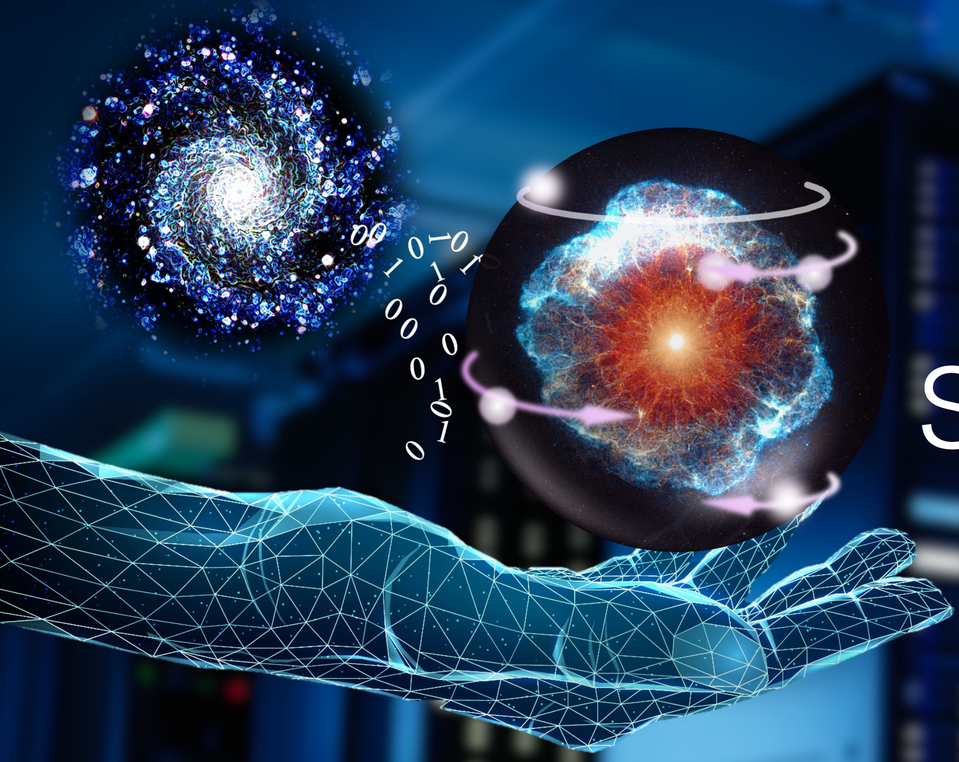

Surrogate Modeling for Computationally Expensive Simulations of Supernovae in High-Resolution Galaxy Simulations

Keiya Hirashima[1]

With Kana Moriwaki[1], Michiko S. Fujii[1], Yutaka Hirai[2,3], Takayuki R. Saitoh[4], Junichiro Makino[4] , and Shirley Ho[5]

[1]University of Tokyo, Japan, [2]Tohoku University, Japan, [3]University of Notre Dame, USA
[4]Kobe University, Japan, [5]CCA, Flatiron Institute, USA

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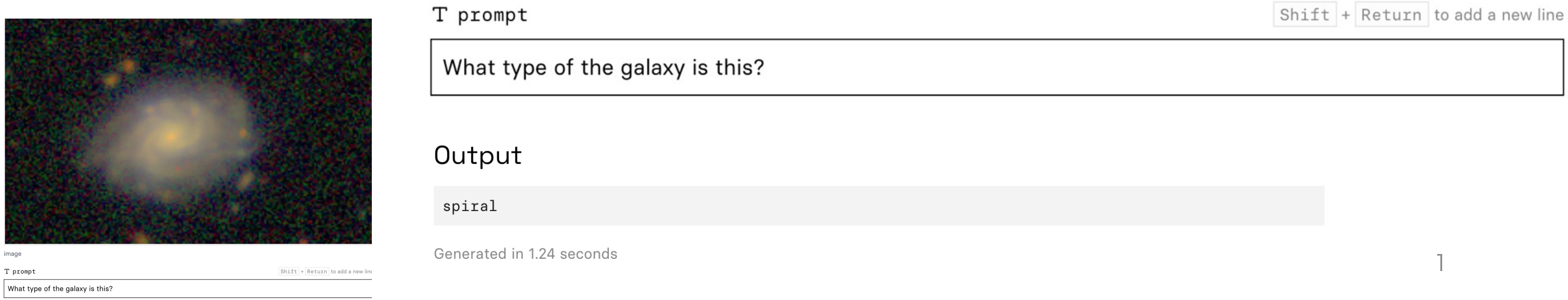
2023/10/19

