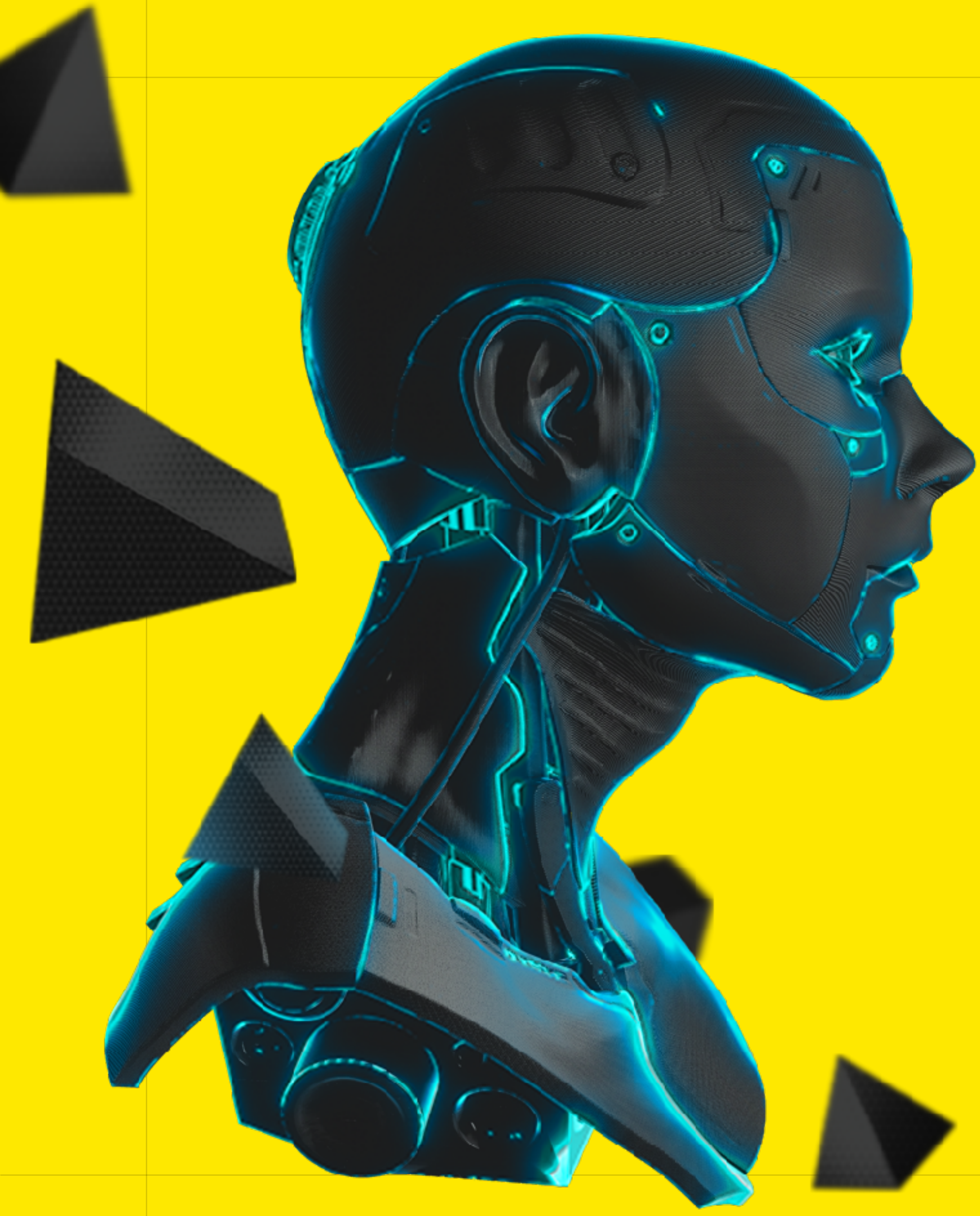

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A MOMENTUM-CONSERVING IMPLICIT MATERIAL POINT METHOD FOR SURFACE TENSION WITH CONTACT ANGLES AND SPATIAL GRADIENTS

Jingyu Chen[1], Victoria Kala[1], Alan Marquez-Razon[1], Elias Gueidon[1], David A. B. Hyde[1], Joseph Teran[2]

[1] UCLA [2] UC Davis

OUTLINE

- **Backgrounds**
- Material Point Method (MPM)
- Conservative Resampling
- Spatially Varying Surface Tension
- Thermomechanical Coupling
- Summary

SURFACE TENSION

Water droplet on a hydrophobic surface

[Source: https://freerangestock.com/photos/61063/milk-crown.html]

Milk crown

[Source: https://news.mit.edu/2013/hydrophobic-and-hydrophilic-explained-0716]

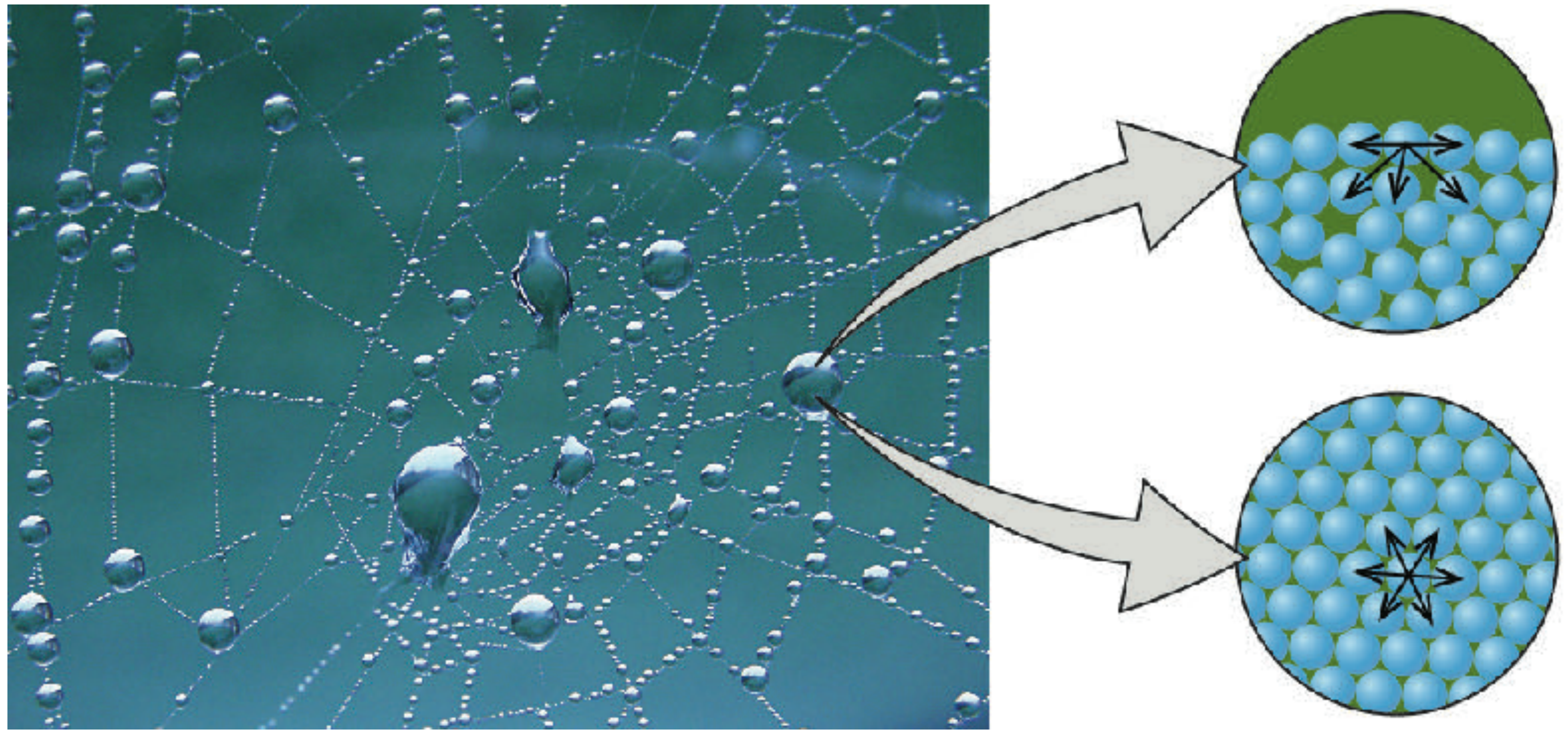
Tears of wine (Marangoni effect)

[Source: https://www.comsol.com/blogs/tears-of-wine-and-the-marangoni-effect/]

SURFACE TENSION

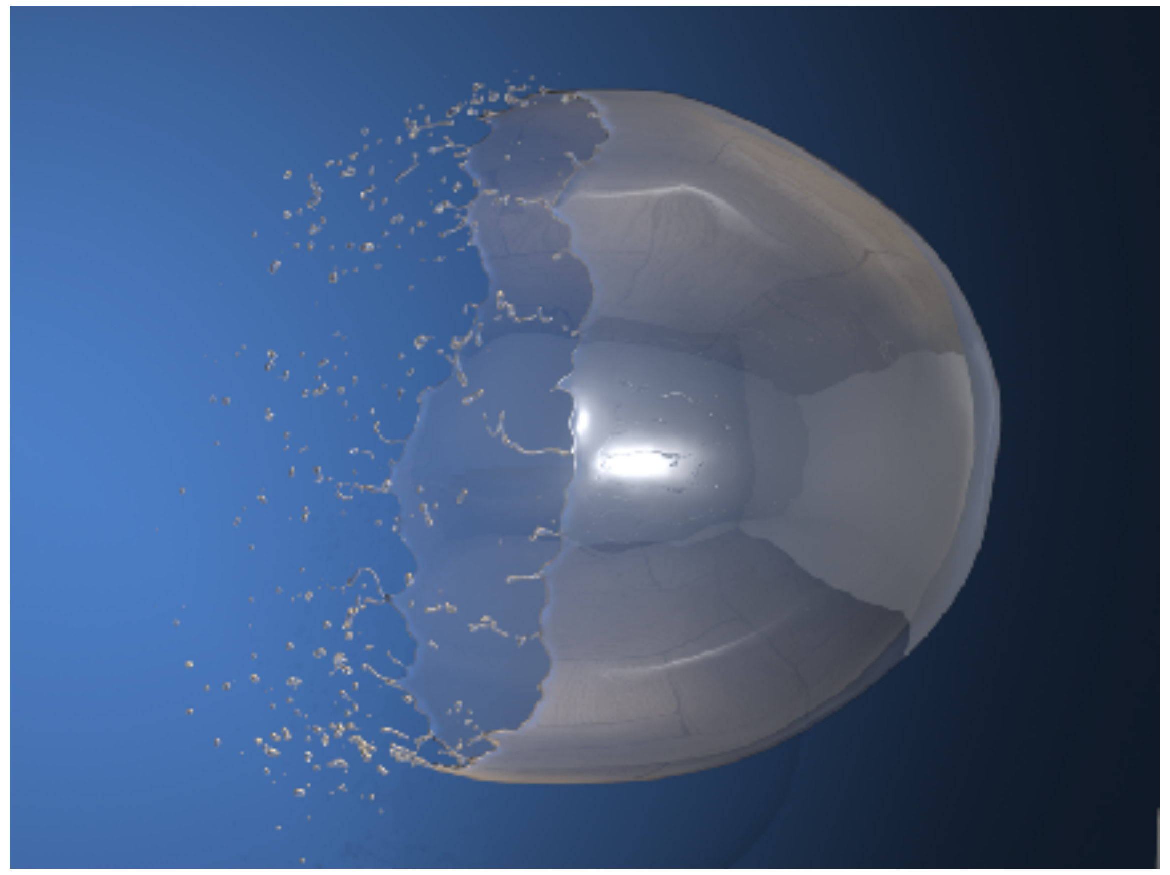
Physics of the surface tension

- Surface tension is caused by the cohesive force between water molecules.
- The liquid surface behaves like elastic membrane.
- The interface is a jump in the fluid density.

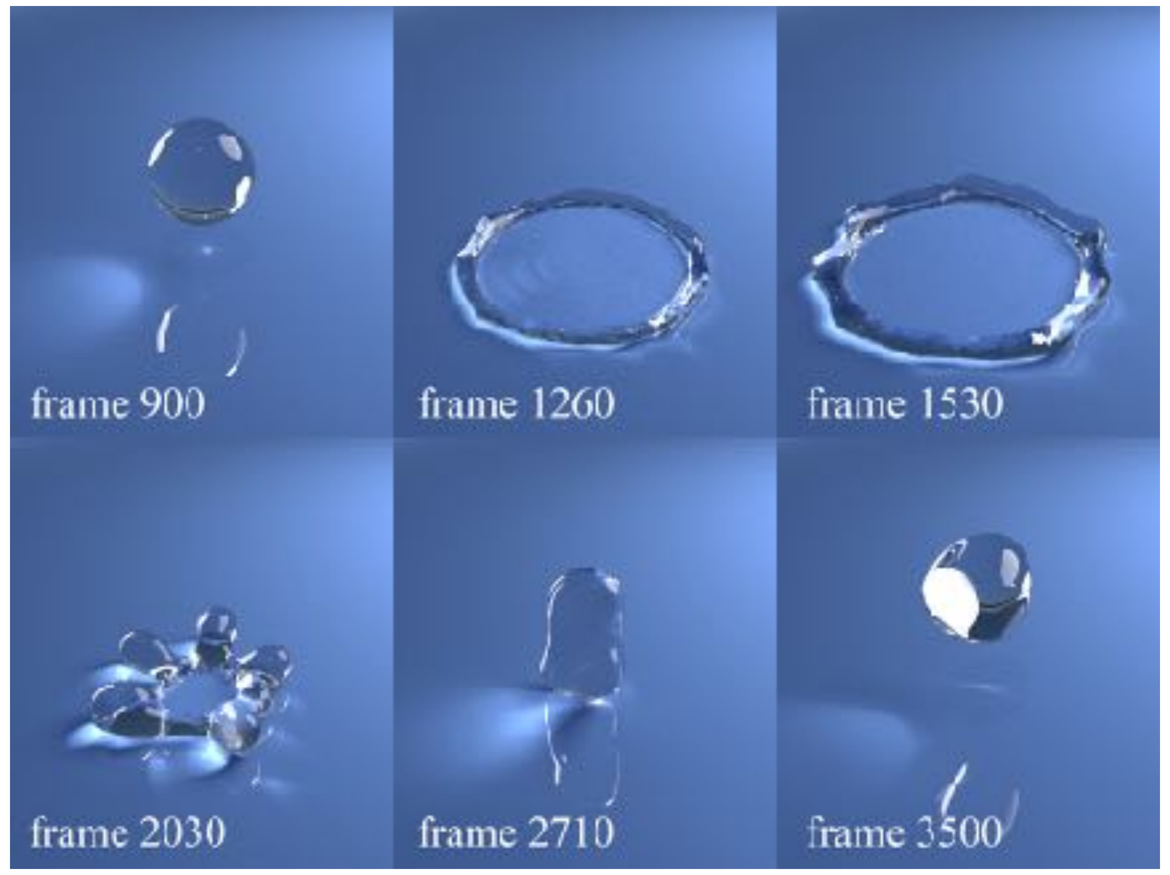


[Source: https://cnx.org/contents/WgINhlpX@3/Properties-of-Liquids]

