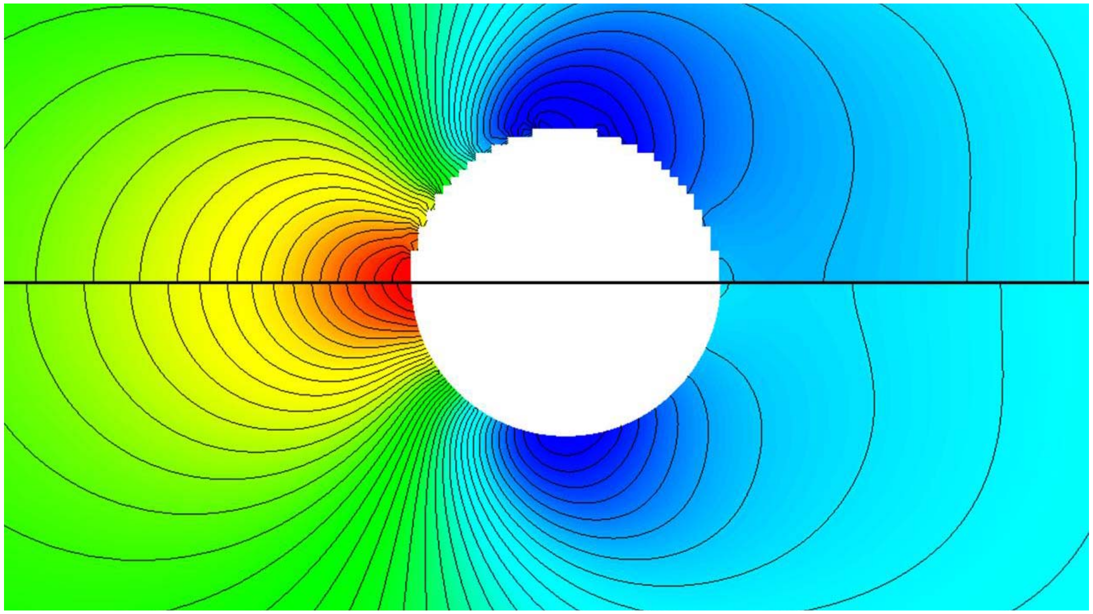
NATIONAL ENERGY TECHNOLOGY LABORATORY



Implementation of Cartesian Cut-Cell Technique into the Multiphase Flow Solver MFIX

Jeff Dietiker

NETL 2009 Workshop on Multiphase Flow Science

Euro-Suites Hotel, Morgantown, WV

April 22-23, 2009

Overview

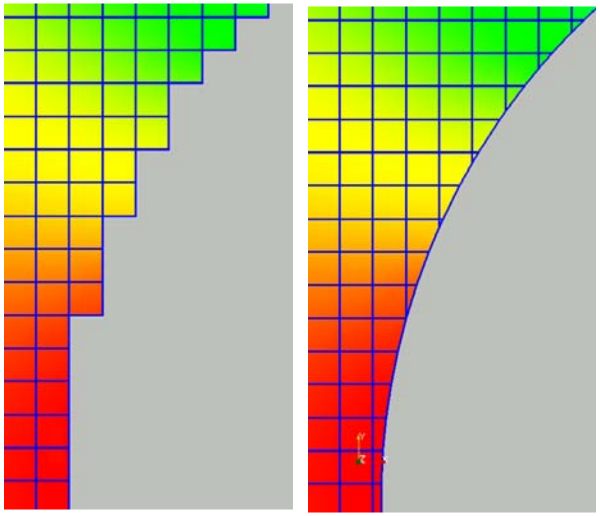
- Introduction
- Cartesian grid cut cell implementation
- Results:
  - Single phase
    - 2D: channel flow, flow over a cylinder
    - 3D: flow over a hemisphere
  - Gas / Solids phase
    - 2D Hourglass flow
    - 2D spouted bed
    - 3D O3 decomposition
- Latest Additions
- Conclusions

Introduction

- **MFIX: Multiphase Flow with Interphase eXchanges**
  - Finite volume , 3D Cartesian or cylindrical coordinate system
  - Continuum model (Interpenetrating fluid and solids phases)
  - Mass and momentum balances equation for gas and solids phases
  - Boundary conditions typically specified along planes, aligned with grid
  - Objective: Add flexibility and accuracy in geometric representation of boundaries

- **Cartesian Grid (Cut-cell) technique:**
  Based on: M.P. Kirkpatrick, S.W. Armfield, J.H. Kent, "A representation of curved boundaries for the solution of the Navier–Stokes equations on a staggered three-dimensional Cartesian grid," Journal of Computational Physics, 184 (2003) 1–36.

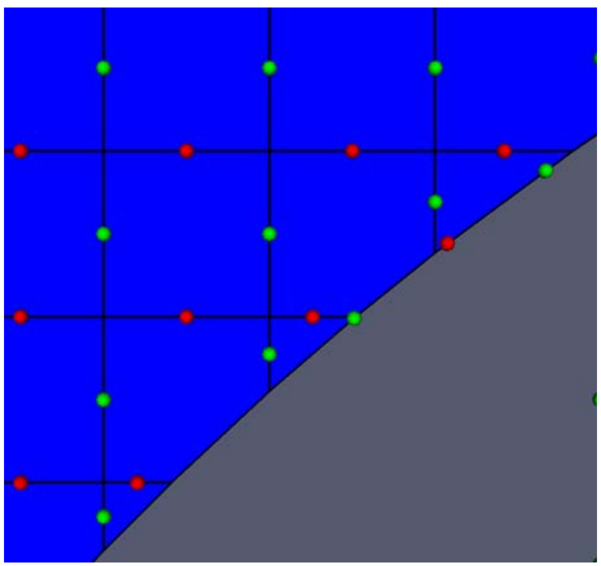
- Representation of curved boundaries
  - Computational cells are truncated at the wall to conform to the shape of the boundaries
  - Preprocessing:
    - Representation of curved or sloping boundary
    - Identify boundary cells (cut cells)
    - Identify "Problematic" cells
    - Computation of cells volumes and face areas
  - Solution
    - Flux computation through cut cell faces
    - Pressure forces
    - Wall shear stress
  - Postprocessing: VTK files (geometry must be saved in every file)

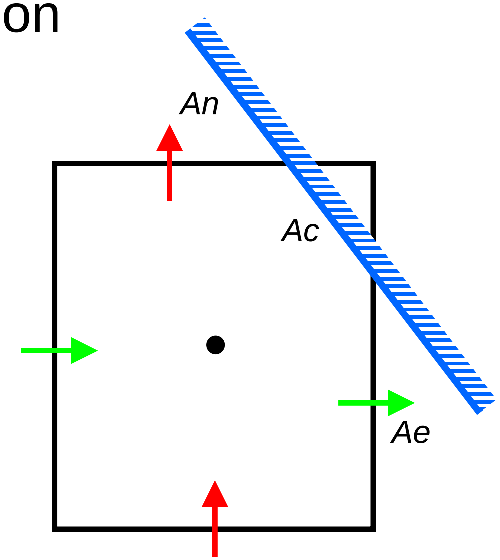


Staircase steps *Cut cells*

Cartesian-Grid Implementation

- **Representation of curved or sloping boundaries**
  - Quadric surfaces (normalized form): $f(\mathbf{x}) = \lambda_1 x_1^{\,2} + \lambda_2 x_2^{\,2} + \lambda_3 x_3^{\,2} + d = 0$
  - Quadric defined by λ_i, d rotation and translation
  - Problematic cells:
    - Velocity cells with only one pressure node
    - Pressure cells with only one velocity node
    - Small cells (stiffness)

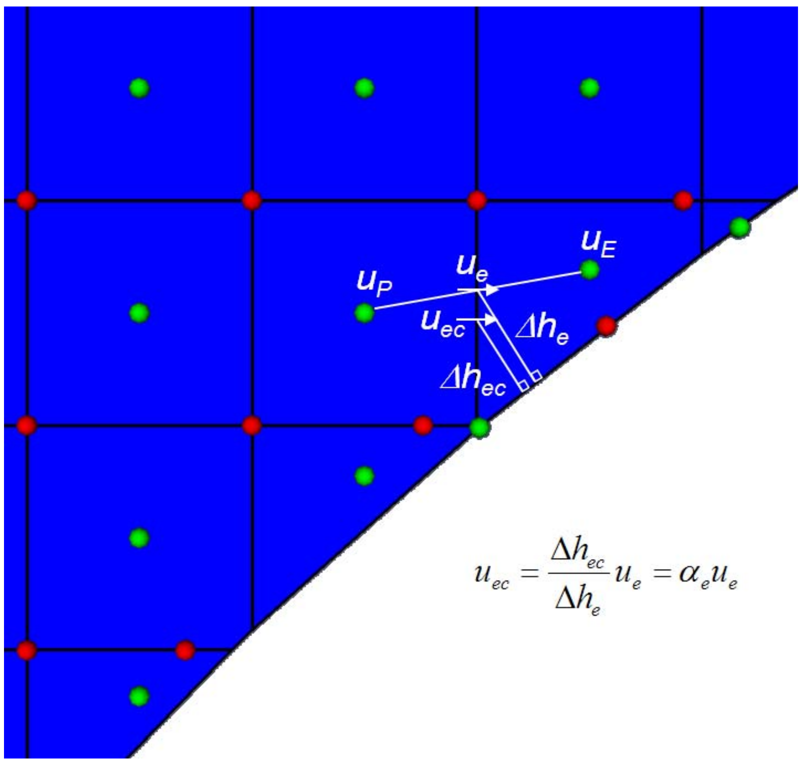




Cartesian-Grid Implementation

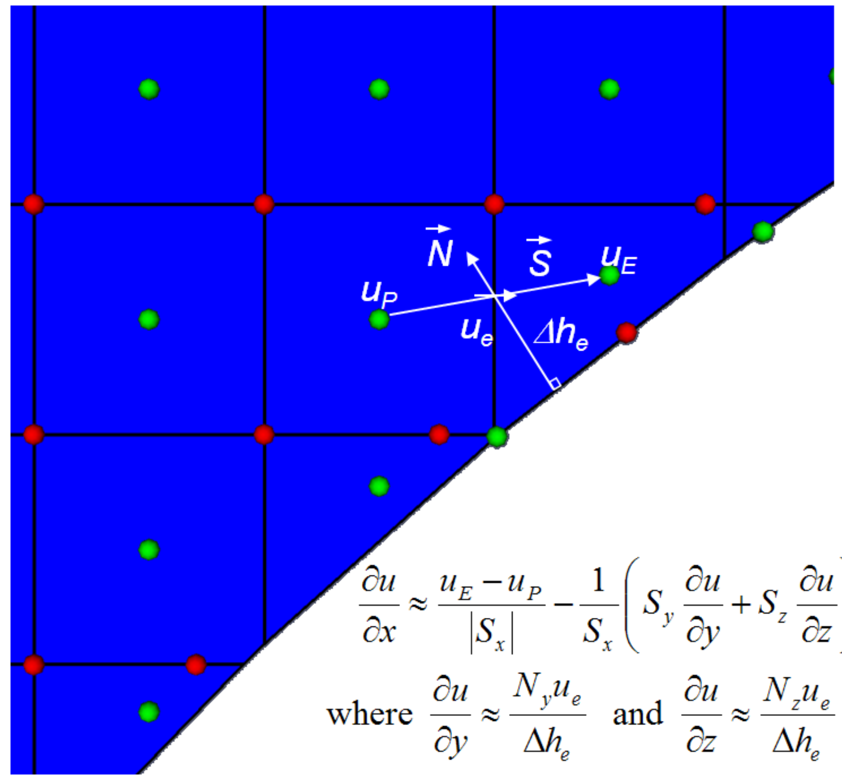
- **Representation of curved or sloping boundaries**

