Conservative & accurate geometric transport methods for discontinuous variables in turbulent multi-physics two-phase flows

MODELING & COMPUTING COMPLEX FLOWS MINISYMPOSIUM
SIAM – CSE 2015

OLIVIER DESJARDINS
SIBLEY SCHOOL OF MECHANICAL AND AEROSPACE ENGINEERING
CORNELL UNIVERSITY

Some acknowledgments

Contributors

- Dr. Mark Owkes (now Assistant Professor in Mechanical Engineering at Montana State University)
- Dr. Jeremy McCaslin (now with ANSYS Fluent)
- Dr. Peter Brady (now at LANL)

Funding sources

- NSF CBET 1034506
- NSF CAREER 1351545

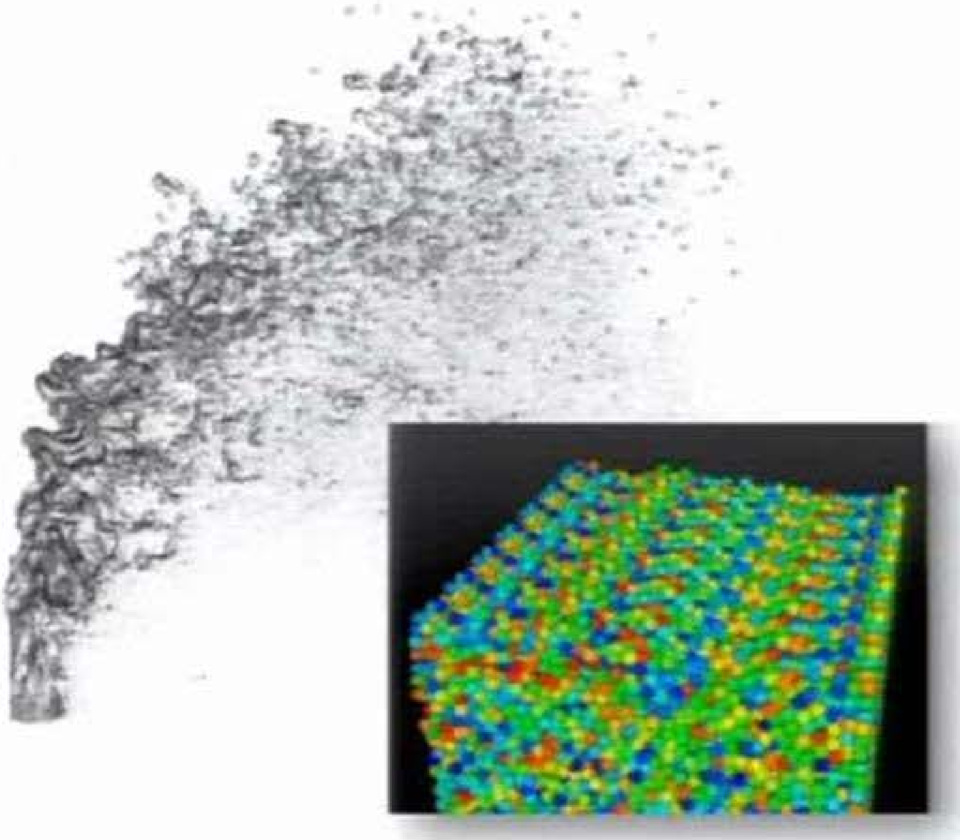
Computing resources

- LLNL – Sequoia & Sierra
- XSEDE – Kraken & Stampede
- ORNL – Titan
- ANL – Mira

