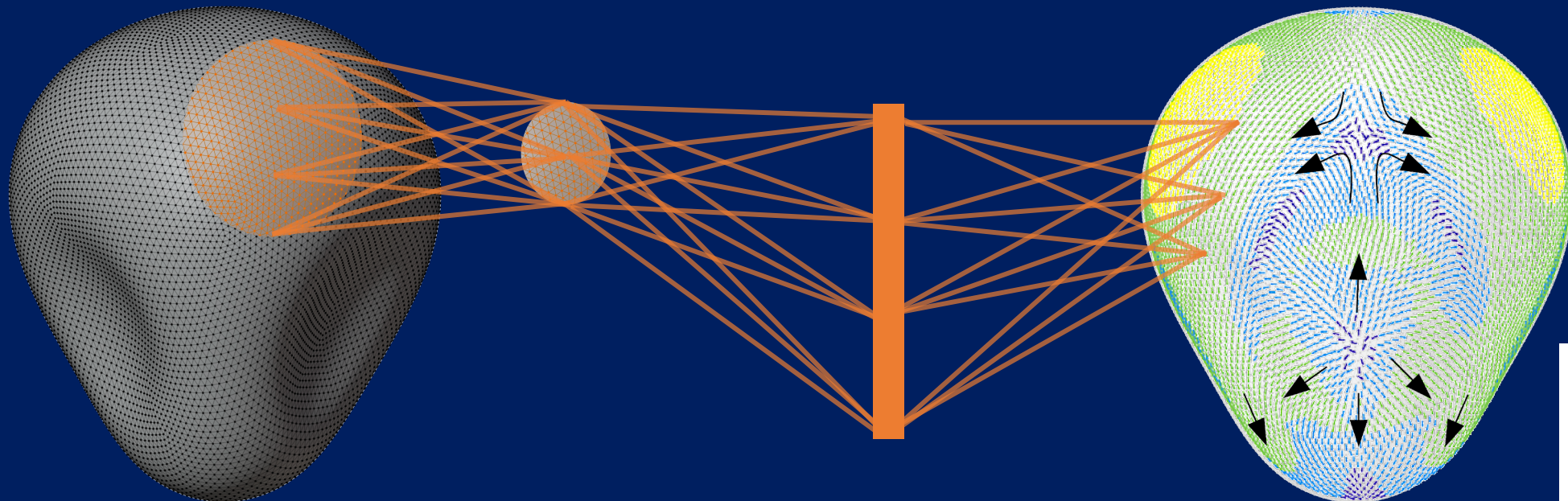


Graph Neural Network Models of Multiphase Flow from Boundary Integral Methods

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APS DFD
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All Images Credit NASA unless
otherwise indicated

