

# Direct Numerical Simulation of Fully Resolved Liquid Droplets in a Turbulent Flow

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NCSA Blue Waters Symposium  
for Petascale Science and Beyond  
May 11, 2015



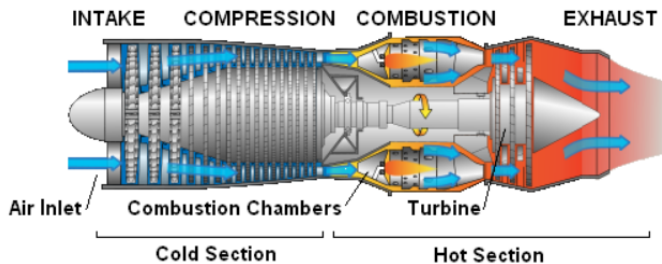
# Objective & motivation

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- Motivation** Dispersed liquid/gas multiphase flows occur in a wide range of natural phenomena and engineering devices, e.g. combustion of liquid fuel sprays.

# Example of application I



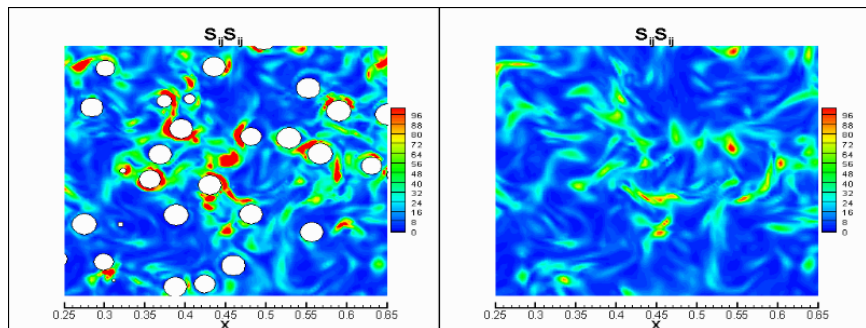


## Example of application II



# Effect of dispersed solid spherical particles on the dissipation rate of TKE ( Lucci, Ferrante & Elghobashi, JFM 2010 )

$Re_\lambda$	$N$	$N_p$	$\Phi_v$	$d/\eta$
75	256	6400	0.1	16



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# Computational requirements

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- ▶ On Blue Waters the simulation required 12 hrs and 65536 processors to advance the solution for about 3 large-eddy turnover times
- ▶ The simulation of dispersed two-phase turbulence requires about double the time of single-phase turbulence

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- ▶ Momentum equations:

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\frac{1}{\rho} \left[ \nabla p + \frac{\nabla \cdot \mathbf{T}}{Re} - \frac{\rho}{Fr} \mathbf{k} + \frac{\mathbf{f}_\sigma}{We} \right]$$

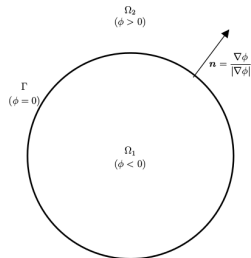
Dimensionless parameters:

$$Re = \frac{\tilde{\rho}_{gas} \tilde{U} \tilde{L}}{\tilde{\mu}_{gas}} \quad Fr = \frac{\tilde{U}^2}{\tilde{g} \tilde{L}} \quad We = \frac{\tilde{\rho}_{gas} \tilde{U}^2 \tilde{L}}{\tilde{\sigma}}$$

# Interface definition & transport

The gas/liquid interface  $\Gamma(t)$  is described as the **zero level set** of a signed distance function  $\phi(\mathbf{x}, t)$  that is transported by the fluid velocity  $\mathbf{u}$  via:

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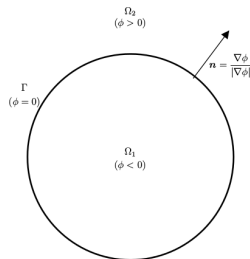
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In order to keep  $\phi$  a signed distance function, a **reinitialization** equation is solved until convergence:

$$\frac{\partial \phi}{\partial \tau} = \text{sign}(\phi_0)(1 - |\nabla \phi|)$$

where  $\tau$  is a fictitious time and  $\phi_0$  is the level set function after the advection step.



