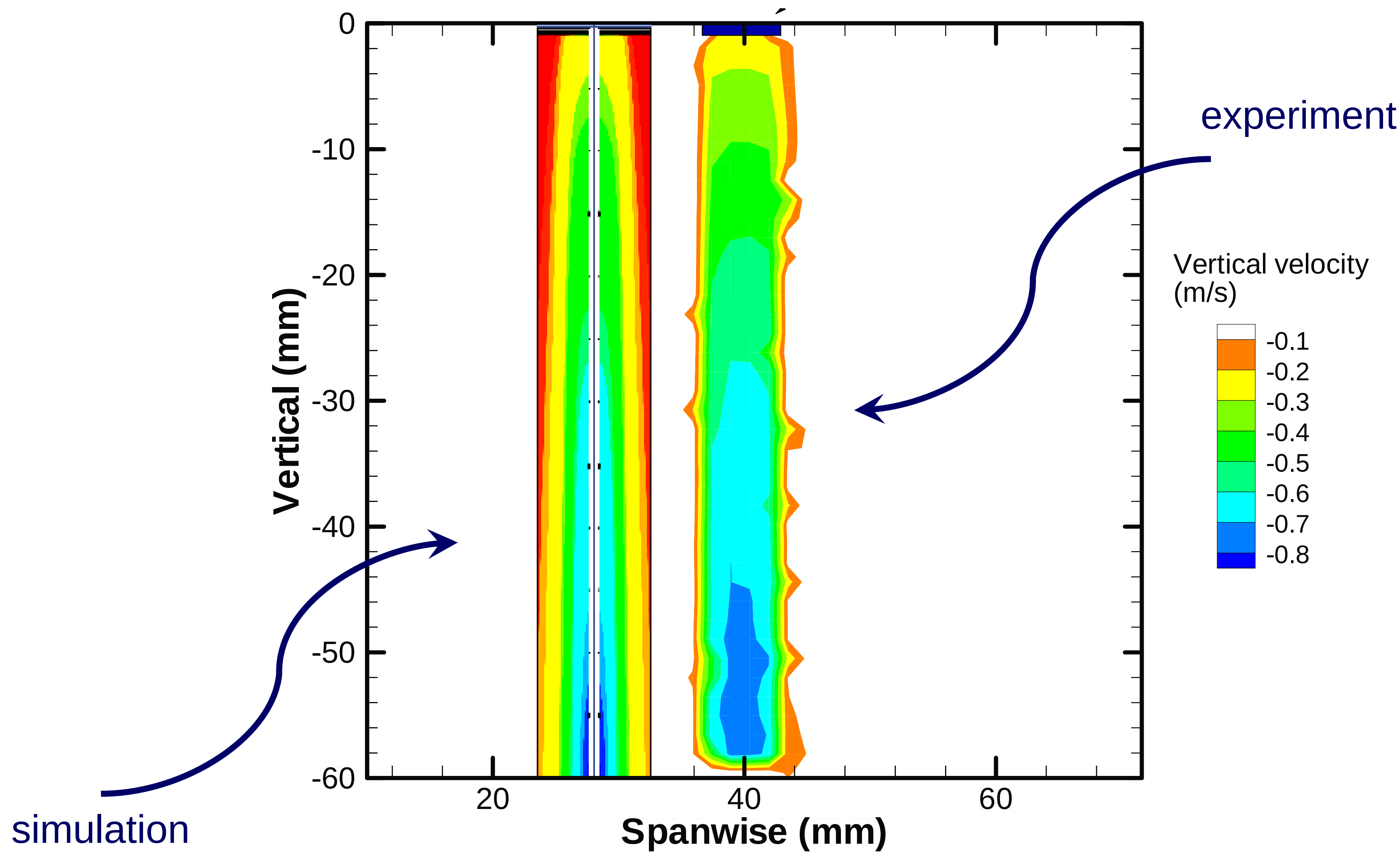
Inlet Y_{SF6} = 0.9315
Inlet v_z = 21.85 cm/s