Drop Squeezing with BIM

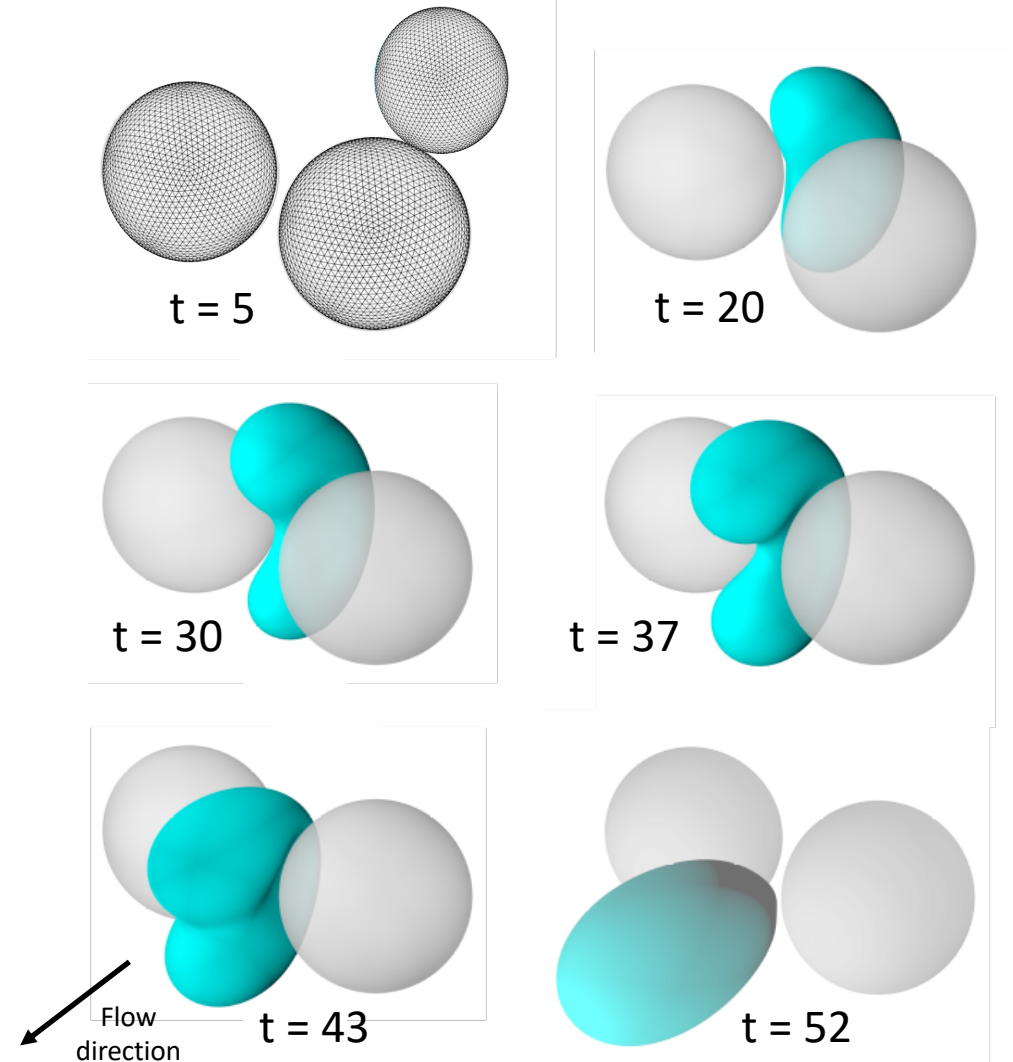


Boundary-Integral Method:

- a powerful tool for multiphase flow
- only interfaces require meshing
- highly accurate, but slow and difficult to parallelize

Drop squeezing (Zinchenko & Davis, 2006)

- tight squeezing and trapping
- stable near critical conditions
 - very computationally expensive!



Why Machine Learning (ML)?



Learning complex functions accelerates simulation bottlenecks

- rapid development of new, more powerful algorithms
- machine learning remains underutilized in CFD

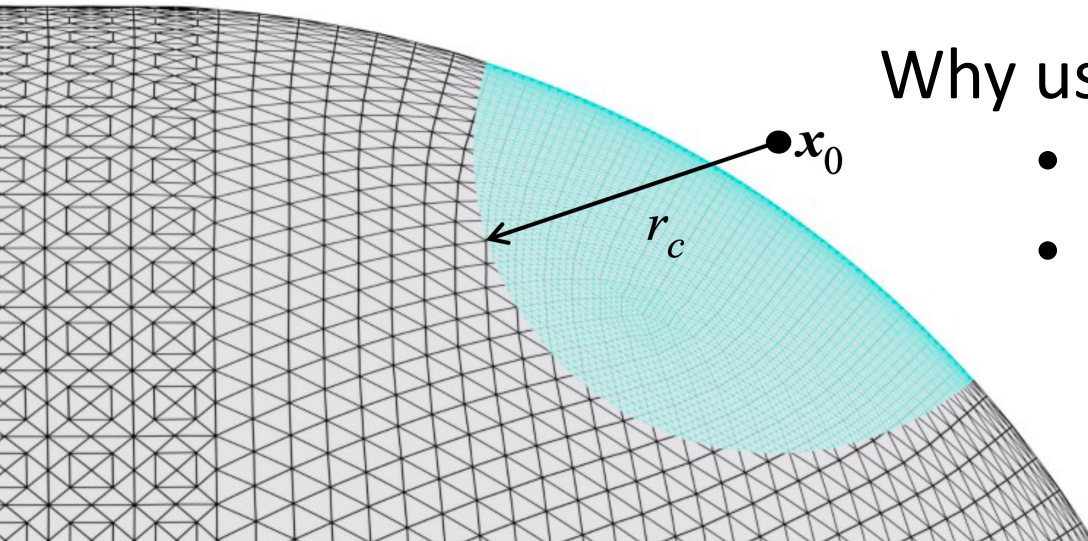
However, machine learning is far from 'universal'

- many choices to be made (software, architecture, hyperparameters)

 TensorFlow →  Keras →  Spektral

Why use graph neural network (GNN) in this case?

- droplet is already meshed, i.e., a graph
- enables convolution over drop surface



Learning Drop Squeezing

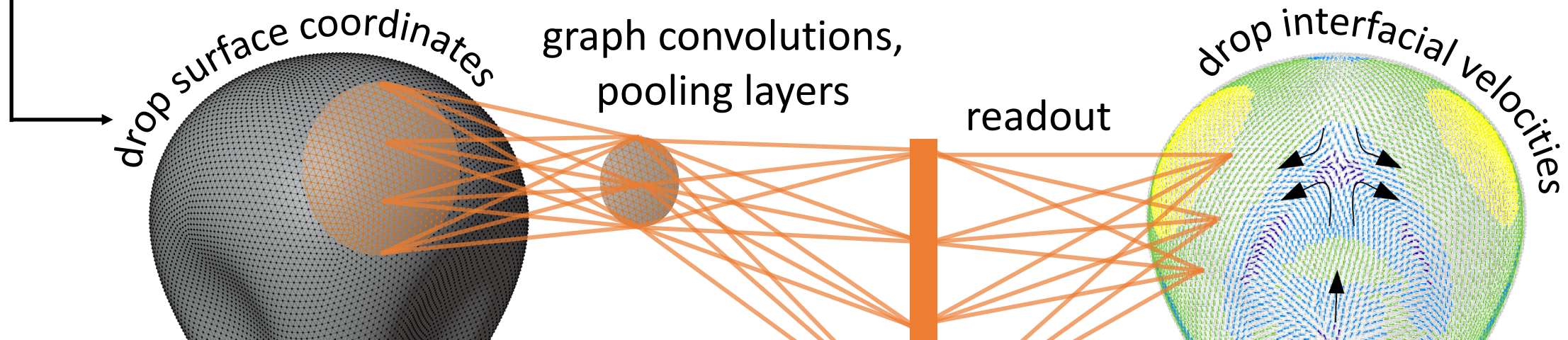


Option 1: Provided interface coordinates, predict velocities

- learn all physics, replace boundary-integral calculation
 - ↳ surface tension, Stokes equation, particle interactions
- once trained, simulation reduces from days to minutes

