

# **Study of Pollutant Dispersion in Urban Environments**

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## **Abstract**

Computational simulations can aid in understanding the complex flows of environmental interests such as the pollutant/chemical dispersion in the urban cityscapes. Computational fluid dynamics (CFD) represents the study of fluid mechanics with the use of computer models and simulations. In this study the simulations of the complex flows involved are created using an open-source parallel CFD framework (the Cactus CFD toolkit). The Cactus CFD toolkit is an open-source problem solving environment for a variety of interdisciplinary fluid dynamics applications.

Specific contributions of this research study have been the implementation of Marker and Cell (MAC) method for the governing equations, transport of passive scalars like the pollutant concentration and the use case definitions for the pollution dispersion problems.

Canonical flows such as jets-in-crossflow (JICF) and flow past obstacles form the physical as well as modeling building-blocks for our application. JICF from elevated sources is used as the model for pollutant release. Flow past an arrangement of obstacles is used as the model for the urban cityscape. Results from these simulations will be presented to elucidate the complex flow physics relevant to the respective problems. Pollutant dispersion in the urban canyon encapsulates all of these complexities as well as their interplay.

**Key words: Pollutant Dispersion, CFD , CACTUS, JICF**

# **1 Introduction**

## **1.1 pollutant dispersion**

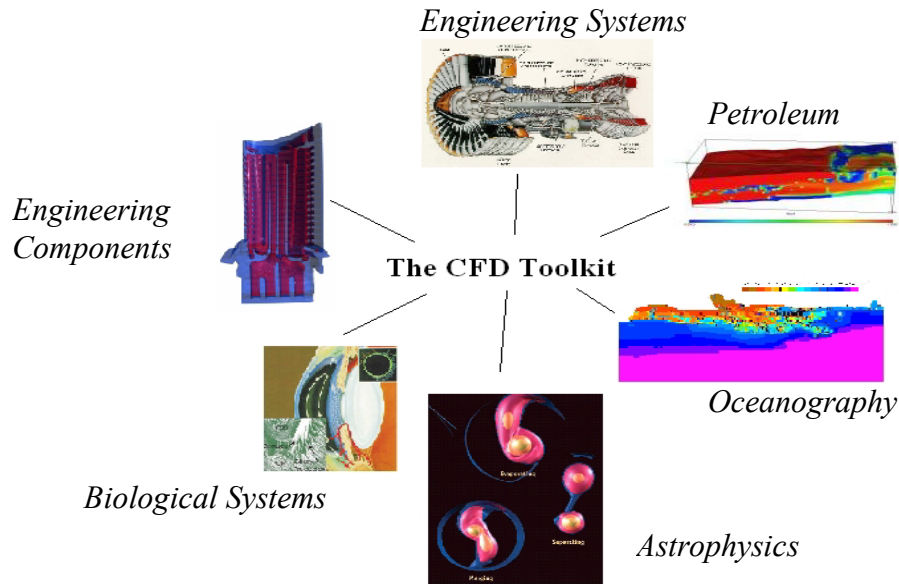
Since the advent of the industrial revolution mankind has started using and creating many compounds that have disturbed the ecological balance of our planet. Some of these compounds are required for the creation of daily life products. A thermal power plant using coal releases great amounts of harmful gases to produce the electric energy that is essential for many day-to-day uses. At times these pollutants are released accidentally such as an oil spill from an oil tanker offshore. Within these contexts reliable predictions of the dispersion of fluids that could represent chemical or pollutant substances within our environment is very important and computer based simulations offer fast, economic solutions rather than experimental simulations. Some extreme events (e.g. accidents and terrorist attacks) are beyond the capabilities of experimental methodologies. Computational fluid dynamics (CFD) offers a reliable and economic solution for planning in such scenarios [2-6, 8-9].

