

Development of Simulation Technique for **Crust Formation** calculation using **Rigid Body Dynamics Model in** **Moving Particle Semi-implicit**

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제주 국제컨벤션 센터 302(3F)



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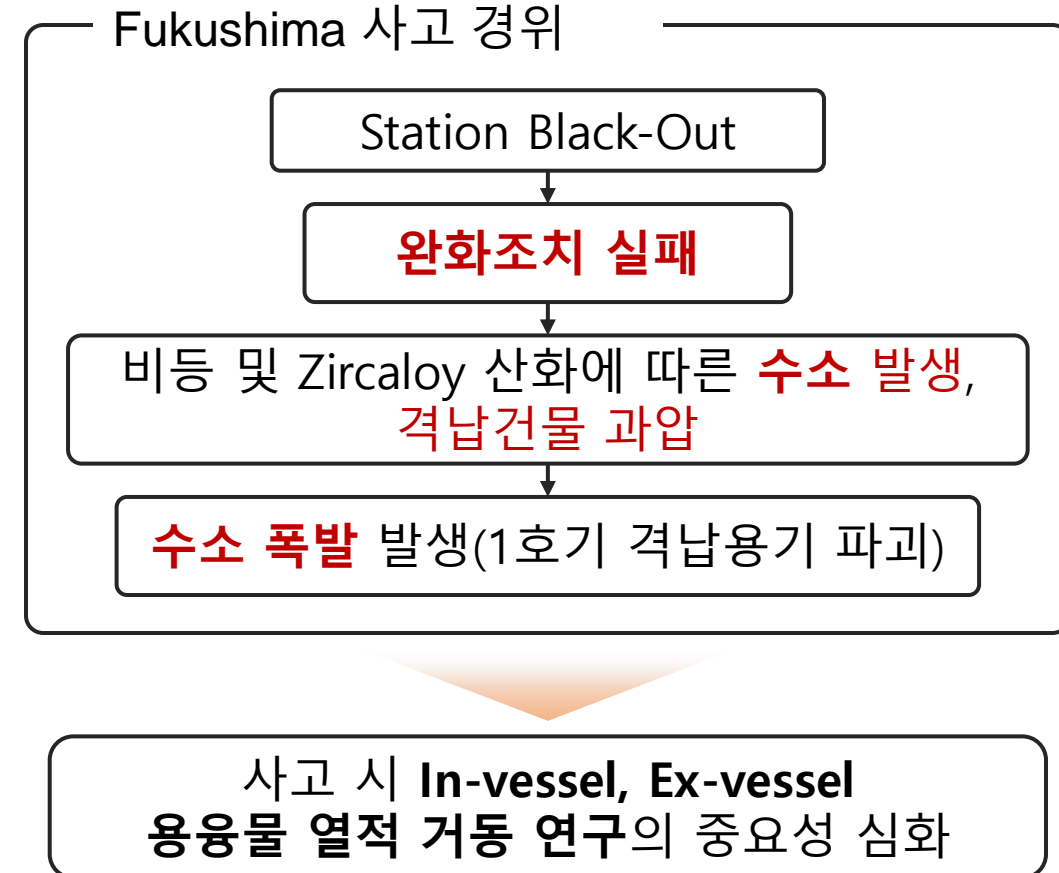
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 - ✓ 상변화(고화 및 용융) 해석 방법론 제안
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- Conclusion



중대사고 해석 연구의 중요성

☑ After Fukushima,.....

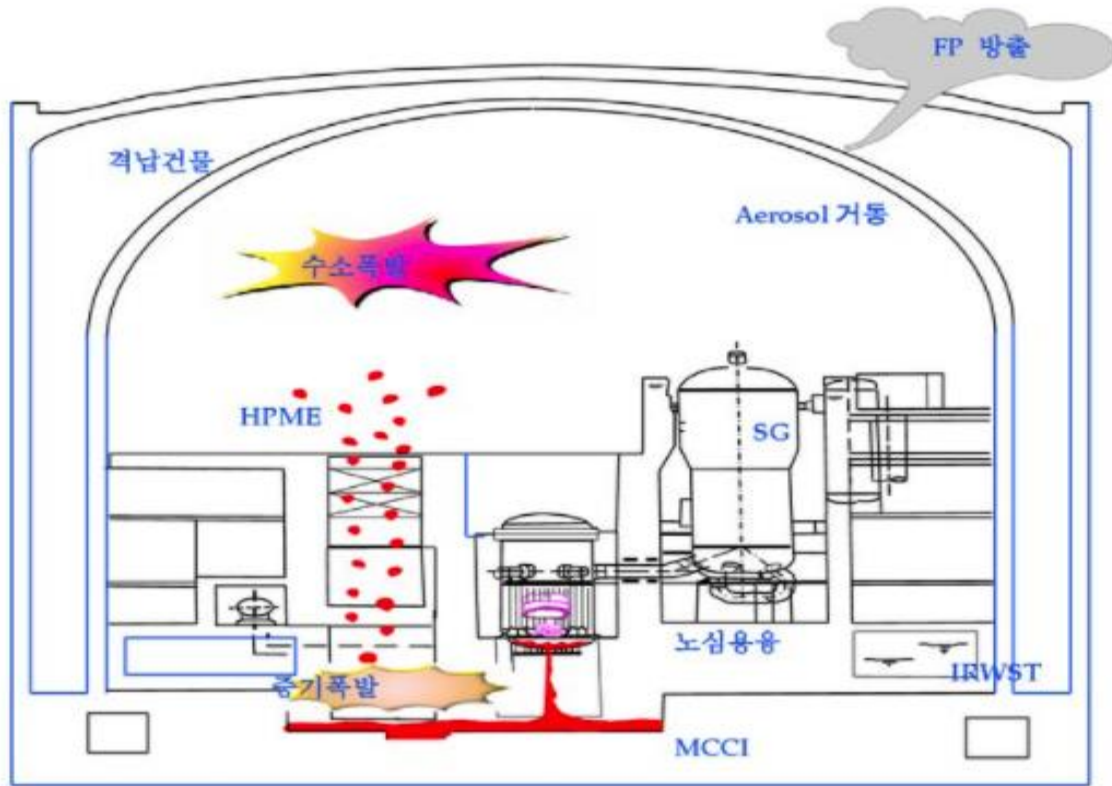
- SBO 사고 완화조치 실패
- 수소 폭발 발생



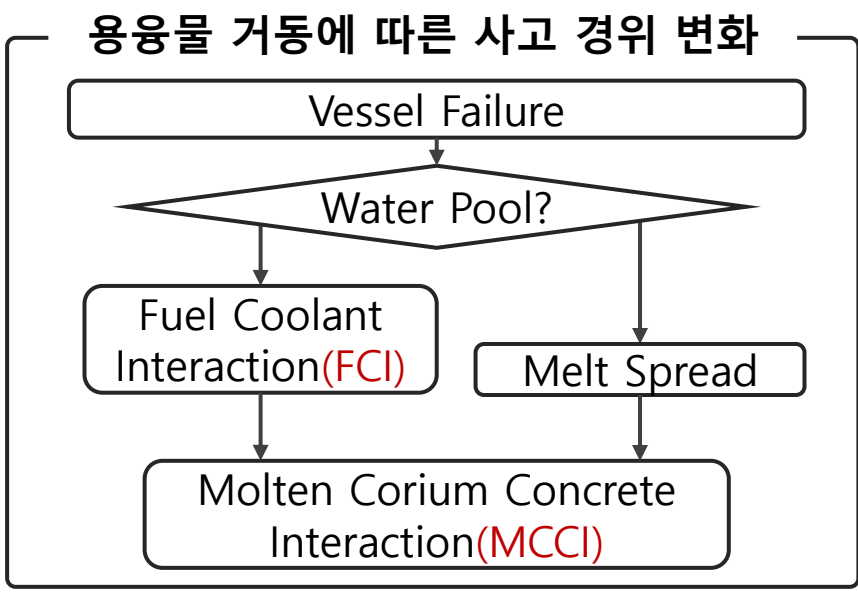
중대사고 해석 연구의 중요성

중대사고 전산 해석 연구

- 중대사고(Severe Accident): 설계 기준사고를 초과하는 사고로서, 심각한 노심손상(용융)을 초래하고 방사성물질의 외부 유출을 억제하는 물리적 방법들의 건전성을 손상시킬 수 있는 사고



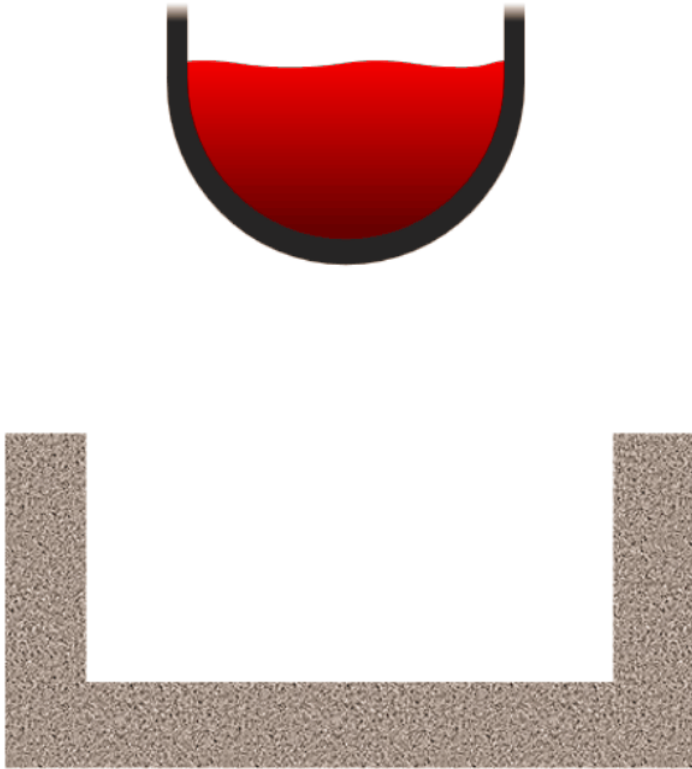
용융물 누설 사고의 가능성



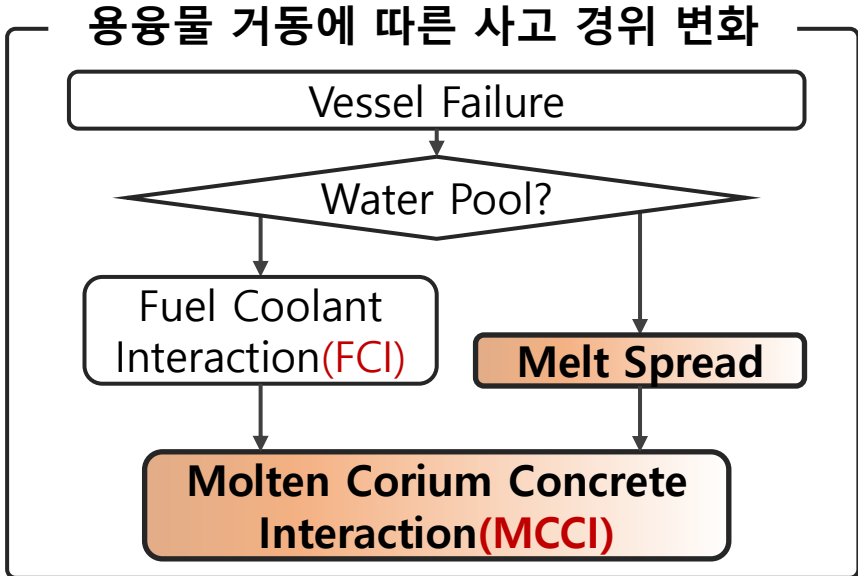
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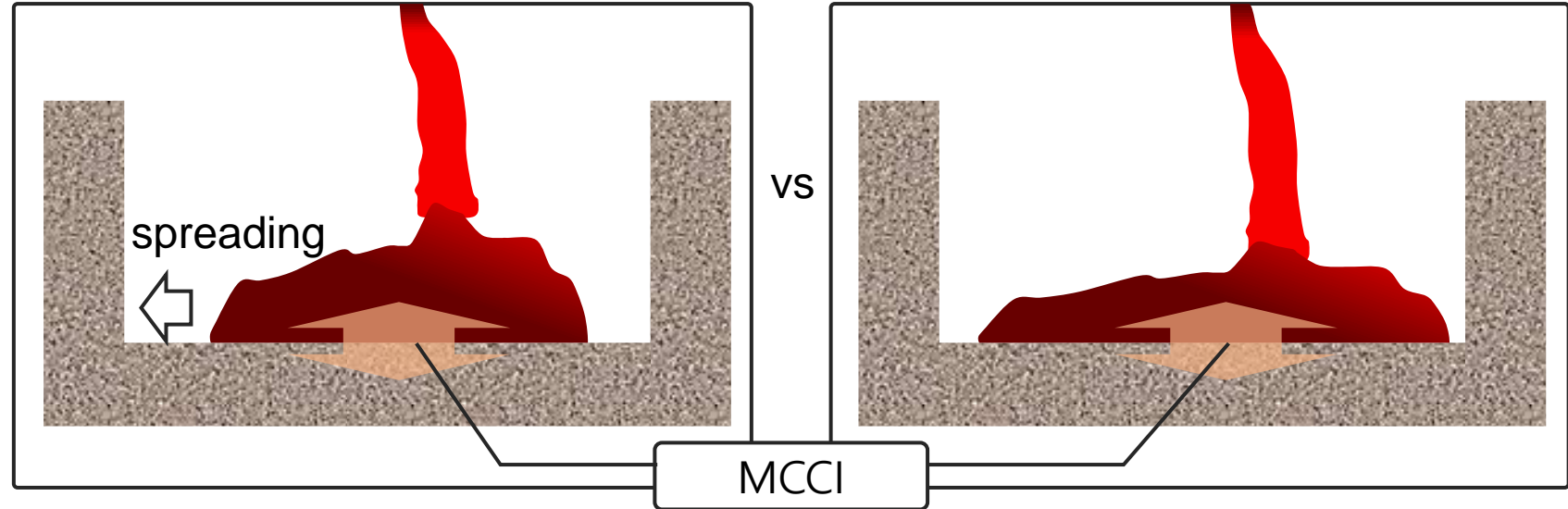
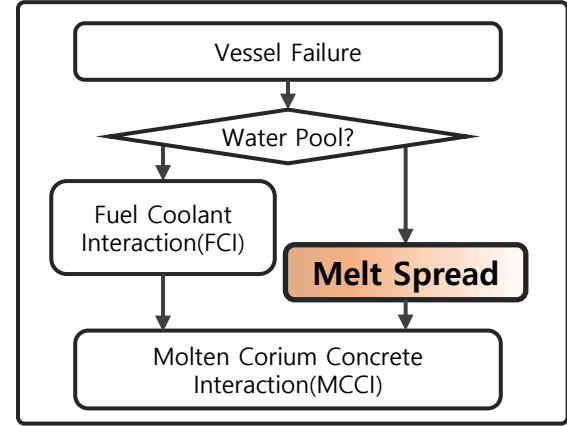
용융물 누설 사고의 가능성