Advection of u-velocity through East face



$$u_{ec} = \frac{\Delta h_{ec}}{\Delta h_e} u_e = \alpha_e u_e$$

Diffusion flux across East face



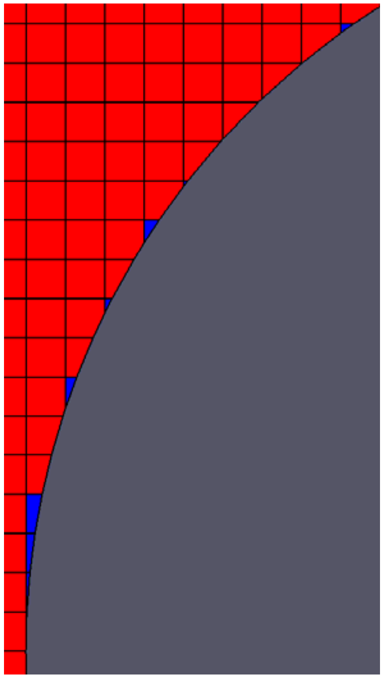
$$\frac{\partial u}{\partial x} \approx \frac{u_E - u_P}{|S_x|} - \frac{1}{S_x}\left(S_y \frac{\partial u}{\partial y} + S_z \frac{\partial u}{\partial z} \right)$$

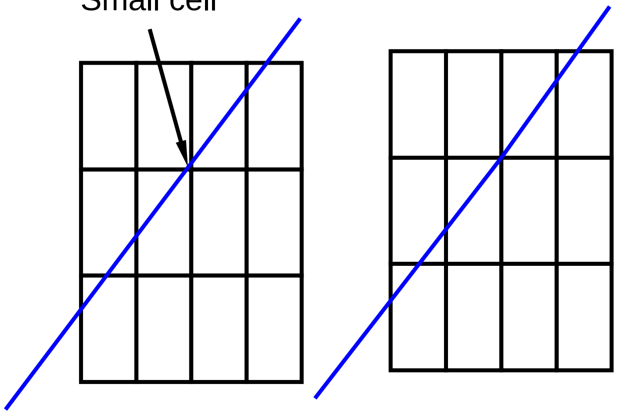
$$\text{where } \frac{\partial u}{\partial y} \approx \frac{N_y u_e}{\Delta h_e} \text{ and } \frac{\partial u}{\partial z} \approx \frac{N_z u_e}{\Delta h_e}$$

Based on zero-velocity at the wall

Cartesian-Grid Implementation

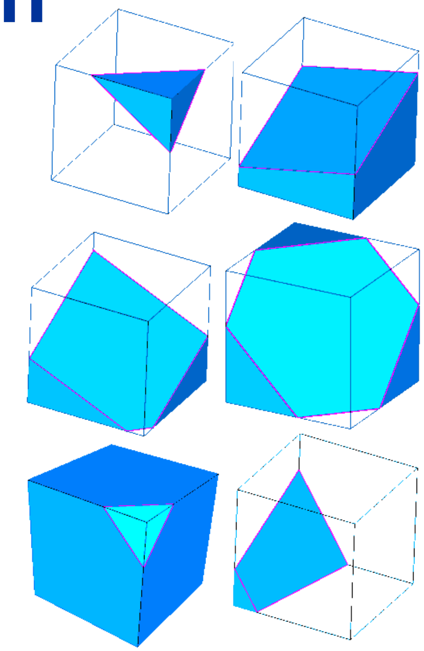
- **Problematic cells:**
  - Velocity cells with only one pressure node
    - Kirkpatrick: Use Master/Slave cell linking procedure: velocity node is moved to adjacent cell
    - Current approach: Velocity node is moved to the center of the cut face (velocity is set to zero)
    - Note: Treating those cells limit their width to half-width of regular cell
  - Pressure cells with only one velocity node
    - Current approach: velocity derivatives (in tr(D)) are computed from $$\frac{\partial u}{\partial x} \approx \frac{N_x u}{\Delta h}$$
  - Small cells (stiffness)
    - Kirkpatrick: Remove pressure node from computation
    - Current approach: Option to move intersection point to nearest corner, based on some user-specified tolerance (e.g., 1% of side length)

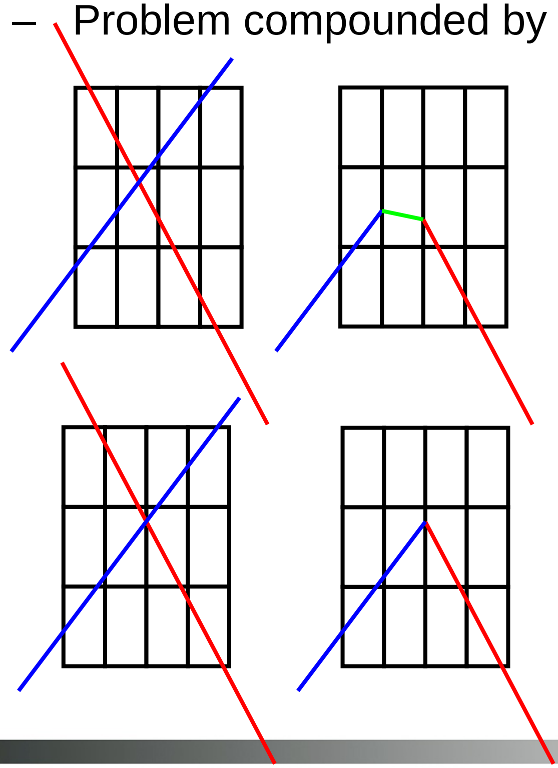




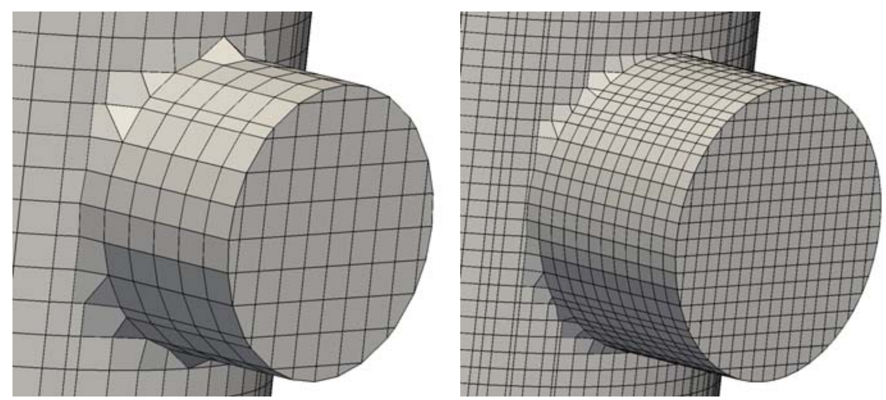
Cartesian-Grid Implementation

- **Limitations:**
  - In 3D, cut face can have between 3 and 6 vertices (visualization)
  - Intersection of quadrics not necessarily well represented
  - Only one cut-face per cell
  - Only one intersection point allowed on each edge
  - Adjusting grid possible only for simple 2D geometries
  - Problem compounded by staggered grid representation





3D cylinder-cylinder intersection



Coarse grid *Fine grid*

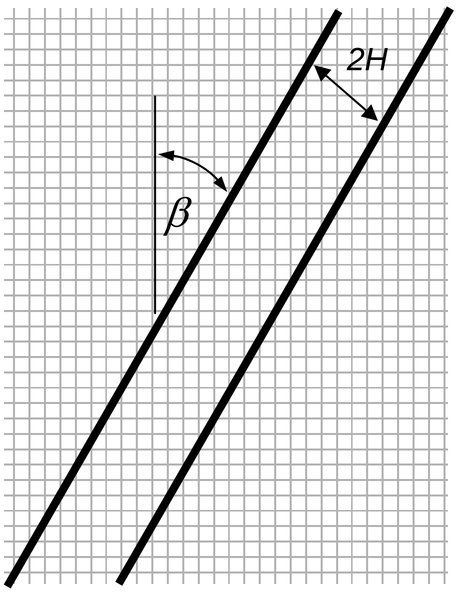
Cartesian-Grid Implementation

- **Cost of Cut-cell Method**
  - Preprocessing:
    - < 1 second for coarse 2D grid
    - ~ 1 minute for fine 3D grid
  - Post-processing:
    - Varies based on number of variables saved and frequency of file saving
    - << 1 second for coarse 2D grid
    - A few seconds for fine 3D grid

Geometry	Grid size	Number of cells	Standard cells	Cut cells	Blocked cells	Overhead	Overhead/ cut cell
2D	40x80	3200	71.50%	7.25%	21.25%	5.52%	0.75
3D	60x100x30	180000	9.55%	3.70%	86.75%	2.49%	0.67

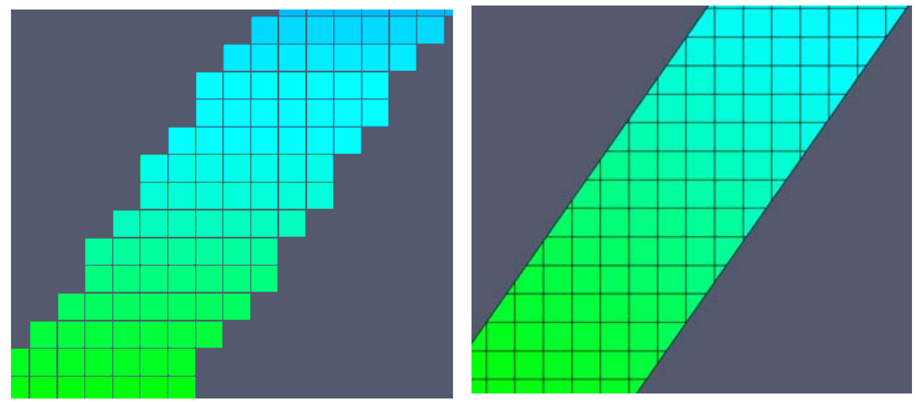
2D Single Phase Channel Flow

- **2D skewed channel flow**



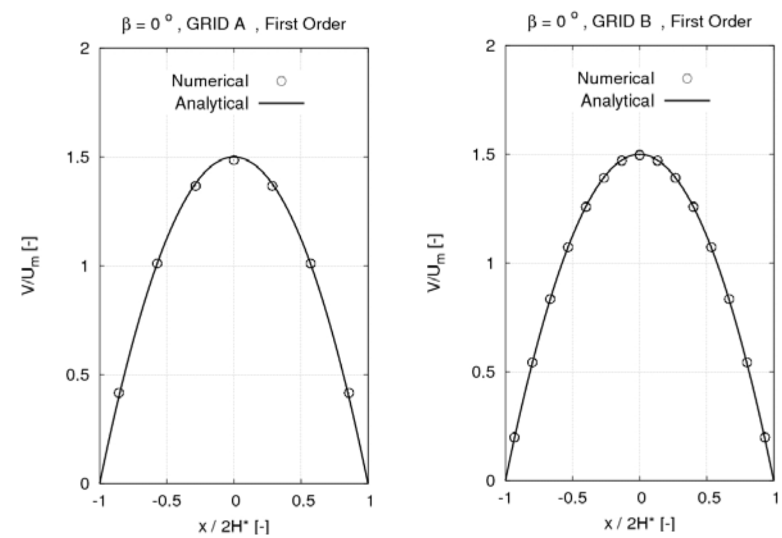
Parabolic velocity profile at Inlet

Staircase steps (β = 35 Deg) *Cut cells (β = 35 Deg)*



β = 0 Deg (channel aligned with grid):