## **1.2 cactus**

Cactus [1] is an open-source, scalable, portable, modular framework for numerically solving partial differential equations on high performance computing (HPC) platforms. Cactus is continually developed at the Center for Computation and Technology (CCT), Louisiana State University (LSU) and at Albert Einstein Institute (AEI). Cactus consists of two parts the “flesh” and “thorns”. The “flesh” offers no true functionality but serves to better integrate and facilitate the interaction between the different components constituting the computational environment. The “thorns” are modules that represent the functional part of Cactus and provide the code that performs the simulation. For example the thorn “CFDConvec” calculates the convective terms in the Navier-Stokes momentum equation (the governing equations for fluid momentum) that are then used by the “CFDEvolver” thorn for evolving the computational fields. Thorns are often categorized into groups called arrangements based on their functionality or on their relation with other thorns, e.g. the CactusBase arrangement offers the basic operation thorns or CactusIO which offers input/output thorns. Cactus flesh can orchestrate a parallel program composed using thorns that is portable across HPC platforms. Cactus is collaboratively used by more than a dozen research groups worldwide (LSU, AEI, Cardiff, GSFC, MPA, Pittsburgh, PSU, Sissa, Soton, UTB, TAT, Thessaloniki, WashU) and continues to be actively developed by a wide community. Implementation of the transport equations relevant to a variety of interdisciplinary applications is being pursued in the Cactus CFD Toolkit project.

### 1.3 CFD

Computational Fluid Dynamics (CFD) is the study of fluid flow phenomena using the computer simulations. A CFD simulation needs the underlying flow description (single or multi phase, compressible or incompressible, laminar or turbulent etc.) using corresponding governing equations, the method of discretizing the individual terms in these equations, solution algorithms and the description of the computational domain discretization (computational mesh). Each one of these components has advanced and CFD has evolved over the several decades into a mature and reliable methodology that is able to handle the multitude of fluid dynamics applications. At LSU, an ongoing IGERT program [7] that addresses applications ranging from flow in the human eye to the evolution of binary stars has been a motivation for the development of an interdisciplinary CFD problem solving environment.



**Fig.1 Various CFD areas of interest for the CFD toolkit (Courtesy IGERT Team at LSU)**

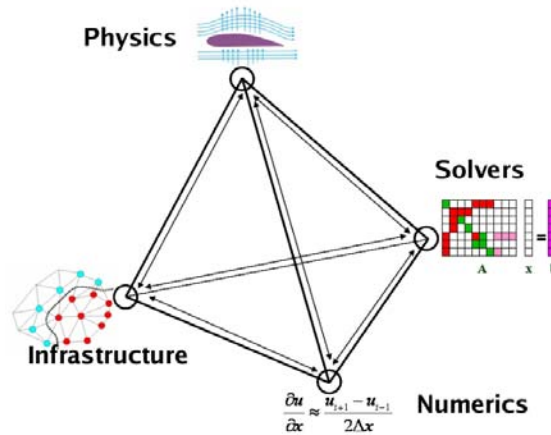
The Navier-Stokes equations represent the governing equations for momentum conservation of a Newtonian fluid. These equations are considered to be valid for a wide variety of fluid flow phenomena and will also be used in this research study.

$$\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = \rho f_i - \frac{\partial P}{\partial x_i} + \mu \left( \frac{\partial^2 u_i}{\partial x_j^2} + \frac{1}{3} \frac{\partial^2 u_j}{\partial x_i \partial x_j} \right)$$

where  $u_i, P, \rho, \mu, f_i, t, x_i$  represent the fluid velocity, pressure field, density, viscosity, body forces, time and spatial dimensions respectively. The numerical discretization of the individual terms in the governing equations and the domain discretization is usually linked and exploited to design efficient and robust flow solvers (section 2).

## 1.4 Cactus CFD toolkit

The Cactus CFD Toolkit is an ongoing research project at the Center for Computation and Technology at Louisiana State University to create a problem solving environment to tackle the multitude of CFD problems in a way that is open-source, portable, scalable and will work on the next generation of High Performance Computing platforms.



*Fig.2 A conceptual view at the design of the Cactus CFD Toolkit*

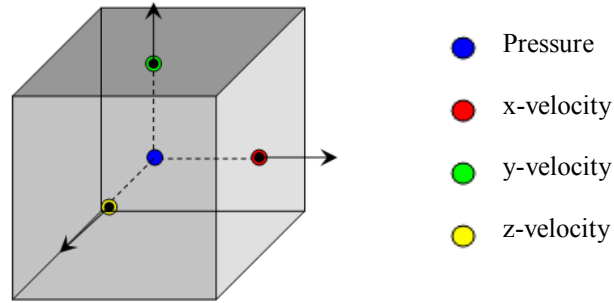
With these goals in mind the Cactus CFD Toolkit is created to take advantage of the capabilities of Cactus and create a modular design with the four main modules: Physics, Infrastructure, Solvers and Numerics. Cactus allows for each of these parts to be written into plug-and-play thorns which in turn allow for the problems to be varied with extreme ease just by changing the relevant thorns. Similarly, using a few parameters the accuracy of a method could be varied or a new method added to do the discretization. Several bench mark problems as well as complex challenging problems are currently being used to verify, validate as well demonstrate the potential of this tool.