Option 2: Learn select computationally-demanding calculations

- slower, but generalizable while still achieving significant speed-up



The 3-Sphere Configuration

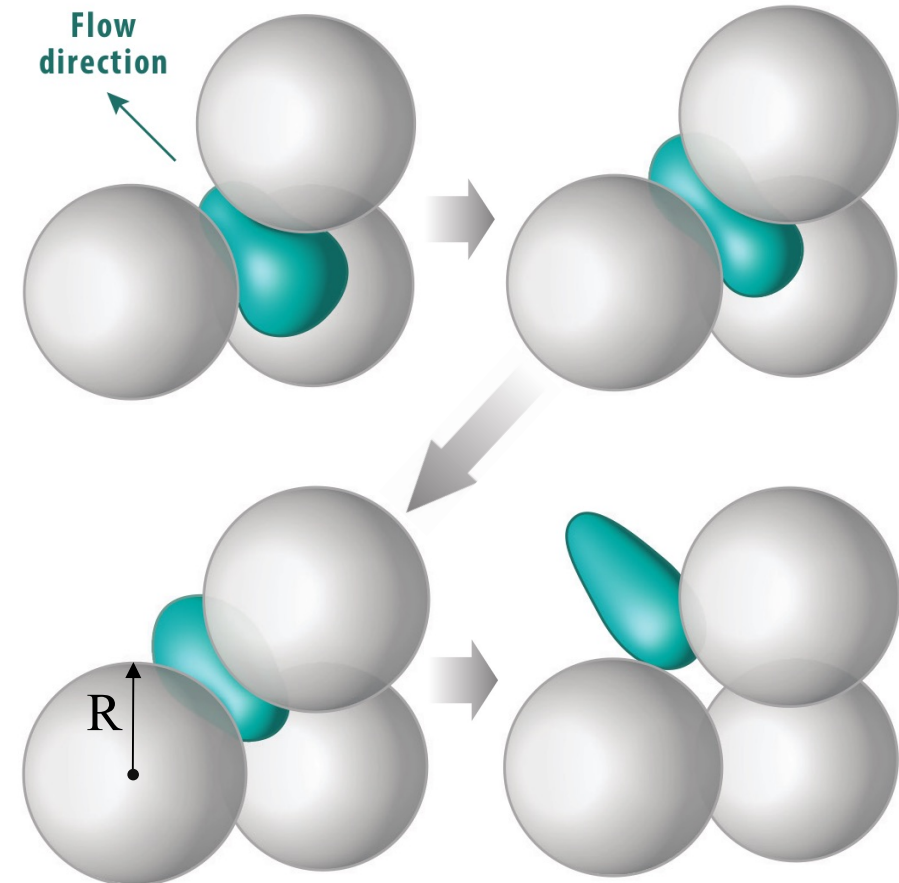


Applications:

- subsurface settings
- microfluidics
- porous media

Uniform far-field flow

Droplet initially $6R$ upstream



Zinchenko & Davis. Annu. Rev. Fluid Mech. 49 (2017): 71-90.

Simulation Parameter	Symbol	Value(s)
Drop:particle radii	$\tilde{a}$	0.6
Interparticle gap	ϵ	0.25
Drop:medium viscosities	λ	4.0

Effect of Capillary Number



Passage vs. trapping behavior

Trapping occurs below Ca_{crit}

BIM data for $Ca = 0.9, 1.1, 1.3, 1.5$

- surface position and velocity
- 2000-3000 frames for each Ca
- 10242 nodes on drop