Molten Corium 해석의 중요성

☑ Melt Spread:

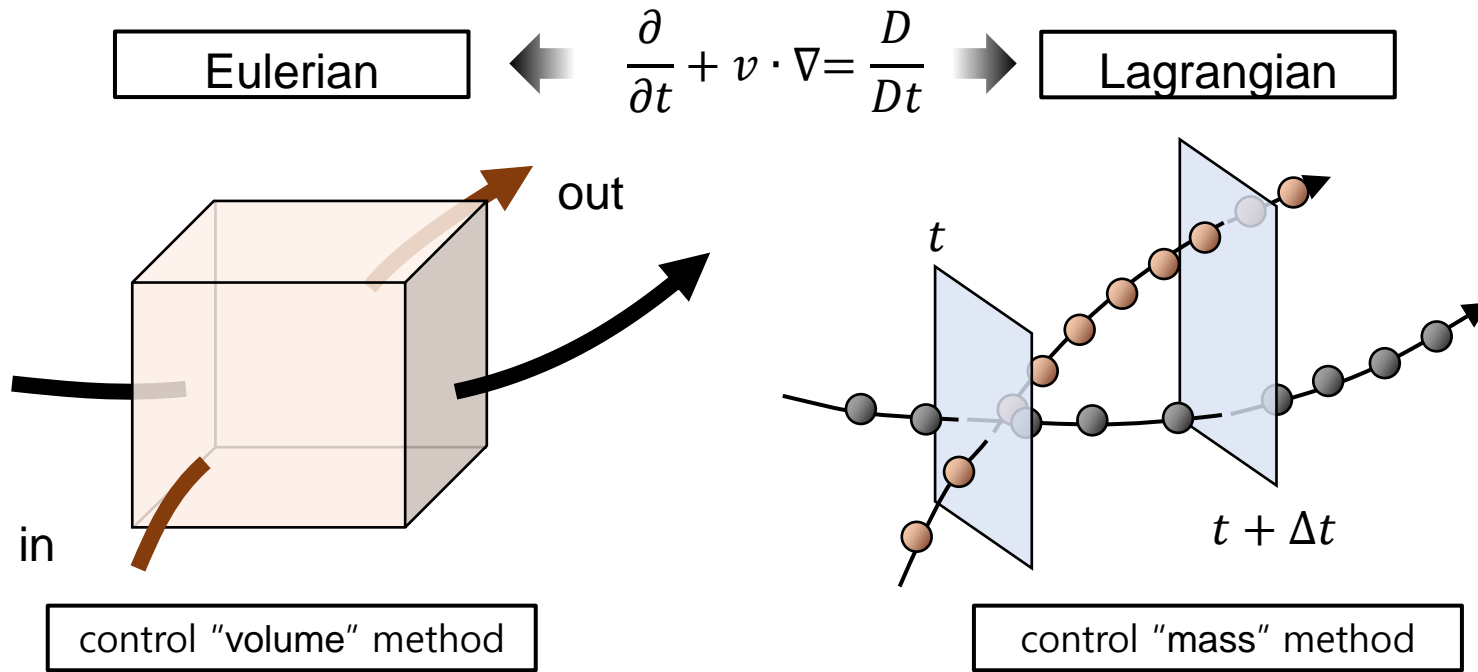
- 용융물 노출 이후 원자로 압력용기 하단 Cavity Pool 에 냉각수가 없을 경우.
- MCCI의 초기 조건으로 사용될 수 있음.



What is Moving Particle Semi-implicit

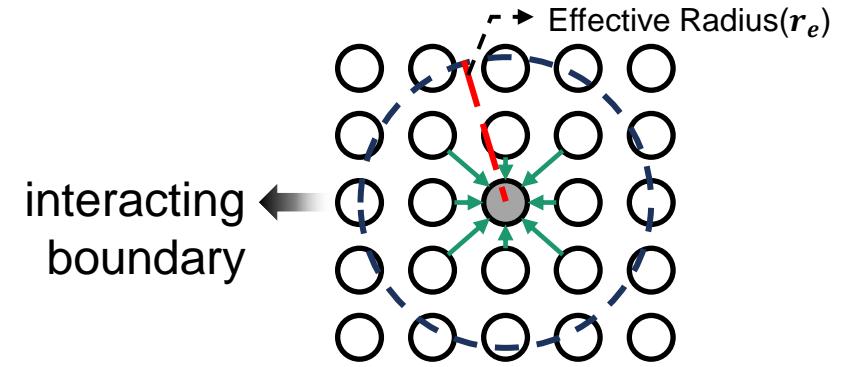
☑ Eulerian 해석과 Lagrangian 해석의 차이

- Control Volume 해석의 관점과 Control Mass 해석의 차이
- 수치모델 구축을 위해 Kernel Function을 활용.

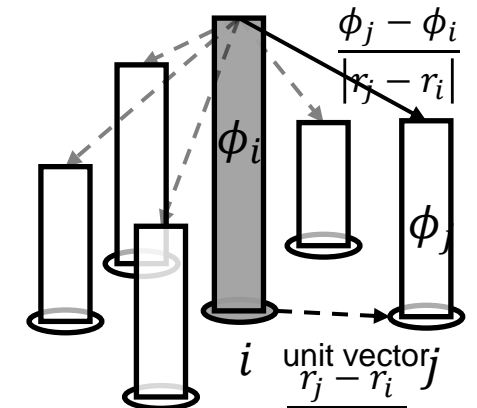


Kernel Function

$$w(r) = \begin{cases} \frac{r_e}{r} - 1 & 0 < r < r_e \\ 0 & r_e < r \end{cases}$$



$\phi = \text{Variable}$
 (ex) Pressure,
 $u_x, u_y,$
 Temperature)



Typical MPS

☑ Governing Equation in MPS

- 상관식이 아닌 가장 기초가 되는 유동 지배 방정식을 이용하여 유체의 유동을 해석

Governing Equation

Continuity Equation:
(Incompressible)

$$\frac{D\rho}{Dt} + \rho \nabla \cdot u = 0$$

Navier Stokes Equation:

$$\frac{Du}{Dt} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 u + g$$

$$\langle \nabla \phi \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \left[\frac{\phi_j - \phi_i}{|r_j - r_i|^2} (r_j - r_i) w(|r_j - r_i|) \right]$$

Numerical Model

Calculate Body Force, Viscous Force

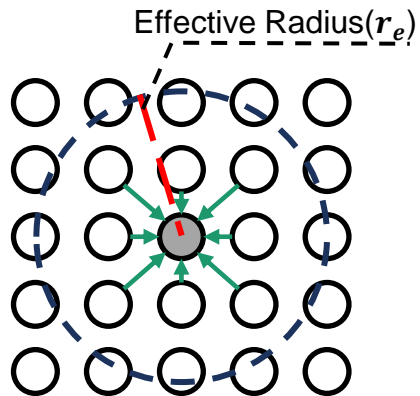
$$u^* = u^t + \Delta t (\nu \nabla^2 u + g)$$

Calculate pressure distribution

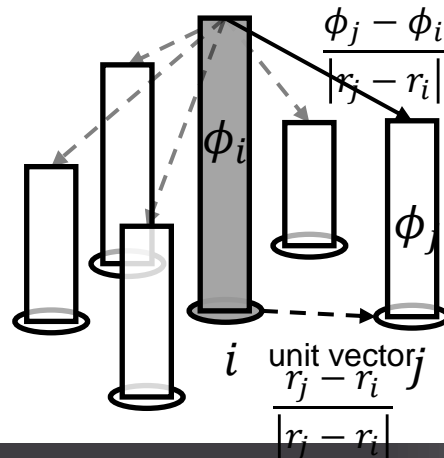
$$\nabla^2 P = \alpha_1 \frac{\rho}{\Delta t} \langle \nabla \cdot u^* \rangle_i + \alpha_2 \frac{\rho}{(\Delta t)^2} \frac{n^* - n^0}{n^0}$$

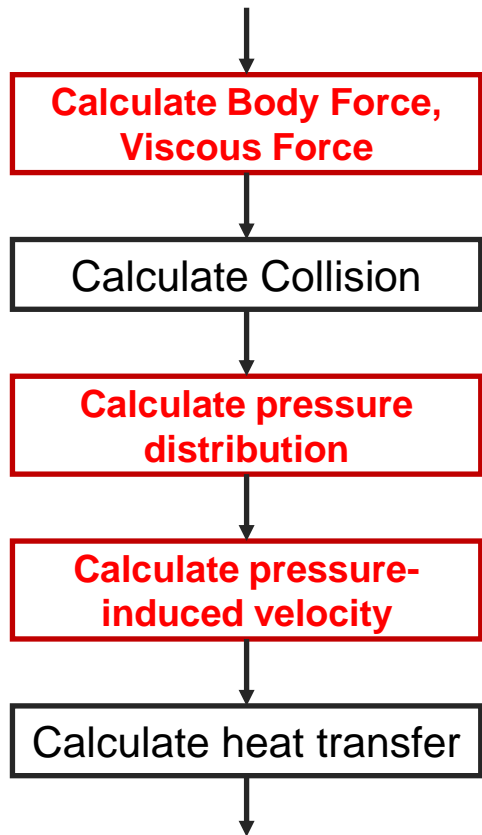
Calculate pressure-induced velocity

$$u^{t+1} = u^* - \frac{\Delta t}{\rho} \nabla P$$



$\phi = \text{Variable}$
(*ex*) Pressure,
 $u_x, u_y,$
Temperature)





Numerical models in Typical MPS

Calculate Body Force, Viscous Force

$$u^* = u^t + \Delta t(v\nabla^2 u + g)$$

Laplacian velocity

$$\left\langle \nabla \cdot \left(\frac{1}{\rho} \nabla u \right) \right\rangle_i^{k+1} = \frac{2d\mu}{\rho n_0 \lambda} \sum (u_j^{k+1} - u_i^{k+1}) w_{ij}$$

Calculate pressure distribution

$$\nabla \cdot u = 0$$

Laplacian Pressure

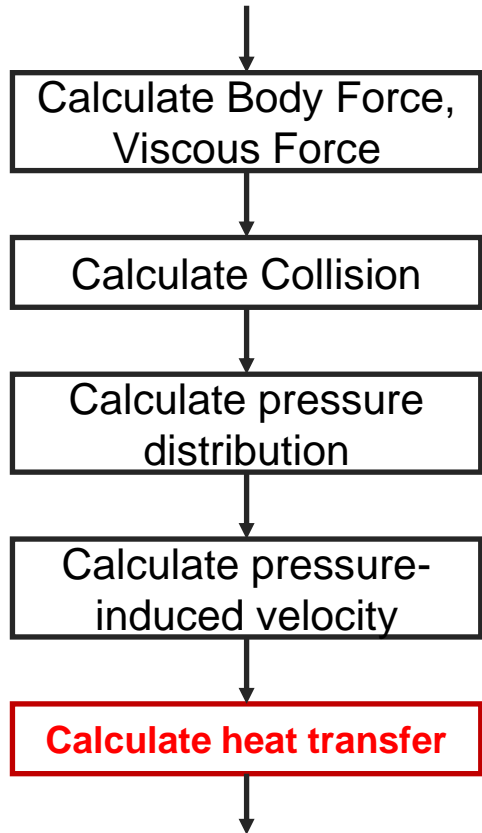
$$\frac{2d\rho}{n_0 \lambda} \sum (P_j^{k+1} - P_i^{k+1}) w_{ij} = \alpha_1 \frac{\rho}{\Delta t} \langle \nabla \cdot u^* \rangle_i + \alpha_2 \frac{\rho}{(\Delta t)^2} \frac{n^* - n^0}{n^0}$$

Calculate pressure-induced velocity

$$u^{t+1} = u^* - \frac{\Delta t}{\rho} \nabla P$$

Gradient Pressure

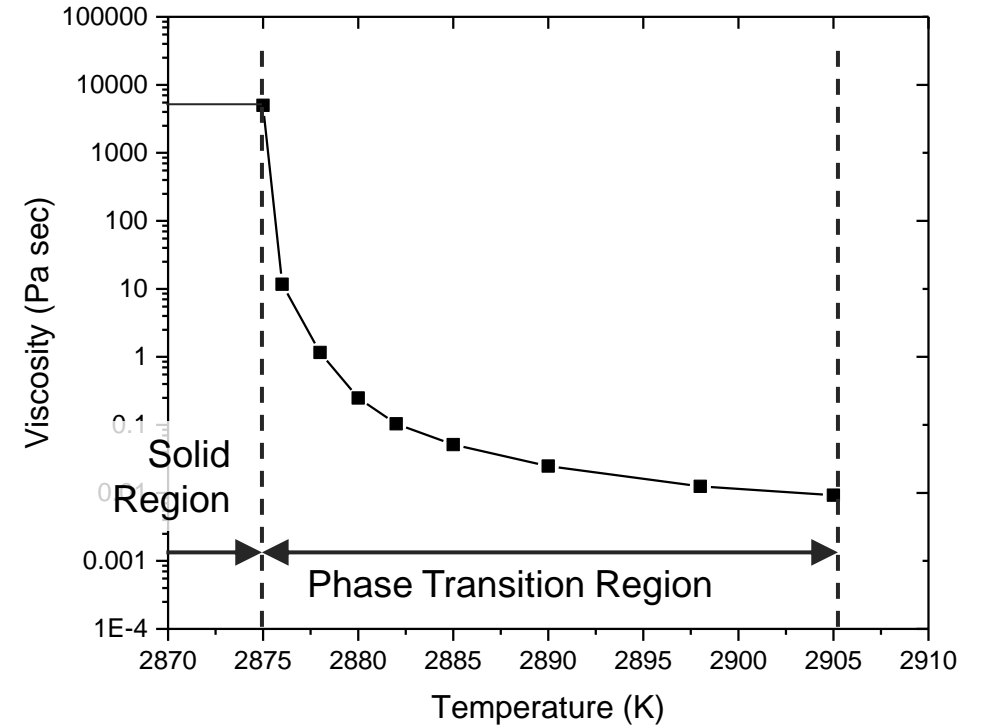
$$\left\langle \frac{1}{\rho} \nabla P \right\rangle_i^{k+1} = \alpha \frac{1}{\rho n_0} \sum \frac{(P_j^{k+1} - P_i^{k+1})(r_j - r_i)}{|r_j - r_i|^2} w_{ij}$$



