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High-Performance Computing & Air Turbulence/Pollution Studies

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GEO-science workshop: Tutorial 2
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Tutorial Outline

• Why high-performance computing?
• Methodology
• LESChem results
  – Ventilation & pollutant removal
  – Buoyancy & temperature stratification
  – Chemically reactive pollutants
• Conclusion
• Upcoming Work
Why high-performance computing? [1/2]

- The atmospheric boundary layer (ABL) is too large to measure
- Broad spectrum of fluid motions
- The variables are uncontrollable
Why high-performance computing? [2/2]

• Turbulence
  – Multi-scale transient motions
• Buoyancy & temperature stratification
  – Instability and chaotic motions
• Coupled physics & chemistry
  – Nonlinear solution
Methodology

• Numerical methods
  – Finite difference
  – Finite volume
  – Finite element

• Parallelization
  – Domain decomposition
Scientific Objective

- Develop large-scale computer models simulating various atmospheric processes
- Elucidate the coupling between air pollution physics & chemistry in urban areas
- Formulate sophisticated parameterizations for chemically reactive pollutant inventory as functions of building morphology
Introduction to CFD

- Currently, 3 types of models are commonly used for resolving/modeling fluid turbulence.
  - $k-\varepsilon$ model (RANS based)
  - Large-eddy simulation (LES)
  - Direct numerical simulation (DNS)

<table>
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<tr>
<th>Model</th>
<th>Accuracy</th>
<th>Computational cost</th>
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<tbody>
<tr>
<td>$k-\varepsilon$ model</td>
<td>Lower</td>
<td>Relatively cheap</td>
</tr>
<tr>
<td>LES</td>
<td></td>
<td>Expensive</td>
</tr>
<tr>
<td>DNS</td>
<td></td>
<td>Very expensive</td>
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Why LES?

• Pollutant dispersion is strongly correlated with atmospheric turbulence
  – $k$-$\varepsilon$ model assumes isotropic turbulent kinetic energy (TKE) but the near-wall turbulence over 2D/3D roughness is highly anisotropic

• Study of the turbulence structure of individual components (i.e.: stream-wise fluctuation component) cannot be achieved using $k$-$\varepsilon$ turbulence model.

• DNS is computationally too demanding (at the moment) for handling turbulence of large length scale.
  – e.g. atmospheric turbulence.
Computational Domain

- **Inlet**: periodic; zero pollutant
- **Top boundary**: symmetry
- **Outlet**: periodic; open boundary for pollutant

**Flow direction**

**Front & Back**: periodic

**AR (Aspect ratio)** = $h/b$

**AR=0.25**

**AR=1.0**
Pollutant Dispersion over Urban Fabrics

A rapid plume rise is clearly depicted

Any “optimum” plot ratio/site coverage in the pollutant removal perspective?
Some Other ARs

AR = 1, single canyon (control)

AR = 0.5, 10 canyons

AR = 2.0, 18 canyons

AR = 1.0, 36 canyons
Pollutant Transport in Stratification

- Contour of wind speed & streamlines

\[ \text{Stable stratification} \quad \text{Ri} = 0.3 \]

\[ \text{Neutral stratification} \quad \text{Ri} = 0 \]

\[ \text{Unstable stratification} \quad \text{Ri} = -0.25 \]

\[ \text{Do we under/over estimate the pollutant removal capability of our cities in daytime/nighttime atmospheric boundary layer?} \]

\[ \text{Ri} = \frac{gh}{U_0^2} \times \frac{\Theta_0 - \Theta_w}{\Theta_0} \]
LES of Chemically Reactive Pollutants

• Simple reversible NO$_x$-O$_3$ chemistry
  \[ \text{NO}_2 \xrightarrow{hv, J_1} \text{NO} + \text{O} \]
  \[ \text{O} + \text{O}_2 + \text{M} \xrightarrow{k_2} \text{O}_3 + \text{M} \]
  \[ \text{O}_3 + \text{NO} \xrightarrow{k_3} \text{NO}_2 + \text{O}_2 \]

How is the non-linear coupling between air pollution physics & chemistry?
Pollutant Removal Mechanism [1/3]

Snap shot of iso-surfaces of streamwise fluctuation velocity at roof level

Large amount of decelerating, up-rising air masses are located along the roof level.

\[ u'' < 0 \text{ represents deceleration} \]

\[ w'' \approx w \text{ at roof level} \]
Pollutant Removal mechanism [2/3]

The accelerating air masses \((u'' > 0)\) carry the background pollutant into the street canyon by sweeps.

The decelerating air masses \((u'' < 0)\) remove the ground-level pollutant to the UBL by ejections.

The primary re-circulation mixes the pollutant within the street canyon.
Pollutant Removal mechanism [3/3]

With pollutant sources

Pollutant removal by ejections

≈

pollutant entrainment by sweeps

Without pollutant source

What is the role of atmospheric turbulence in pollutant removal over urban areas?
Laboratory Validation

• Wind tunnel (neutral + unstable) & water channel experiments (stable) to assess the LES results

• Other wind tunnels & water channels in HKU

Complementary solutions to the air pollutant transport over urban areas.
Future Work (in the next 2 years)

• Large-scale scientific computing
  – Increase the computation size by 1 to 2 order of magnitudes (100 to $10^3$ million grid points)
  – Fundamental understanding of turbulent flow, & heat & mass transfer over urban roughness

• Use Asian cities & Hong Kong as platforms/models to examine the urban climate & pollutant transport characteristics
  – Demonstrate the feasibility of using computer models for urban climate & air quality studies
  – Applicable to other developing cities in China & the world

• Deliverables & long-term impact
  – Non-CFD models/parameterizations for other air quality applications
  – Accidental/emergency/health risk assessments