20 velocity profiles extracted at constant y-values



GRID A: 7 Cells across channel (x-direction)

GRID B: 15 Cells across channel (x-direction)

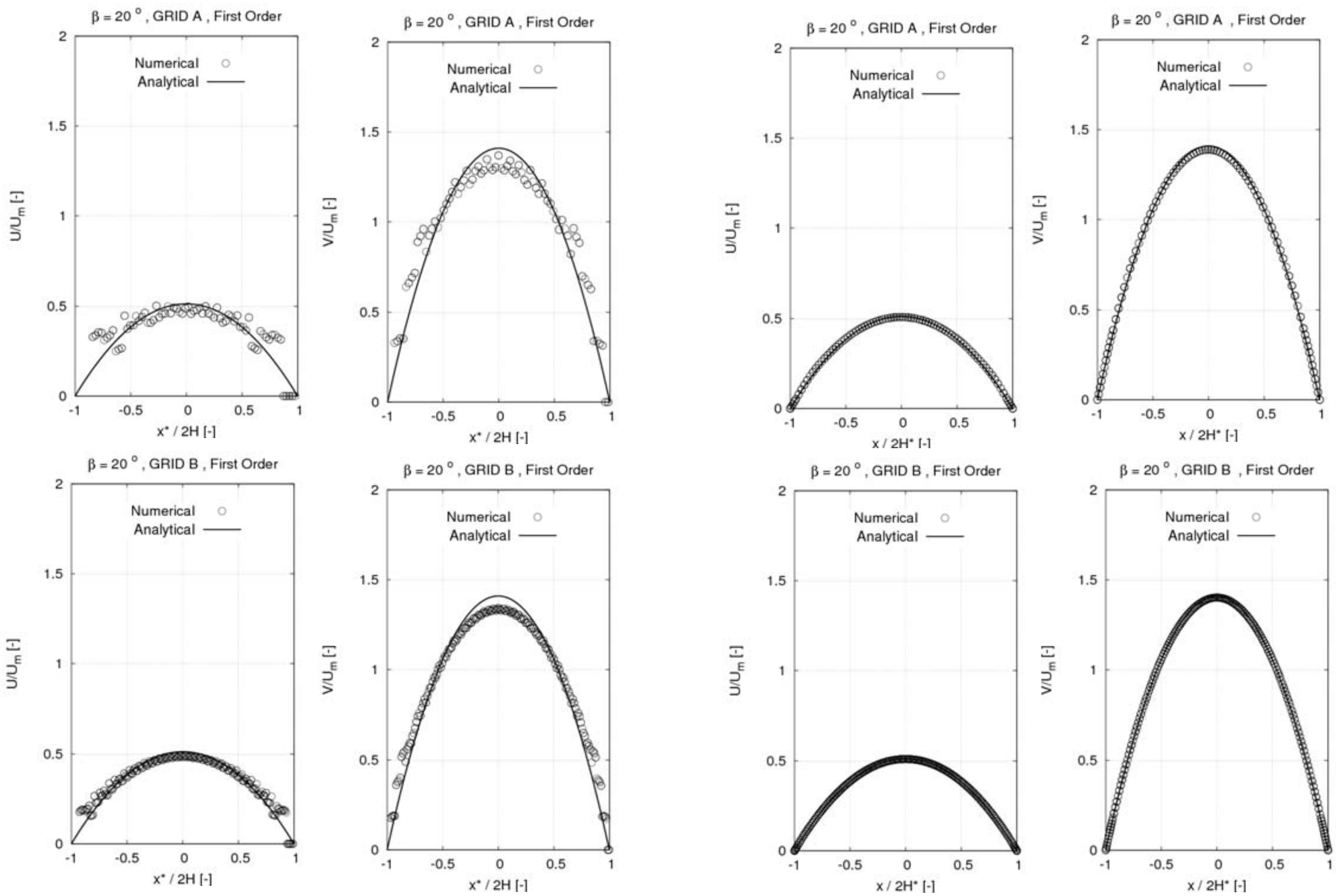
2D Single Phase Channel Flow

- **2D skewed channel flow, Re = 1, First Order**

Staircase ***Cut-cell***

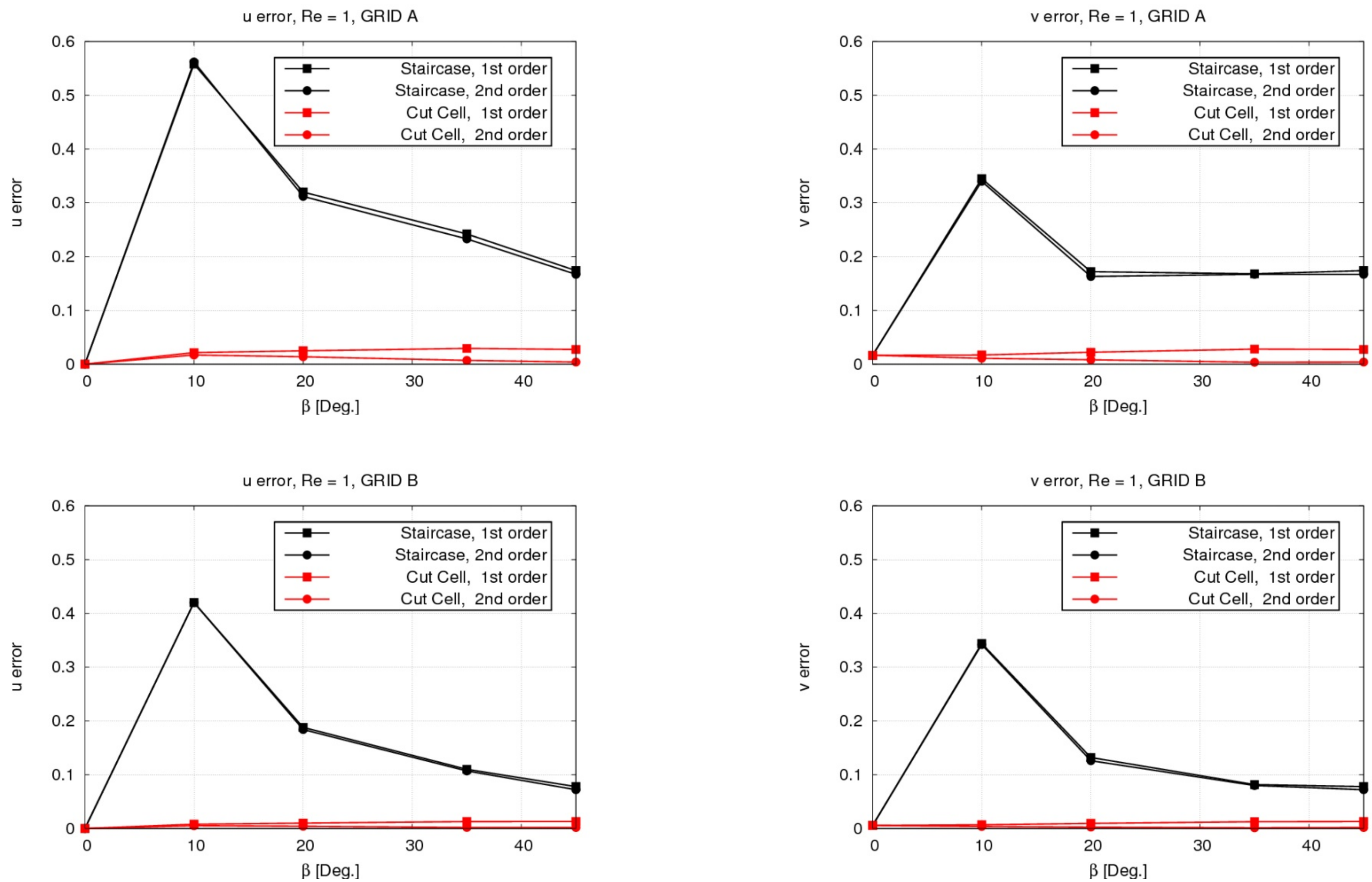
GRID A

GRID B



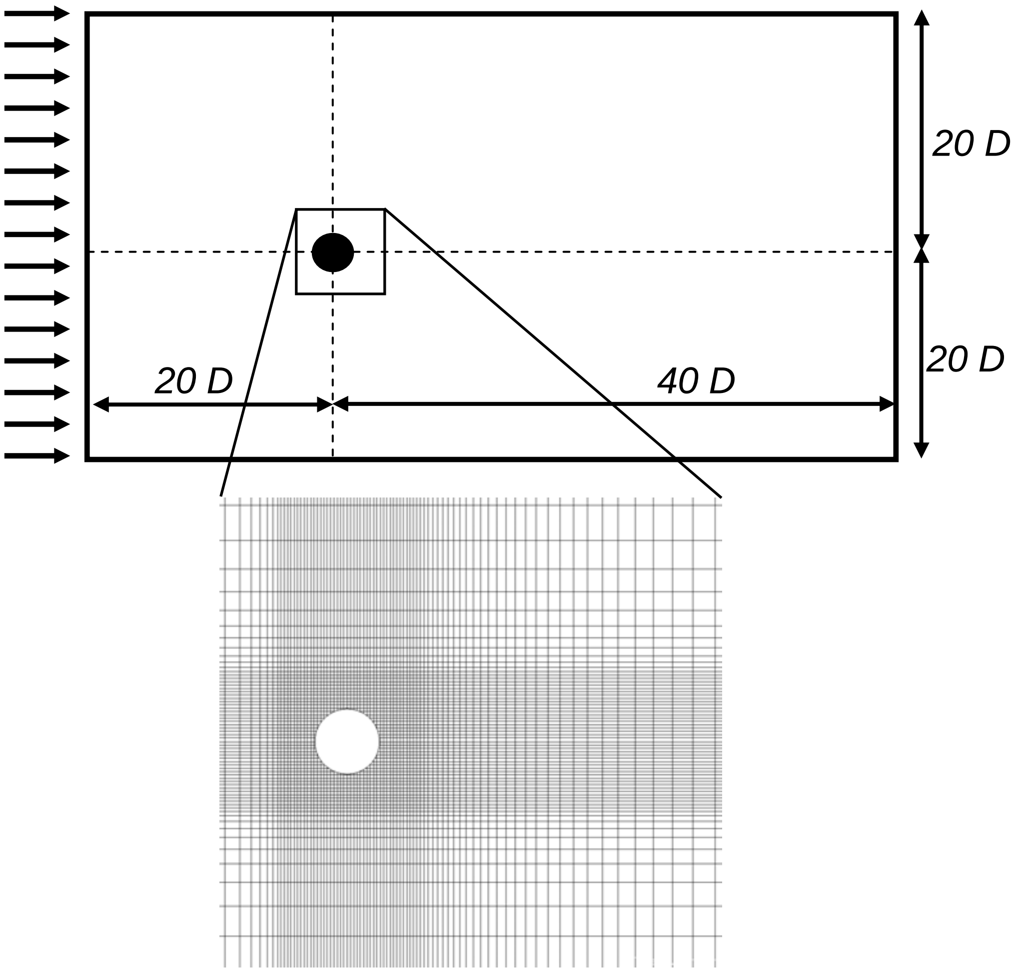
2D Single Phase Channel Flow

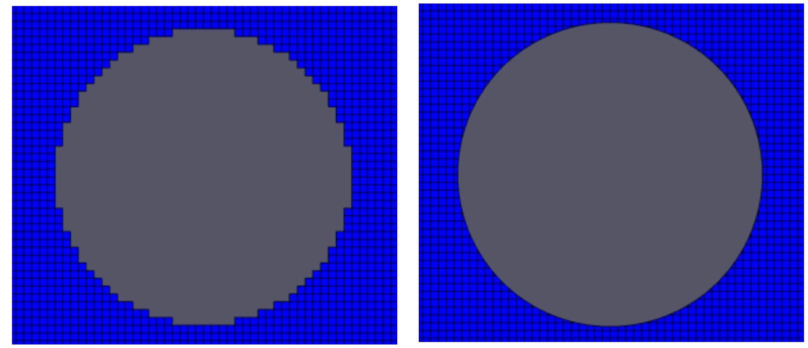
- **2D skewed channel flow, Re = 1 error**



