Direct Numerical Simulations of Droplet-Laden Flows*

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Outline

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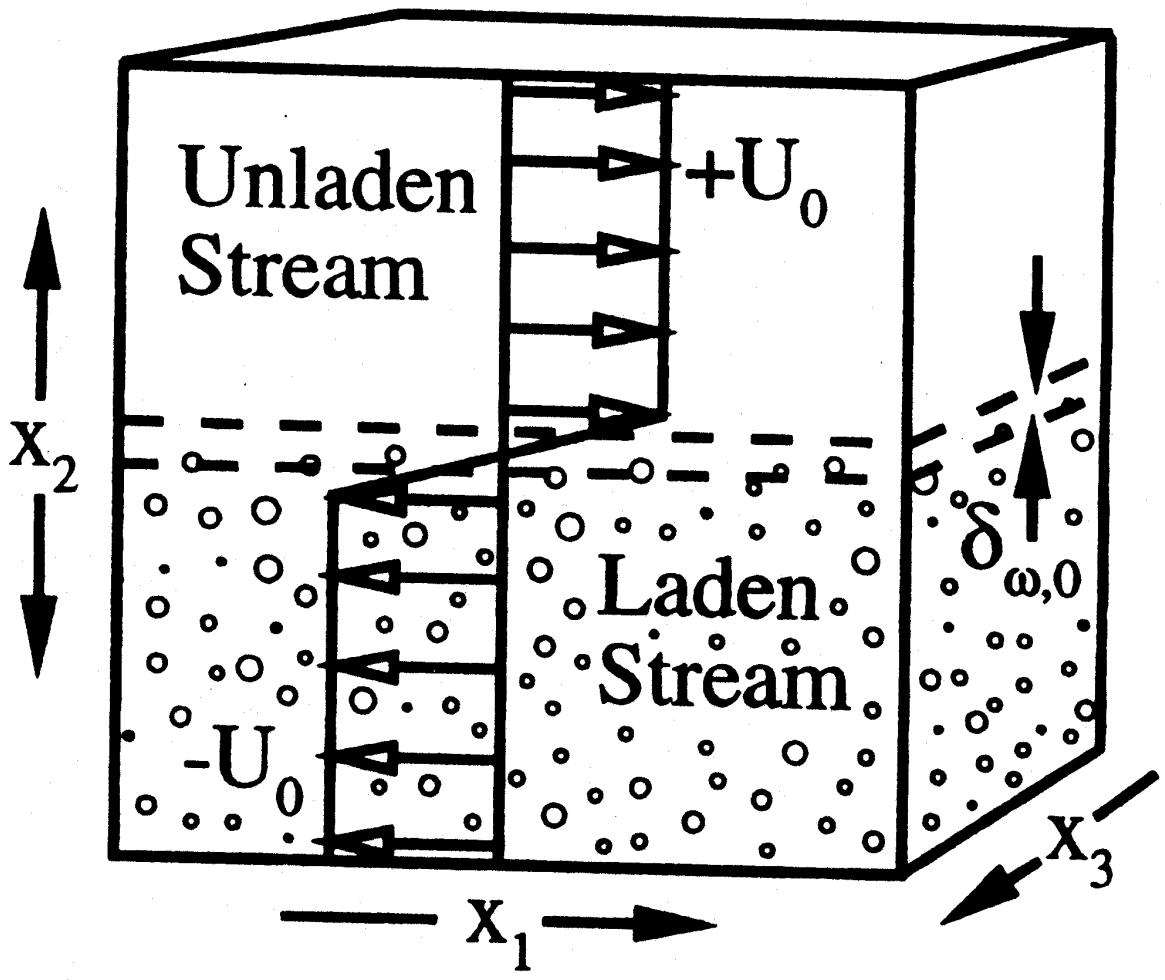
Summary of Flow Problem

- Three-dimensional mixing layer: two parallel streams at different velocities, the interface is the mixing region
- Spatial mixing layer: fixed region in space
- Temporal mixing layer: follow a coherent structure in time
- Initially, the lower stream is droplet-laden, the upper stream is droplet-free
- As the layer evolves, it undergoes rollup and pairing and growth, entraining droplets
- The carrier gas is hotter than the droplets, causing the droplets to evaporate