$$Ca = \frac{\mu_e |\mathbf{u}_\infty| \tilde{a}}{\sigma_{eq} L}$$

capillary number

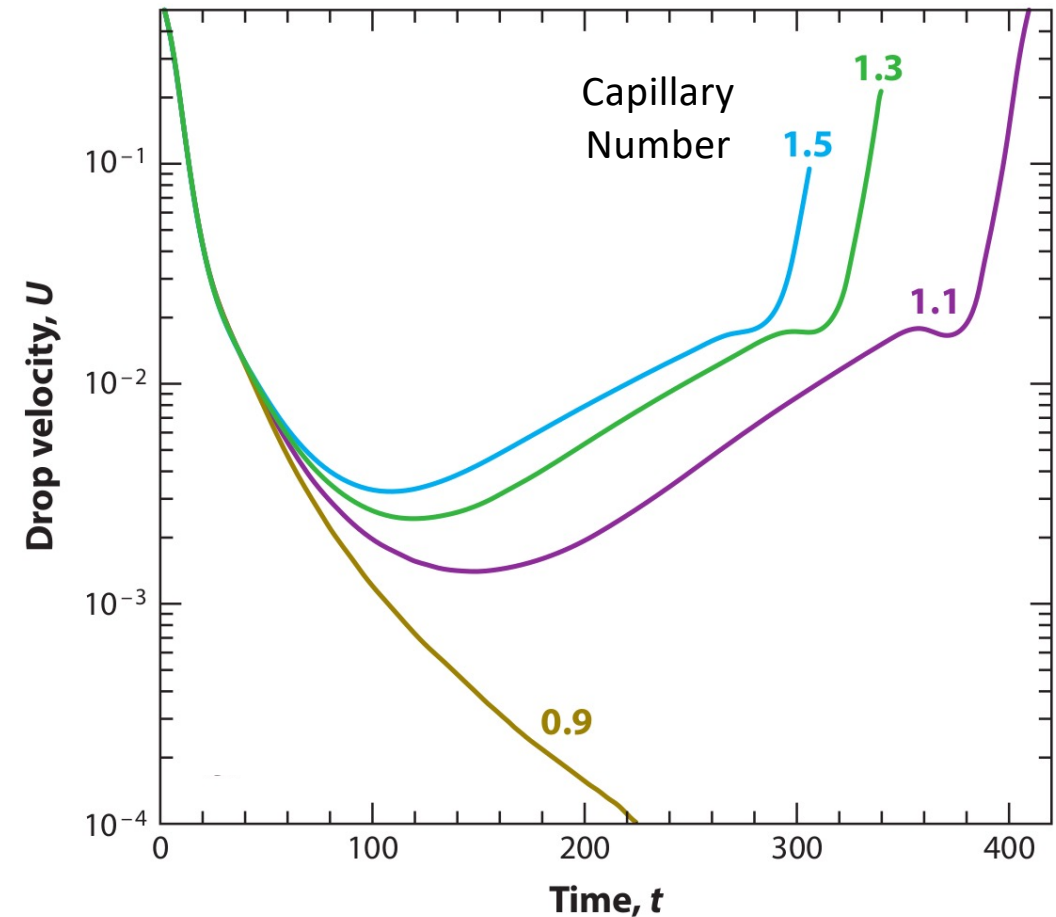
viscosity of medium μ_e

magnitude of far-field velocity $|\mathbf{u}_\infty|$

undeformed drop radius $\tilde{a}$

equilibrium surface tension σ_{eq}

characteristic length $\equiv$ solid particle radius L



Zinchenko & Davis. Annu. Rev. Fluid Mech. 49 (2017): 71-90.

Physical Considerations



BIM is a nonlocal technique

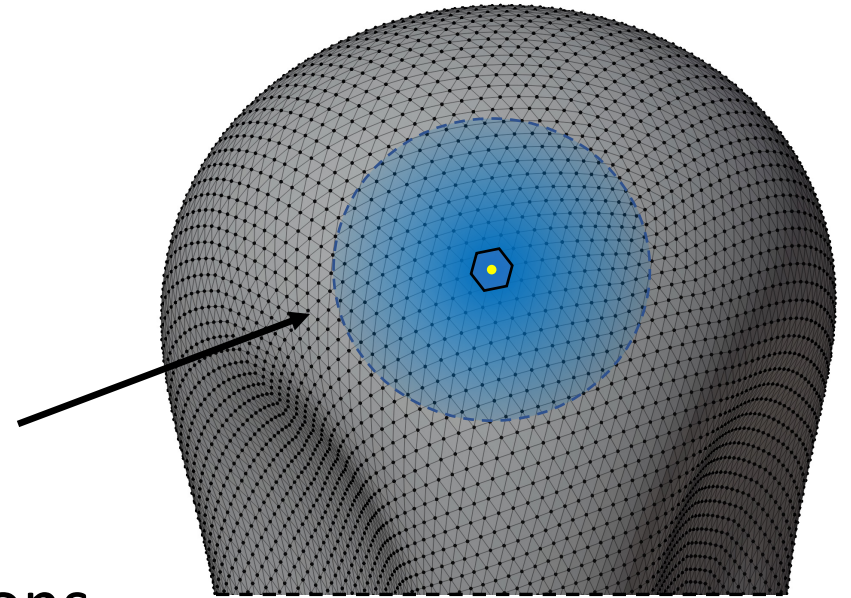
- all nodes influences each other

Vanilla graph convolutional network (GCN):

- struggles to learn non-local contributions
- attempted solution: k-hop adjacency matrix

GCN with skip connection: ARMA filter¹

- effectively learns local and global contributions



ARMA -> TopK(0.143) -> ARMA -> TopK(0.7) -> Dense(1024) -> Readout

Output (interfacial velocity) ranges over four orders of magnitude

- velocity data normalized by log scaling for accurate learning

GNN Model of Trapped Drop



GNN model (ARMA-TopK):

