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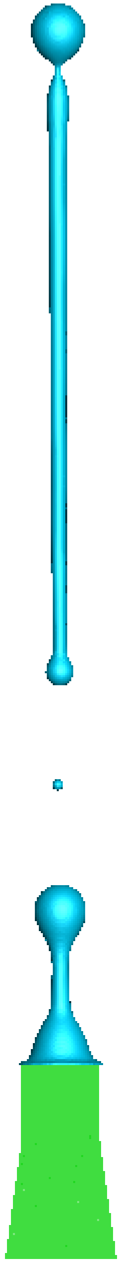

Gerris: a Powerful Modeling Tool for Capillary Flows

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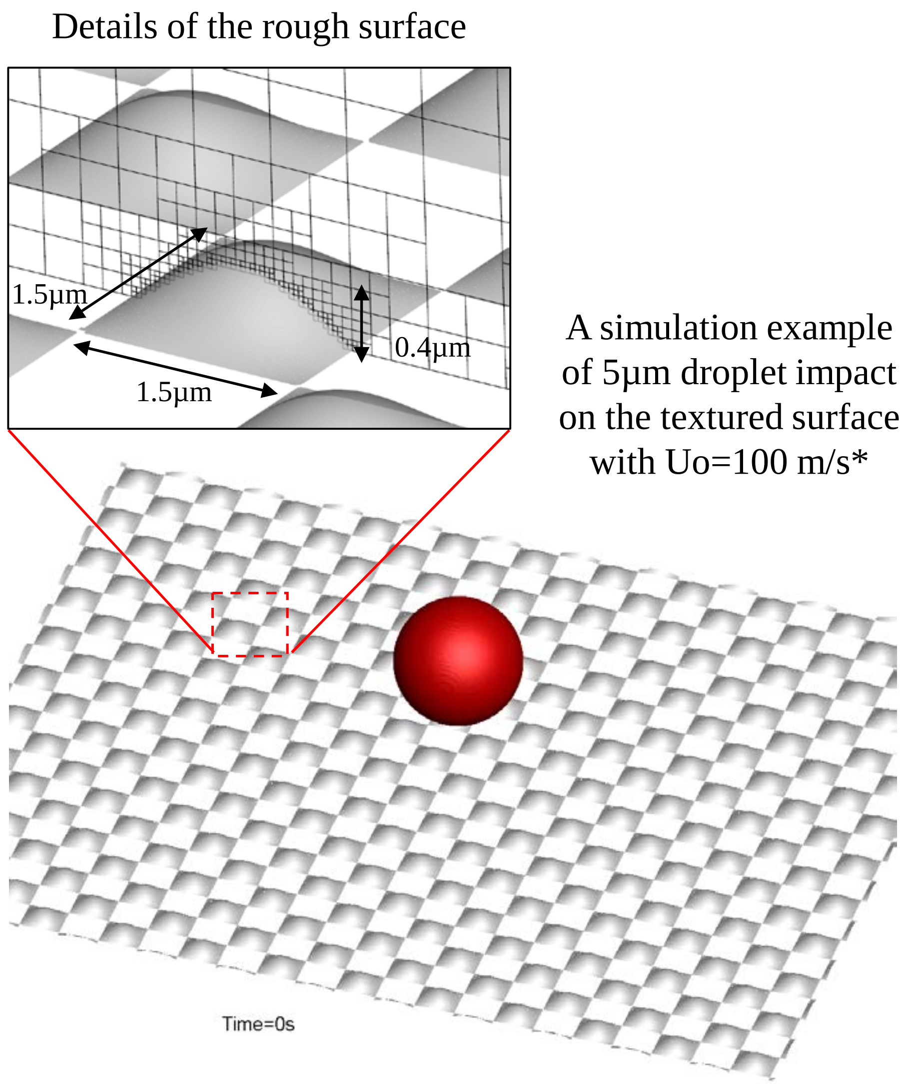
Outline

- How do I get started with Gerris
- Droplet formation in Inkjet process
- Capillary flow in low-gravity
- Droplet-media interaction
- Future work



A simulation example of 5μm droplet impact on the textured surface with Uo=100 m/s*

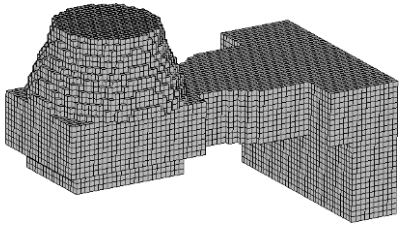
*H. Tan, Numerical study on splashing of high-speed microdroplet impact on dry microstructured surfaces. *Computers & Fluids*, 2017. 154: p. 142-166.

How do I get started with Gerris

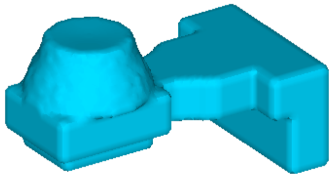
HP's drop-ejection simulation tool: CFD3*

- Uniform Cartesian grid
- Stair-step method for solid geometry
- Naiver-Stokes for liquid phase
- Drive-bubble dynamics
- Contact angle model
- Algebraic calculation based Volume of Fluid
- Height-function for curvature calculation
- Surface-tension directly applied to interface cells

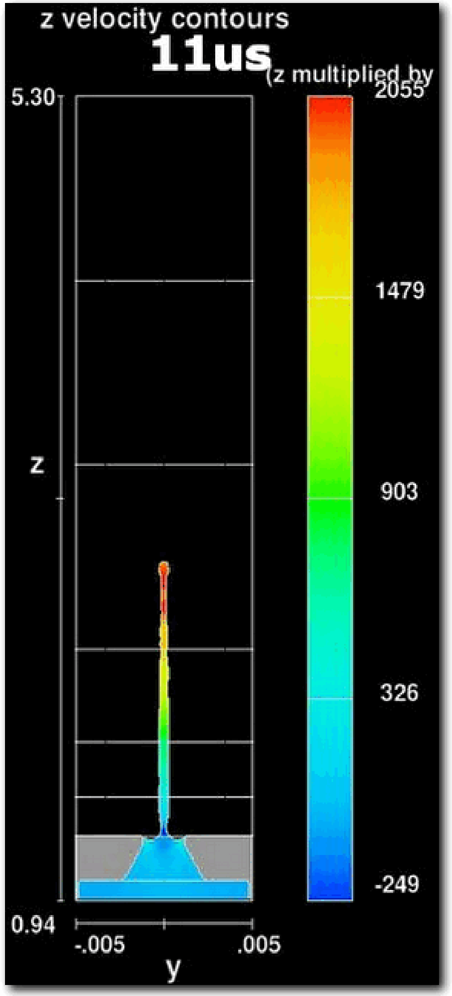
Original CFD3 has a problem in conserving the momentum!



*H. Tan, et al., Numerical simulation of droplet ejection of thermal inkjet printheads. *International Journal for Numerical Methods in Fluids*, 77(9), 544-577, 2015.
H. Tan, et al, Validation of an in-house 3D free-surface flow solver in inkjet printing, *the 2nd ASME Verification and Validation Symposium*, May 22-24, Las Vegas, Nevada, 2013.



CFD3 simulation



Flow3D simulation

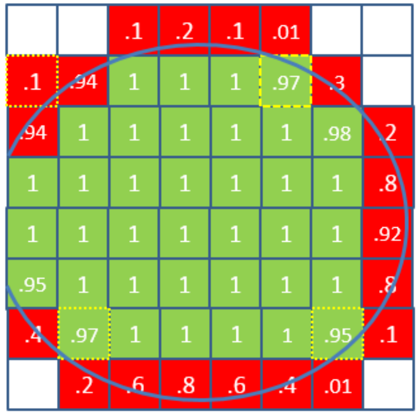
How do I get started with Gerris

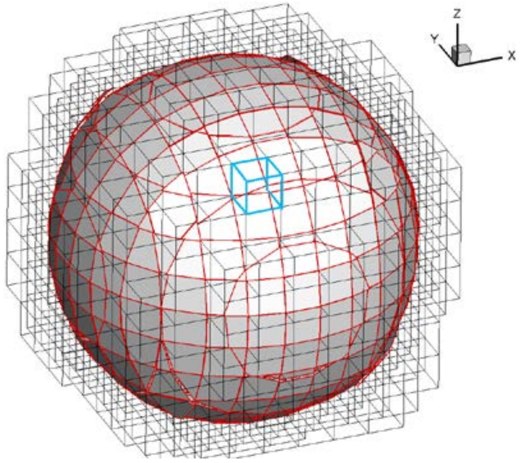
- Curvature calculation for under-resolved cells

  paraboloid-fitted method[1]

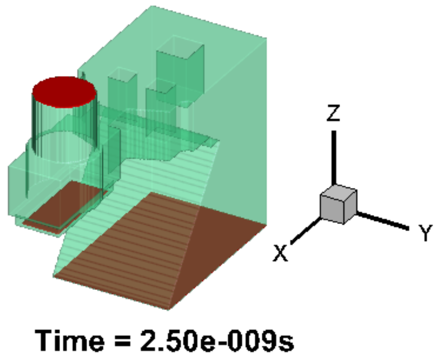
- Geometrical calculation based VOF

  Piecewise Linear Interface Calculation[2]





κ (height function): -0.373
κ (parabola-fitting): 0.404
Analytical: 0.42



[1]Popinet, S., An accurate adaptive solver for surface-tension-driven interfacial flows. *Journal of Computational Physics*, 2009. **228**(16): p. 5838-5866.

[2]Gueyffier, et al., Volume-of-Fluid Interface Tracking with Smoothed Surface Stress Methods for Three-Dimensional Flows. *Journal of Computational Physics*. **152**(2), 423-456, 1999.

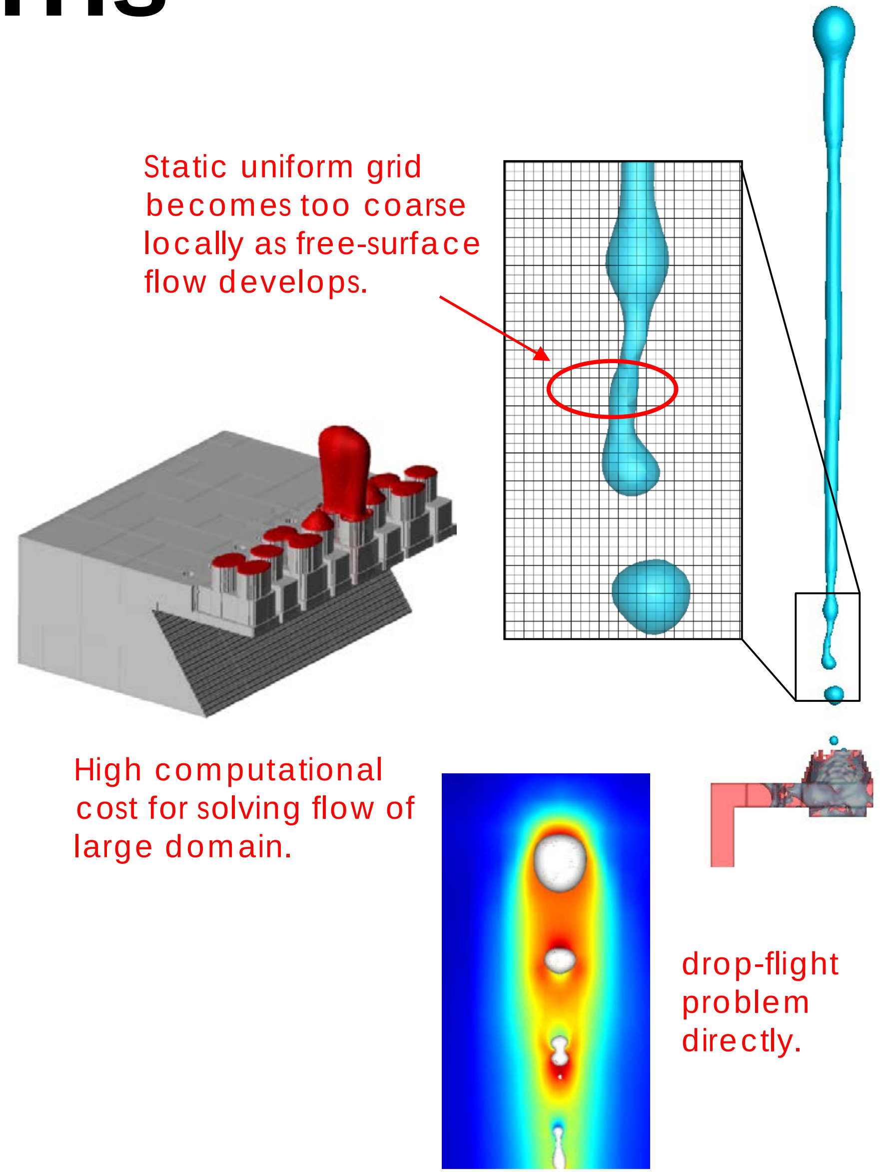
How do I get started with Gerris

Can Gerris be used to simulate droplet ejection in thermal inkjet process?

Need to know…

- Various numerical methods implemented in Gerris, including NS solver, VOF, cut-cell for solids, boundary conditions, parallel implementation, Oct-tree adaptation, ...
- Gerris style for program flow (e.g. GfsVariable, GfsEvent, GfsSource, GfsFunction, GfsOutput,...)
- Object-oriented programming using only ANSI-C*;

Learning curve is steep if you want to adapt Gerris for modest complex problems!



* Object Oriented Programming with ANSI C, Axel-Tobias Schreiner,1993

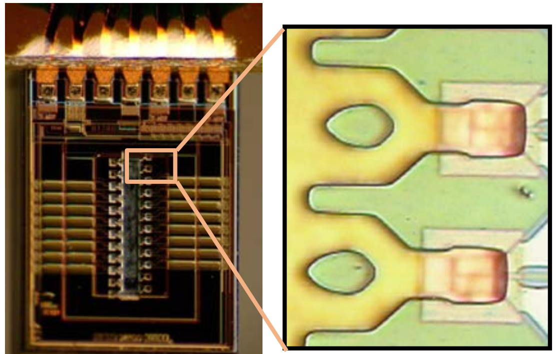
Washington State University Vancouver

Outline

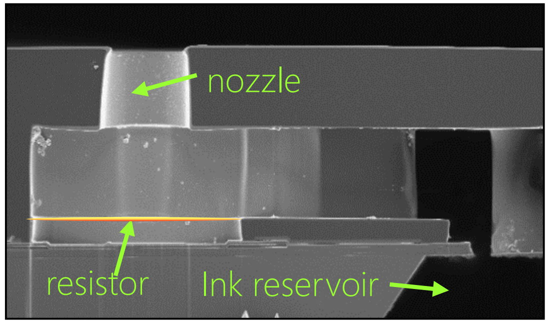
- **How do I get started with Gerris**
- **Droplet formation in Inkjet process**
- **Capillary flow in low-gravity**
- **Droplet-media interaction**
- **Future work**

Droplet formation in Inkjet process

Drop-on-Demand (DOD) Thermal Inkjet (TIJ)

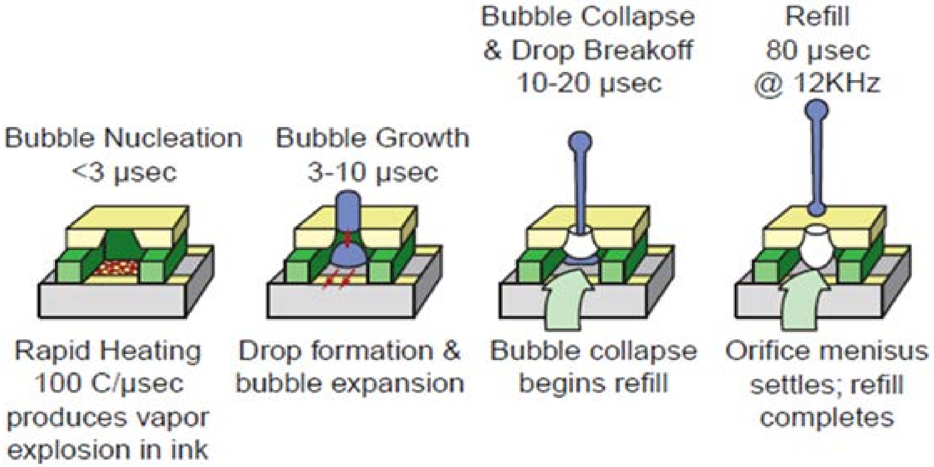


Top view

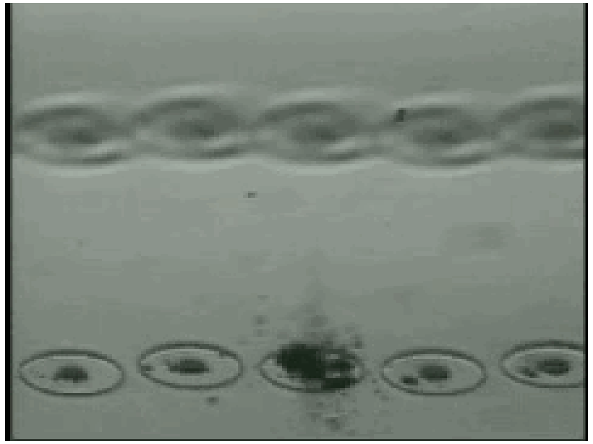


Cross-section

Schematic of a firing chamber structure



Droplet-ejection sequence in TIJ

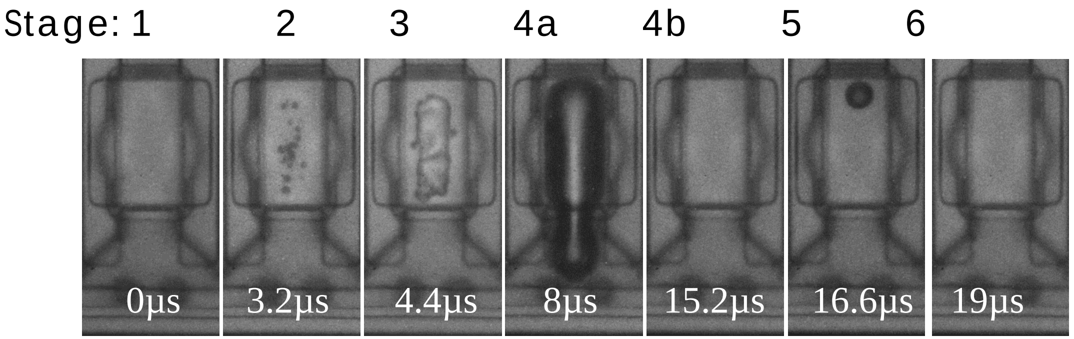


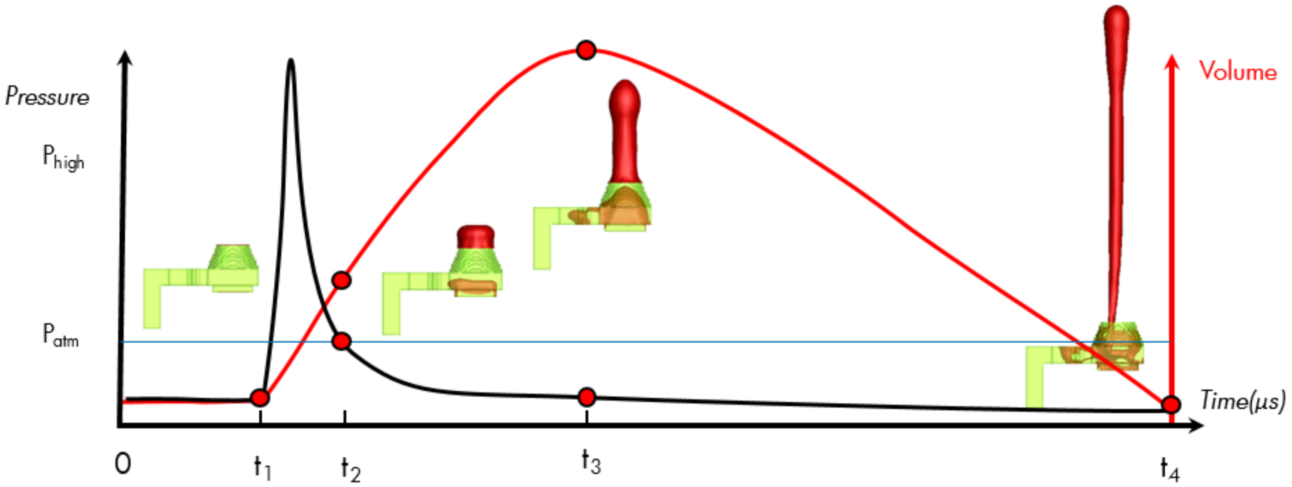
High-speed imaging of TIJ

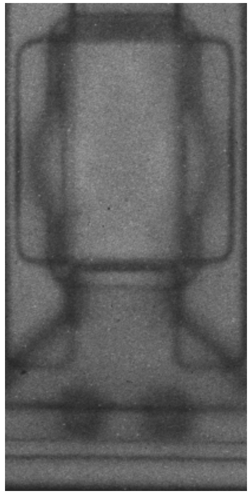
Droplet formation in Inkjet process

TIJ boiling: heat flux1-2 x10^9 W/m^2. (Sun surface ~6.58 x10^7 W/m^2)

1. Thin film heating
2. Boiling incipience (pre-nucleation)
3. Boiling
4. Vapor bubble expansion & collapse
5. Rebound
6. Vapor bubble disappears