SURFACE TENSION SIMULATIONS

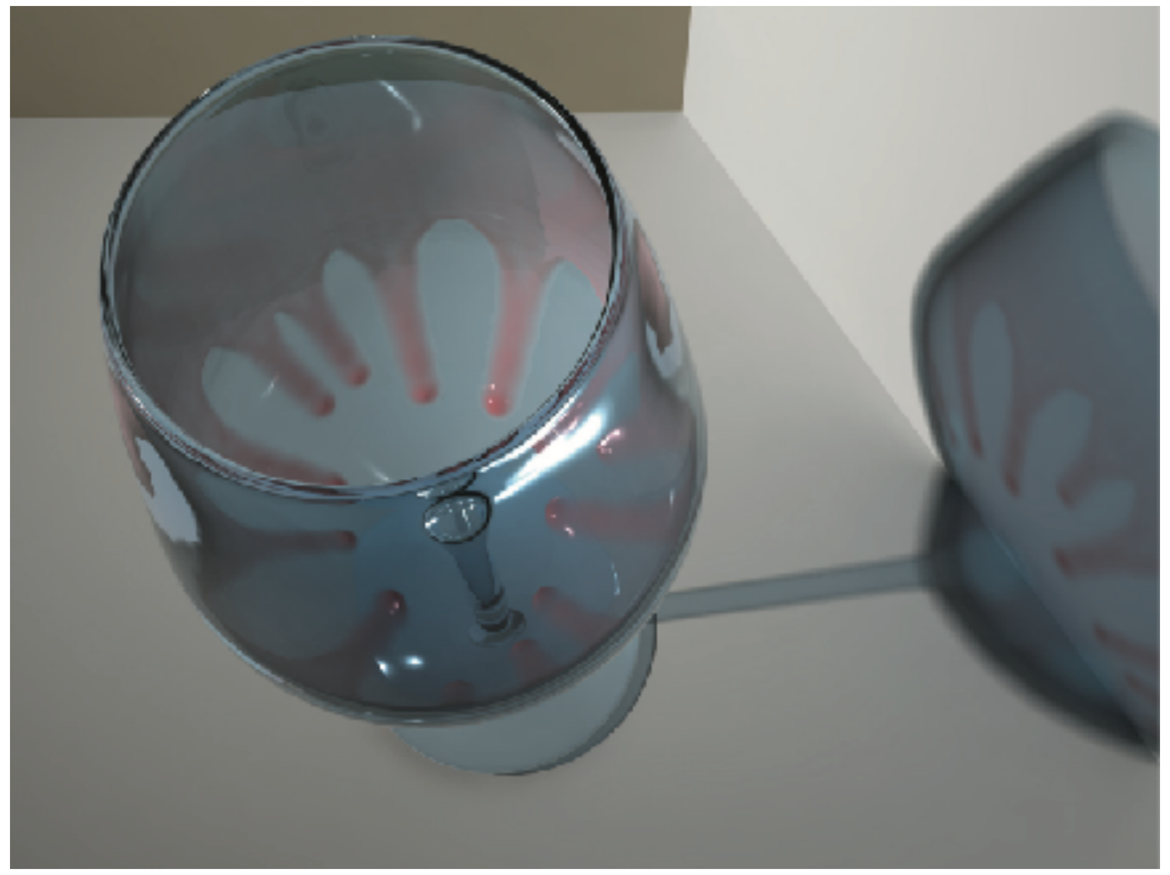


[Zhu et al. 2014]



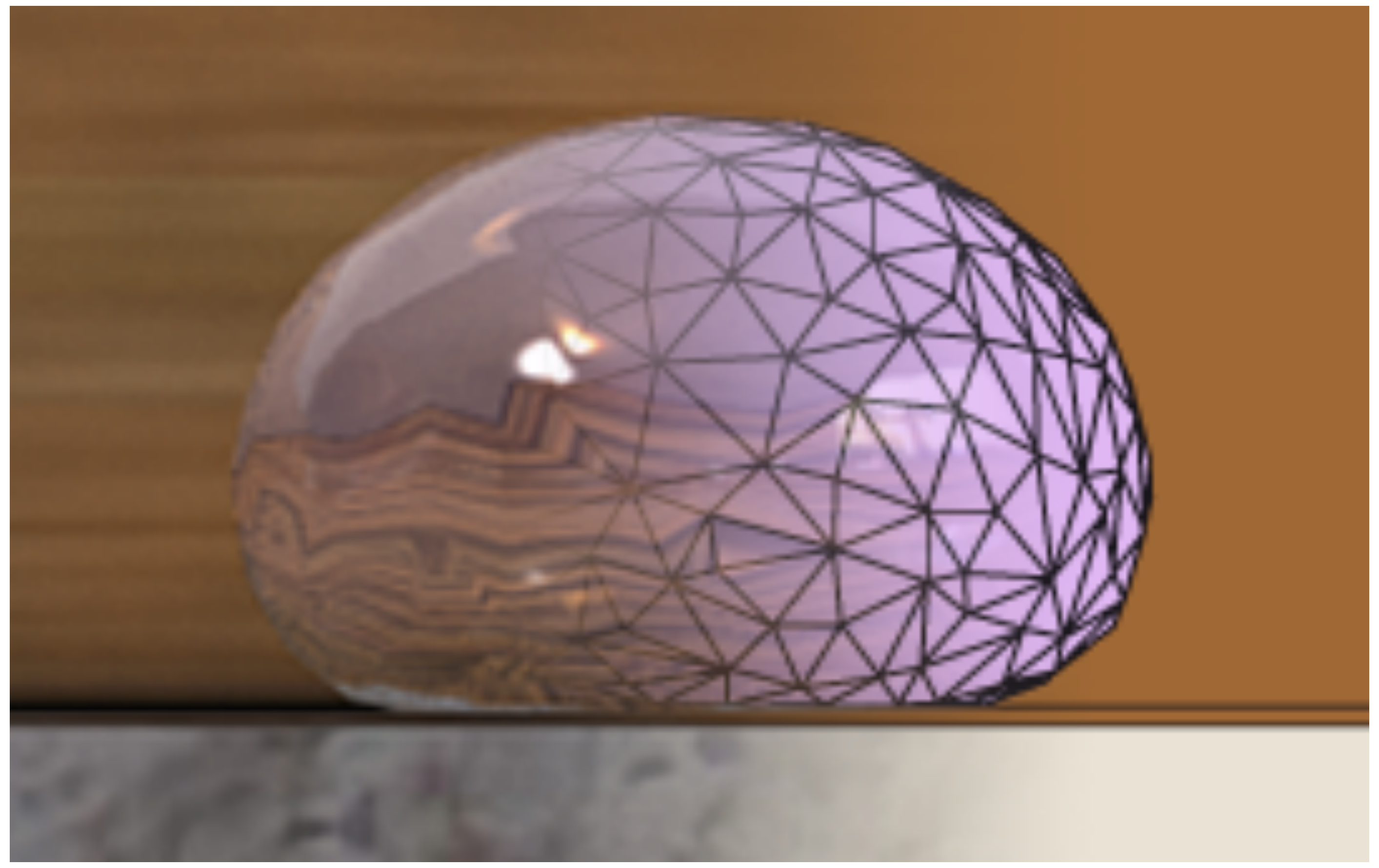
[Da et al. 2016]

[Clausen et al. 2013]

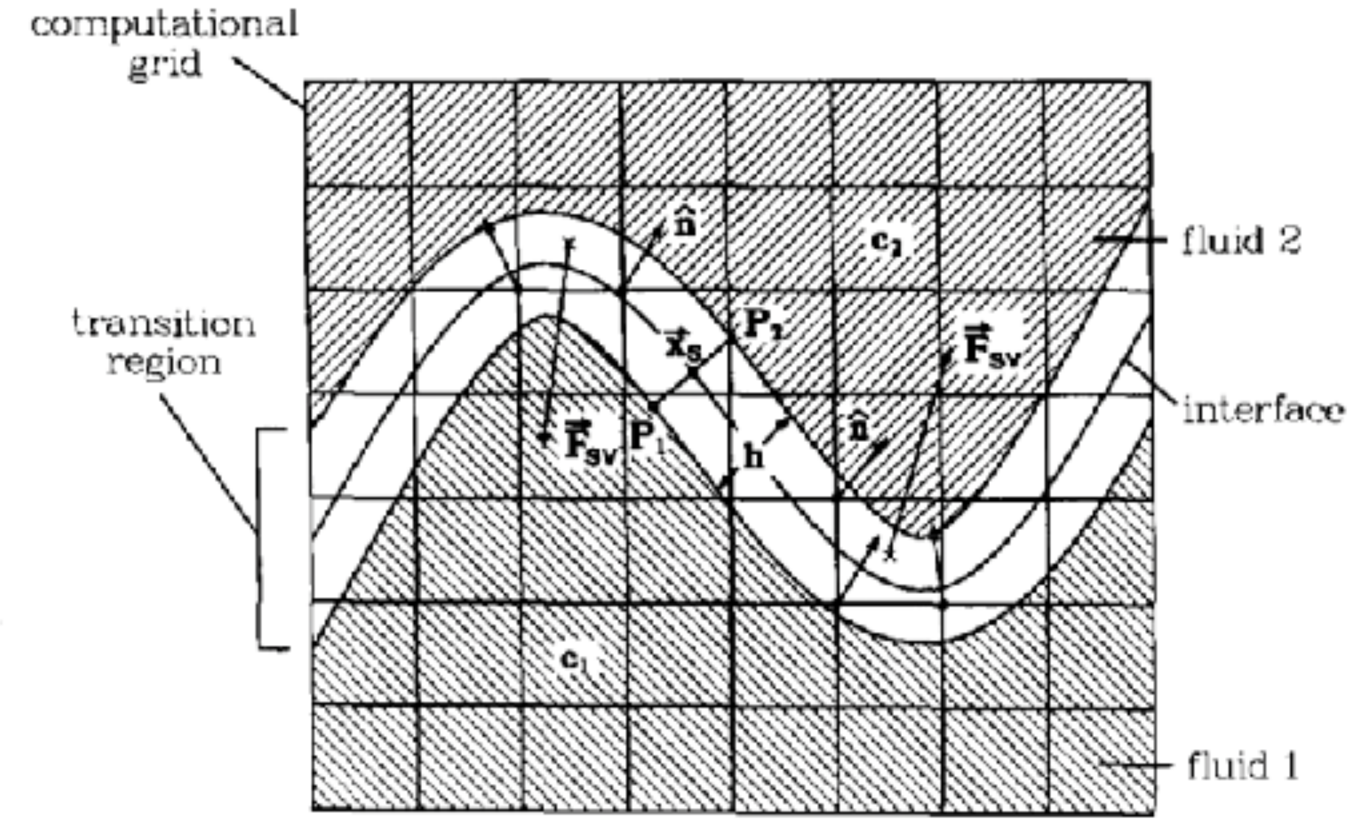


[Azencot et al. 2015]

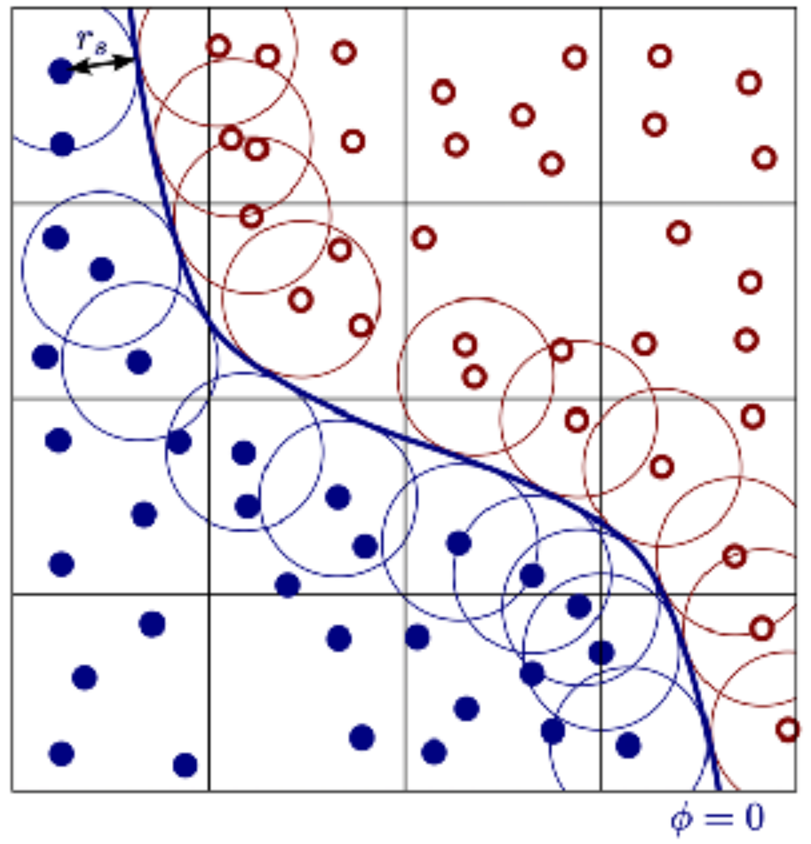
DEFINING THE SURFACE



Surface tracking with explicit mesh
[Clausen et al. 2013]



Continuum Surface Force with color function
[Brackbill et al. 1992]



Particle-derived level sets
[Boyd and Bridson 2012]

SURFACE TENSION MODEL

Continuum Surface Force

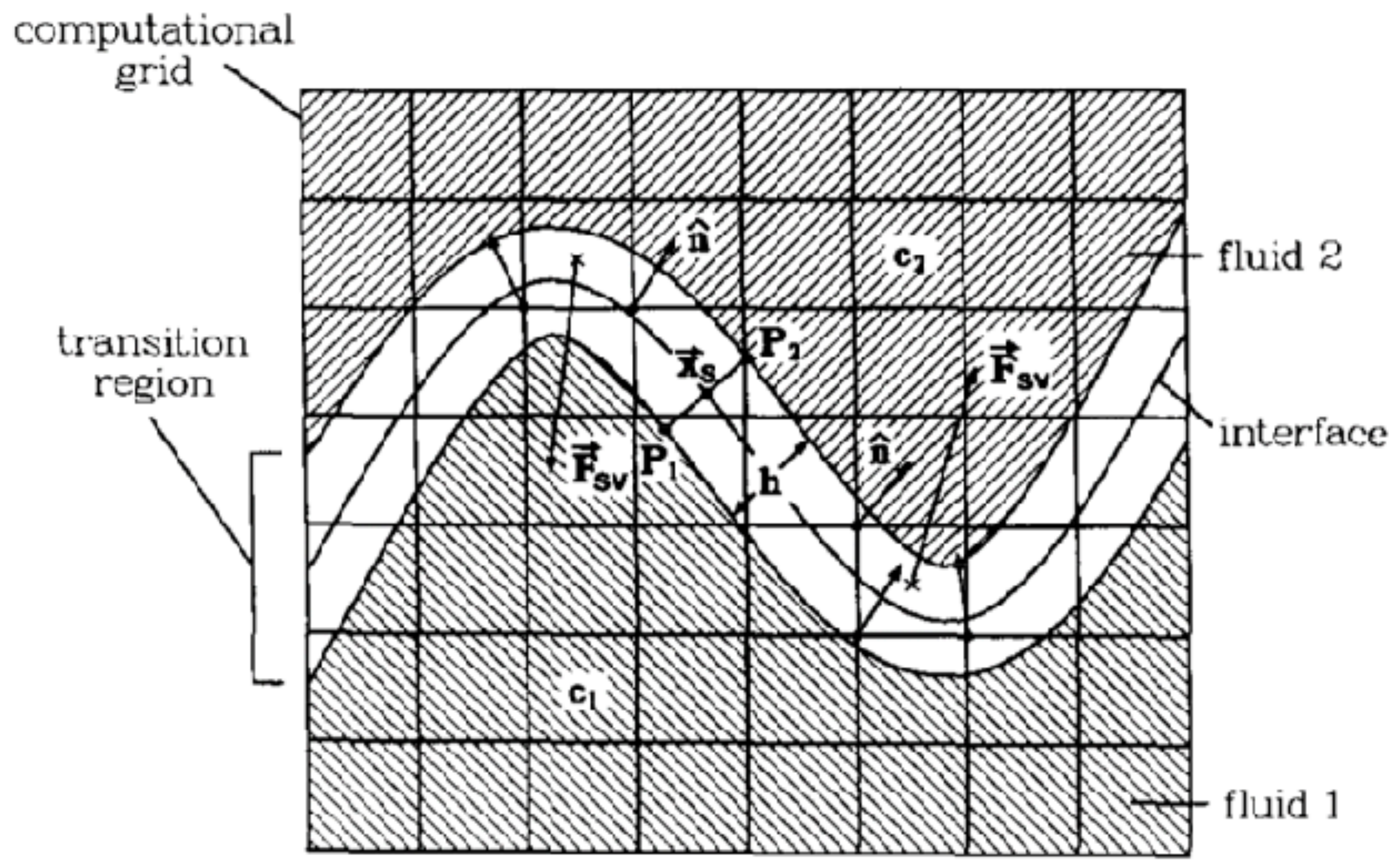
- Interfacial traction [Brackbill et al. 1992]

Surface tension coefficient

$$\mathbf{t} = k^{\sigma}\kappa\mathbf{n} + \nabla^{s}k^{\sigma}.$$

Curvature Surface normal

- Curvature is calculated from the unit normal based on the color function.
- Challenging for implicit time marching schemes.