About us…

Computational Thermo-Fluids Laboratory

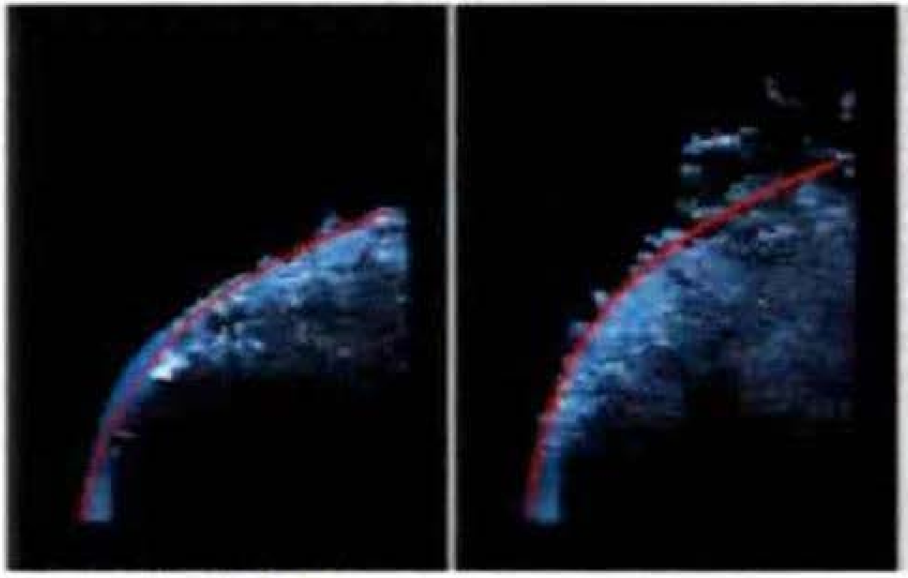
- http://ctflab.mae.cornell.edu
- Focus on multiphase reacting turbulent flows
- Massively parallel computing

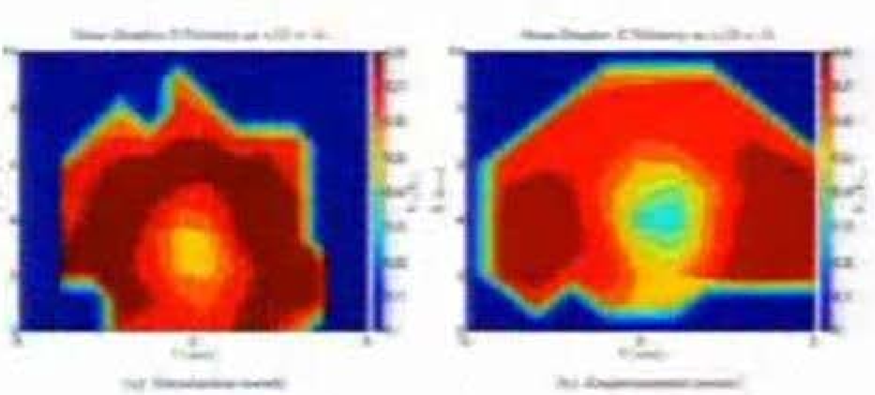


About us…

Computational Thermo-Fluids Laboratory

- http://ctflab.mae.cornell.edu
- Focus on multiphase reacting turbulent flows
- Massively parallel computing





Mean droplet velocity at $z/D = 15$

Importance of liquid-gas turbulent flows

Many questions remain unanswered on liquid atomization

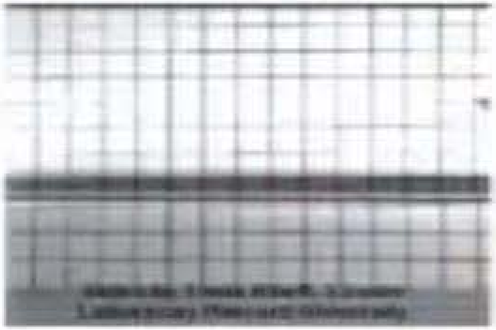
- What is the drop size distribution?
- Where do drops form?
- By what mechanisms?
- Can predictive models be developed?

Photo courtesy of C. T. Bowman, Stanford University

Some of the challenges associated with two-phase flows

Liquid-gas flows are discontinuous

- Phase-interface is extremely thin and exhibits a singular surface tension force
- Fluid properties vary significantly across the interface



Liquid-gas flows are strongly multi-scale

- From microscopic droplets to cm (even meters in many flows)
- Complex and frequent topology changes
- Turbulence

Liquid-gas flows are often multi-physics

- Dirty interfaces, surfactants
- Non-isothermal, Marangoni flows, phase change, supercritical effects
- Electrostatic effects