## 2 Methodology

### 2.1 Domain discretization

For all the computational simulations in this research study, the domain of interest is represented by Cartesian meshes. Cartesian meshes are collection of cubical (or hexahedral) cells. In collocated approach, all the sought variables are stored at the center of the cell. While this discretization is simple to implement, it poses certain problems such as velocity and pressure de-coupling. In order to get a correct estimate for the flow flux into the cell velocity values have to be interpolated onto the cell faces and this requires the use of more grid points when calculating second or higher order accurate approximations for convection terms. Another method of discretizing

that alleviates the de-coupling problem is the Marker and Cell (MAC) method. This method places the velocity values of the faces of the computational cell and the pressure at the center of the cell.



*fig.3 Schematic of the MAC cell*

For single-phase fluid flow problems, the Navier-Stokes equations are used for the simulation. The flow speeds of fluids in urban canyons allows us to simplify these governing equations by assuming that the fluid is incompressible and simplifying the governing equations.

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\text{Re}} \frac{\partial^2 u_i}{\partial x_j^2}$$

where Re is the non-dimensional Reynolds number based on the characteristic fluid velocity and length scale which for this prototype simulation was set to a relatively low value of 100 to maintain laminar flow. The evolution of pollutant concentration field ( $\Phi$ ) is calculated by treating the concentration as a passive scalar field [10].

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = \frac{1}{\text{Sc Re}} \frac{\partial^2 \phi}{\partial x_j^2}$$

## 2.2 Boundary conditions

The boundary conditions are used to specify the conditions at the inflow/outflow around the computational domain or represent the vicinity of a bluff body wall (such as building facades). These boundary conditions along with the governing equations define a well-posed problem. For example, in this research study inflow boundary condition is used at the entrance of the computational domain along the flow direction, and outflow boundary condition at the computational domain exit, inflow boundary condition inside the jet region represents the pollutant release, wall boundary condition on the lowest plane represent the ground, freeslip boundary conditions on the top plane represent the sky, the wall conditions are also used on all faces of the buildings and elevated pollutant source. The freeslip boundary conditions along spanwise directions constrain the flow from moving out of the computational domain at that those respective positions by setting the normal component of the flow to zero.

## 2.3 Algorithm

The pressure field does not have any explicit evolution equation. Therefore an alternate way of calculating the pressure gradient and the pressure field must be used (the fractional-step procedure).

Problem Statement: Solve 
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = C_i^n + D_i^n - \nabla p$$

**such that** 
$$\nabla \cdot u_i^{n+1} = 0$$

Step 1: Calculate an intermediate velocity field by dropping the pressure term in the momentum equations

$$\frac{u_i^{n+1/2} - u_i^n}{\Delta t} = C_i^n + D_i^n$$

Step 2: Calculation of pressure by the Gauss-Seidel SOR algorithm

$$\nabla^2 p = \frac{\nabla \cdot u_i^{n+1/2}}{\Delta t}$$

Step 3: Update new velocity (ensures mass conservation)

$$\frac{u_i^{n+1} - u_i^{n+1/2}}{\Delta t} = -\nabla p$$

## 2.4 Numerical discretizations

The terms that require discretizing in the simplified Navier-Stokes equations are the time derivative of velocity, the diffusive terms, the convective terms and the pressure gradient.