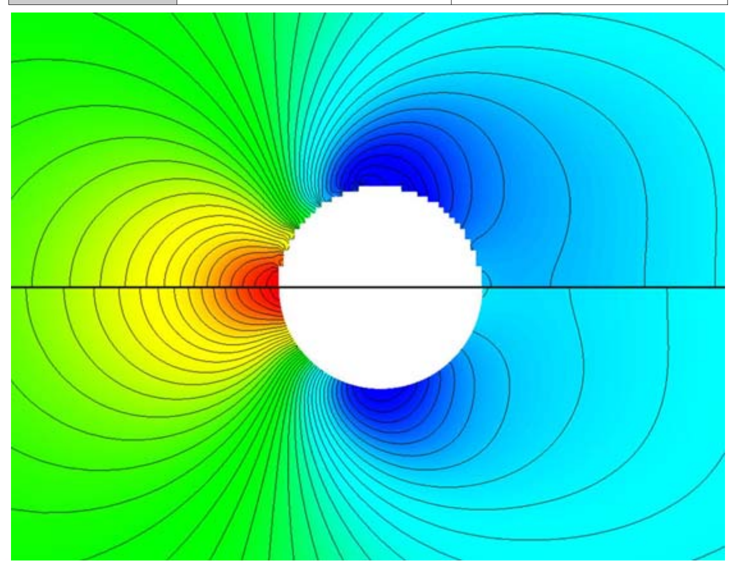
2D Single Phase Cylinder Flow

- **2D flow over a cylinder, Re = 40 (Steady case)**





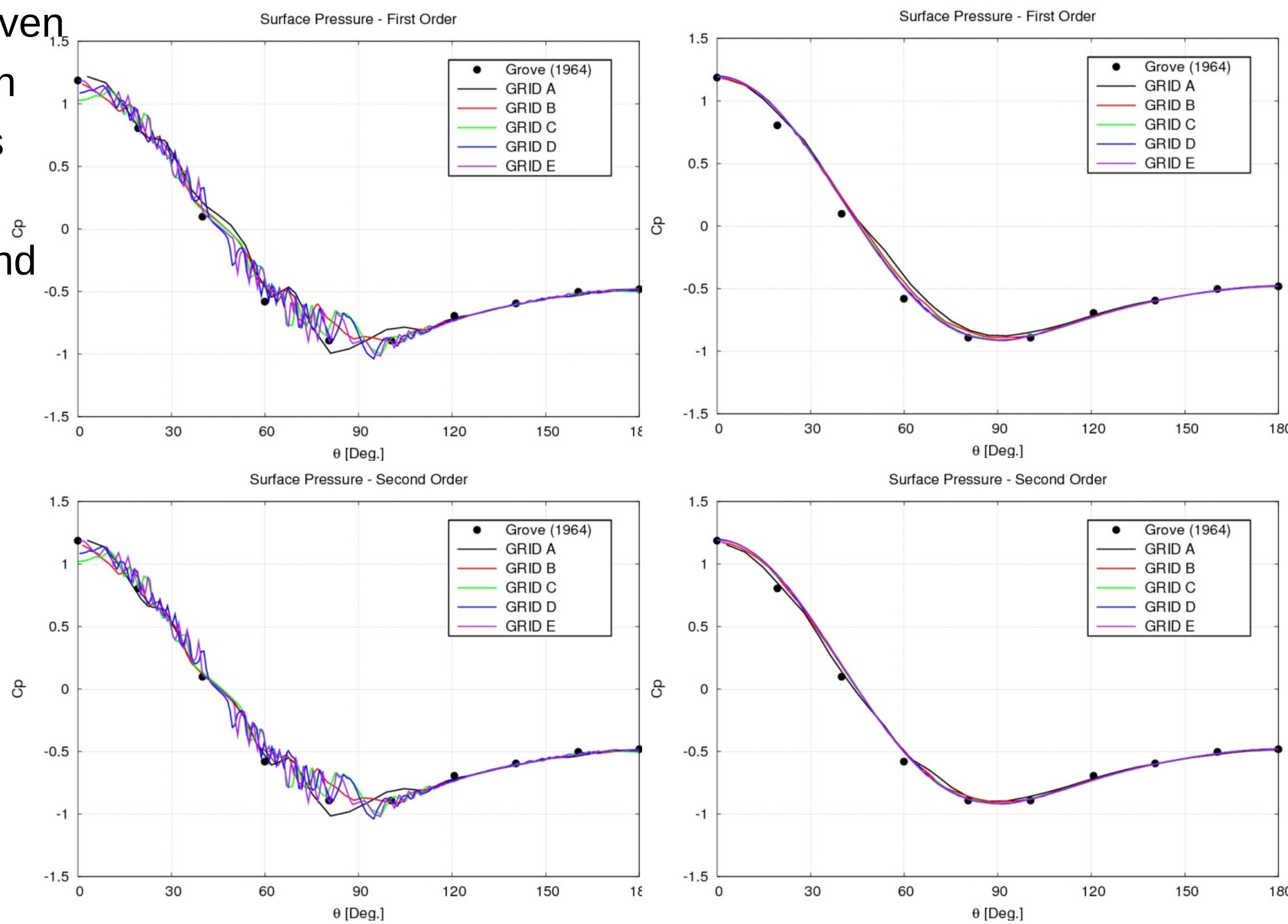
GRID	IMAX x JMAX	cells/diameter
A	120x80	20
B	200x140	40
C	320x240	80
D	420x320	120
E	520x420	160



2D Single Phase Cylinder Flow

- **Surface Pressure Distribution**
- General trend captured by Staircase method, even with coarse grid, with pressure oscillations
- Cut-cell technique provides accurate and smooth surface pressure distribution

