15 Computational fluid-dynamics models

15.1 Background

The expression Computational Fluid Dynamics (CFD) modeling comes from engineering, and refers to methods that can be used for the simulation of very-fine scales of motion. The terminology is confusing in the context that weather and climate modeling also involves the use of computational methods to solve the dynamic equations for a fluid. When the term CFD modeling is used in its conventional way in the atmospheric sciences, it refers to the simulation of motions that can synonymously be referred to as occurring on the sub-mesogamma scale, the microscale, or the turbulence scale.

Because we are revisiting the concept of the scales of motion that are represented by a model solution, a reminder of the pertinent discussions in Chapter 3 is appropriate. There is a tendency to think of the $2\Delta x$ length scale as the resolution limit of a model, although it has been shown by Skamarock (2004) (e.g., Fig. 3.36) and others that spatial filters associated with the finite-differencing scheme and the explicit diffusion in a model can cause the effective resolution to be quite different from this limit. Motions unresolved by the model can generally be referred to as the subfilter-scale (SFS).

15.2 Types of CFD models

There are three general categories of CFD models, although there are myriad methods for solving the equations, just as with larger-scale models.

- Reynolds'-Averaged Navier–Stokes (RANS) equations serve as the basis for one type, where, as described in Chapter 2, averaging operations relegate the turbulence effects on the mean motion to Reynolds-stress terms that must be parameterized, and the dependent variables in the equations pertain to the nonturbulent part of the motion. These RANS-type CFD models resolve small-scale flows around obstacles such as complex terrain and buildings, but the solution represents an average over the turbulent eddies that can dominate the motions in these situations. Thus model solutions remain steady, as long as the large-scale conditions defined by the LBCs do not change. An example of a RANS CFD model is described in Coirier *et al.* (2005).
- Large-Eddy Simulation (LES) models do not use averaging to eliminate the turbulence, but explicitly simulate the larger energy-containing eddies. A SFS parameterization

(also called a model) is used to represent the effects of the smallest-scale turbulence on the resolved scales.

- Direct Numerical Simulation (DNS) models capture all of the relevant scales of turbulent motion, so no parameterization is needed of the effects of unresolved scales. This is by far the most computationally demanding type of CFD modeling, and has limited use for complex processes.

The LES-type models are the ones most commonly used for research and practical applications in the atmospheric sciences. As an example of LES-model applications, an intercomparison of simulations of the stable boundary layer by eleven LES models was undertaken as part of the Global Energy and Water-cycle EXperiment (GEWEX) Atmospheric Boundary-Layer Study (GABLS). See Holtslag (2006) for a description of GABLS and Beare *et al.* (2006) for a summary of the LES models used in the study.

15.3 Scale distinctions between mesoscale models and LES models

Using the terminology of Wyngaard (2004), let Δ represent the scale of the spatial filter associated with the solution of the equations of motion and l be the scale of the energy-containing turbulence. Figure 15.1 shows a schematic of a turbulent-energy spectrum, as

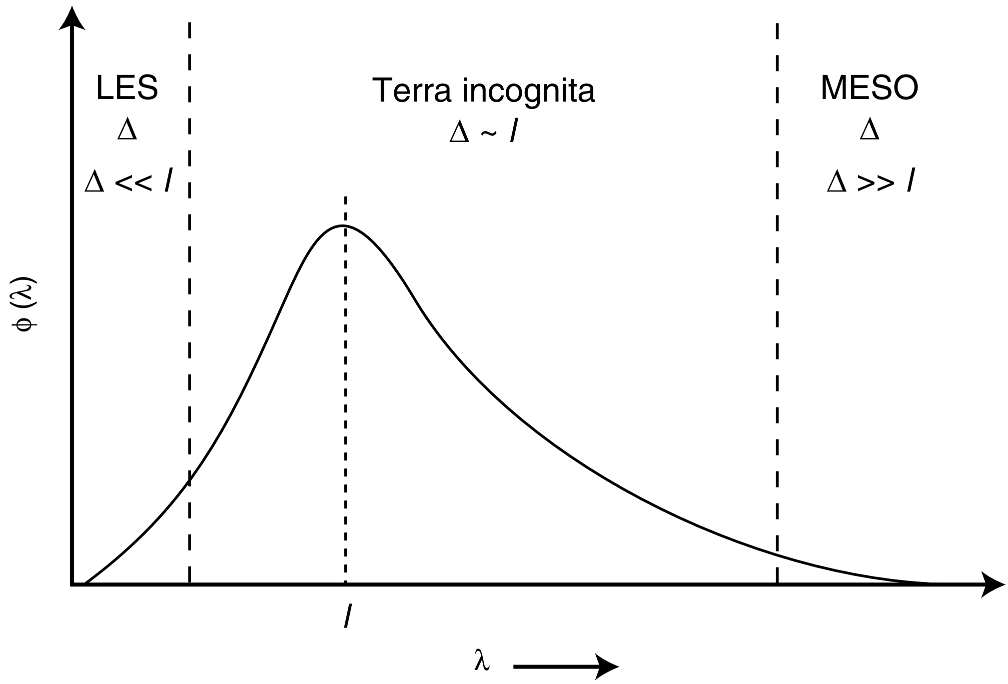

Fig. 15.1 Schematic of a turbulent-energy spectrum, as well as spatial-filter length scales (Δ) for LES and mesoscale (MESO) models. The variable l is the scale of the energy-containing turbulence, Φ is turbulent energy, and λ is wavelength. See the text for details. Adapted from Wyngaard (2004).