As a consequence, liquid-gas flows are…

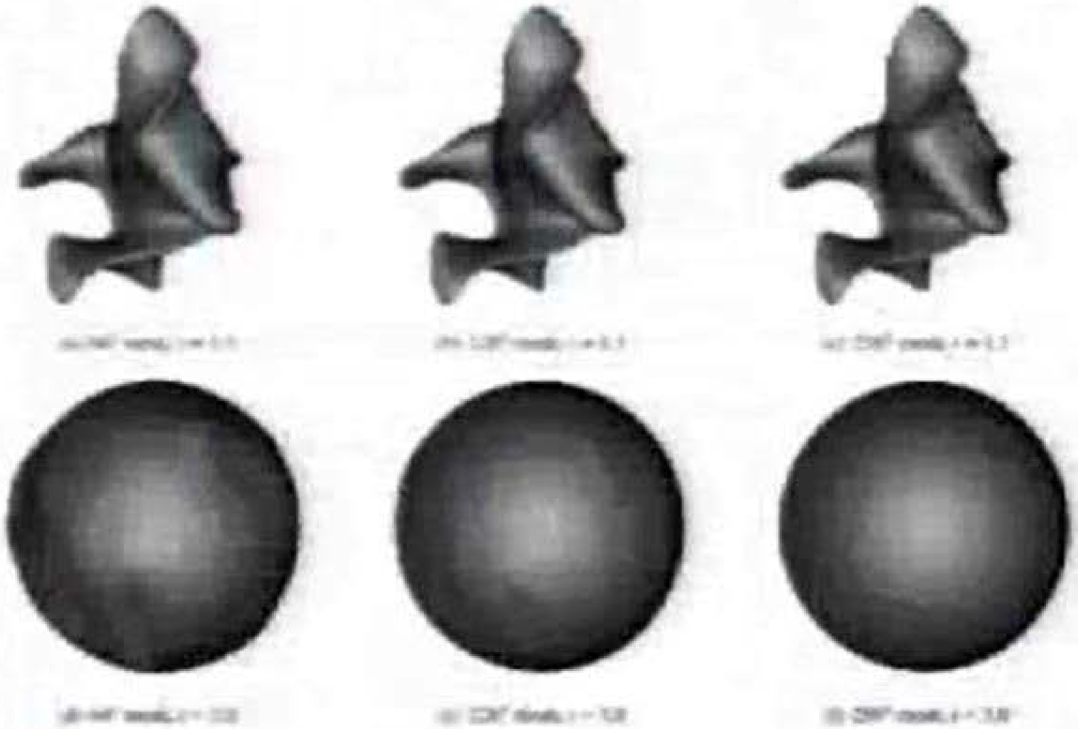
… difficult to characterize experimentally

… difficult to simulate and model accurately

Verification exercise – Volume fraction transport

Properties of the interface transport scheme

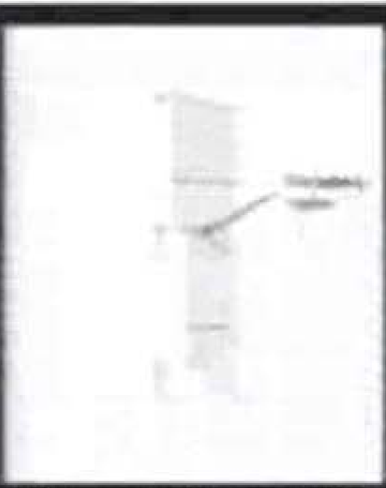
- Exactly conservative
- Exactly bounded
- Second order accurate



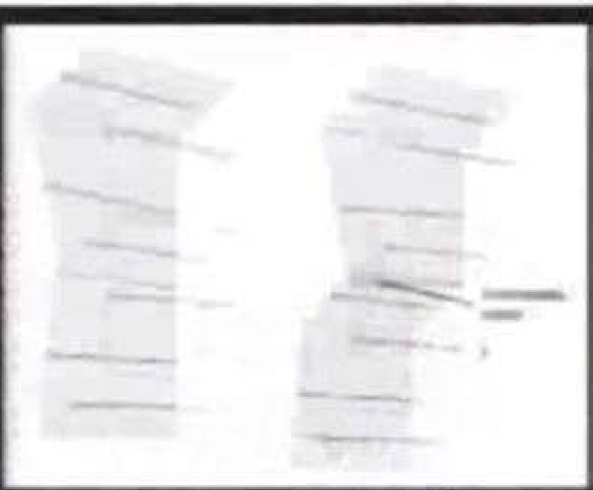
N_x	E_{shape}	E_{mass}	E_{bound}	Time/Timestep (s)
64	5.281e-01	5.472e-16	1.124e-17	1.61
128	9.357e-02	1.198e-15	1.198e-17	3.70
256	2.300e-02	1.290e-14	7.598e-17	12.0