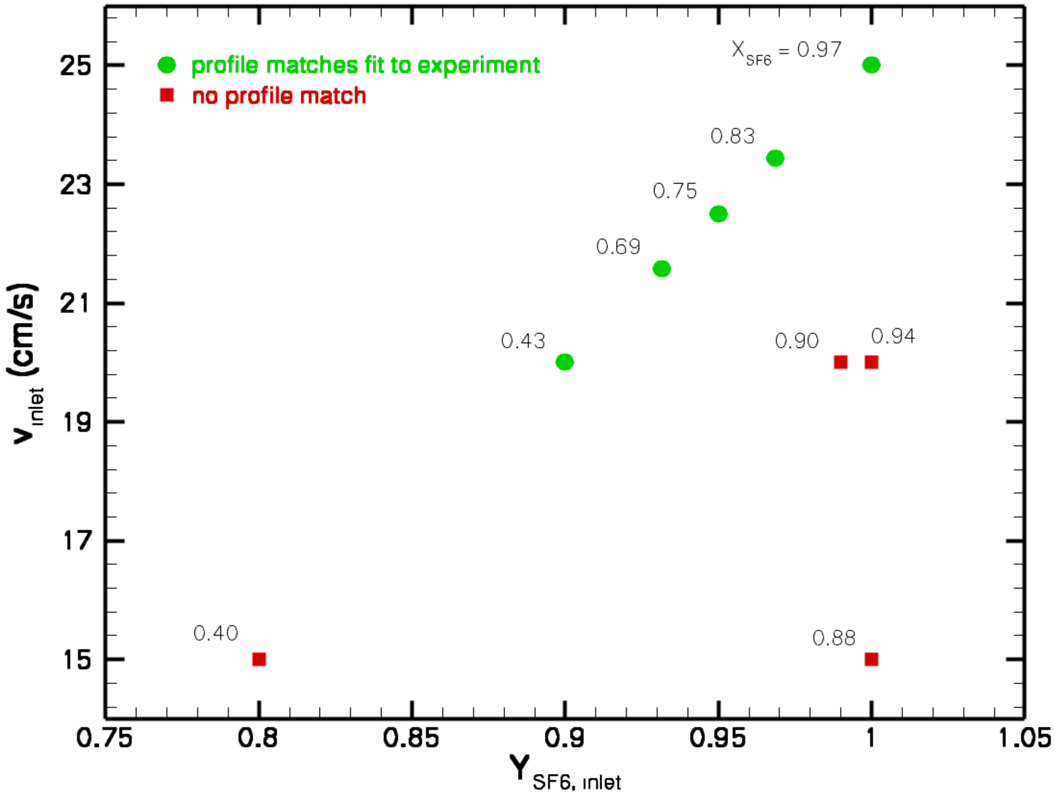
Inlet Y_{SF6} = 0.9685
Inlet v_z = 23.43 cm/s



Initial Vertical Velocity: Comparison



Simulations of Initial Conditions



- It's not so easy to determine the initial conditions!
- Profile "matches" collapse on a line on the plane: one parameter family
- Should quantify error in matching experimental fit

The Need For A Better Metric

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

Possible Metrics

Some possibilities

- Self-induced vortex velocity
- Circulation

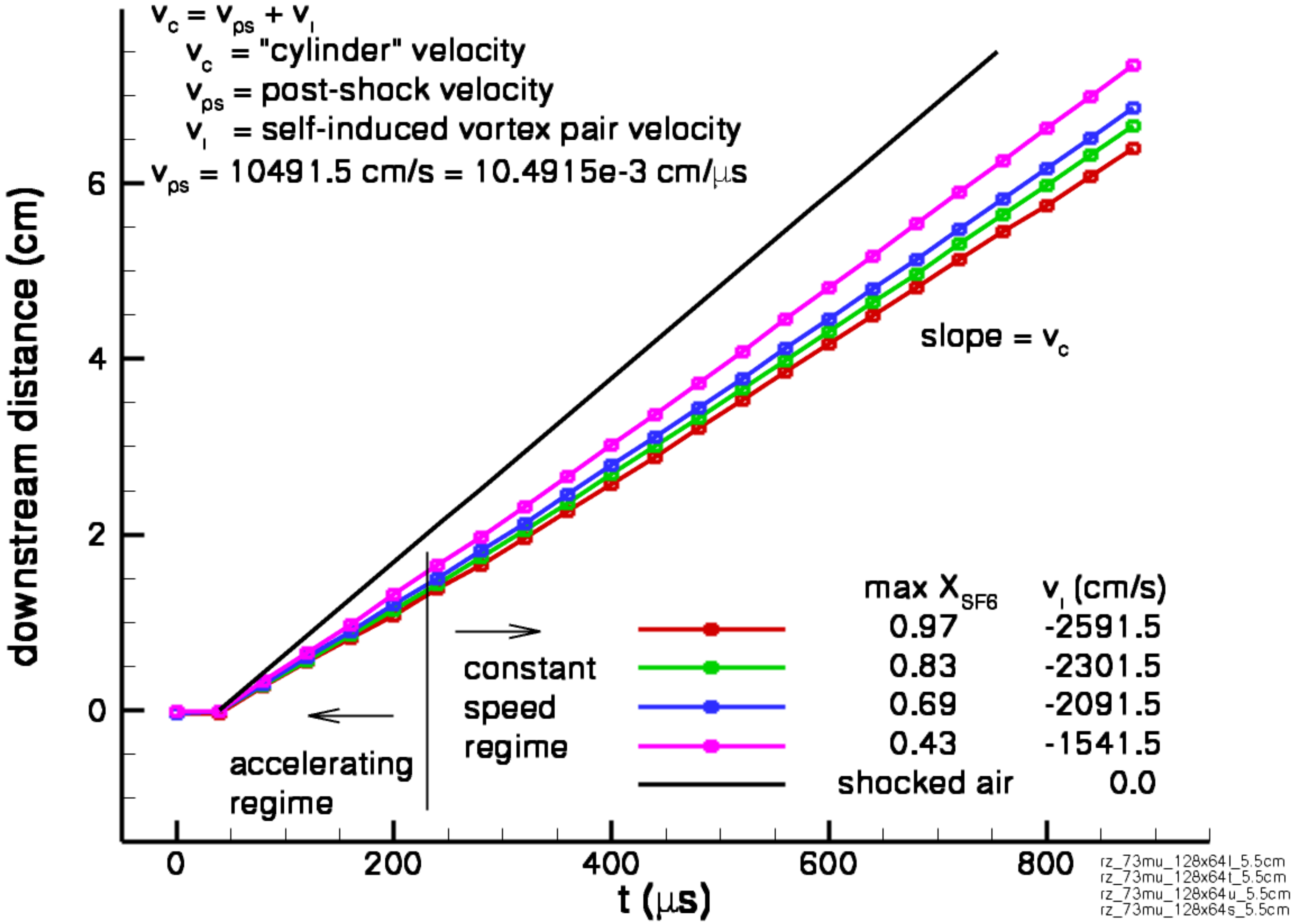
Properties

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

Application

- A way to probe the initial composition gradients (X_{SF6}), a necessary step before studying evolution on small scales (secondary instabilities, turbulence, diffusion)