Mixing Layer Configuration



Flow Modeling

DNS/LES/SGS Protocol

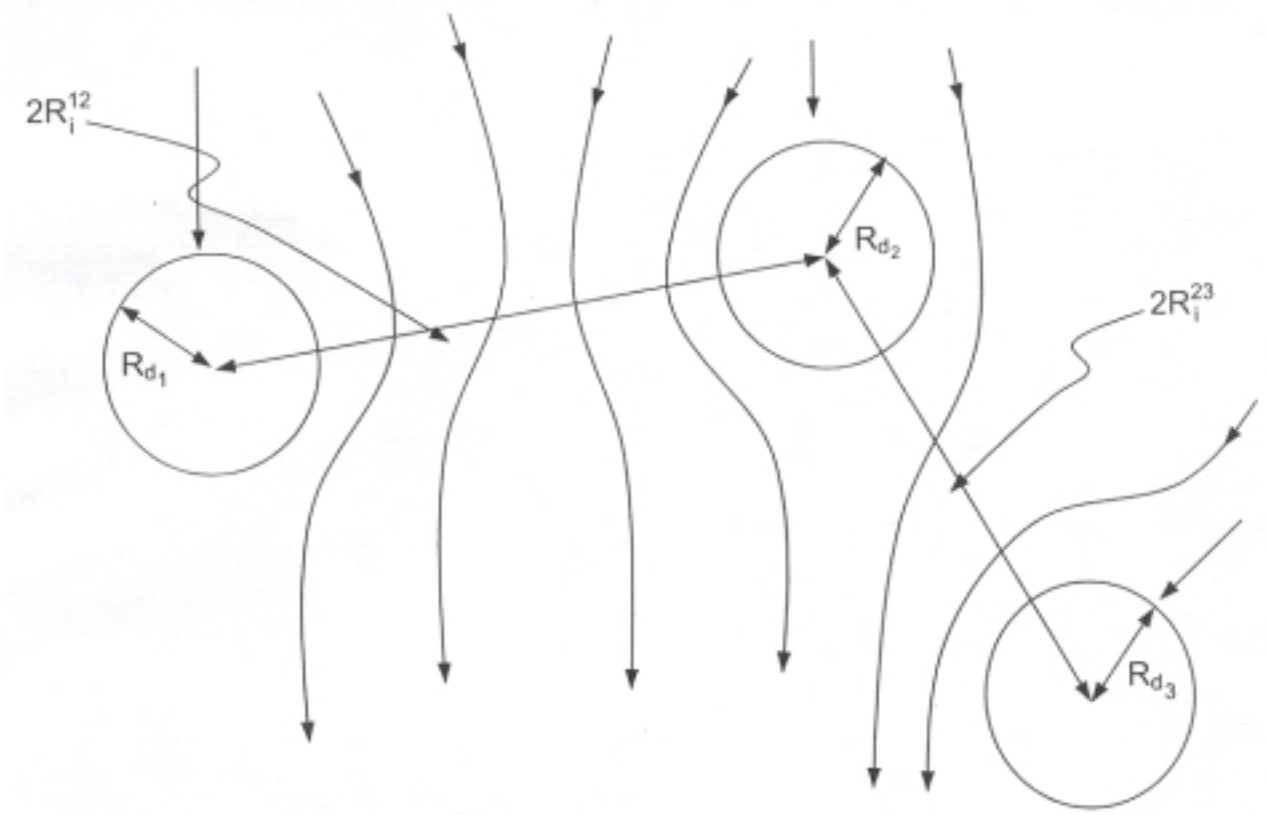
- Direct Numerical Simulation (DNS) requires resolving all relevant length scales
- Large Eddy Simulation (LES) assumes that an ordering of scales exists such that large scales can be resolved on the computational grid whereas the subgrid scales (SGS) can be modeled
- Since in LES only the large scales need to be resolved, the resolution can be much less than the comparable DNS
- The equations for the large scales (i.e. for LES) are derived by spatially filtering the DNS equations; the filtering introduces SGS terms which need to be modeled

Flow Modeling (continued)