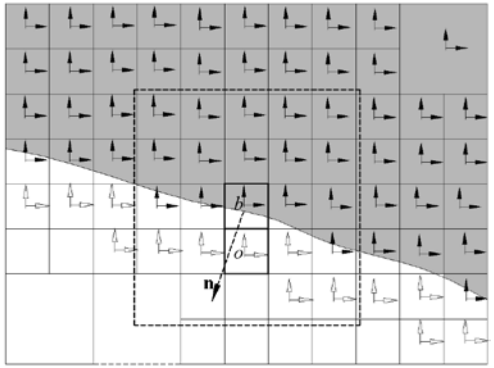


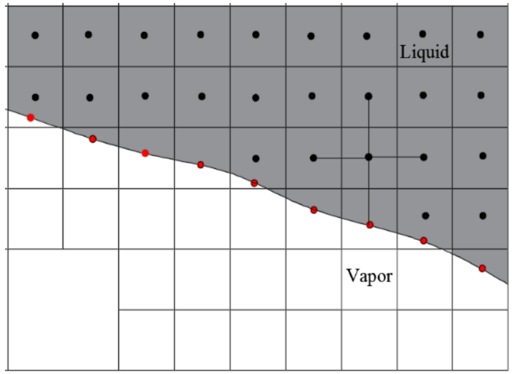
Droplet formation in Inkjet process

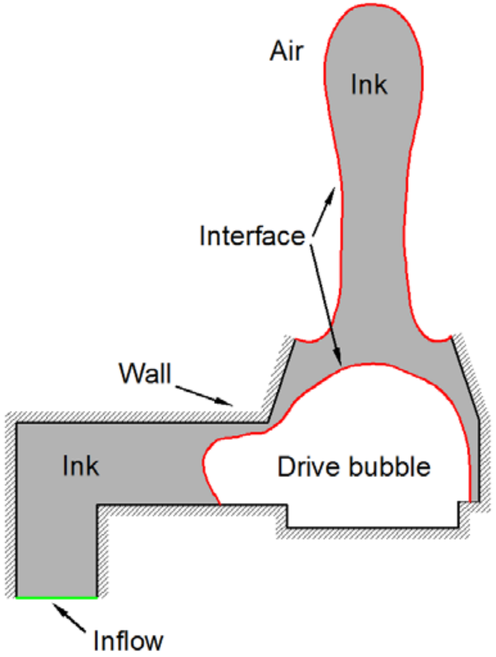
Drive bubble dynamics

- Assume that the adiabatic expansion and collapse of the drive bubble follow a polytropic process (pV^n = constant).
- Bubble can split and merge due to geometry constrains.
- Velocity in empty cells adjacent to vapor-liquid interface is extrapolated for calculation the advection and viscous terms conveniently without the irregular computing stencils*

$$\Gamma = \sum_{k=1}^{N} \left(\mathbf{u}_o + \mathbf{A} \cdot \mathbf{x} - \mathbf{u}_k \right)^2 + \lambda \, \mathbf{t} \cdot \left(\mathbf{A} + \mathbf{A}^T \right) \cdot \mathbf{n}$$







$$-p = -p_g + \sigma\kappa - \mathbf{n} \cdot \boldsymbol{\tau} \cdot \mathbf{n}$$

$$\mathbf{t} \cdot \boldsymbol{\tau} \cdot \mathbf{n} = 0$$

*Popinet, S. and S. Zaleski, *Bubble collapse near a solid boundary: a numerical study of the influence of viscosity*. Journal of Fluid Mechanics, 2002. **464**: p. 137-163.

Droplet formation in Inkjet process

Contact angle model

Capillary force plays an important role in the refill of the firing chamber.

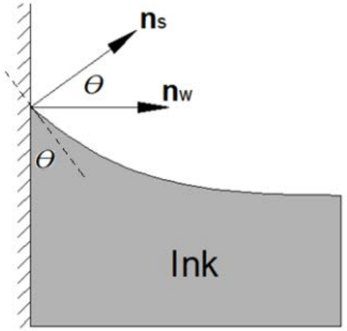
A fictitious height function in the solid wall can be calculated by

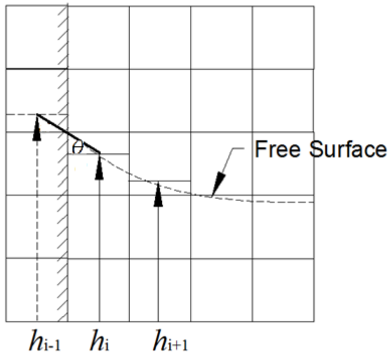
$$h_{i-1} = h_i + \frac{\Delta}{\tan\theta}$$

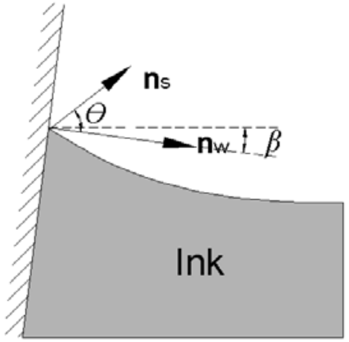
When the normal direction $\mathbf{n}_w$ of the wall is not aligned with the Cartesian directions.

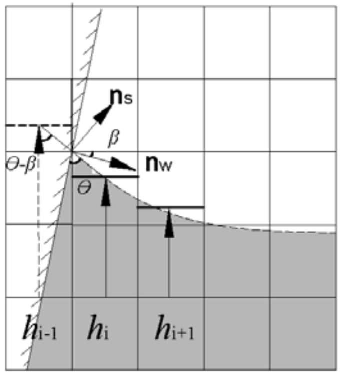
$$h_{i-1} = h_i + \frac{\Delta}{\tan(\theta - \beta)}$$

Calculation of 3D case is more complicated than that for 2D case, especially when $\mathbf{n}_w$ is not aligned with the Cartesian direction.









Droplet formation in Inkjet process

Gerris implementation

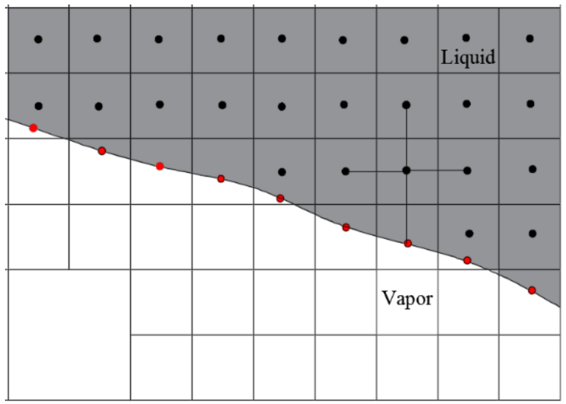
- Create a new event class ‘**drive_bubble_event**’ to handle the drive bubble dynamics (e.g. initialize the drive bubble parameters, flag drive bubble, calculate drive bubble volume, pressure, track the bubble state, etc.).
- Create a new method ‘**gfs_diffusion_bubl**’ to handle the solution of provisional velocity (in fractional-step projection method for NS equations) involving vapor-liquid interface.

$$\rho^{n+1/2}\left[\frac{\mathbf{u}^*-\mathbf{u}^n}{\Delta t}+\left(\mathbf{u}^{n+1/2}\cdot\nabla\right)\mathbf{u}^{n+1/2}\right]=\nabla\cdot\left[\mu^{n+1/2}\left((2-\beta)\mathbf{D}^n+\beta\mathbf{D}^*\right)\right]+\left(\sigma\kappa\delta_s\mathbf{n}\right)^{n+1/2}$$

- Create a new method ‘**gfs_poisson_solve_bubl**’ to handle the solution of the Poisson equation involving vapor-liquid interface.

$$\nabla\cdot\left[\frac{\Delta t}{\rho^{n+1/2}}\nabla p^{n+1/2}\right]=\nabla\cdot\mathbf{u}^*$$

- Implement a 3D version of **GfsVariableTracerVOFHeight** in vof.c
- Create a new class ‘**surface_angle_bc_class**’ to specify the contact angle for solid walls and implement relevant curvature calculation adjustment in vof.c.
- Create a few new methods in GerrisOutput (e.g. statistics of droplets, interface segments, tecplot output, etc.)
- Clean bugs especially when a complex solid geometry present.



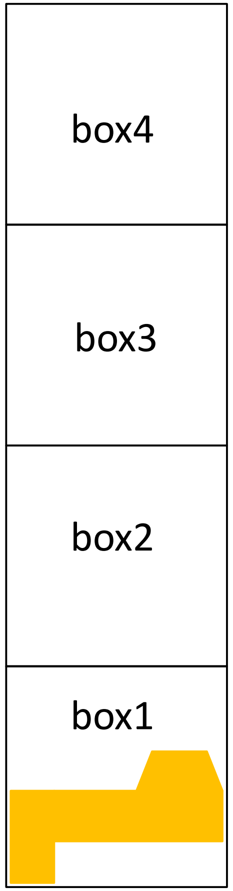
Droplet formation in Inkjet process

Gerris implementation

```
4 3 GfsSimulation GfsBox GfsGEdge {} {
  Global {
    #define LEVEL 7
    #define GRAVITY 980
    #define MU_L  1.3e-2
    #define MU_G  1.8e-4
    #define RHO_L 1.
    #define RHO_G 1.e-3
    #define var(T,min,max) (CLAMP(T,0,1)*(max - min)
+ min)
    #define rho(T) var(T, RHO_G/RHO_L, 1.)
    #define mu(T)  var(T, MU_G/MU_L, 1.)
    #define Z_t  22e-4
    #define Noz_t -10e-4
    #define PA 1.01e6
    #define P_back 9950
//  back pressure
    static double pressure_refill (double x, double y,
double z, double P) {
       if (x < -27e-4 && y <= -48e-4 && fabs(z) < Z_t)
return -P_back;
       return P;
    }
// vof boundary
   static double vof_bc (double x, double y, double z) {
    if (y < -48e-4 && fabs(z) <= Z_t)  return 1.;
    else return -1.;
  }
```

```
// initial drive bubble
    static double drive_bubble (double x, double y, double z)
{  if (fabs(z) >= Z_t)
           return -1.;
        else if (y < Noz_t && !(x > -11e-4 && y < -37.9e-4))
           return 1.;
        else
           return -1.; }
  }
  GfsTime { end  = 40.e-6 }
  GfsRefine 1
  GfsRefineSolid LEVEL
  GfsSolid solid.gts
  VariableTracerVOFHeight {} T
  Variable T0
  InitFraction T0  (vof_bc(x, y, z))
  VariableFiltered T1 T 3
  InitFraction {} T (drive_bubble(x, y, z))
  PhysicalParams {L = 100.e-4 alpha =  1/rho(T1)/RHO_L }
  SourceViscosity MU_L*mu(T1)
  VariableCurvature K T Kmax
  SourceTension T 50 K
AdaptFunction { istart = 1 istep = 1 } {cmax = 0.1 maxlevel =
LEVEL cfactor = 2 } (T > 0 && T < 1)
 GModule drive_bubble
  DriveBubble {} T {direction = 2 crit_factor = 8. p_high =
8e6 p_floor = 3.e5  pa = PA}
SurfaceAngleBc T 40
```

```
EventBalance {istep=1}   0.1
  OutputBalance {istep = 1} balance
  GfsOutputSimulation { step = .25e-6} file-inkjet-vof-%ld.gfs
  GfsOutputSimulation { step = .25e-6 } tecplot-%ld.dat
{variables= U,V,W,P,Tsolid=0 format = Tecplot}
  GfsOutputTiming { istep  = 20 } stdout
}
GfsBox {bottom = Boundary {
BcDirichlet T T0 BcDirichlet P pressure_refill(x,y,z,P)
BcNeumann V 0 BcDirichlet U 0 BcDirichlet W 0 }
     right = BoundaryOutflow    left  = BoundaryOutflow
      front = BoundaryOutflow back  = BoundaryOutflow
}
GfsBox { pid = 1
       right = BoundaryOutflow left  = BoundaryOutflow
       front = BoundaryOutflow back  = BoundaryOutflow
}
GfsBox { pid = 2
       right = BoundaryOutflow left  = BoundaryOutflow
       front = BoundaryOutflow back  = BoundaryOutflow
}
GfsBox { pid = 3
       right = BoundaryOutflow left  = BoundaryOutflow
       front = BoundaryOutflow back  = BoundaryOutflow
       top   = BoundaryOutflow
}
1 2 top
2 3 top
3 4 top
```

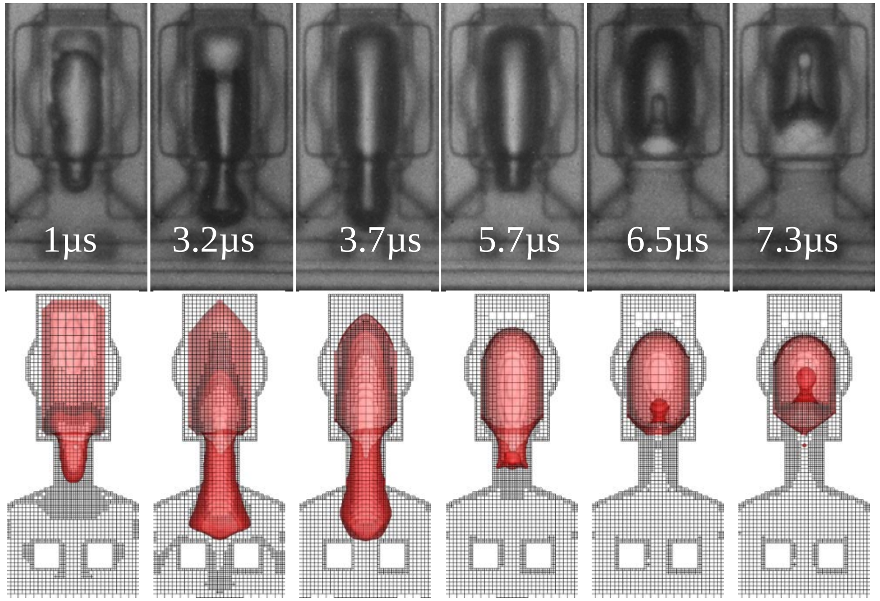


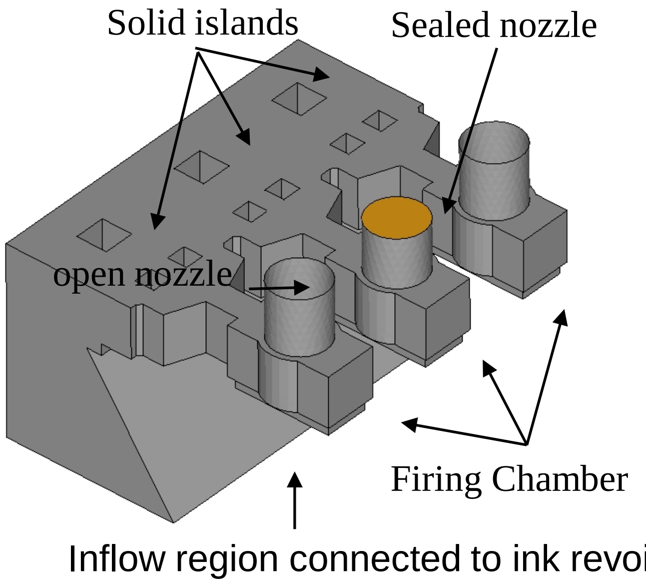
Droplet formation in Inkjet process

Simulation Examples*

Vapor bubble behavior in TIJ firing chamber

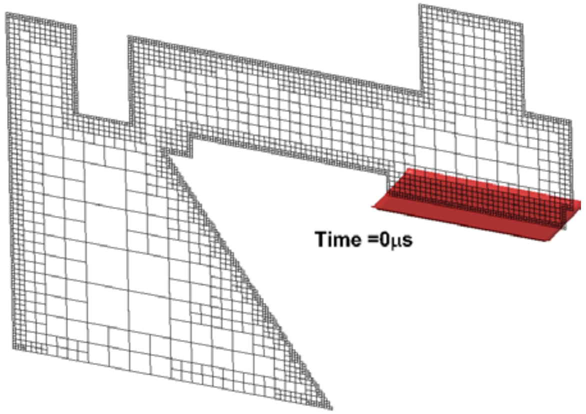
Voltage 26V, pulse width 3us, water at 25^{o}C, Domain size is 130 μm×130 μm×130 μm, the finest level L= 8, Δ_{min}=0.75 μm.





Input parameters

Variable	value
Viscosity μ	0.001 kg/ms
Surface tension σ	0.07 kg/s2
Density ρ	1000 kg/m3



* H. Tan, An adaptive mesh refinement based flow simulation for free-surfaces in thermal inkjet technology. *International Journal of Multiphase Flow*. 82, 1-16, 2016.

Droplet formation in Inkjet process

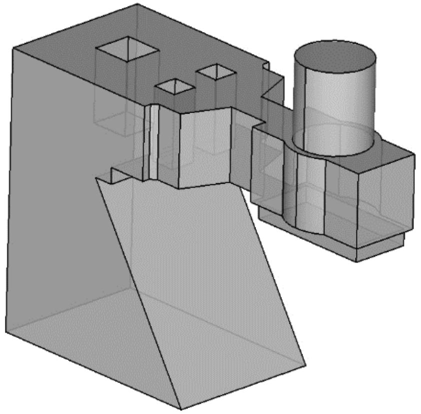
Simulation Examples*

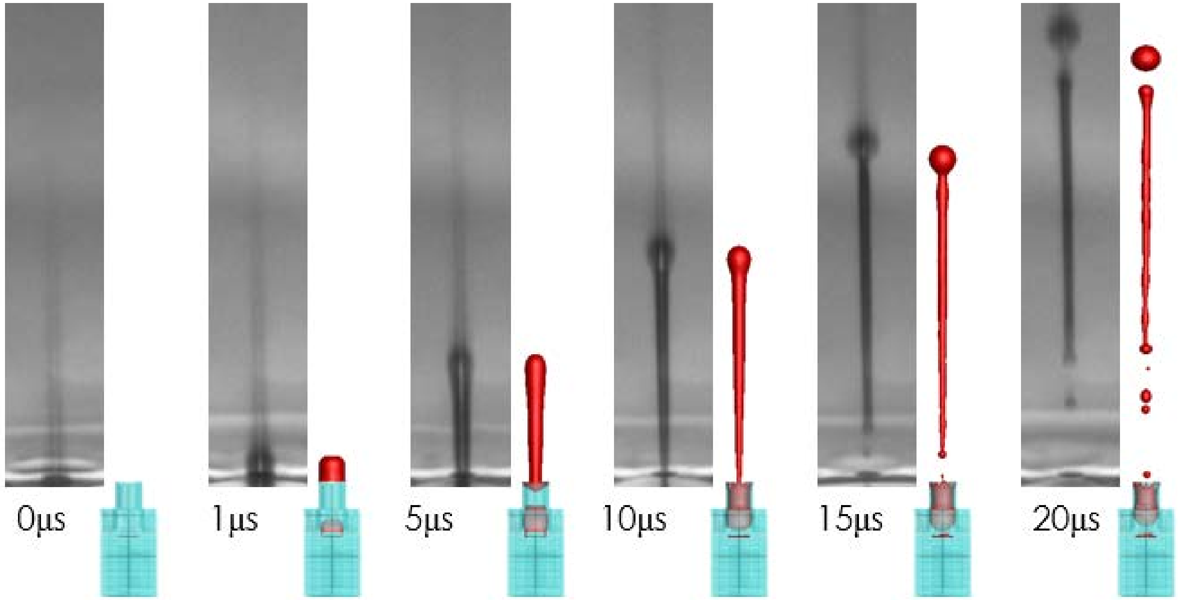
droplet-ejection simulation

- Domain size:125μmX125μmX625μmL_{max}: 8, Δ_{min}: 0.5μm. The mesh is adaptive to the interface curvature and local velocity gradient.
- Summary of results

	Experiment	Simulation
Droplet weight(ng)	9.8	10.1
Droplet speed (m/s)	15.4	15.3
Refill frequence (kHz)	20	16

Variable	value
Viscosity γ	0.011 cm^2/s
Surface tension σ	40 dyn/cm
Density ρ	1.0 g/cm3
Contact Angle	45^0