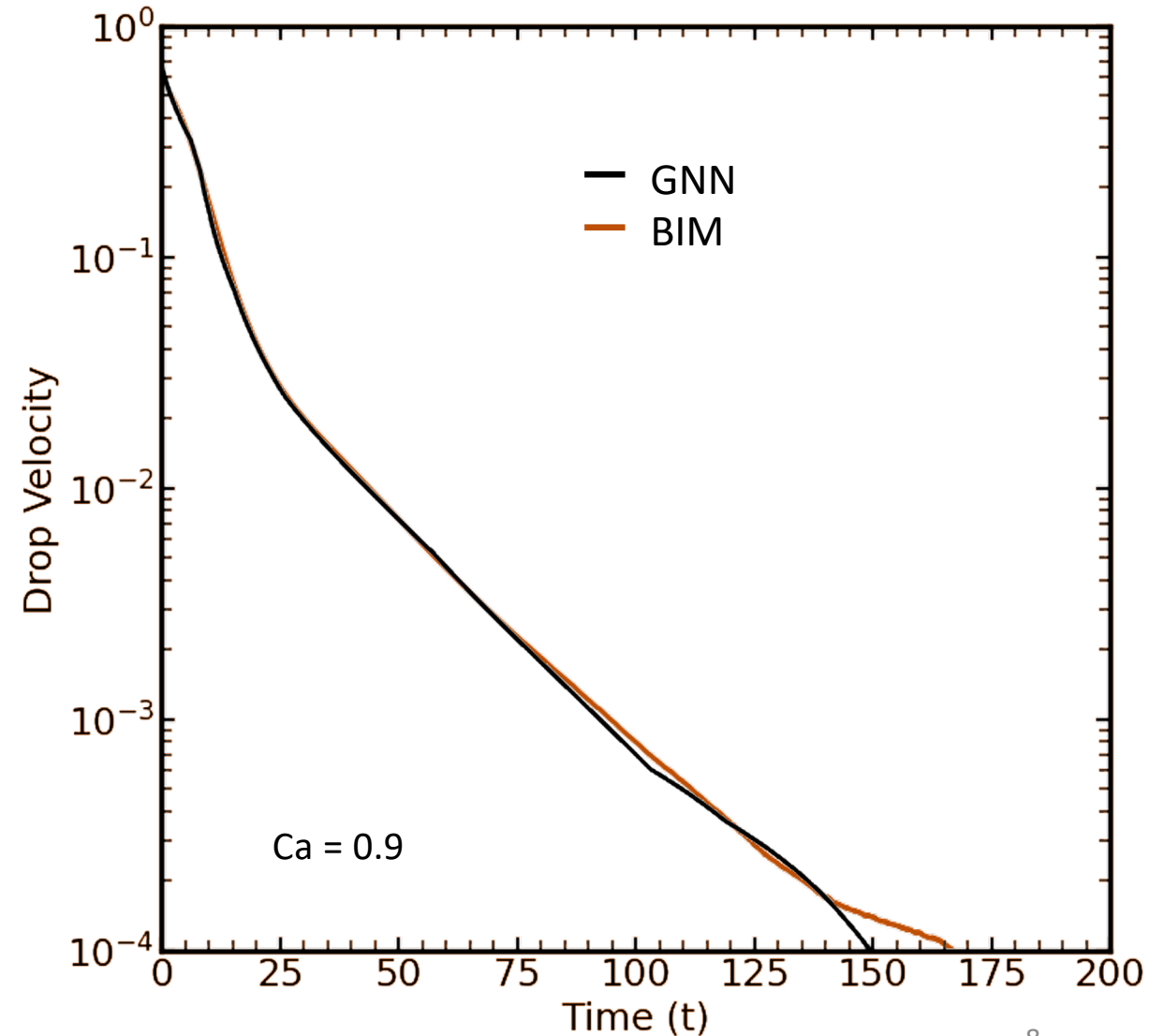
- accurate prediction of interfacial velocities
- successful trapped droplet
- velocity output ranges over four orders of magnitude