Induced Velocity vs. Initial Composition



Circulation

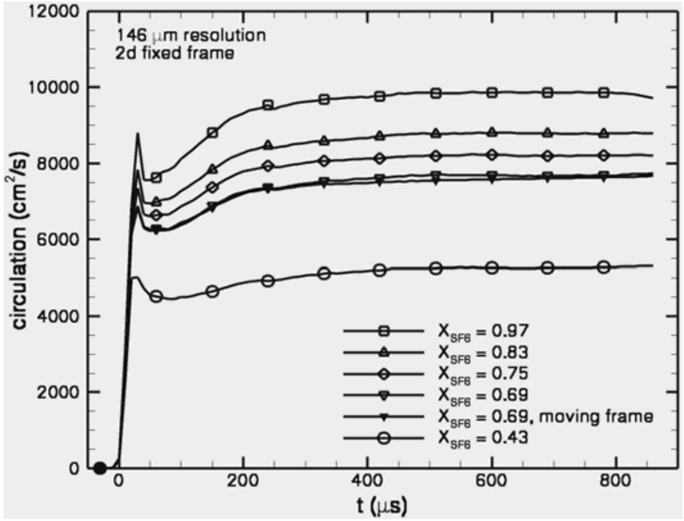
Circulation is the integral of vorticity:

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

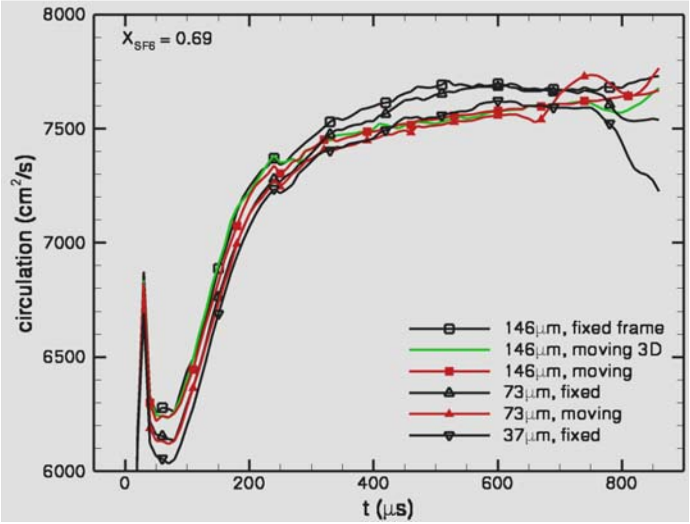
- We consider only the z-component of vorticity
- We integrate over the lower-y half of the domain (lower half in the spanwise dimension)