The time derivative is handled by simple first order forward Euler scheme.

$$\frac{\partial u_l}{\partial t} \approx \frac{(u_l)_{i,j,k}^{n+1} - (u_l)_{i,j,k}^n}{\Delta t}$$

The diffusive terms are calculated by second order accurate central differencing scheme.

$$\frac{\partial^2 u_l}{\partial x_1^2} \approx \frac{(u_l)_{i+1,j,k}^n - 2(u_l)_{i,j,k}^n + (u_l)_{i-1,j,k}^n}{(\Delta x_1)^2}$$

The convective terms are calculated by using a skew-symmetric second order accurate scheme as follows.

$$u_1 \frac{\partial u_1}{\partial x_1} \approx \frac{(u_1)_{i+1,j,k}^n \left( (u_1)_{i,j,k}^n + (u_1)_{i+1,j,k}^n \right) - (u_1)_{i-1,j,k}^n \left( (u_1)_{i,j,k}^n + (u_1)_{i-1,j,k}^n \right)}{4\Delta x_1} \quad (i = j)$$

$$u_2 \frac{\partial u_1}{\partial x_2} \approx \frac{1}{2} \left( \frac{\left( (u_1)_{i,j,k}^n + (u_1)_{i,j+1,k}^n \right) \left( (u_2)_{i,j,k}^n + (u_2)_{i+1,j,k}^n \right) - \left( (u_1)_{i,j,k}^n + (u_1)_{i,j-1,k}^n \right) \left( (u_2)_{i,j-1,k}^n + (u_2)_{i+1,j-1,k}^n \right)}{4\Delta x_2} \right)$$

$$+ \frac{1}{2} \left( \frac{\left( (u_2)_{i,j,k}^n + (u_2)_{i+1,j,k}^n + (u_2)_{i,j-1,k}^n + (u_2)_{i+1,j-1,k}^n \right) \left( (u_1)_{i,j+1,k}^n - (u_1)_{i,j-1,k}^n \right)}{8\Delta x_2} \right) \quad (i \neq j)$$

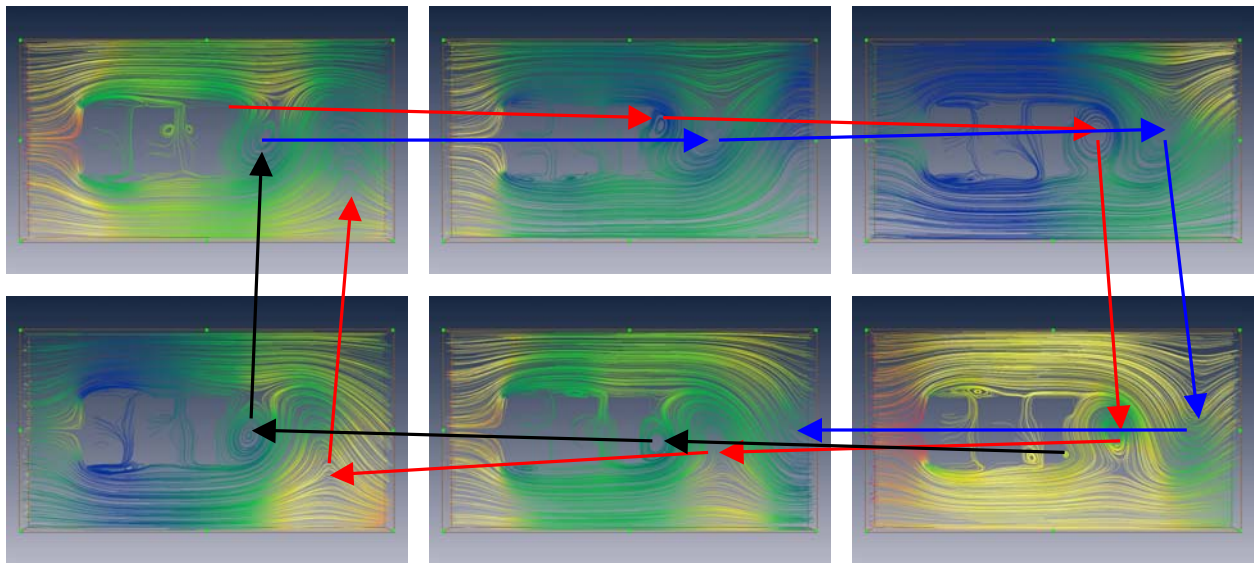
The pressure terms are calculated by a second order accurate central differencing scheme around the velocity location.

$$\frac{\partial p}{\partial x_1} \approx \frac{(p)_{i+1,j,k}^n - (p)_{i,j,k}^n}{\Delta x_1}$$

