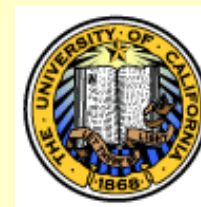


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# RELEASE and ATMOSPHERIC DISPERSAL of LIQUID AGENTS

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Theo Theofanous (PI)  
University of California, Santa Barbara

Rich Couch, Program Manager  
Lawrence Livermore National Laboratory

***S&T CBIS October 25-28, 2005***



# Operational Capability to be Provided

**Source Term**

**Aerobreakup**

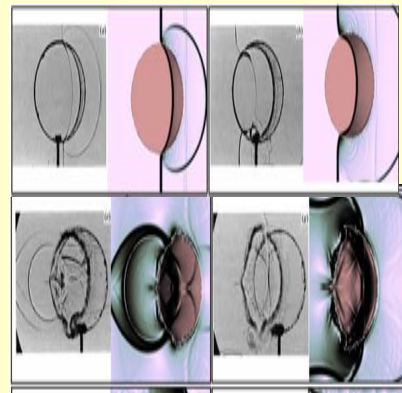
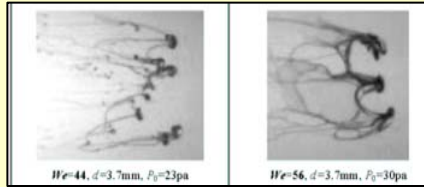


**Experiments**

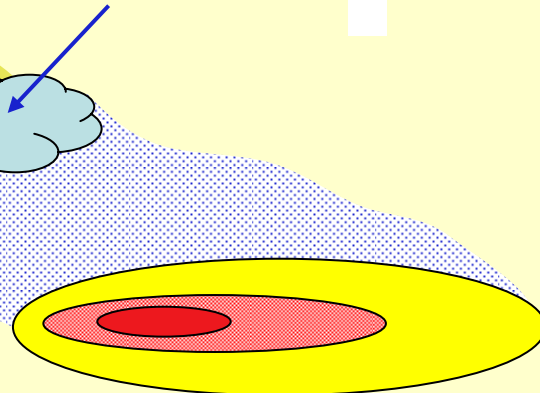


+

**Numerical Simulations**

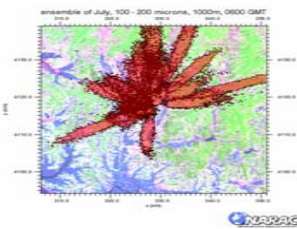


**Atmospheric Dispersion**



**Deposition and Exposure**

**Consequence Assessments**

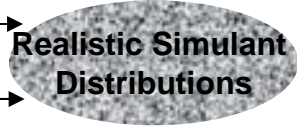


**Source Term Model**

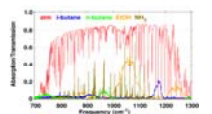
Optical



Radar

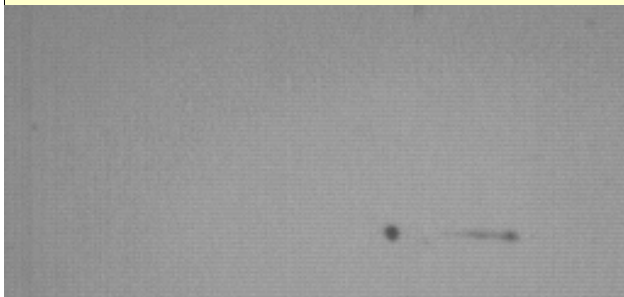


**Signatures**



## Controlling Mechanisms: VISCOELASTICITY

Rather than breaking into droplets, viscoelastic liquids tear into threads and sheets that resist pinch-off



Newtonian



Viscous



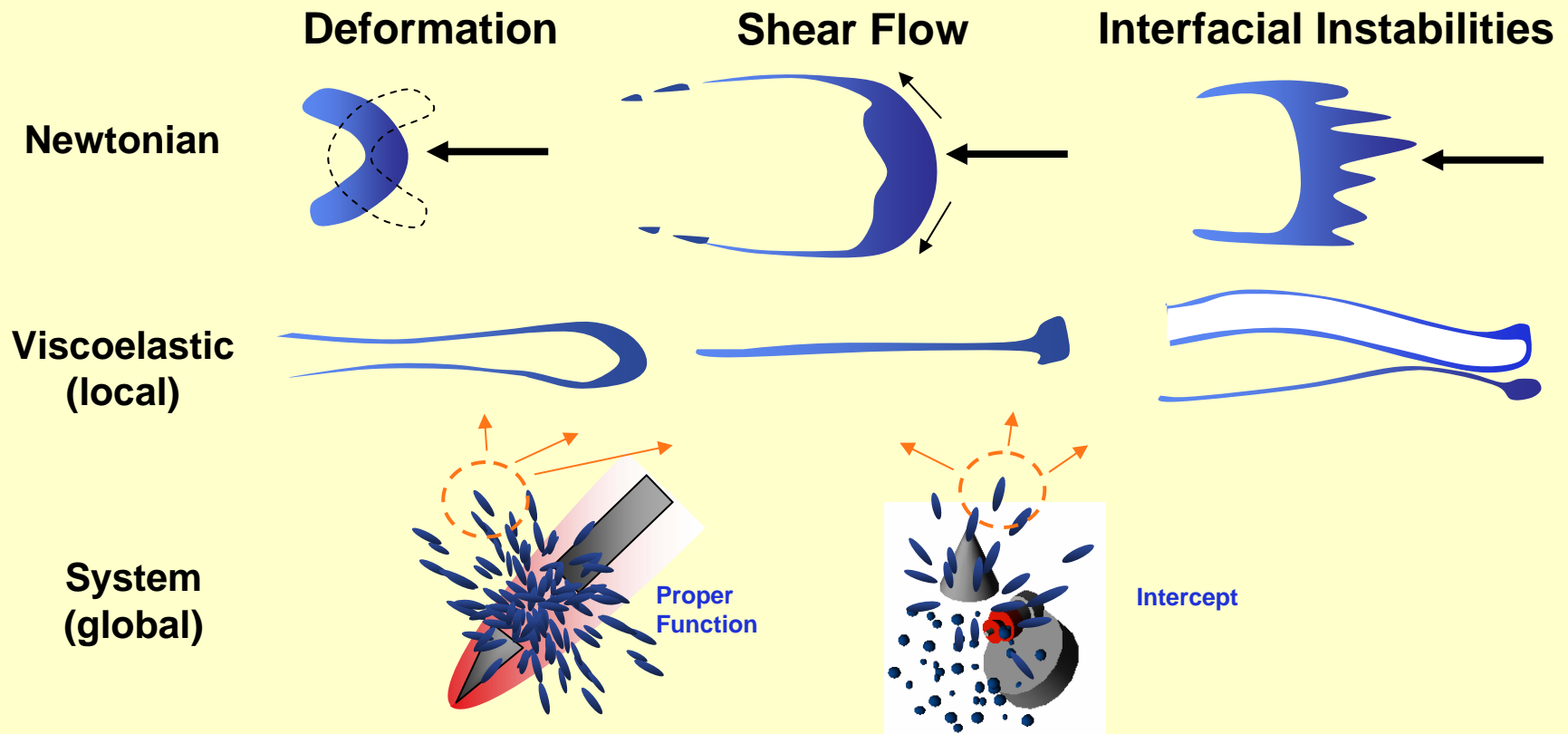
Viscoelastic

“Thickener” is added precisely for the purpose of controlling atomization . . .

**Concentration and Length of Polymer Chain  
selected to “Tailor” Effect**

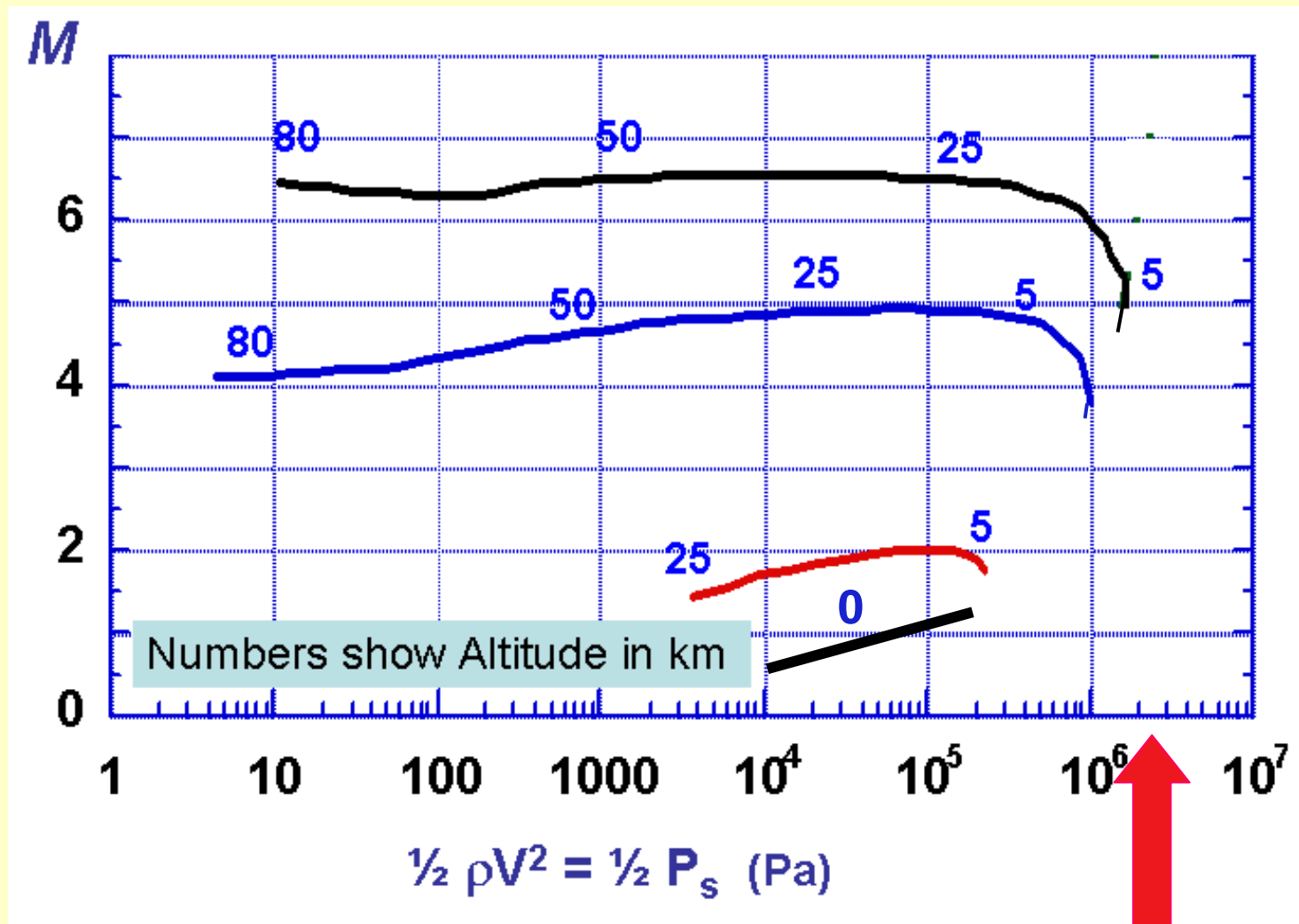
# Controlling Mechanisms: Aerodynamic History

Aerodynamic interactions result in a complex superposition of mechanisms that are highly sensitive to  $\rho v^2$ .