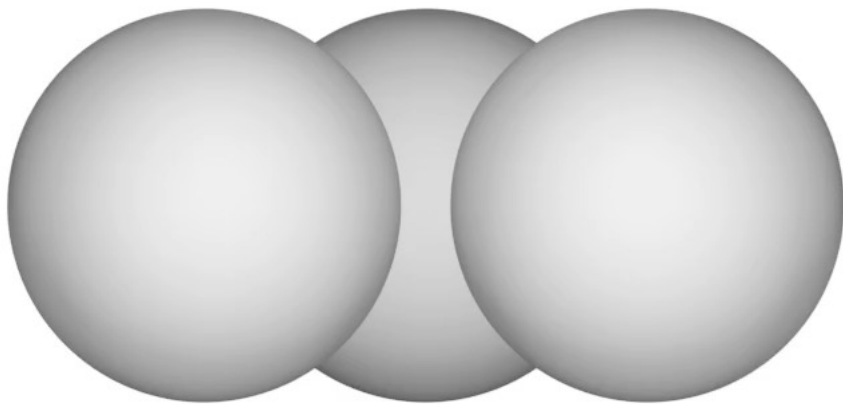
BIM runtime: 4-7 days

GNN model runtime: ~1 hour

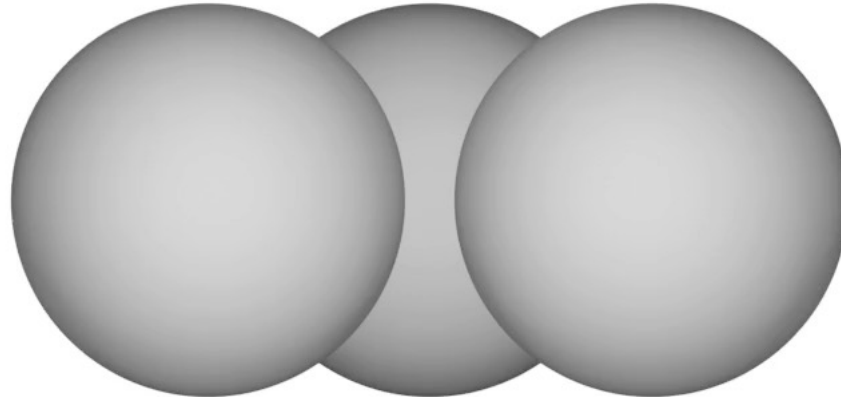
- constant runtime
- >100x speedup

Training time: 1 day





BIM



GNN

Drop-to-medium
viscosity ratio: 4.0

$Ca = 0.9$

Drop radius = 0.6

Far-field vel. = 1.0

Min. drop vel. = $1e-4$

Model for Drop Passthrough



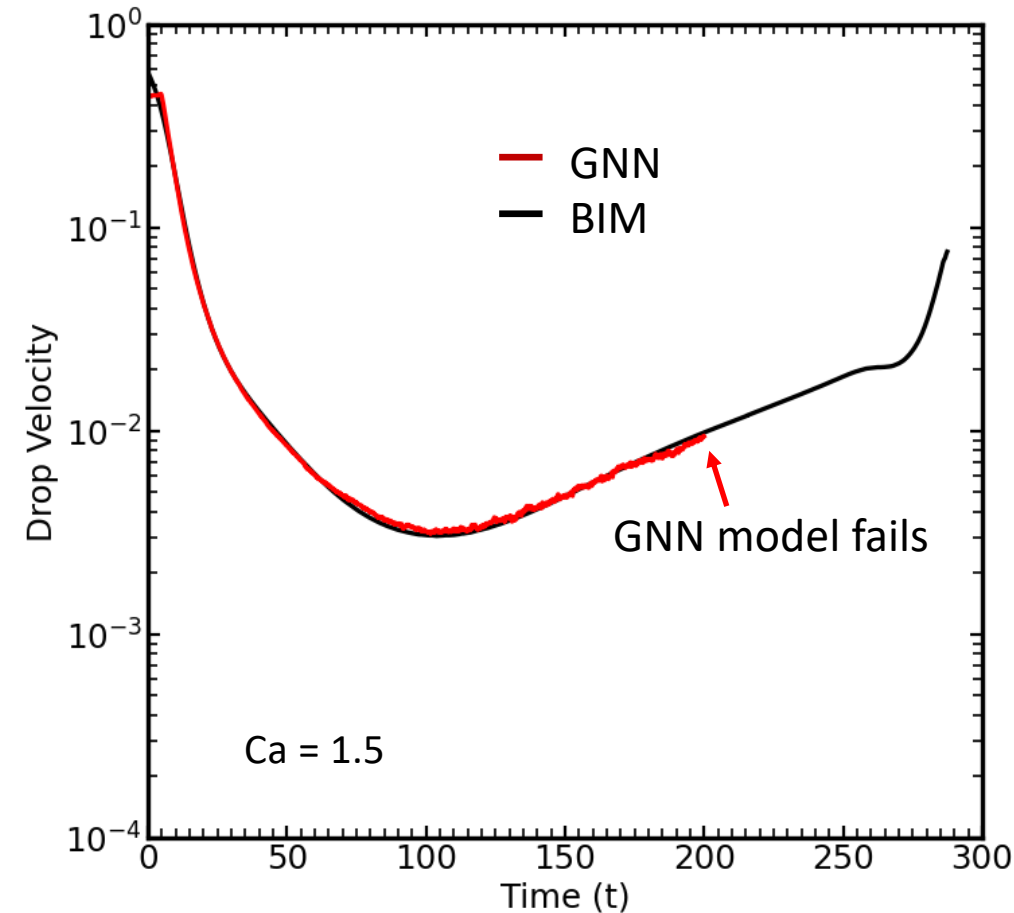
Drop passthrough more challenging to learn

- inverse situation from BIM simulations
- unable to model complete passthrough
 - instabilities develop in surface mesh

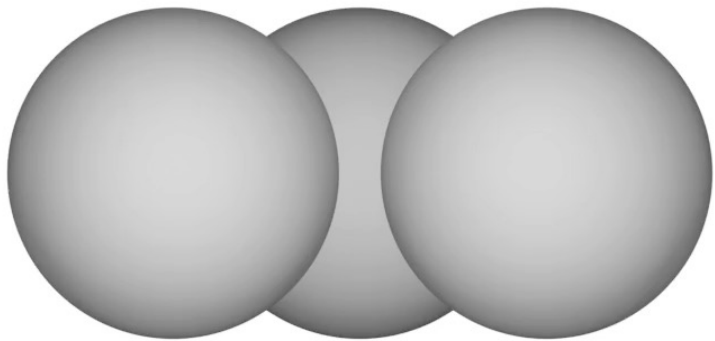
Tens of architecture combinations attempted

Possible ways forward:

- dedicated network for each node
 - significantly slower ML model
- physics-informed ML
 - difficult with integral formulation