DNS/LES/SGS Protocol

- With the exception of the SGS terms, the form of the LES equations (for filtered variables) is the same as that of the DNS equations (for unfiltered variables)
- SGS models can be obtained by performing DNS, and filtering the DNS results--*a priori* modeling
- SGS models can be tested by using them in performing LES--*a posteriori* modeling

Typical Drop Interactions in Laminar Sprays



Flow Modeling (continued)

Length scales:

- Interstitial distance R_i
- Droplet radius R_d
- Kolmogorov scale $\__K$ (smallest length scale of turbulence)
- Scale of energy containing eddies l

Reynolds number:

$$\mathrm{Re}_d \ldots \frac{|u_{drop} - u_{gas}| R_d}{\nu_{gas}} = O(10)$$

$$\mathrm{Re}_l \ldots \frac{u_{gas} l}{\nu_{gas}} ? O(10^4), \quad \eta_K = \frac{l}{\mathrm{Re}_l^{3/4}}$$

Typically: $R_d \sim 10^{-5}$m, $R_i \sim 10^{-3}$ m, $R_d/R_i \sim 10^{-2}$

Flow Modeling (continued)

Pertinent models according to Λ_K/R_i and Λ_K/R_d

	Dilute Spray $R_d/R_i=O(10^{-2})$		Dense Spray $R_d/R_i=O(1)$	
Λ_K/R_d	Λ_K/R_i	Pertinent model	Λ_K/R_i	Pertinent model
$O(10^4)$	$O(10^2)$	Point source; drops see laminar flow	$O(10^4)$	Granular flow; drops see laminar flow
<<1 $O(1)$	<<1 $O(10^{-2})$	Resolve details of surface-eddy interactions	<<1 $O(1)$	Granular flow; drops see turbulent flow

Numerics

Flow modeling considerations

- Spatial vs. temporal mixing layer: the temporal mixing layer is simpler to simulate as periodic boundary conditions can be used; it has important features in common with the spatial mixing layer
- Droplet model: the flow around each drop is represented by a validated, laminar, model. Thus DNS in two-phase flow has different meaning from DNS in single phase flow wherein all scales are solved. Also, the droplet-carrier gas interaction needs to be modeled consistently.
- Reynolds number: the simulation viscosity, which is much higher than the physical one, is computed based on the Reynolds number

Numerics (continued)

Numerical algorithm considerations

- Explicit fourth Runge-Kutta time-integration: explicit time-integration requires less memory than an implicit method, is faster to derive and code, but has smaller maximum timesteps
- Eighth-order finite difference: higher order means fewer grid points to attain the same accuracy, but higher-order methods are less numerically stable and require larger stencils
- Physical grid: using uniform grid spacing in each direction reduces errors due to variable grid spacing, but requires high resolution even in smooth regions

Experiences

Not enough memory...

- DNS: maximum Reynolds number was 200; for transition to turbulence, estimated Reynolds number was 600; resolution proportional to Reynolds number so needed 3^3=27 times as many grid points
- LES: feasible but needed SGS models for two-phase coupled flow
- Solution: modify DNS code to run on a parallel machine, perform DNS at higher Reynolds number, derive SGS models based on DNS

Experiences (continued)

Parallelization

- Compiler directives--could keep same code, but would be restricted to available shared memory on the computer
- Message passing--domain decomposition; would need change code but would have more memory available on the computer.
- The main modification was the addition of ghost cells at the boundaries, requiring subroutines that only updated the ghost cells.
- In the parallel code, these subroutines would be replaced by interprocessor communication

Experiences (continued)

Programming strategy

- Rewrite the DNS code to make it easier to parallelize and to convert for LES (added terms in equations)
- Develop a parallel code that can be converted to a serial code
- Develop a code that can be easily modified since as part of ongoing research, the basic equations will undergo continual modification
- Keep the code modular so that different versions of a subroutine can be implemented
- Develop a code that is memory as well as CPU efficient

Experiences (continued)

Optimization

- The code generally vectorizes well, because much of it involves loops over all gridpoints (IJK) and loops over all droplets (N).
- However, the coupling terms between flowfield and droplets vectorize only moderately because the droplets move relative to the grid and are not coincident with the grid points.
- We chose an algorithm wherein the droplets are tied to the grid that they are physically located in, with the intention of minimizing communication in the parallel version.