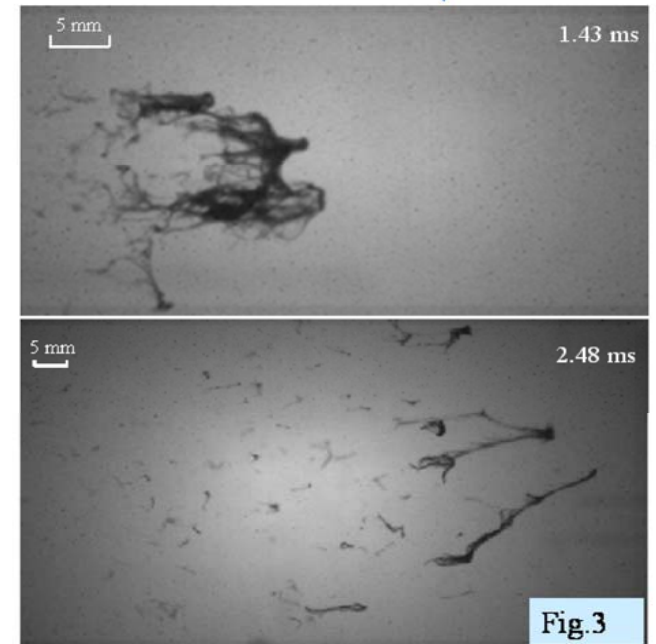
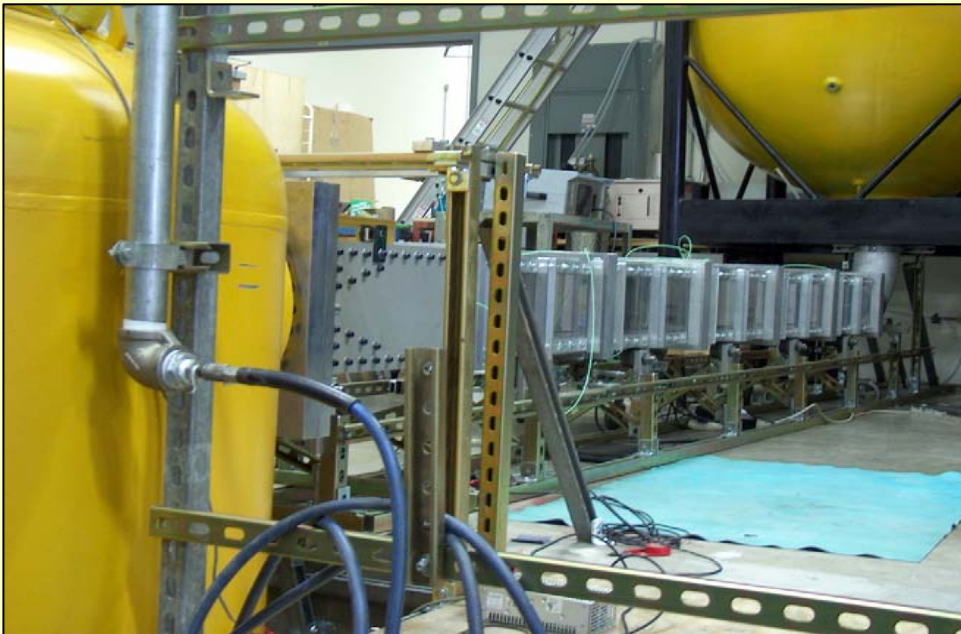
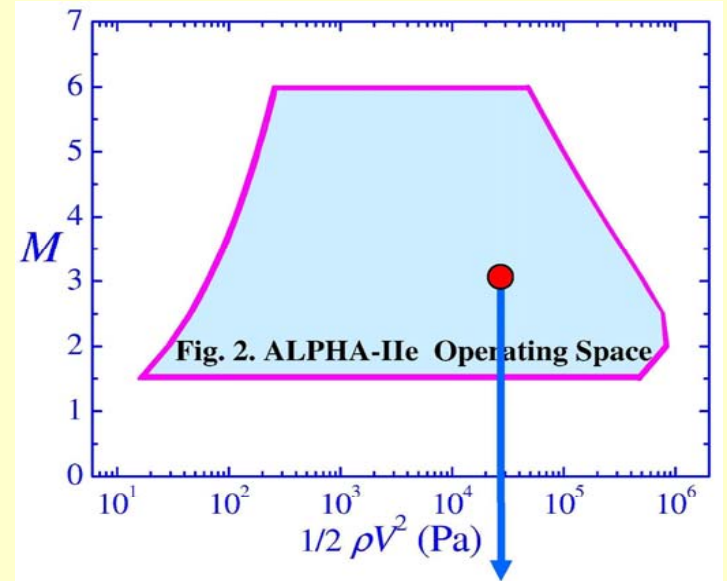
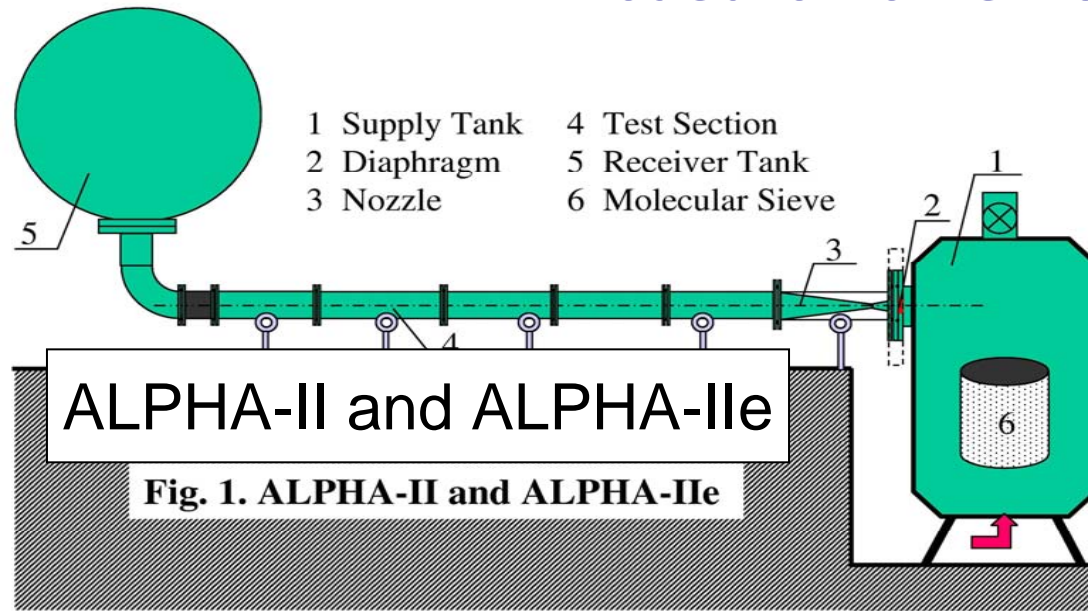
**Scaling:** From Droplet.....to Beer Can..... to Warhead Quantities

# All Release Conditions are Achievable in Experiments



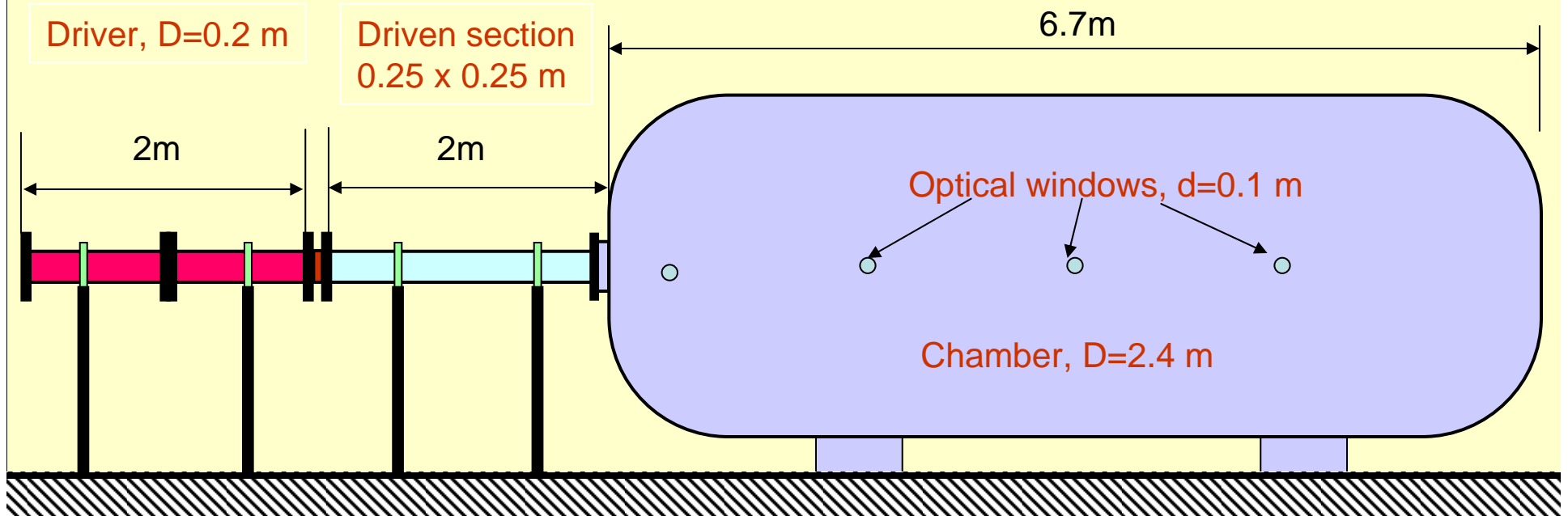


# Using the Laboratory as Frame of Reference Makes Measurements Possible

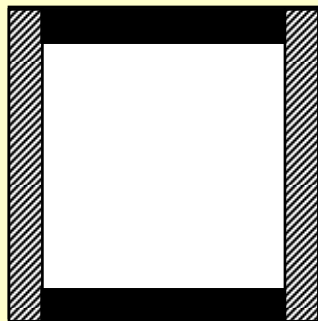




# ASOS Overall (1: 45)



Cross section of Expansion section (1:8)



Transparent

Special : He-N<sub>2</sub> & Discontinuity  
Aerodynamic History





# A Hierarchy of Objectives

**Local Scaling** .....  $We, M, Oh, R_\tau$  ..... **Lower Bound**  
Principally with Experiments/Theory/DNS

**System Scaling** ..... **Realistic/Predictive/Adaptable**

mass ratio

release (boundary) conditions

aerodynamic history.....

*shielding*

*coalescence*

*shock dynamics*

*cloud permeability*

*length scales (  $We, M, Oh, R_\tau$  )*

Principally with Experiments/Theory/EFM

# Major Results

- On Data Base development we have proven all aspects of the experimental technique and begun Production Runs (well ahead of schedule),
- We have shown experimentally that VE drops can survive intact at  $We \sim 4,000!$  Or  $1/2\rho v^2 = 2 \cdot 10^5 !$
- We developed a theoretical understanding of the mechanisms for Newtonian/Viscous liquid breakup over the whole range of regimes, unified all data, and corrected major, long-standing misconceptions,
- On DNS we achieved the sharp treatment of interfaces, and established capability to compute instabilities on shocked, high acoustic impedance mismatch interfaces.

# Scope of this Presentation

- Develop Data Bases (Experiments)  
 $10^4 < \frac{1}{2} rv^2 < 10^5$ ,  $M=3$  (ALPHA II); ND, VD ;
- Understand Key Physics (Discrete/Dilute)  
Break-up Regimes with Newtonian (Viscous) Liquids
- Understand Key Physics (Discrete/Dilute)  
Break-up Regimes with Viscoelastic Liquids (Small Drops)
- Sharp Treatment of Interfaces  
Fidelity of Instability Prediction by DNS

# Scope of this Presentation

- Develop Data Bases (Experiments)

$$10^4 < \frac{1}{2} rv^2 < 10^5, \quad M=3 \quad (\text{ALPHA II}); \quad \text{ND, VD} ;$$

- Understand Key Physics (Discrete/Dilute)

Break-up Regimes with Newtonian (Viscous) Liquids

- Understand Key Physics (Discrete/Dilute)

Break-up Regimes with Viscoelastic Liquids (Small Drops)