### 3 Results

#### 3.1 flow past buildings (bluff bodies)

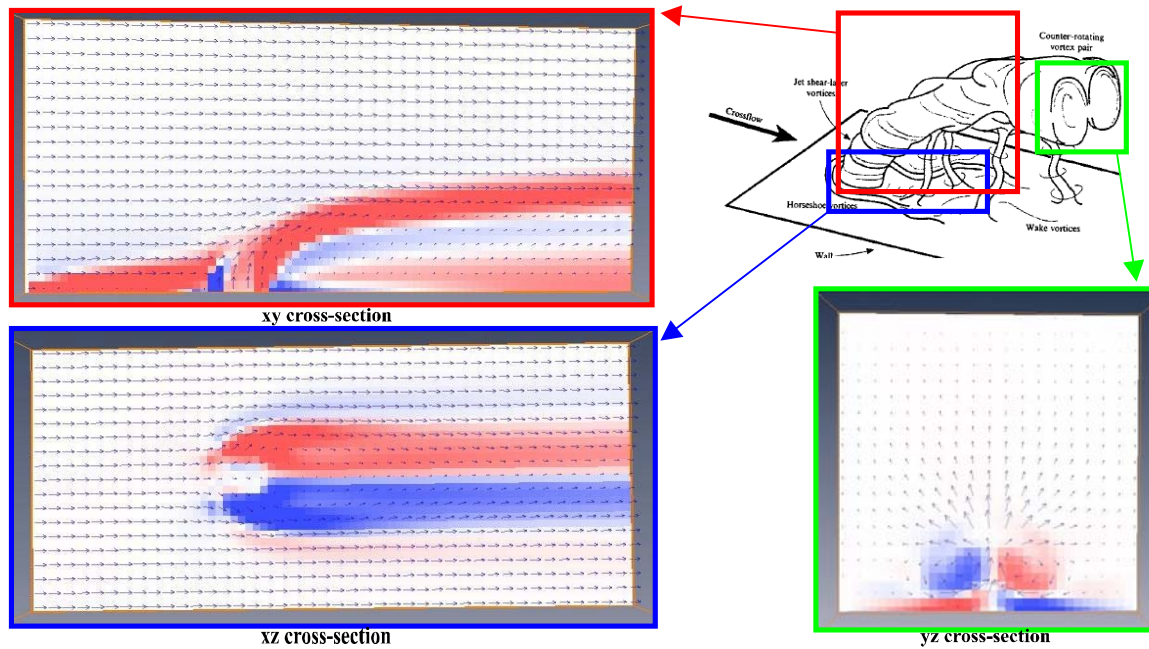
Flow past bluff bodies causes flow separation, recirculating eddies and convecting vortices to appear in fluid flows. To highlight these flow features an example of flow past obstacles arranged to form the letters “CCT” was studied. The flow past CCT show the periodic vortex shedding that occurs around bluff bodies immersed in a moving fluid. The arrows (red, blue and black) follow the “life-cycle” of these vortices.



*Fig.4 Periodic vortex shedding by flow past CCT (pictures arranged in clockwise order starting from top-left)*