Phase Change model in Typical MPS

$$T = \begin{cases} T_m + \frac{H - H_{latent}}{\rho C_p} & H > H_{latent} \\ T_m & 0 < H < H_{latent} \\ T_m + \frac{H}{\rho C_p} & H < 0 \end{cases}$$

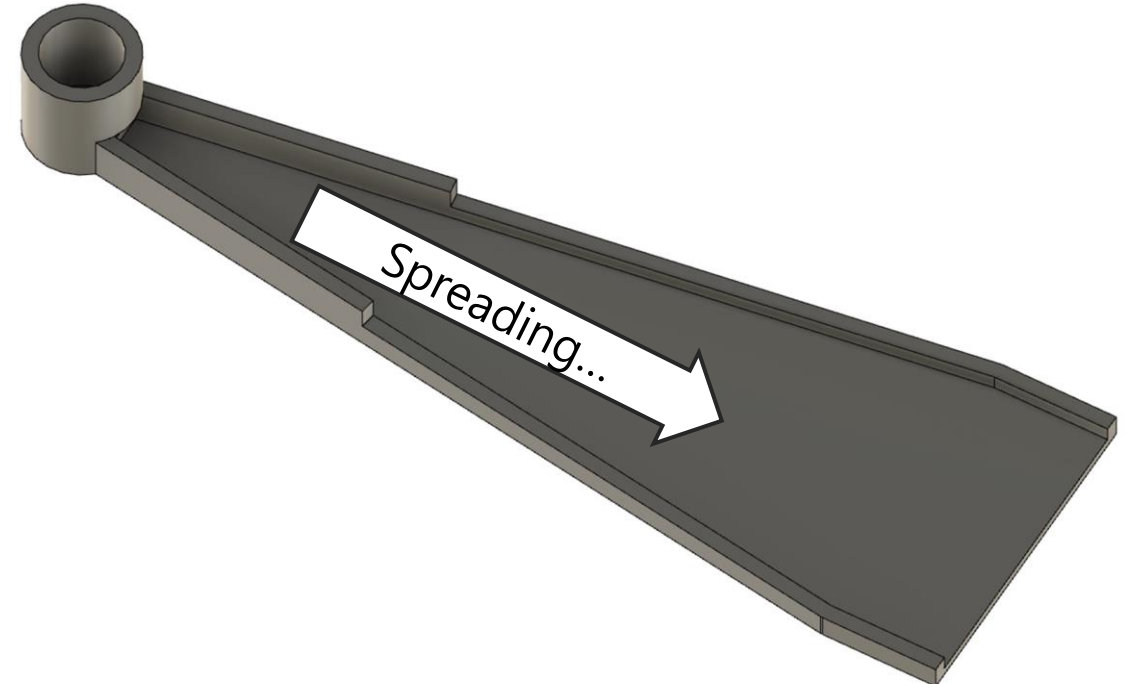
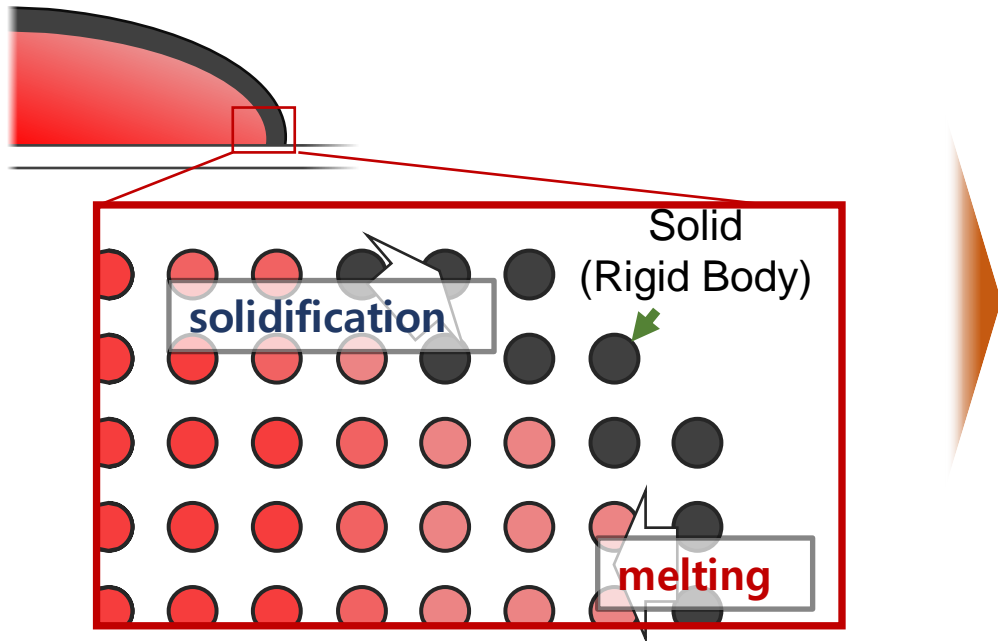
Enthalpy에 따른 입자 온도 계산 및 상 결정

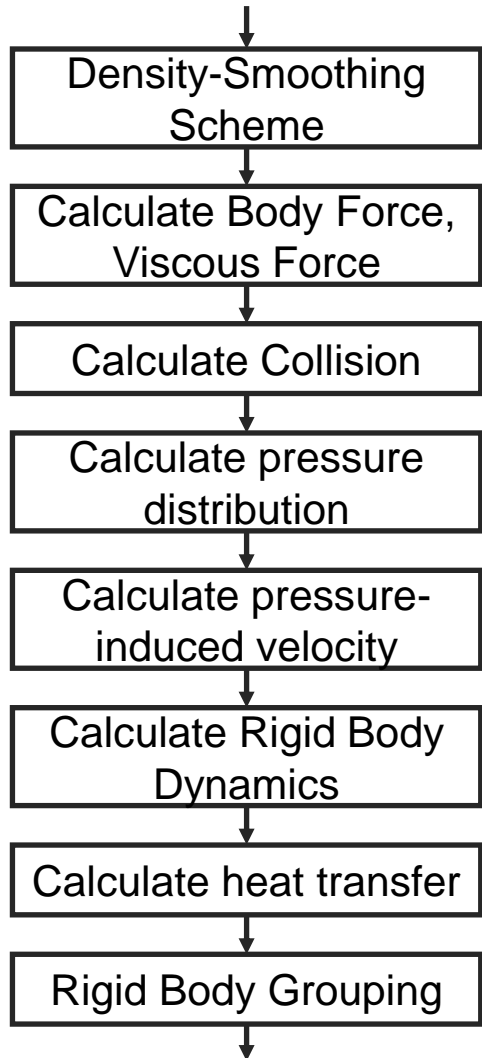


계산 편의를 위해 고체 영역은 점도가 매우 큰 유체로 해석

Objective

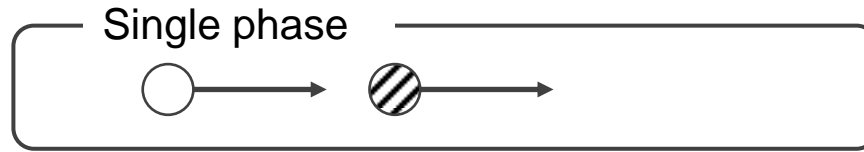
- ☑ 다상유동 및 상변화 해석 알고리즘 구축
 - 다상 유동 해석에 활용 가능한 적절한 모델 선정
 - 용융물 상변화 해석에 활용하기 위한 적절한 방법론 개발
- ☑ 대표 Corium 해석 예인 FARO 실험 해석을 통한 모델 검증 및 비교 분석





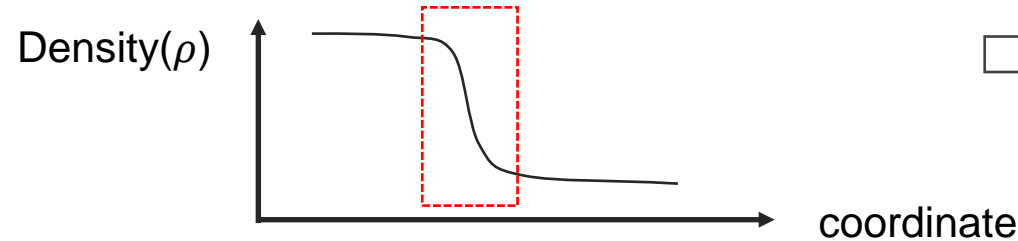
Multi-phase MPS

In Single phase condition

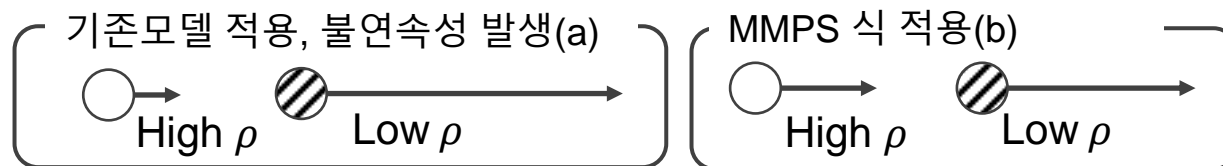


Single Phase 계산(동일 Property) 내에서는 인접한 입자끼리 상호작용 시 **연속적인 속도장이 형성**

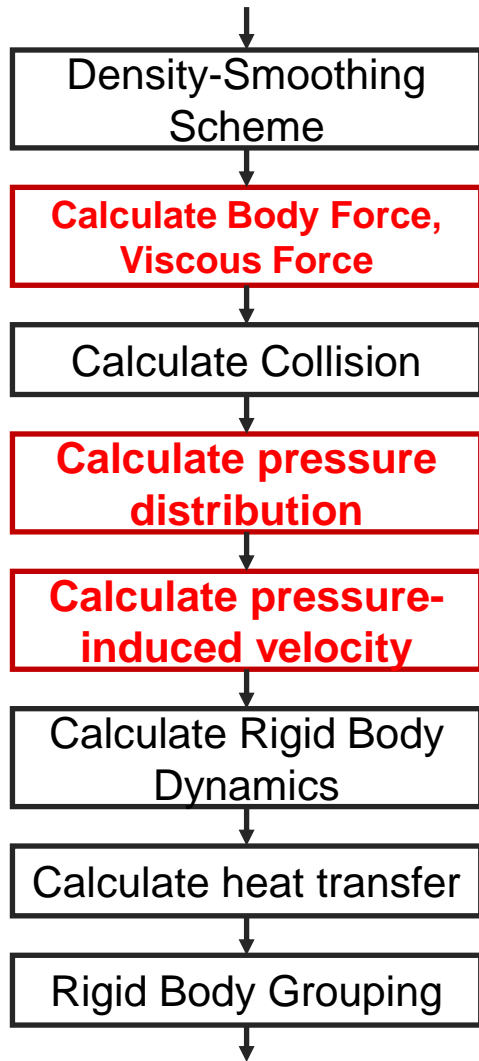
In Multi-phase condition or Temperature-dependent property, simulation with structure(wall)



인접한 두 입자간 밀도차가 크게 나타날 경우, **큰 밀도차에 의해 불연속적인 속도** 분포가 나타남 (가속도 \propto 힘(= 압력차)/밀도)



불연속성을 상쇄



Multi-phase MPS

Laplacian velocity

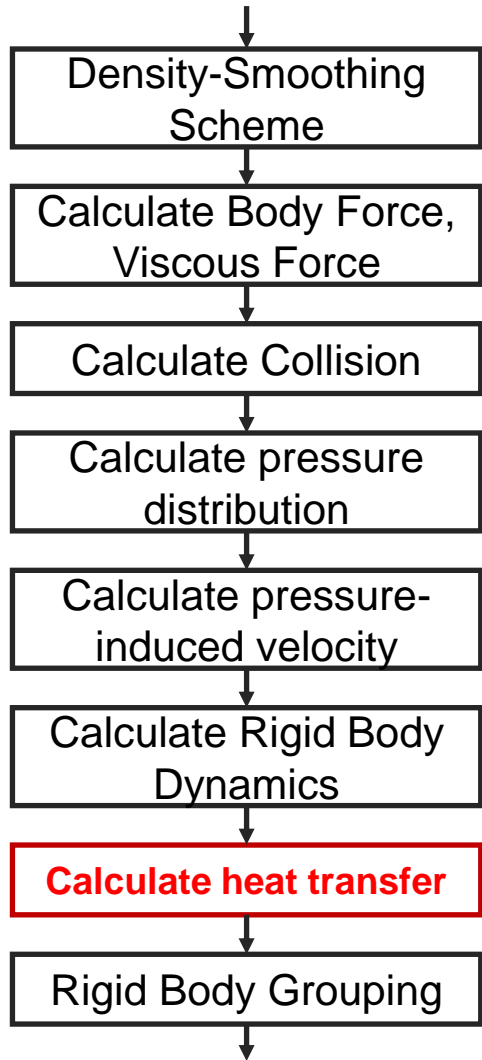
$$\left\langle \nabla \cdot \left(\frac{1}{\rho} \nabla u \right) \right\rangle_i^{k+1} = \frac{2d}{n_0 \lambda} \sum \frac{2\mu_i \mu_j}{\mu_i + \mu_j \hat{\rho}_i + \hat{\rho}_j} \frac{2}{2} (u_j^{k+1} - u_i^{k+1}) w_{ij}$$