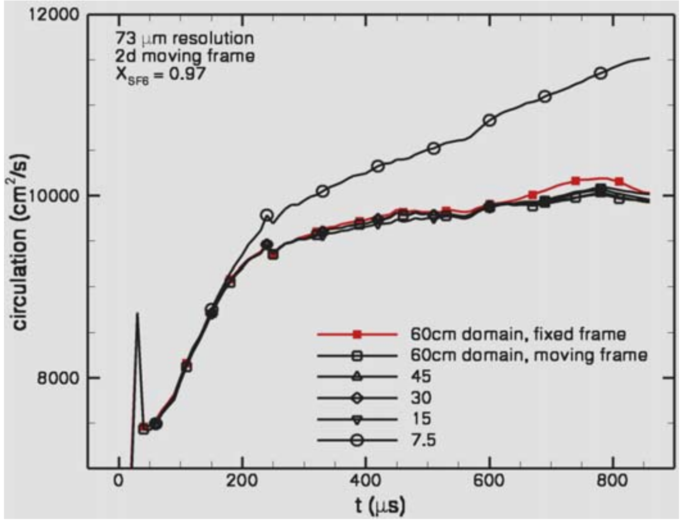
Circulation Sensitivity

Initial SF_6 Mole Fraction



Resolution, Ref. Frame





Domain Size

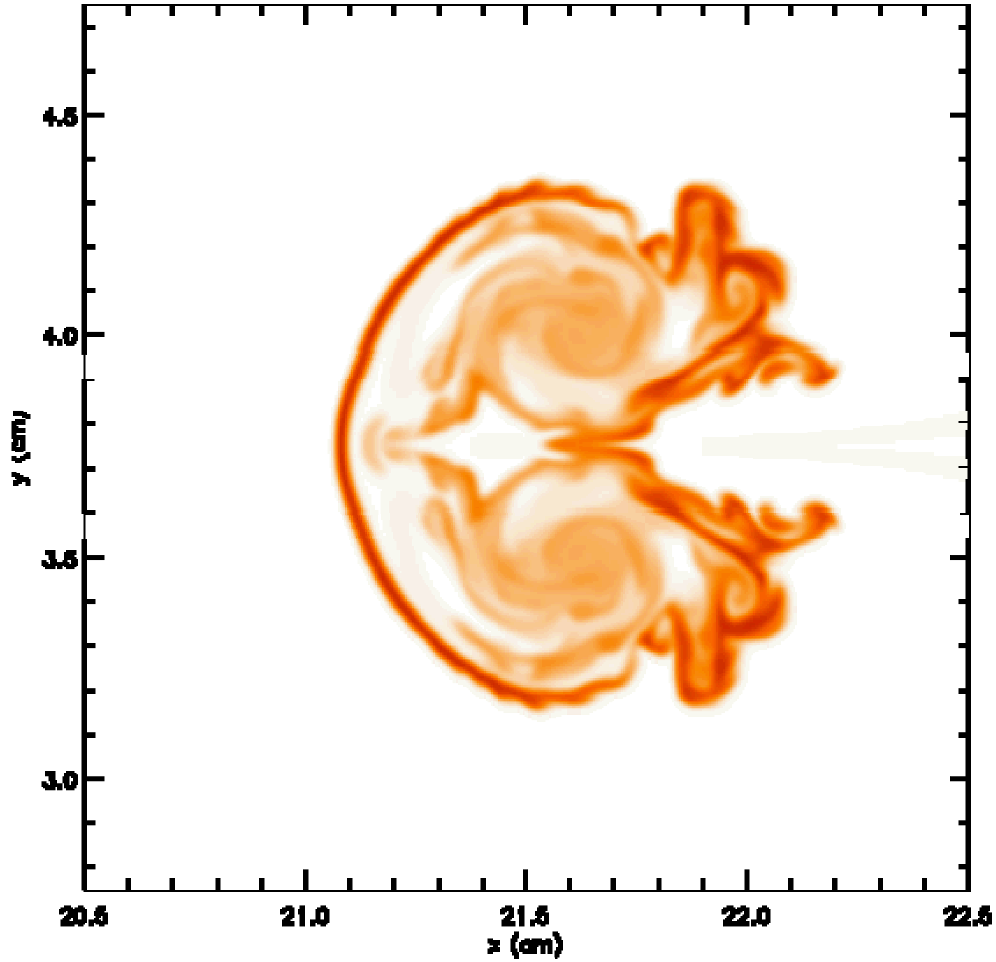
3-D Simulations

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

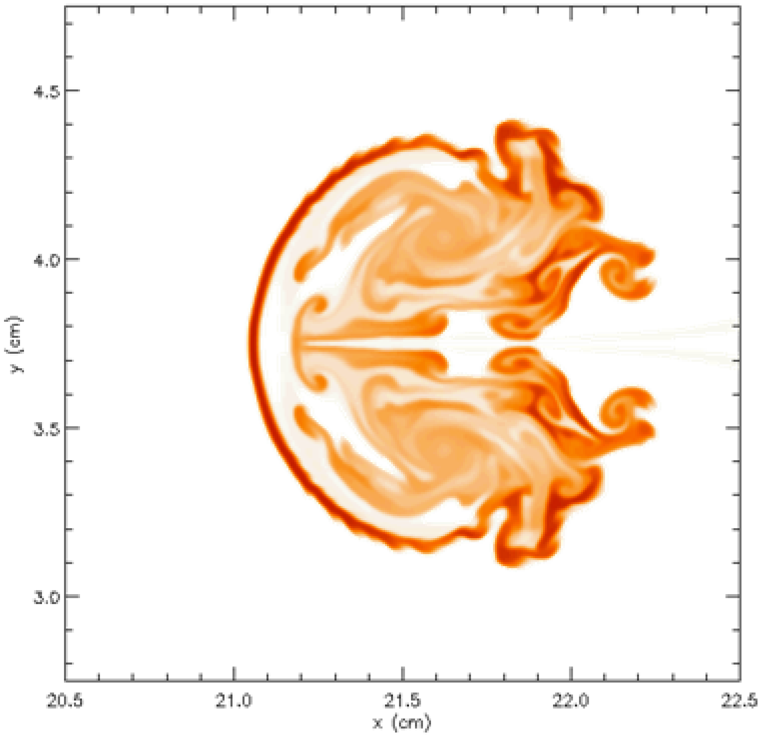
We have left the validation program proper – no experimental data.