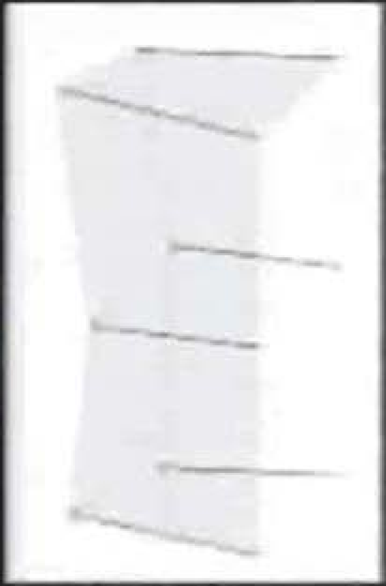
Geometric transport strategy


Noh & Woodward 1976


Rider and Kothe 1998


López et al. 2004


Hernández et al. 2008


Owkes & Desjardins 2013

- \+ **Three-dimensional**
- \+ **Discretely conservative**
- \+ **Bounded**

- \- **Leads to many complex geometric operations**

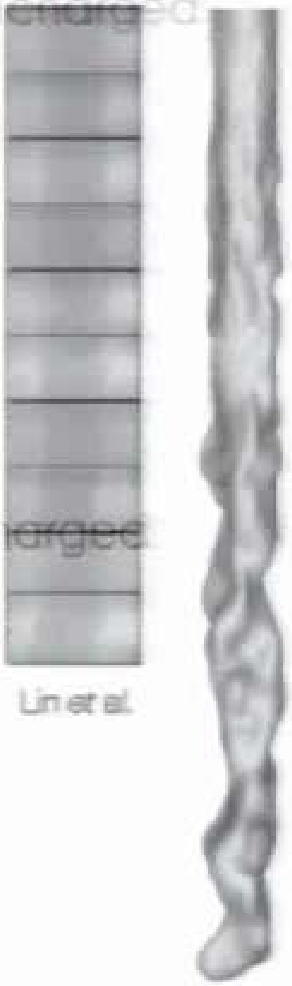

Owkes & Desjardins, JCP 270: 587 – 612, 2014

See also:
Le Chenadec & Pitsch 2013
Ivey & Moin 2012
Marić et al 2013
Zhang 2013

Simulation of turbulent EHD atomization

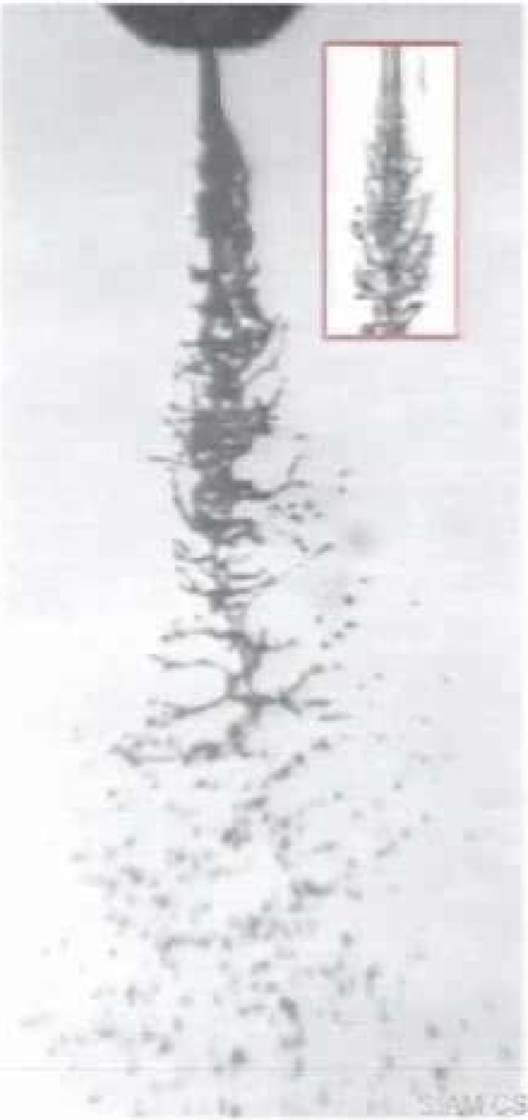
Simulation of turbulent EHD atomization

Uncharged



Lin et al.