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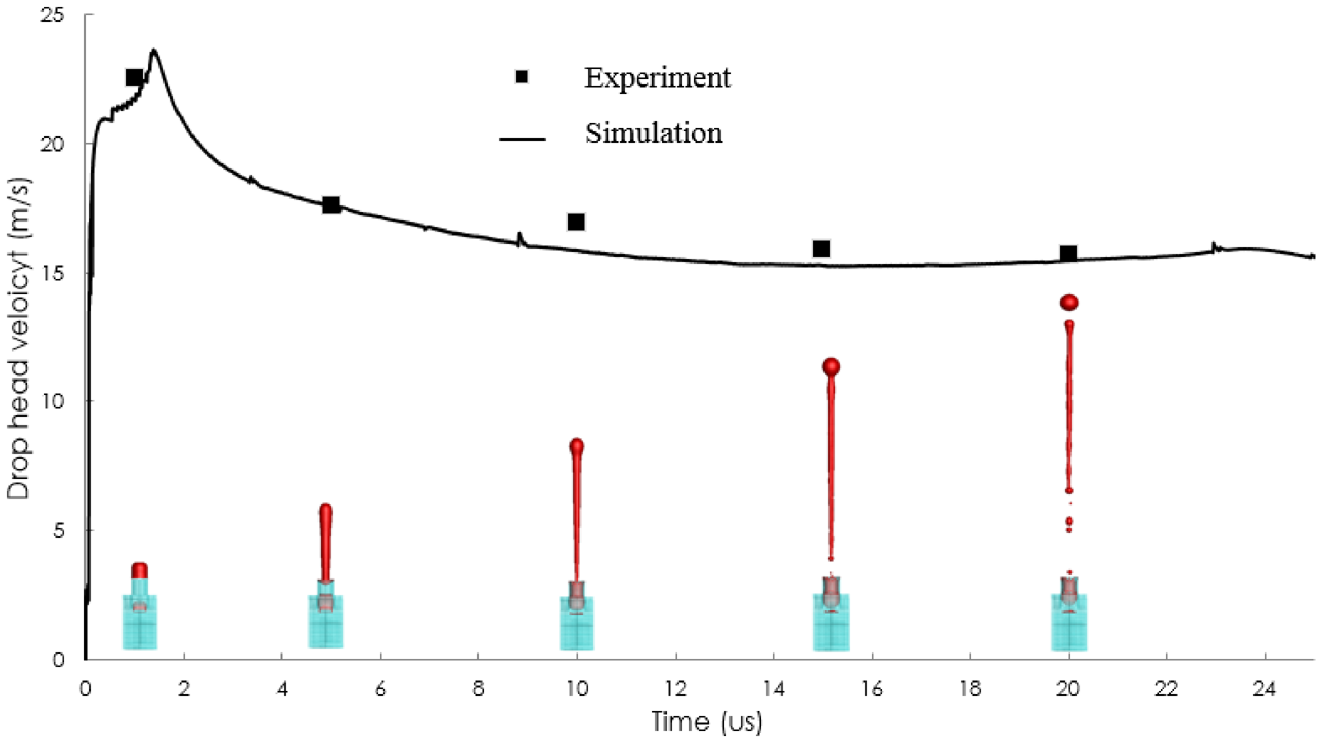
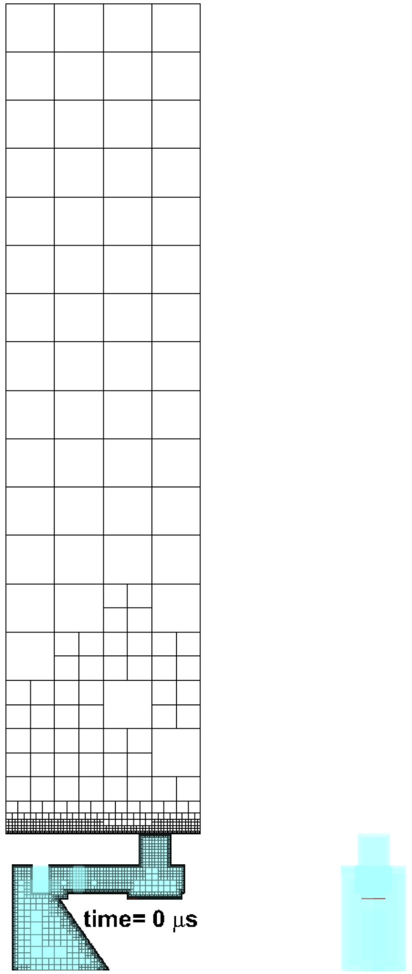
Droplet formation in Inkjet process

Simulation Examples*

droplet-ejection simulation





Side view Front view

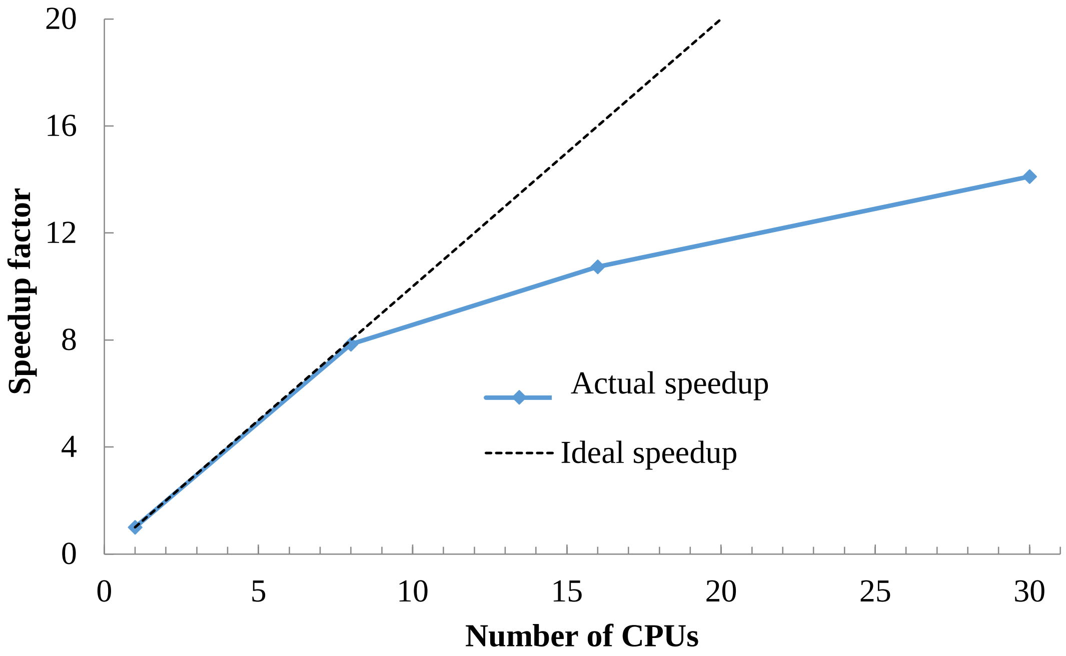
* H. Tan, An adaptive mesh refinement based flow simulation for free-surfaces in thermal inkjet technology. *International Journal of Multiphase Flow*. 82, 1-16, 2016.

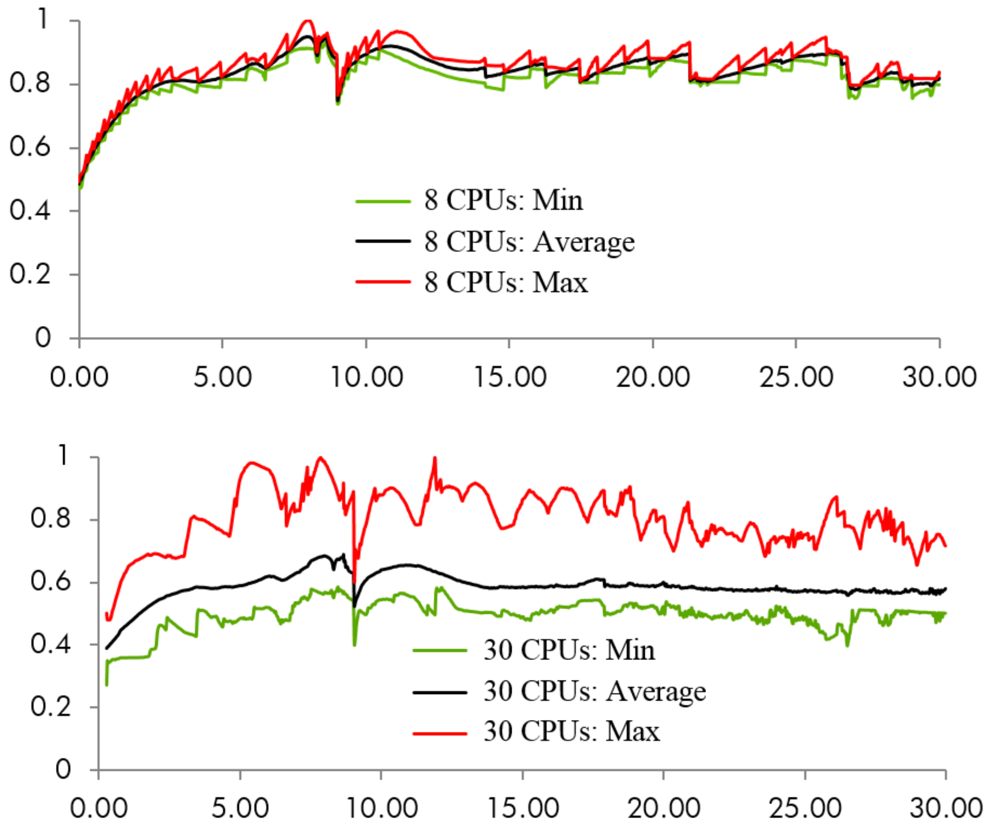
Droplet formation in Inkjet process

Simulation Examples*

droplet-ejection simulation

Parallel performance





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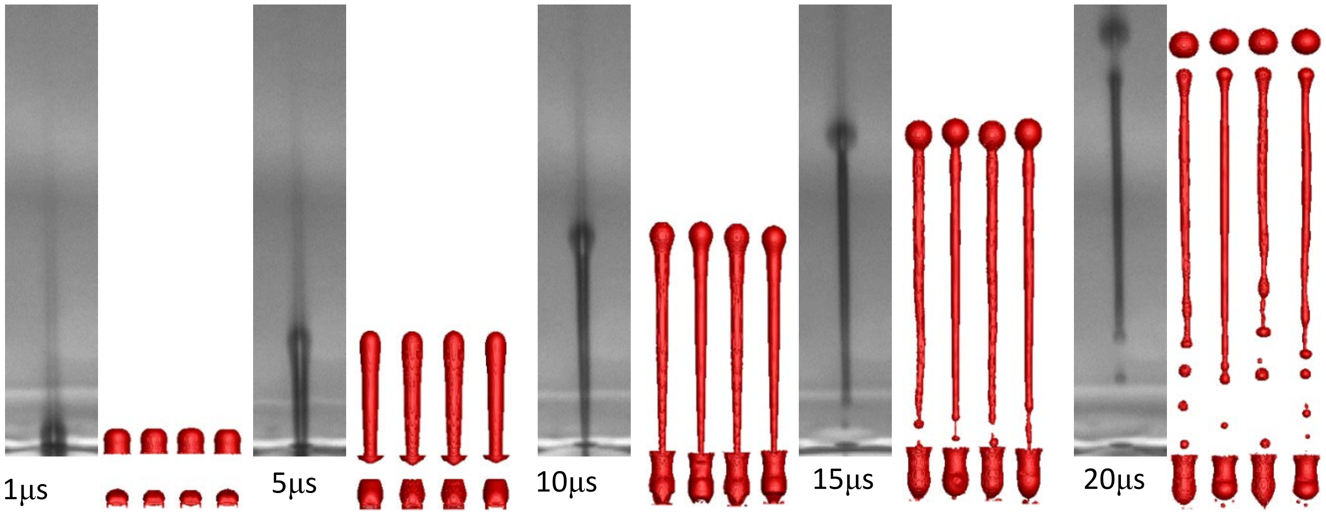
Droplet formation in Inkjet process

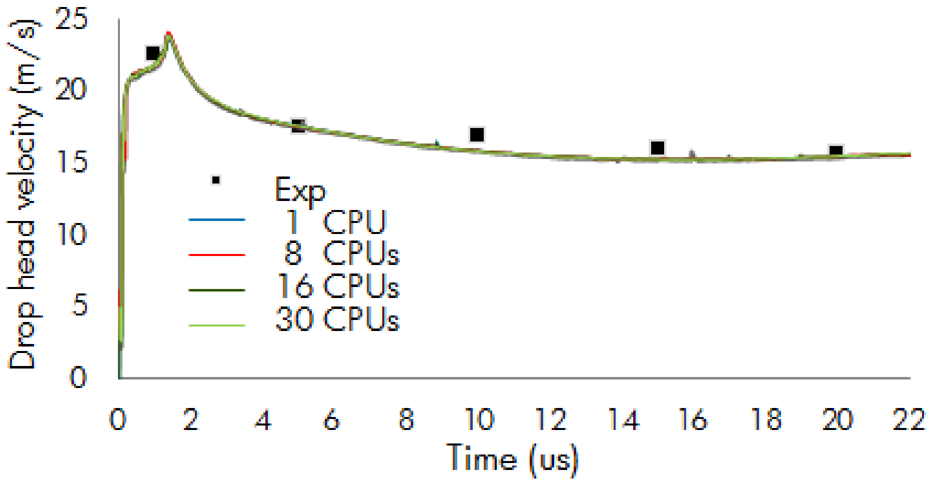
Simulation Examples*

droplet-ejection simulation

Effect of parallel computation on solution



#CPUs: 1 8 16 30 1 8 16 30 1 8 16 30 1 8 16 30 1 8 16 30



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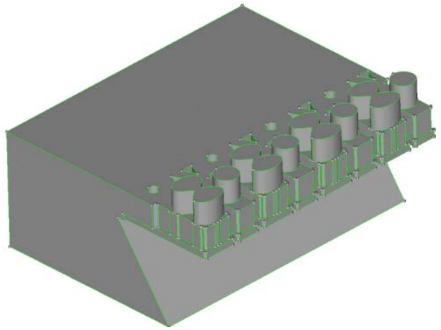
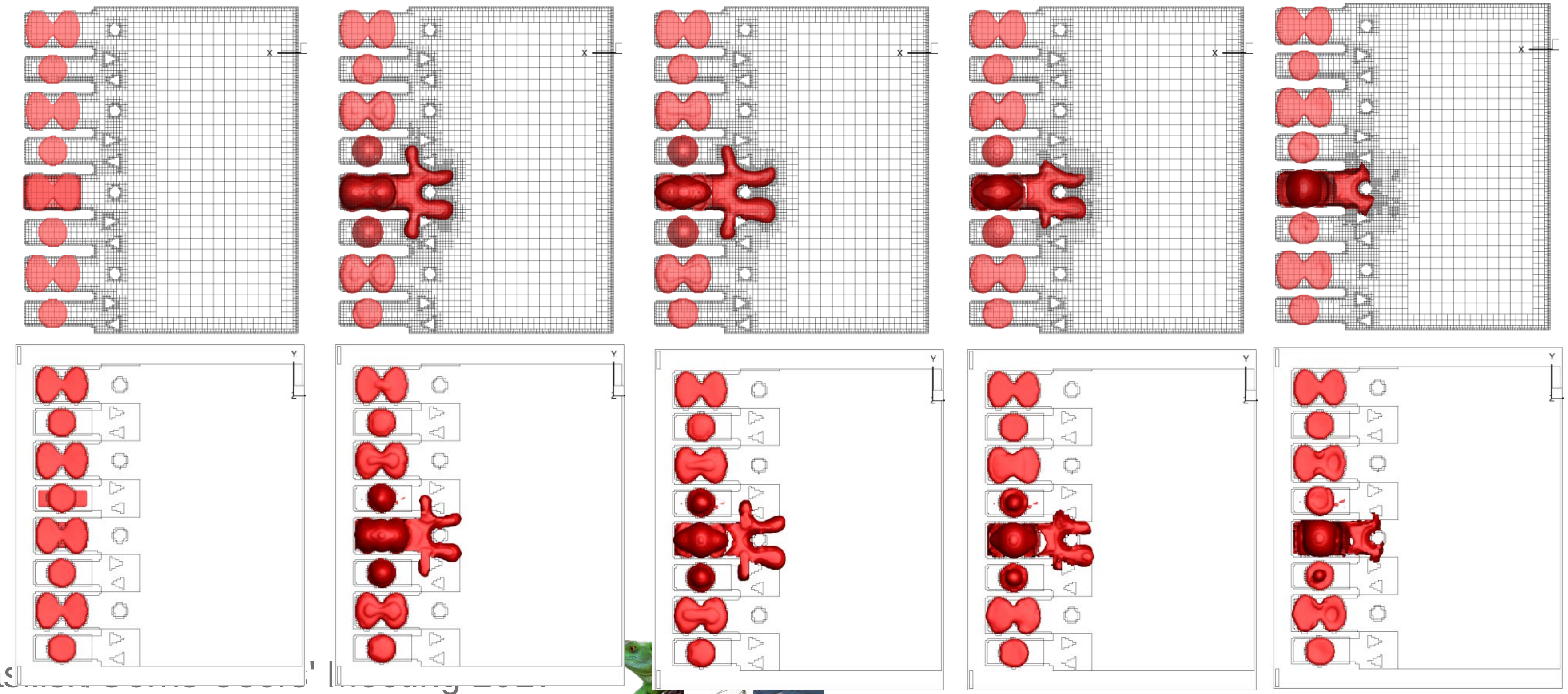
Droplet formation in Inkjet process