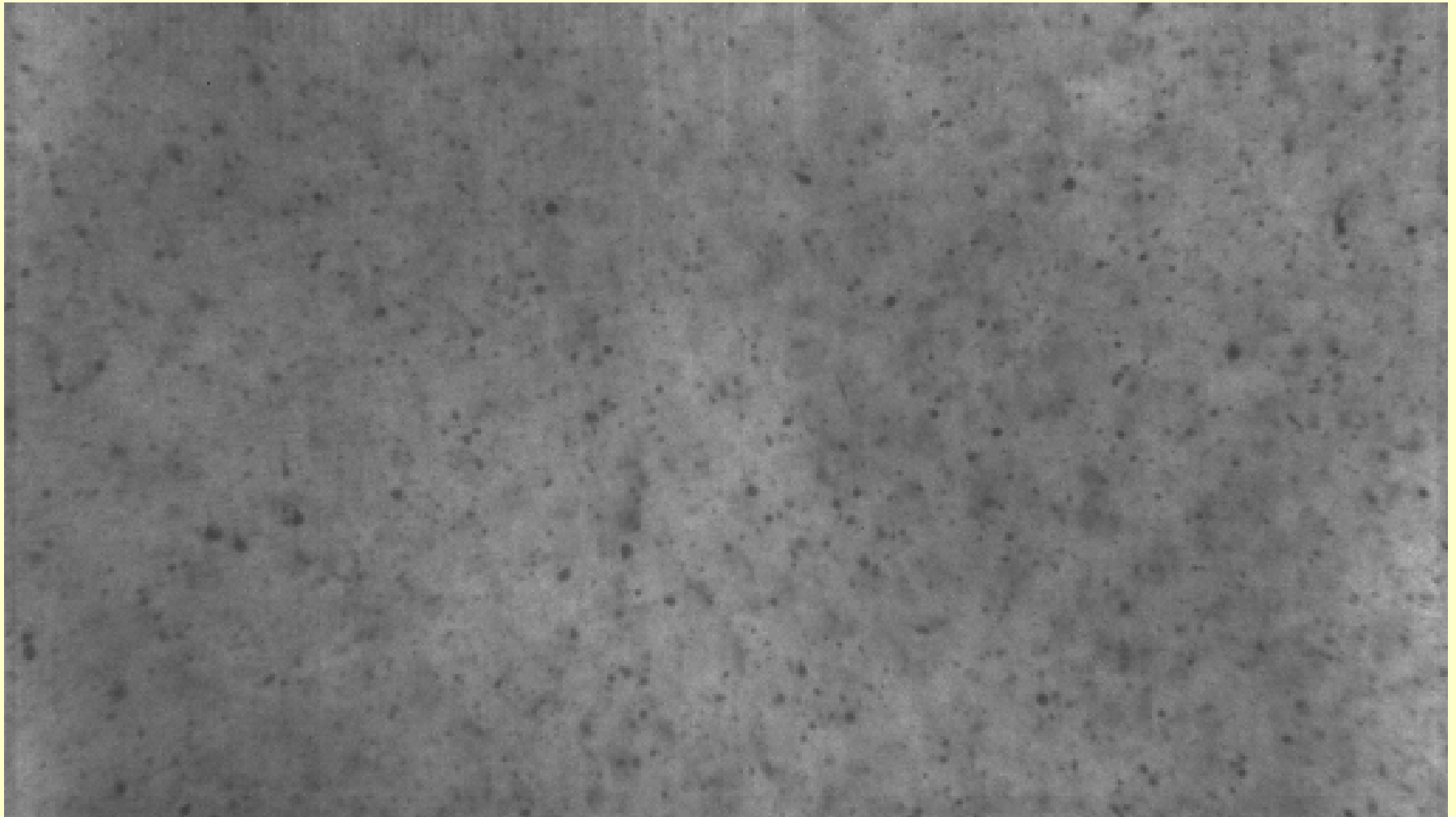
- Sharp Treatment of Interfaces

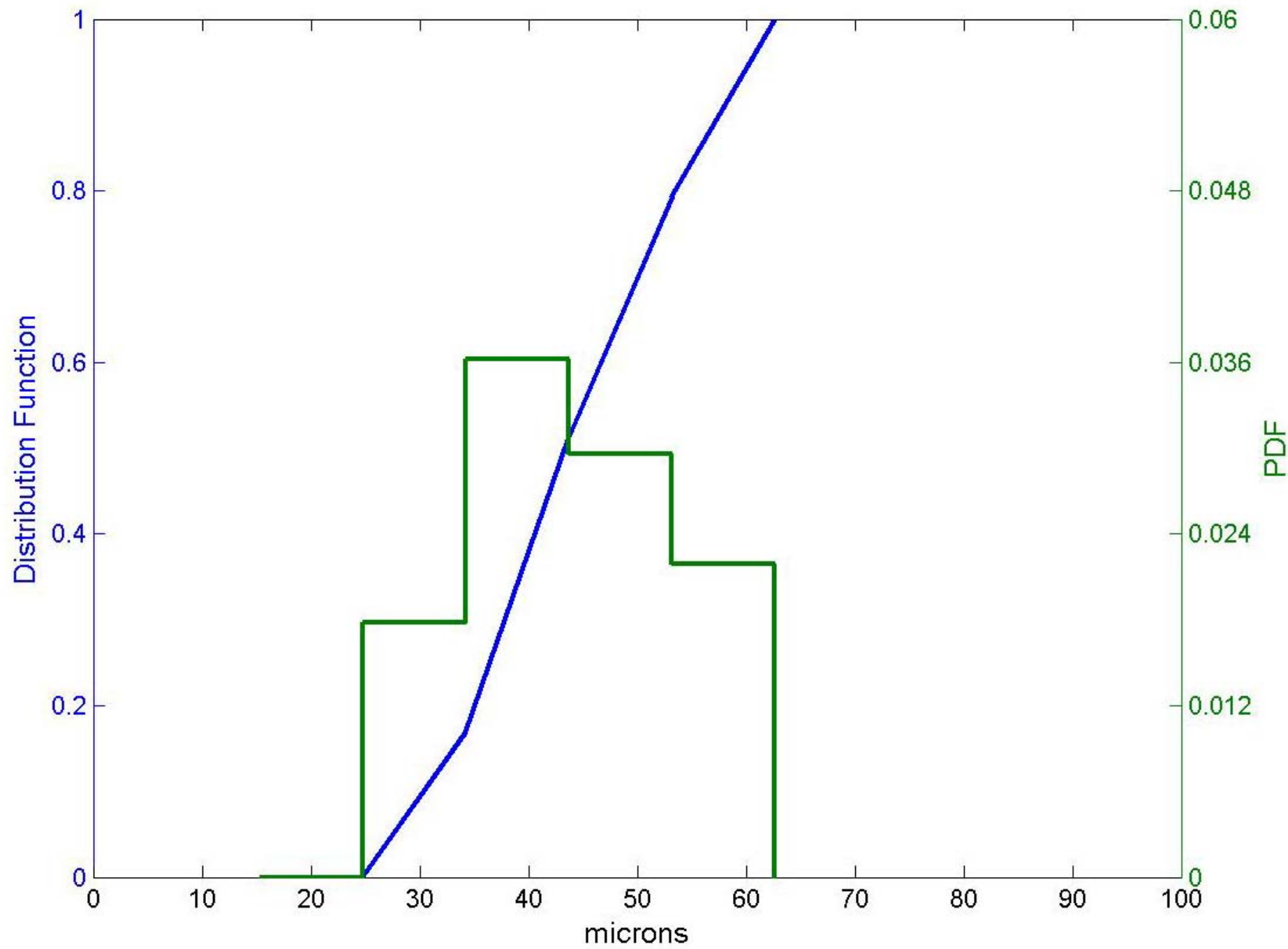
Fidelity of Instability Prediction by DNS



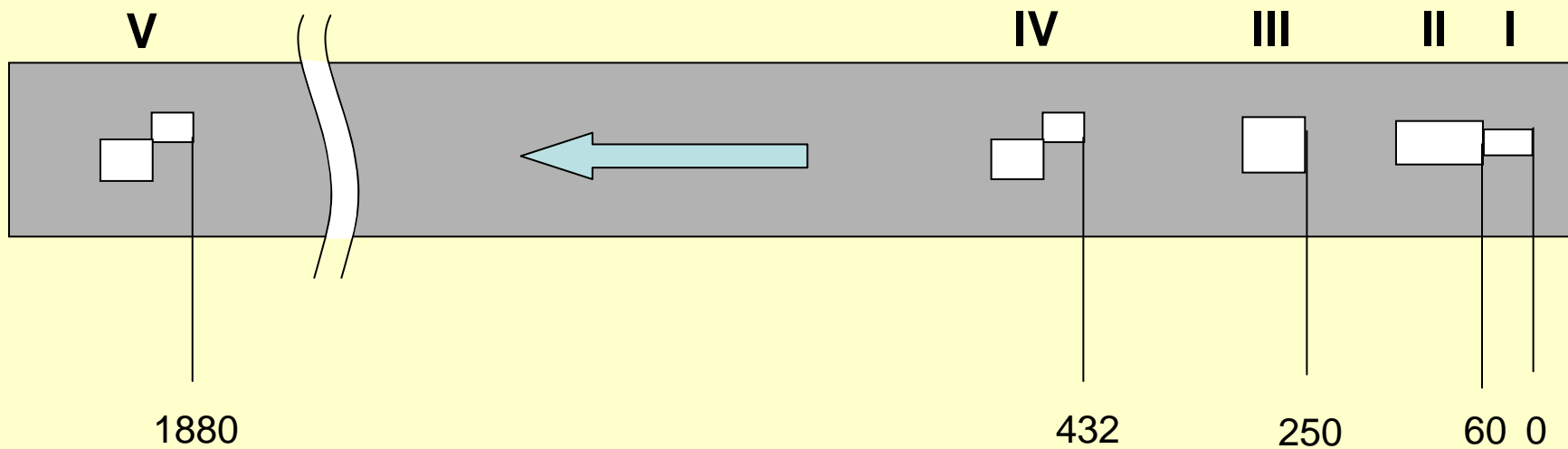
# We have the first Newtonian Particle Size Distributions in the shear regime

100  $\mu\text{m}$





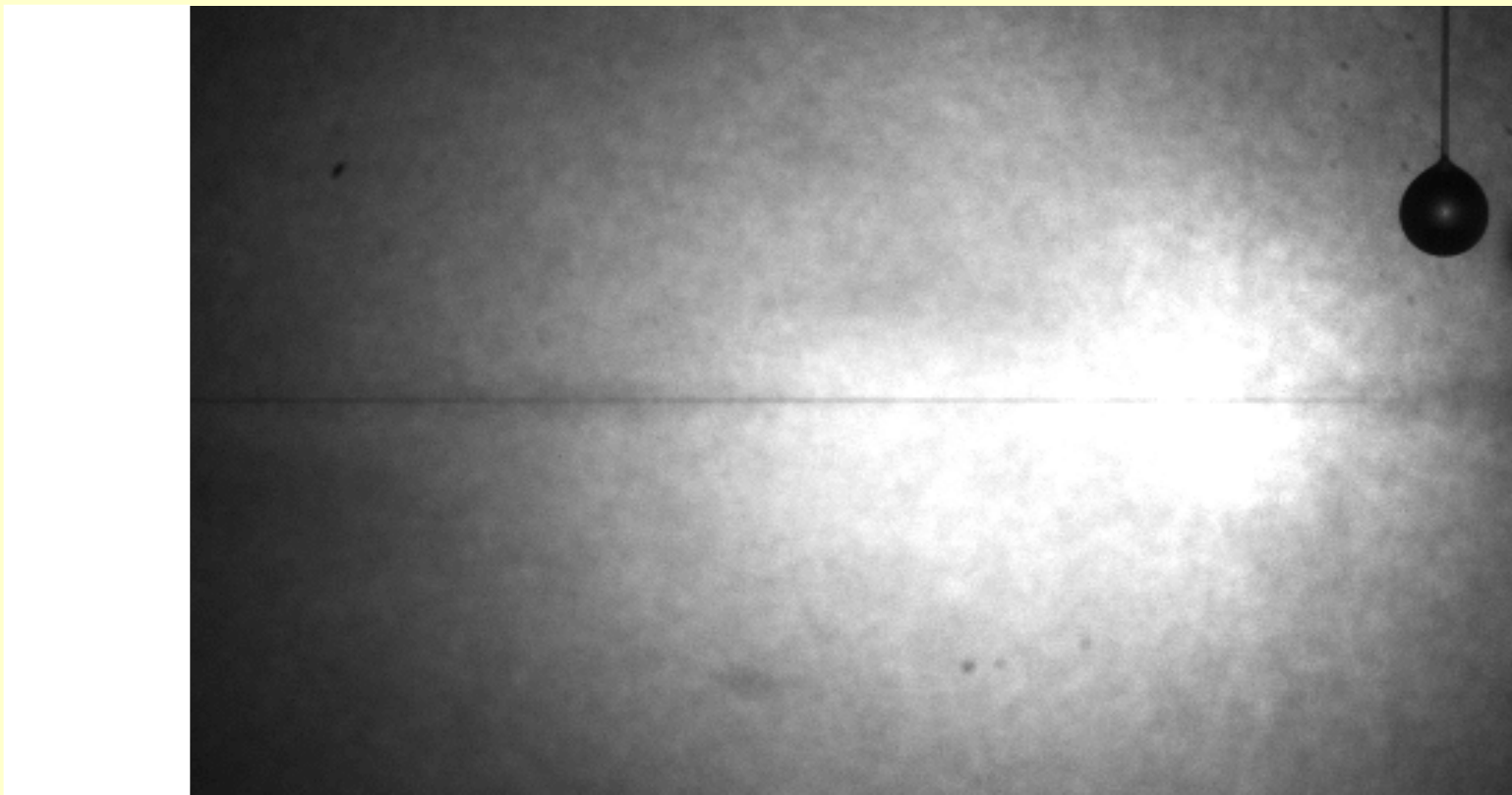
# Stage Arrangement



Stages I – V are sampling stages using high-speed cameras.

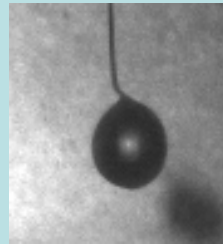
Unit: mm

**Breakup at  $\frac{1}{2} \rho V^2$  of  $10^5$  Pa**

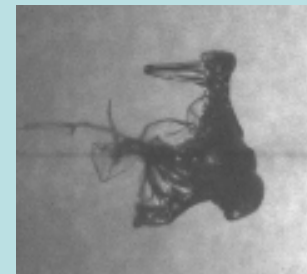
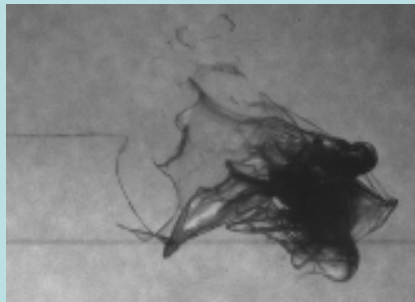


**3.8%PSBMA+TBP**  
 **$d = 3.4$  mm,  $We=29,000$**

## *Breakup History at the Dynamic Pressure of $10^4$ Pa*



Stage I



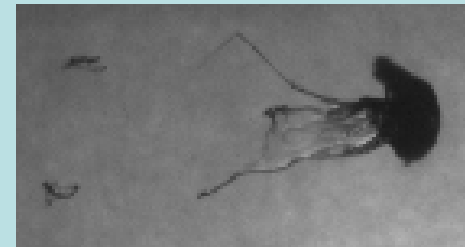
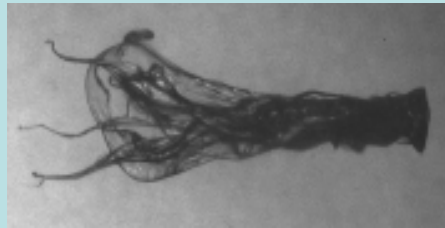
10 mm



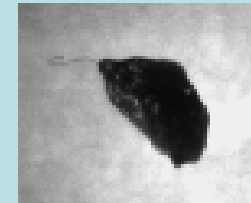
# *Breakup History at the Dynamic Pressure of $10^4$ Pa*

Stage II

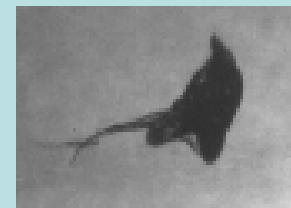
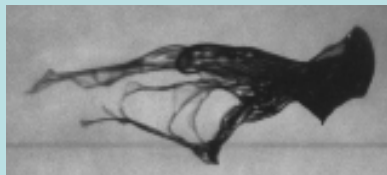
Run 1



Run 2



Run 3



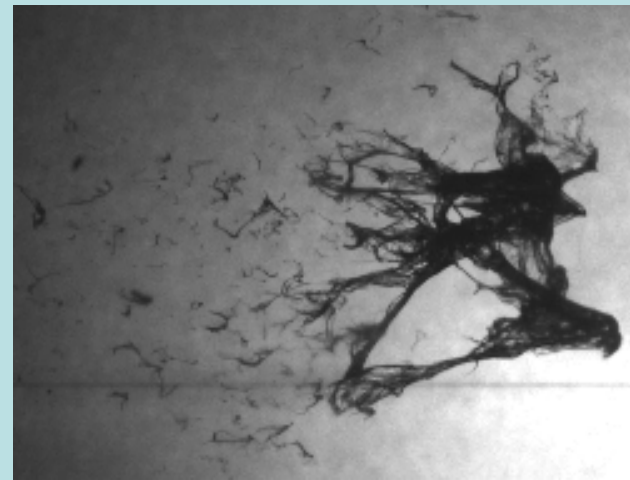
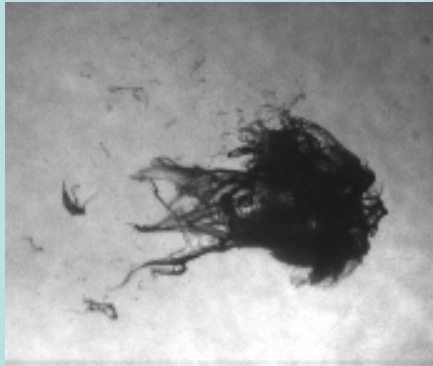
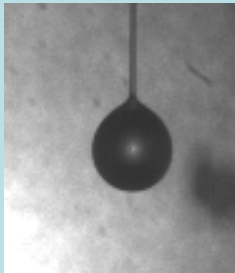
Camera I