Laplacian Pressure

$$\frac{2d}{n_0 \lambda} \sum \frac{\hat{\rho}_i + \hat{\rho}_j}{2\hat{\rho}_i \hat{\rho}_j} (P_j^{k+1} - P_i^{k+1}) w_{ij} = \alpha_1 \frac{\rho}{\Delta t} \langle \nabla \cdot u^* \rangle_i + \alpha_2 \frac{\rho}{(\Delta t)^2} \frac{n^* - n^0}{n^0}$$

Gradient Pressure

$$\left\langle \frac{1}{\rho} \nabla P \right\rangle_i^{k+1} = \alpha \frac{d}{n_0} \sum \frac{2}{\hat{\rho}_i + \hat{\rho}_j} \frac{(P_j^{k+1} - P_i^{k+1})(r_j - r_i)}{|r_j - r_i|^2} C_{ij} w_{ij} + (1 - \alpha) \frac{d}{n_0} \sum \frac{1}{\hat{\rho}_i} \frac{(P_j^{k+1} - P_i^{k+1})(r_j - r_i)}{|r_j - r_i|^2} C_{ij} w_{ij}$$



Heat transfer calculation

Heat transfer model in multi-properties condition

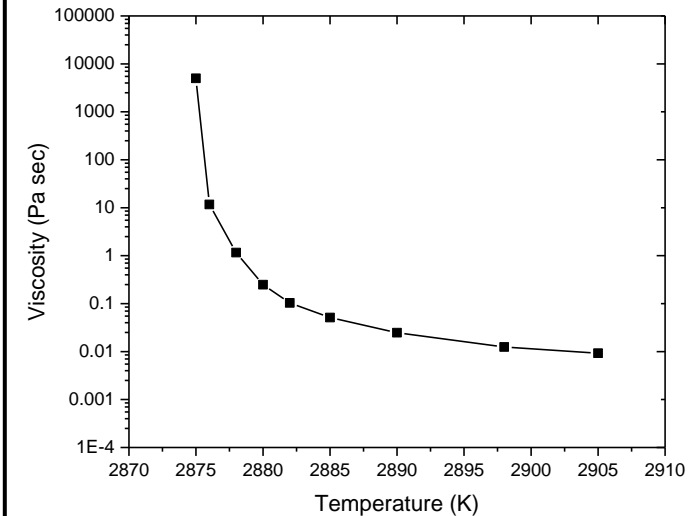
$$H_i^{t+1} = H_i^t + \Delta t \frac{2d}{n_0 \lambda} \sum \frac{2k_i k_j}{k_i + k_j} (T_j^{k+1} - T_i^{k+1}) w_{ij}$$

Boundary Condition(Radiative Heat Transfer)

$$Q = \varepsilon \sigma A T_i^4 \quad A = 6 \left(1 - \frac{n_i}{n_0} \right) l_0^2$$

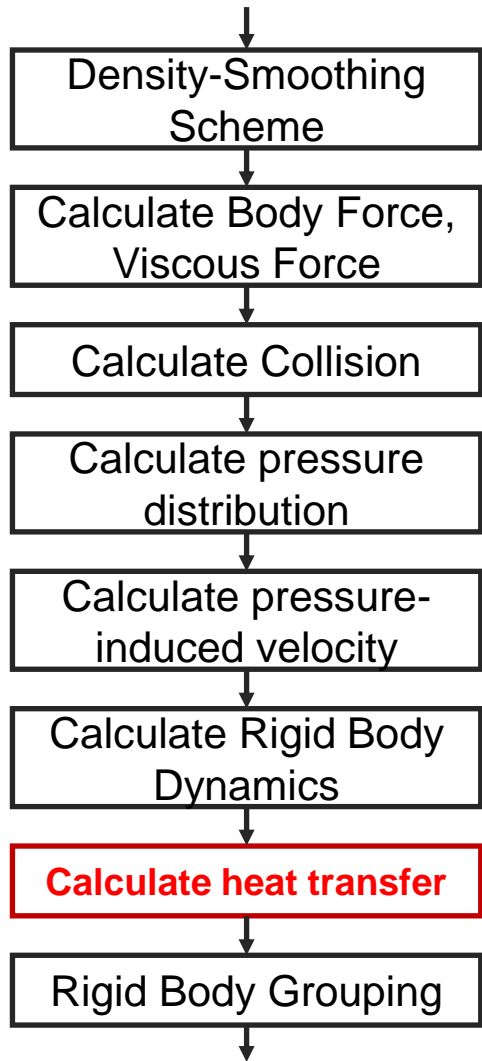
$$\varepsilon(\text{emissivity}) = 0.2 \quad \sigma(\text{Stefan-Boltzmann const}) = 5.67\text{E-}8$$

Multi-viscosity above melting temperature

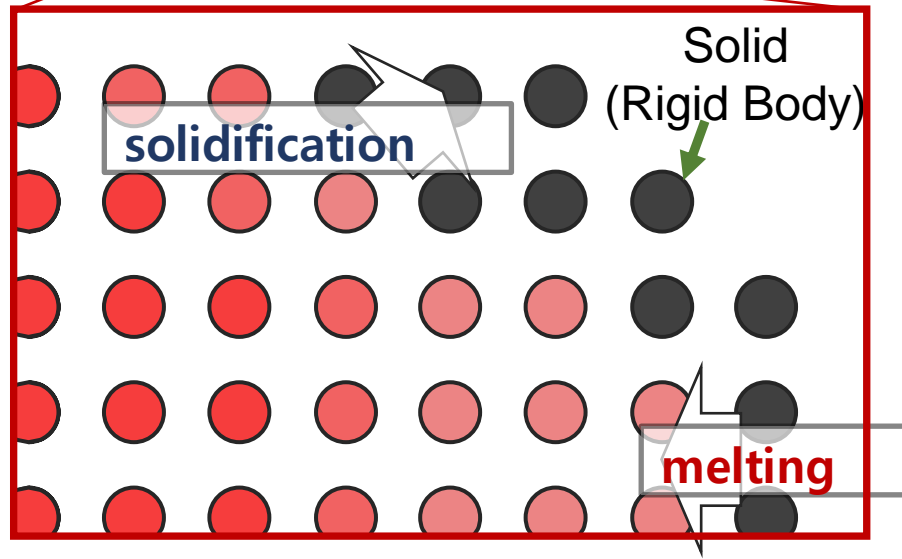
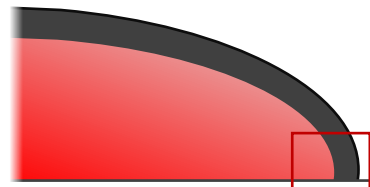


Linearly interpolated

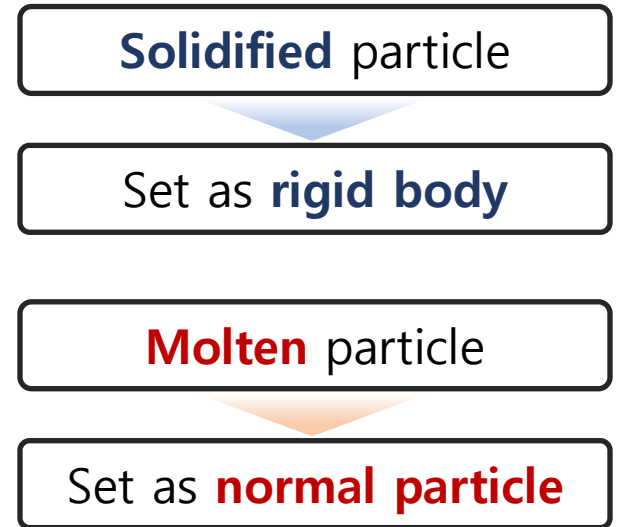
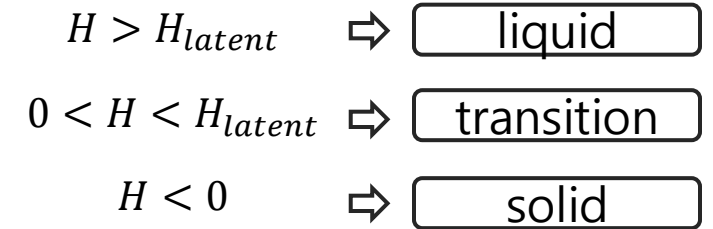
Construction of Phase Change Algorithm



열전달 해석 결과를 반영한 고화 층 조성



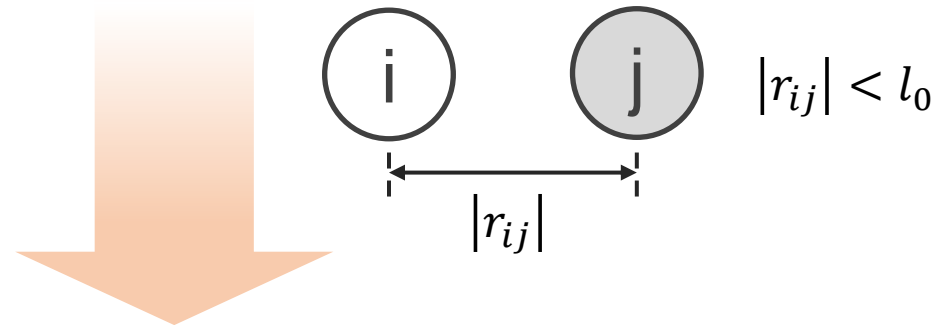
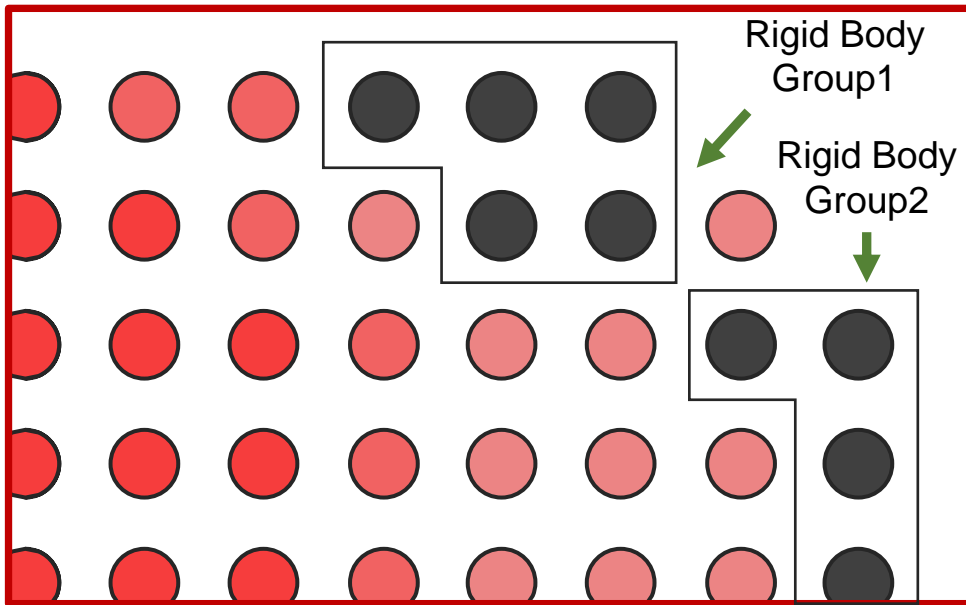
$$T = \begin{cases} T_m + \frac{H - H_{latent}}{\rho C_p} & H > H_{latent} \\ T_m & 0 < H < H_{latent} \\ T_m + \frac{H}{\rho C_p} & H < 0 \end{cases}$$



상변화 해석을 위한 고화 층 그룹화

☑ Rigid Body 계산을 수행하기 위해 각 Solid 입자들에 대한 그룹화를 수행

- **Rigid body sticking distance** 정의: 하나의 Rigid Body Group이 유지되는 최소 거리($1.1l_0$)
- **Rigid body sticking rules**: 이웃 입자가 아래 조건을 만족할 시, 같은 group으로 정의함.

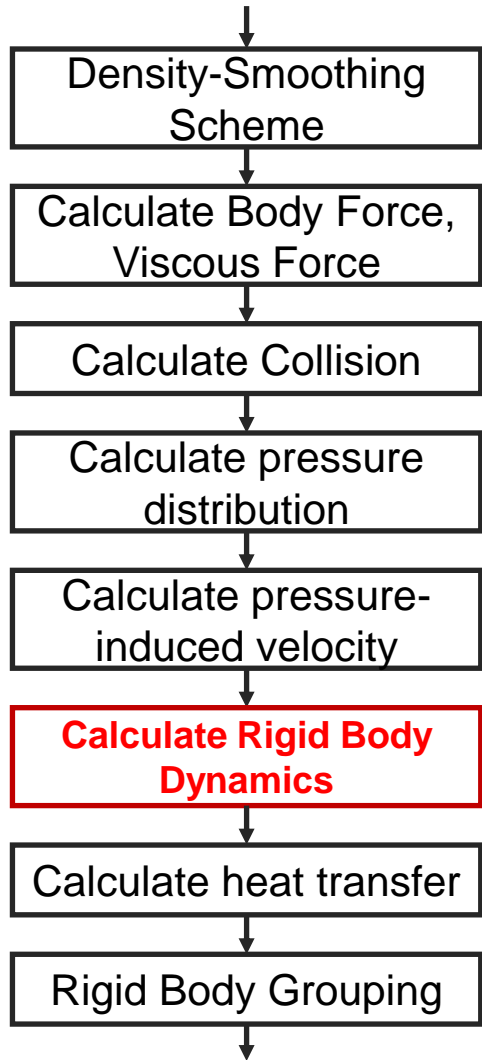


Rule. 0: 대상 입자와 이웃입자가 **모두 Solid 입자임**

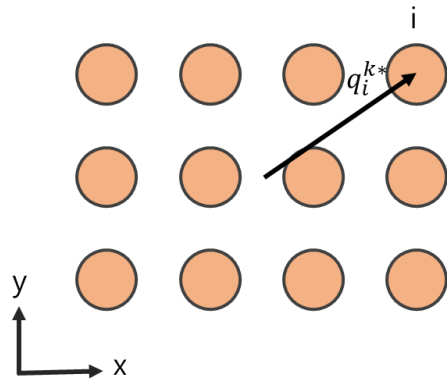
Rule. 1: 대상 입자(i)가 이번 timestep 에서 액체에서 고체로 고화된 경우