Continuum Surface Force
[Brackbill et al. 1992]

SURFACE TENSION MODEL

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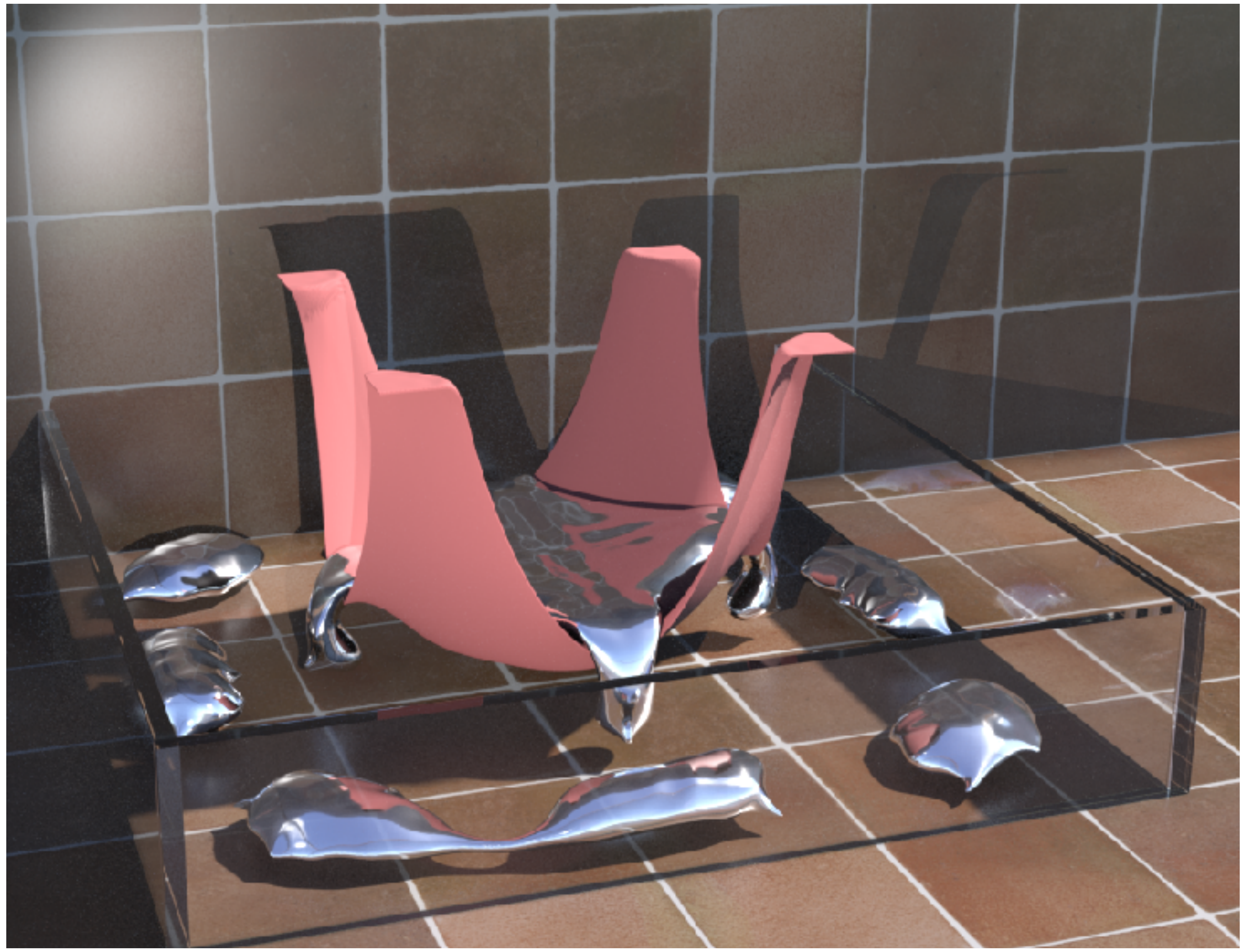
Energy-based Approach

- The surface tension is modeled as a potential energy associated with the surface area [Hyde et al. 2020]

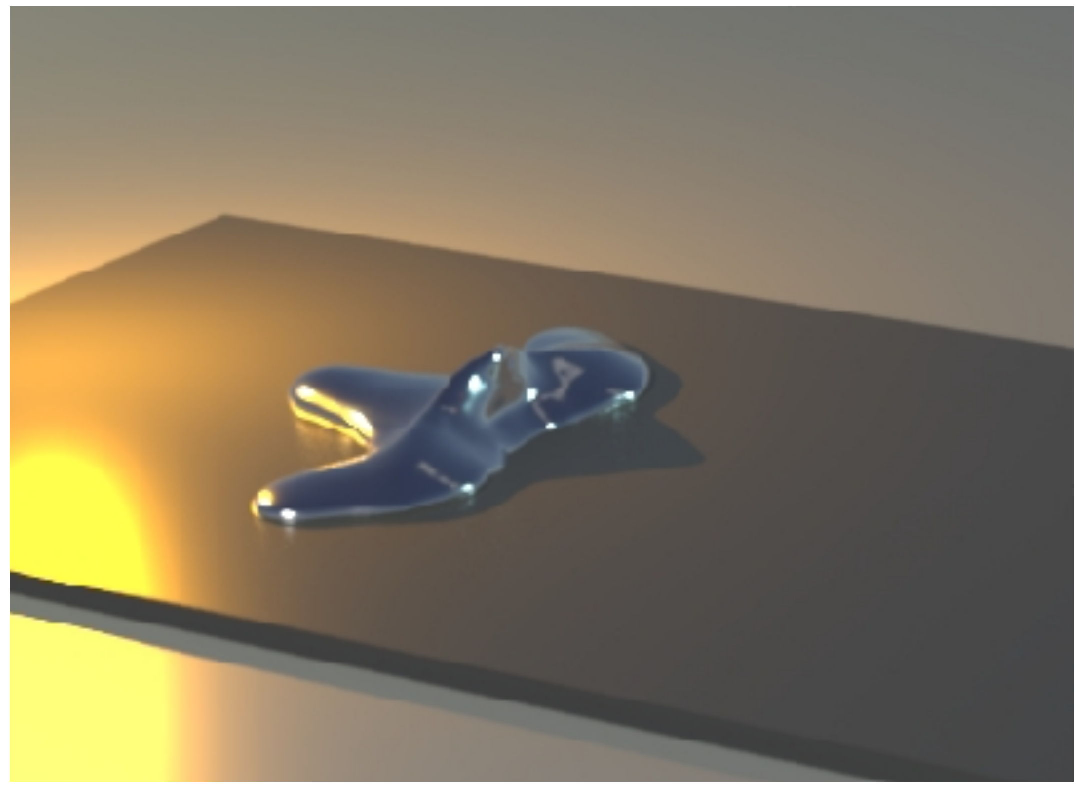
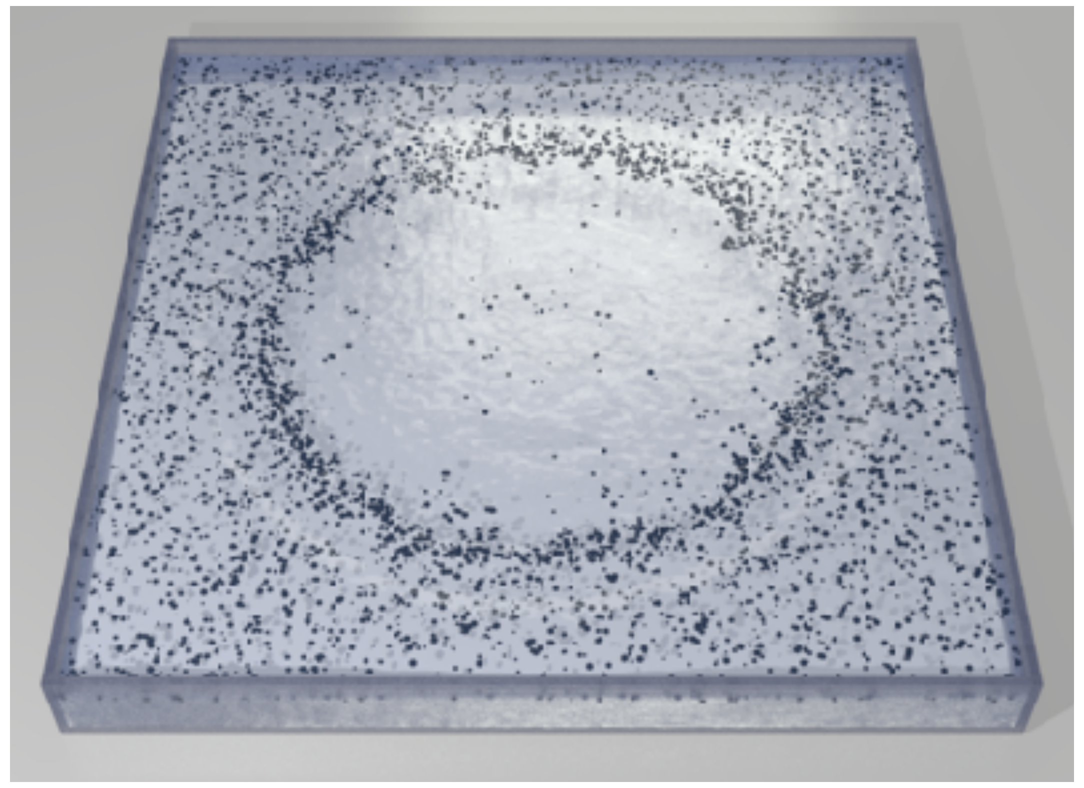
$$\Psi^{\sigma}(\mathbf{x}) = k^{\sigma} \int_{\partial\Omega^t} ds(\mathbf{x}).$$

- The surface tension force is defined as the gradient of surface energy.
- Benefits:
  - No need for mean curvature estimation.
  - Allows the implicit time stepping scheme with large Δt.



[Hyde et al. 2020]

OVERVIEW


CONTRIBUTIONS

- A novel implicit MPM discretization of spatially varying surface tension forces.
- A momentum-conserving particle resampling technique for particles near the liquid interface.
- An implicit MPM discretization of the convection/diffusion evolution of temperature/concentration coupled to the surface tension coefficient including a novel particle-based Robin boundary condition.

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GOVERNING EQUATIONS

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Conservation of mass

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}$$

Conservation of momentum

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}$$

σ is the Cauchy stress. For fluid, $\boldsymbol{\sigma} = -p\mathbf{I} + \mu \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}^T \right)$, $p = -\frac{\partial \psi^p}{\partial J}$.

Conservation of energy

$$\rho c_p \frac{DT}{Dt} = K \nabla^2 T + H$$

$$K \nabla T \cdot \mathbf{n} = -h(T - \bar{T}) + b$$

GOVERNING EQUATIONS

SIGGRAPH 2021

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Conservation of energy

$$\rho c_p \frac{DT}{Dt} = K \nabla^2 T + H$$

$$K \nabla T \cdot \mathbf{n} = \underbrace{\boxed{-h(T - \bar{T})}}_{\text{Convection}} + \underbrace{\boxed{b}}_{\text{Heat flux}}$$

CONSTITUTIVE MODELS

SIGGRAPH 2021

- (Compressible) fluid potential energy density:

$$\psi^p(J) = \frac{\lambda^l}{2}(J-1)^2, \quad p = -\frac{\partial \psi^p}{\partial J}.$$

- Fixed-corotated solid [Stomakhin et al. 2012]:

$$\psi^h(\mathbf{F}) = \mu^h \sum_{\alpha=0}^{d-1} (\sigma_\alpha - 1)^2 + \frac{\lambda^h}{2}(J-1)^2.$$

- Our surface tension potential energy:

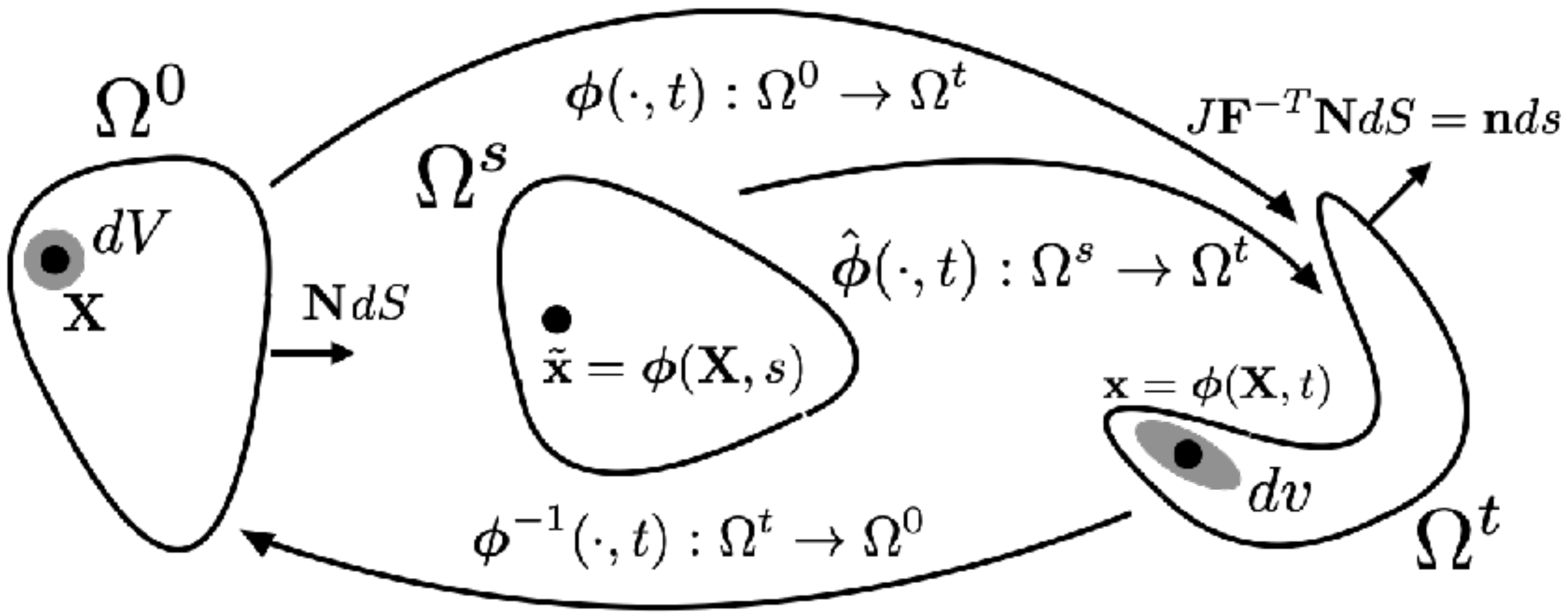
$$\Psi^\sigma(\mathbf{x}) = \int_{\partial\Omega^t} k^\sigma(\mathbf{x}, t) ds(\mathbf{x}).$$

  - $k^\sigma(\mathbf{x}, t)$ can vary in space as a function of temperature or concentration.
  - No special treatment is required for the ∇^s term in $\mathbf{t} = k^\sigma \kappa \mathbf{n} + \nabla^s k^\sigma$.