10 mm

Camera II

*Breakup History of a Polymeric drop at the  
dynamic pressure of  $10^5$  Pa*

Stage I

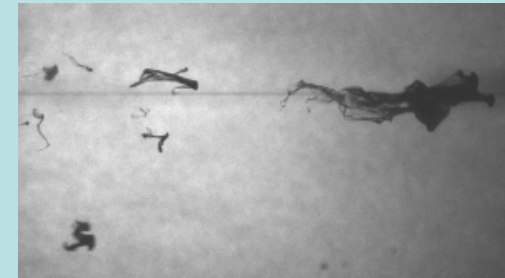
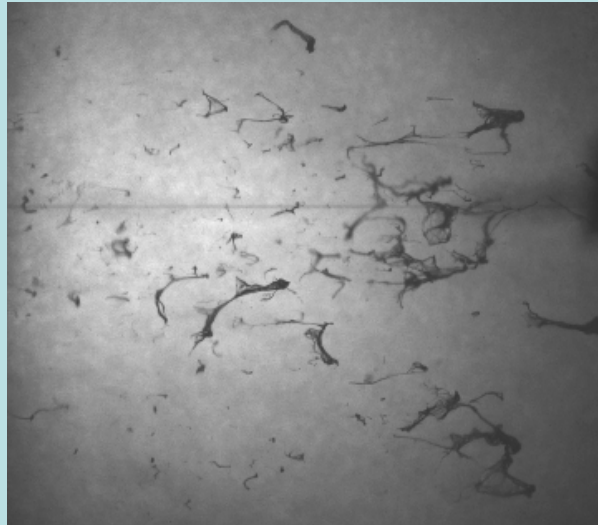


10 mm

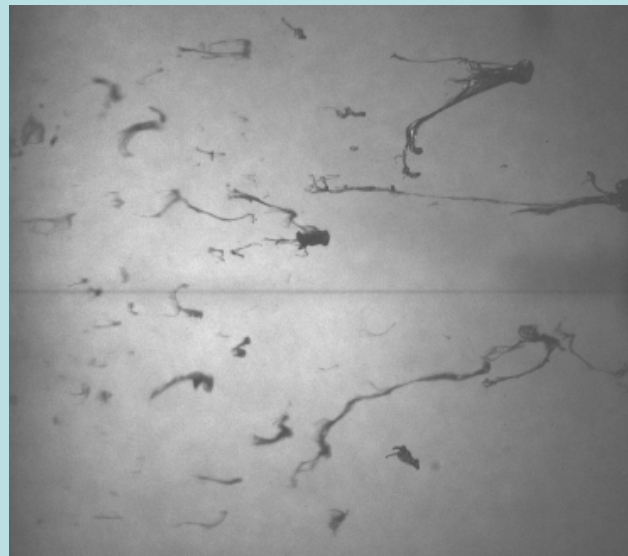
# *Breakup History at Dynamic Pressure of $10^5$ Pa*

Stage II

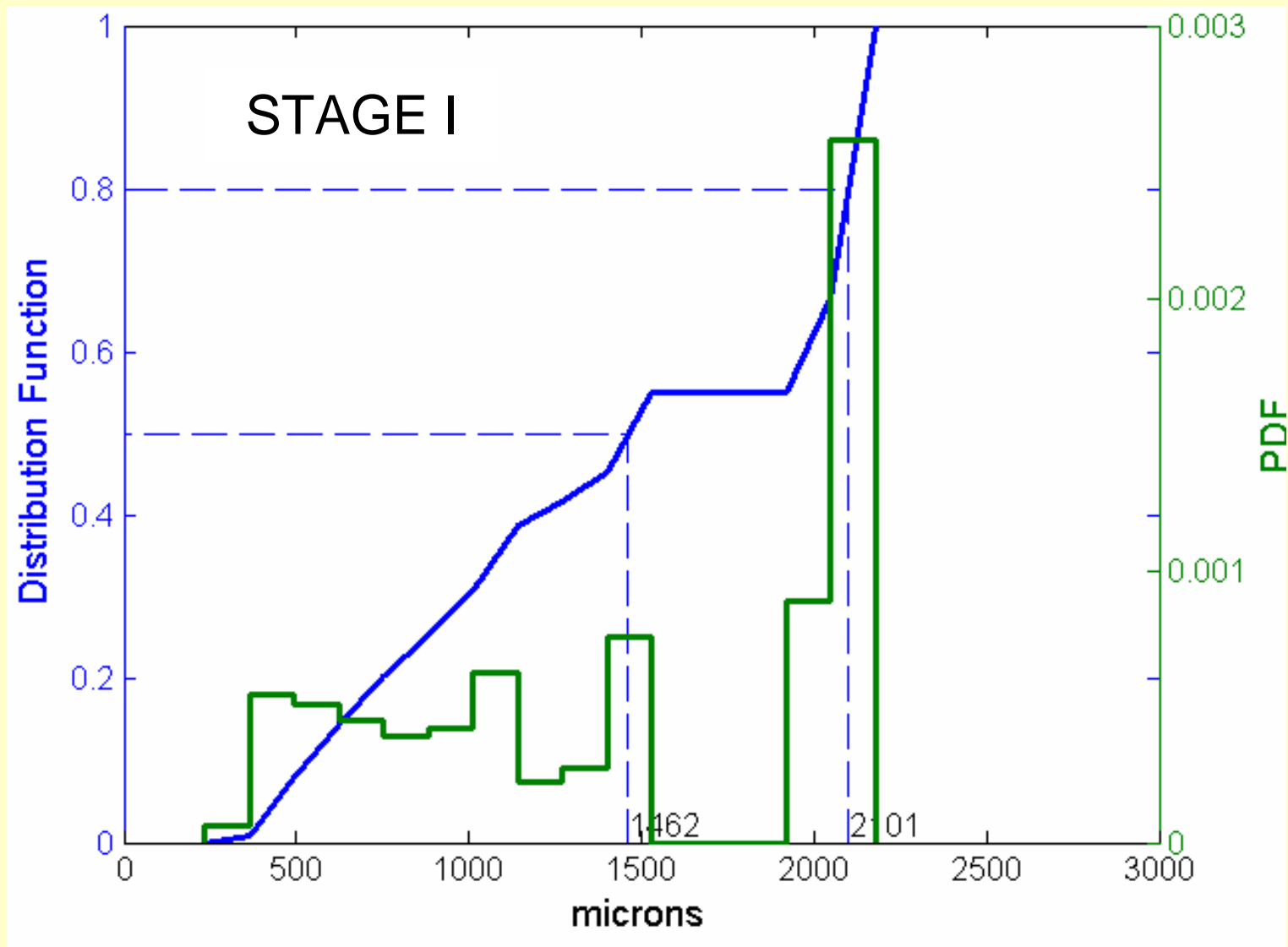
Run 2



Run 3



10 mm

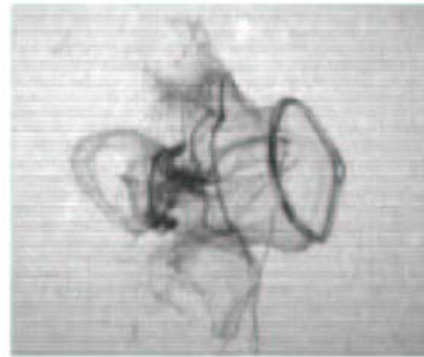


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- Understand Key Physics (Discrete/Dilute)  
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- Sharp Treatment of Interfaces  
Fidelity of Instability Prediction by DNS