CPS Seminar

Self-Introduction

Keiya Hirashima

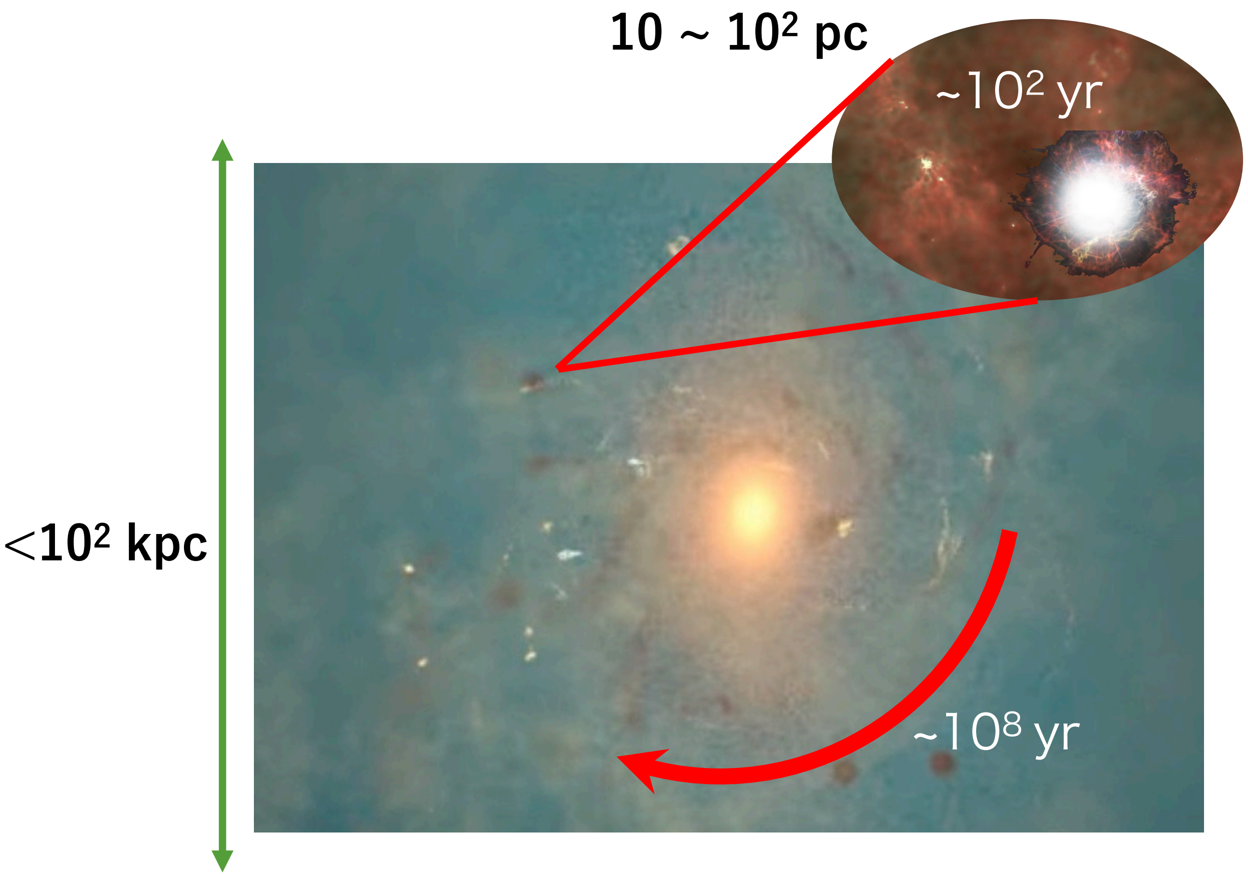
- PhD student (the University of Tokyo)
- Research interest
  - Galaxy formation and evolution
  - Surrogate modeling for SN feedback with machine learning
- Some other projects…
  - Surrogate modeling with GNNs/transformers
  - Foundation model to describe the morphology of galaxies