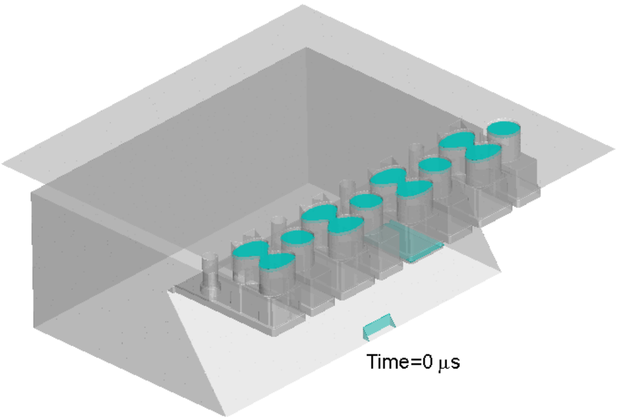


Simulation Examples

droplet-ejection simulation

Multi-nozzle case



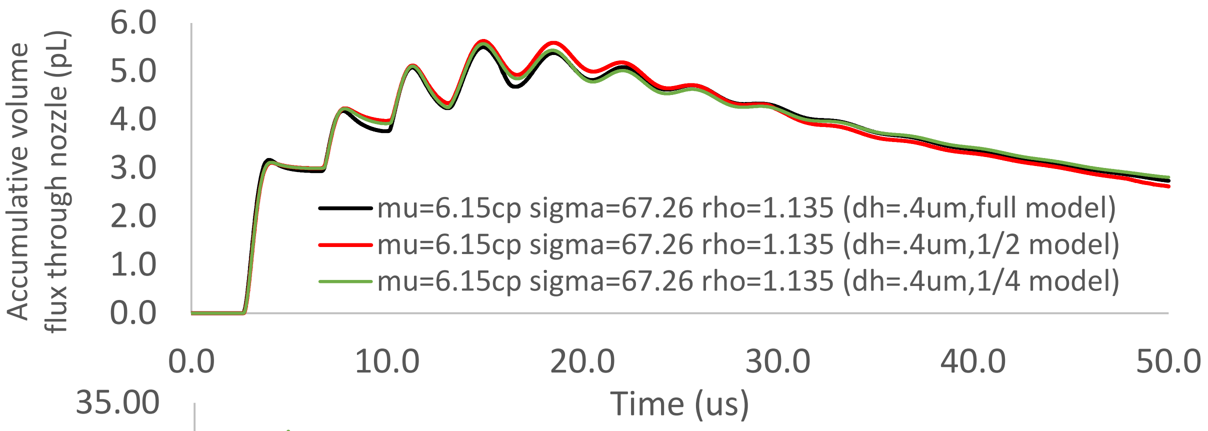


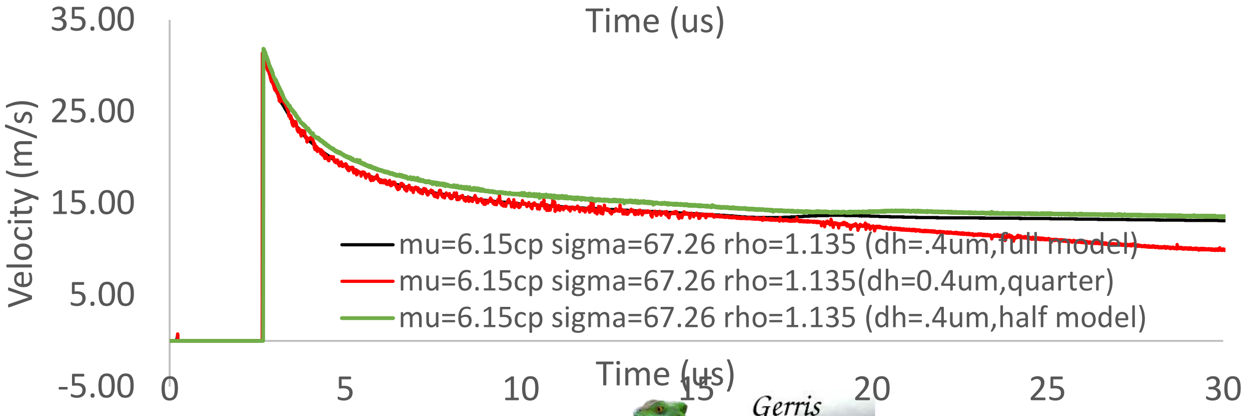
Droplet formation in Inkjet process

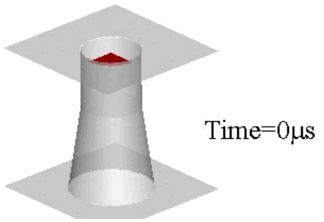
¼ model **½ model** **full model**

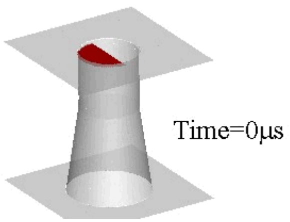
Simulation Examples

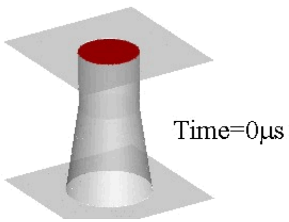
full-model, ¼-model, and ½-model









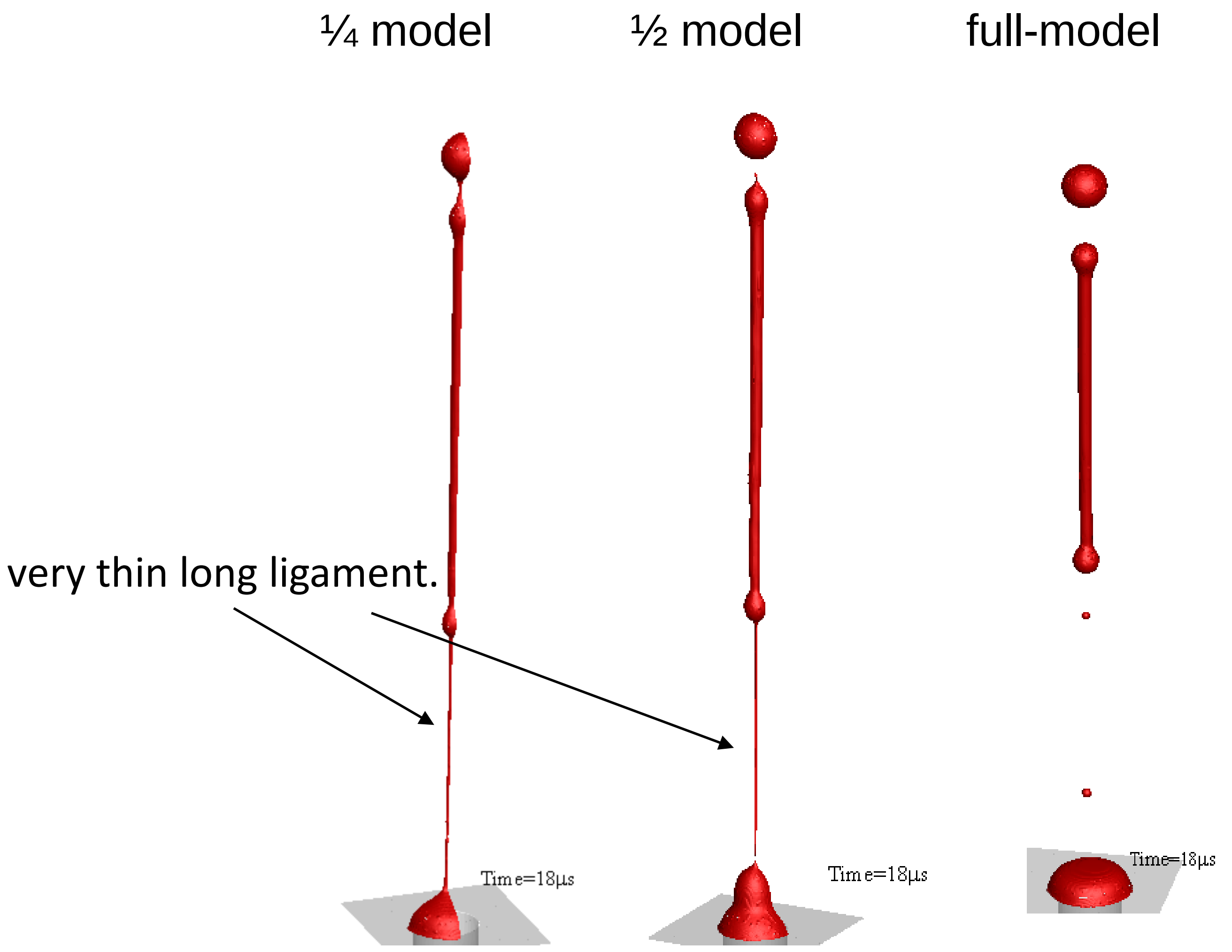


Droplet formation in Inkjet process

Simulation Examples

For drop velocity and volume, all three models give very close results.

Both ½- and ¼-models predict a very thin and long ligament after the end blob in the tail, whereas full-model predicts two very small satellite droplets.



Outline

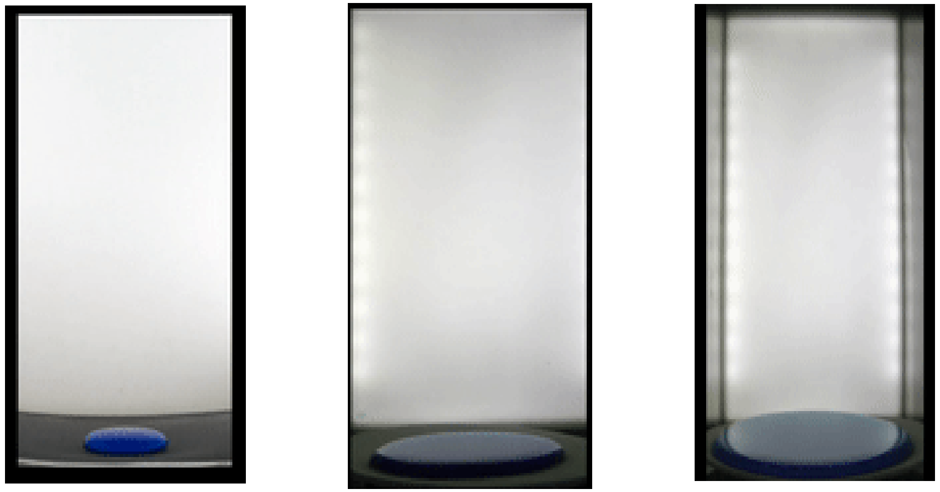
- How do I get started with Gerris
- Droplet formation in Inkjet process
- Capillary flow in low-gravity
- Droplet-media interaction
- Future work

Capillary flow in low-gravity

Puddle jump*

2.1-s drop tower facility at Portland State University ($g \leq 2\times10^{-4} g_o$).

Vol=2 mL 30mL 95mL



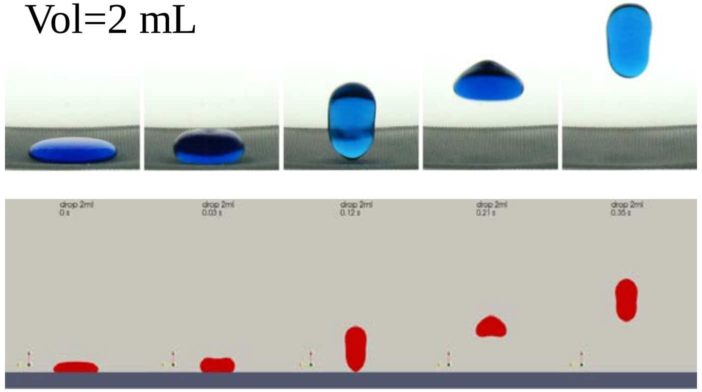
A puddle jumps from superhydrophobic surface in low-g condition.

*Wollman, A. and M. Weislogel, *New investigations in capillary fluidics using a drop tower.* Experiments in Fluids, 2013. **54**(4): p. 1499.

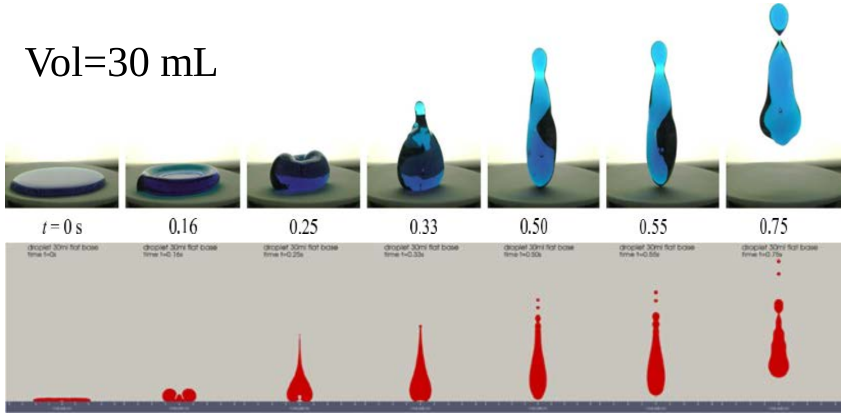
Capillary flow in low-gravity

Puddle jump*

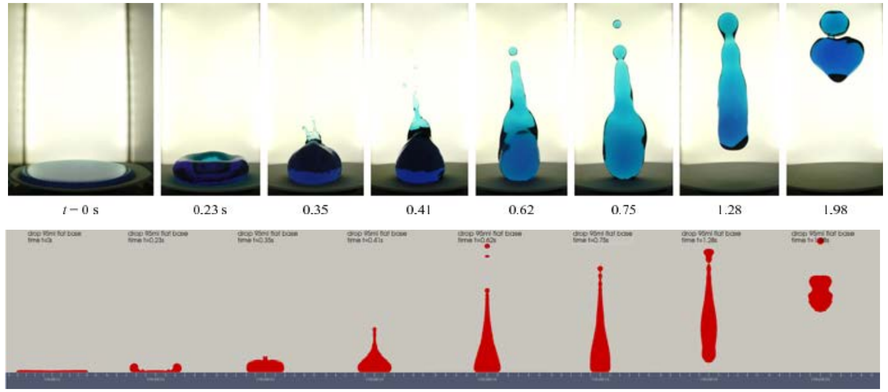
Vol=2 mL

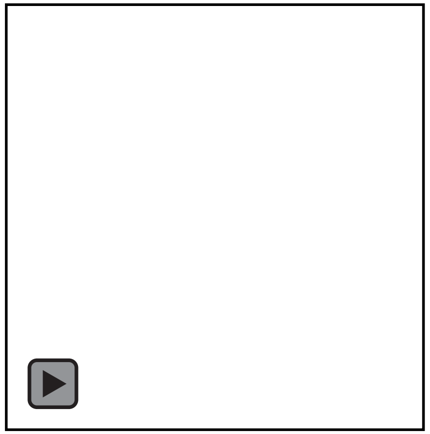


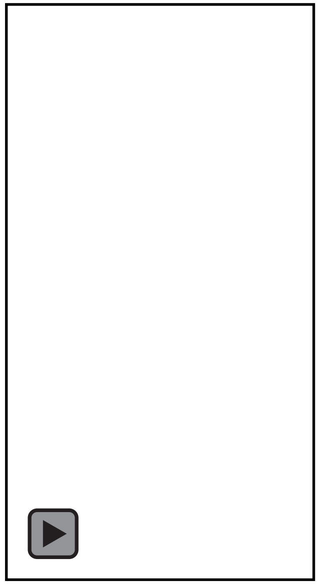
Vol=30 mL



Vol=95 mL



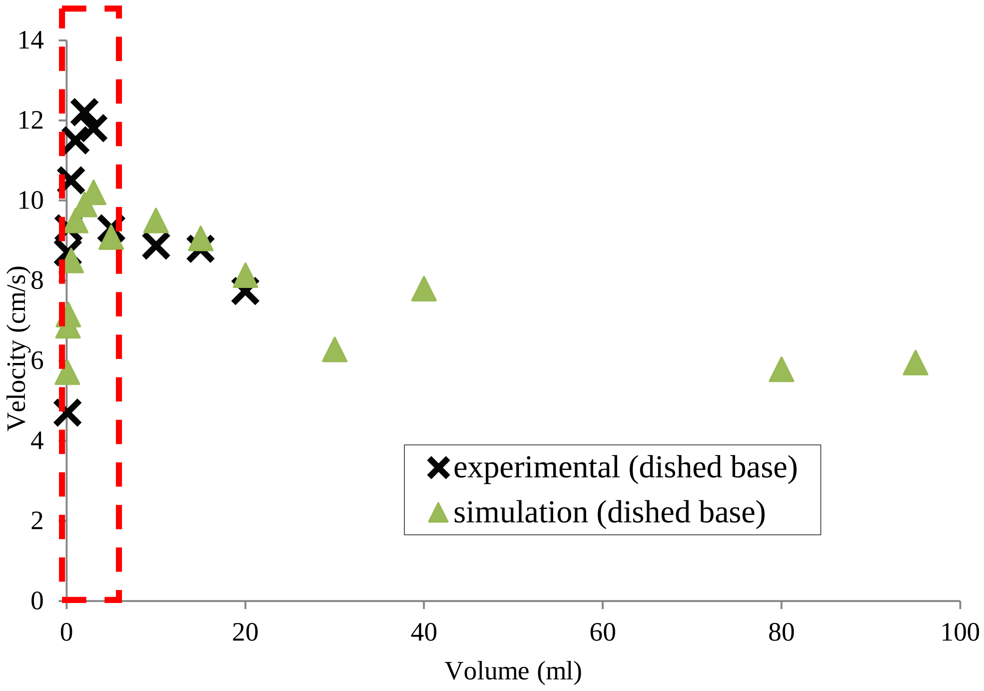


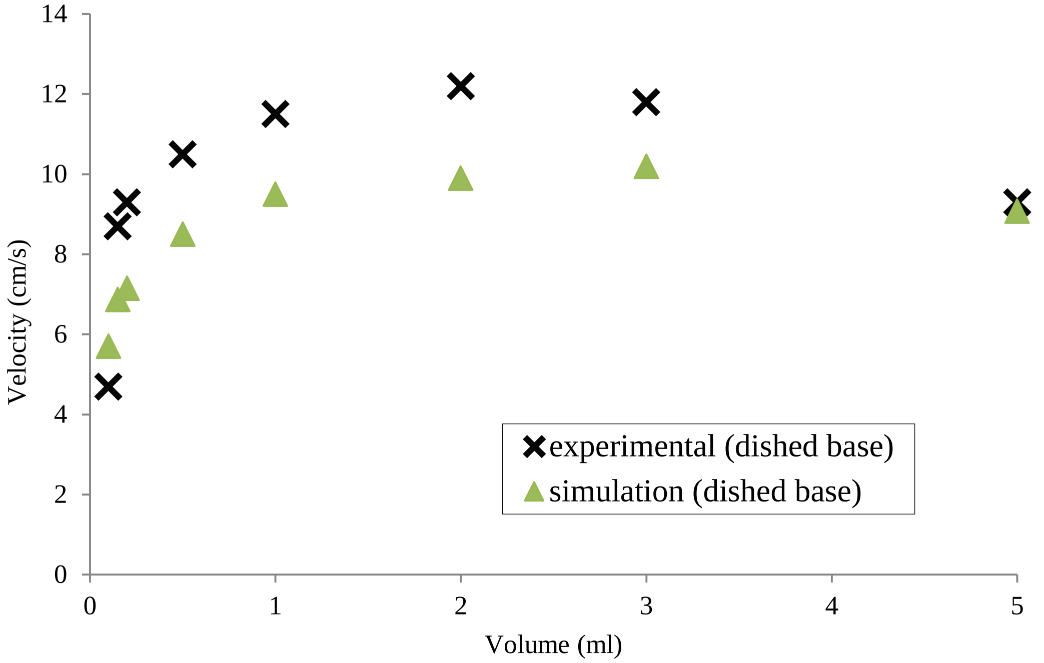


*Attari, B., et al, *Puddle jumping: Spontaneous ejection of large liquid droplets from hydrophobic surfaces during drop tower tests.* Physics of Fluids, 2016. **28**(10): p. 102104.

Capillary flow in low-gravity

Puddle jump

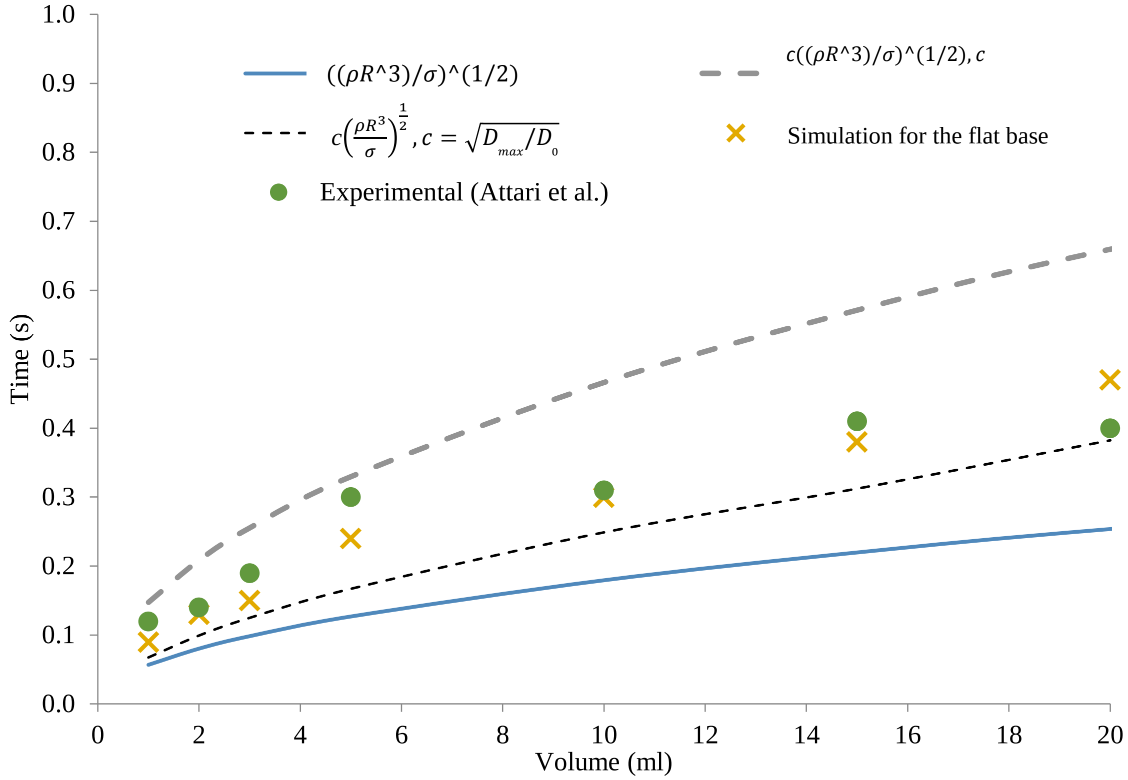


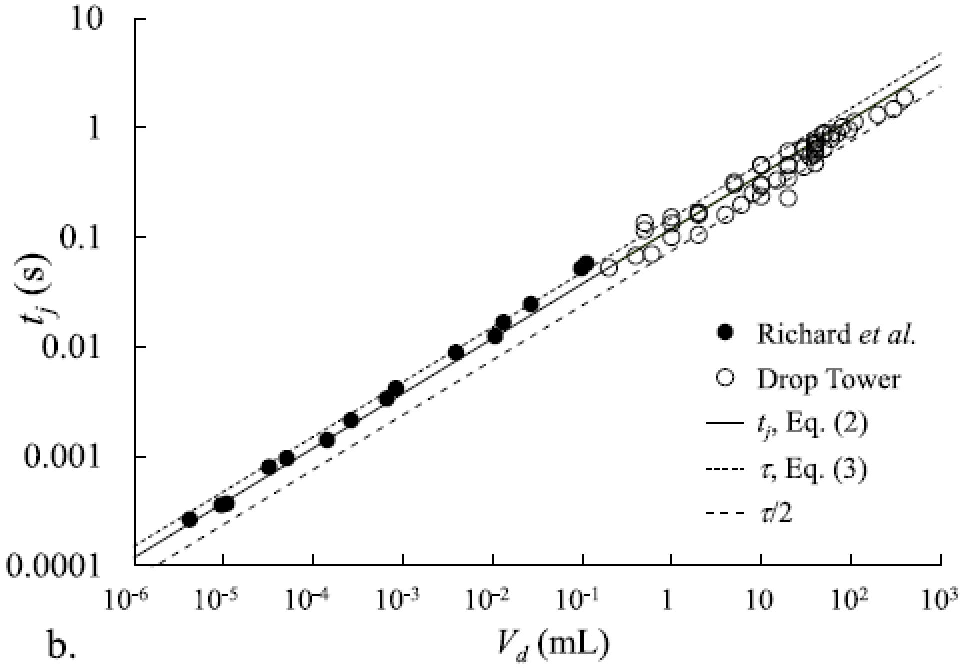


Capillary flow in low-gravity

Puddle jump

$$\tau_c = c\left(\frac{\rho R^3}{\sigma}\right)^{\frac{1}{2}}$$





*Attari, B., et al, *Puddle jumping: Spontaneous ejection of large liquid droplets from hydrophobic surfaces during drop tower tests.* Physics of Fluids, 2016. **28**(10): p. 102104.