Experiences (continued)

Optimization (continued)

- At the highest optimization level, the compiler will perform the obvious optimizations e.g. remove redundant code, rearrange computations, unroll short loops.
- It is best to write the code in the simplest, most natural, most readable way and then use performance tools to guide optimization.

Experiences (continued)

Optimization (continued)

- PARAMETER statements: used to set global variables that will not change during the computation, e.g. the number of grid points
- Short utility routines: these make the code more readable; the compiler will inline them.
- Performance tools (e.g. flowview) : these will indicate which subroutines take the most time and which may need to be inlined. Be sure to check input/output routines.
- Usually just a few subroutines take the most time. Focus on optimizing these.

Experiences (continued)

Moving ...

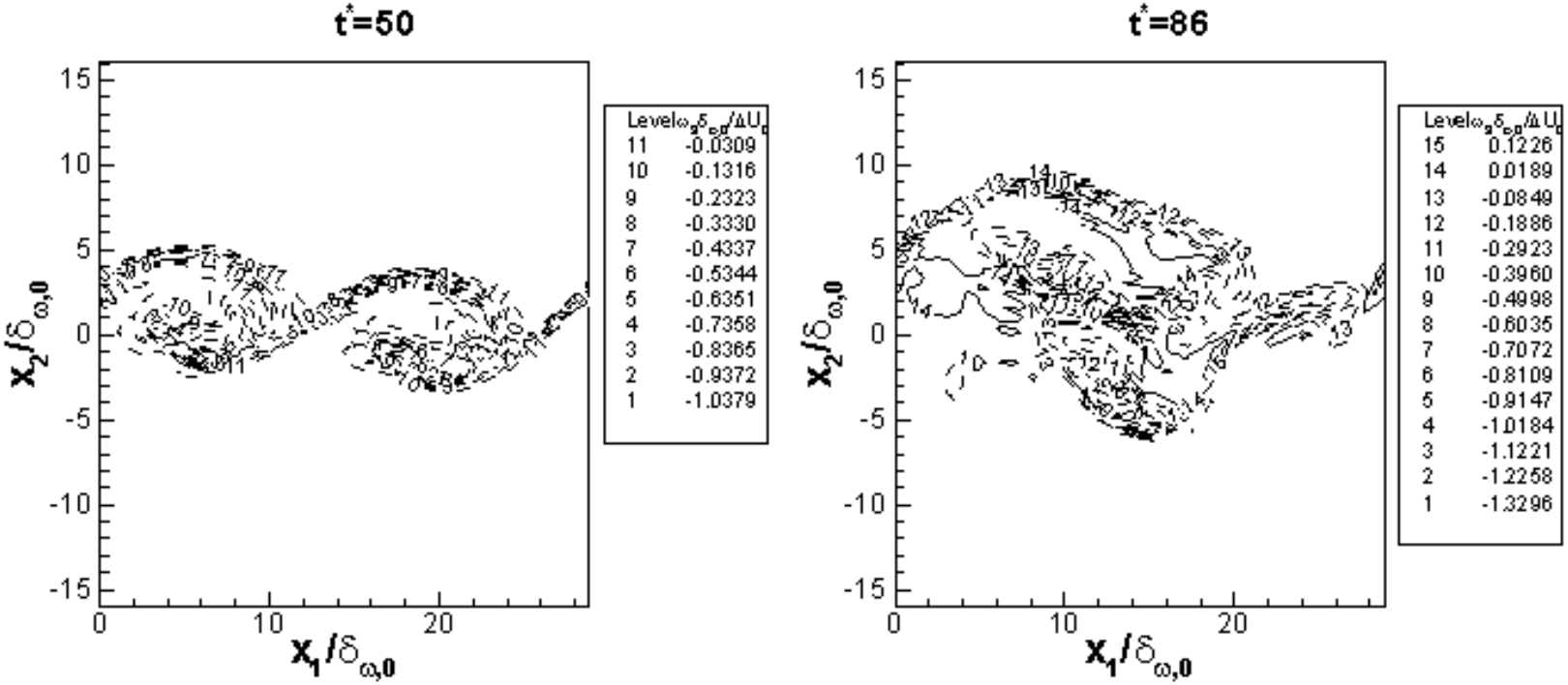
- The transition from the J90 to the SV1A was seamless.
- Although FORTRAN90 is backward compatible with FORTRAN77, differences between the compilers necessitated some minor changes to the code.
- Some sections of the code benefited from being rewritten to take advantage of FORTRAN90 features, e.g. the Poisson solver used to compute the initial condition using FORTRAN90 array syntax is over four times faster than the FORTRAN77 version.