#### 3.2 jets in cross flow

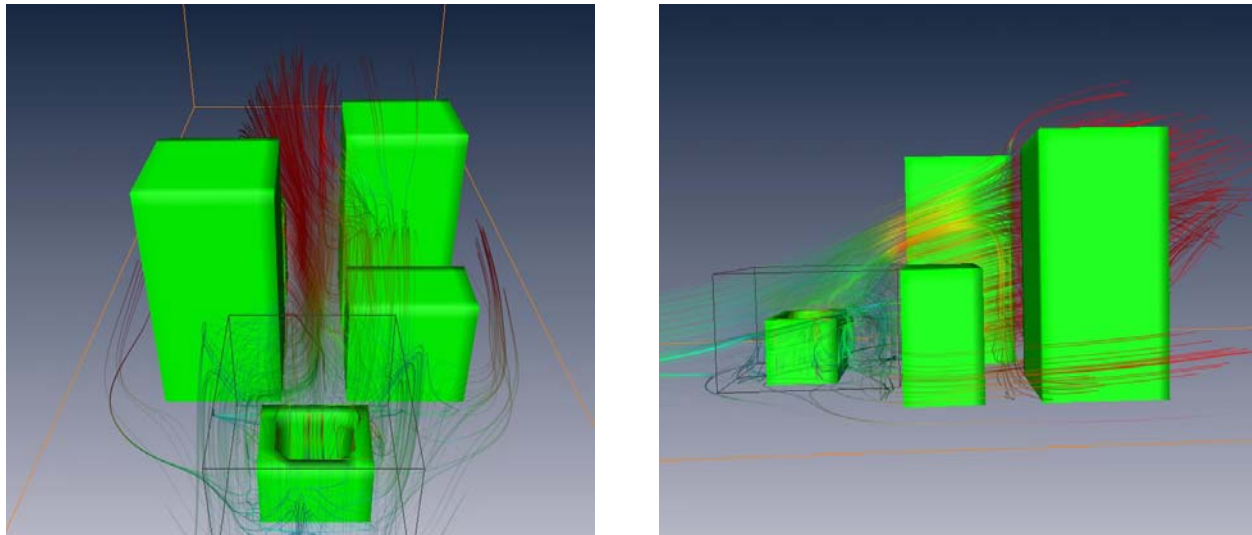
Jets in Cross Flow (JICF) contains complex flow phenomenon and serves a bench mark for CFD programs [10]. The impingement of crossflow on the transverse jet creates complex flow features. JICF is used to model the pollutant release since the flows of the surrounding fluid interacts with the pollutant fluid as it leaves the edge of the elevated sources (such as chimney stacks). Salient features of JICF contains: The counter-rotating pair of vortices or a kidney shaped circulation in cross-sectional projected view, horseshoe shape recirculation around the jet injection and shear layer vortices. Several orthogonal projection views are presented here to demonstrate that all the relevant salient flow features were resolved in these simulations. The curl of the velocity field (also called vorticity field) represents the rotation rate of the flow and the contours of the vorticity component that is normal to the projection view are also shown along with the velocity vectors (red levels correspond to CW rotation and blue levels correspond to CCW rotation).



*Fig.6 Vectors and Curl of velocity field on orthogonal projection views*

### 3.3 pollutant dispersion

To study the pollutant dispersion in urban environment, a jet is released from an elevated source (to model a chimney stack) around the cluster of four buildings (two short and two tall buildings arranged in an anti-symmetric fashion).

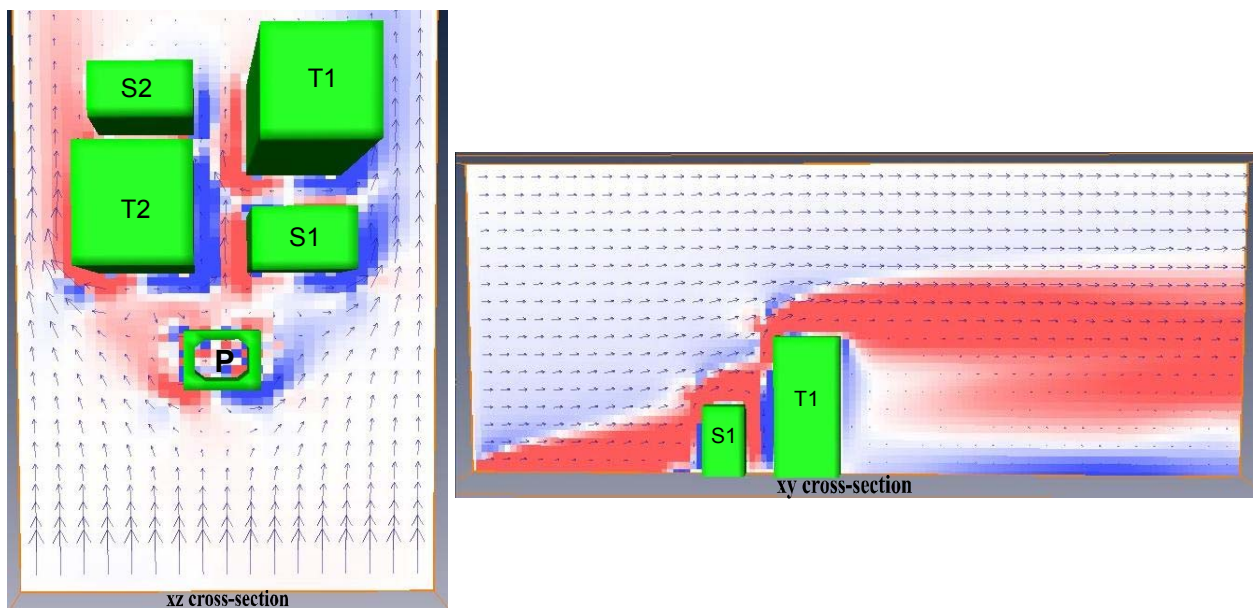


*Fig.7 Streamlines showing the flow details near the jet*

In this study, the flow patterns are analyzed using streamlines, velocity vectors as well as the curl of the velocity field. Further, a time sequence of pollutant concentration field displays the manner in which it is dispersed across