Rule. 2: 이웃 입자(j)이 이번 timestep 에서 액체에서 고체로 고화된 경우

Rule. 3: 대상 입자(i)와 이웃 입자(j)가 이전 timestep 에서 또한 같은 group이었을 경우



Rigid Body Dynamics Calculation



Rigid Body 평균 좌표 및 속도 계산

$$r_g = \frac{1}{N} \sum_i r_i$$

$$q_i^{k*} = r_i - r_g$$

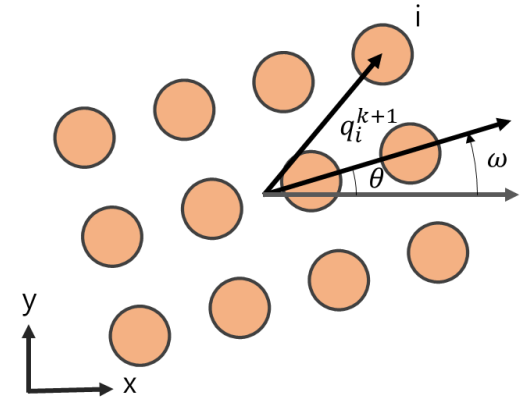
$$u_g = \frac{1}{N} \sum_i u_i^{k*}$$

회전관성을 통한 Rigid Body 회전량 계산

$$\omega = \frac{1}{I} \sum_i q_i^{k*} \times u_i$$

$$I = \sum_i |q_i^{k*}|^2$$

$$\frac{d\theta}{dt} = \omega$$



Rigid Body 속도 수정

$$u_i^{k+1} = u_g + q_i^{k*} \times \omega$$

$$q_i^{k+1} = R(\theta) q_i^{k*}$$

Calculation Condition

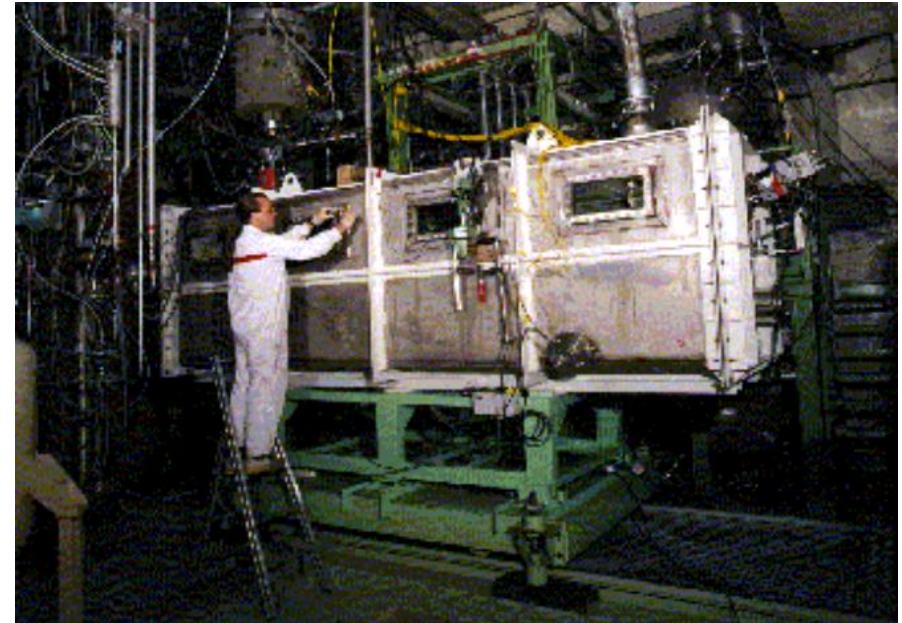
Schematics of FARO-L26S

☑ Schematics of FARO facility

- FARO(Furnace And Release Oven) program: A large **multi-purpose test facility** in which several phenomena can be studied under **simulated accident conditions in IAEA at 1987~1989**
- The FARO Program include “Melt spreading in Dry or Wet substrate”, “Quenching”, “Fuel Coolant Interaction(FCI)”, etc...



FARO Facility:
the FAT test vessel for melt quenching experiments

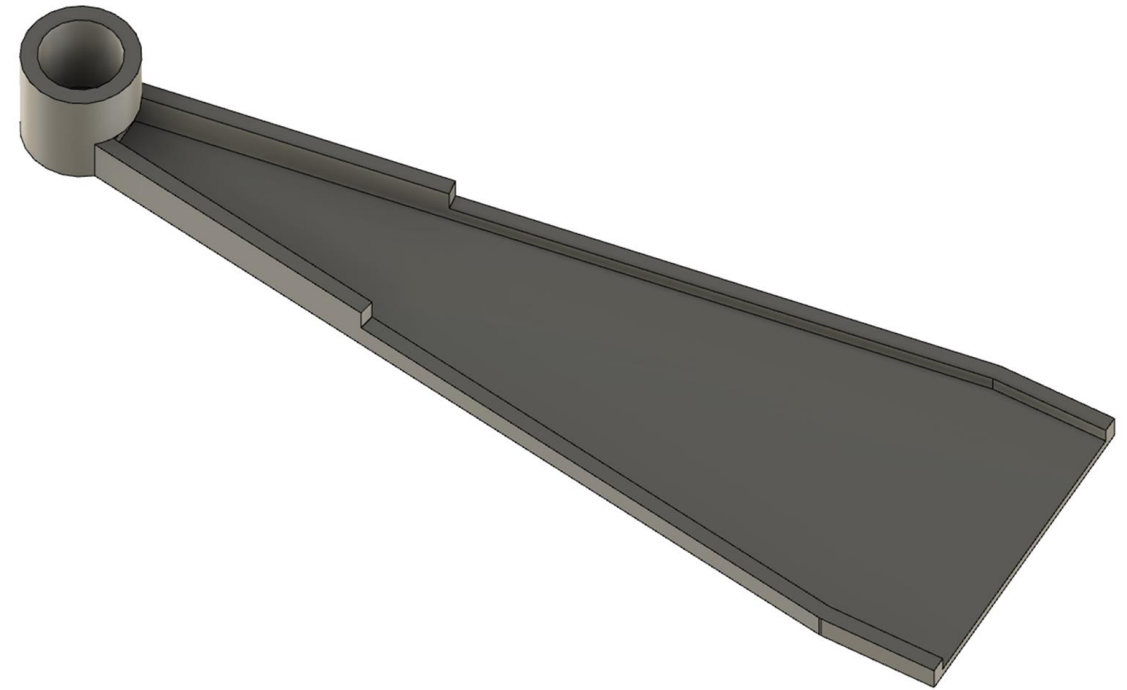
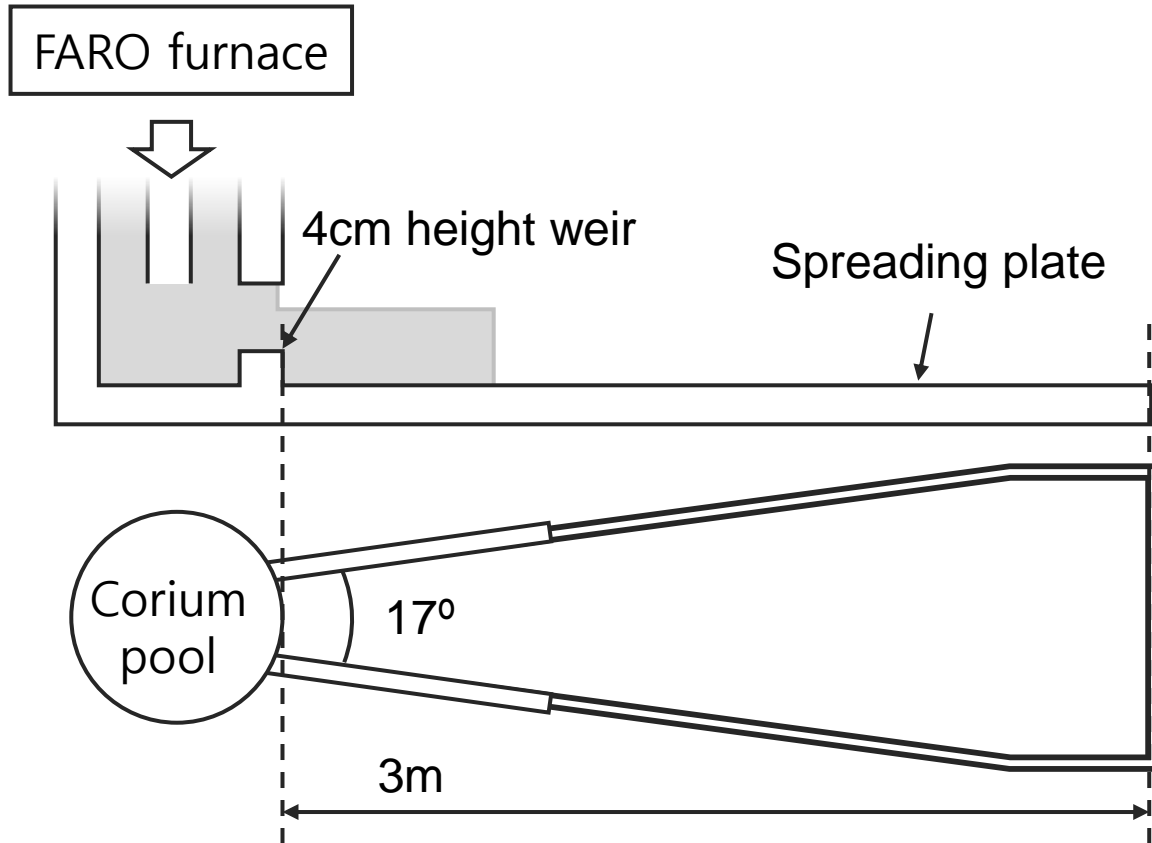


FARO Facility:
the SARCOFAGO test vessel for melt spreading experiments

Calculation Condition

Schematics of FARO-L26S

☑ Schematics of FARO-L26S experiment



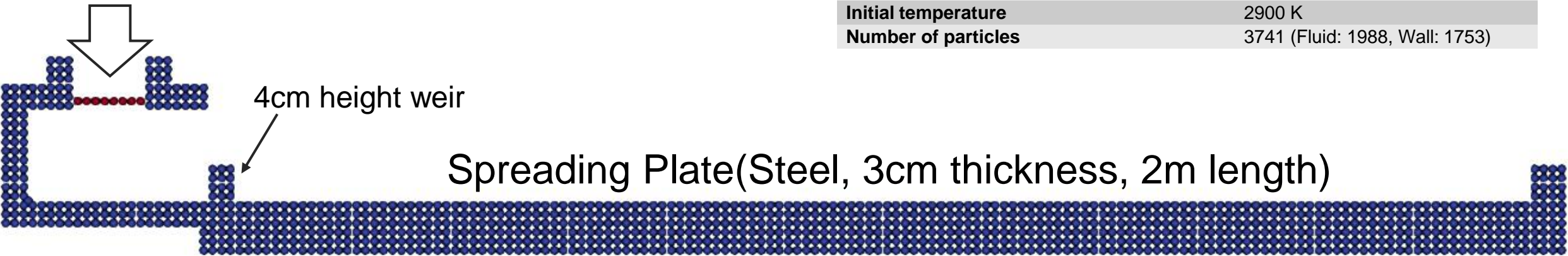
Calculation Condition

Melt Spread Calculation in FARO facility

☑ Calculation Condition

- Injected mass flow rate : 160.3kg/sec
- Injected velocity: 0.17m/sec
- Initial temperature: 2900K

주입 경계조건 적용(160.3kg/sec Corium)



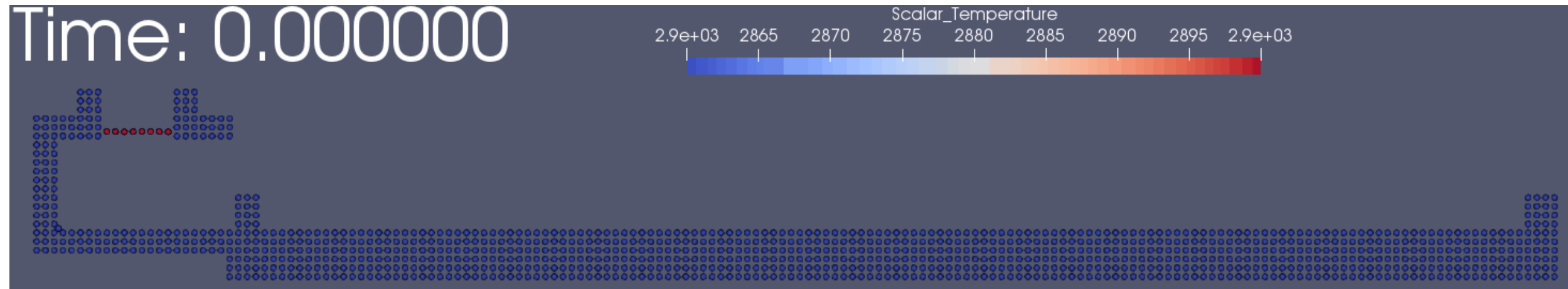
Property	
Composition	UO ₂ /ZrO ₂ (80/20 weight percent)
Density	8000 kg/m ³
Thermal Conductivity	3.0 W/m K
Heat Capacity	0.5 J/kgK
Latent Heat	3.0 kJ/m ³
Effective radius Factor	
Number density calculation (n_0 or n_i)	3.1
Gradient calculation ($\nabla\phi$)	3.1
Laplacian viscosity calculation ($\nu\nabla^2u$)	4.0
Laplacian pressure calculation (∇^2P)	4.0
Laplacian temperature calculation (∇^2T)	3.6
Free surface threshold (β)	0.95
Initial temperature	2900 K
Number of particles	3741 (Fluid: 1988, Wall: 1753)

Calculation Result

Melt Spread Calculation in FARO facility

☑ Calculation Result

- Number of particle: (Gradually increasing) 1099 at 0sec, 2352 at 16sec
- Computation Time: about 18.7hr for 16sec(current time)
- Computation Environment: GPU Tesla A100*3ea