Experiences (continued)

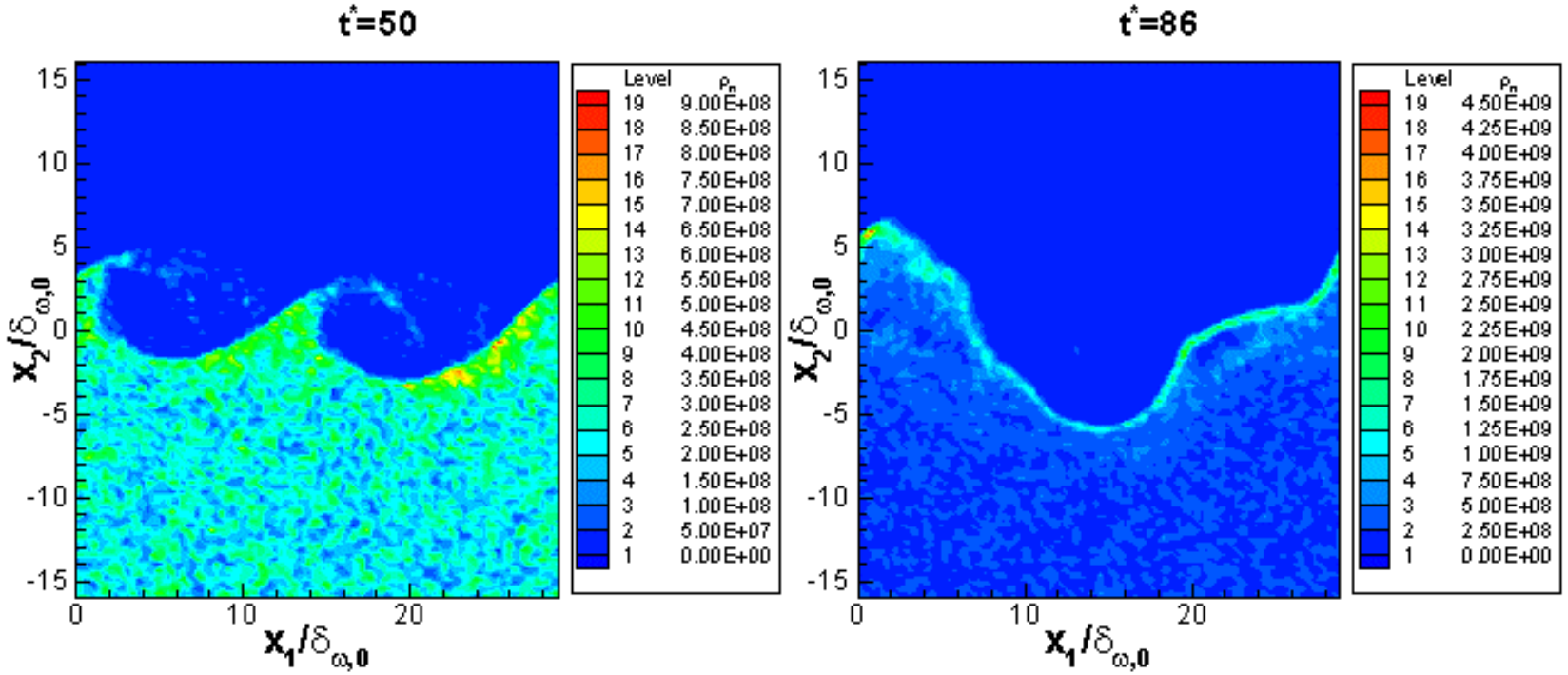
Reynolds Number	200
Physical Domain	0.2mx0.25mx0.12m
Grid size	96x18x64=786,432 points
Number of droplets	700,000
Number of timesteps	630

Machine	Language	Compiler Options	Memory	CPU Time Per step
CrayJ90	FORTRAN77	-Zv	64Mw	138s
Cray SV1A	FORTRAN90	-O2	74Mw	134s
Cray SV1A	FORTRAN90	-O3	91Mw	86s

