APPLICATIONS OF THE MSS (MICRO-SWIFT-SPRAY) MODEL TO LONG-TERM REGULATORY SIMULATIONS OF THE IMPACT OF INDUSTRIAL PLANTS

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The MSS Model

- MSS is the combination of:
  - a simplified CFD model (Micro SWIFT) coupled to
  - a LPDM (Lagrangian Particle Dispersion Model) (Micro SPRAY)

- MSS was designed to model urban or industrial micro-scale dispersion phenomena with CPU times significantly shorter than the full CFD solutions.

- Typical initial MSS emergency response applications:
  - Domain size: 1 to 5 km dimension / Cell size: 1 to 10 meters
  - Single PC processor CPU time about 1/10th of real simulated time
  - Response time: few minutes

- MSS is operational into the US-DOD HPAC 5 suite of models
  - Coupled to SWIFT meteorological assimilation model
  - Coupled to SCIPUFF (Particle to Puff conversion and handoff)
MSS Development Group

- MSS is developed by several organizations:
  - ARIA Technologies (F)
  - ARIANET (I)
  - ISAC / CNR (I)
  - SAIC (USA) for DTRA
  - CEA (F)
  - MOKILI (F)
  - CAIRN Développement (F)
MSS initial Domain of application

Role of MSS in the HPAC system
MSS is an urban/industrial site scale tool

Example on Salt Lake City

MSS Urban Dispersion Simulation

Resolution in HPAC: 3 to 5 m

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MSS applications in PARIS
CBRN emergency response

- Release in the City Center: Place de la Concorde

Elysée: French President’s Residence
US Embassy in Paris

Courtesy of CEA
Dr. Patrick ARMAND

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Recent MSS Developments

Funded by DTRA CEA INERIS

- N-SWIFT (Nested-SWIFT) Development
- Deposition processes
- Dense gas simulation
- Explosion cloud simulation
- Multi-phase jets / Evaporation processes
- Concentration variances
- Generalized geometries
- Pressure distributions > Infiltration
- Parallel version of MSS
N-SWIFT Development

- **SWIFT: a meteorological data assimilation tool**
  - Time & space interpolation of several surface and profile data (Wind, Temperature, Humidity) from gridded data (model) or sparse data (experimental)
  - Use of high-resolution complex terrain and land-use
  - Mass consistent adjusted flow solution
  - Stability influence on adjustment
  - Diagnostic of vertical velocity of the mean flow
  - Estimation of mixing height evolution (h)
  - Diagnostic of BL turbulent quantities (u*, L)
  - Diagnostic of 3D turbulence fields
  - Used in HPAC to drive dispersion model (SCIPUFF)

*Nested SWIFT (N-SWIFT) : multi-scale upgrade*
N-SWIFT: why a Multi-Grid version?

- N-SWIFT: downscaling from 1km to 3m resolution
  - Nesting used by major meso-scale prognostic models (MM5, WRF) to downscale from standard NWP resolution to about 1km resolution.
  - Nesting allows to smoothly transfer information down to the Micro-scale, thus reducing the errors related to inflow data approximations.
  - Nesting may use different approximations at different scales:
    - Urbanized bulk surface layer formulation at 500 m resolution
    - Use of porous cells at 100m resolution
    - Use of actual buildings at 3m resolution
  - Nesting allows to make use of different meteorological input datasets at different scales.
N-SWIFT Multi-Grid development

OKC 4-Level Nesting application.

1120 m resolution
N-SWIFT Multi-Grid development

OKC 4-Level Nesting application.

300 m resolution

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N-SWIFT Multi-Grid development

OKC 4-Level Nesting application.

75 m resolution

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N-SWIFT Multi-Grid development

OKC 4-Level Nesting application.

4 m resolution
N-SWIFT Multi-Grid development

**Principle and advantages.**

- **MM5/WRF solution** (1.87 km resolution)
  - Additional observed data (300 m scale)
  - Additional observed data (75 m scale)
  - Additional observed data (urban canopy scale)

- **SWIFT 1** (1120 m) Free cells

- **SWIFT 2** (300 m) Free cells

- **SWIFT 3** (75 m) Porous cells

- **SWIFT 4** (4 m) Full cells

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N-SWIFT Multi-Grid development

OKC 4-Level Nesting application.

N-SWIFT: Domain 3 (75m) and Domain 4 (4m)
Dense gas simulation with MSS

Experiment 8 Thorney Island : images
Dense gas simulation with MSS

Experiment 8 Thorney Island
Multi-phase jets

Cooling tower plumes: primary evaporation/condensation

Air, water vapor, liquid water (several droplet size classes)

White iso-surface: water vapor 5.E-05 kg/m3
Light blue iso-surface: water droplets 1E-10 kg/m3
Concentration variances

New scheme, tested on CONFLUX and FFT07

\[ R = \frac{\sigma_c}{C_{\text{mean}}} \]

Concentrations computed « on the fly »

Order of magnitude and general behavior are correct.