UPDATED LAGRANGIAN FORMULATION

- From $\partial\Omega^s$ to $\partial\Omega^t$, using Nanson's formula, the infinitesimal area is $ds(\mathbf{x}) = |\hat{J}\hat{F}^{-T}\tilde{\mathbf{n}}|\, ds(\tilde{\mathbf{x}})$.
- Surface tension potential energy becomes

$$\Psi^\sigma(\mathbf{x}) = \int_{\partial\Omega^t} k^\sigma(\mathbf{x}, t) ds(\mathbf{x}) = \int_{\partial\Omega^t} k^\sigma(\hat{\phi}(\tilde{x}, s, t), t)\,|\hat{J}\hat{F}^{-T}\tilde{\mathbf{n}}|\, ds(\tilde{\mathbf{x}}).$$



[Hyde et al. 2020]

DISCRETIZATION

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MPM

- We discretized the governing equations using MPM with backward Euler scheme.
- Why MPM?
  - Based on continuum mechanics.
  - Good for fluid-solid interactions.
  - Easily handle large topological change.

UPDATE SCHEMES

- Momentum update

$$m_{\mathbf{i}}^n \frac{\hat{\mathbf{v}}_{\mathbf{i}}^{n+1} - \mathbf{v}_{\mathbf{i}}^n}{\Delta t} = \mathbf{f}_{\mathbf{i}}(\mathbf{x} + \Delta t \hat{\mathbf{q}}) + m_{\mathbf{i}}^n \mathbf{g}.$$

- Temperature update

$$\begin{aligned} c_p m_{\mathbf{i}} \frac{\hat{T}_{\mathbf{i}}^{n+1} - T_{\mathbf{i}}^n}{\Delta t} = & - \sum_p K \frac{\partial N_{\mathbf{i}}}{\partial x_\alpha}(\mathbf{x}_p^n) \hat{T}_{\mathbf{j}}^{n+1} \frac{\partial N_{\mathbf{j}}}{\partial x_\alpha}(\mathbf{x}_p^n) V_p^n \\ & - \sum_r h N_{\mathbf{i}}(\mathbf{s}_r^n) \hat{T}_{\mathbf{j}}^{n+1} N_{\mathbf{j}}(\mathbf{s}_r^n) \, | \, d\mathbf{A}_r^n \, | \\ & + \sum_r N_{\mathbf{i}}(\mathbf{s}_r^n) \left[h \bar{T}(\mathbf{s}_r^n) + b(\mathbf{s}_r^n) \right] | \, d\mathbf{A}_r^n \, | \\ & + \sum_p N_{\mathbf{i}}(\mathbf{x}_p^n) H(\mathbf{x}_p^n) V_p^n \end{aligned}$$

MPM SIMULATION LOOP

ALGORITHM 1: Time integration loop for MPM simulations using APIC transfers.

begin Particle-to-Grid Transfers
- Transfer time t^n mass to grid by evaluating Equation 6, $m_{\mathbf{i}}^n = \sum_p m_p N_{\mathbf{i}}(\mathbf{x}_p^n)$;
- Transfer time t^n momentum to grid by evaluating Equation 6, $m_{\mathbf{i}}^n \mathbf{v}_{\mathbf{i}}^n = \sum_p m_p N_{\mathbf{i}}(\mathbf{x}_p^n)\left(\mathbf{v}_p^n + \mathbf{A}_p^n(\mathbf{x}_{\mathbf{i}} - \mathbf{x}_p^n)\right)$;

end

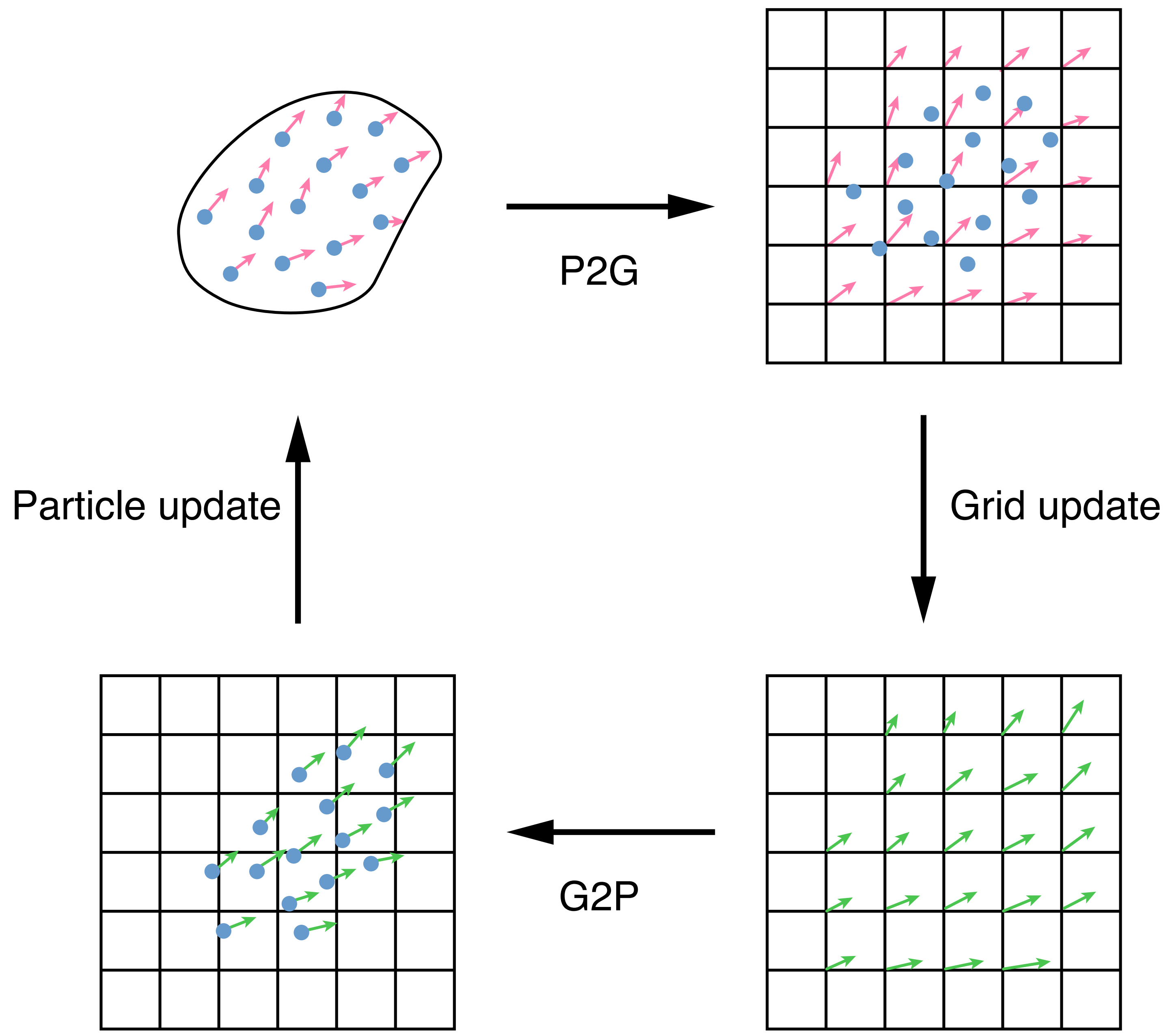
begin Momentum Update
- Update momentum on the grid from t^n to t^{n+1} by solving Equation 8, $m_{\mathbf{i}}^n \frac{\hat{\mathbf{v}}_{\mathbf{i}}^{n+1} - \mathbf{v}_{\mathbf{i}}^n}{\Delta t} = \mathbf{f}_{\mathbf{i}}(\mathbf{x} + \Delta t \hat{\mathbf{q}}) + m_{\mathbf{i}}^n \mathbf{g}$, either explicitly (set $\hat{\mathbf{q}} = 0$) or implicilty (set $\hat{\mathbf{q}} = \hat{\mathbf{v}}^{n+1}$);

end

begin Grid-to-Particle Transfers
- Evaluate time t^{n+1} particle velocity via Equation 10, $\mathbf{v}_p^{n+1} = \sum_{\mathbf{i}} N_{\mathbf{i}}(\mathbf{x}_p^n)\hat{\mathbf{v}}_{\mathbf{i}}^{n+1}$;
- Evaluate time t^{n+1} particle affine information via Equation 10, $\mathbf{A}_p^{n+1} = \frac{4}{\Delta x^2} \sum_{\mathbf{i}} N_{\mathbf{i}}(\mathbf{x}_p^n)\hat{\mathbf{v}}_{\mathbf{i}}^{n+1}(\mathbf{x}_{\mathbf{i}} - \mathbf{x}_p^n)^T$;
- Update particle positions to t^{n+1} via $\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \mathbf{v}_p^{n+1}$;

end

[Hyde et al. 2020]



OUTLINE

SIGGRAPH 2021

- Backgrounds
- Material Point Method (MPM)
- **Conservative Resampling**
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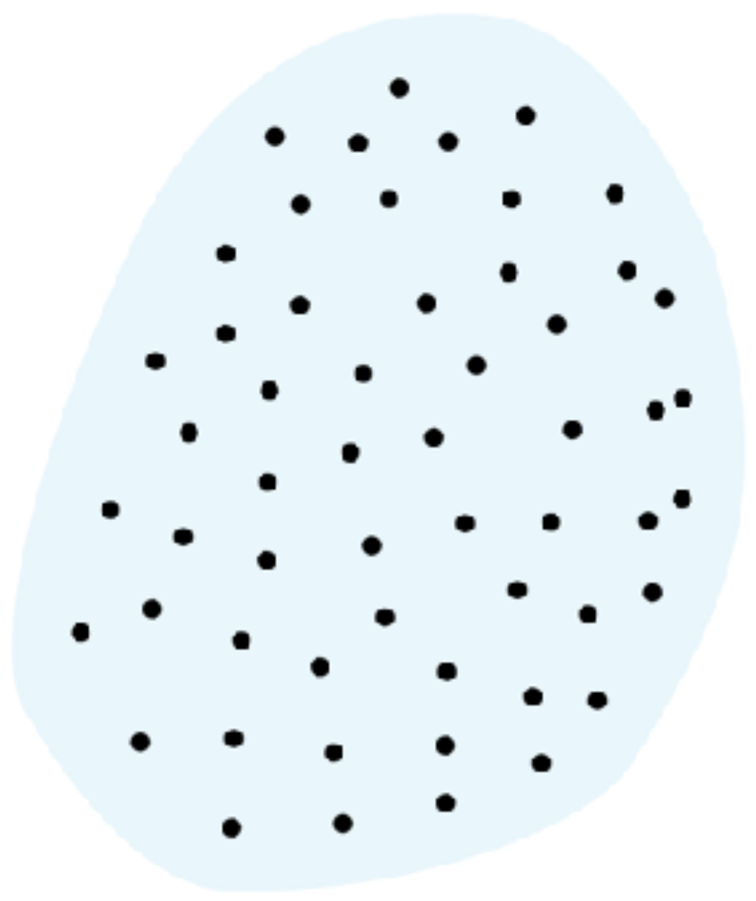
- Summary

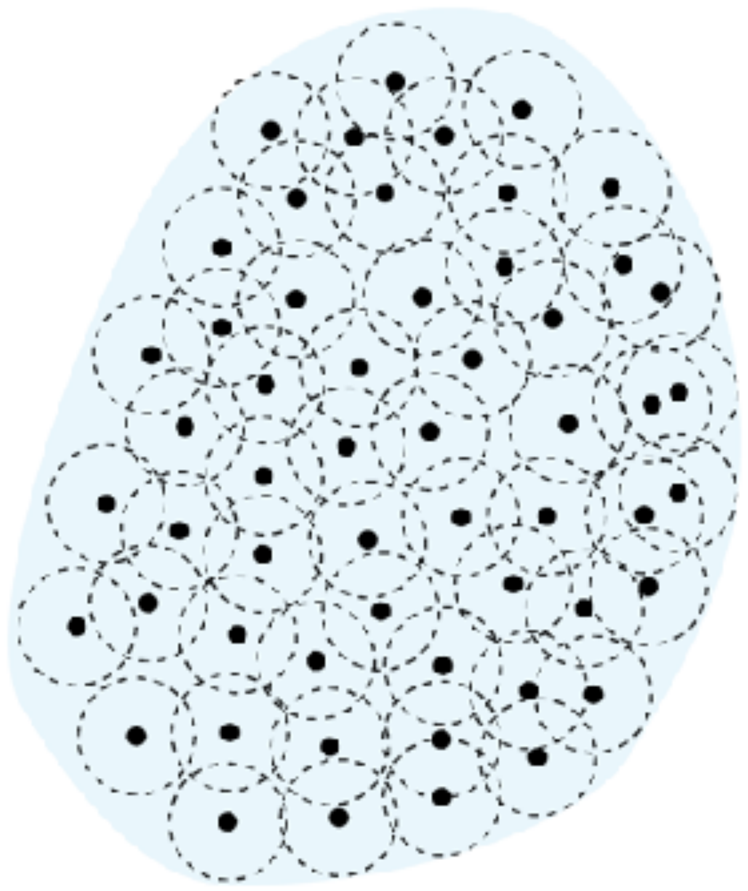
CONSERVATIVE RESAMPLING



PROCEDURE

- Build particle level sets.
- Generate isocontour from particle level sets.
- Sample surface particles on the isocontour.
- Find the closest interior particles for each surface particles.
- Build balance particles $\boldsymbol{b}_r^n = \boldsymbol{s}_r^n + 2\left(\boldsymbol{x}_{p(\boldsymbol{s}_r^n)}^n - \boldsymbol{s}_r^n\right)$.
- Remapping (within each particle group).
  - Assign mass, linear and affine velocity (momentum splitting).
  - Remove the temporary particles and merge the momentum.