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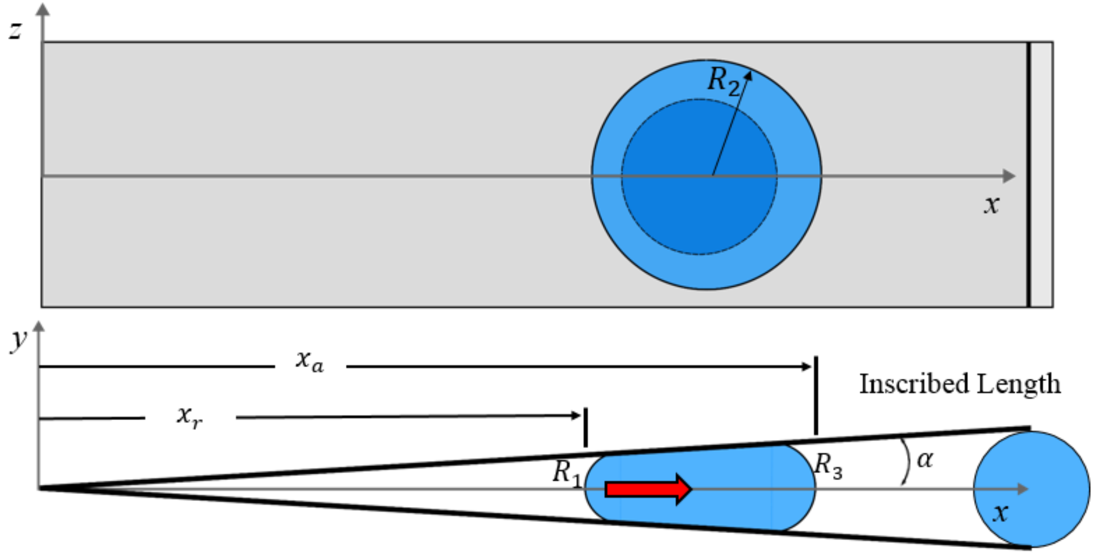
Capillary flow in low-gravity

Capillary migration in super-hydrophobic wedges*



$$\Delta P_{net} \approx \sigma \left(\frac{1}{R_1} - \frac{1}{R_3} \right)$$

$$U \approx \left(\frac{\sigma g}{\rho}\right)^{1/4} \left[-2\cos\theta + 2\left(\frac{\pi H}{V}\right)^{1/2} - 6^{2/3}\left(\frac{\pi H}{V}\right)^{1/3}\right]^{1/2}$$

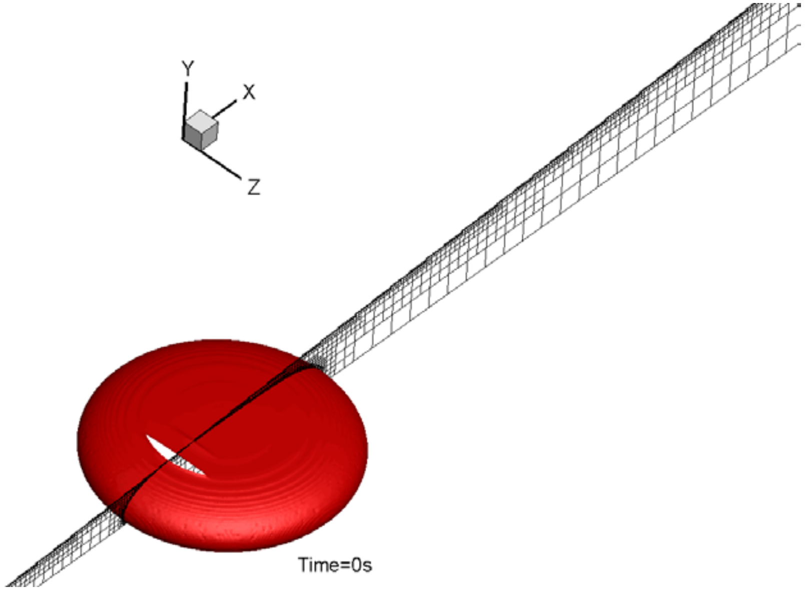
$$t_{jw} \approx \left(\frac{3V}{4\pi}\right)^{1/3} \left(\frac{\rho}{\sigma g}\right)^{1/4} \frac{1}{-2\cos\theta \cdot \sin\alpha}$$

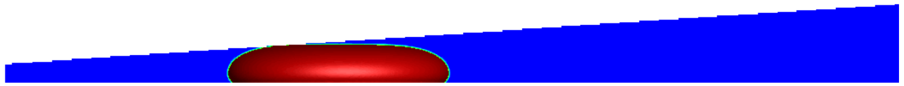
*Torres, L., et al., Large droplet generation by capillary migration in super-hydrophobic wedges, 33rd Annual Meeting of the American Society for Gravitational and Space Research, ID306, Seattle, Oct. 25-28, 2017.

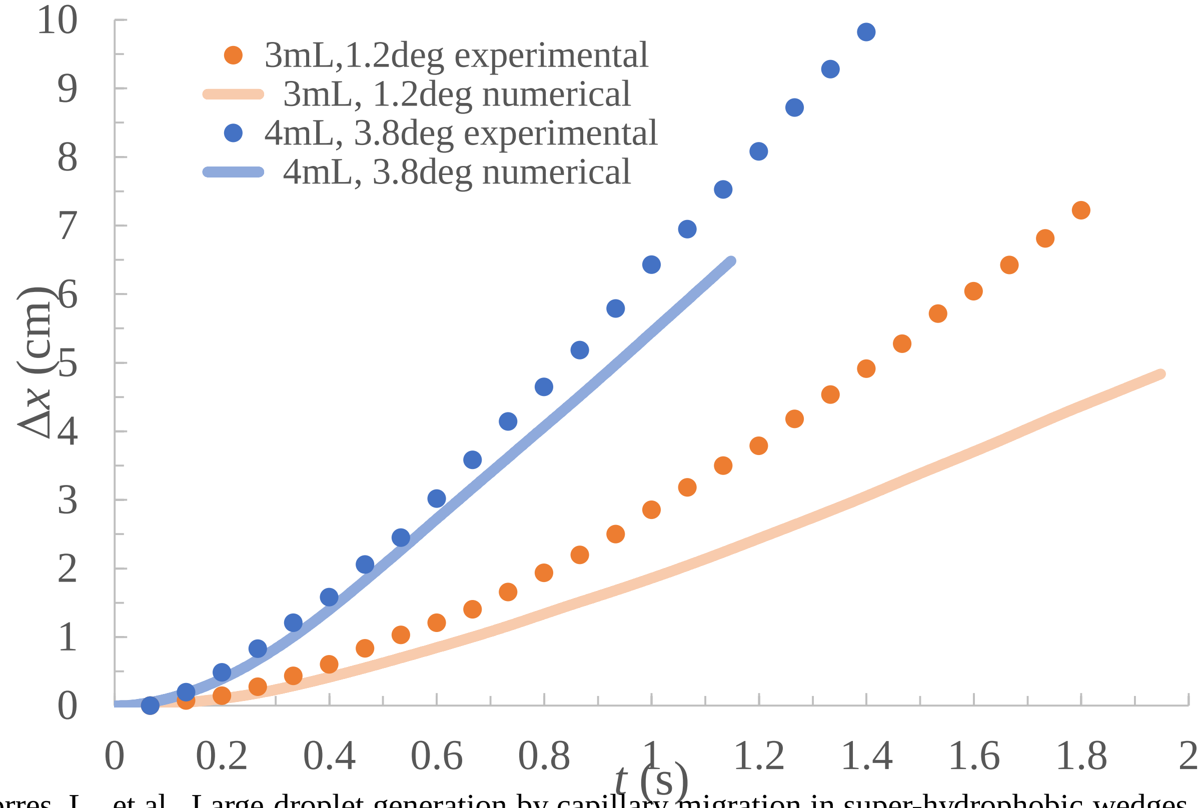
Capillary flow in low-gravity

Capillary migration in super-hydrophobic wedges*

4ml α=3.8⁰





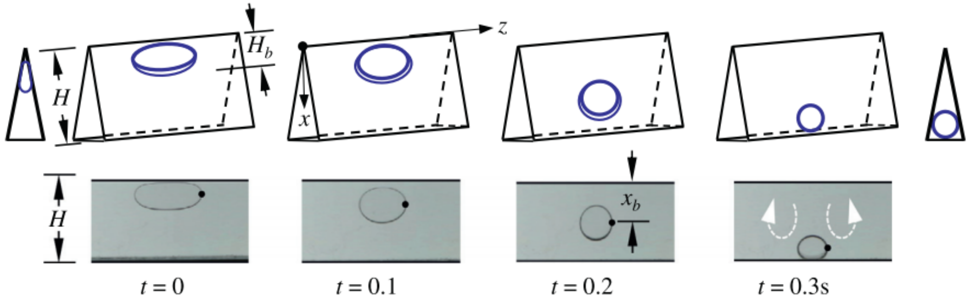


*Torres, L., et al., Large droplet generation by capillary migration in super-hydrophobic wedges, 33rd Annual Meeting of the American Society for Gravitational and Space Research, ID306, Seattle, Oct. 25-28, 2017.

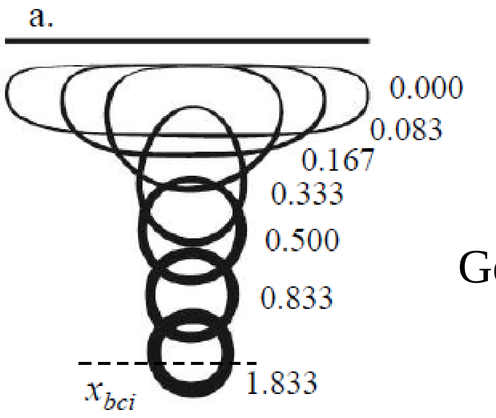
Capillary flow in low-gravity

Capillary migration in super-hydrophobic wedges*

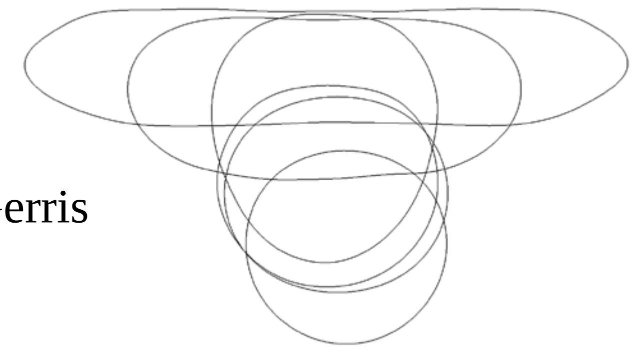
Jensen *et al.* 2014

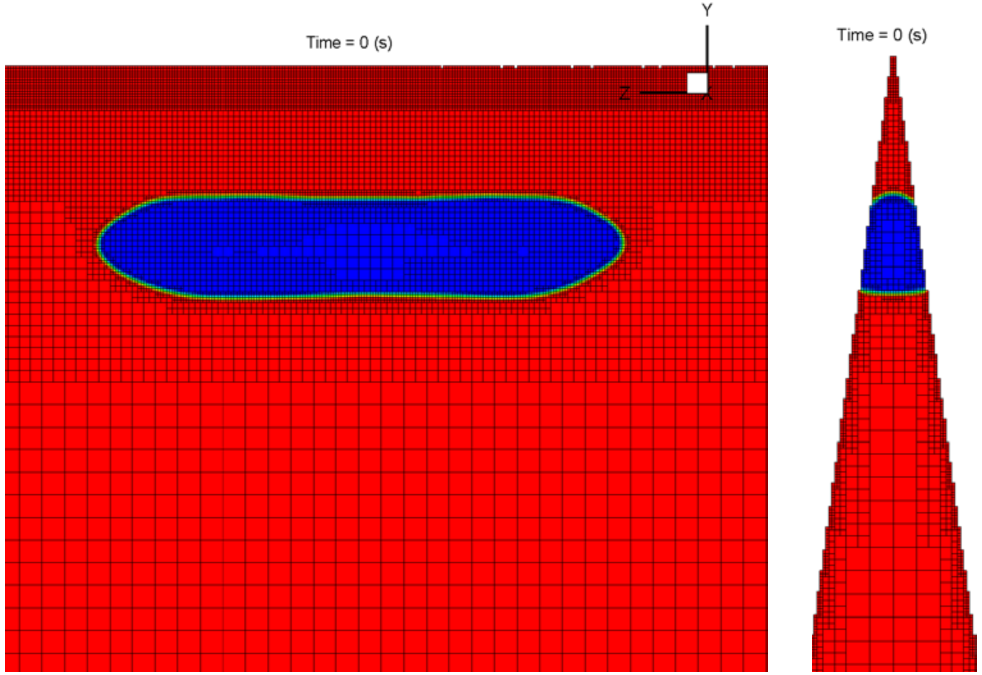


Exp.



Gerris

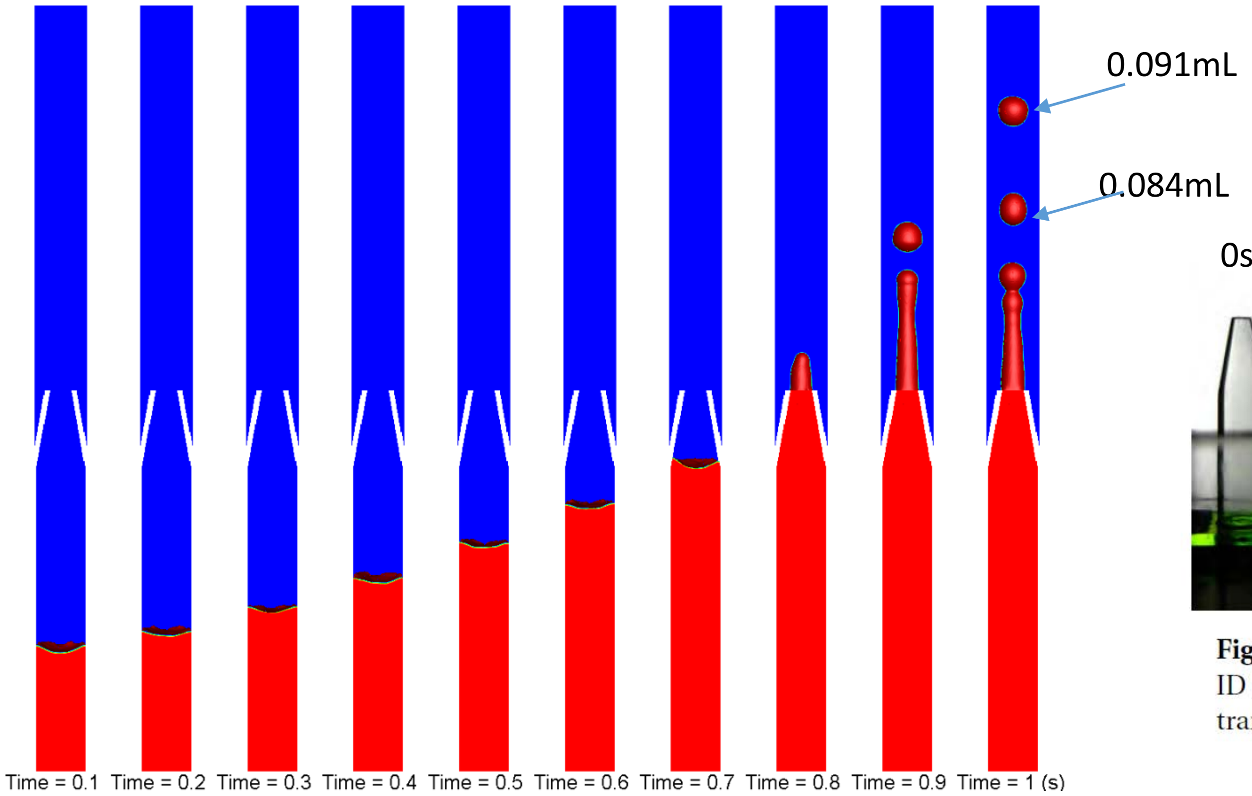




*Weislogel., et al., Capillary channel flow EU2-02 on the international space station: an experimental investigation of passive bubble separations in an open capillary channel, NASA/TM-20150218720.

Capillary flow in low-gravity

Auto-ejection*



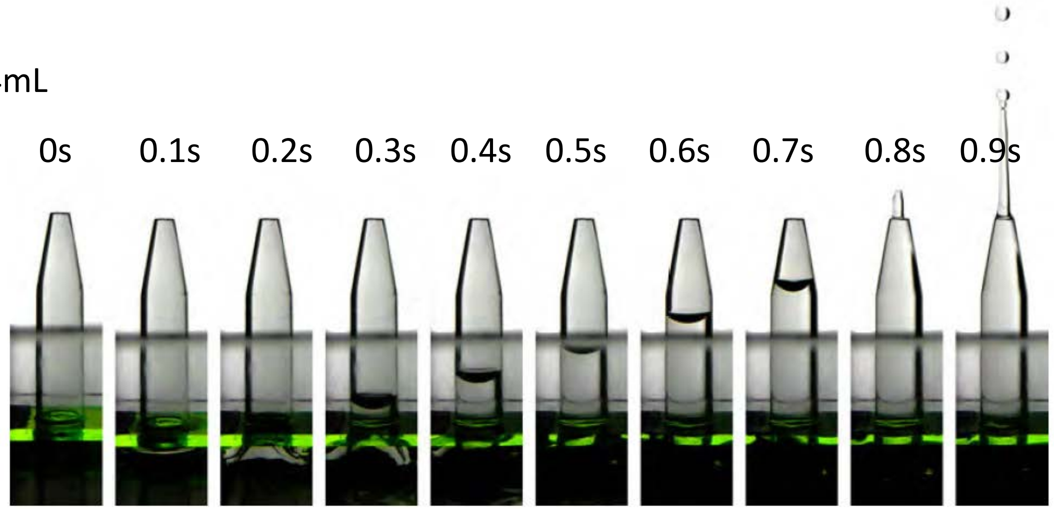


Figure 3.3: Spontaneous capillary rise of 0.65cS PDMS in a 73.5mm long, 9.2mm ID circular tube (images at 10Hz). The 3.88mm tube nozzle exit ID produces a transient jet which eventually breaks up into 6 $\approx$ 0.02ml drops.

*Wollman, A. and M. Weislogel, *New investigations in capillary fluidics using a drop tower.* Experiments in Fluids, 2013. **54**(4): p. 1499.

Outline

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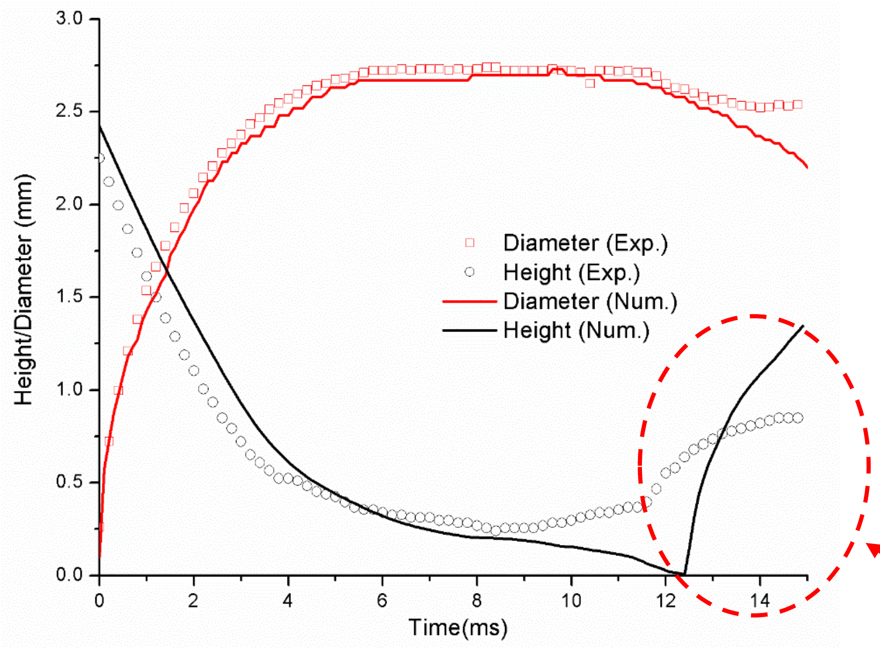
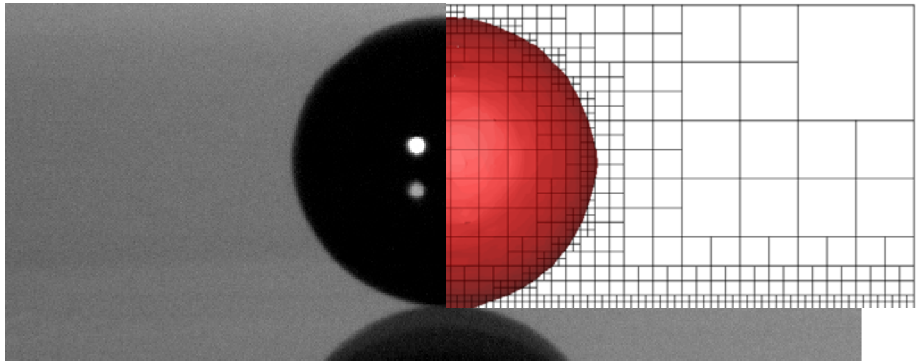
Droplet-media interaction

Droplet impact on glass surface*

Ink droplet



U_0=0.57m/s (We=27)



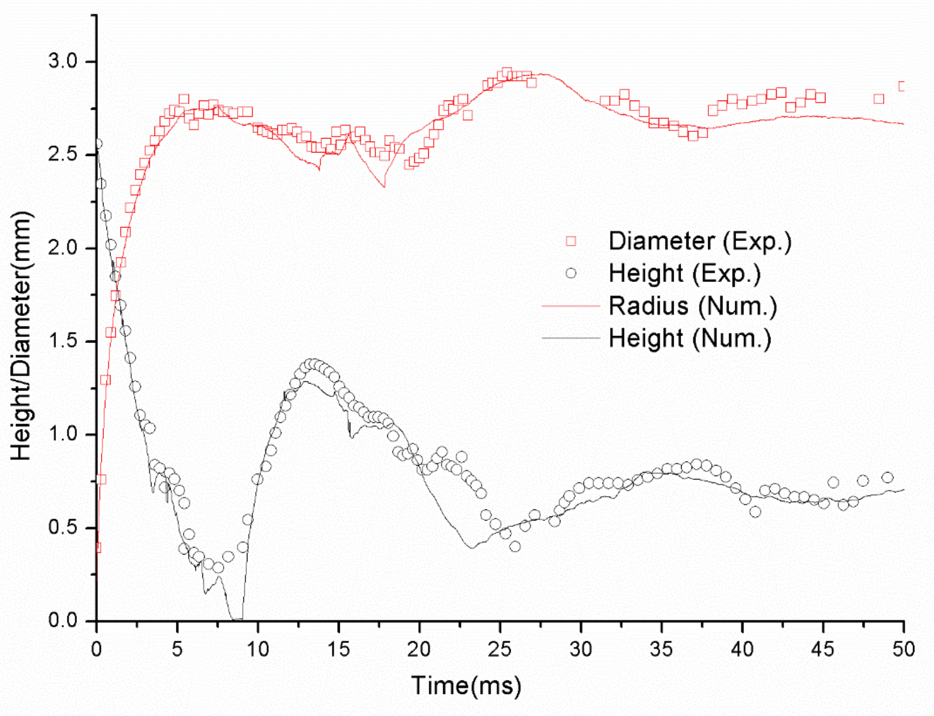
Simulation predicts much higher rebound. Dynamic surface tension plays an important role.