Variance to mean increases towards the edges of the plume.

Quantitative comparisons are very difficult: plumes are often very thin and show strong meandering. Averaging time is an issue.
Generalized geometries
MSS applied to Urban Planning Tunnel studies

Case of an Urban Tunnel where TiO2 coating is considered (courtesy Ciments Calcia).

Reference Case
Average NOx concentration inside tunnel: 744 µg/m³

Coating applied
Average NOx concentration inside tunnel: 589 µg/m³

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Pressure distribution > Infiltration

Pressure diagnostic in MSS

- In MSS, Micro-SWIFT computes a diagnostic pressure field on buildings (façades and roofs), giving Delta(P) on each facet of a building (method suggested by Mike BROWN & als, LANL)

Poisson solver for:

\[ \frac{1}{\rho} \Delta p = -\text{div} \left( \partial_j (\bar{U}_j \bar{U}_i) \right) \]

→ Dynamic pressure coefficient \( C_p \)

\[ C_p = \frac{\bar{P} - \bar{P}_0}{1/2 \rho V_0^2} \]
Pressure distribution > Infiltration

Development of infiltration schemes in MSS

- Infiltration parameters set for different building blocks exactly as texture elements in a GIS, governing transfers.
Pressure distribution > Infiltration

Development of infiltration schemes in MSS

- Example of infiltration in different building blocks. Paris real urban landscape, test on traffic emissions.
Parallel version of MSS

Current status

- Funded by CEA
- **Target configurations:**
  - Large Linux clusters (2048 processors) for real-time Urban simulation over Paris
  - Standard multi-core laptops (Windows): Air Quality applications where MSS is run hourly for several years
- **Separate parallel architecture for Micro SWIFT and Micro SPRAY:**
  - Parallel *time frames* and *tiles* (domain separation) for Micro SWIFT
  - Parallel *particle clouds* per each tile for Micro SPRAY
  - Simpler if no P-P interaction (dense gases with P-M interaction,)
Parallel version of MSS

General scheme

- Exchange of particles at lateral boundaries of each tile needs to be introduced (lateral boundary conditions) => significant upgrade to the MicroSPRAY code structure.
Letter to Santa Claus

- We seek a dispersion model able to simulate:
  - the micro-scale between buildings (obstacle aware)
  - with relatively complete physics
  - sequentially (hour after hour) several years of plant operation (or of traffic emissions in cities),
  - with a time-domain approach and a short time step (1 hr or less)

- And we want to drive this model:
  - With modern regional scale meteorological codes (e.g.: WRF)
  - With a realistic meteorology (not single point but 3D),
  - To open the way to forecast applications.
MSS Long Term applications

- MSS is a good trade-off which can:
  - be driven by WRF + Nested SWIFT to go down from the 1km scale to the metric scale
  - simulate the micro-scale flow between buildings (obstacle aware) with relatively complete physics
  - provide 80% of the solution in 1% of the CPU
  - Iterate on long time series of model input (meteorology, emissions)

- In a hierarchy of increasing quality and complexity (hence of CPU load) one could set:
  - MERCURE, FLUENT: Full CFD
  - MSS, AUSTAL, QUIC: Lagrangian Particles Model
  - CALPUFF, SCIPUFF: Trajectory Puff Model
  - AERMOD, ADMS: Straightline Gaussian Model
Car factory example

Real-world permitting application

- Evaluation of Health Impact
- Determination of the dispersion of several VOCs.
- The site comprises many large buildings and is surrounded by several residential tall towers.
- Simulation of the dispersion over a period of 3 years, hourly input meteorological data
- Solution: two nested grids.
  - The inner grid covers a square domain of about 2x2 km size, with a resolution of 10 m. MSS is used
  - The outer grid covers a square domain of 6x9 km size, with a resolution of 20 m.
- On the outer grid, a transition to a puff model was used, and clusters of particles are converted into puffs when they come out of the inner domain.
The systematic **blocking effect of the large buildings** is clearly visible on the concentration map on the right. As far as CPU is concerned this type of simulation involves about a week of elapsed time on a 10 processors machine, per year simulated.
Hospital heating system example

Real-world situation
AIR CITY Project
Applying MSS to Paris Air Quality
Conclusions

- **Obstacle aware LPDM models** like MSS may be run in long term mode (one or several years hourly simulations)

- **The physical completeness** of these models is quite attractive

- The existence of **parallel versions**, as well as the generalization of multi-core processors and small clusters is currently **breaking the CPU barrier**, opening the way to **routine applications**

- An EU working group on **long term small scale 3D simulations** might be useful.
Thank you for your attention

Questions?