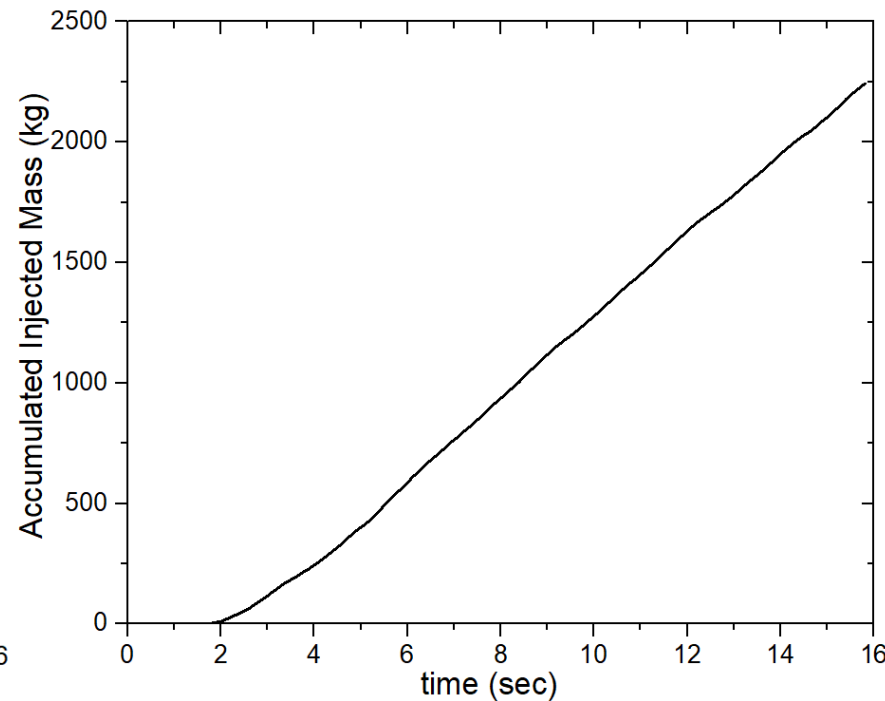
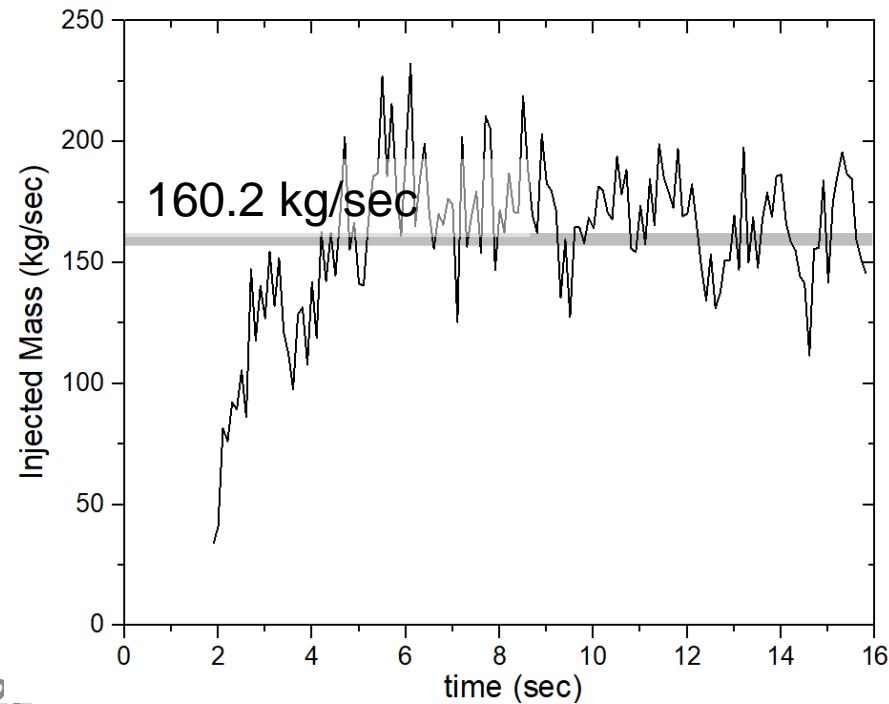
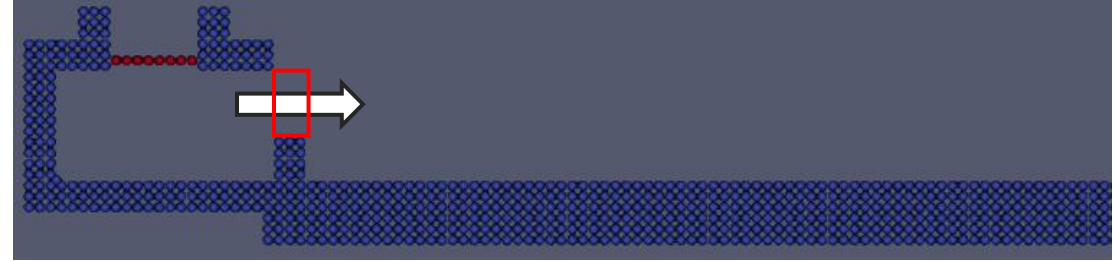


Calculation Result

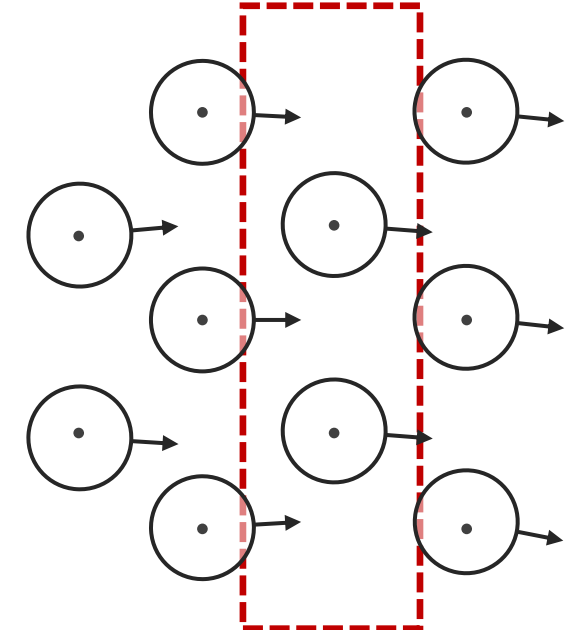
Melt Spread Calculation in FARO facility

Analysis of Calculation Result

- 기판(Steel Substrate)로의 진입 유량



Example)



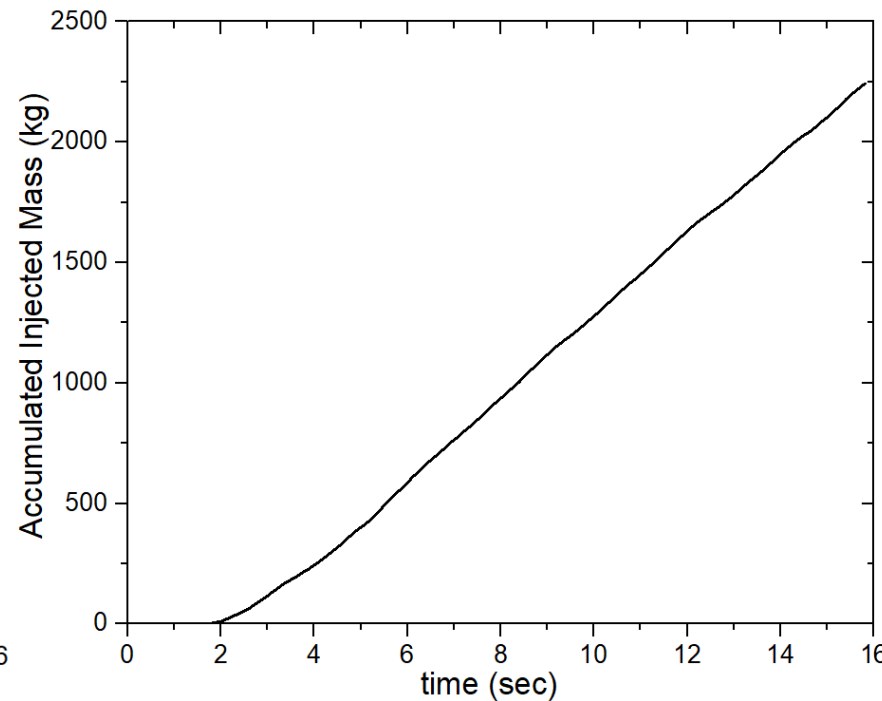
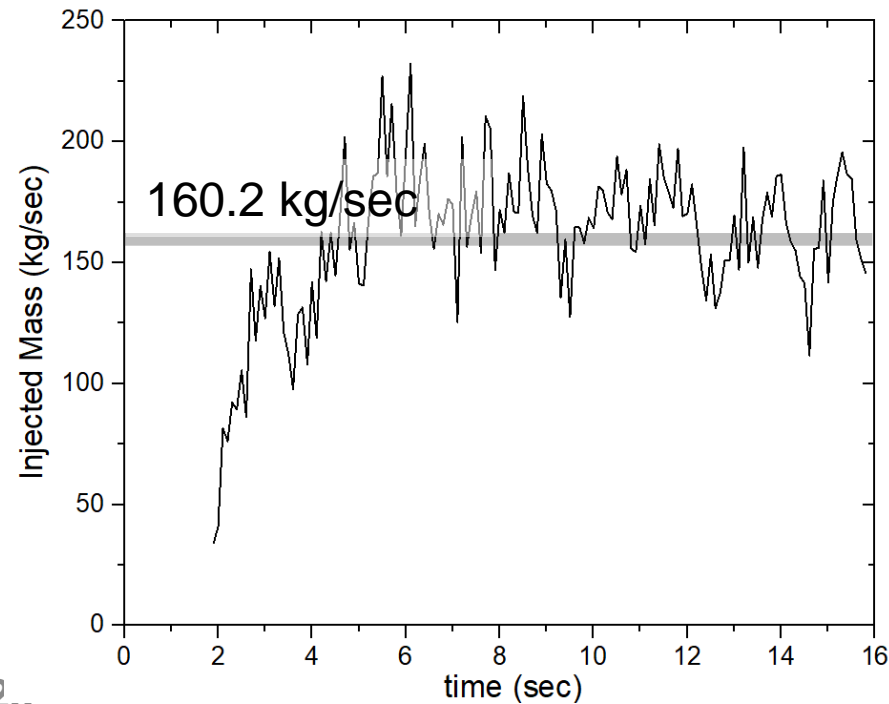
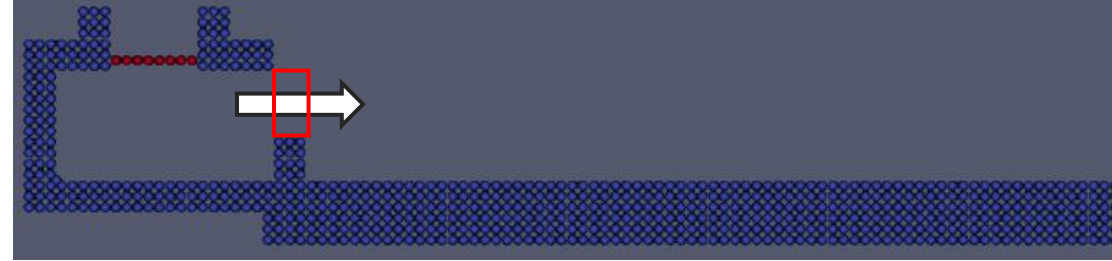
Number of particle in
Control volume = 2

Calculation Result

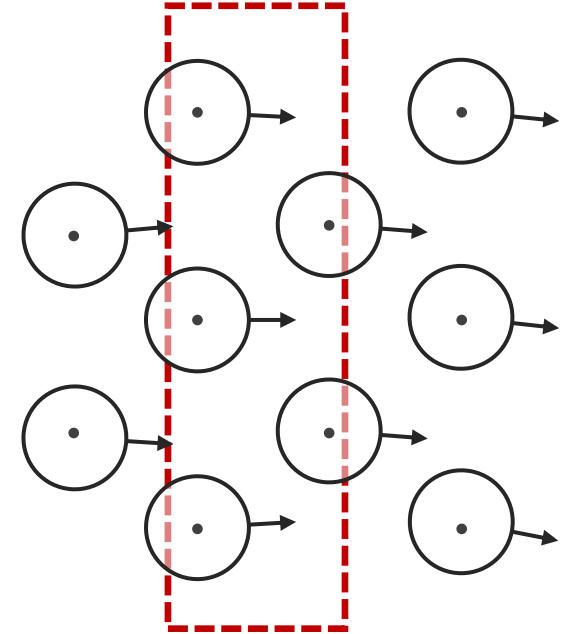
Melt Spread Calculation in FARO facility

Analysis of Calculation Result

- 기판(Steel Substrate)로의 진입 유량



Example)