2-D vs. 3-D Flow Morphology

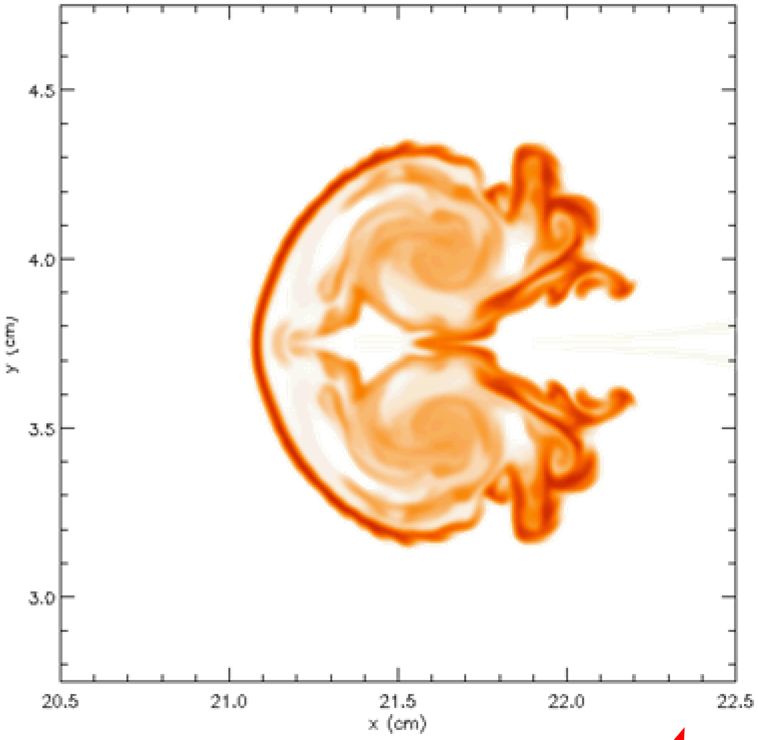


3-D

2-D vs. 3-D Flow Morphology



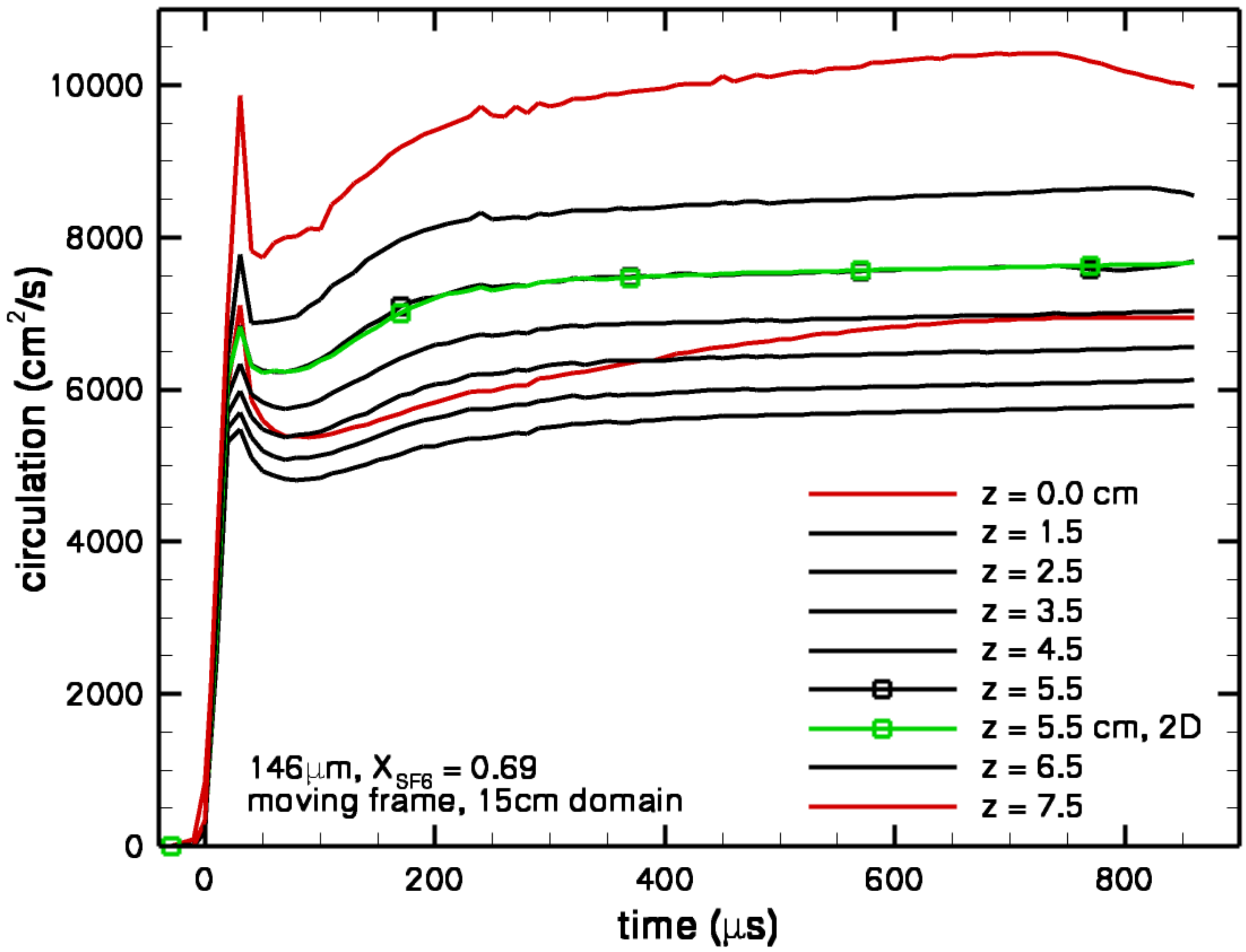
2-D, t = 750 μs



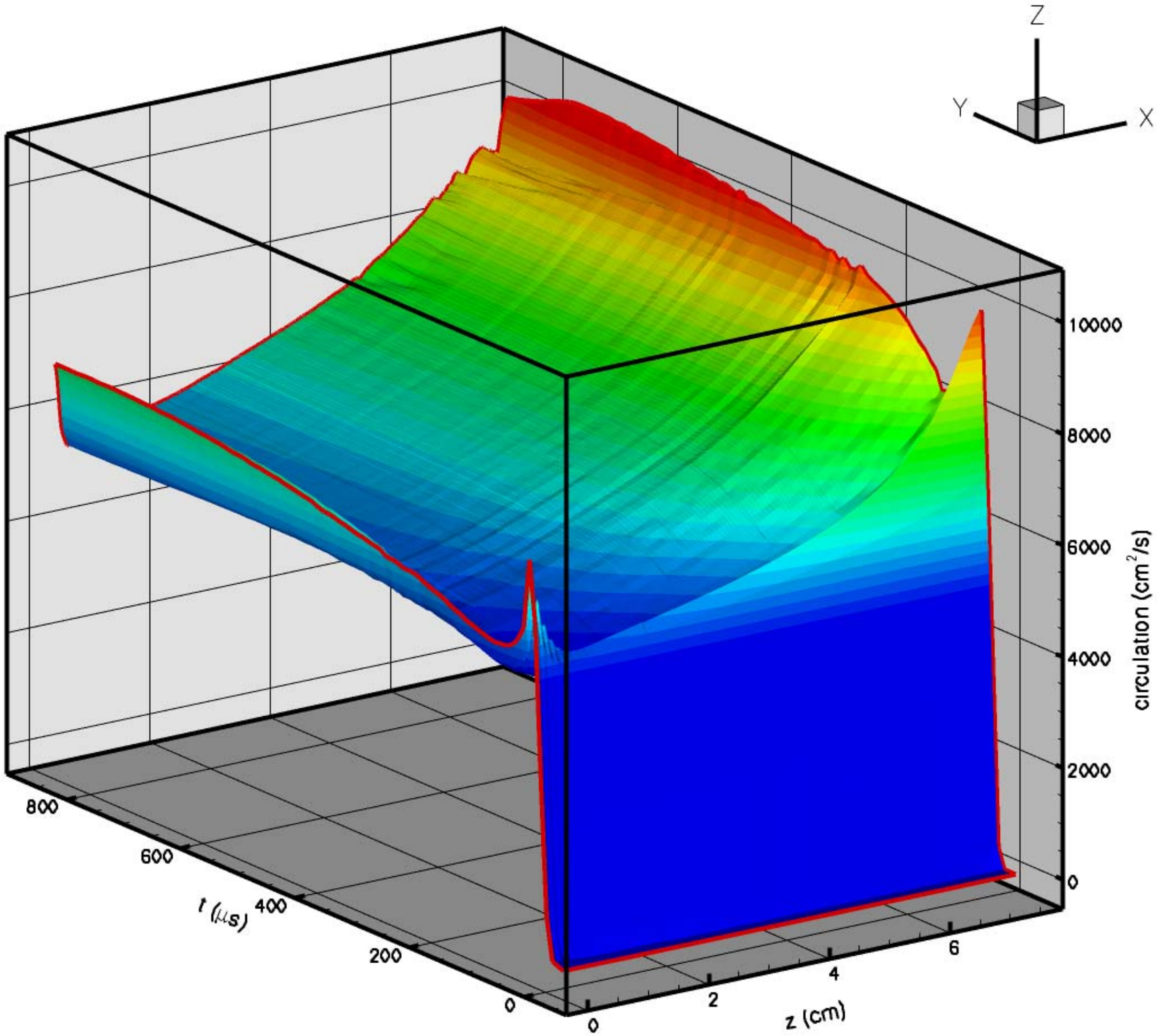
3-D, t = 750 μs

…simulation demonstrates that nature is…

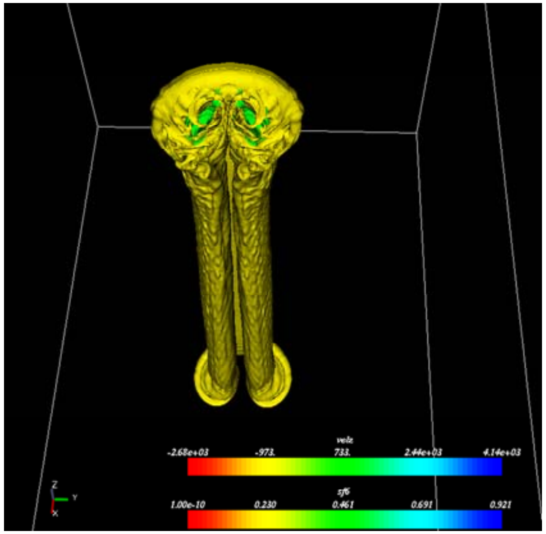