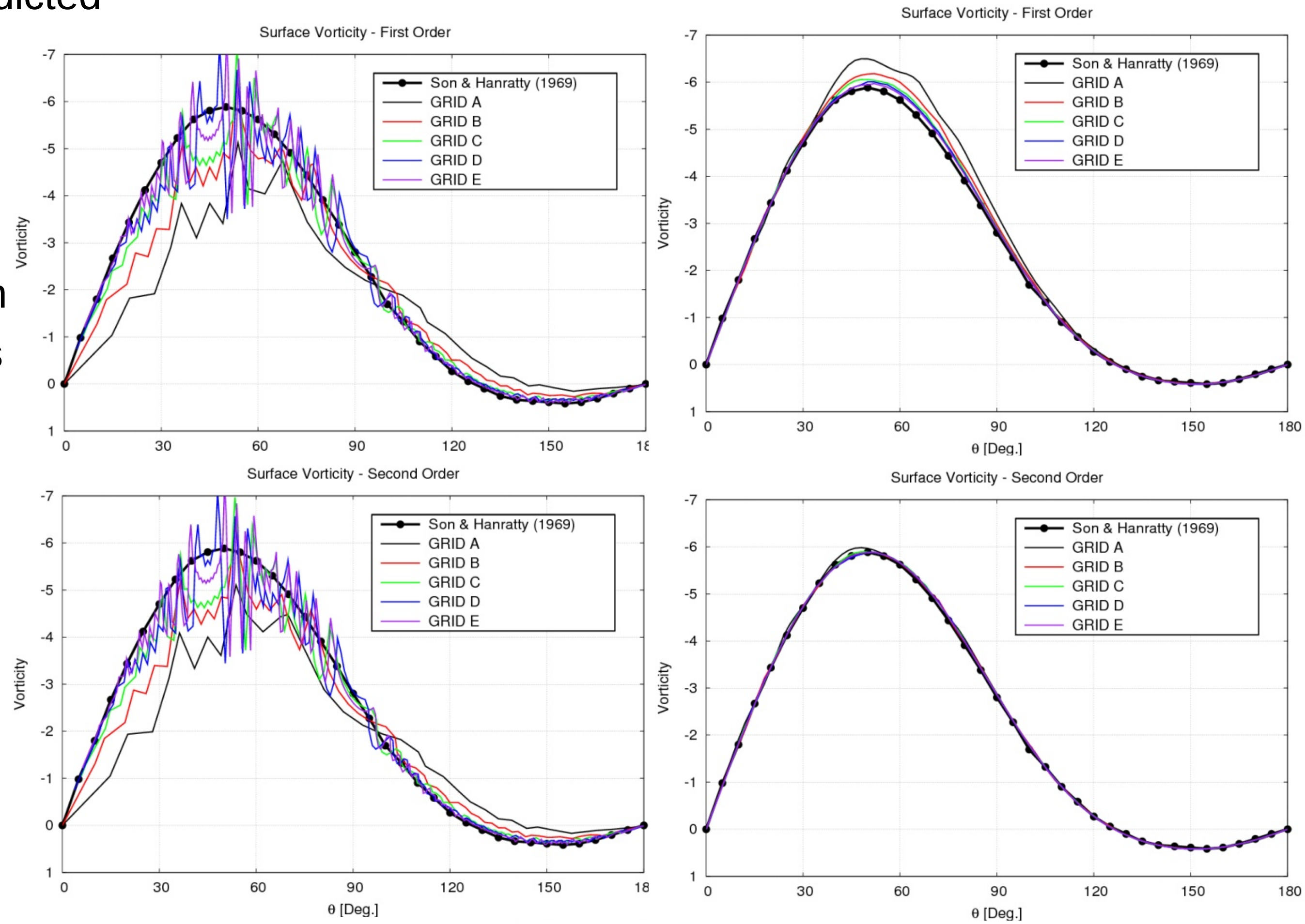
Staircase ***Cut-cell***



2D Single Phase Cylinder Flow

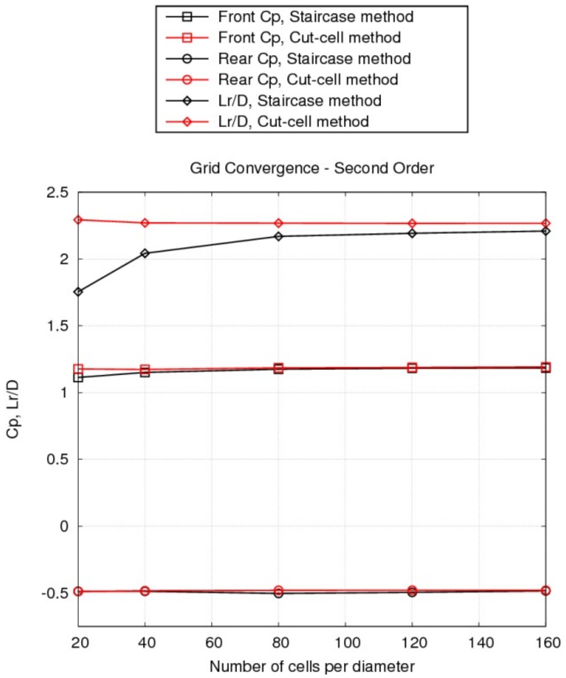
- **Surface Vorticity Distribution**
- Staircase:
  - Vorticity under-predicted with coarse grid.
  - Large oscillations even with fine grid
- Cut-cell :
  - Smooth distribution
  - Accuracy improves as grid is refined

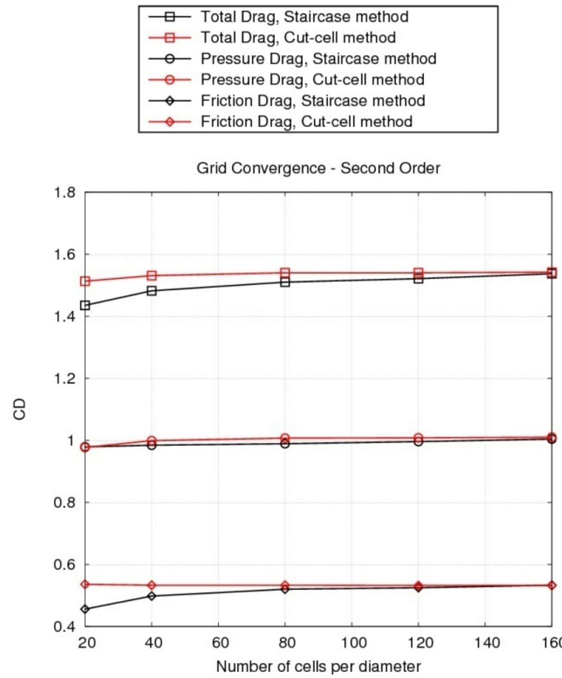
Staircase ***Cut-cell***

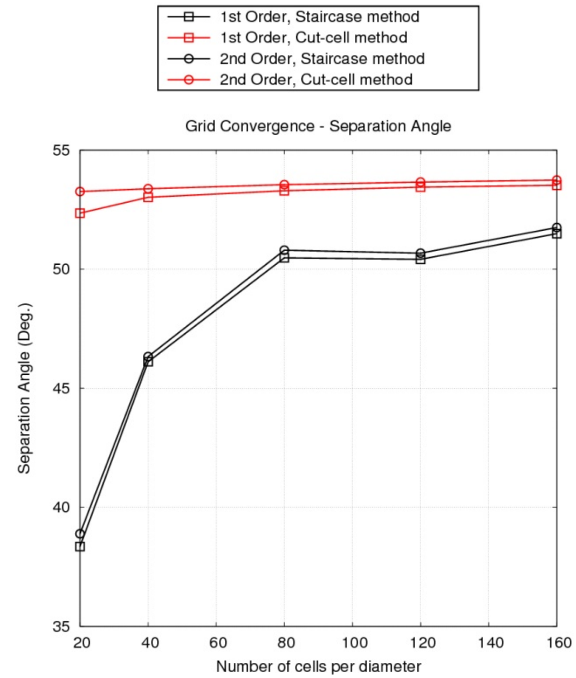


2D Single Phase Cylinder Flow

- **Grid Convergence Analysis**



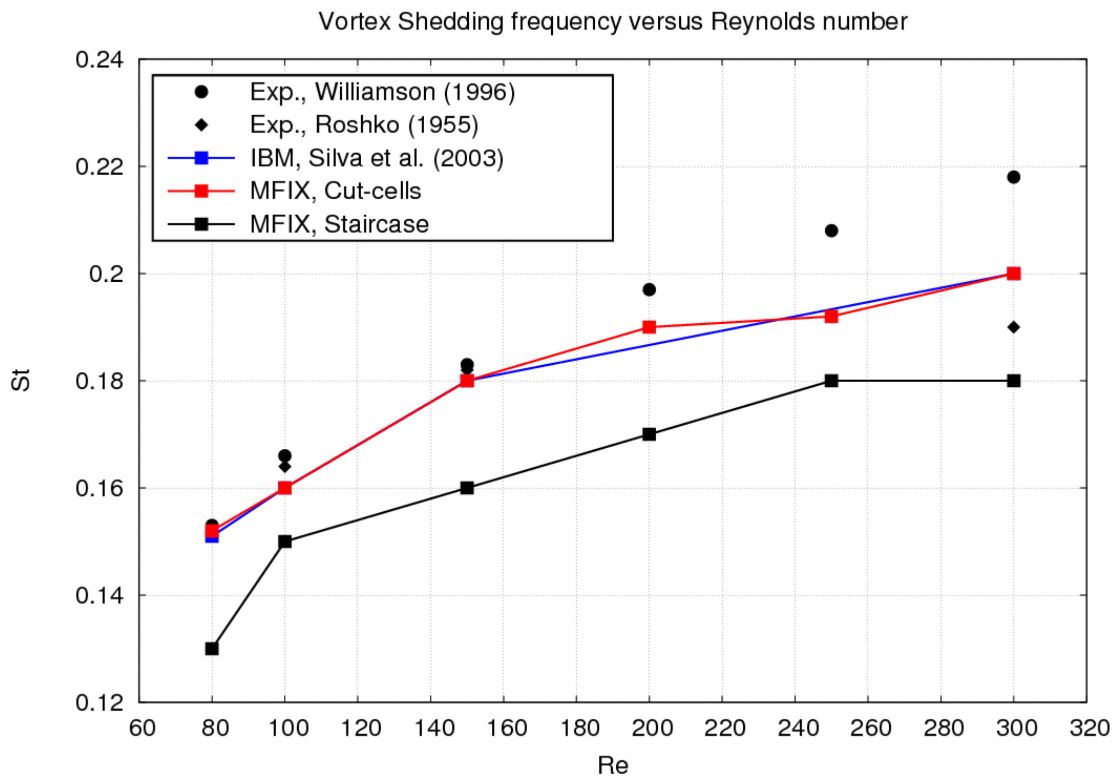


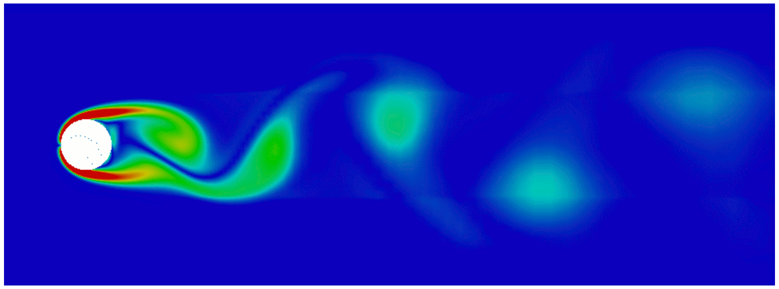


Author(s)	Method	CD	CD,P	CD,F	Front Cp	Rear Cp	Sep. Angle (Deg.)	Lr/D
Grove et al. (1963)	Experimental		0.935		1.190			
Takami & Keller (1969)	Numerical	1.536			1.141		53.55	2.35
Son & Hanratty (1969)	Numerical	1.510					53.90	
Dennis & Chang (1970)	Numerical	1.522	0.998	0.524	1.144		53.80	2.35
Collins & Dennis (1973)	Numerical	1.560					53.60	2.15
Dennis (1973)	Numerical	1.494			1.142			
Nieuwstadt & Keller (1973)	Numerical	1.550			1.120		53.34	2.18
Fornberg (1980)	Numerical	1.498			1.140		55.00	2.24
Kirkpatrick et al. (2003)	Numerical	1.535			1.0 *		53.55	2.26
MFIX, Staircase, GRID E, 2^{nd} Order	Numerical	1.537	1.004	0.533	1.184	-0.484	51.75	2.21
MFIX, Cut Cell, GRID E, 2^{nd} Order	Numerical	1.542	1.010	0.532	1.192	-0.480	53.74	2.27

2D Single Phase Cylinder Flow

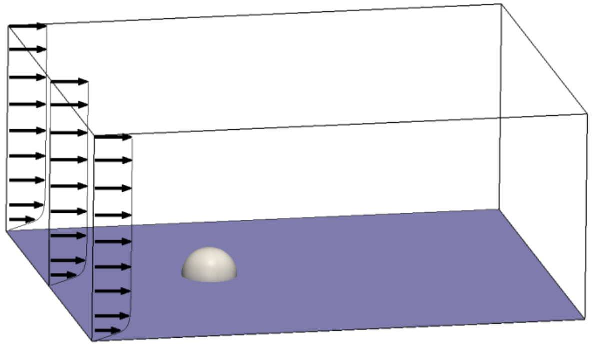
- **2D flow over a cylinder, Re = 80 to 300 (Unsteady case)**
  - Staircase method tends to under-predict vortex shedding frequency
  - Cut cell technique compares well to experimental data, and results obtained by Immersed Boundary Method (Silva et al., 2003)