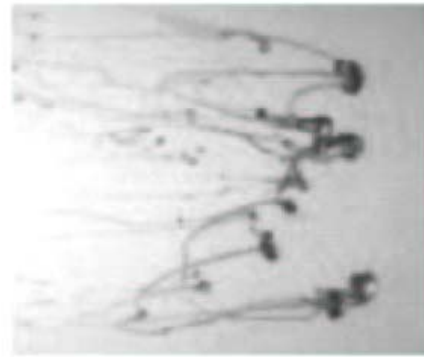


R  
T  
P



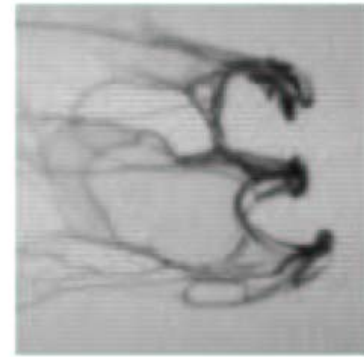
2

$We=28, d=3.8\text{mm}, P_0=15\text{pa}$



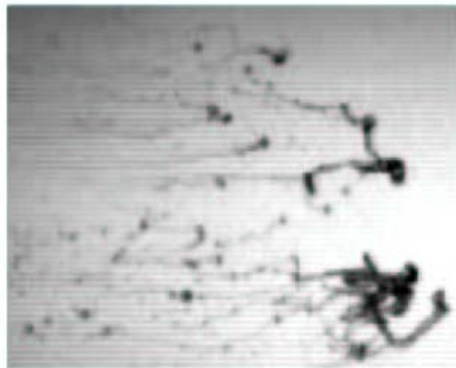
3

$We=44, d=3.7\text{mm}, P_0=23\text{pa}$



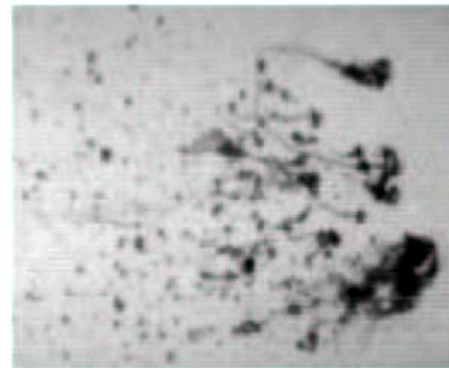
4

$We=56, d=3.7\text{mm}, P_0=30\text{pa}$



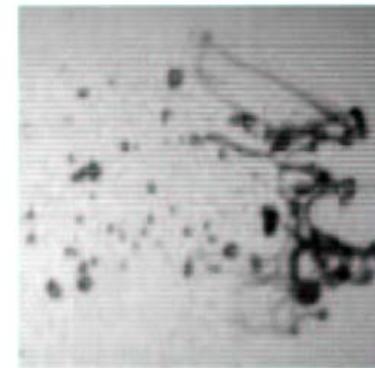
2-3

$We=58, d=3.7\text{mm}, P_0=31\text{pa}$



3

$We=63, d=3.7\text{mm}, P_0=35\text{pa}$



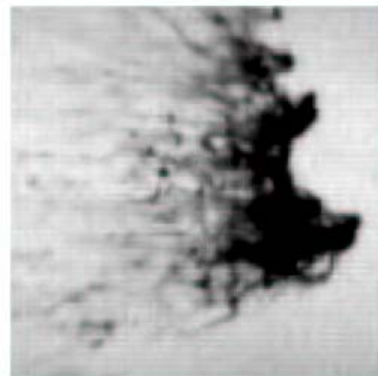
3-4

$We=68, d=3.7\text{mm}, P_0=37\text{pa}$



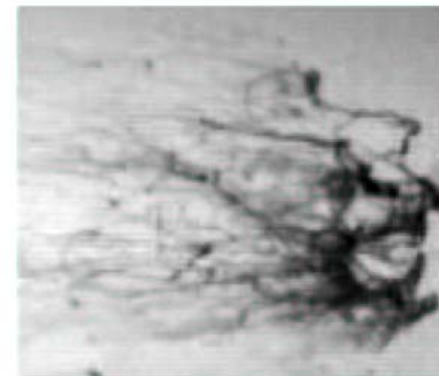
4-5

$We=109, d=3.9\text{mm}, P_0=55\text{pa}$



4-5

$We=183, d=3.7\text{mm}, P_0=100\text{pa}$

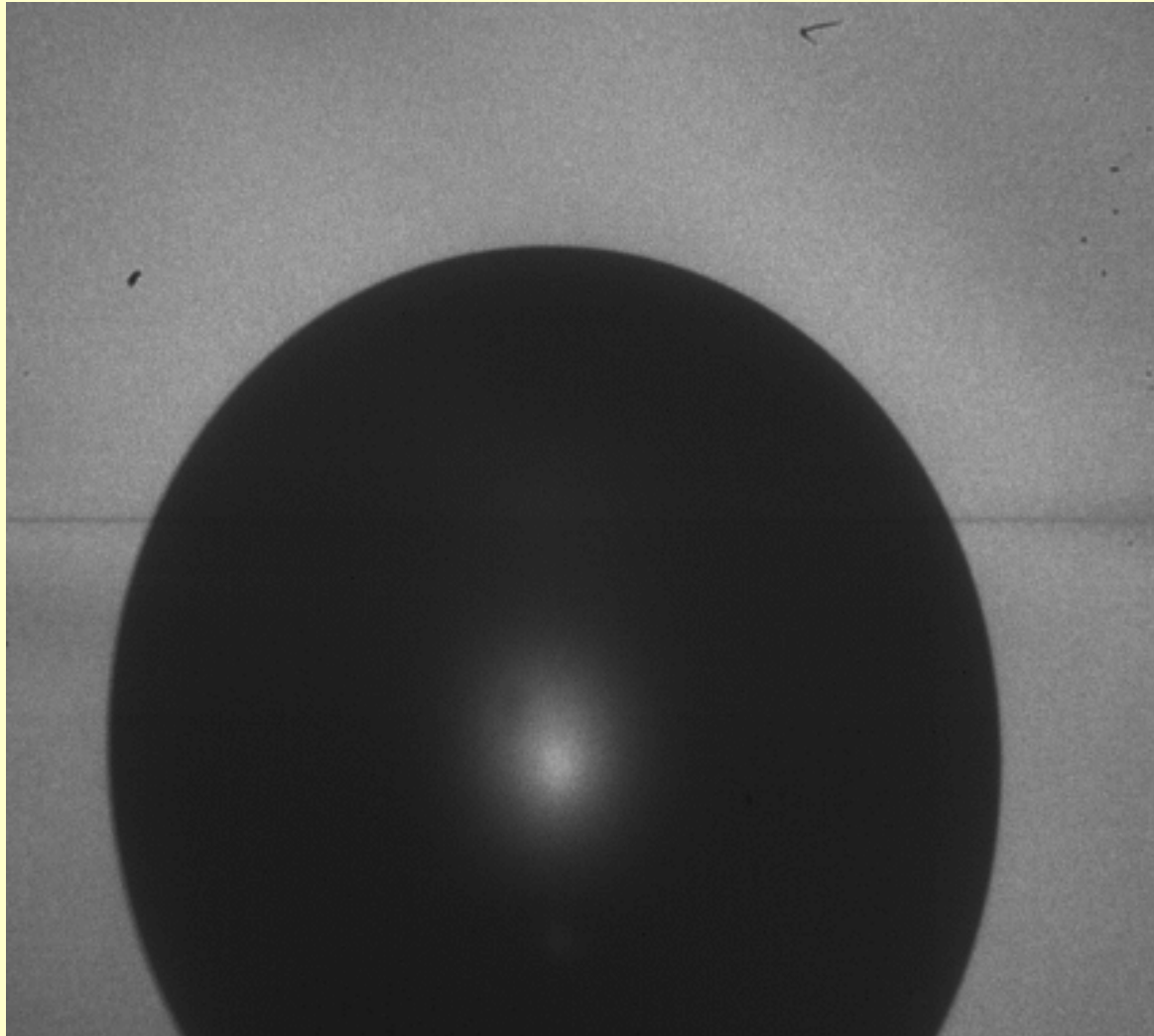


9

$We=299, d=3.7\text{mm}, P_0=160\text{pa}$

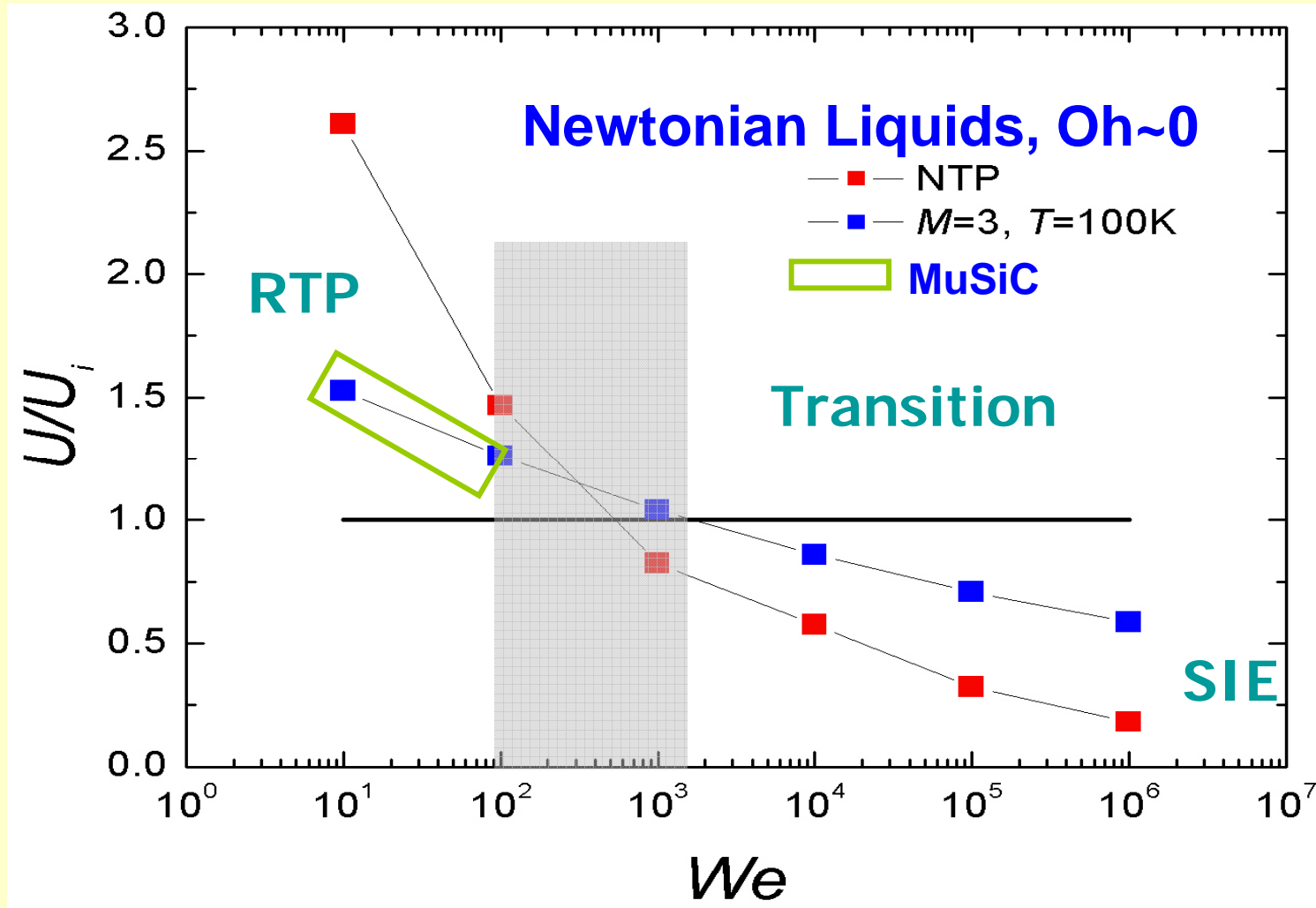
*Close-up of a TBP drop at Dynamic Pressure of  $10^5$  Pa*

**S  
I  
E**



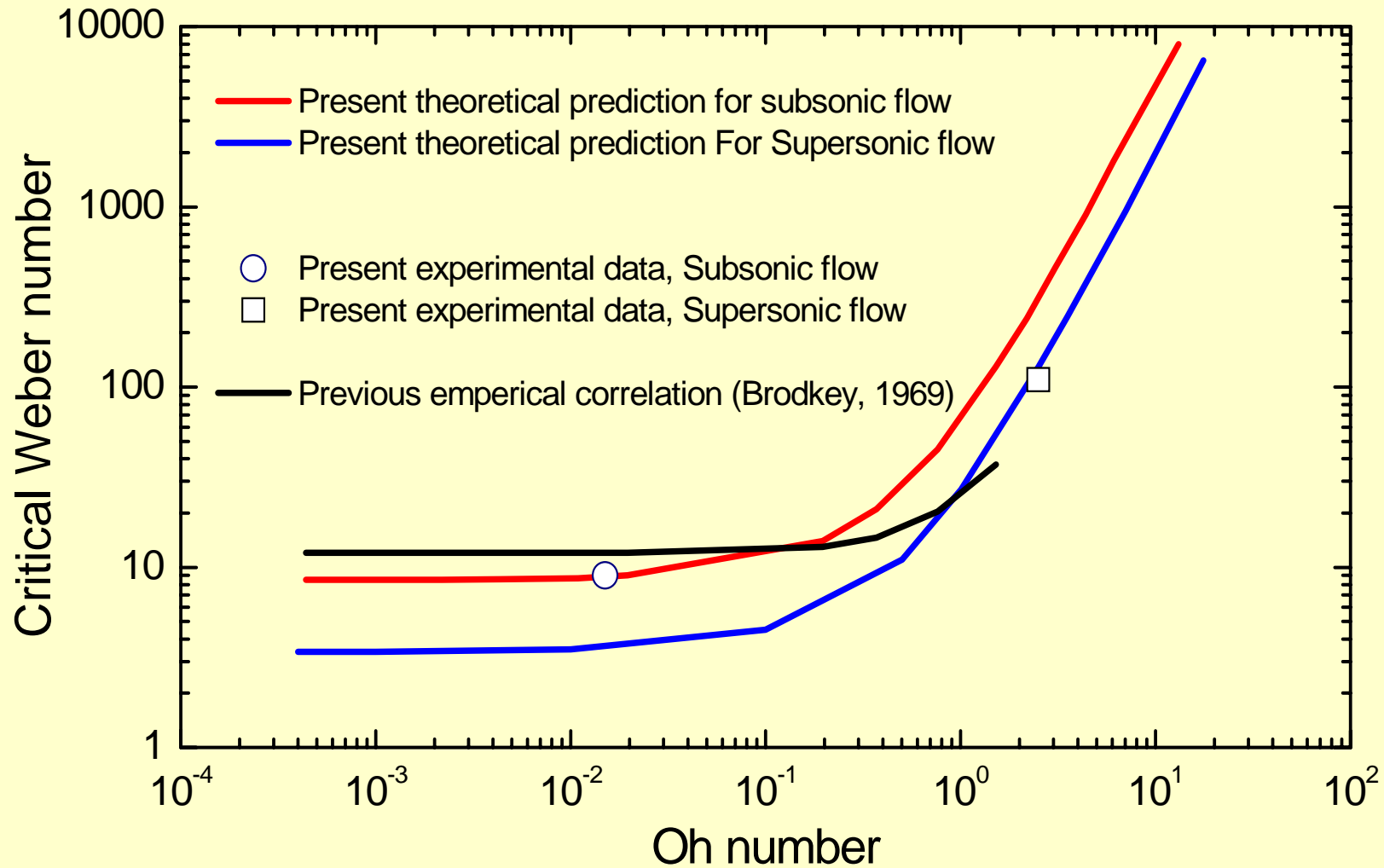
TBP drop,  $d=3.5$  mm,  $We=31,000$   
(Movie) Frame-frame time interval= $80 \mu\text{s}$

# We now have a Comprehensive Understanding of the Regimes of Aerobreakup for Newtonian Liquids



T.G.Theofanous, et al., *ASME JFE*, 2004 and IUTAM Elsevier, 2006.

# We now Understand how Viscous, Newtonian Liquids Break up.



Theory: Single Taylor Wave Penetration  
the Timing works out too.

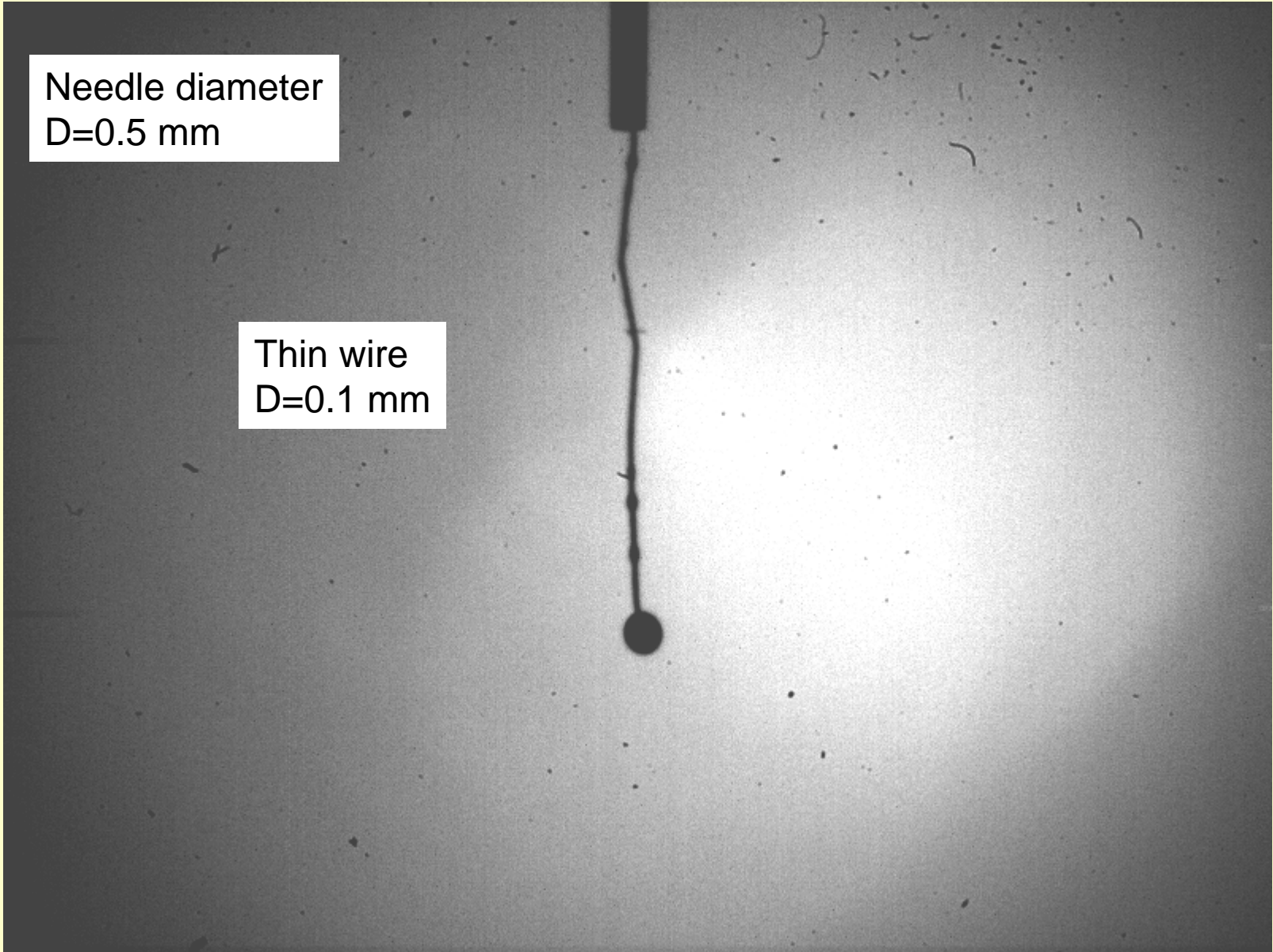
# Scope of this Presentation

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- Understand Key Physics (Discrete/Dilute)  
**Break-up Regimes with Viscoelastic Liquids (Small Drops)**
- Sharp Treatment of Interfaces  
Fidelity of Instability Prediction by DNS