Circulation: 2-D vs. 3-D



3-D Simulation: Circulation

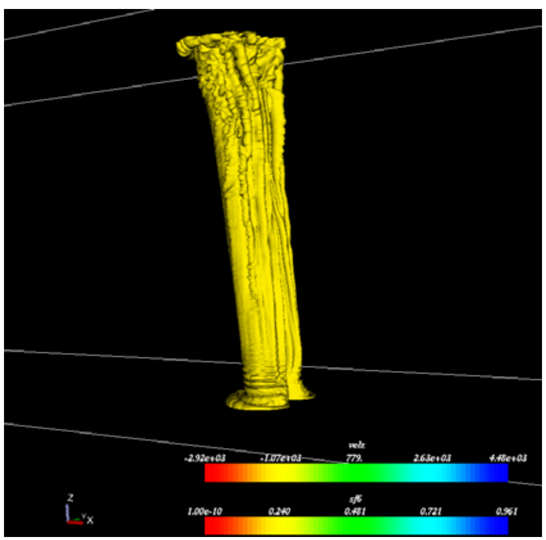


3-D Simulation: SF_6 Density Morphology



$X_{SF6} = 0.69$
$t = 750\ \mu s$

Mild structures are visible on the back of the cylinder

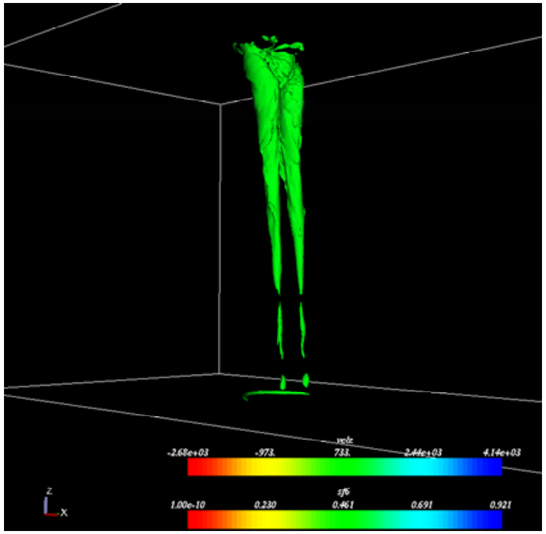


$X_{SF6} = 0.97$
$t = 750\ \mu s$