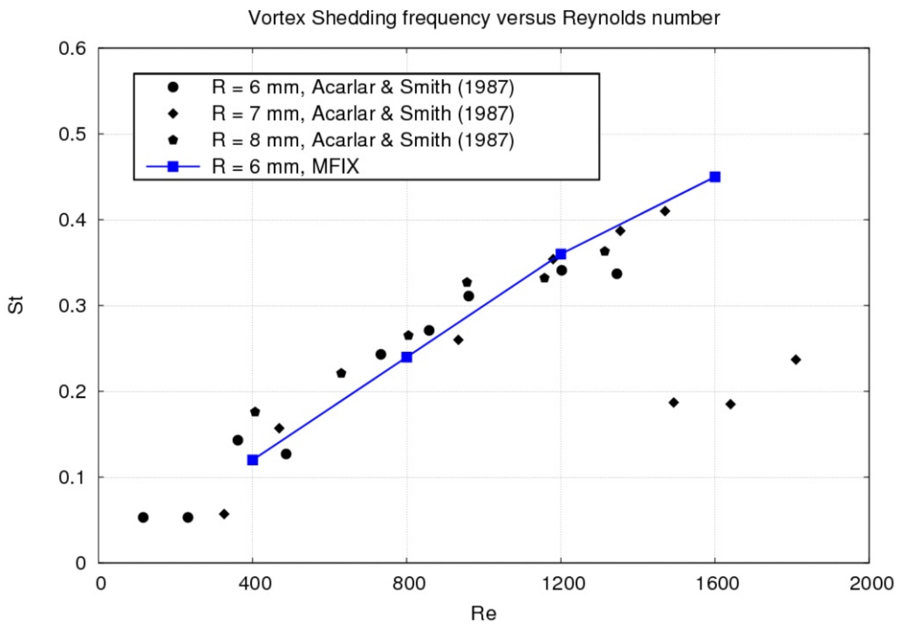


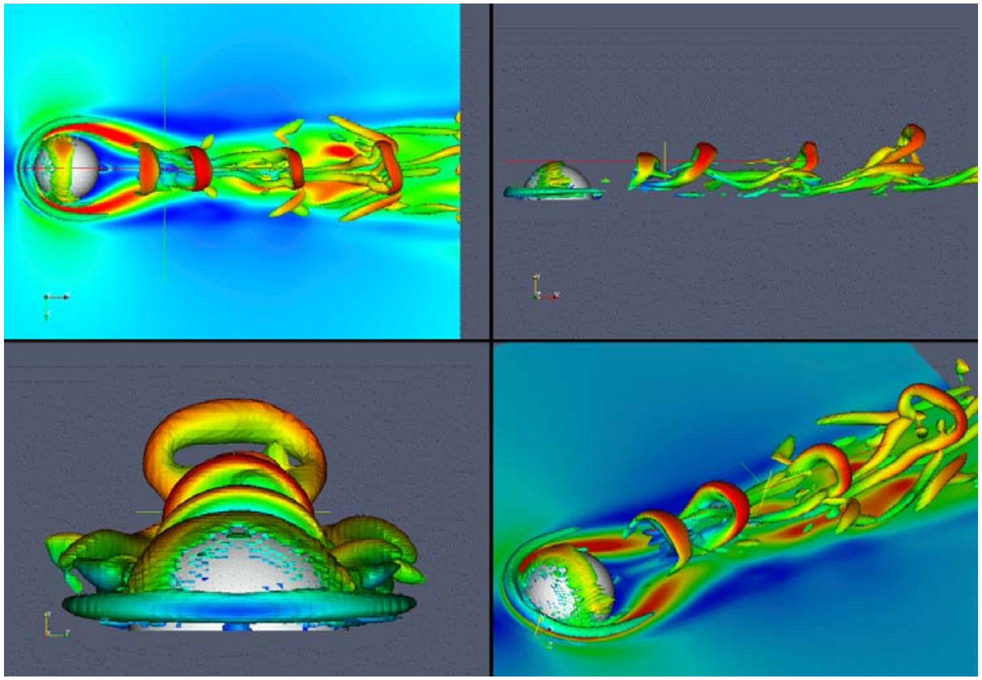


3D Single Phase Hemisphere Flow

- **Formation of Hairpin Vortices over a Hemispheric protuberance (Gas phase only)**
- Incoming laminar BL
- Grid size = 500,000 cells, 30 cells per diameter
- Hairpin vortices are captured
- Vortex shedding frequency compares well with experimental data

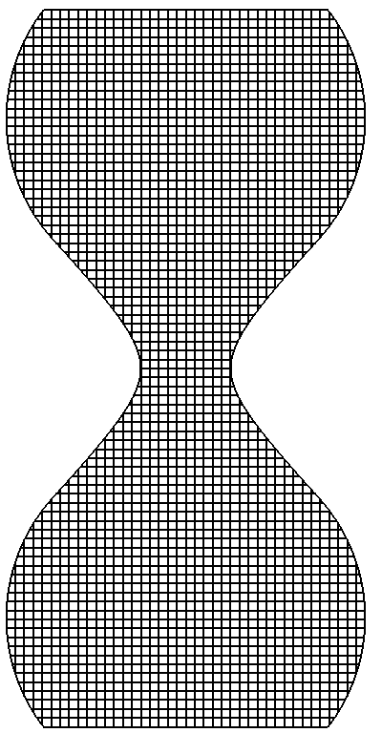


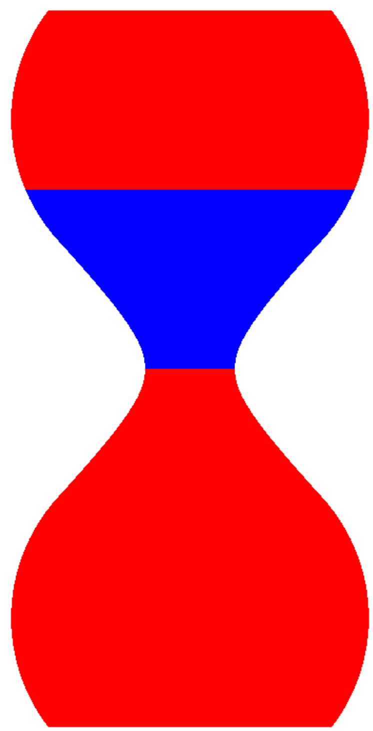


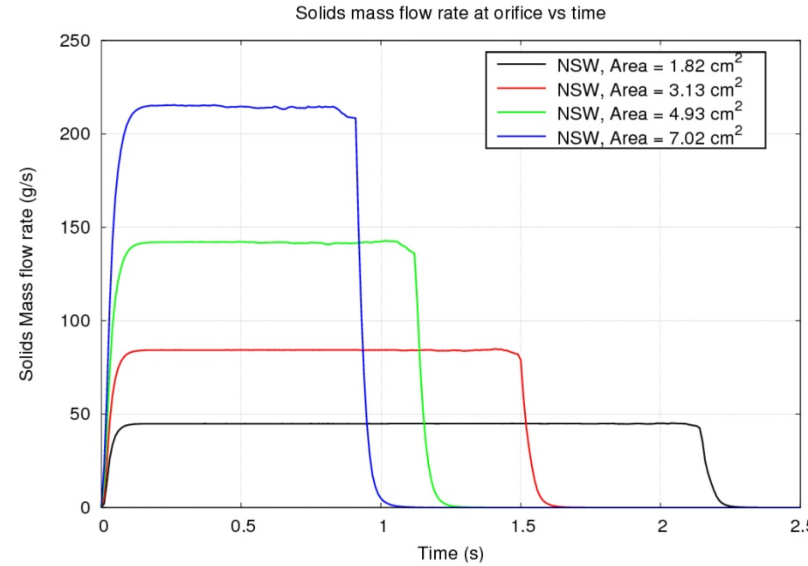


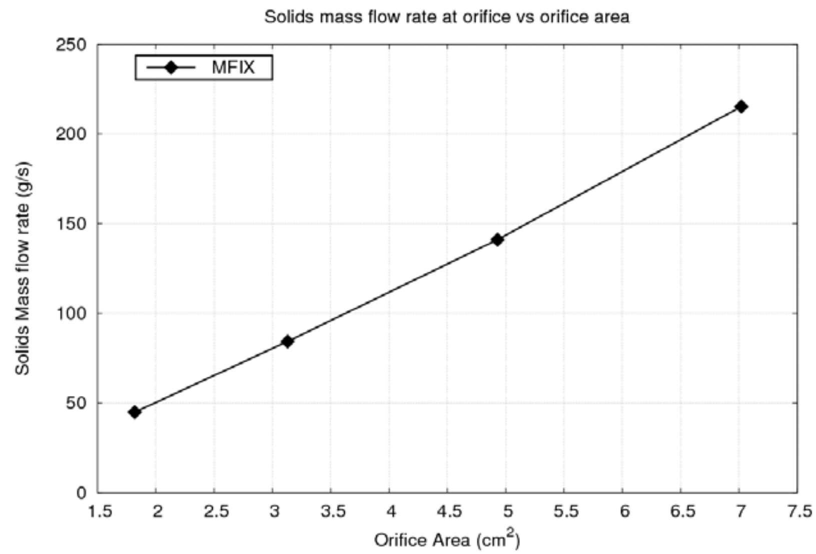
2D Gas/Solids Phase Flow

- **2D Hourglass flow**
  - Coarse grid (40x80)
  - Geometry represented by 3 quadrics
  - Proper behavior observed



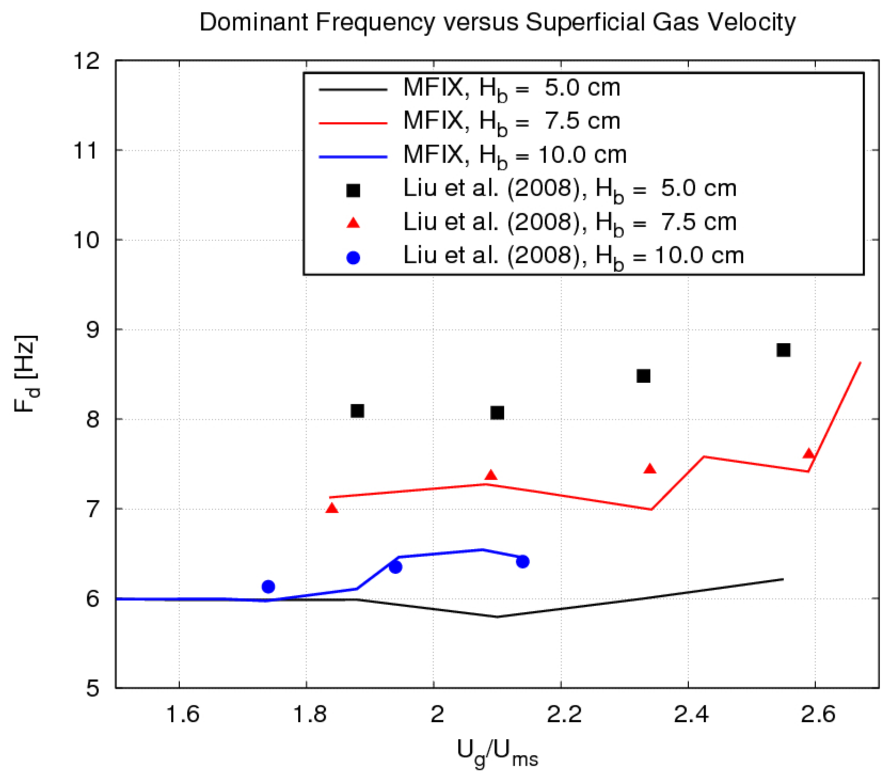


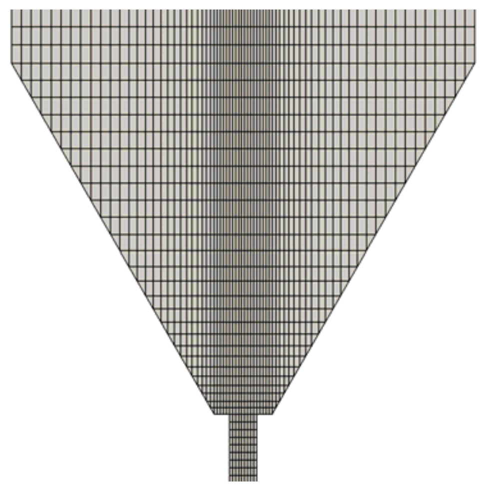


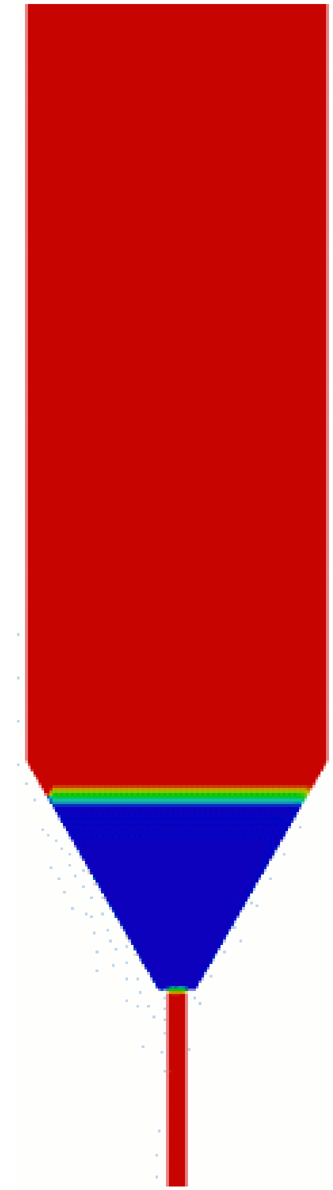


2D Gas/Solids Phase Flow

- **2D Spouted bed**
  - Grid size = 71x108
  - Ratio width / depth = 10
  - Dominant frequency well predicted for Hb =7.5 and 10.0 cm