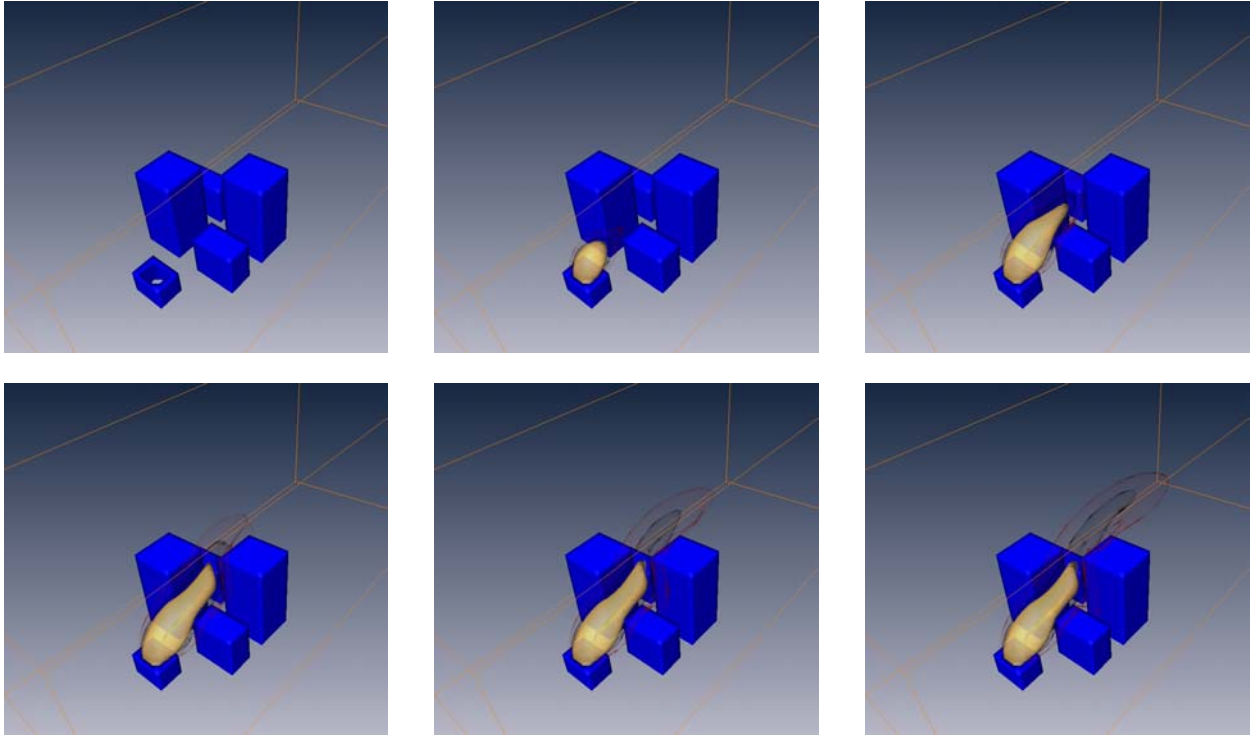
these buildings. The domain size for the chosen problem was  $120 \times 40 \times 40$  grid points. The elevated pollutant source contains  $8 \times 5 \times 8$  grid points with the jet being  $4 \times 4$  grid points at the y-min plane. The buildings are  $8 \times 18 \times 9$ ,  $6 \times 9 \times 9$ ,  $7 \times 9 \times 9$  and  $9 \times 18 \times 9$  grid points. The physical lengths of the domain are non-dimensionalized with respect to jet injection dimension and are  $12 \times 4 \times 4$ . The time step for the simulation is 0.01 with 30000 iterations. All inflow velocities are normalized with respect to jet velocity and set to 1.