CONSERVATIVE RESAMPLING



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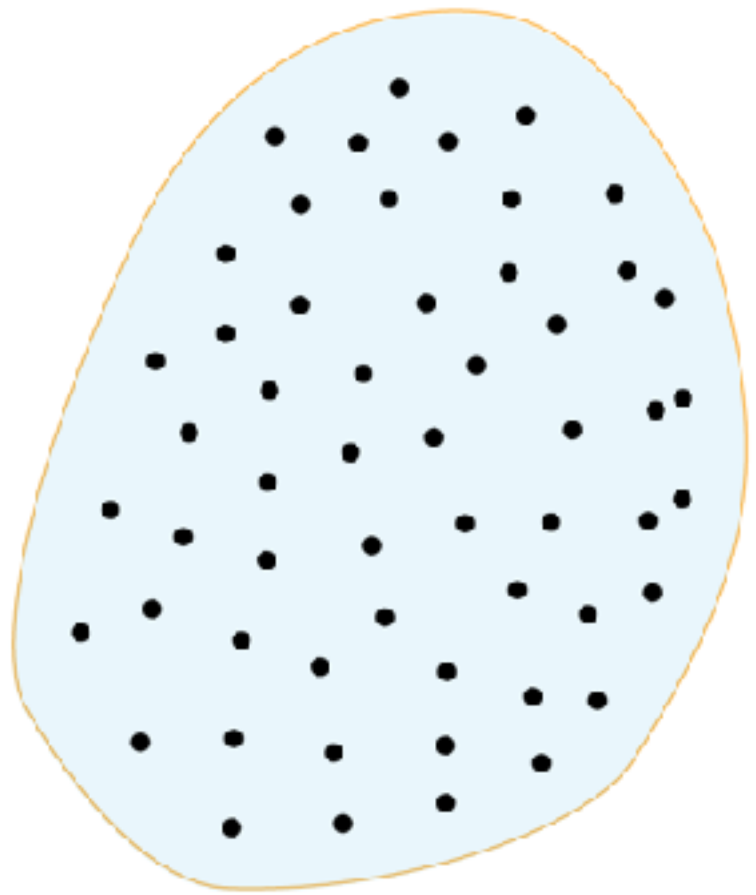

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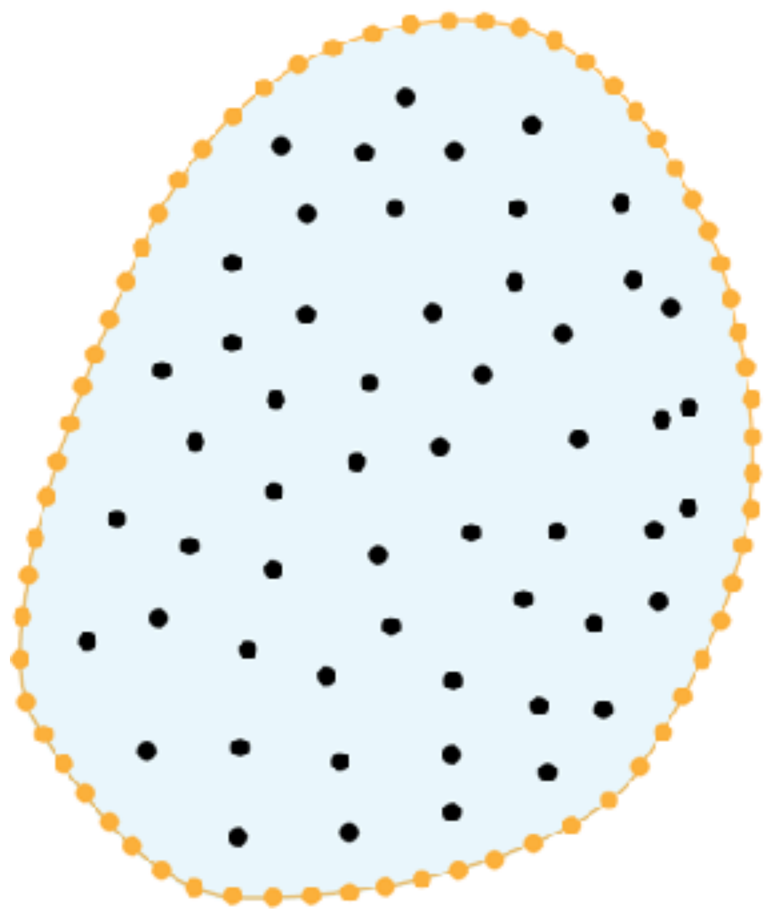

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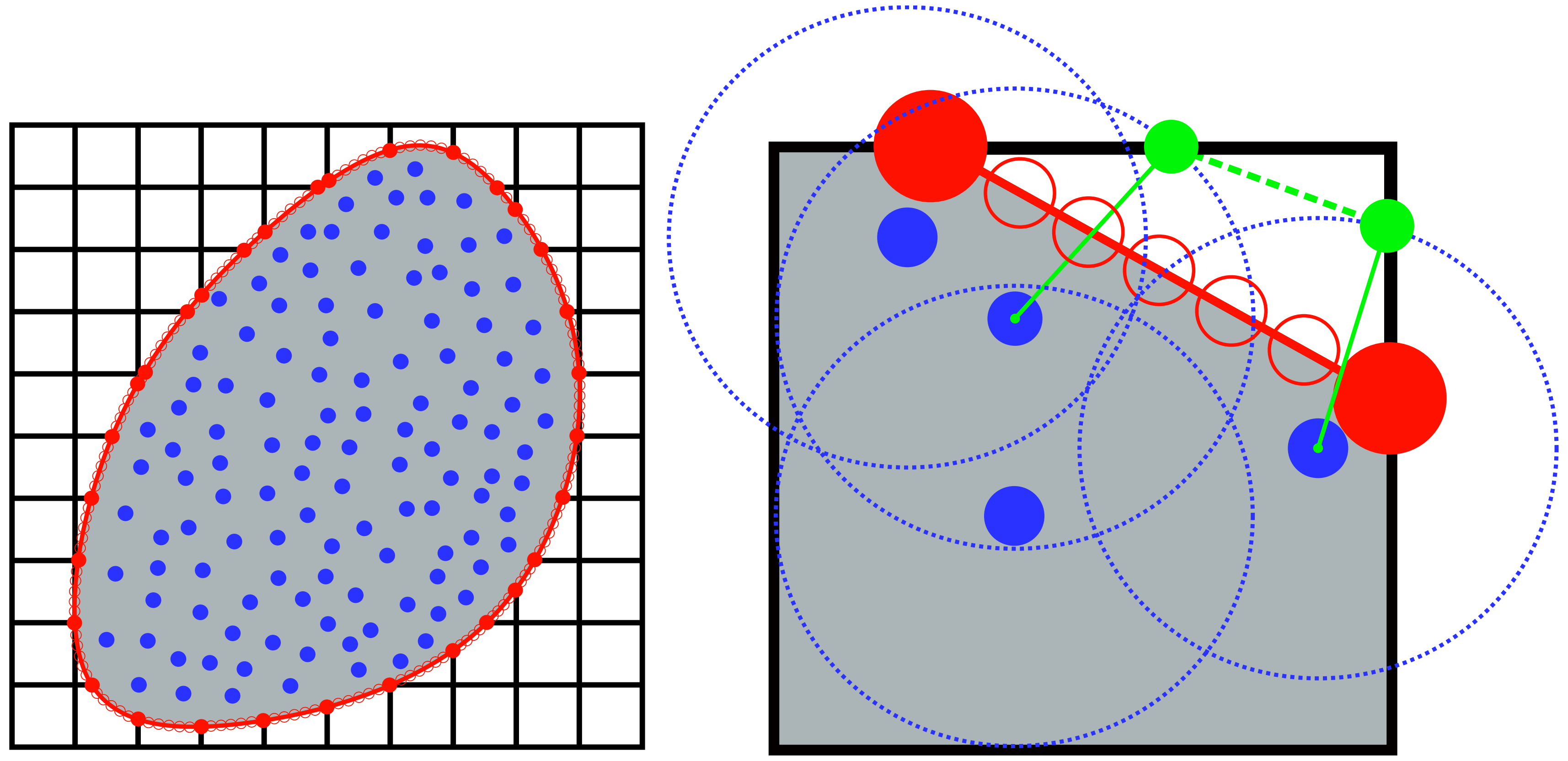
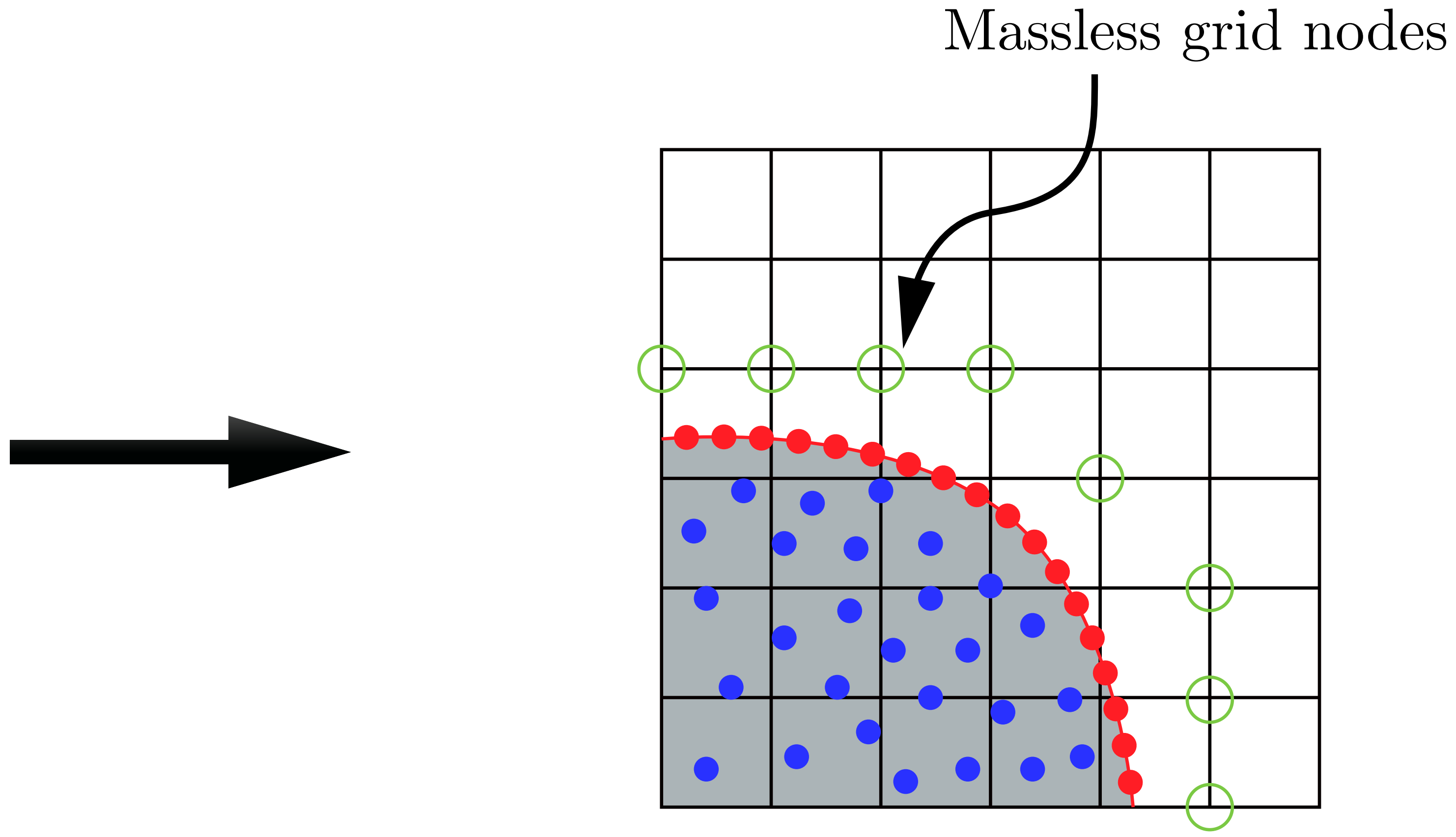
NONCONSERVATIVE RESAMPLING

- Surface tension forces are applied through the surface particles.
- Hyde et al. [2020] proposed a method to sample the boundaries with massless surface particles.
  - Guarantee the mass conservation
  - Lose the momentum conservation



Resampling in [Hyde et al. 2020]



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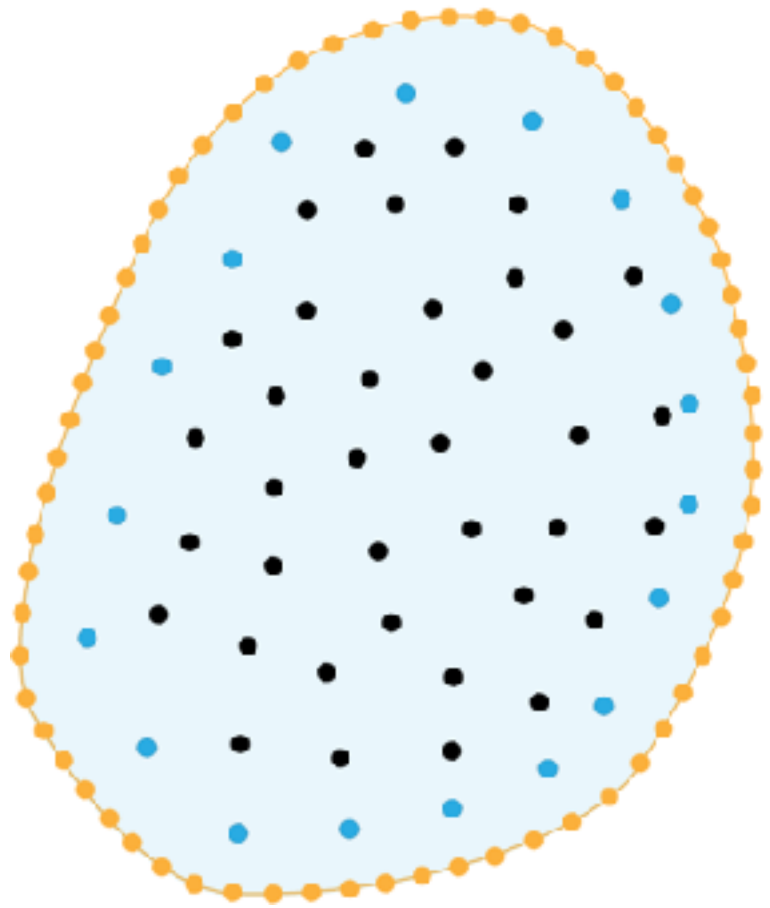

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CONSERVATIVE RESAMPLING

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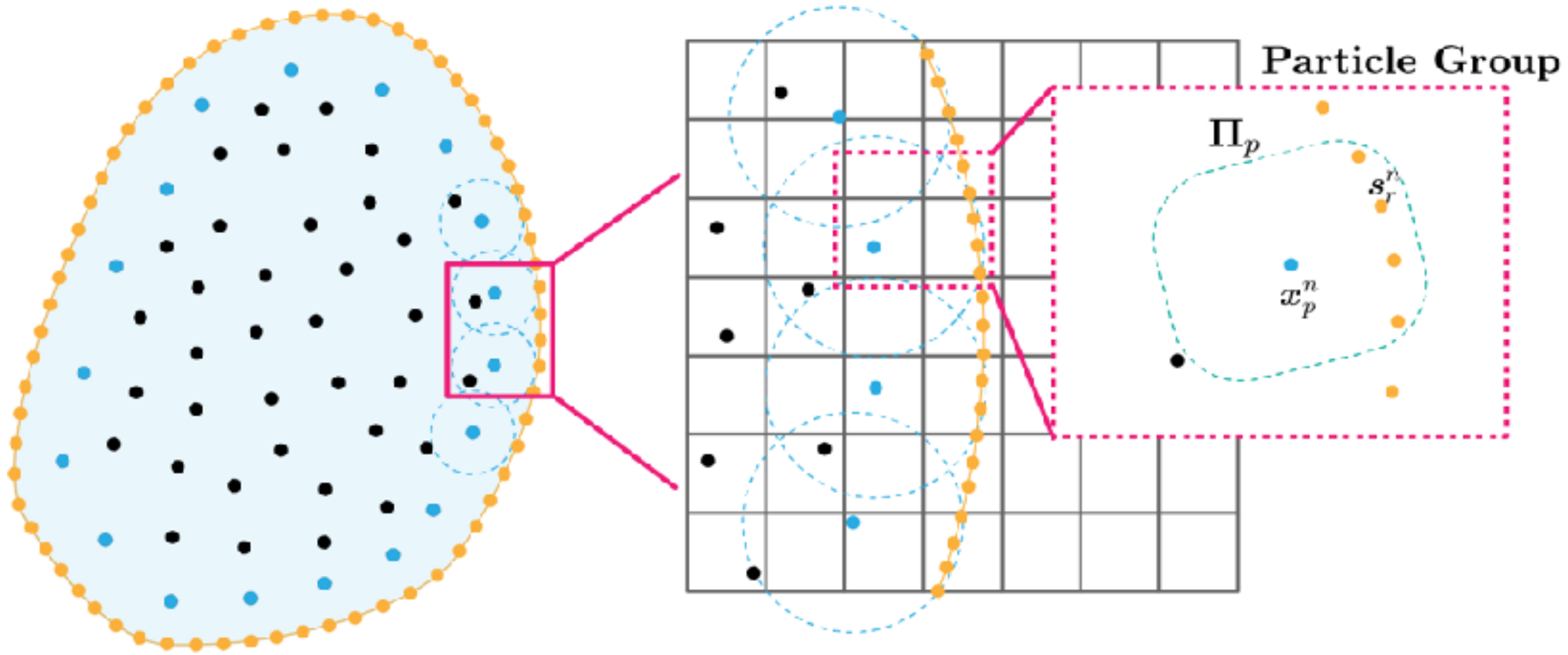