Outline

- Introduction: Overheads of galaxy simulations
- #1 A Hamiltonian splitting with deep learning
- #2 Surrogate modeling for the SN feedback
- Summary

Galaxy Simulations Using SPH*



The formation of the galaxy [1].

*SPH: Smoothed Particle Hydrodynamics

[1] https://www.youtube.com/watch?v=DDsUXRfs6ZQ

[2] Applebaum et al. (2021)

[3] Grand et al. (2021)

ASURA-FDPS (N-body/SPH)

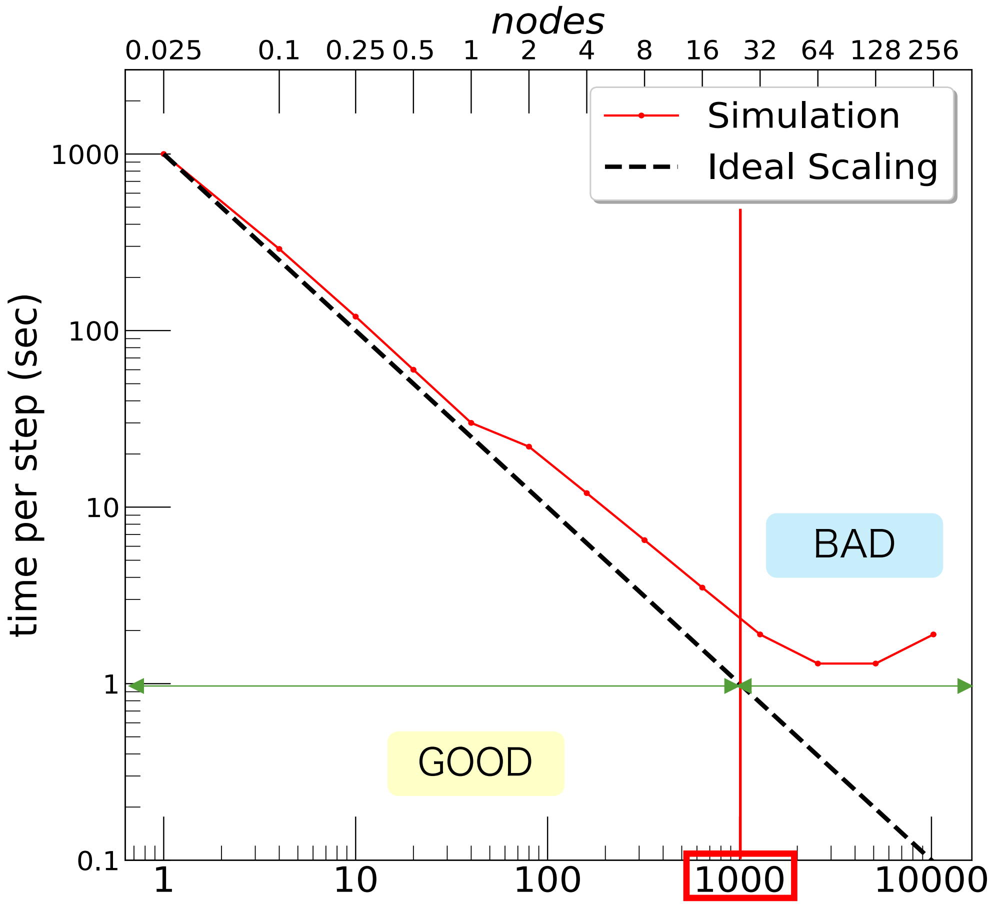
(based on Saitoh+08,09, Iwasawa+16)