The fluid evolution in the problem combines some patterns from the two canonical cases and adds some new patterns due to the interaction between JICF and the flow past buildings. The buildings also create small vortices around the faces of the buildings that trap certain fluid particles.

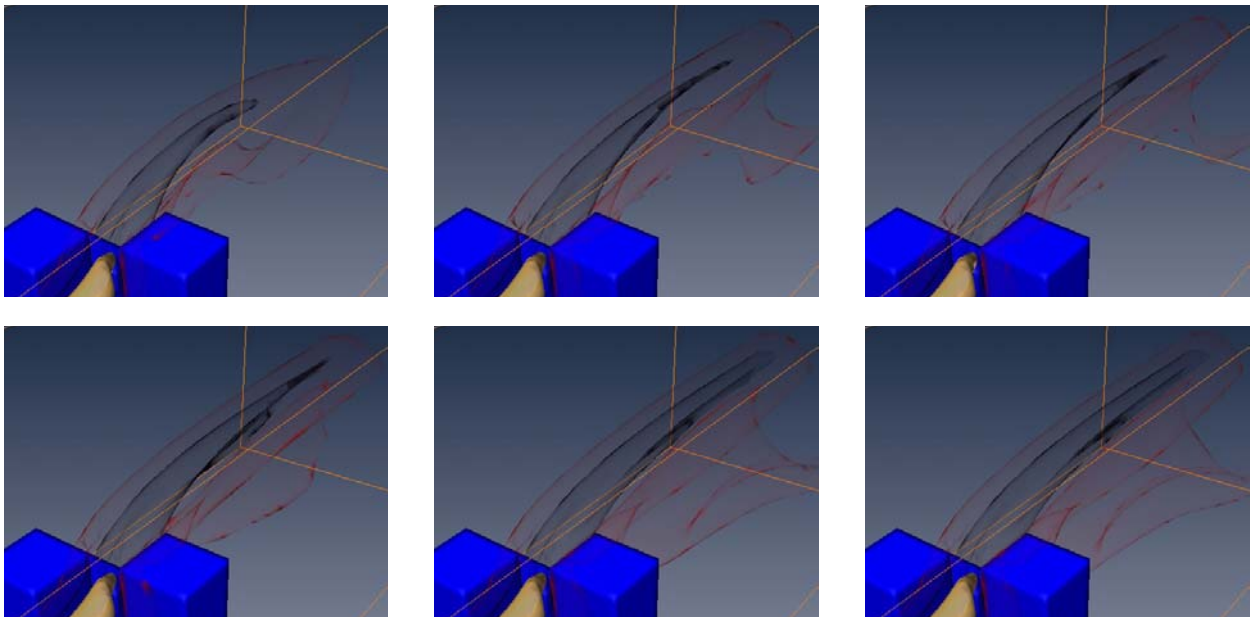


**Fig.8 Velocity vectors and curl of velocity field: Top-view (left) and Side-view (right)**

The pollutant concentration evolution initially follows the flow streamlines around the release region. The concentration mixes rapidly with the fluid as it exits the elevated source and therefore no high-concentrations were observed beyond the release area. The flow of the fluid through the small space between the tall buildings further lowers the concentration because the fluid then proceeds to disperse in all directions and the concentration also follows this by covering a higher volume of computational domain but at a lower concentration level. Though the pollutant concentration in the vicinity of the elevated source seems relatively static, the pollutant concentration in the far field is remarkably unsteady. In the wake of the tall building (the right side of the domain) the lower concentration also presents a flapping/periodic movement. This is similar to the periodic vortex shedding around the flow past obstacles.



*Fig.8 pollutant concentration field ( dispersion near the source)*



*Fig.9 pollutant concentration isosurfaces periodic movement (far field dispersion behind buildings)*

#### **4 Conclusions and Future Directions**

A prototype simulation was carried out to understand the pollutant dispersion process around the complex arrangement of the buildings in an urban environment. Building block problems were also analyzed in detail to

demonstrate the capabilities of the computational tool. In future, we plan to simulate realistic cityscapes using GIS datasets with CFD Toolkit on HPC platforms [3]. The physical models, numerical discretization schemes as well as computational mesh handling capabilities are also being enhanced for such complex grand challenge problems.

## **5 Acknowledgments**

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