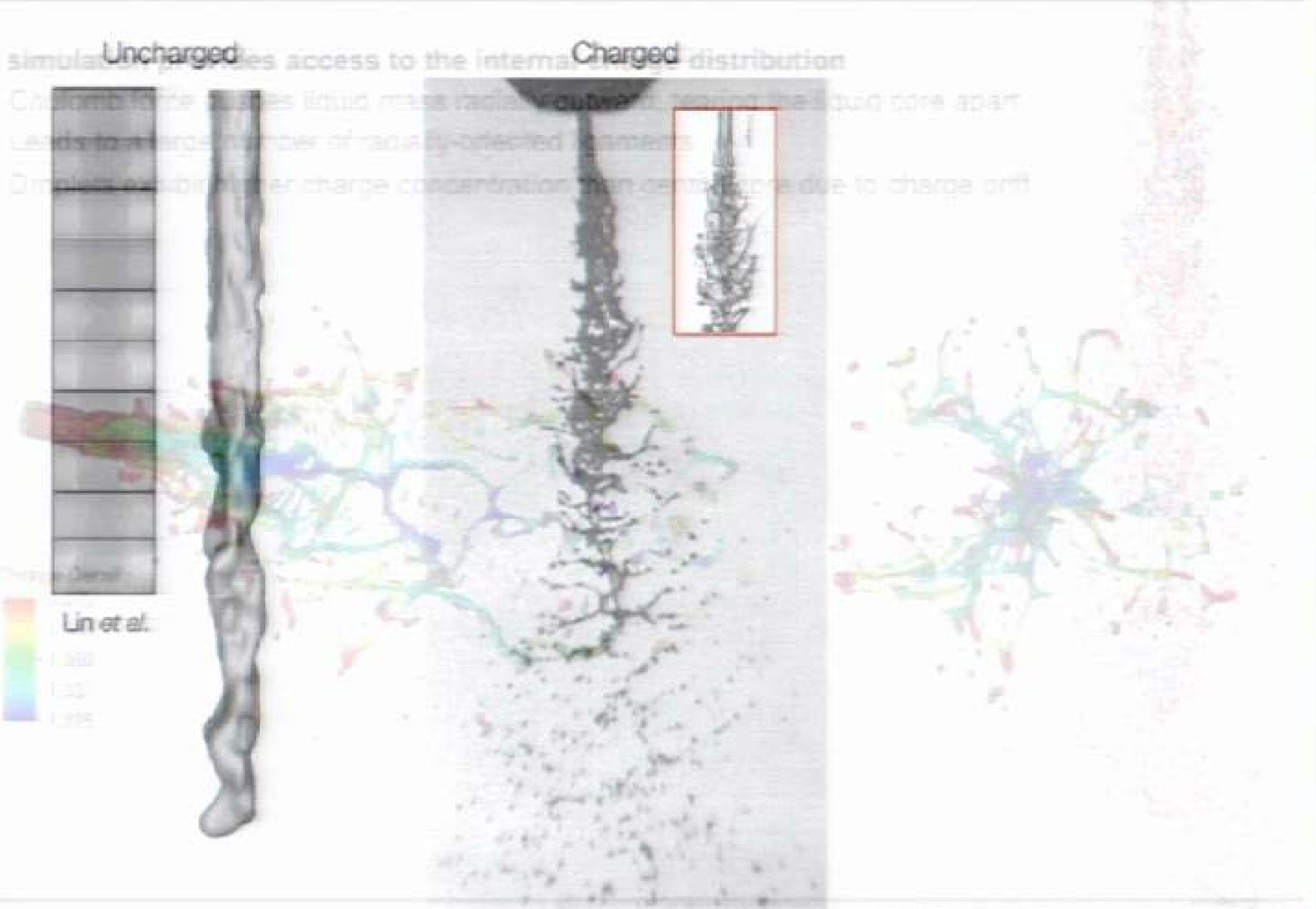
Charged



Simulation of turbulent EHD atomization

3D simulation provides access to the internal charge distribution

- Coulomb force pushes liquid mass radially outward, tearing the liquid core apart
- Leads to a large number of radially-oriented ligaments
- Droplets exhibit higher charge concentration than central core due to charge drift



Summary

- Discussed a novel **2nd order, fully conservative, consistent methodology** to transport discontinuous variables
- Accounts explicitly for flow discontinuities using
  - Planar interface representation
  - Simplex-based computational geometry toolbox
- Application to an emerging complex flow problem
  - Electrohydrodynamic atomization
- *Looking forward: focus on including phase change within the same framework*