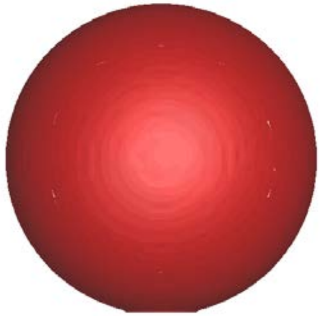
*H. Tan, Absorption of Picoliter Droplets by Thin Porous Substrates. *AIChE Journal*, 2017, 63(5): p. 1690-1703.

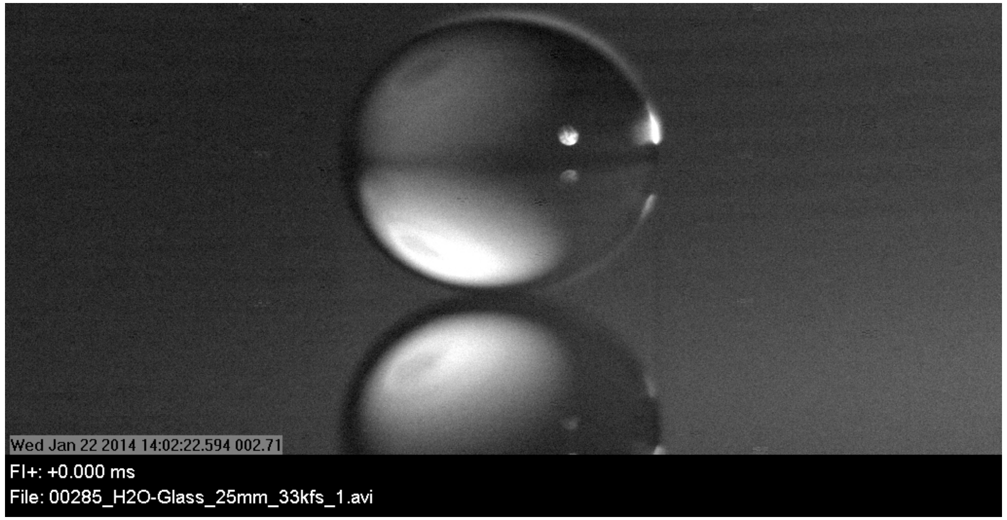
Droplet-media interaction

Droplet impact on glass surface*

Water droplet





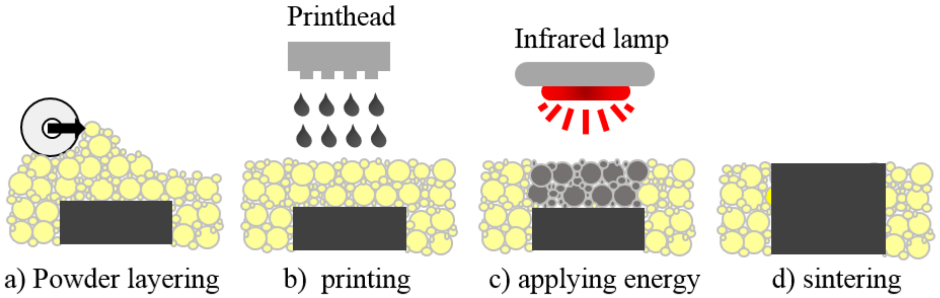


*H. Tan, Absorption of Picoliter Droplets by Thin Porous Substrates. *AIChE Journal*, 2017, 63(5): p. 1690-1703.

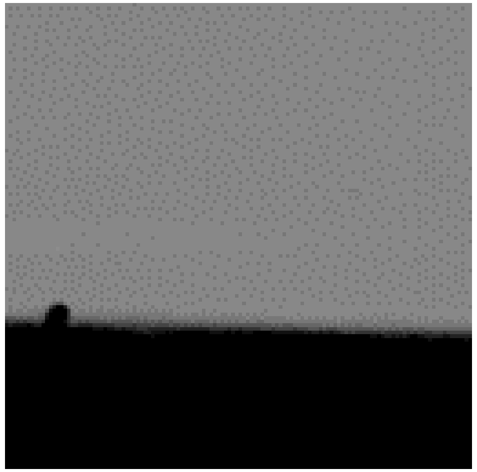
Droplet-media interaction

Droplet impact on powders

High-speed sintering 3D printing machine



HSS 3D printing process: (a) powder is deposited on the build area by a roller; (b) A radiation absorbent ink is printed on desired area of the powder layer; (c) An infrared radiation source scans the entire build area; (d) The powder area masked by the ink is sintered and the entire process is repeated until the part is completed.

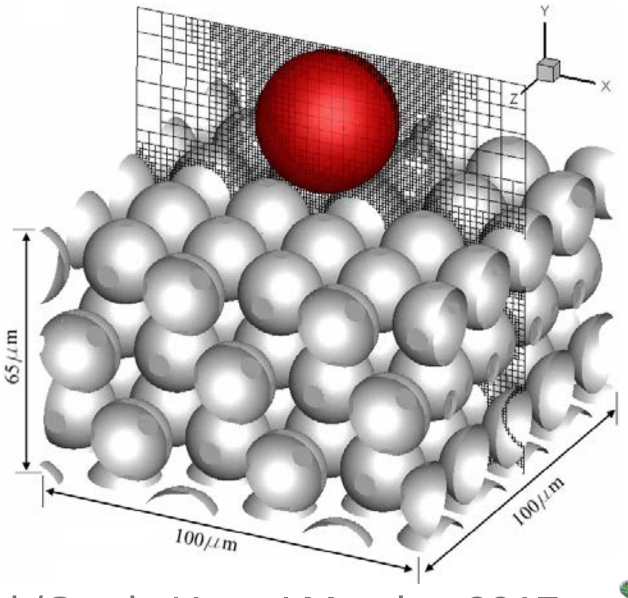


Drop impact on loose powder

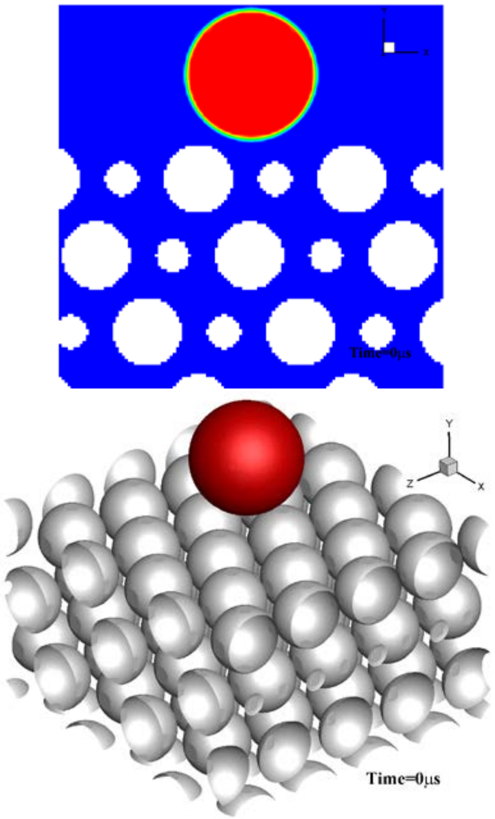
Droplet-media interaction

Droplet impact on powders*

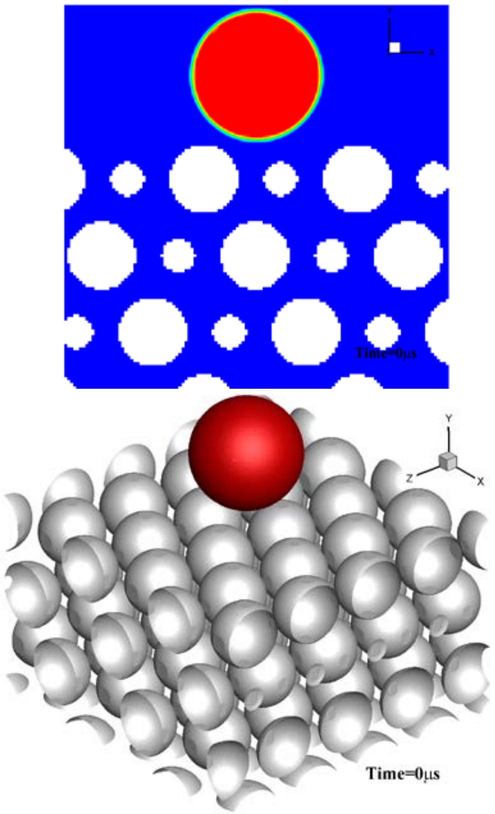
- impact velocities U_0=1m/s, U_0=5m/s, U_0=10m/s.
- Powder pack density is 0.4869, particle diameter=20µm
- Ink droplet diameter 36.68µm



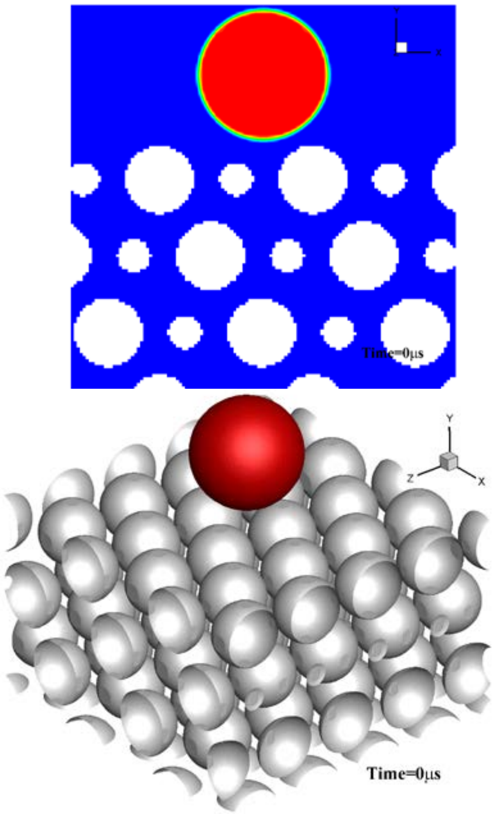
U_0=1m/s (We=0.611)



U_0=5m/s (We=15.3)



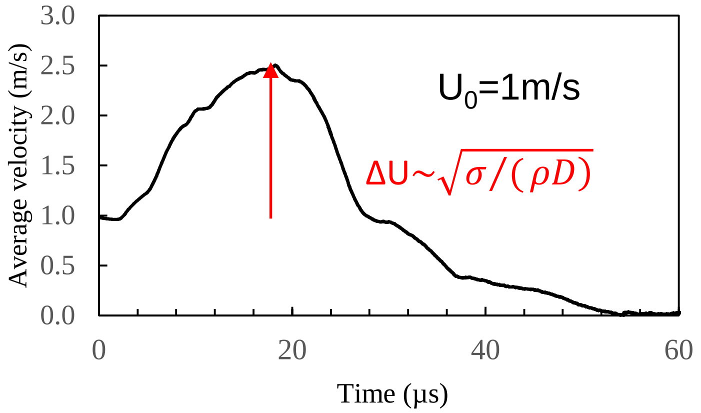
U_0=10m/s(We=61.1).

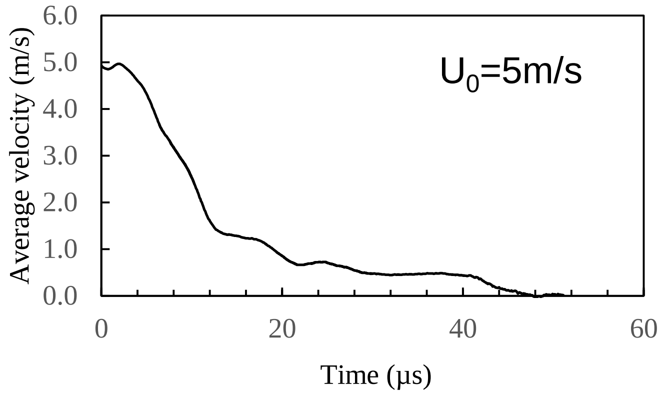


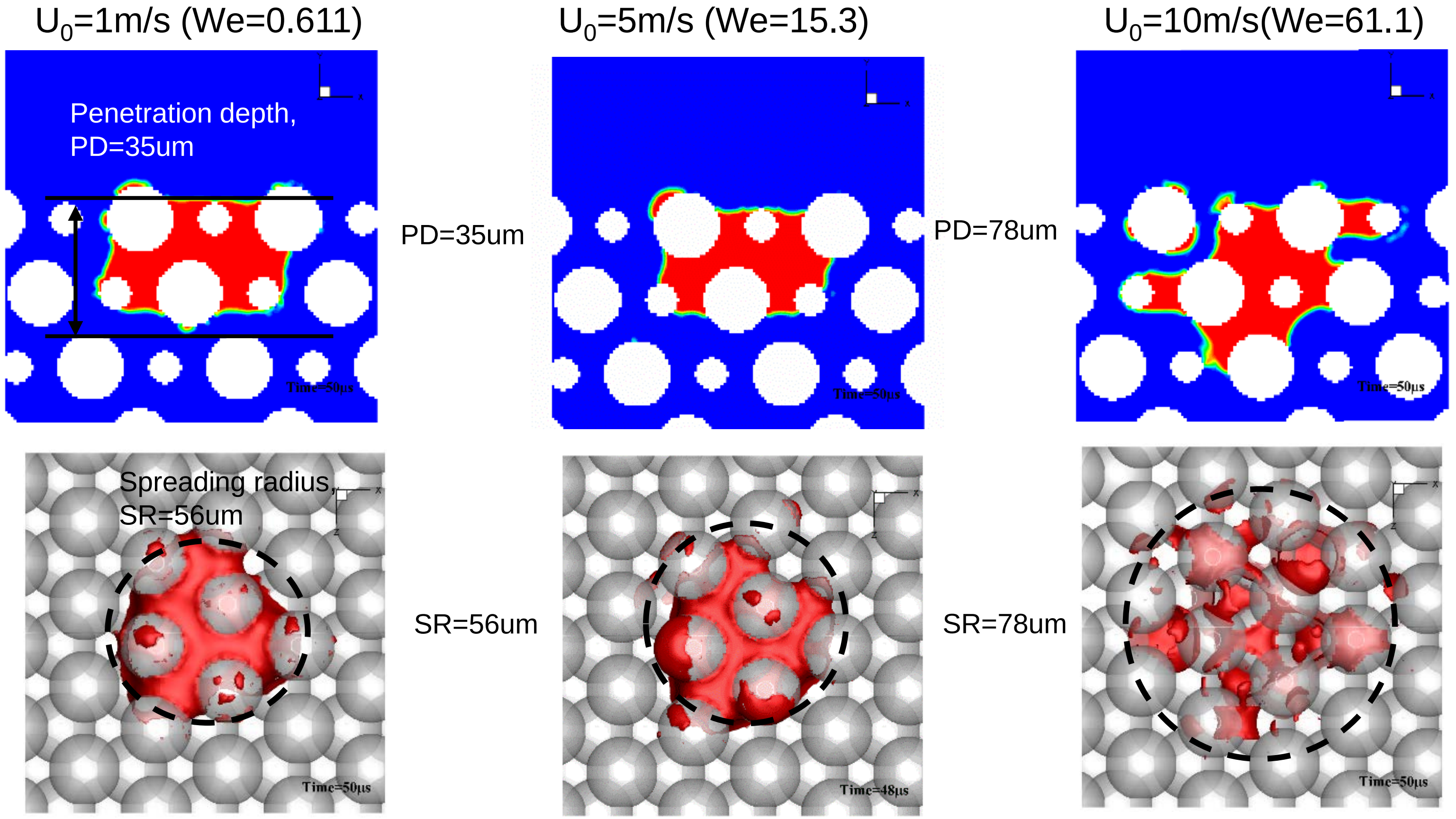
*H. Tan, Three-dimensional simulation of micrometer-sized droplet impact and penetration into the powder bed. *Chemical Engineering Science.* 2016, 153: 93-107.

Droplet-media interaction

Droplet impact on powders*







*H. Tan, Three-dimensional simulation of micrometer-sized droplet impact and penetration into the powder bed. *Chemical Engineering Science.* 2016, 153: 93-107.

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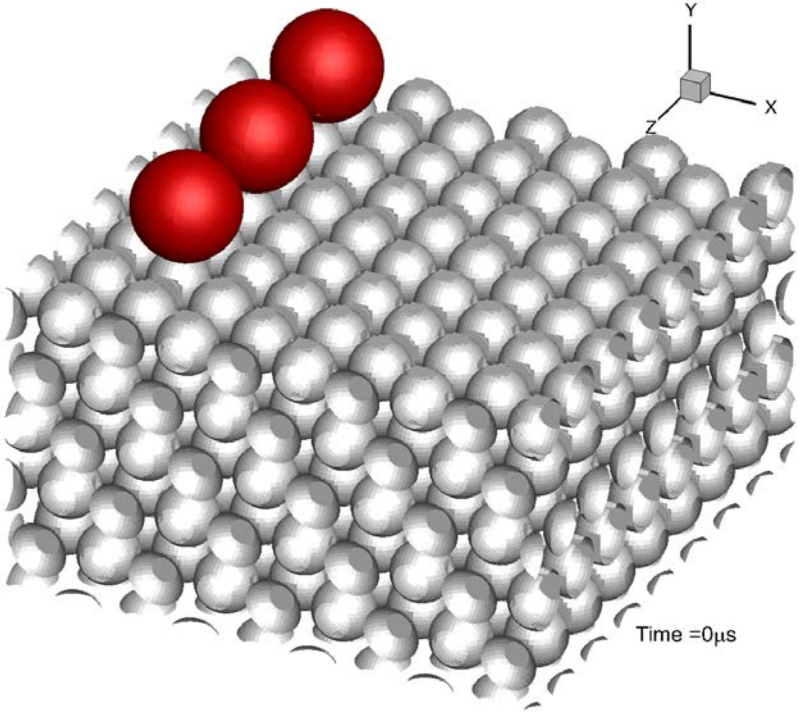
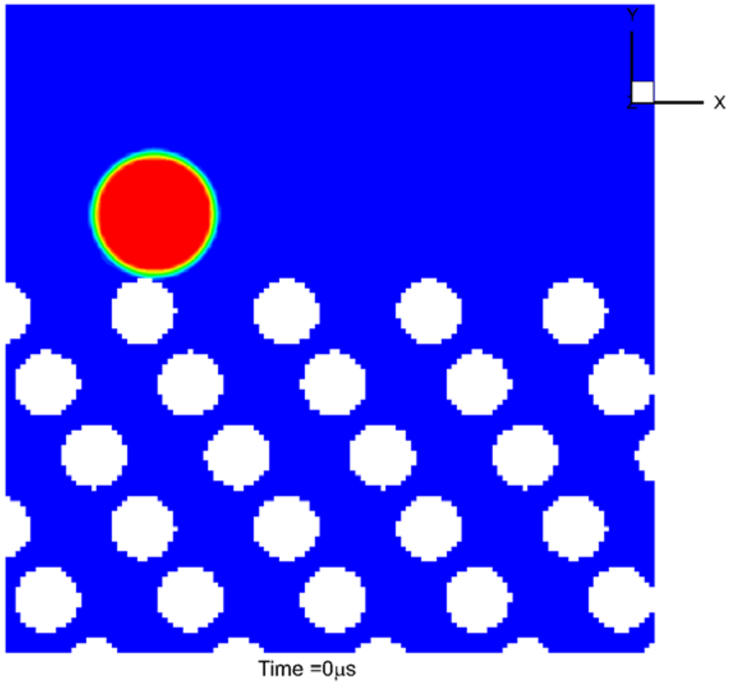
Droplet-media interaction

Droplet impact on powders*

Impact velocities U_0=5m/s
Powder pack density is 0.4869
particle diameter=20µm
Ink droplet diameter 36.68µm





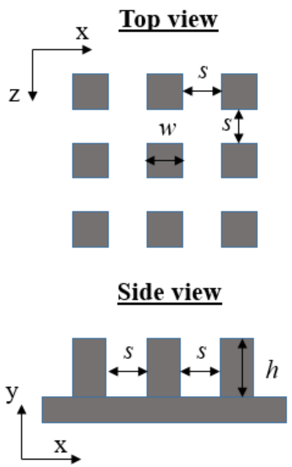
*H. Tan, Three-dimensional simulation of micrometer-sized droplet impact and penetration into the powder bed. *Chemical Engineering Science.* 2016, 153: 93-107.