## Drop Generator – Polymer Drop

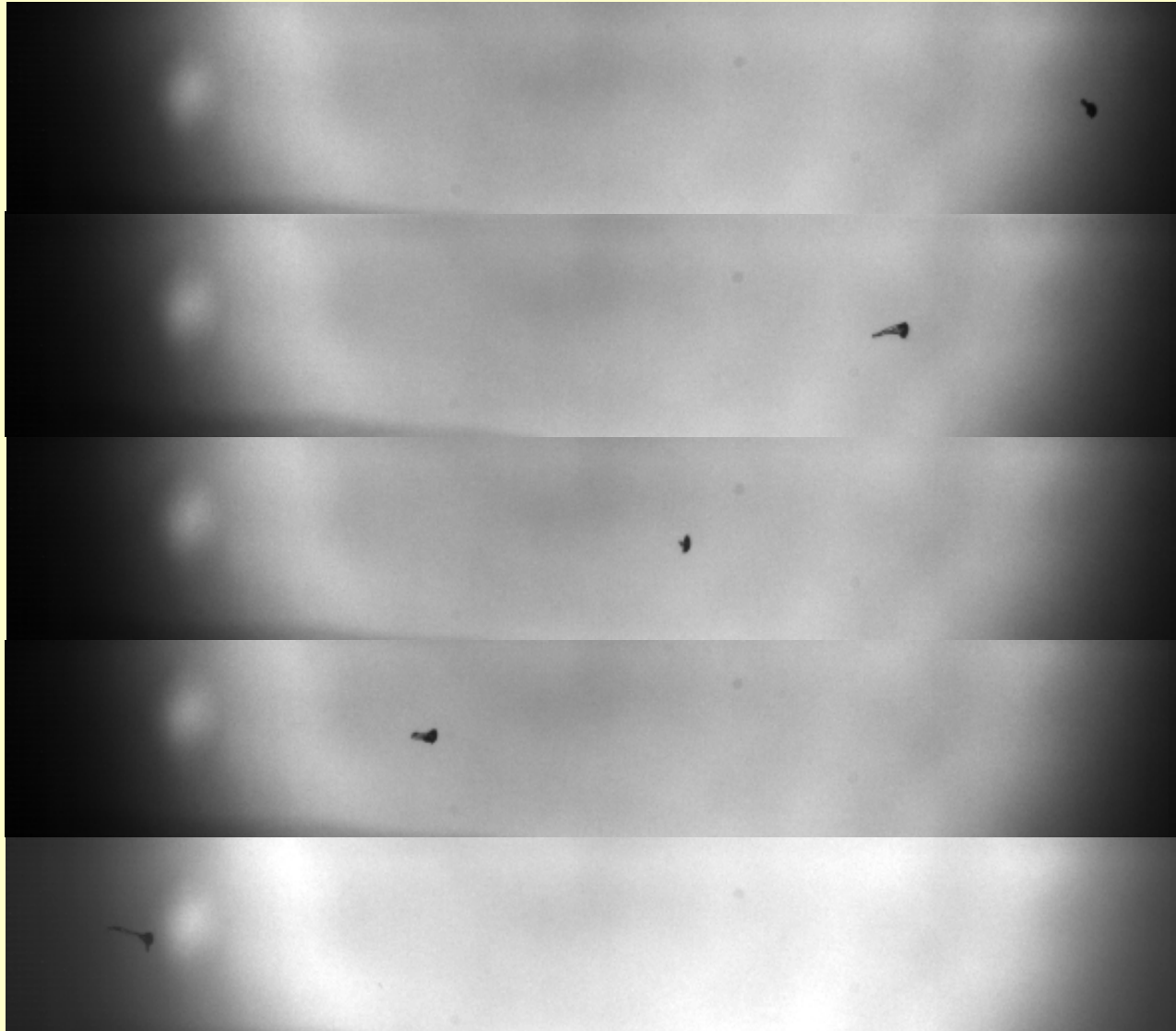
Needle diameter  
 $D=0.5$  mm

Thin wire  
 $D=0.1$  mm





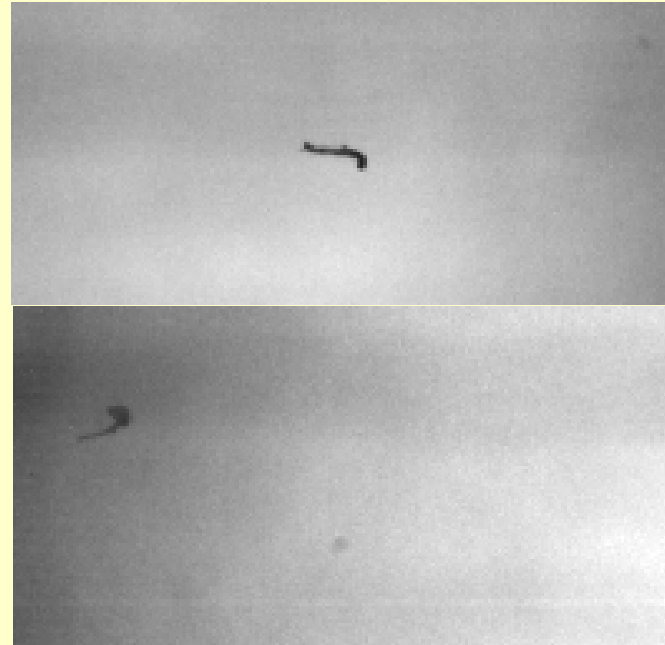
Polymer drop at  $We_0 = 4500$



$d=0.6$  mm, Drop velocity  $V=200$  m/s



## Polymer drop at $We_0 = 4100$ , 153mm Downstream



$t = 1.175$  ms

$t = 1.254$  ms

$d = 0.5$  mm, Drop velocity  $V = 335$  m/s,

$$We = 0.21 We_0$$

# Scope of this Presentation

- Develop Data Bases (Experiments)  
 $10^4 < \frac{1}{2} rv^2 < 10^5$ ,  $M=3$  (ALPHA II); ND, VD ;
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**Fidelity of Instability Prediction by DNS**

# Delta-formulation

## Transition from one fluid to another

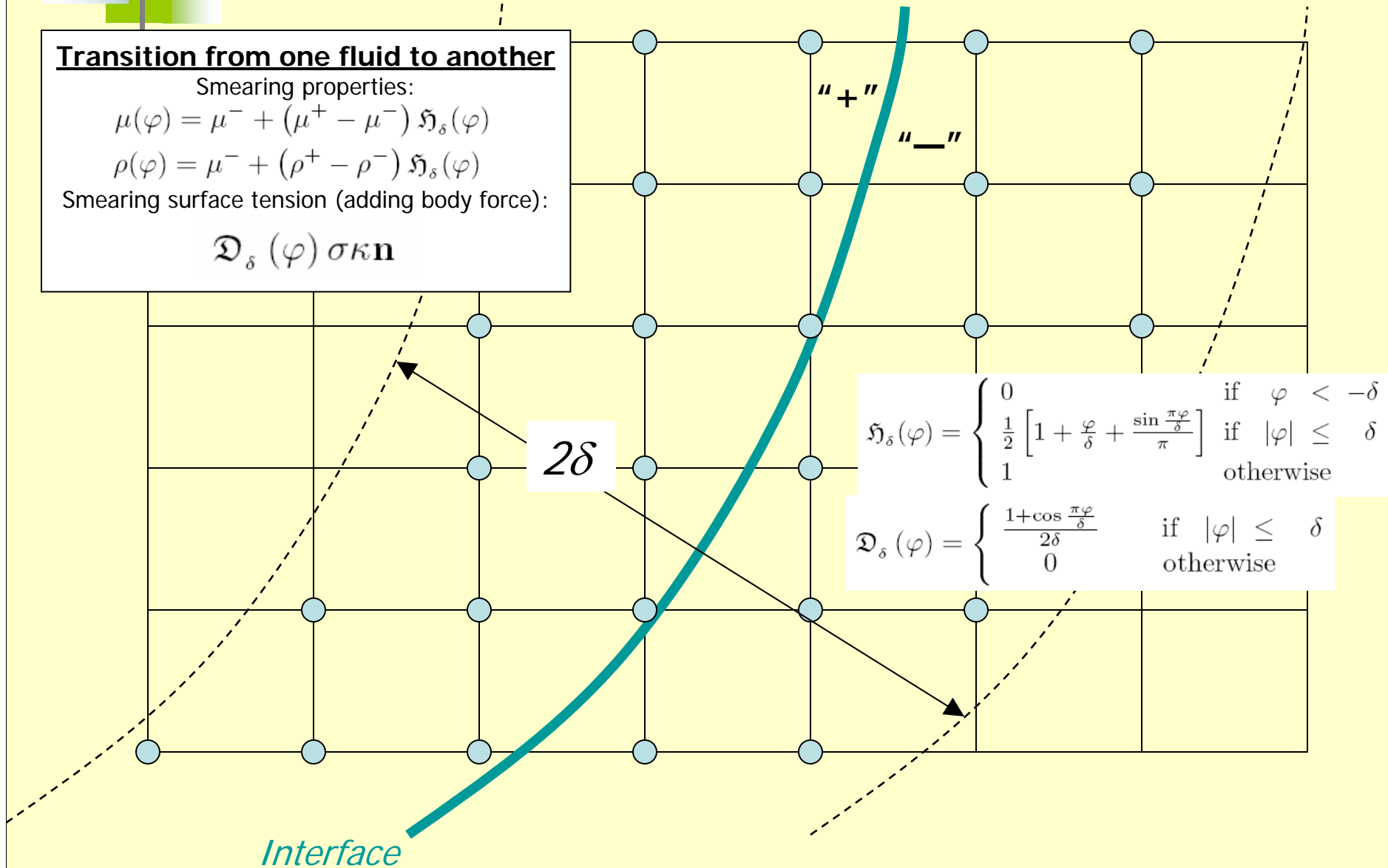
Smearing properties:

$$\mu(\varphi) = \mu^- + (\mu^+ - \mu^-) \mathfrak{H}_\delta(\varphi)$$

$$\rho(\varphi) = \rho^- + (\rho^+ - \rho^-) \mathfrak{H}_\delta(\varphi)$$

Smearing surface tension (adding body force):

$$\mathfrak{D}_\delta(\varphi) \sigma \kappa \mathbf{n}$$

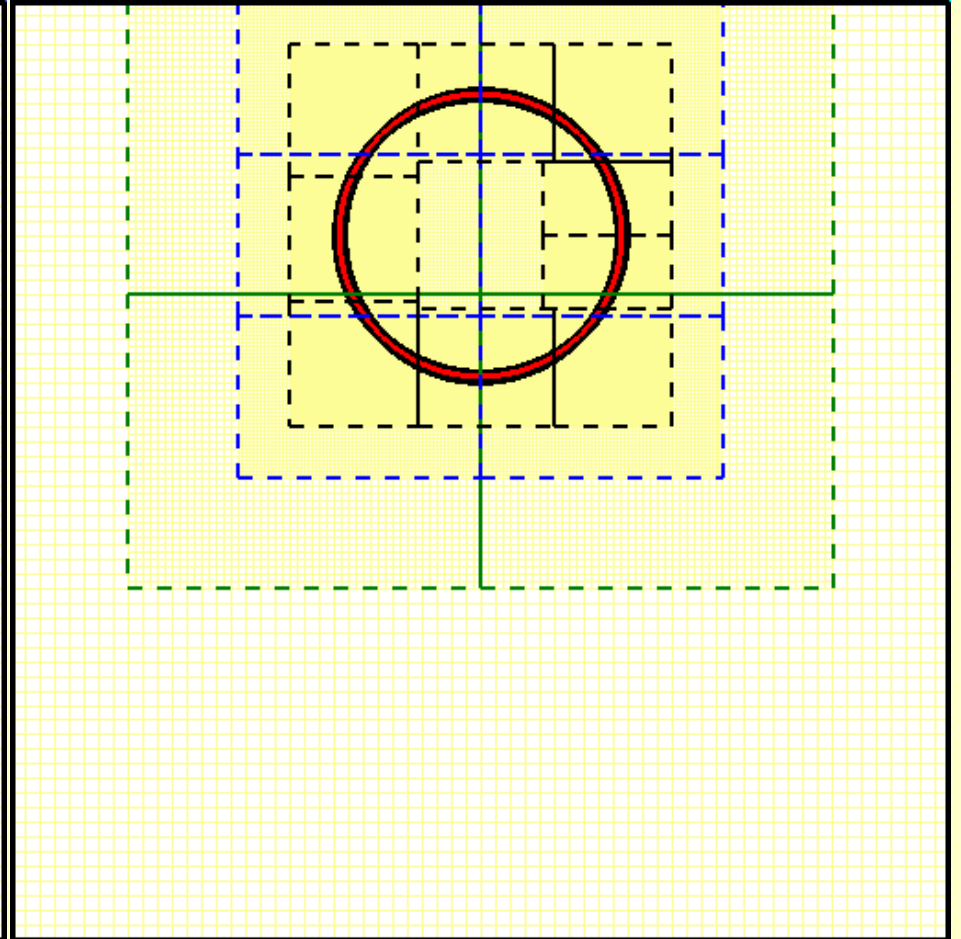
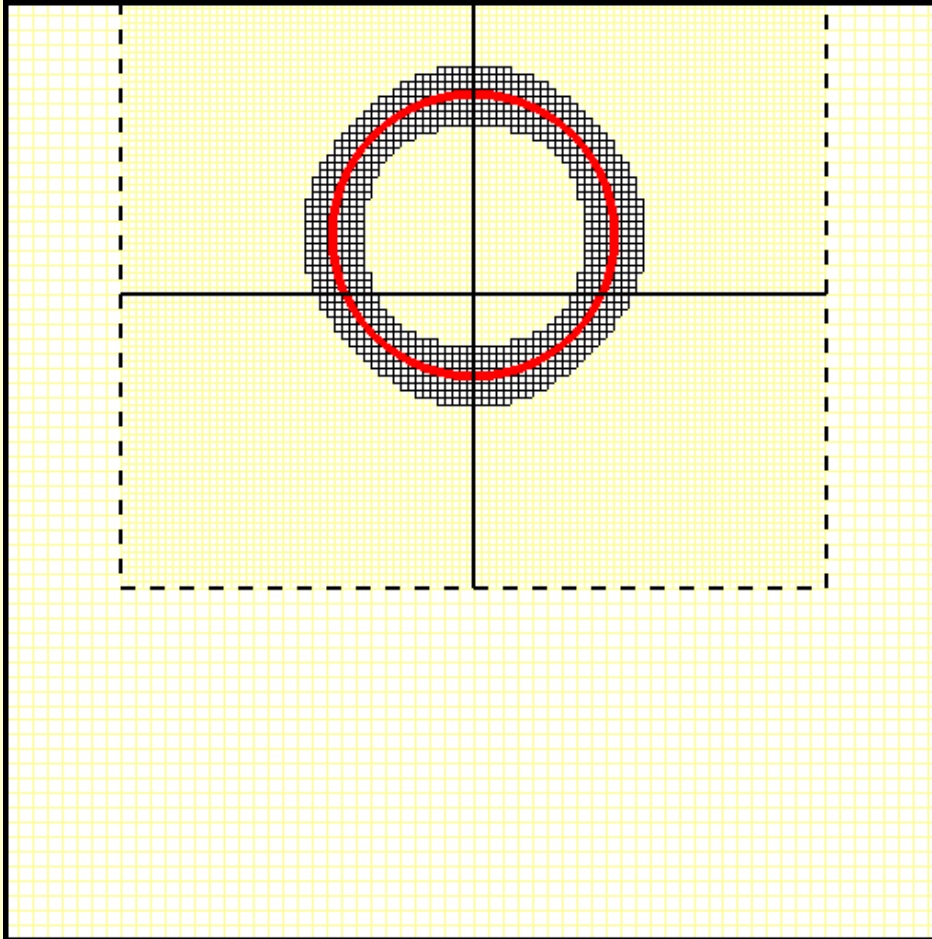