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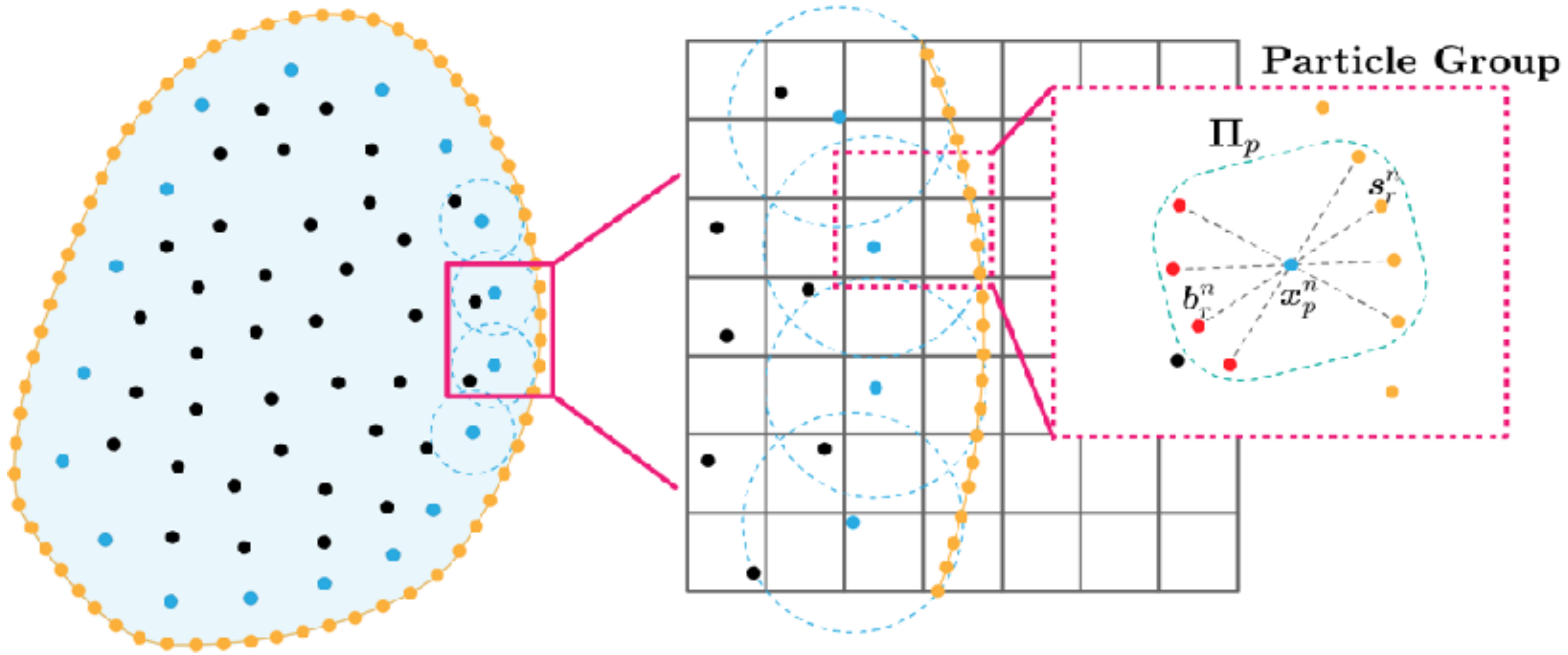

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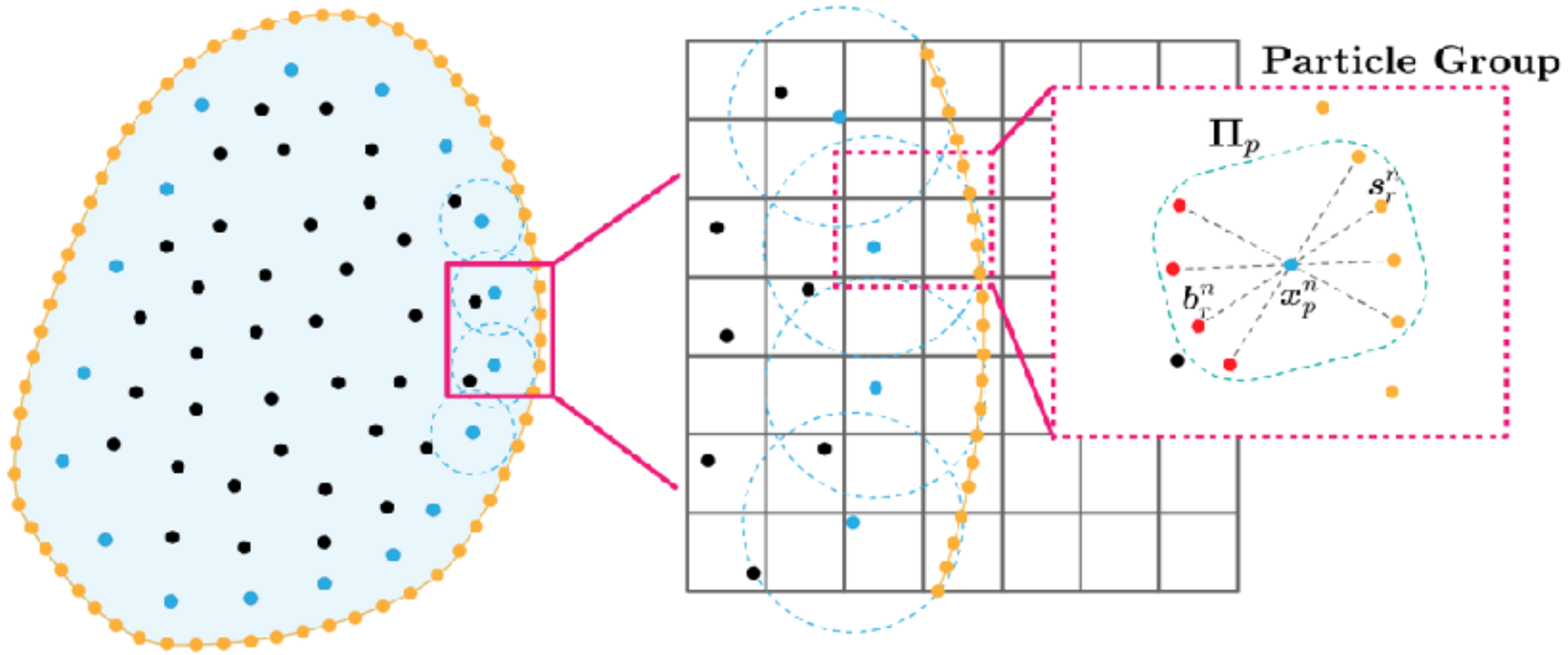

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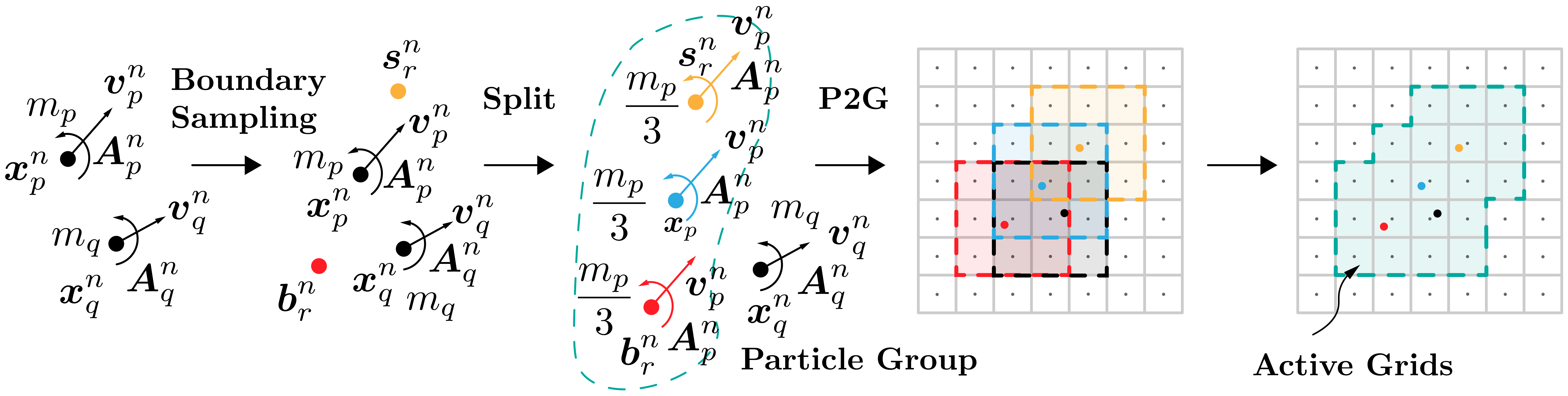
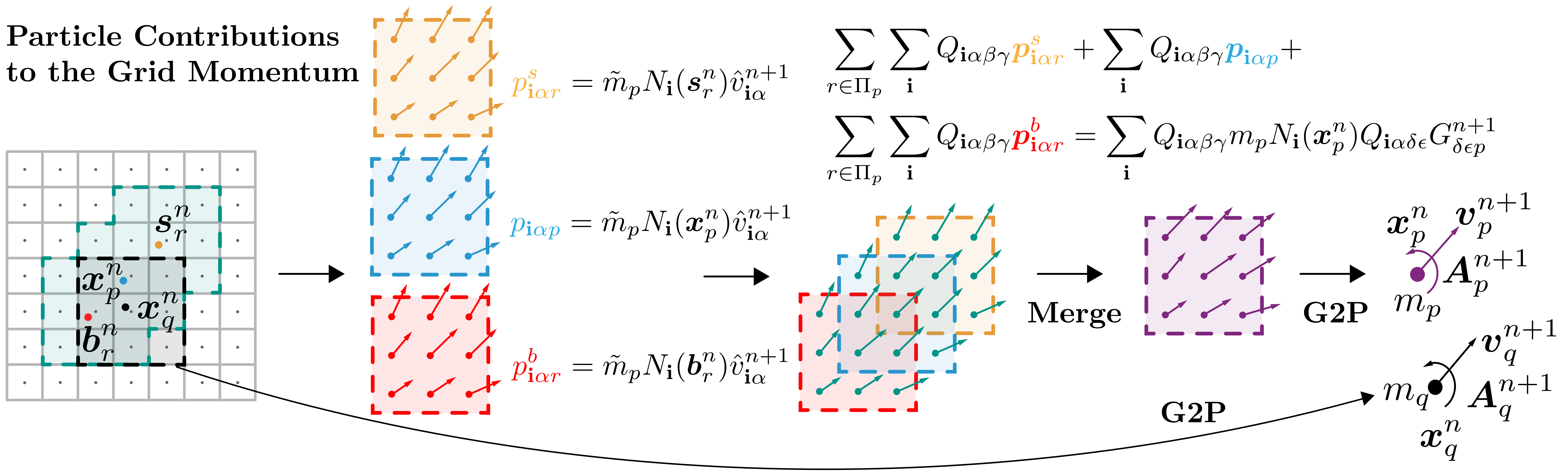
REMAPPING: SPLITTING



- Split the mass m_p of the original $\boldsymbol{x}_p^n$ to surface particles $\boldsymbol{s}_r^n$ and balance particles $\boldsymbol{b}_r^n$.
- Assign linear velocity $\boldsymbol{v}_p^n$ and affine velocity $\boldsymbol{A}_p^n$ to $\boldsymbol{s}_r^n$ and $\boldsymbol{b}_r^n$.
- This technique avoids massless grid nodes and conserves the total linear and angular momentum.

REMAPPING: MERGING



- Temporary particles are deleted before the advection.
- Mass and momentum of surface particles $\boldsymbol{s}^n_r$ and balance particles $\boldsymbol{b}^n_r$ are merged into the interior particles $\boldsymbol{x}^n_p$ before the removal.

EXAMPLE: MOMENTUM CONSERVATION

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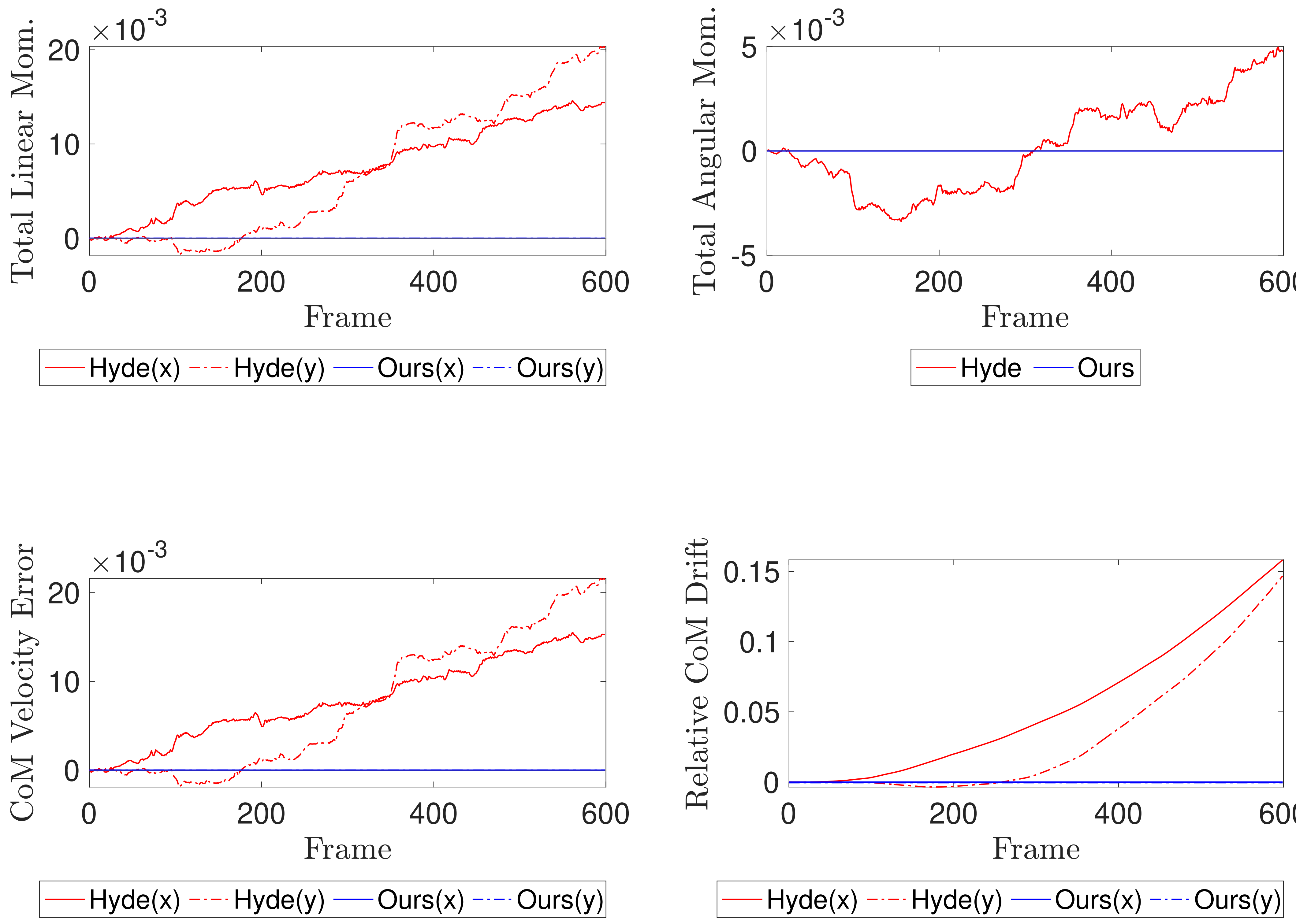

Left: Our conservative resampling.
Right: Nonconservative resampling from Hyde et al. [2020]