- Gravity + Hydrodynamics
  - (DISPH; saitoh+13)
- Radiative Cooling/Heating (Ferland+17)
- Star formation (Hirai in prep.)
- Feedback
  - SNe Ia/IIb, AGB, Neutron star merger
- Chemical evolution (CELib; Saitoh17)
- FUV background

- About to accomplish star-by-star simulations… but…
  - Previous work [2, 3] : $10^3 M_\odot$
  - Our goal (ASURA-FDPS) : $10 M_\odot$

Overheads in Galaxy Formation Simulations

The parallelization efficiency saturates at ~10^3 CPU cores.



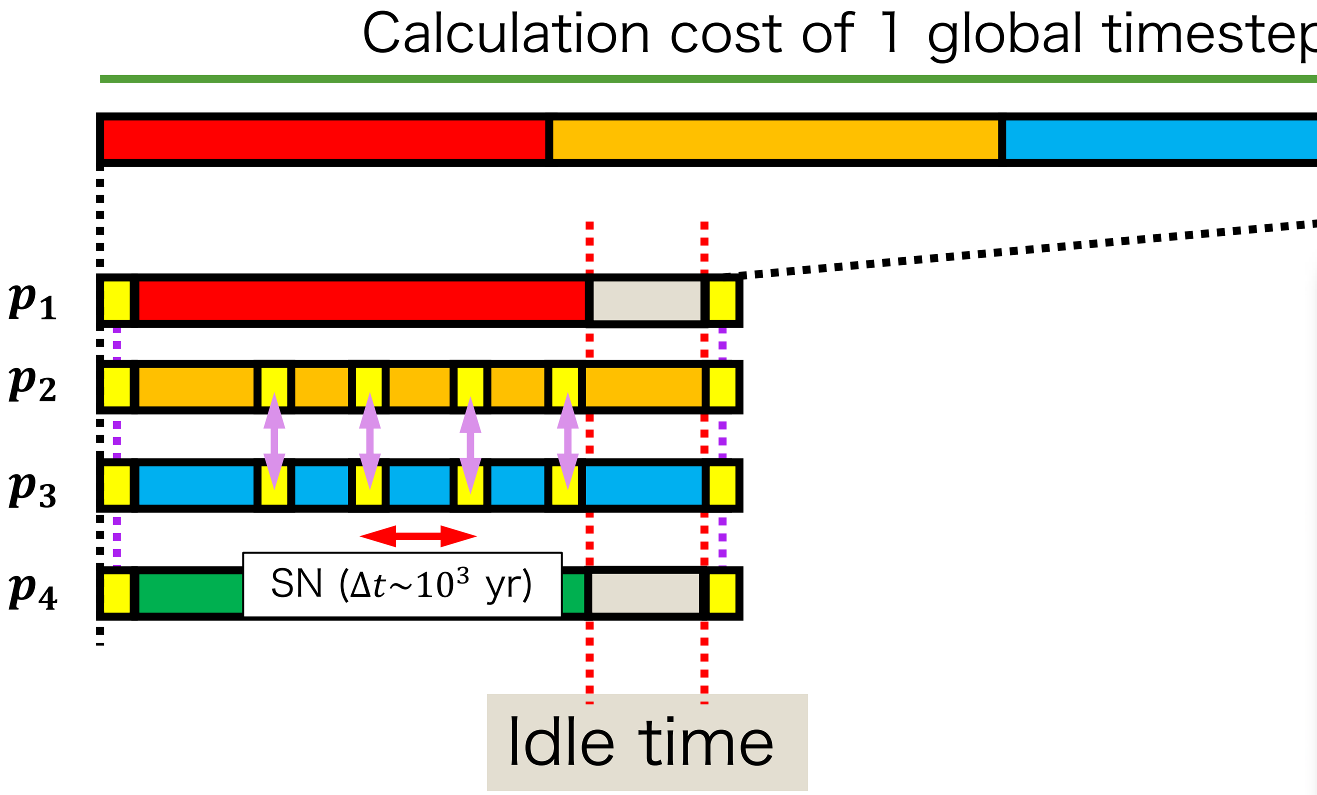
Strong Scaling of GADGET-4
(Based on Figure 63 in Springel et al. 2021)