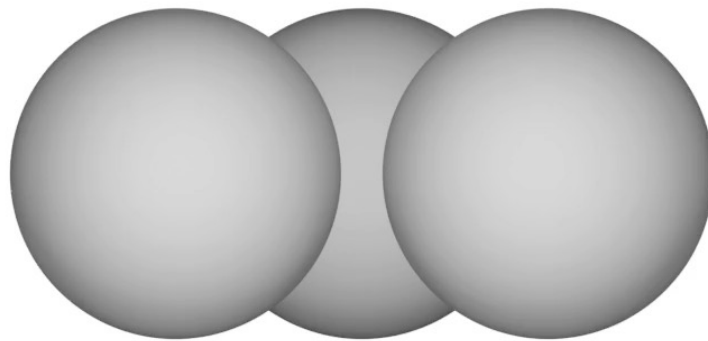


Modeling Drop Passthrough

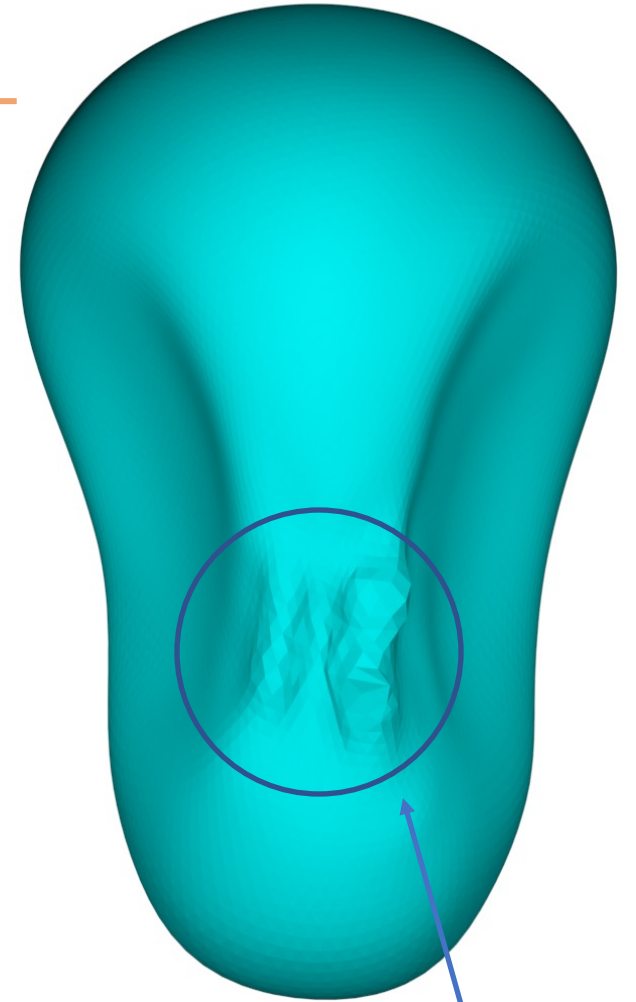


BIM (ground truth)

$Ca = 1.5$



GNN (up to instability)



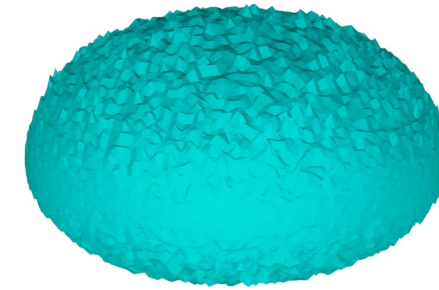
GNN mesh instability

Inherent Limitations of ML



Learned regression less accurate than BIM

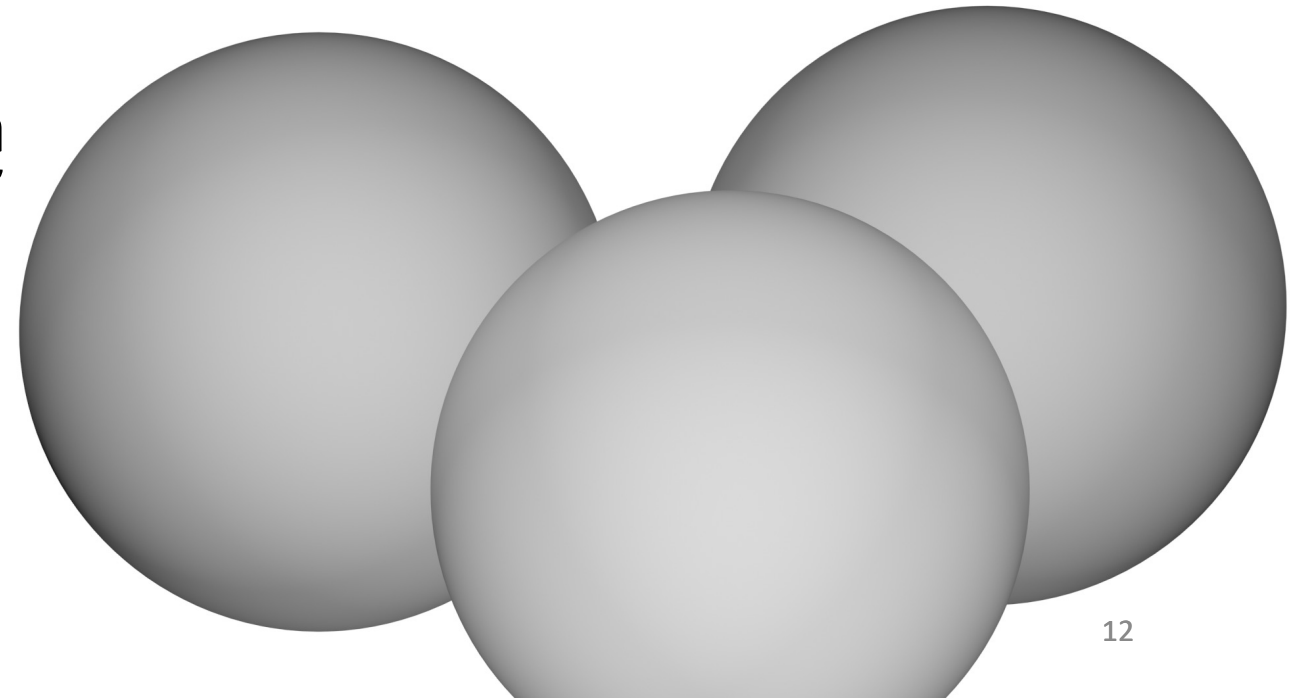
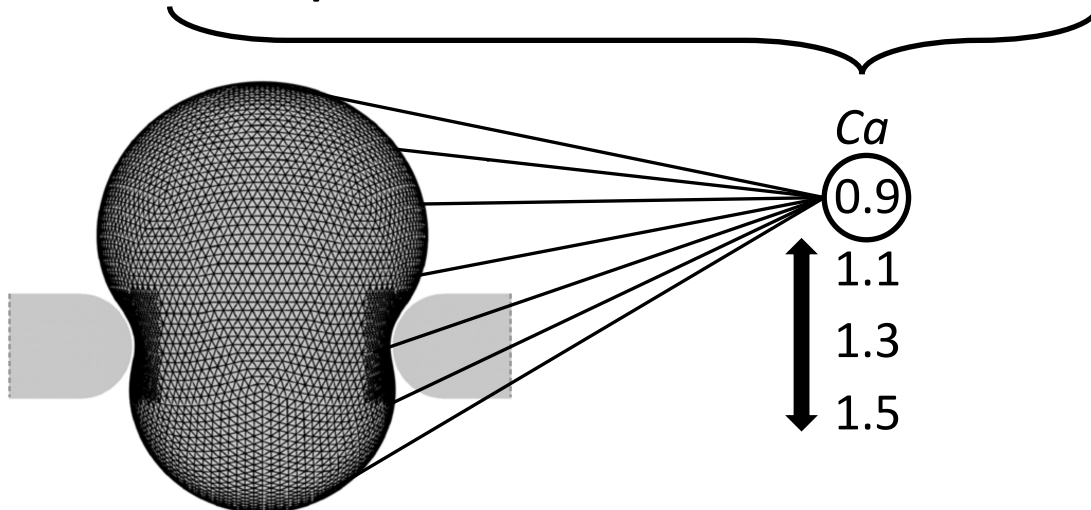
- unlike BIM simulations, drop surface required smoothing
- nodes smoothed via best-paraboloid fit