well as spatial-filter length scales for LES and mesoscale (or larger scale) models. For model spatial-filter scales in the "MESO" region on the right, long-wavelength, side of the graph, the turbulent energy is clearly in the unresolvable SFSs ($\Delta \gg l$). This is appropriate because for meso- and larger-scale models, the turbulence should be parameterized and not resolved. But, for LES models that resolve the energy-containing turbulence, the scale of the spatial filter must be sufficiently small relative to the turbulence scales ($\Delta \ll l$). Thus LES spatial filters should be in the short-wavelength region on the left side of the graph. The point of Wyngaard (2004) is that it is not clear how to apply models with spatial-filter scales within the part of the spectrum containing the turbulent energy (the terra incognita).

15.4 Coupling CFD models and mesoscale models

Because CFD model domains only span a limited area, they must obtain their LBCs from observations, analyses of observation, or larger-model grids with perhaps resolutions on the mesoscale. The CFD model may be run with temporally constant LBCs, or the LBCs may vary as the large-scale flow evolves. Initial conditions are typically defined from a relatively smooth, or even horizontally uniform, variable field. The local forcing, e.g. from orography or structures, will then allow microscale features to develop. For example, when CFD models are used to simulate the impact of a building on the winds in an urban area, the initial conditions will represent the "skimming flow", well above the rooftops, and the forcing from the building will generate channeling in the street canyons, and vortices on all sides of the building, during the simulation.

In some cases, the same dynamical core can be run as a traditional mesoscale model and as an LES model, with inner grids using LES closures and the outer grids run with standard mesoscale-model closures. In this case, there is generally two-way interaction between the mesoscale and the LES scale. In contrast, when distinct models simulate the two scales, it is more typical to use one-way coupling. Note that the use of the same model dynamical core to span the LES scale and the mesoscale with a series of nested grids can lead to the scale-separation issues described in the last section, if a standard ratio of 3–5 is used for the resolution of adjacent grids.

A significant issue with LES-model LBCs is that the inflow boundary will generally be defined by an atmosphere in which the turbulence effects are parameterized. Thus, there will be no turbulence structures entering the grid, and because of the short residence time of the air flowing over such small computational grids there may not be sufficient time for the turbulence to develop before the air exits at the outflow boundary. This situation is similar, in principle, to that discussed in Section 3.5, where a significant buffer zone is needed between the upwind boundary and the area of meteorological interest on the grid. This allows small-scale processes to spin up as the air enters the central region of the grid. Unfortunately, the advective time scales are the same for mesoscale and LES-scale models, even though the sizes of the computational grids are much smaller in the latter case. For example, an LES model may have a grid increment of 5 m and a computational domain with a length scale of 1 km. If the inflow wind speed is 5 m s^{-1}, the air will reach the center of the computational grid in 100 s, quite possibly an insufficient amount of time to develop the turbulence. This would render the LES inadequate for the intended purpose. One approach to this problem is to try to specify turbulence structures in the inflowing air, but this is challenging.

As with any system of coupled models, a situation-dependent aspect of the coupling between LES and larger-scale models is the sensitivity of the LES model solution to errors in the LBCs. For example, wind-direction errors in a mesoscale model may be consistent with the state of the science, and these errors may not have a significant negative impact on the value of forecasts of sensible weather. But, there may be particular applications of a CFD model such that this error in the initial conditions and LBCs produces a profound error on the CFD-model scales. For example, Fig. 15.2 shows the simulated concentration of a plume of hazardous material that has been released at street level into the atmosphere on the south side of Oklahoma City, USA. A large-scale wind was used as the input to a RANS-type CFD model (Coirier *et al.* 2005), and the resolved wind flow within the street canyons was used as input to a transport and diffusion model. In one case, the large-scale wind was from the south-southwest, in which case the plume covered the east side of the urban area (a). When the large-scale wind direction was changed by 22.5°, to southerly, the plume's impact changed from the eastern half to the western half of the city (b). Here, the existence of the street canyons causes a large response in the low-level flow of the plume to a small change in the large-scale wind direction. Note that this wind-direction difference is consistent with the expected errors in forecasts of low-level winds from mesoscale models.