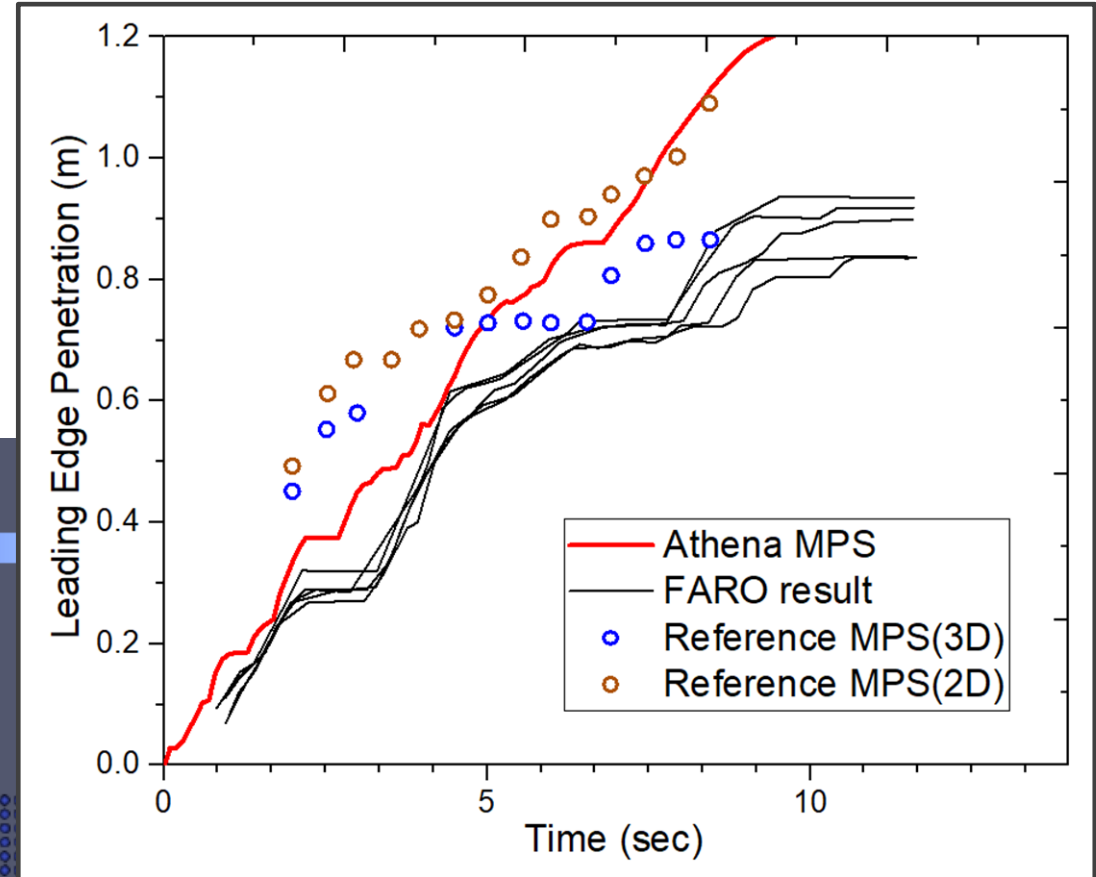
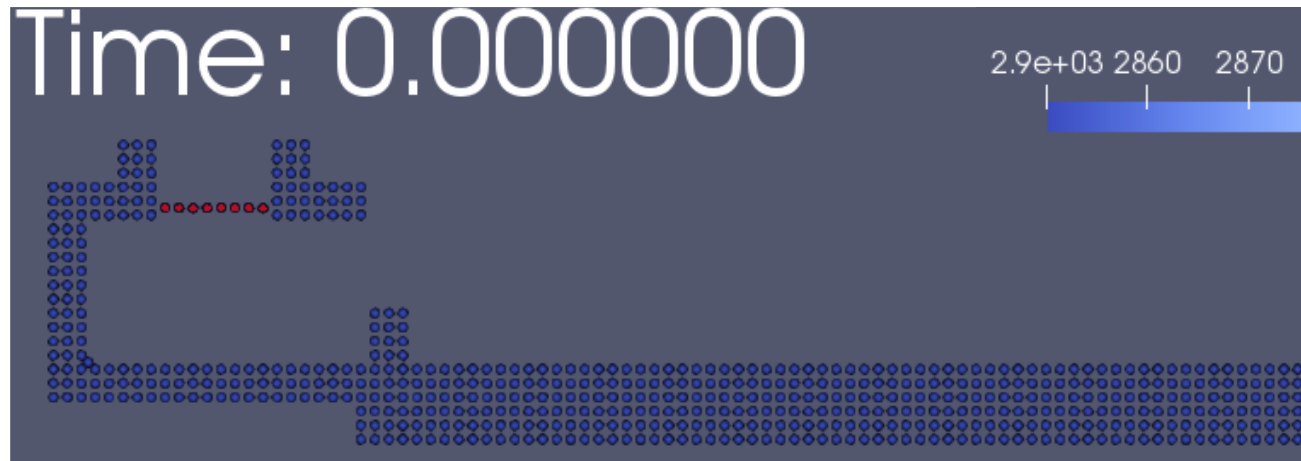
Number of particle in Control volume = 5

Calculation Result

Melt Spread Calculation in FARO facility

Analysis of Calculation Result

- Leading Edge Penetration:
용융물의 전진 거리, 기판 위에서의 이동 거리

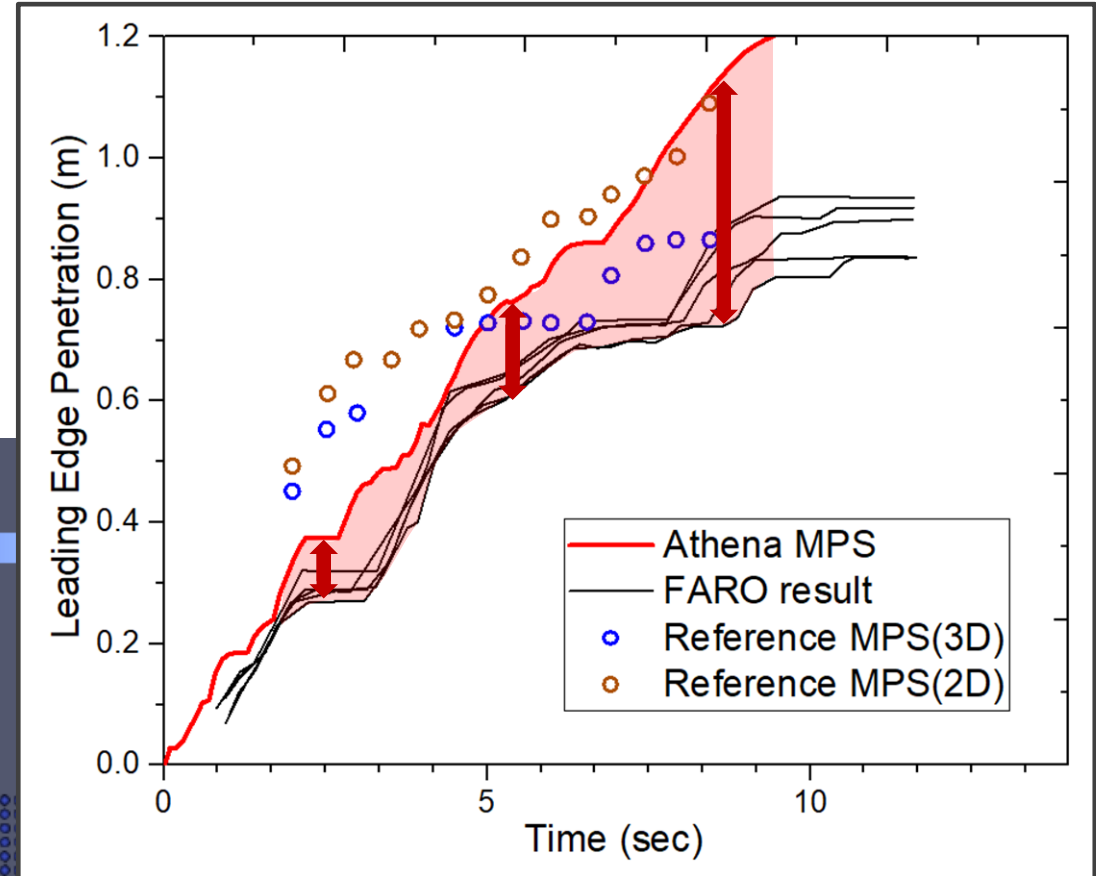
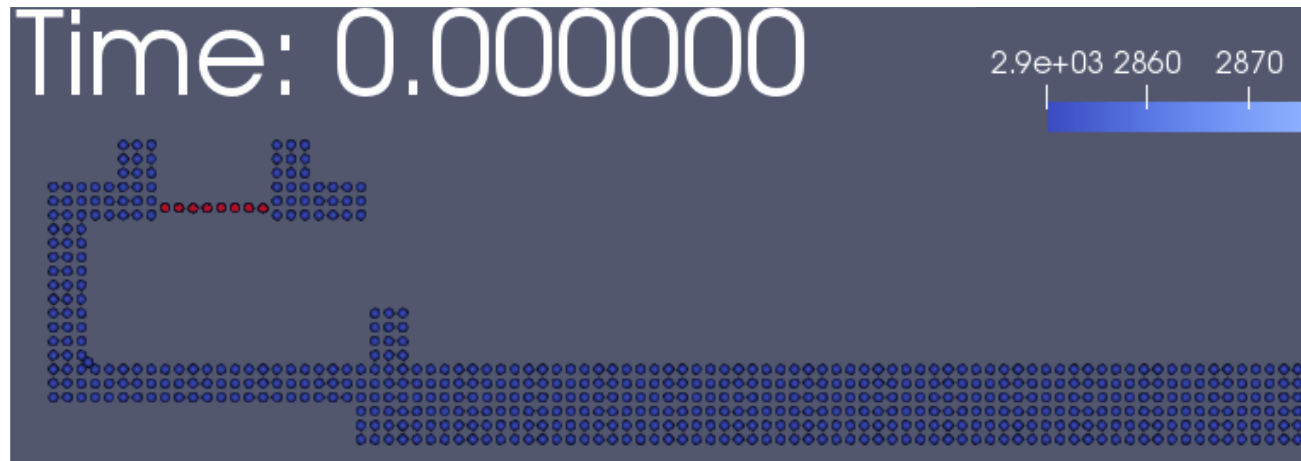


Calculation Result

Melt Spread Calculation in FARO facility

Analysis of Calculation Result

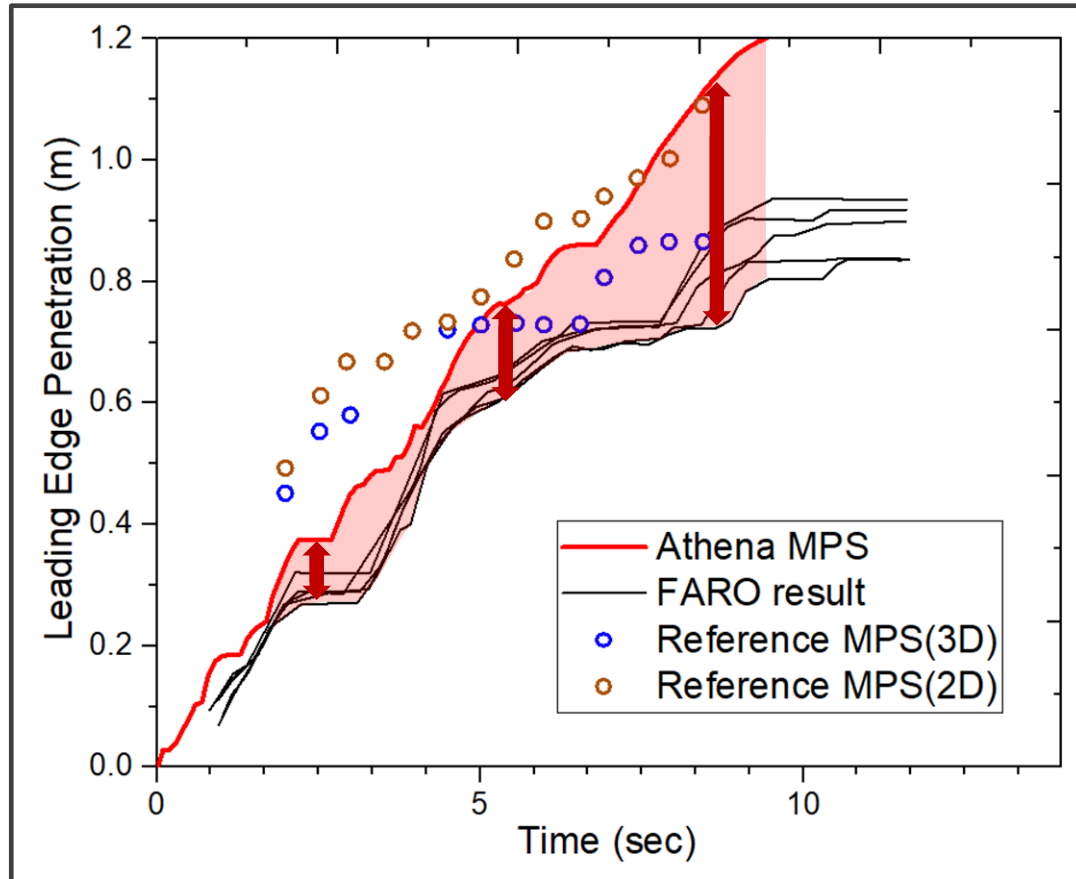
- Leading Edge Penetration:
용융물의 전진 거리, 기판 위에서의 이동 거리