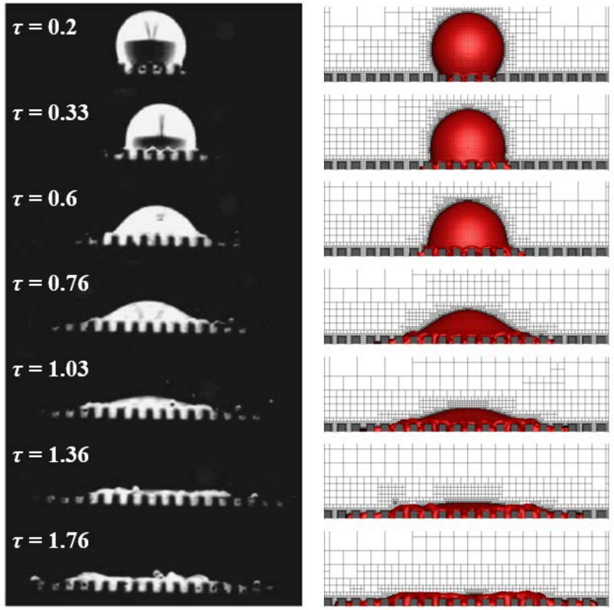
Droplet-media interaction

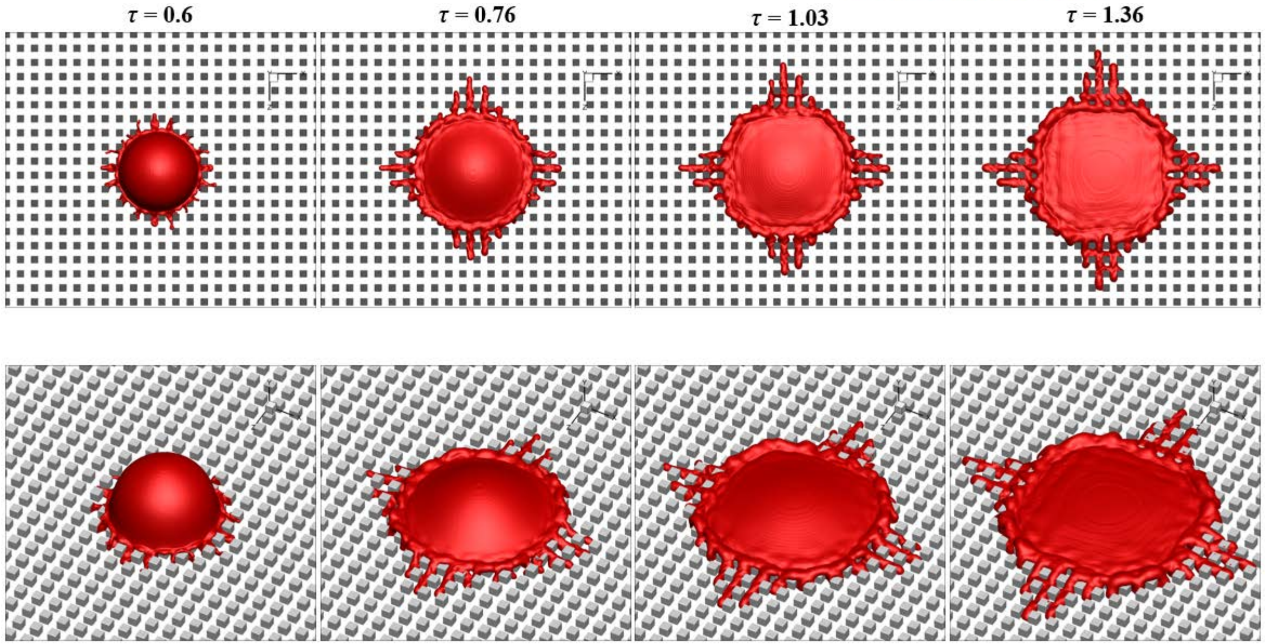
Droplet impact on microstructured surfaces

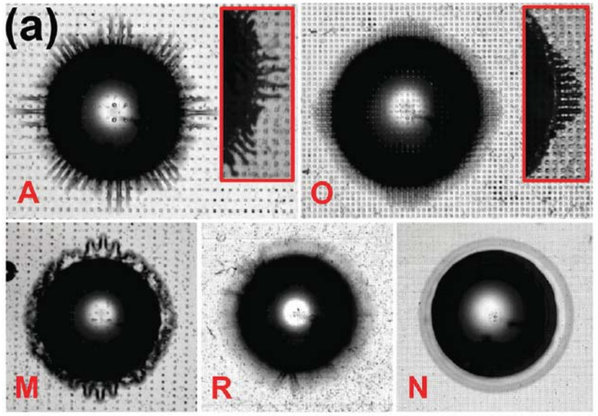
Water droplets impact on substrates that consist of square-shaped pillars of w=0.3mm h=0.3mm s=0.3 mm between pillars. (Sivakumar, et al. Physics of Fluids, 2005)

D_o=2.99mm, U_o=1.96 m/s. The corresponding We=158.3 and Re= 5895









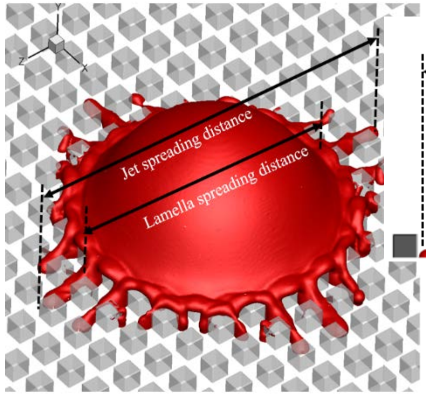
Robson and Willmott. Soft Matter, 2016

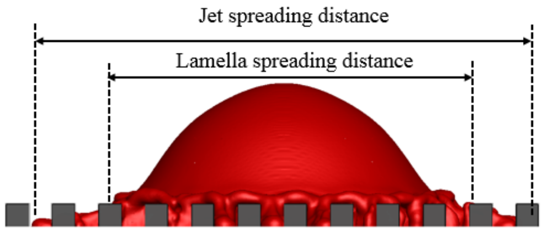
Droplet-media interaction

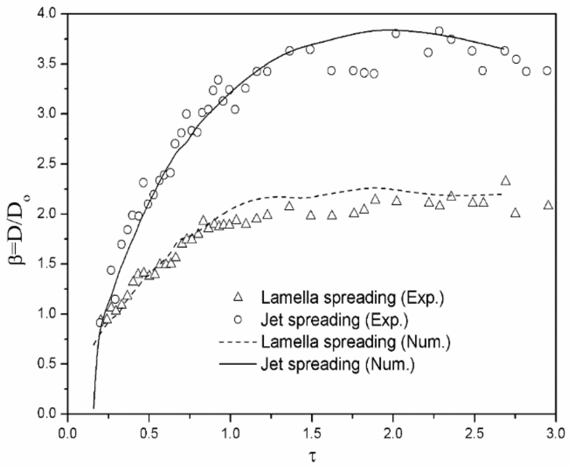
Droplet impact on microstructured surfaces

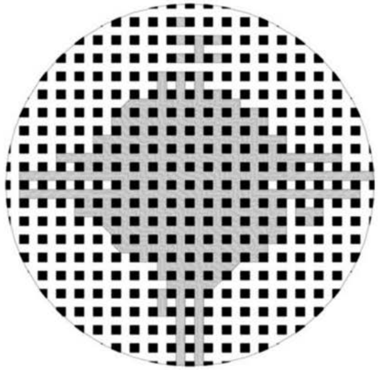
Water droplets impact on substrates that consist of square-shaped pillars of w=0.3mm h=0.3mm s=0.3 mm between pillars. (Sivakumar, et al. Physics of Fluids, 2005)

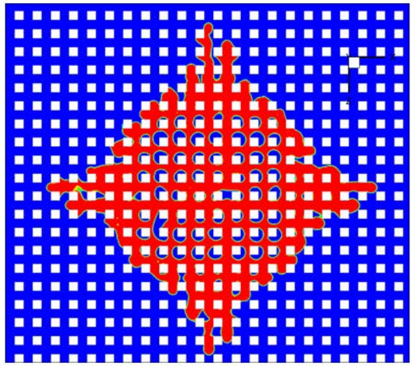
D_o=2.99mm,
U_o=1.96 m/s.
(We=158.3 and Re= 5895)

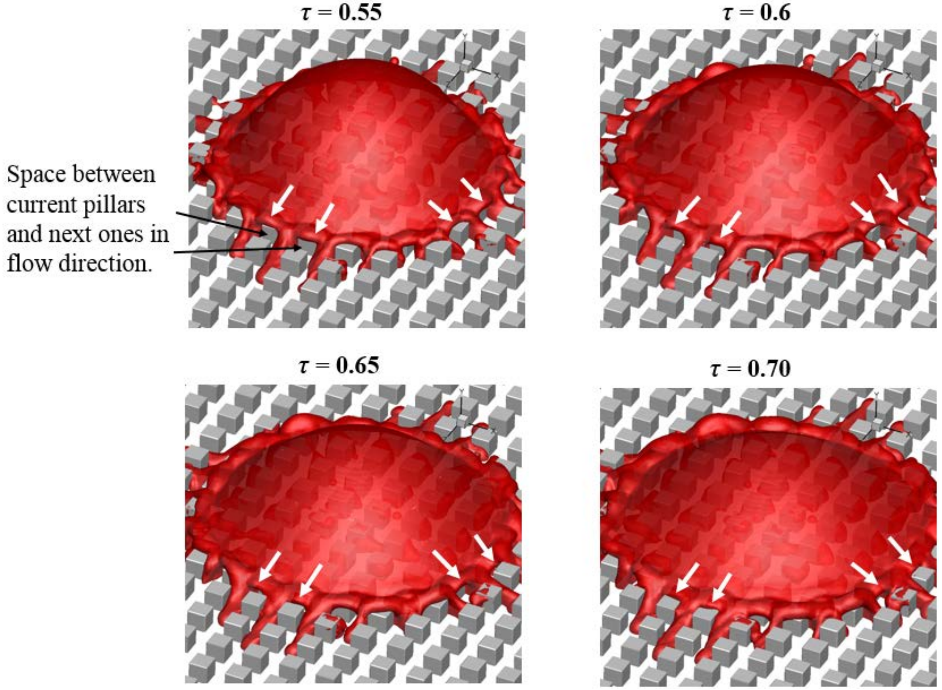










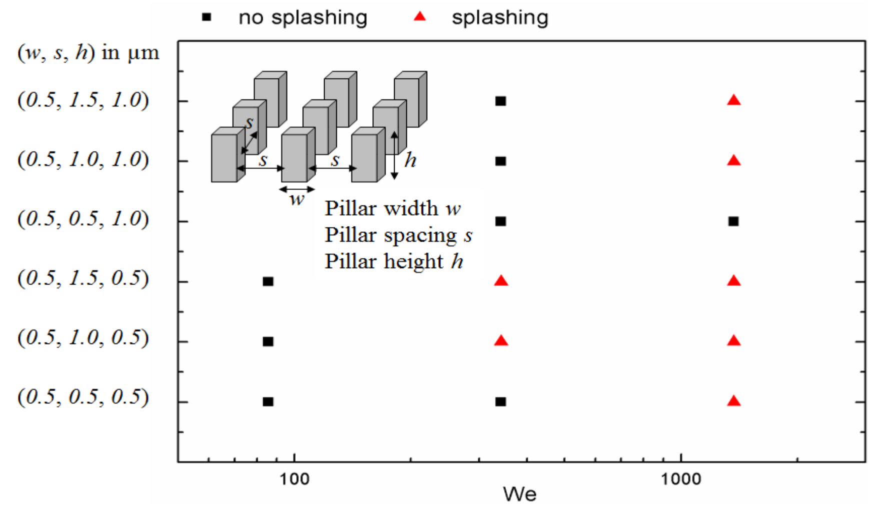


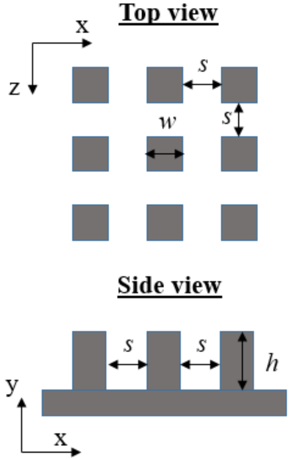
Droplet-media interaction

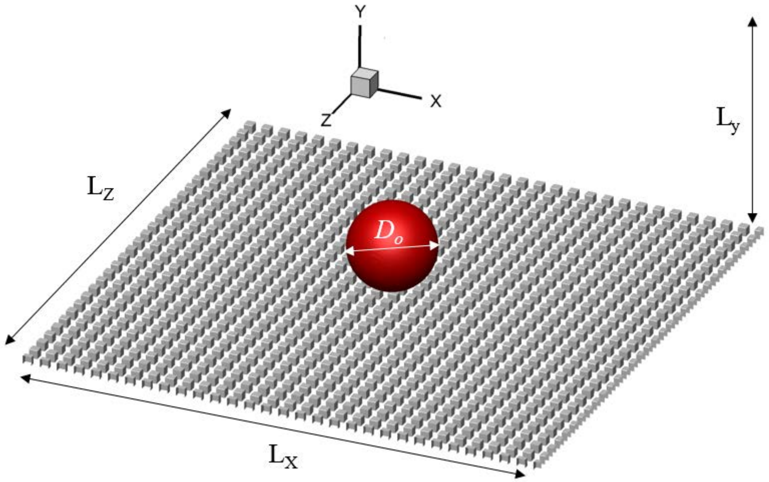
Droplet impact on microstructured surfaces*

D_o=10 µm

Uo (m/s)	We	Re	w (µm)	s (µm)	h (µm)
25	86.6	250	0.5	0.5	0.5
			0.5	1.0	0.5
			0.5	1.5	0.5
50	342.5	500	0.5	0.5	0.5
			0.5	1.0	0.5
			0.5	1.5	0.5
			0.5	0.5	1.0
			0.5	1.0	1.0
			0.5	1.5	1.0
100	1369.9	1000	0.5	0.5	0.5
			0.5	1.0	0.5
			0.5	1.5	0.5
			0.5	0.5	1.0
			0.5	1.0	1.0
			0.5	1.5	1.0







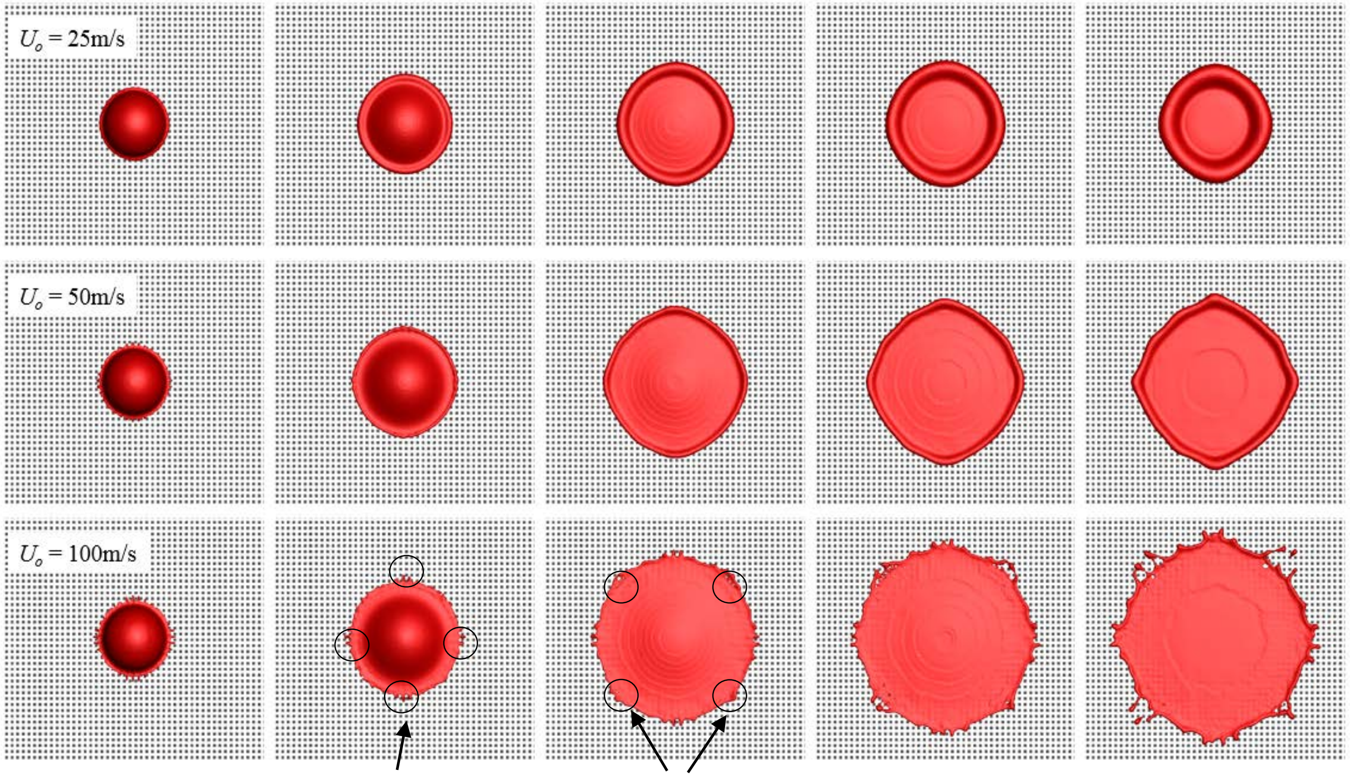
*H. Tan, Numerical study on splashing of high-speed microdroplet impact on dry microstructured surfaces. *Computers & Fluids*, 2017. **154**: p. 142-166.

Gerris

Droplet-media interaction

Effect of impact velocity

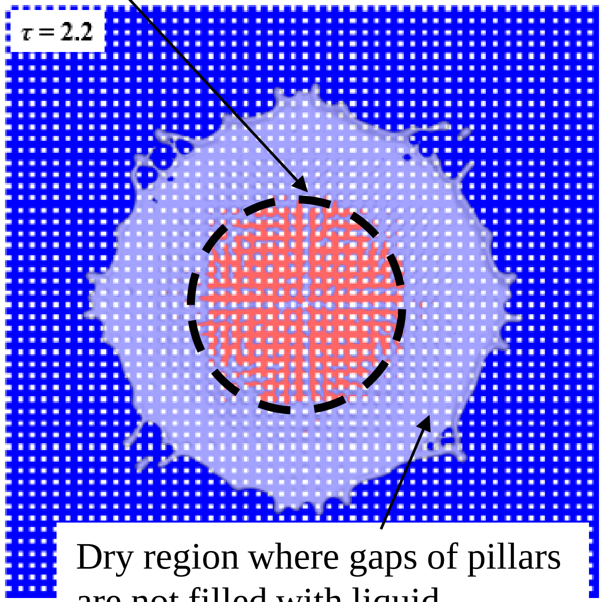
Snapshots of a droplet of D_o=10 μm impact on the dry microstructured surface (s=h=w=0.5 μm)



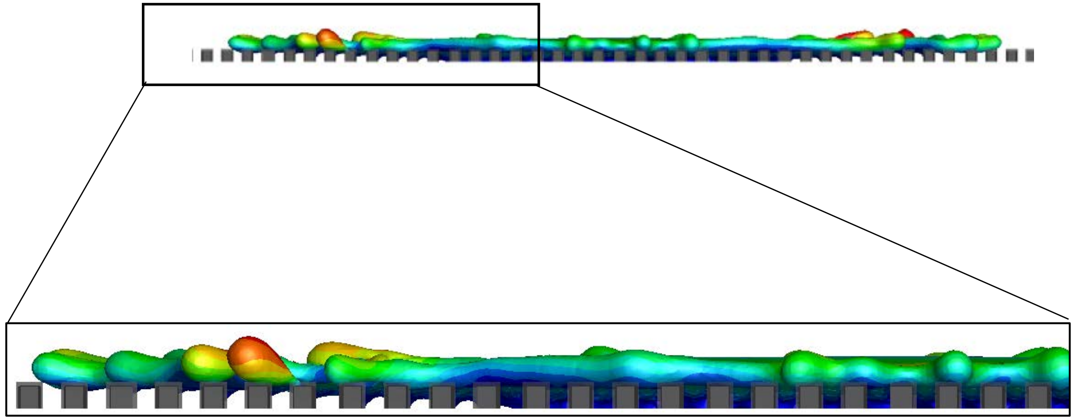
Jets in on-axis directions.

Thin lamella becomes unstable.

Wetted region where gaps of pillars are nearly filled with liquid.



Dry region where gaps of pillars are not filled with liquid.