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

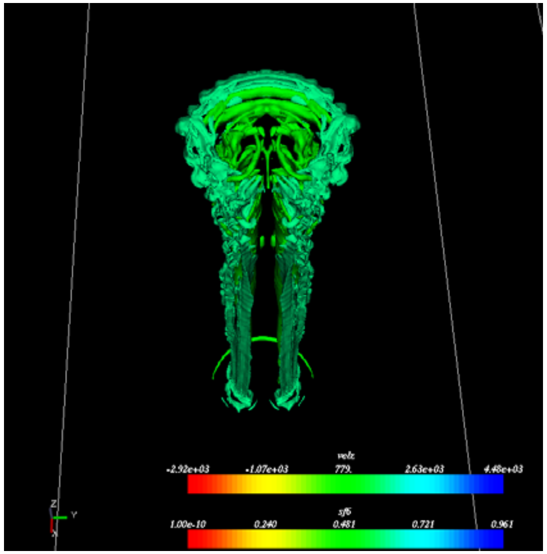
3-D Simulation: Vertical Velocity Morphology



X_{SF6} = 0.69
t = 750 μs

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

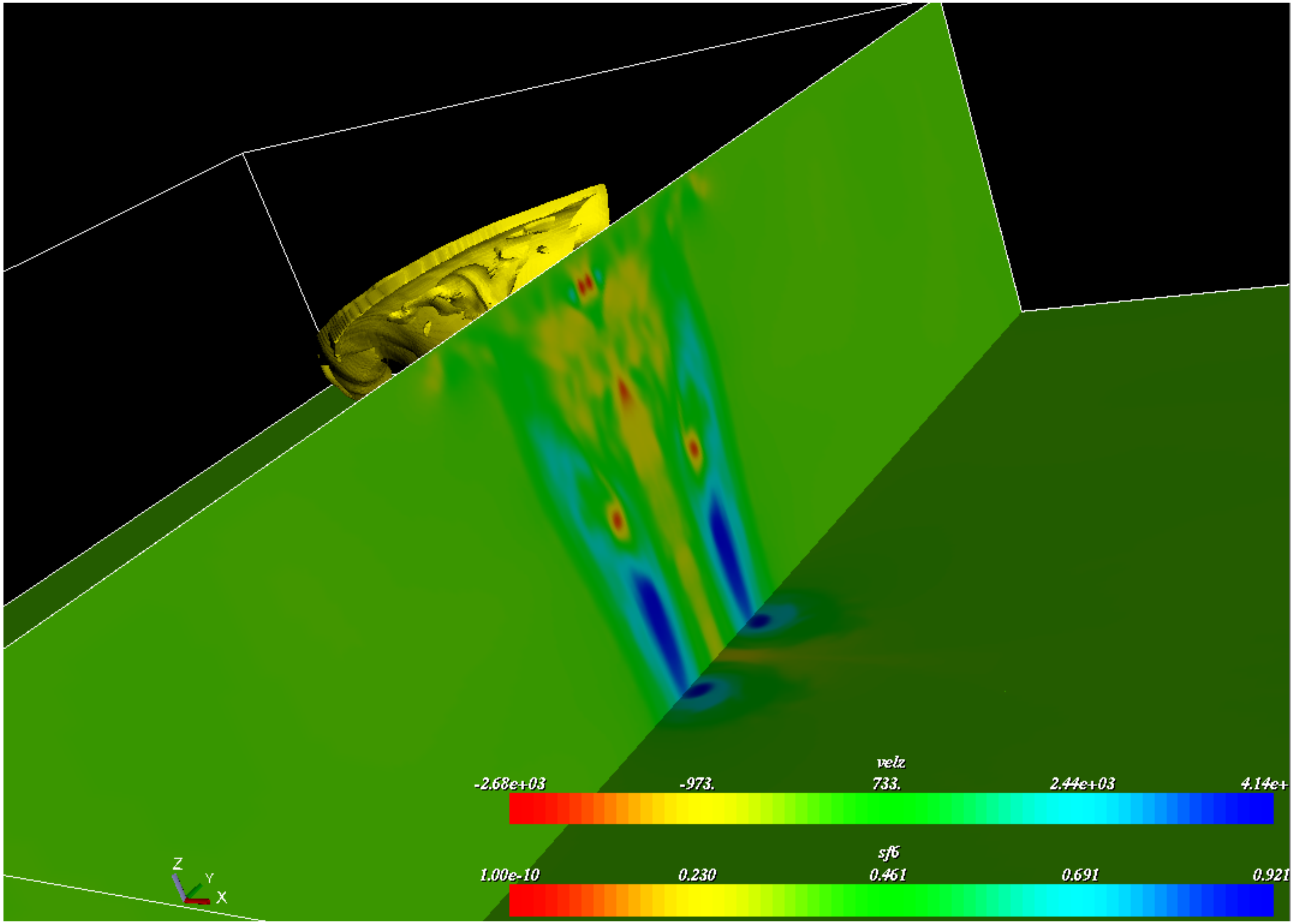
Spreading as the top wall is approached indicates acceleration