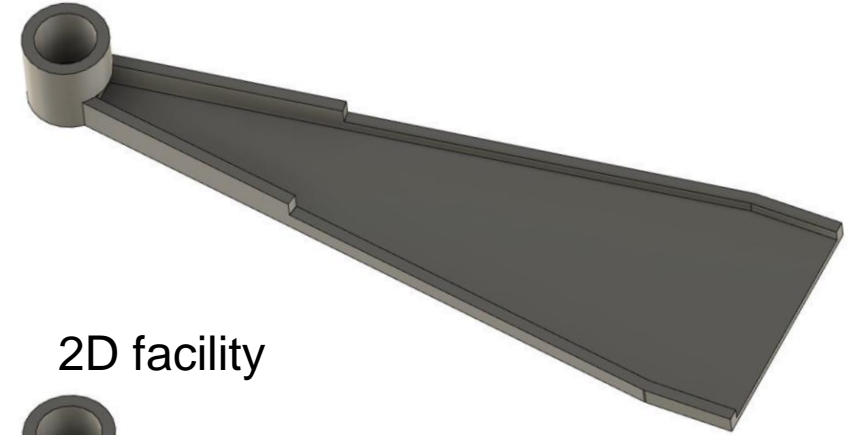
Calculation Result

Schematics of FARO-L26S

Analysis about Calculation Result



Real(3D) facility



2D facility



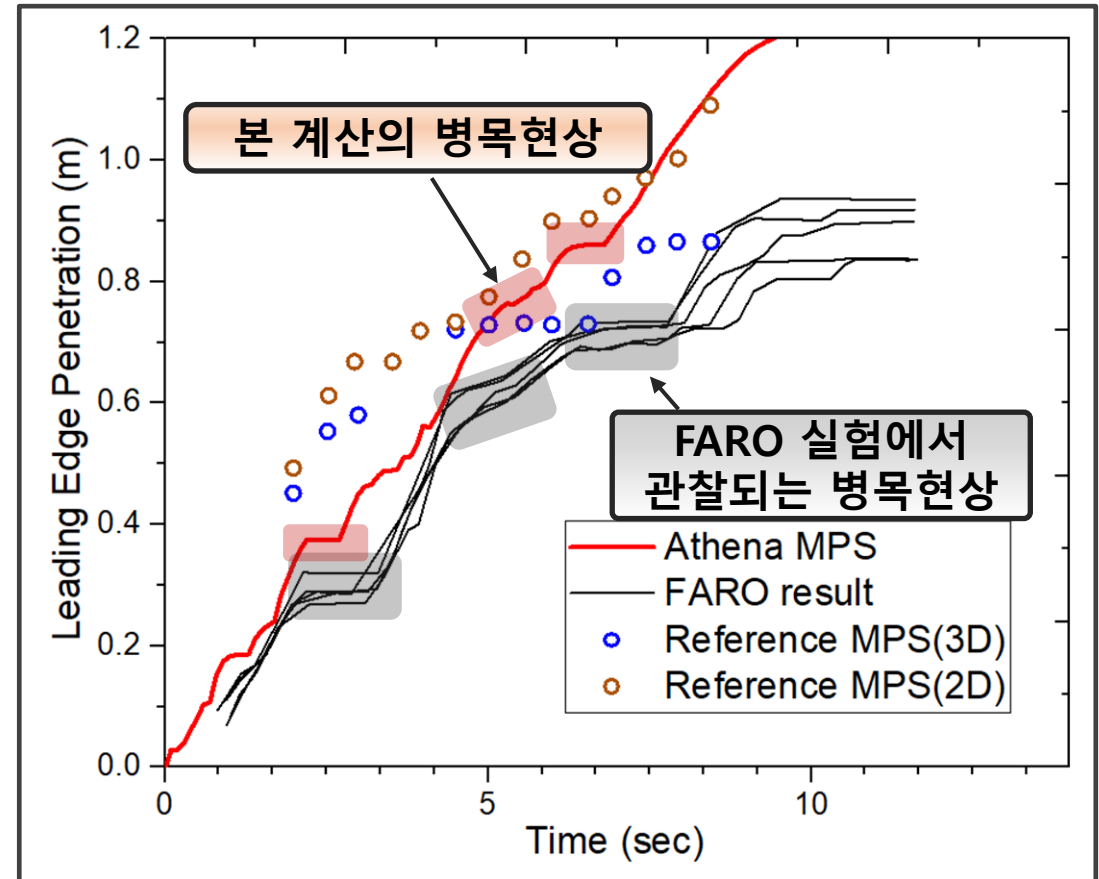
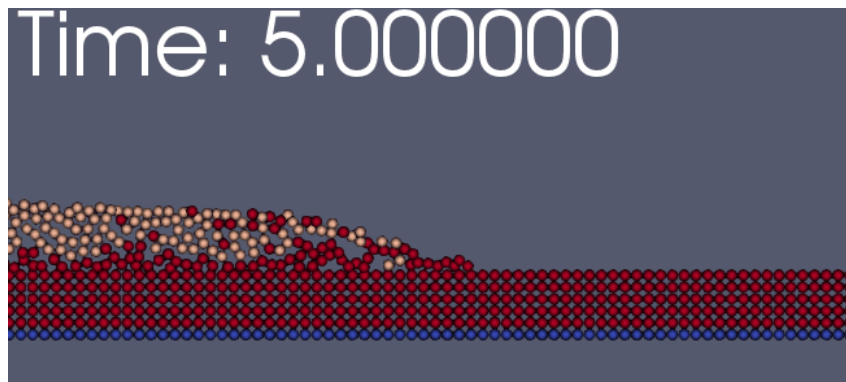
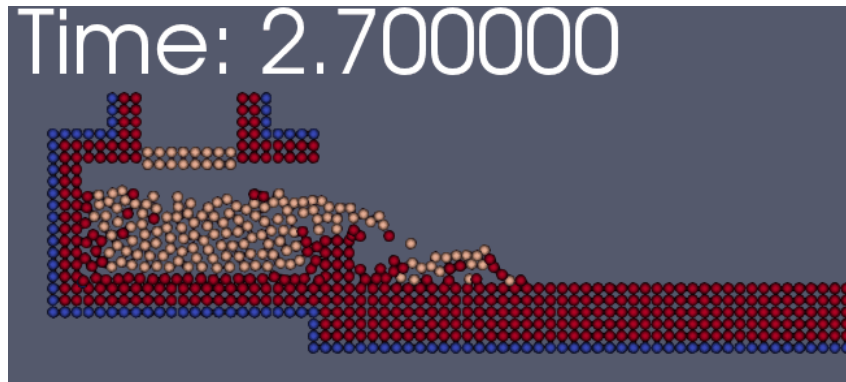
2D 계산의 한계점, 전진할 수록 오차가 심화

Calculation Result

Melt Spread Calculation in FARO facility

Analysis of Calculation Result

- 주기적으로 나타나는 병목현상과 해소
- Crust 벽의 생성에 의한 병목현상



Conclusion

Summary

Algorithm Development

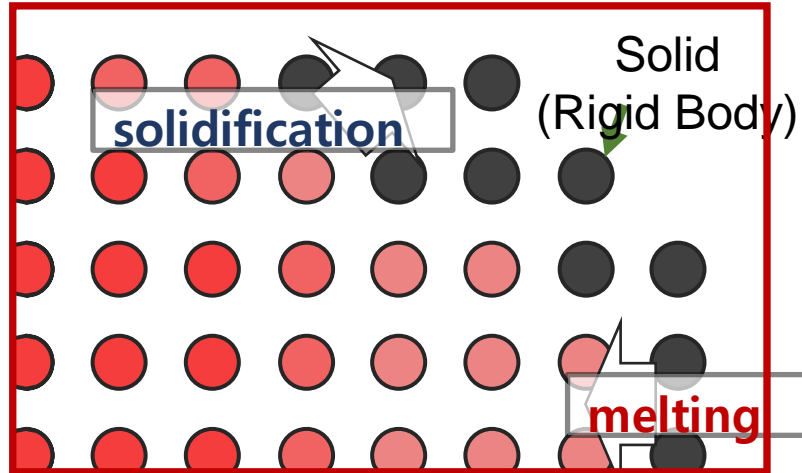
Multi-phase MPS

+

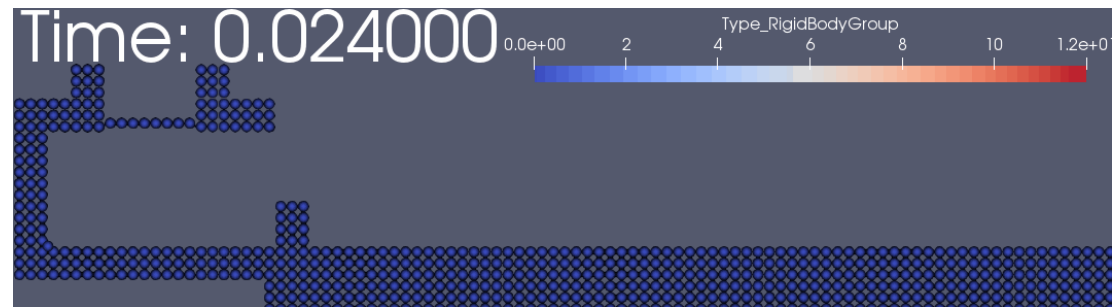
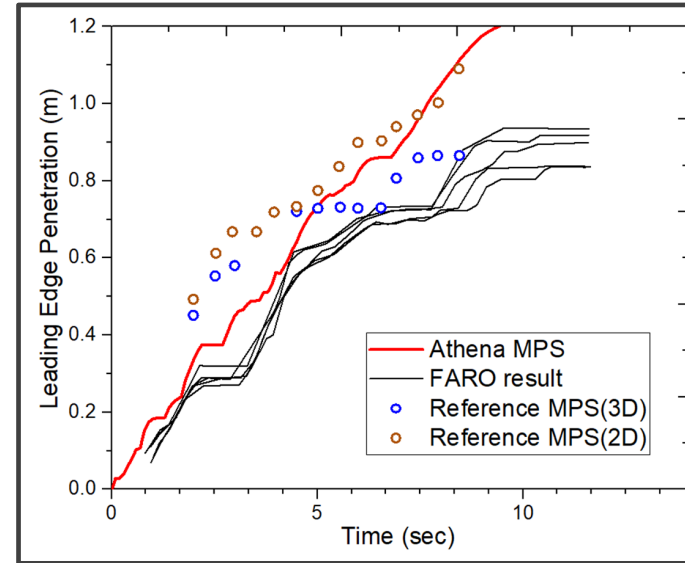
Rigid Body Dynamics

+

Phase Transition Grouping



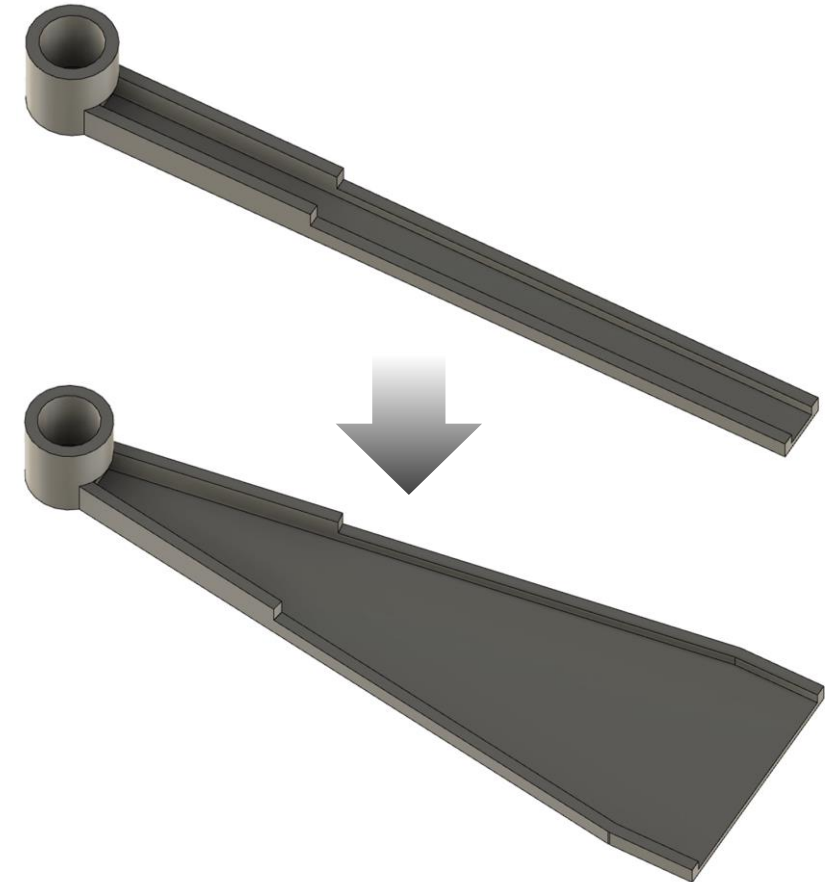
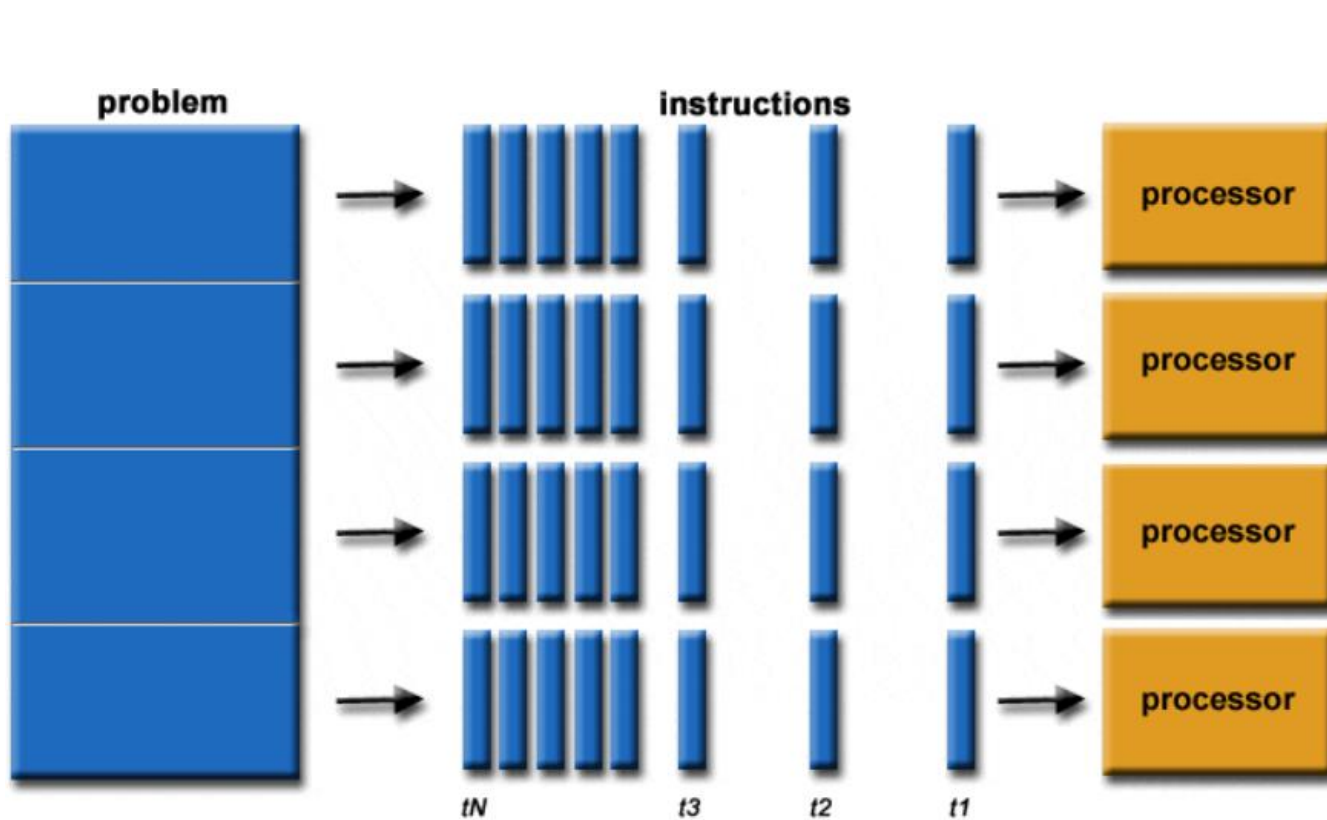
Verification with FARO example



Future Works

3D 해석으로의 확장 기반 마련

- 3D 해석으로의 발전 및 계산 정확도 향상을 위한 병렬컴퓨팅 해석 체계 개발



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Thank you for your attention

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Rigid Body Group(RBG) Tracking algorithm
(재귀함수 알고리즘)