without
surface
smoothing

Generalizing ML models is difficult

- ultimate objective is to interpolate to new values of Ca



GNN-BIM: Summary and Outlook

Graph convolutional NNs are promising for modeling dynamic interfaces

- High-accuracy regression for node-level prediction
- GCNs with skip connections and pooling capture global contributions

Able to accurately model droplet trapping

- More powerful networks required for passthrough

Massive speedups when running models

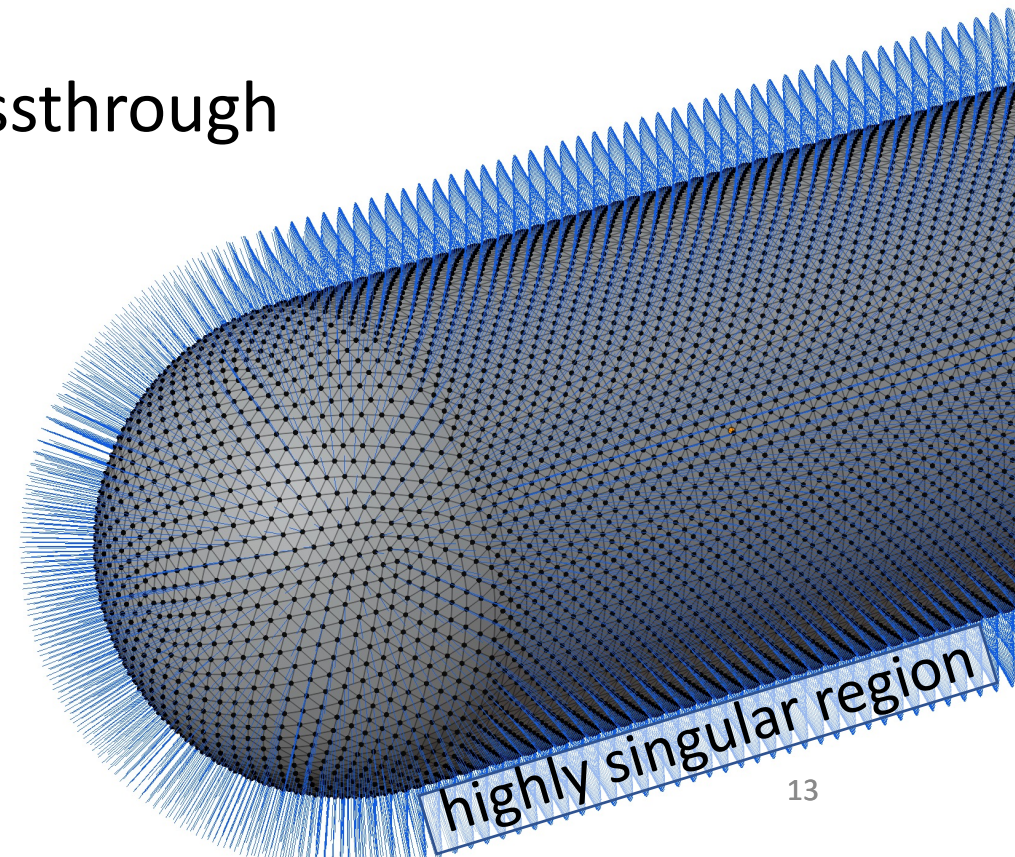
- Two to three orders of magnitude

Limitation of the architectures tested:

- Unable to generalize to new parameters

Future ML application to BIM:

- Apply only to select computationally-intensive aspects of BIM



Thank You!