# Variable-Density Projection Method

1. A provisional velocity  $\mathbf{u}^*$  is computed from  $\mathbf{u}^n$ , the velocity field at time  $n$ :

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\delta t} = \mathbf{R}^n$$

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3.  $\mathbf{u}^*$  is corrected to obtain  $\mathbf{u}^{n+1}$ , the velocity field at time  $n + 1$ :

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \delta t \frac{\nabla p^{n+1}}{\rho^{n+1}}$$

# Solution of the Variable-Coefficients Poisson's equation

$$\nabla \cdot \left( \frac{\nabla p^{n+1}}{\rho^{n+1}} \right) = \frac{\nabla \cdot \mathbf{u}^*}{\delta t}$$

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- ▶ A **Geometric Algebraic Multigrid** preconditioner is used
- ▶ We rely on the PETSc library for the solution of the linear system

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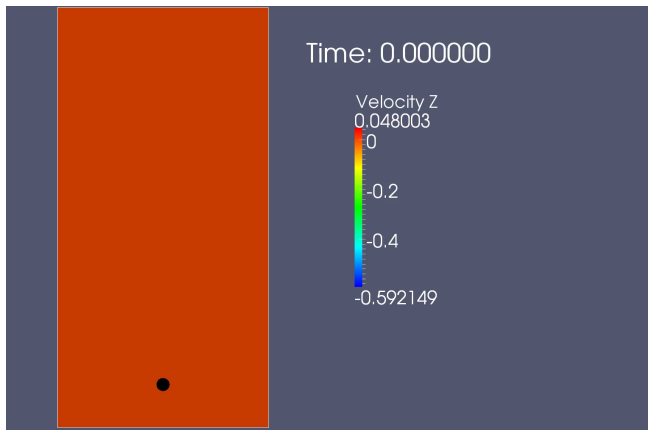
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- ▶ We will try different solutions, e.g. OpenMP/MPI, improve communication topology ...

# Falling droplet test I

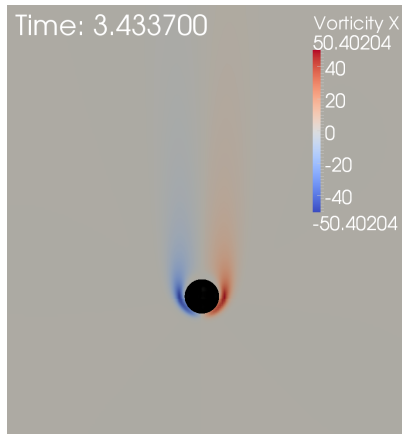
$Re_D$	$Fr_D$	$We_D$	$\rho_l/\rho_g$	$\mu_l/\mu_g$
96	1009	0.06	829	54





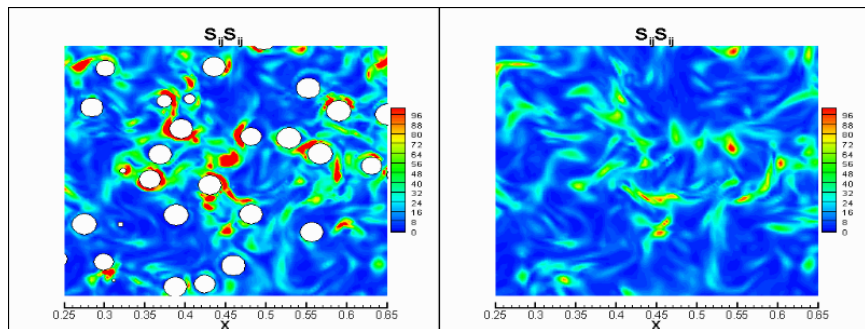
# Falling droplet test II

## VORTICITY ALONG X-AXIS



# Future developments

We will replace the solid particles with droplets, and examine the effect on the turbulence structure.



# Aknowledgments

- ▶ NSF Award Number: 0933085  
Program Officer: Ashok Sangani
  
- ▶ NSF-PRAC Award 1144323  
Program Officer: Irene Qualters
  
  
- ▶ BW Support: Dr. Bill Kramer & Manisha Gajbe