**I. ac<sup>3</sup>MR**

# Single Vortex

2 AMR levels:  $128^2$

4 AMR levels:  $512^2$  (8 processors)

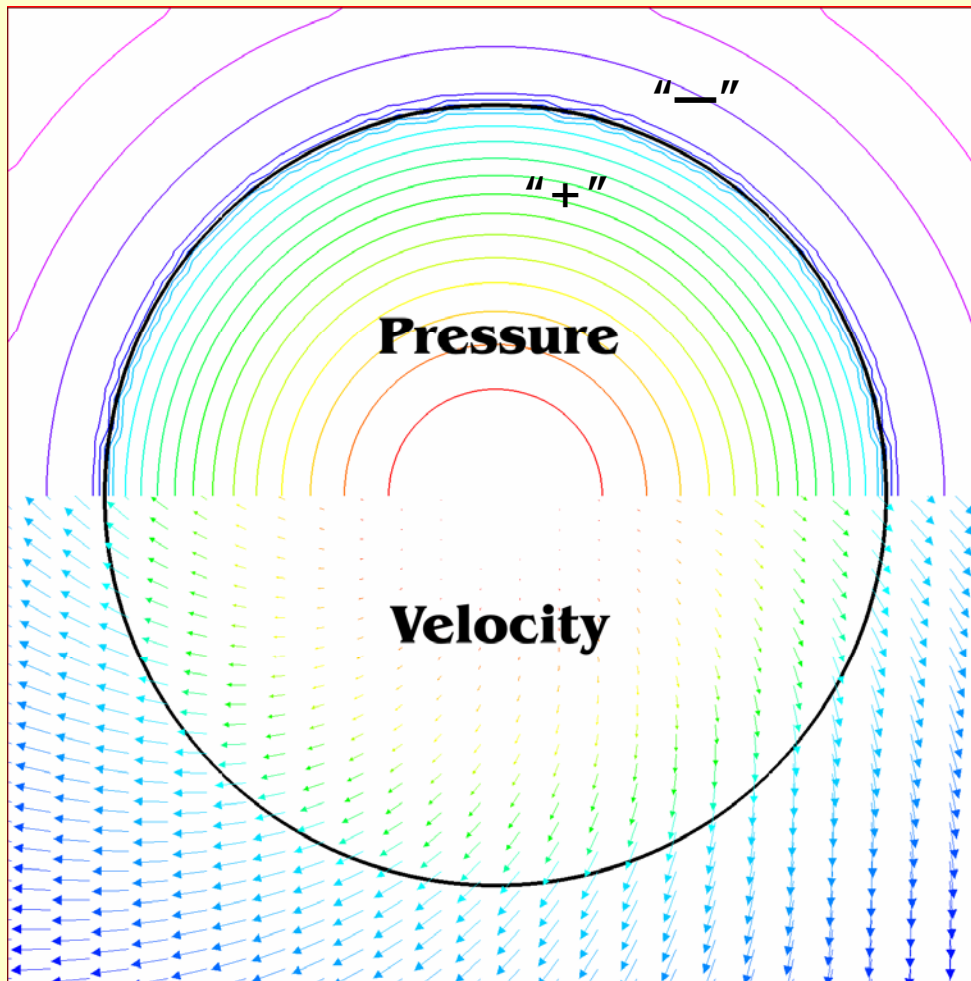


High-resolution simulations

**aC<sup>3</sup>MR**

# **V. Sharp Reconstruction (SR) of interface jump conditions**

# Grid convergence test



## Exact solution:

$$P^+(r) = P_0 + (P_1^+ - P_0) \left(\frac{r}{R}\right)^2$$

$$V_\xi^+(r) = V_{\xi I} \left(\frac{r}{R}\right)^2$$

$$V_\eta^+(r) = V_{\eta I} \left(\frac{r}{R}\right)^3$$

$$P^-(r) = P_1^- \frac{R}{r}$$

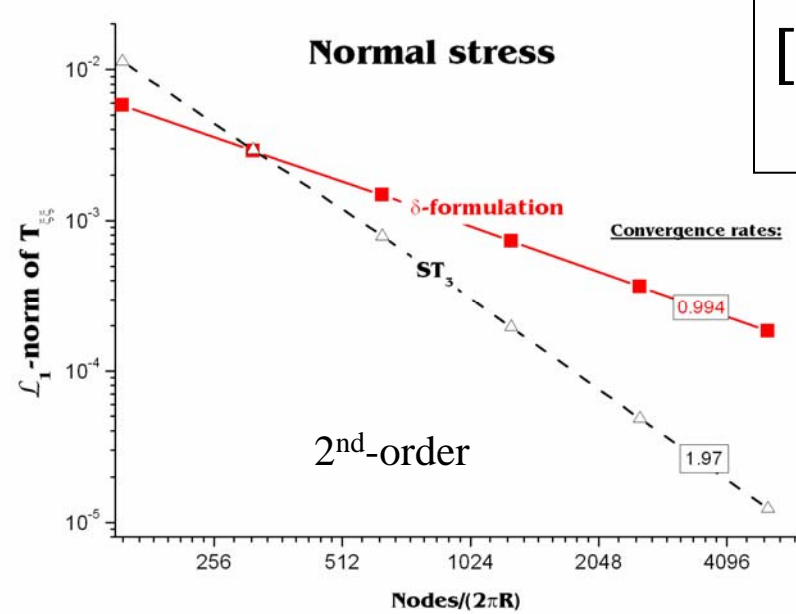
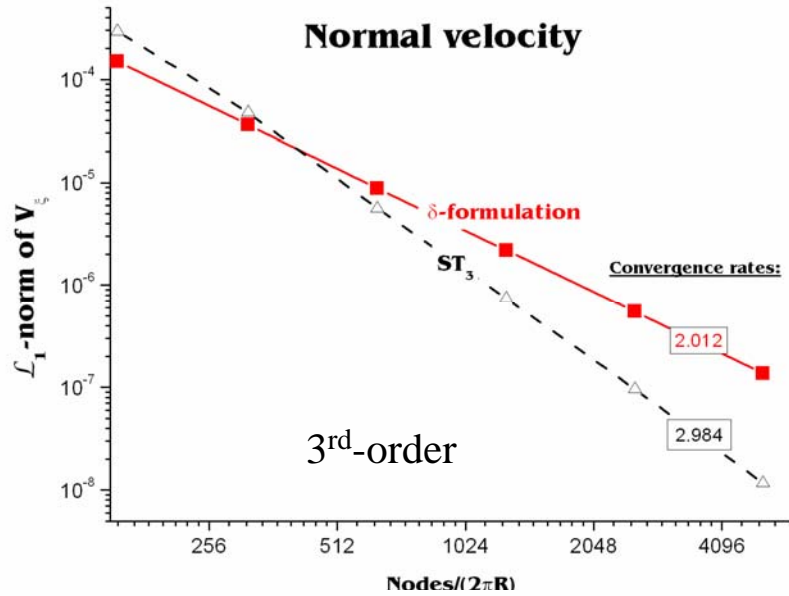
$$V_\xi^-(r) = V_{\xi I} \left(1 - 2 \langle \mu \rangle \frac{r}{R} \left(1 - \frac{r}{R}\right)\right)$$

$$V_\eta^-(r) = V_{\eta I} \left(1 - 3 \langle \mu \rangle \left(1 - \frac{r}{R}\right)\right)$$

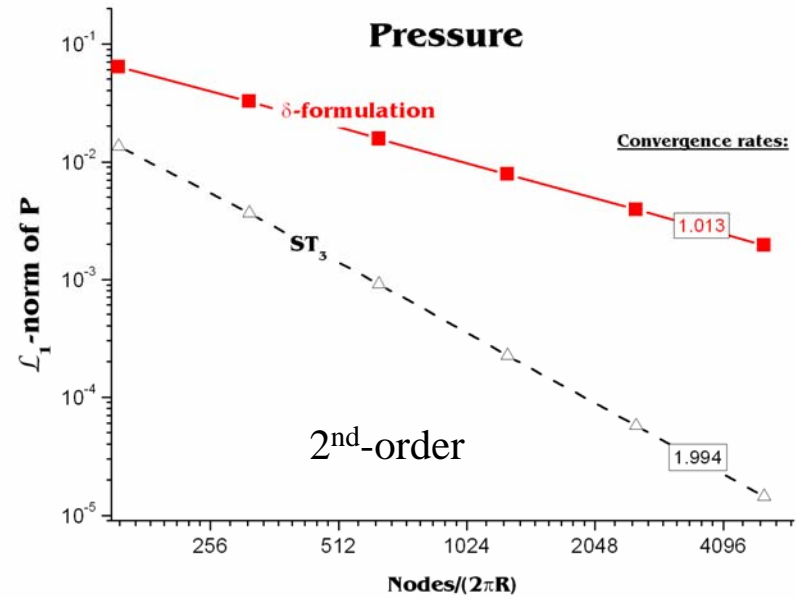
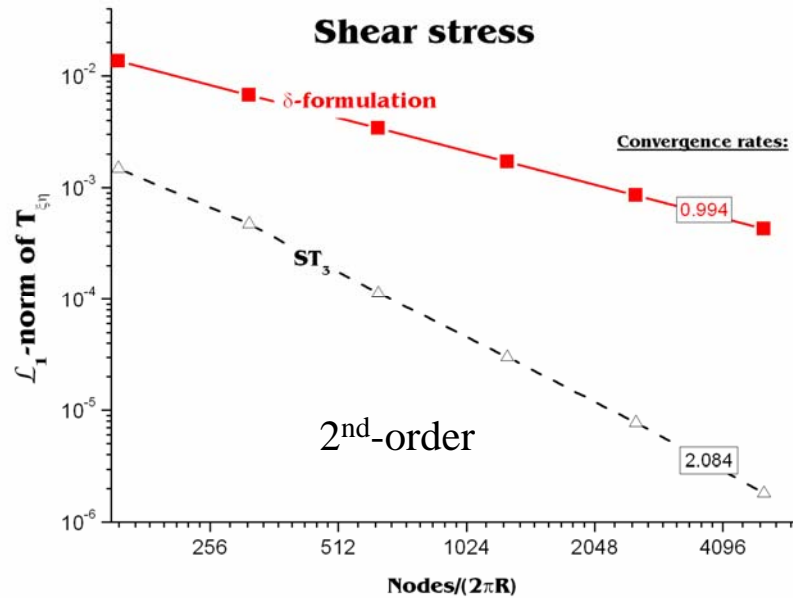
where  $P_0 = 20$ ,  $P_1^+ = 10$ ,  $P_1^- = P_1^+ - \frac{\sigma}{R}$ ,  $\sigma = 1$ ,  $V_{\xi I} = 1$ ,  $V_{\eta I} = 1$



# Grid convergence test

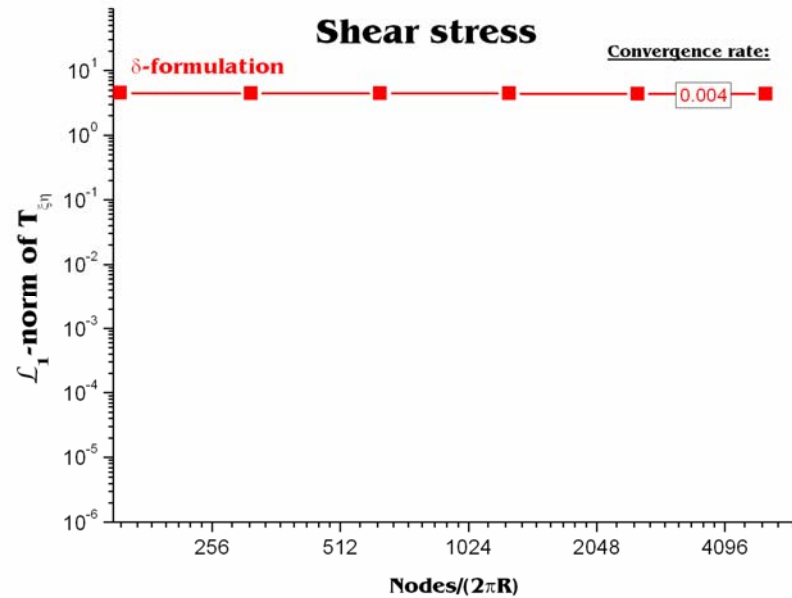
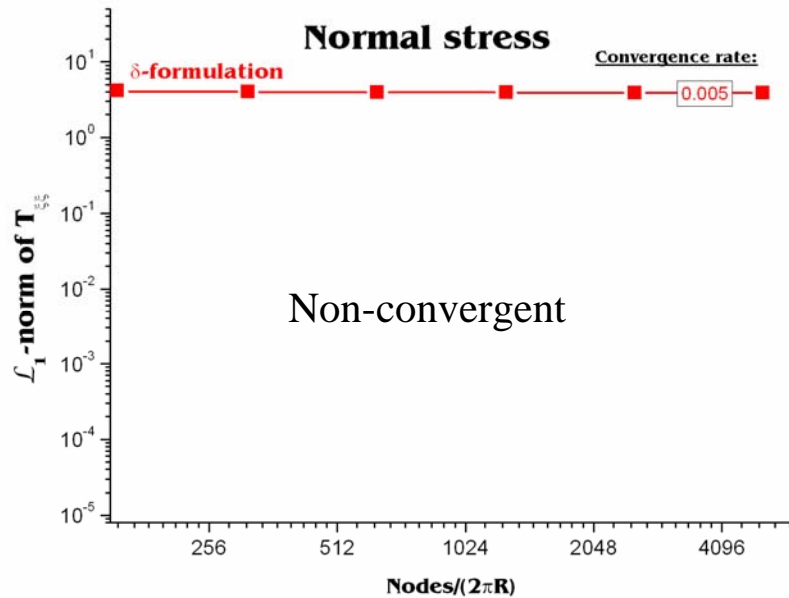
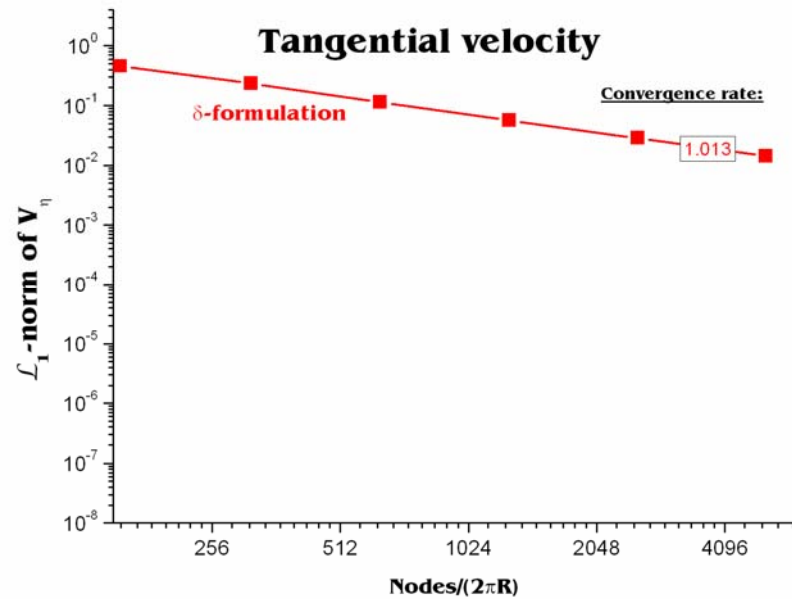
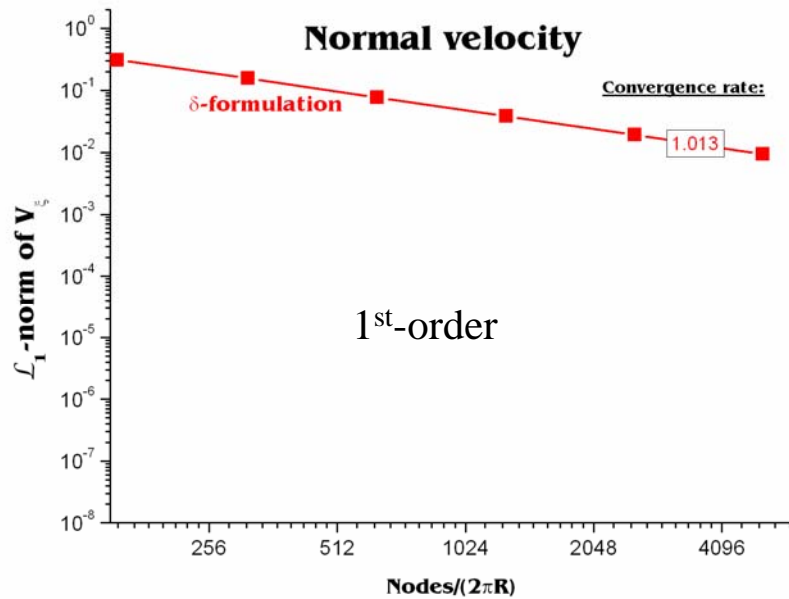