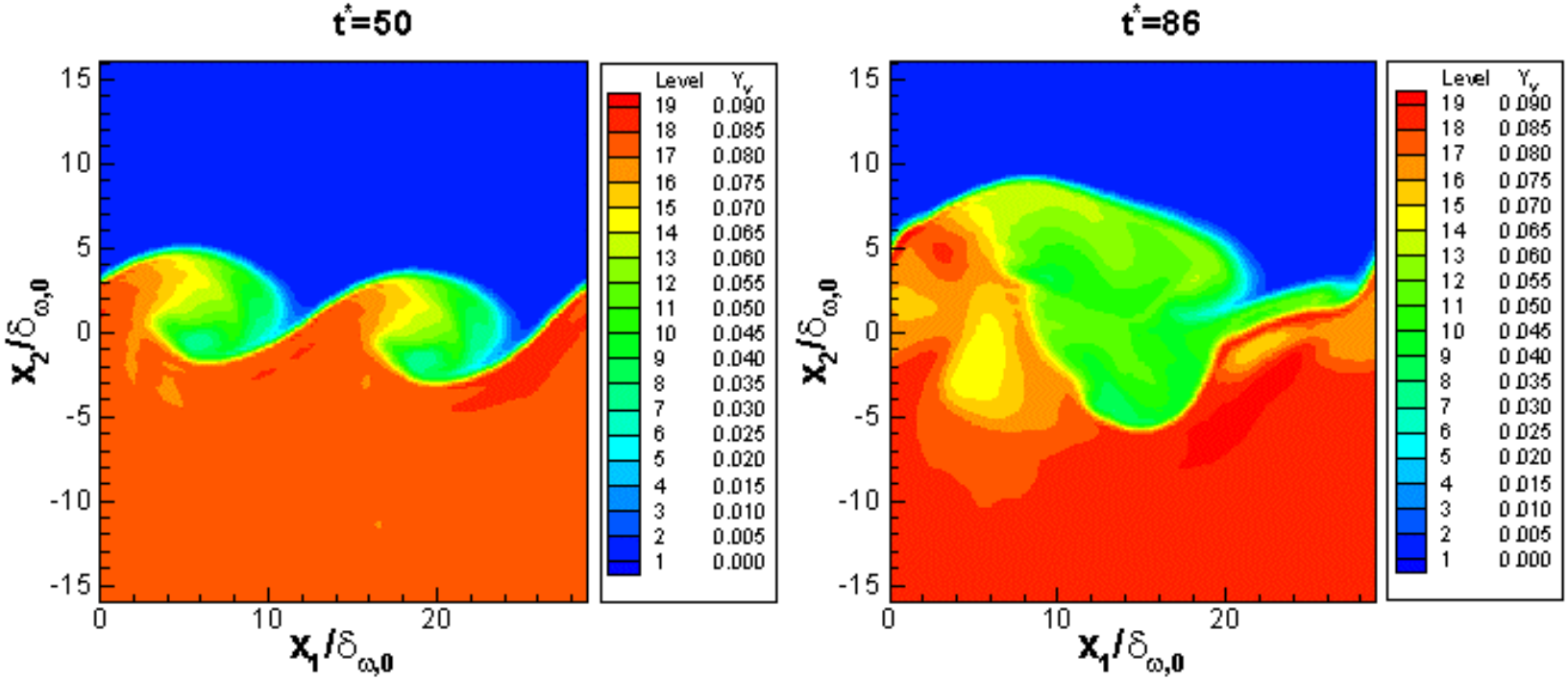
Mixing Layer Evolution--Spanwise Vorticity



Mixing Layer Evolution--Droplet Number Density



Mixing Layer Evolution—Vapor Mass Fraction



Conclusions

- We have developed an efficient code for performing numerical simulations of fluid flow carrying evaporating droplets.
- We have maintained a flexible code that can been easily parallelized for performing direct numerical simulations at higher Reynolds numbers and can be converted for performing large eddy simulations by the inclusion of subgrid scale models.
- Our experiences illustrate how the available computational resources influence not only the selection of the numerical method, but also the physical model used.