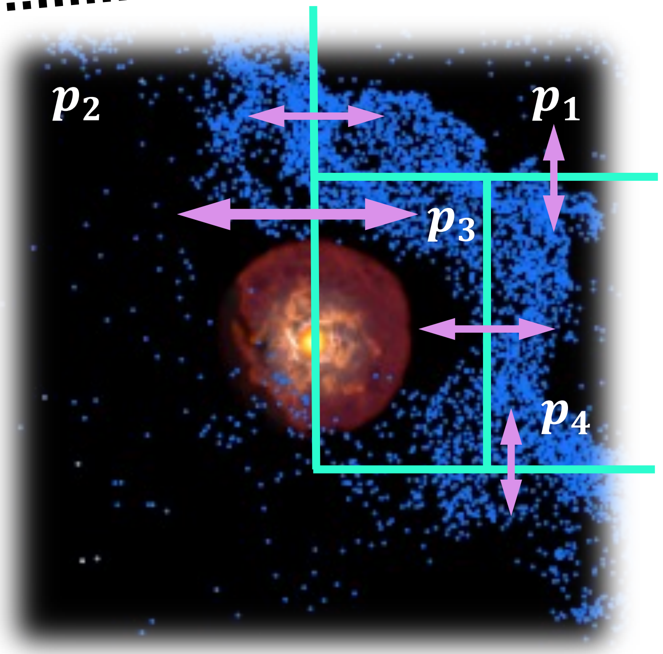
e.g.,
- GADGET-4(Springel+21)
- DC Justice League (Applebaum+21)
- Fire-2(Hopkins+18)

- Due to small timescale regions (e.g. SNe), the communication overhead occurs.
- Even the latest supercomputers cannot solve it (e.g., Fugaku has ~10^6 CPU cores).

Communication Overheads

The integration with short timesteps needs a huge number of calculations and inter-node communications.





Credit: NAOJ

How can I avoid the bottleneck?