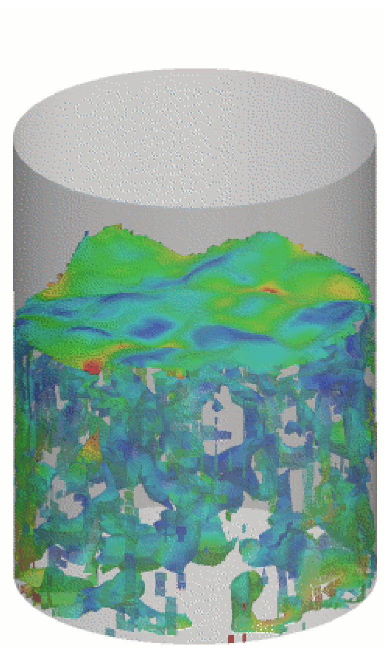


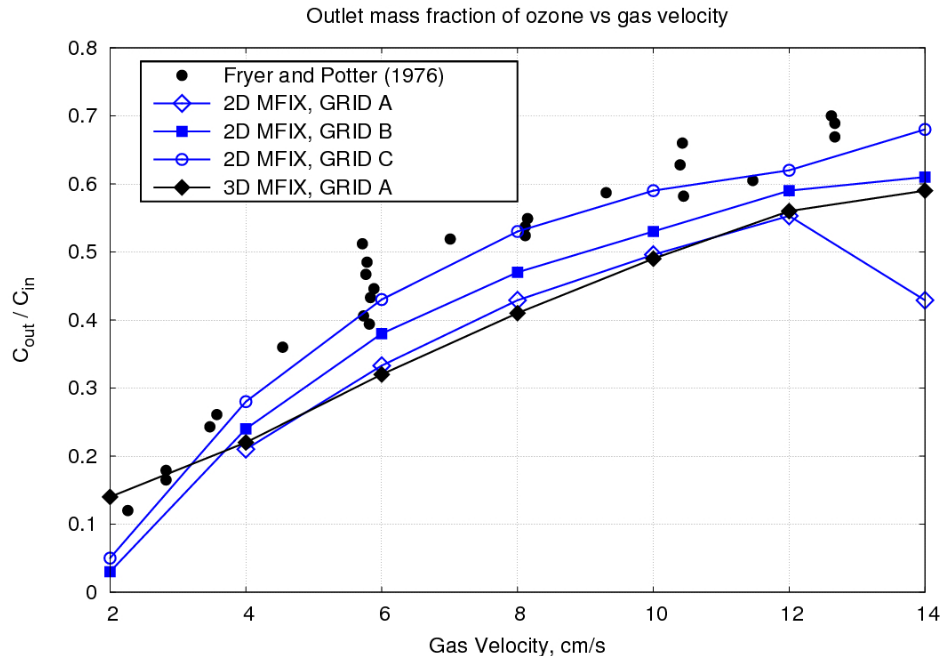


3D Gas/Solids Phase Flow

- **3D Ozone decomposition**
  - Simple 3D geometry (cylinder)
  - Second order spatial discretization
  - O3 mass fraction at inlet = 0.1 (O3 – air mixture)
  - Full 3D simulation gives similar results to 2D-axisymmetric simulation, with better prediction for smallest and largest superficial velocities
  - Simulation with finer grid under way

GRID	2D Axisymmetric	3D
A	18 x 56	36 x 56 x 36
B	36 x 56 *	
C	72 x 112 *	

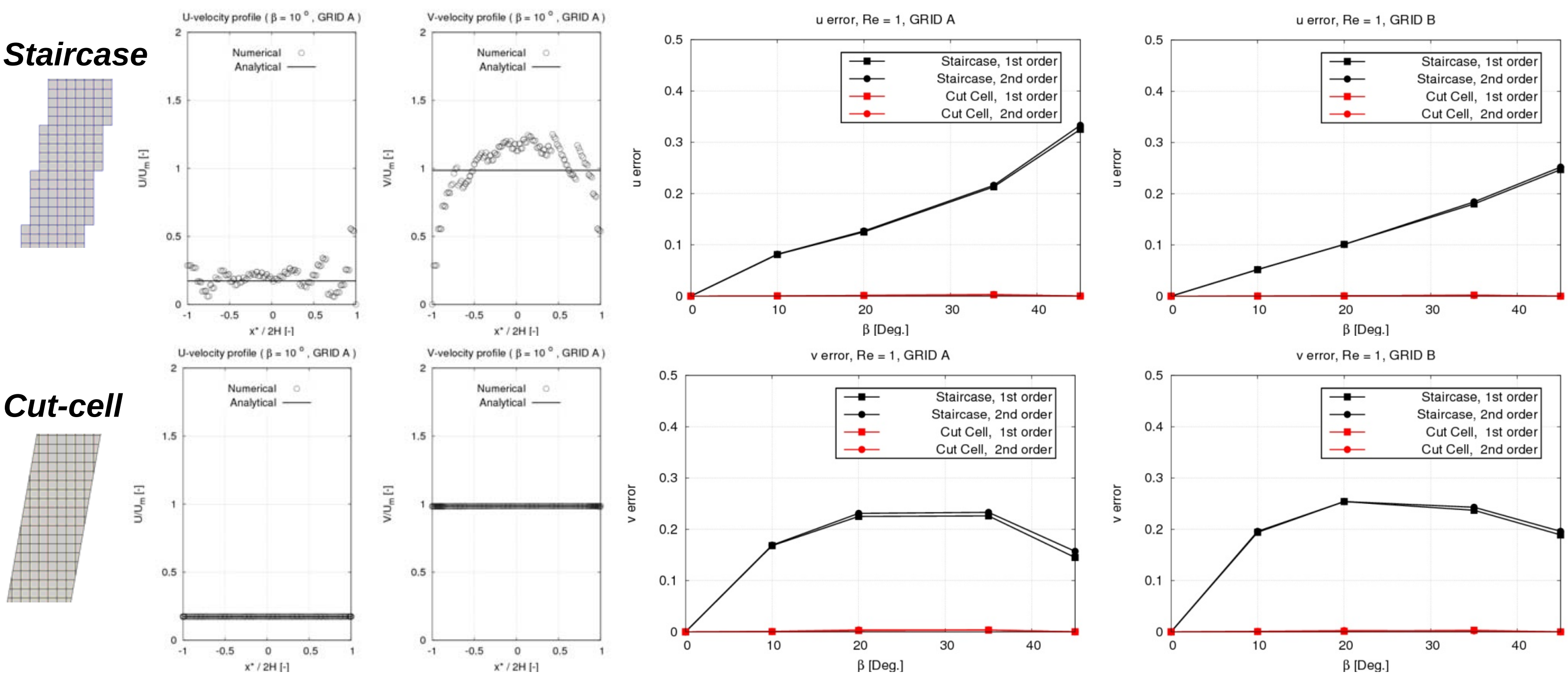




** From "Fluid Dynamic Simulation of O3 Decomposition in a Bubbling Fluidized Bed", Syamlal, M., and O'Brien, T.J., AIChe Journal, Vol. 49, No 11 (2003)*

Latest Additions

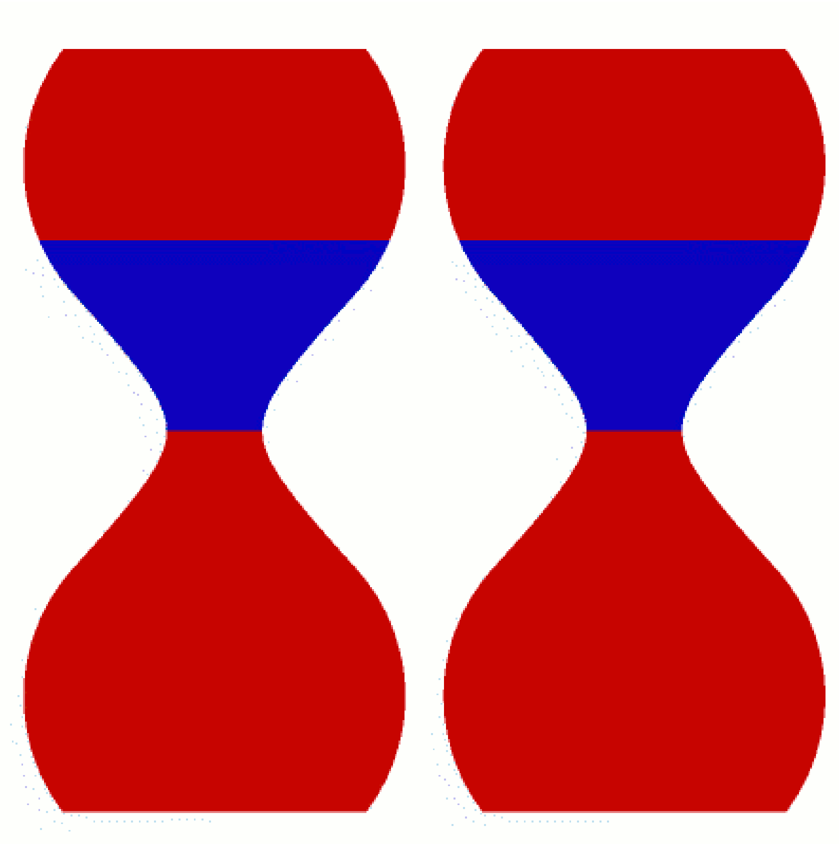
- **Free-slip boundary conditions**
  - All terms implying zero velocity at wall are turned off (e.g, $\alpha_e = 0$)
  - **2D Channel flow** (Gas phase only): Cut cell technique shows clear improvement over the staircase representation for coarse and fine grid