$[\mu] = 0$   
 $\sigma = 0$



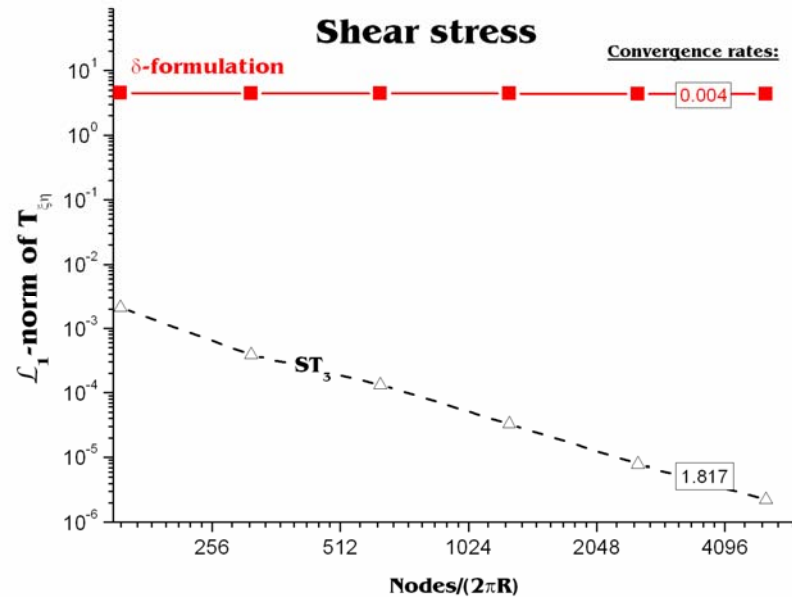
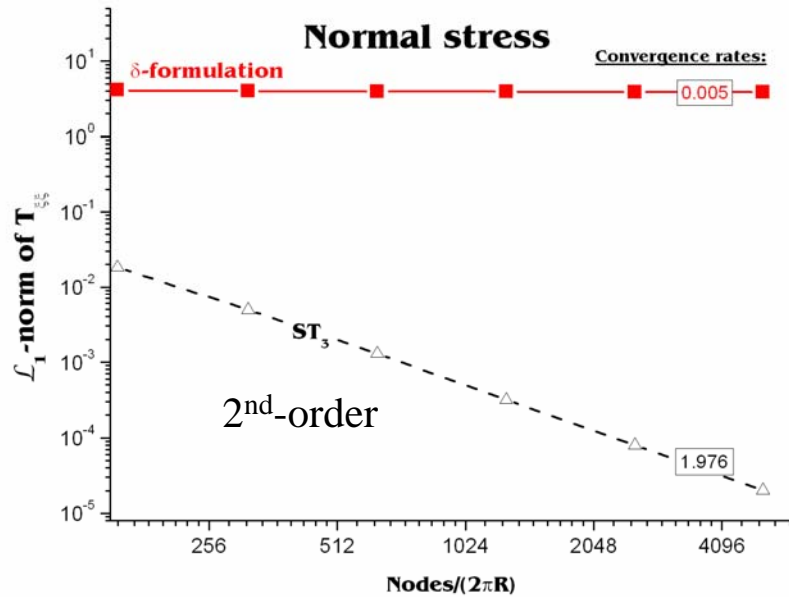
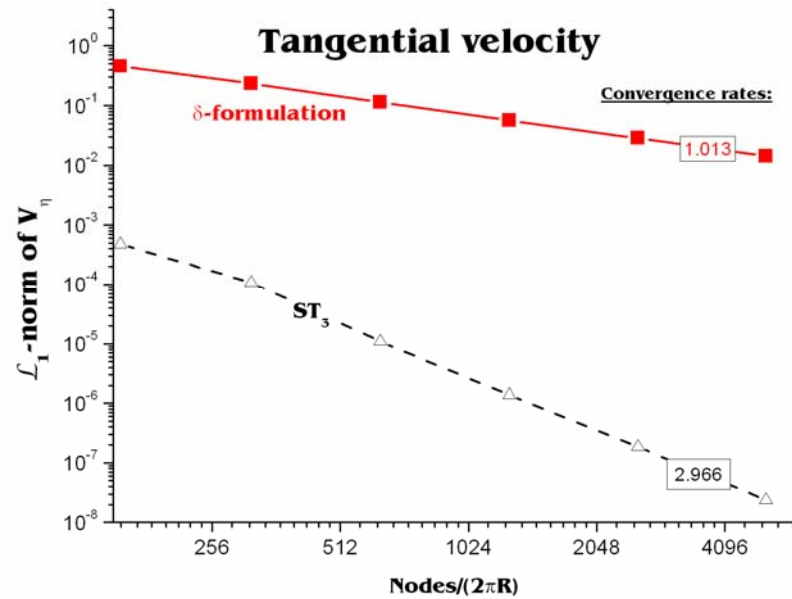
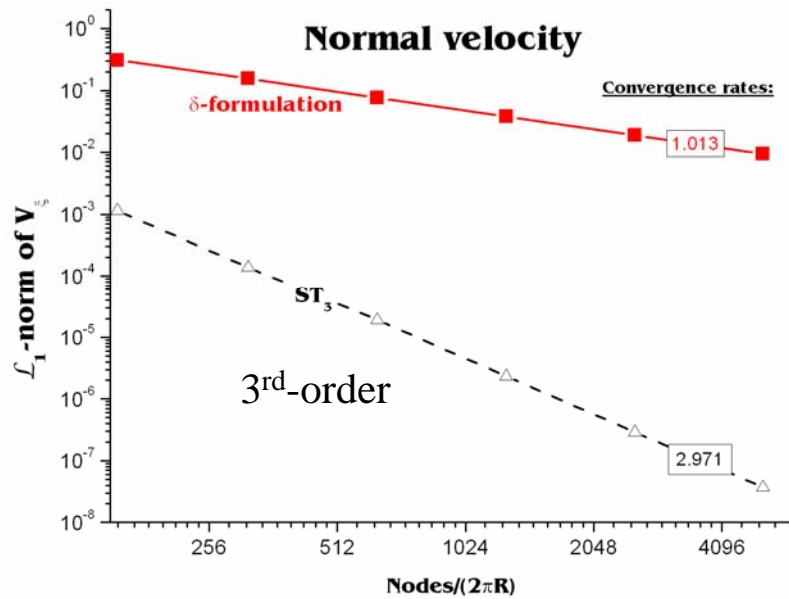
# Grid convergence test

$$\langle \mu \rangle = 25$$
$$\sigma = 1$$

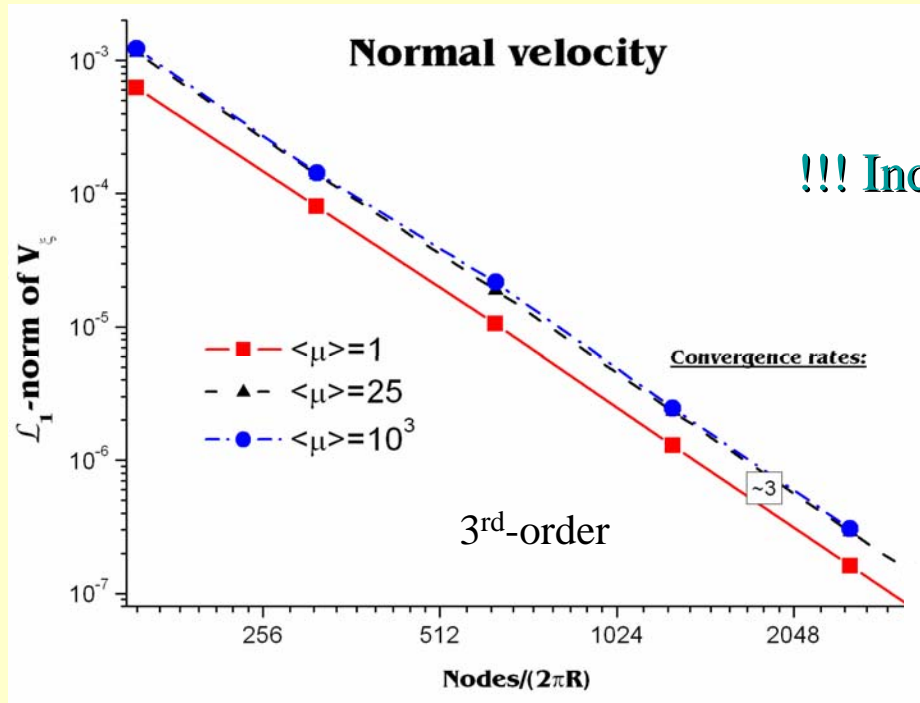


# Grid convergence test

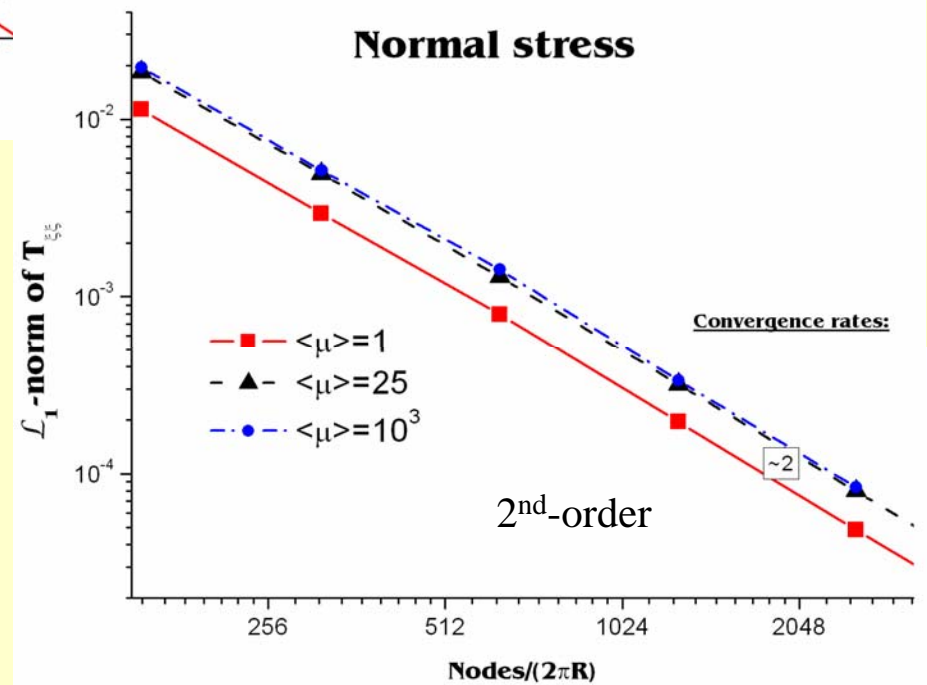
$$\langle \mu \rangle = 25$$
$$\sigma = 1$$



# Grid convergence test



!!! Independent of viscosity ratio !!!



# Major Results

- On Data Base development we have proven all aspects of the experimental technique and begun Production Runs (well ahead of schedule),
- We have shown experimentally that VE drops can survive intact at  $We \sim 4,000!$  Or  $1/2\rho v^2 = 2 \cdot 10^5 !$
- We developed a theoretical understanding of the mechanisms for Newtonian/Viscous liquid breakup over the whole range of regimes, unified all data, and corrected major, long-standing misconceptions,
- On DNS we achieved the sharp treatment of interfaces, and established capability to compute instabilities on shocked, high acoustic impedance mismatch interfaces.