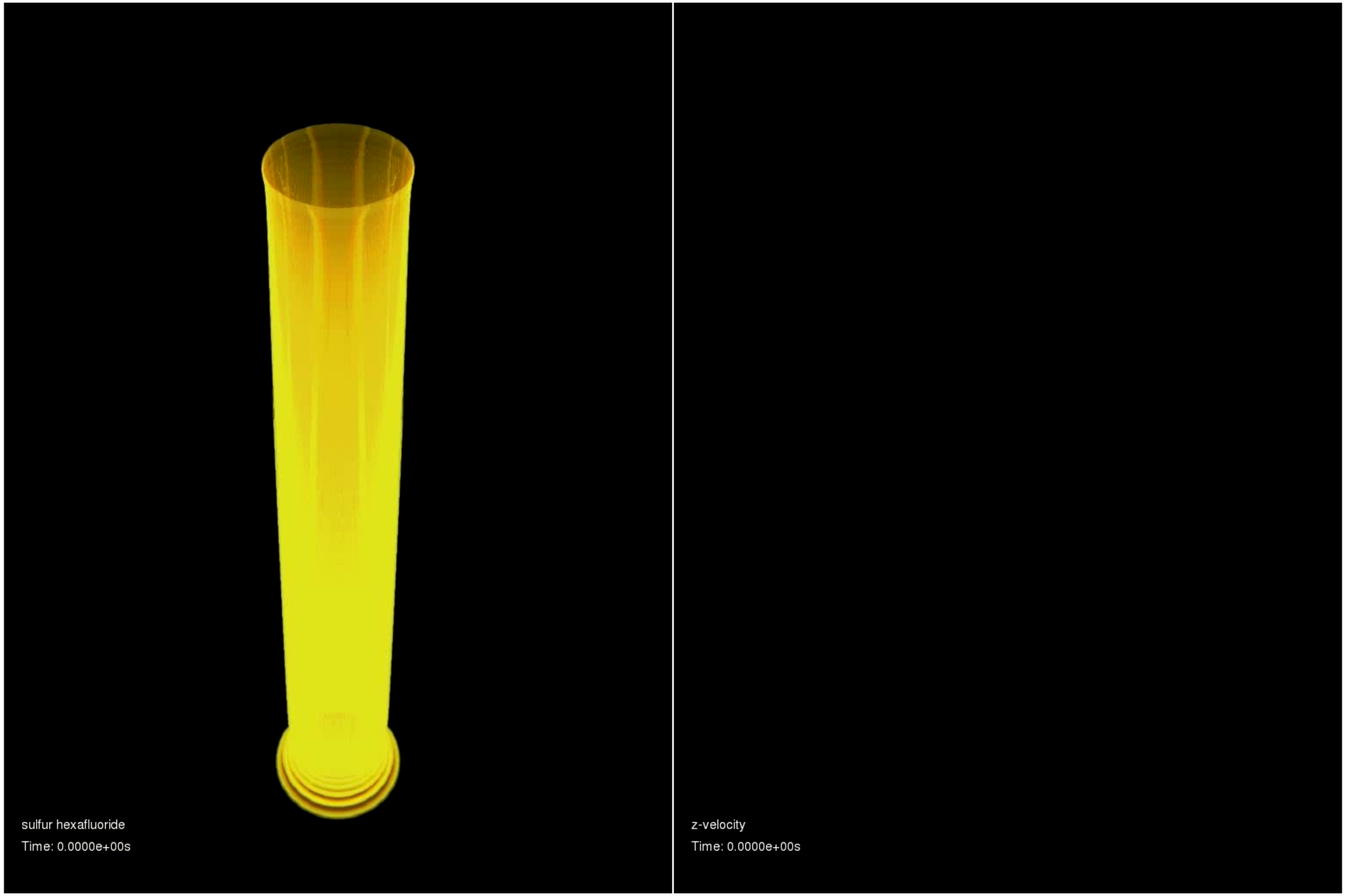
X_{SF6} = 0.97
t = 750 μs

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

3-D Simulation: Vertical Velocity Flowfield



3-D Simulation: Flow Visualization



Summary and Future Plans

- Initial validation for the shock-cylinder interaction was ***qualitative*** and focused on the influence of simulation parameters
- Led to a discovery of time-dependent ***error component*** in the AMR-aided simulations allowing for possible code improvement
- Attracted interest of experimentalists, led to the modifications of the experimental setup
- This will offer us data allowing for making ***quantitative comparison*** and ***optimizing future experiments***