$k^\sigma = 20$ $k^\sigma = 5$ $k^\sigma = 1$ $k^\sigma = 0.1$ $k^\sigma = 0.05$

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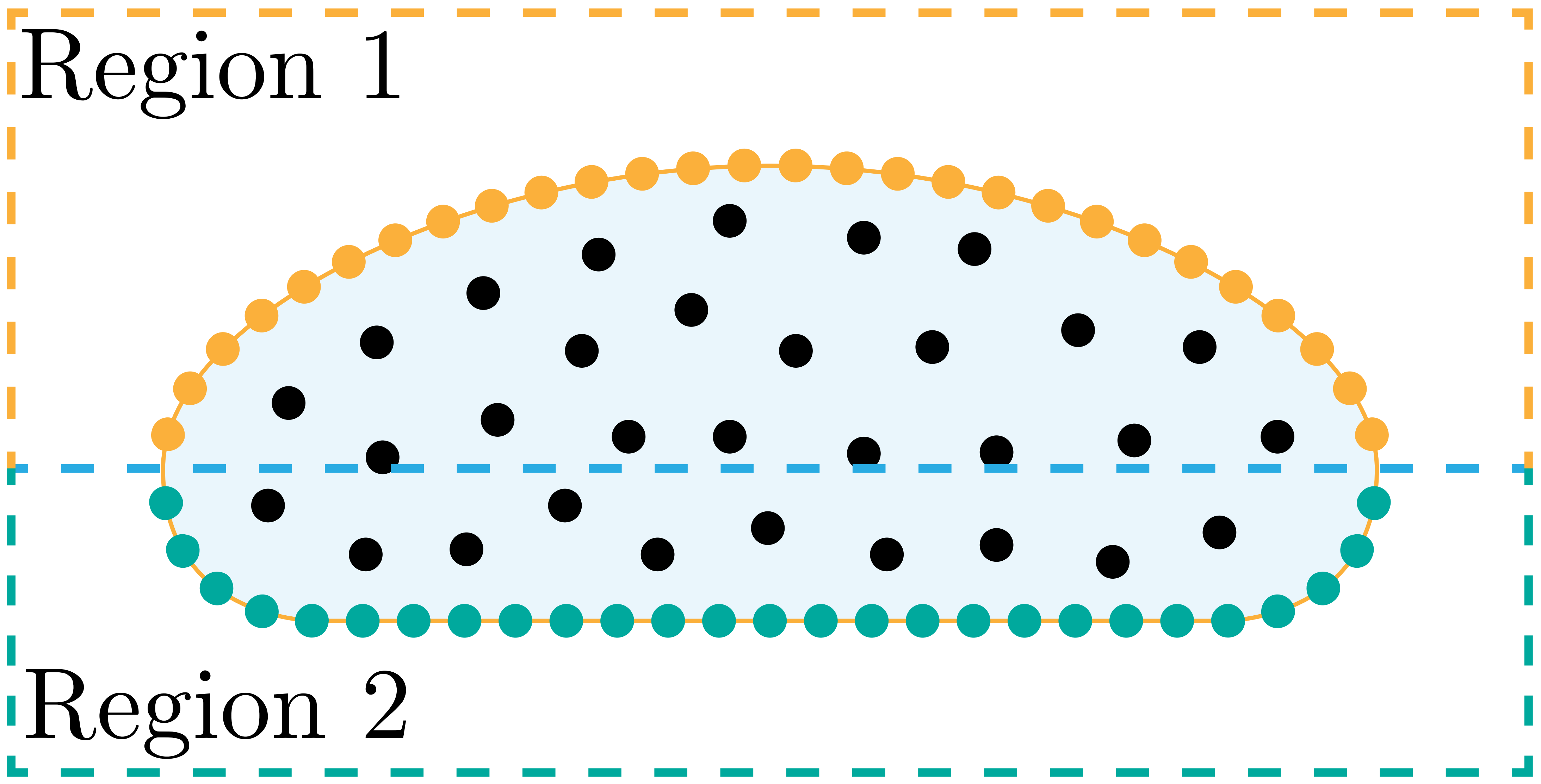
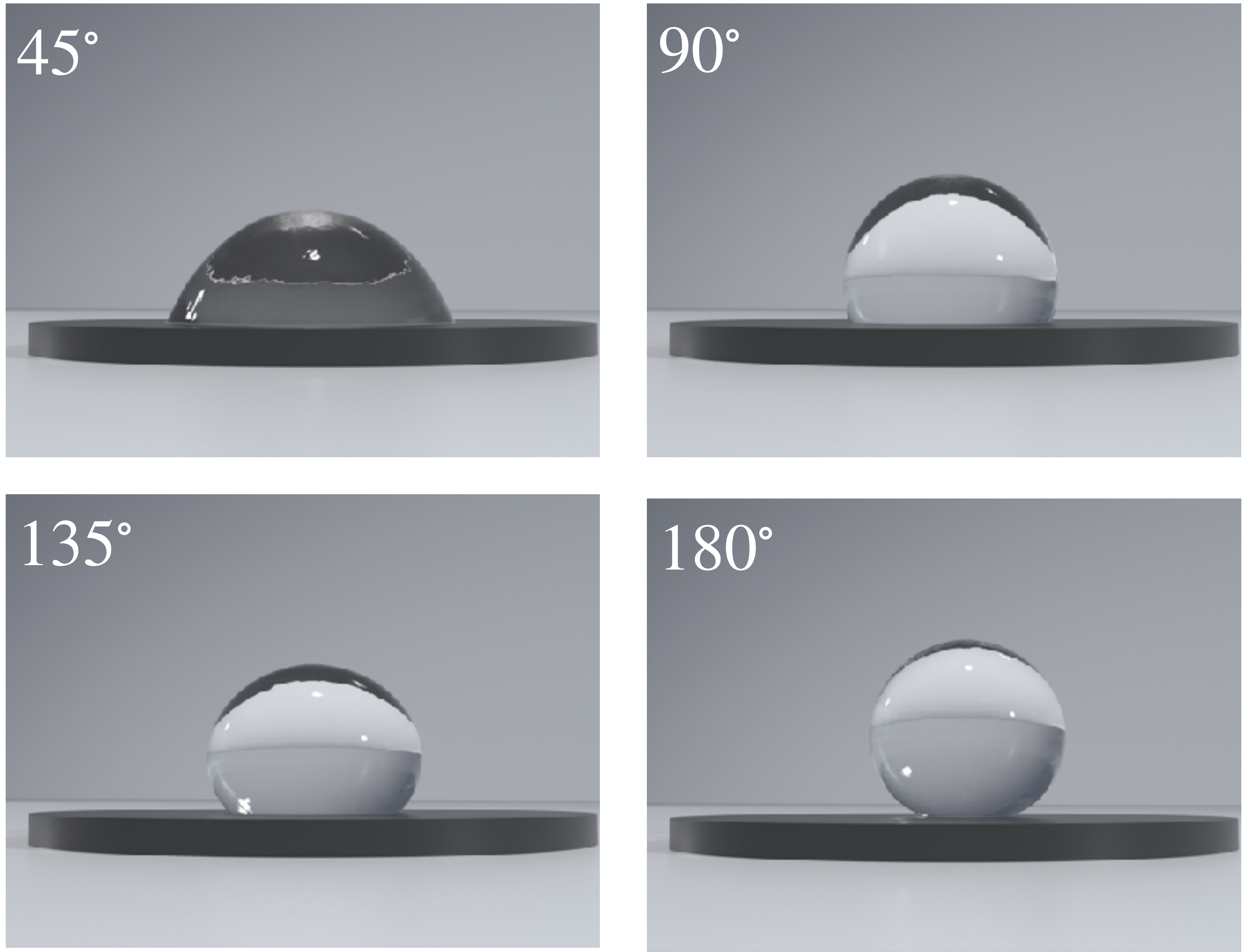
SPATIALLY VARYING SURFACE TENSION

SURFACE TENSION PER PARTICLE

- Each surface particles s_r^n can have different surface tension coefficient k^σ based on:
  - position
  - time
  - temperature / concentration
- Allow controlling the contact angle or dynamic spreading on the surface.
- Enable surface tension driven flow.



EXAMPLE: CONTACT ANGLE



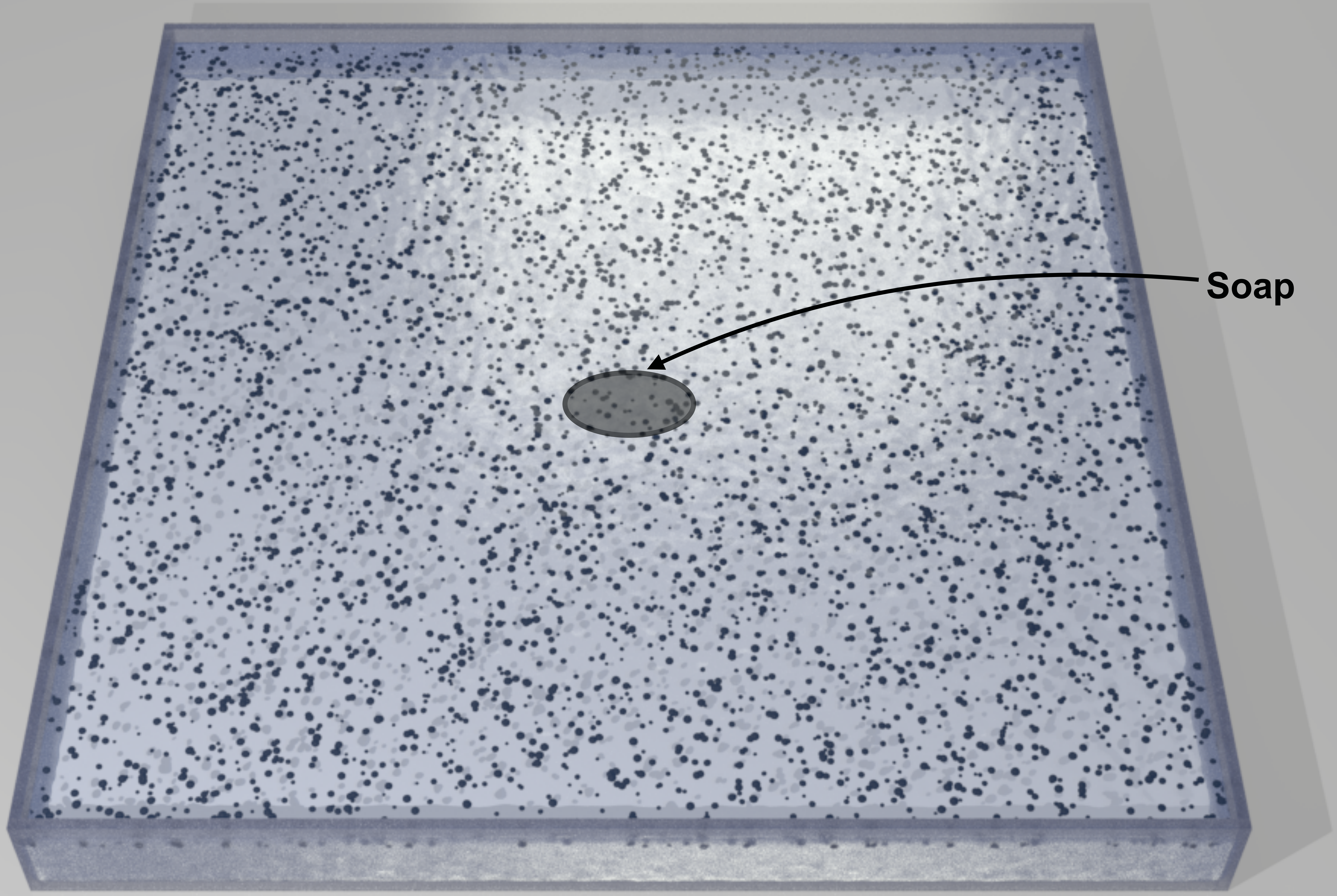
CONTACT ANGLE

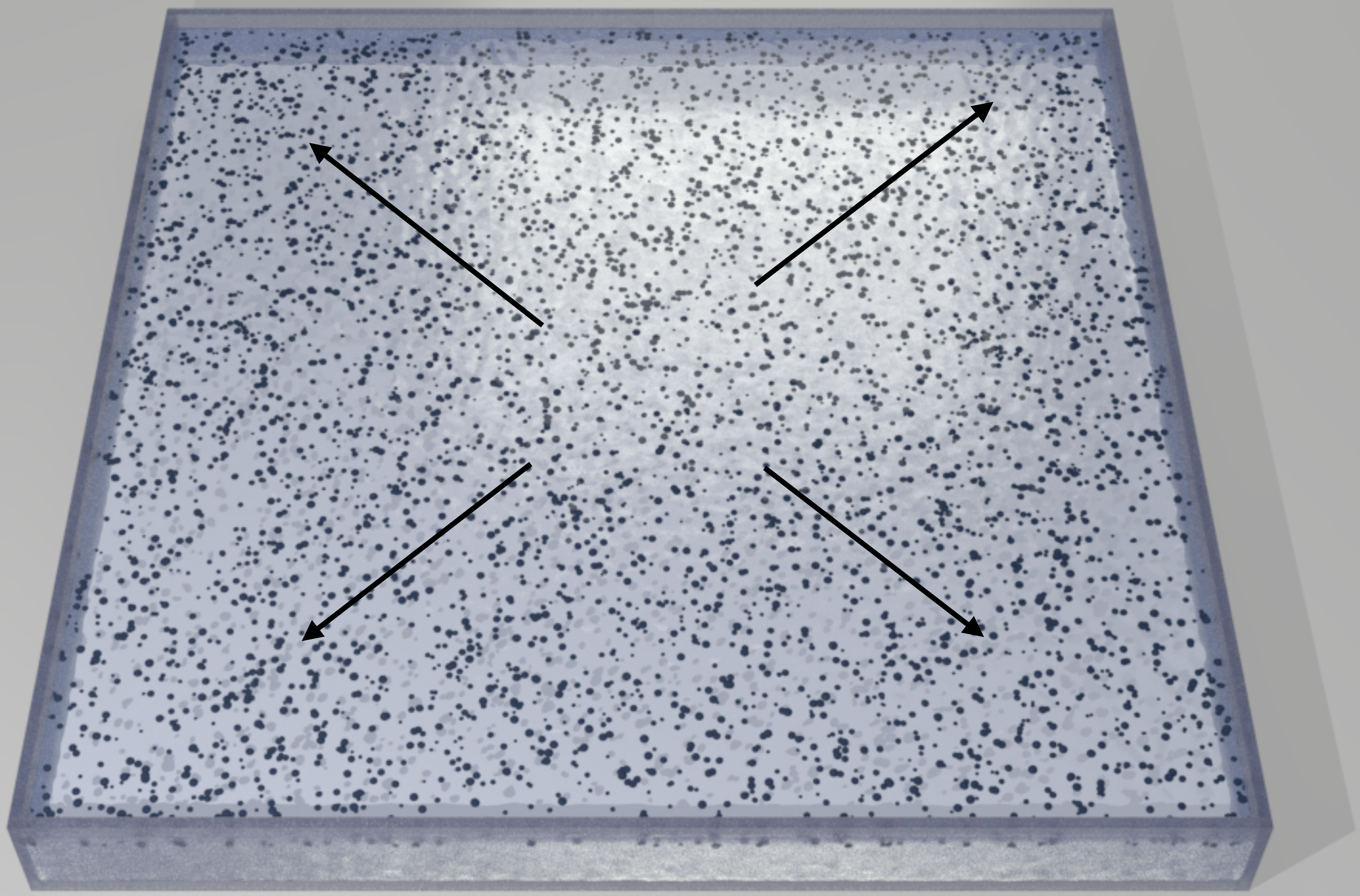
- The contact angle can be determined by Young's equation

$$k^{\sigma}_{SG} = k^{\sigma}_{SL} + k^{\sigma}_{LG}\cos(\theta).$$

  - Further simplify by ignoring k^{σ}_{SG} [Clausen et al. 2013].
- The desired contact angle is achieved by setting a proper surface tension ratio $k^{\sigma}_{SL}/k^{\sigma}_{LG}$.