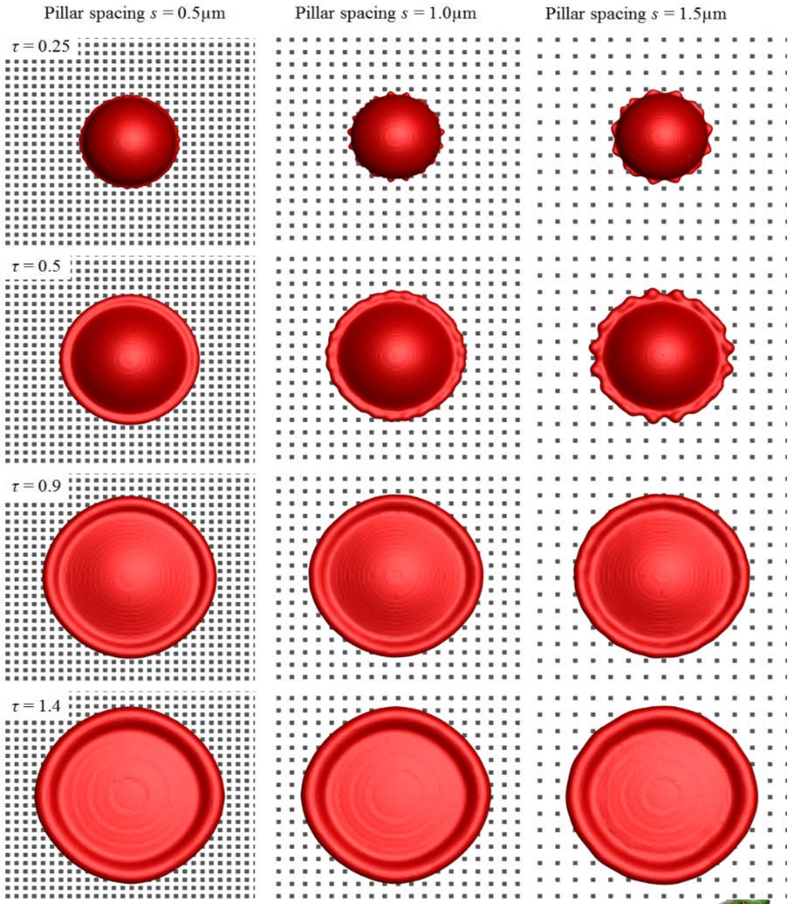


*H. Tan, Numerical study on splashing of high-speed microdroplet impact on dry microstructured surfaces. *Computers & Fluids*, 2017. **154**: p. 142-166.

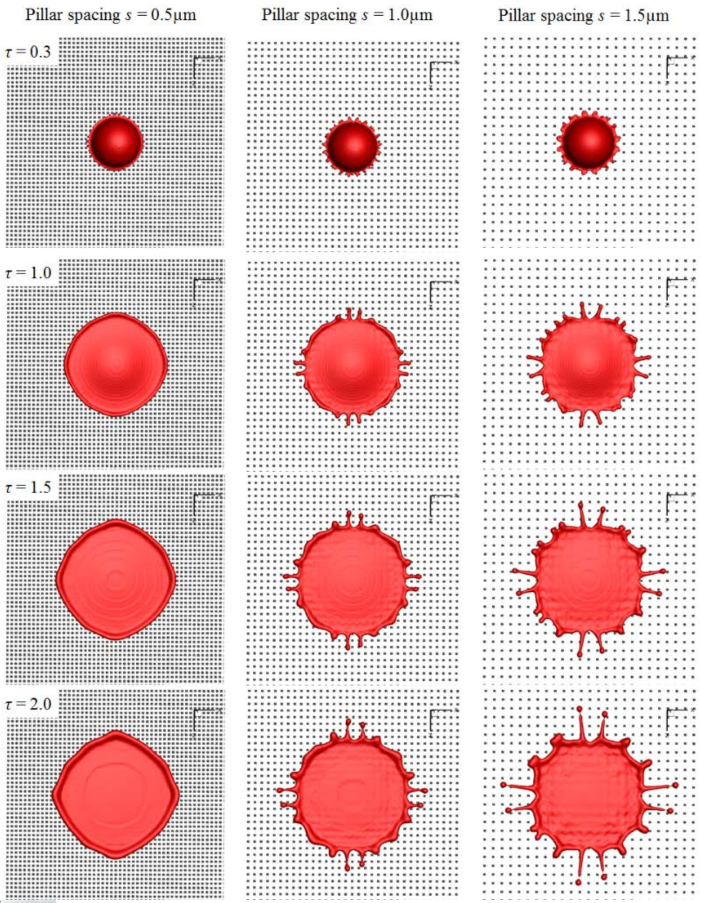
Droplet-media interaction

Effect of microstructures-Pillar spacing

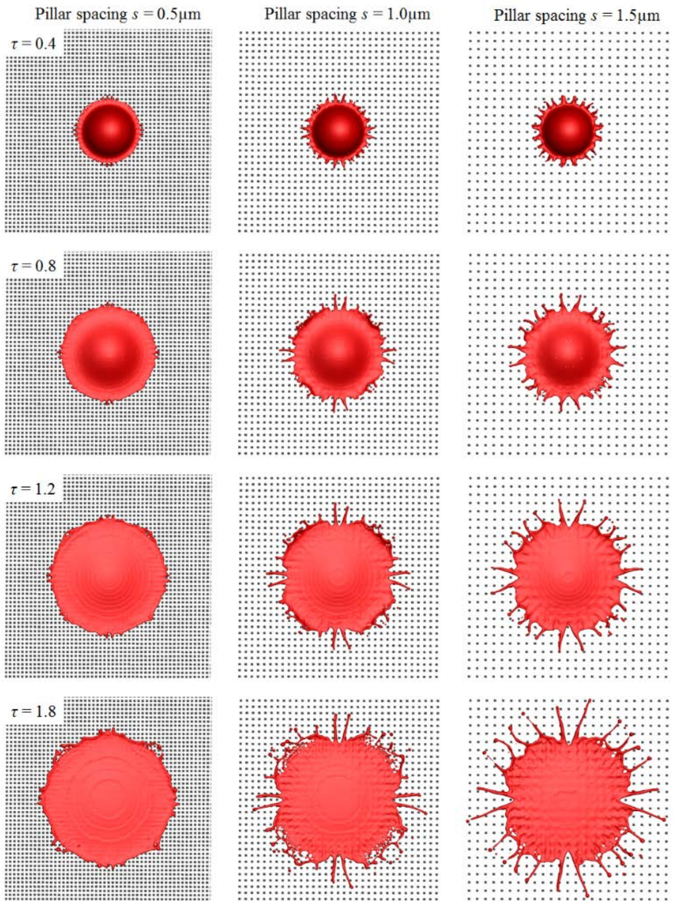
U_o= 25 m/s



U_o= 50 m/s



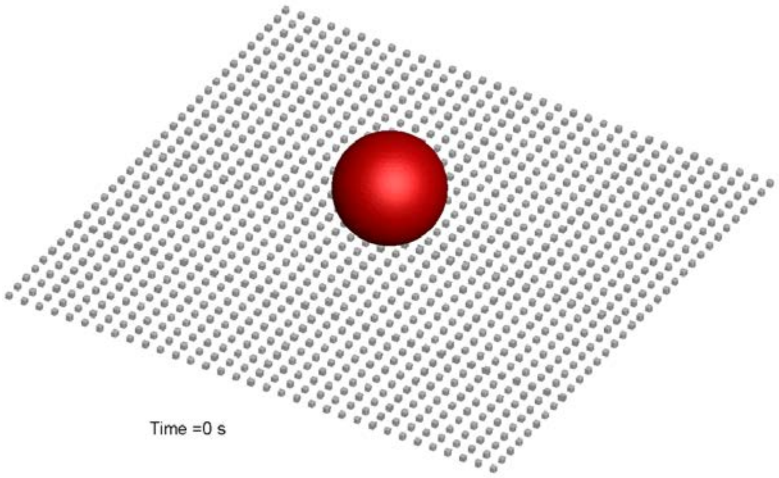
U_o= 100 m/s



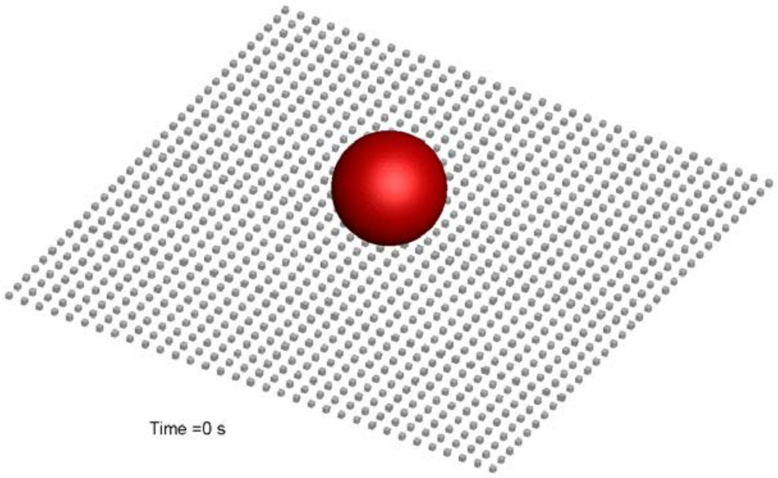
Droplet-media interaction

Droplet impact on microstructured surfaces*

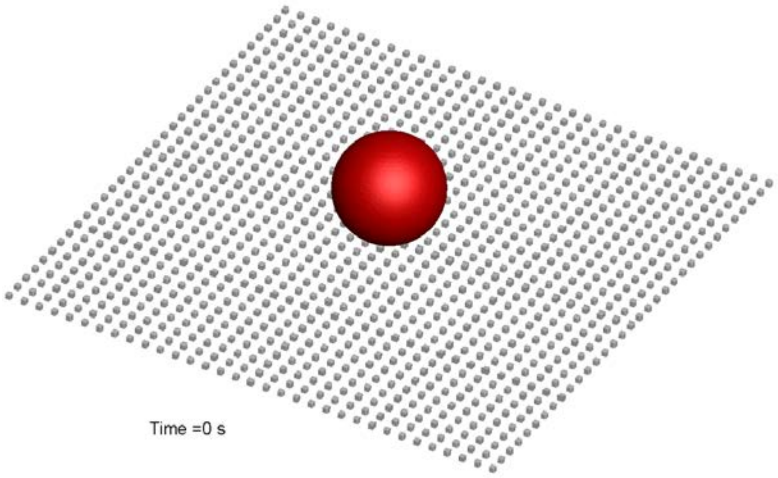
U_o= 25 m/s



U_o= 50 m/s



U_o= 100 m/s



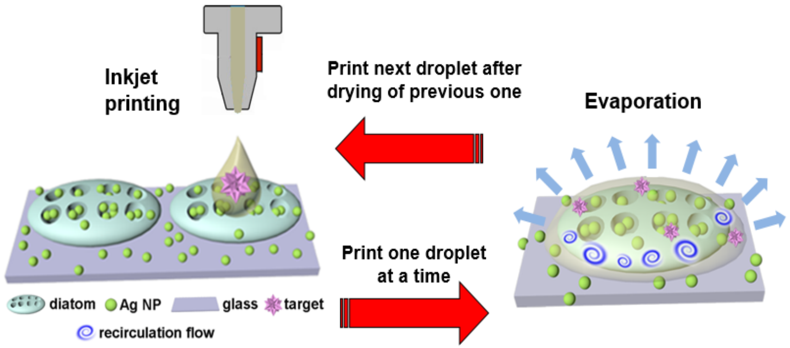
*H. Tan, Numerical study on splashing of high-speed microdroplet impact on dry microstructured surfaces. *Computers & Fluids*, 2017. **154**: p. 142-166.

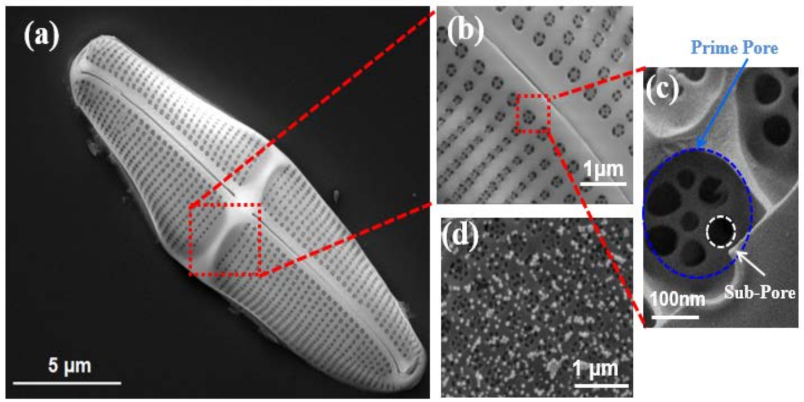
Outline

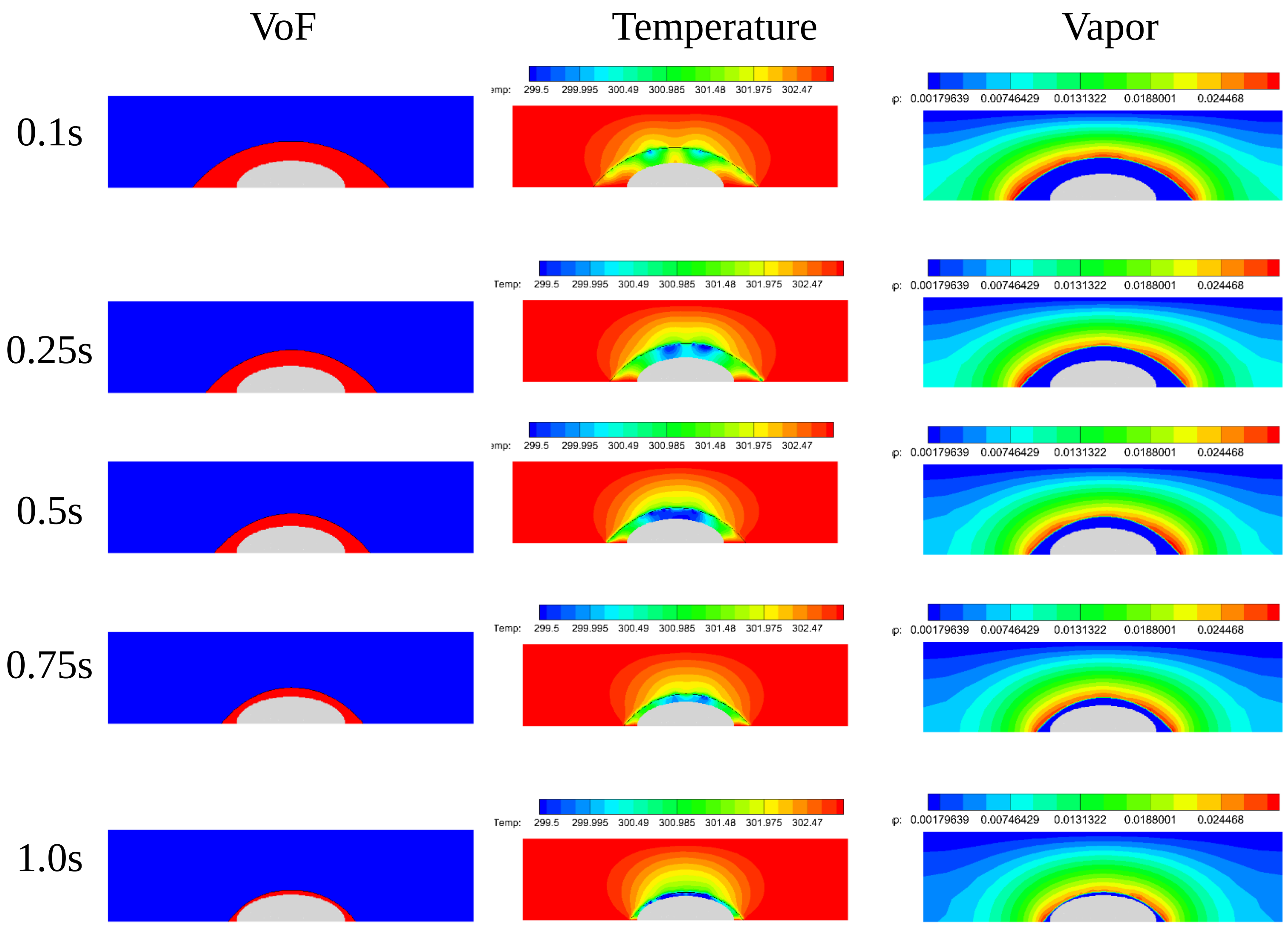
- How do I get started with Gerris
- Droplet formation in Inkjet process
- Capillary flow in low-gravity
- Droplet-media interaction
- Future work

Future work

Thermocapillary flow*



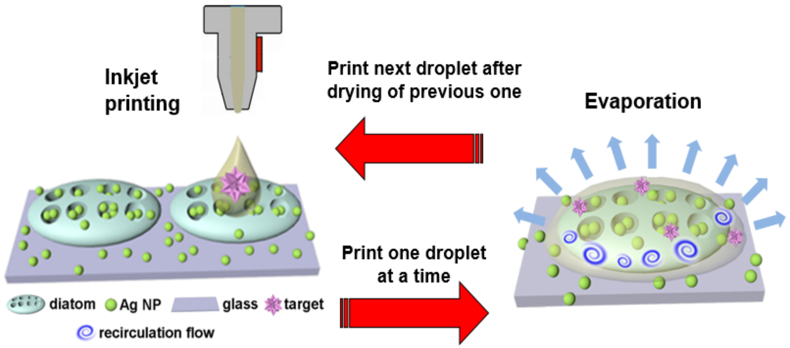


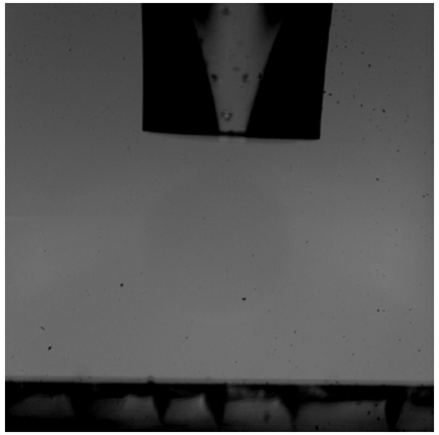


Kong X, et al., Optofluidic Sensing from Inkjet-Printed Droplets: the Enormous Enhancement by Evaporation-Induced Spontaneous Flow on Photonic Crystal Biosilica. *Nanoscale*. 2016, **8**(39): p. 17285-17294

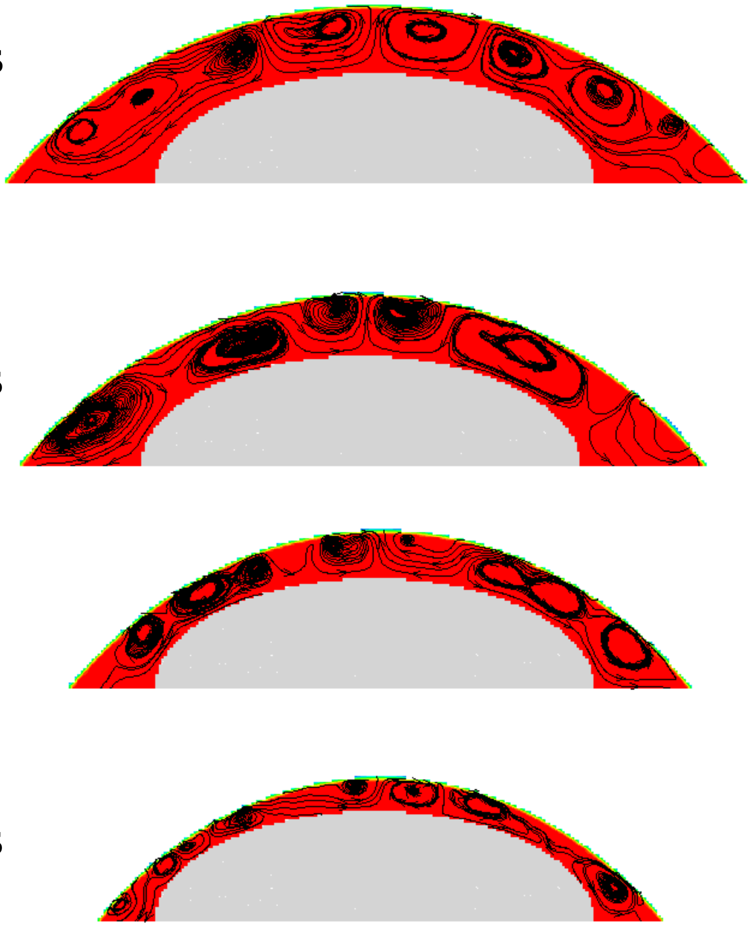
Future work

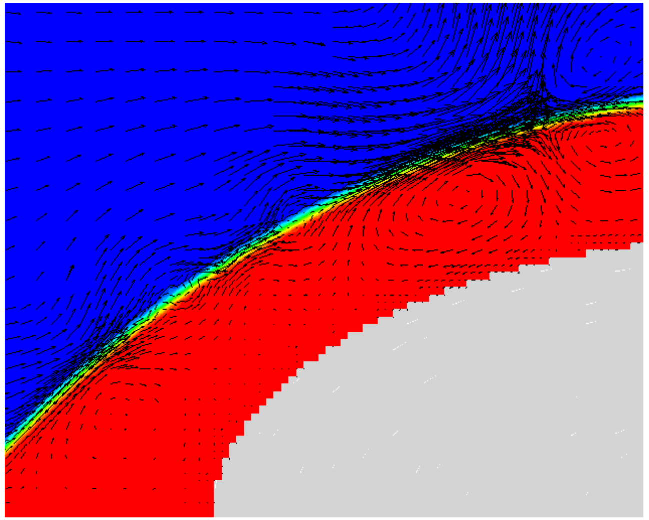
Thermocapillary flow





0.1s
0.25s
0.5s
0.75s





Thank you for your attention!