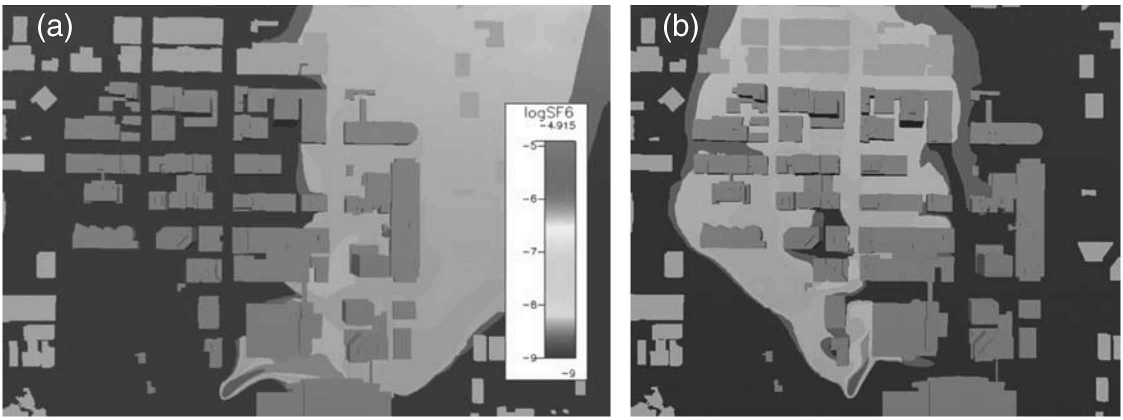

Fig. 15.2 A large-scale wind was used as the input to a RANS-type CFD model (Coirier *et al.* 2005), and the resolved wind flow within the street canyons (black area between rectangular buildings) was used as input to a transport and diffusion model. In one case, the large-scale wind was from the south-southwest, in which case the plume (irregular gray shapes) covered the east side of the urban area (a). When the large-scale wind direction was changed by 22.5°, to southerly, the plume's impact changed from the eastern half to the western half of the city (b). Provided by William Coirier, Kratos/Digital Fusion, Inc.

15.5 Examples of CFD-model applications

Applications of CFD models fall into two categories, as do the uses of NWP models – they are used for scientific discovery (knowledge generation) as well as for addressing practical problems. Practical applications are of course abundant in the engineering area, such as simulating the flow over an aircraft as part of the design process. In the context of microscale atmospheric science, some examples follow.

- Studies that are aimed at better understanding turbulence can lead to improved parameterizations of the effects of the turbulence on fluxes, for example in the nocturnal stable boundary layer, or within a tree canopy during the day.
- The wind loading on tall buildings is studied by design engineers, to enable safer construction.
- Wind turbines must be located to maximize the available power as well as to minimize the turbulence load on the generator. Decisions about the general area for locating wind farms are often made using analyses that are based on mesoscale models. But, optimizing the locations of the individual turbines in complex terrain requires the use of CFD models.
- Wake turbulence produced by specific types of aircraft on takeoff is studied to define the requirements for safe distances that must be maintained between aircraft in a takeoff sequence.
- The transport in the urban boundary layer of hazardous gases or aerosols, released for example from a transportation or industrial accident, can be studied.

Many, many other examples exist.

15.6 Algorithmic approximations to CFD models

Because of the small grid increments, CFD models are very computationally demanding to run. Thus, when solutions are required quickly to meet operational needs of some type, algorithmic approximations to CFD-model solutions are used. For example, if forecasts are needed of street-level winds between buildings in an urban area, say based on the input of rooftop winds from an operational mesoscale model, LES or RANS CFD models may be too computationally demanding to provide building-scale solutions on usable time scales. An approach that has been used to address this problem is to employ LES-model solutions and wind-tunnel studies to define the patterns of the airflow around a variety of obstacle shapes, for different wind directions, stabilities, and vertical shears of the horizontal wind. The resulting catalogue of flow patterns can be used to develop algorithms that define the building-aware wind flow under variable large-scale conditions. An example of such a rule-based system is the Quick Urban & Industrial Complex (QUIC) model (Pardyjak *et al.* 2004), which has a wind-flow component (QUIC-URB) and a QUIC-PLUME code that tracks plumes of air pollutants among buildings.

SUGGESTED GENERAL REFERENCES FOR FURTHER READING

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Moin, P., and K. Mahesh (1998). Direct numerical simulation: A tool in turbulence research. *Annu. Rev. Fluid. Mech.*, **30**, 539–578.

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PROBLEMS AND EXERCISES

1. Describe additional practical applications of LES models.
2. Speculate about the challenges associated with using LES models to simulate the stable boundary layer, versus the neutral or unstable boundary layer. Confirm your ideas with a literature search.
3. What are the similarities between the turbulence-modeling scale issues described in Wyngaard (2004), and the fact that 1–10 km grid increments are considered to be too small for parameterizing convection but too large to resolve it in a model?
4. When CFD models run fast enough in the future to be used operationally, discuss whether there will be a role them in predicting urban weather – that is, the specific weather conditions within the street canyons.