$k_{SL}^{\sigma}/k_{LG}^{\sigma} = 0.05$
$k_{SL}^{\sigma}/k_{LG}^{\sigma} = 0.3$
$k_{SL}^{\sigma}/k_{LG}^{\sigma} = 0.6$
$k_{SL}^{\sigma}/k_{LG}^{\sigma} = 1.0$


Soap



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THERMOMECHANICAL SIMULATIONS WITH MPM

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RELATED WORKS

- MPM for the thermomechanical simulations:
  - Stomakhin et al. [2014] simulated the phase change and applied the voxalized thermal boundary conditions directly on the grid.
  - Ding et al. [2019] used a temperature and porosity-dependent viscoelastoplastsic model.
- Our method resolves the sub-cell boundary geometry by applying boundary conditions through particles.

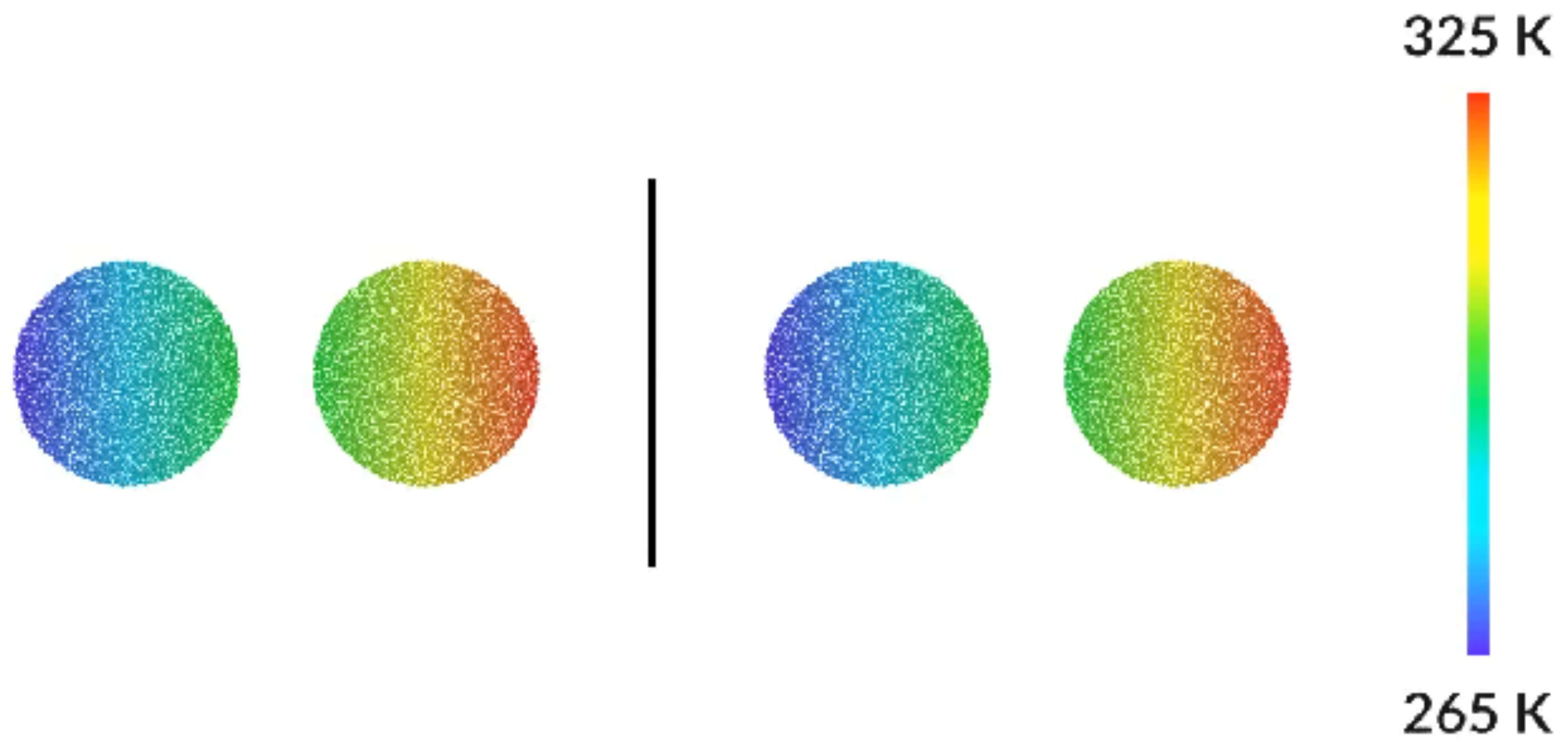
[Stomakhin et al. 2014]

[Ding et al. 2019]

THERMAL BOUNDARY CONDITIONS

ROBIN BC

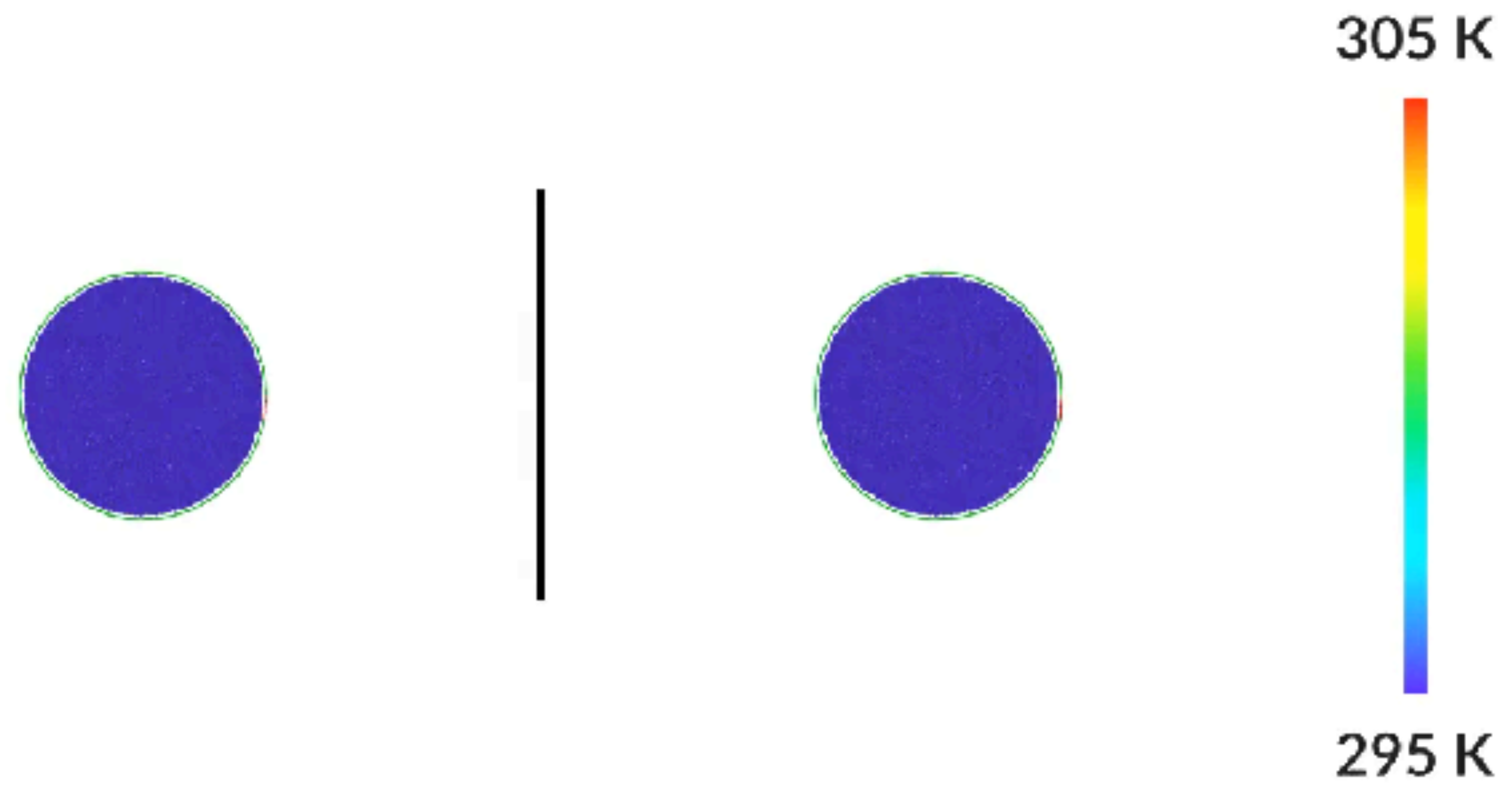
- The Robin boundary condition equilibrates material temperature to the ambient temperature.



Left: with Robin bc.
Right: without Robin bc.

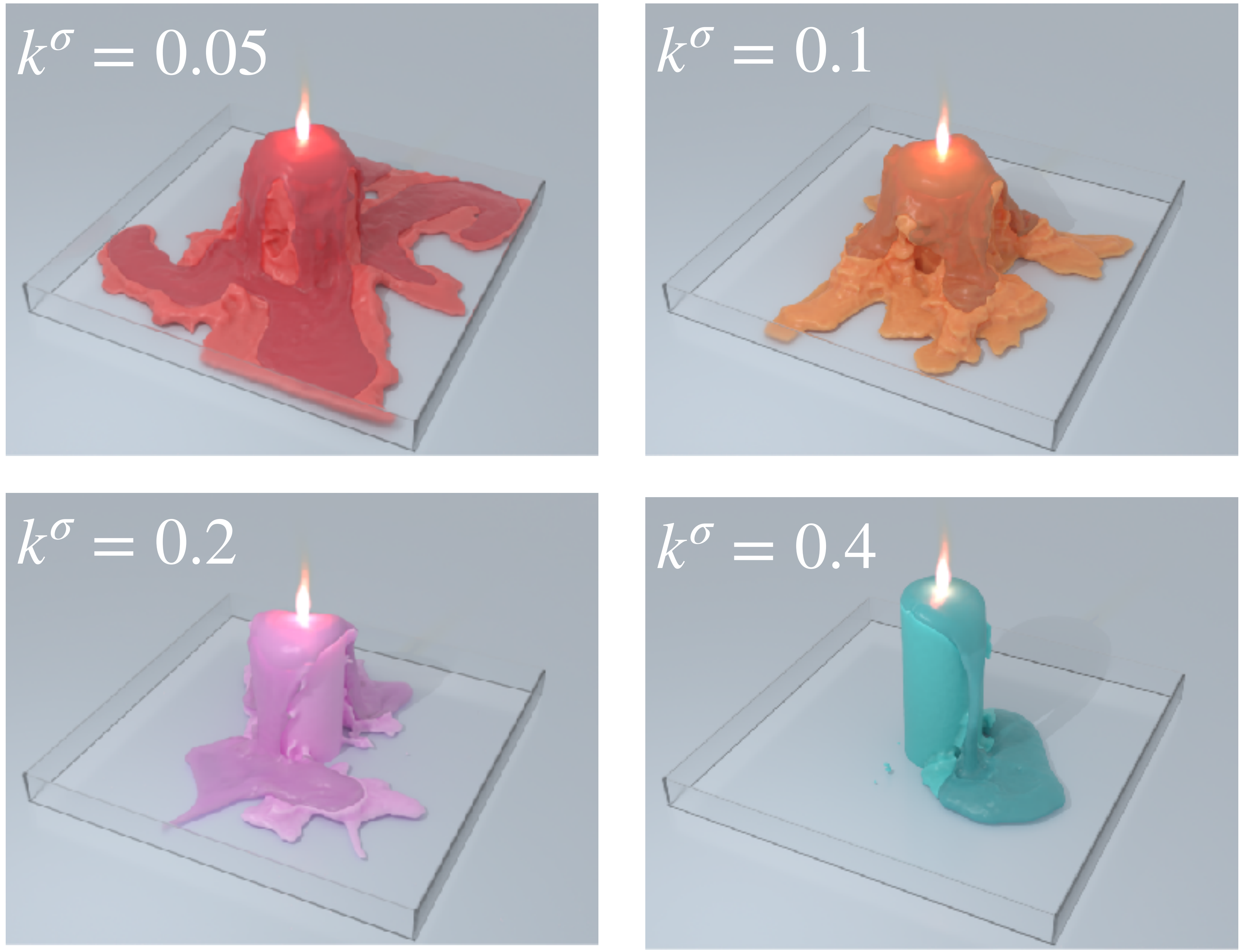
BC THROUGH PARTICLES

- Easy to apply complex boundary conditions



Left: heating (Neumann) + convection (Robin).
Right: heating (Neumann) only.

PHASE CHANGE



MELTING AND RESOLIDIFYING

- The flame is modeled as a Neumann boundary condition (heating).
- The resolidification is enabled by the Robin boundary condition (convective heat transfer).
- The wax changes phase based on its temperature:
  - melt if the temperature is above the melting point.
  - solidify if the temperature is below the melting point.


SIGGRAPH

OUTLINE

- Backgrounds
- Material Point Method (MPM)
- Conservative Resampling
- Spatially Varying Surface Tension
- Thermomechanical Coupling
- **Summary**

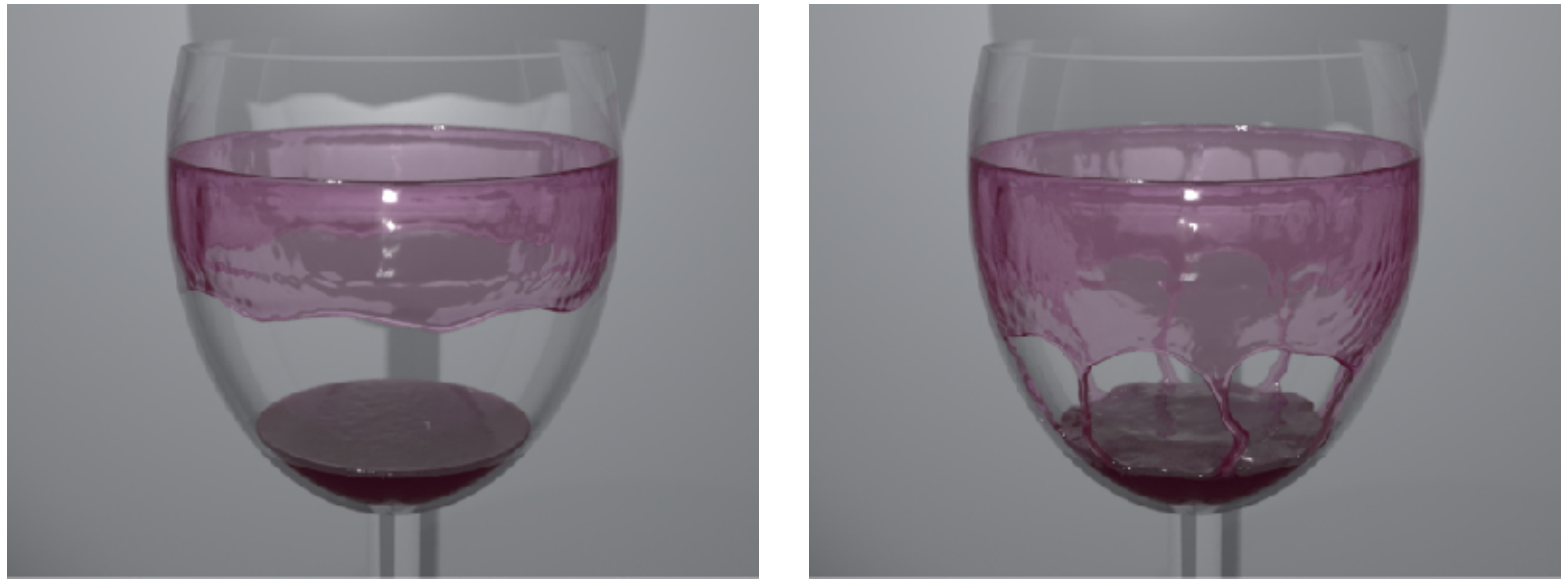
SUMMARY

Contributions

- Our implicit MPM allows for simulating spatially varying surface tension.
- Our approach provides perfect conservation of the total linear and angular momentum.
- We coupled the surface tension simulation with the particle-base thermal boundary conditions.

Future directions

- Adding mixture model like [Ding et al. 2019].
- Simulating evaporation of alcohol, wax, etc.
- Generalizing our approach to SPH.



The falling wine forms tears and ridges.

SIGGRAPH 2021

THANK YOU!