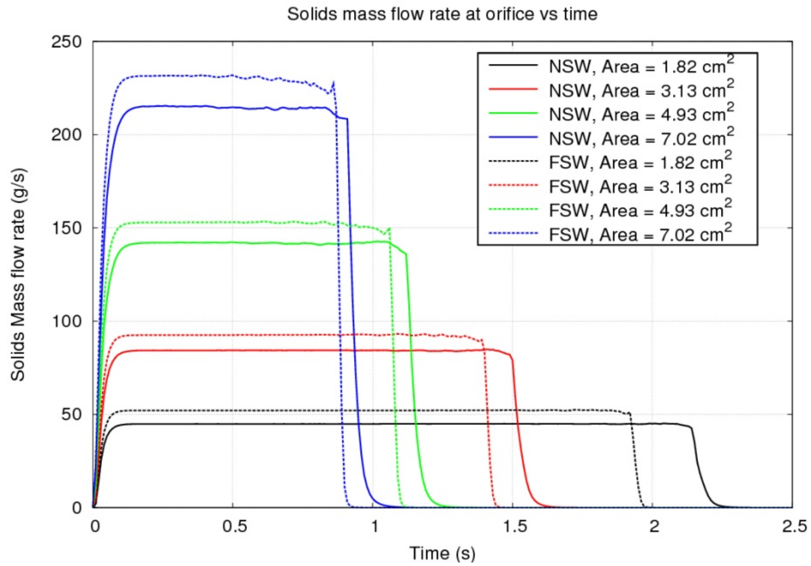
Latest Additions

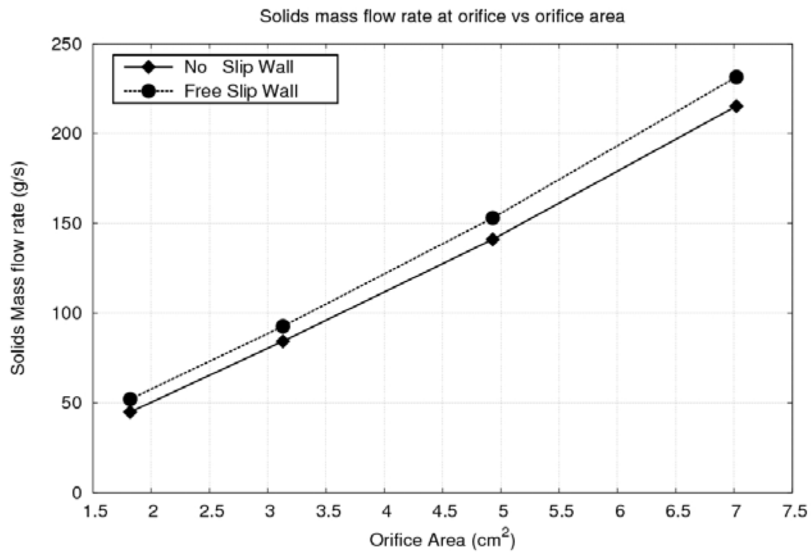
- **Free-slip boundary conditions**
  - **2D Hourglass flow:**

    Solids mass flow rate larger than with NSW



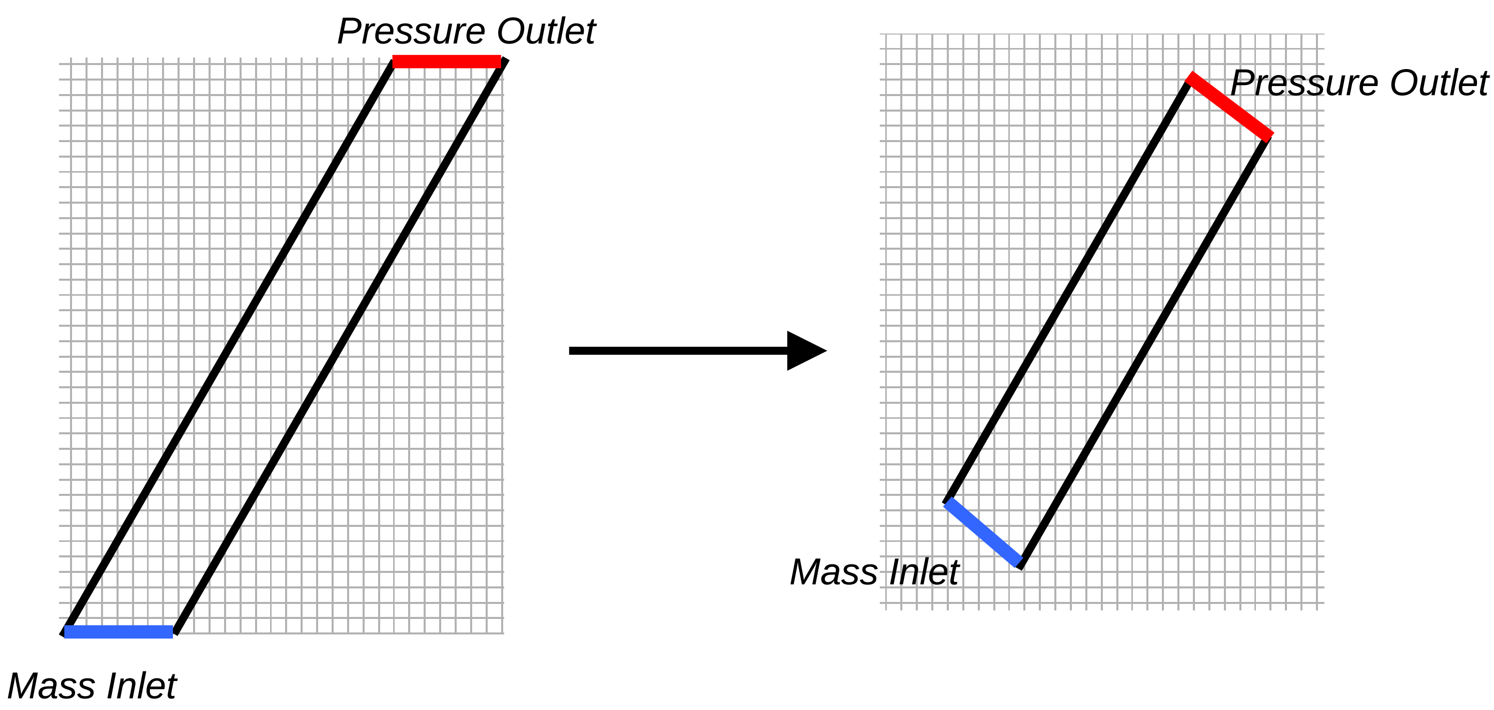
No-Slip Wall *Free-Slip Wall*





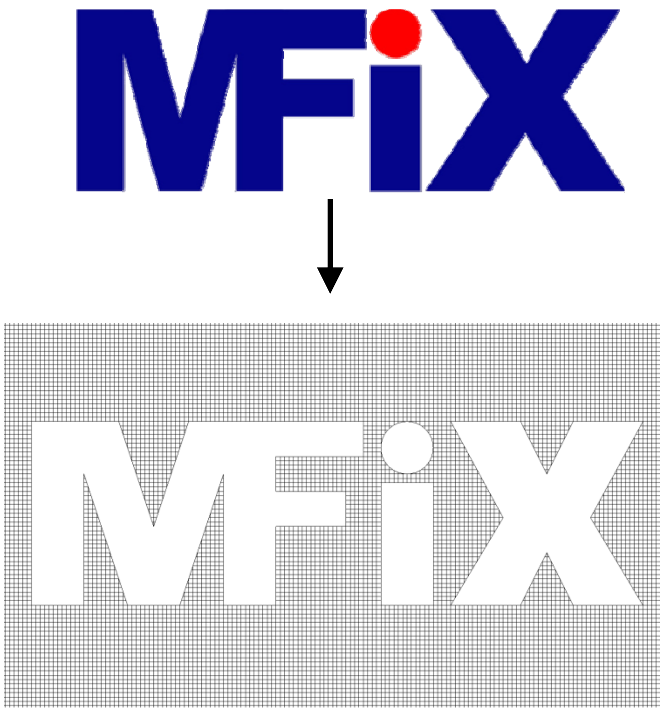
Latest Additions

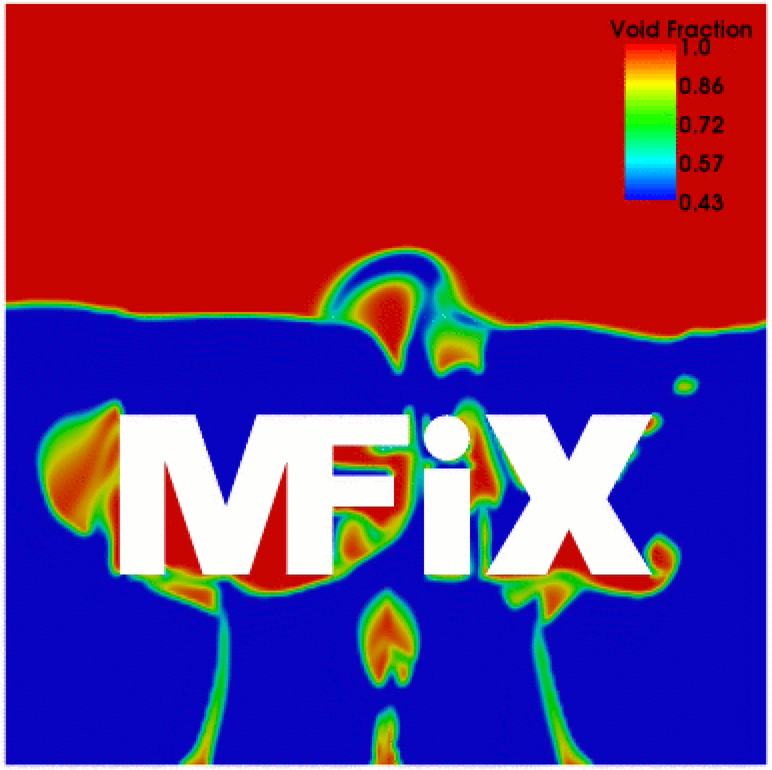
- **Other boundary conditions (in progress)**
  - Mass Inflow (MI) and Pressure Outflow (PO) boundary conditions can be specified along quadric surfaces (2D and 3D)
  - Less stable than original MFIX BC's for PO (Gas/ Solids phase)



Latest Additions

- **Boundary Geometry**
  - Boundary geometry can be specified from:
    - Quadric surfaces (2D and 3D), with intersections
    - User-defined function (2D and 3D)
    - A series of vertices defining a polygon (2D only)





Conclusions

- Successful Implementation of Cartesian grid Cut-cell technique into MFIX
- Method tested for:
  - Internal flow
  - External flow
  - Single phase
  - Gas/solids phase

- The 3 steps (Preprocessing, flow solution, post-processing) are efficient

- Future work (short term):
  - Parallelization of the code
  - Partial slip boundary conditions
  - Remove the dead cells and perhaps use a space-filling curve to index the cells

- Future work (long term):
  - Ability to define boundaries using surface triangulations
  - Ability to accept mesh information from an external Mesh generator such as Gambit
  - Hanging-nodes
  - Adaptive mesh refinement
  - Moving boundaries and immersed objects