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- Introduction: Overhead of galaxy simulations
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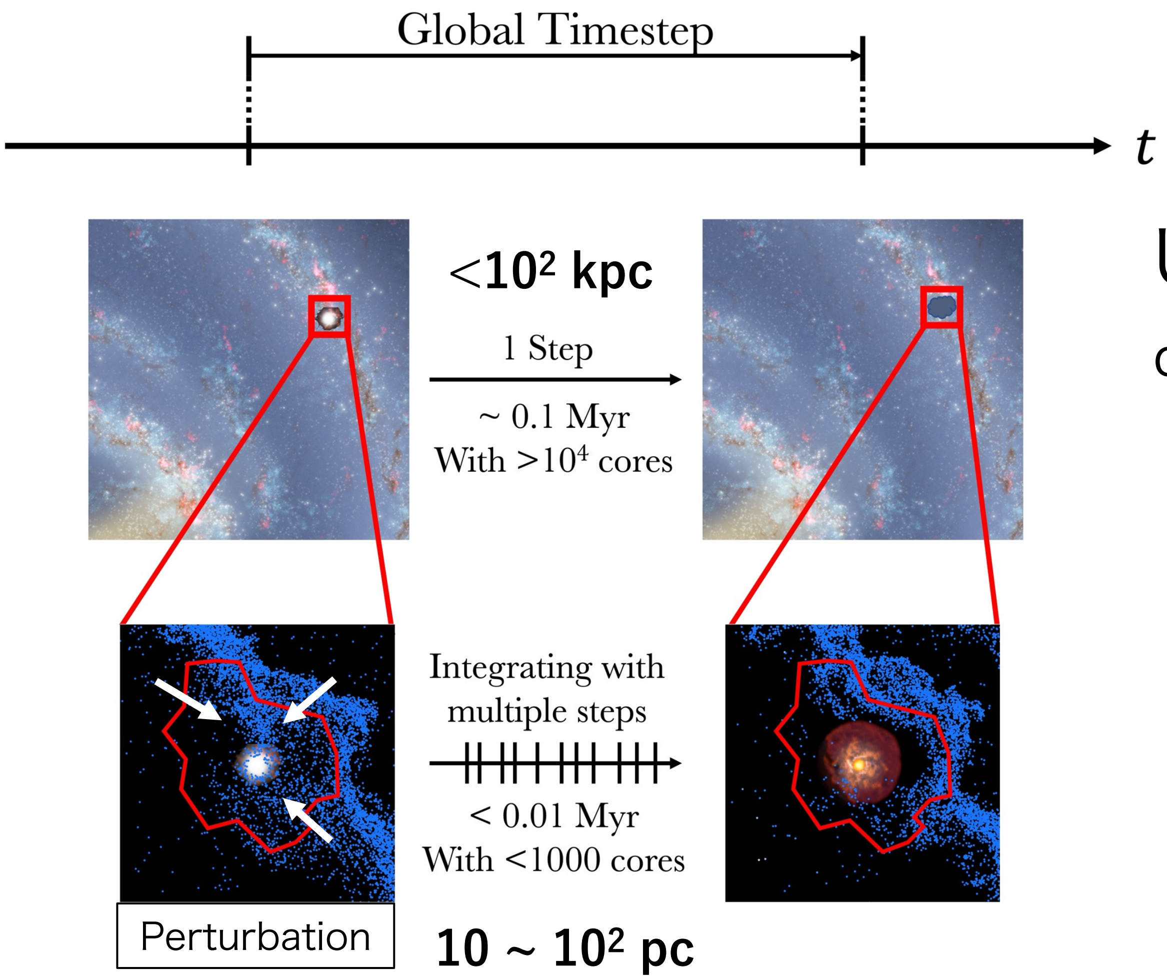
Hamiltonian Splitting Method



credit:[Upper: NASA/JPL-Caltech/ESO/R. Hurt,
Lower-Right: NAOJ, Lower-Left: ESO/M. Kornmesser]

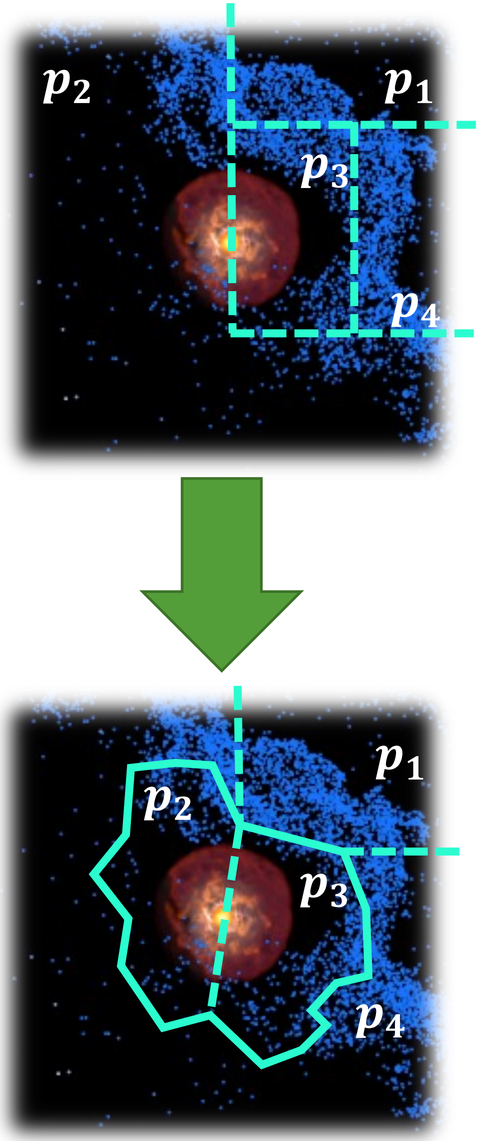
Use multiple integration methods

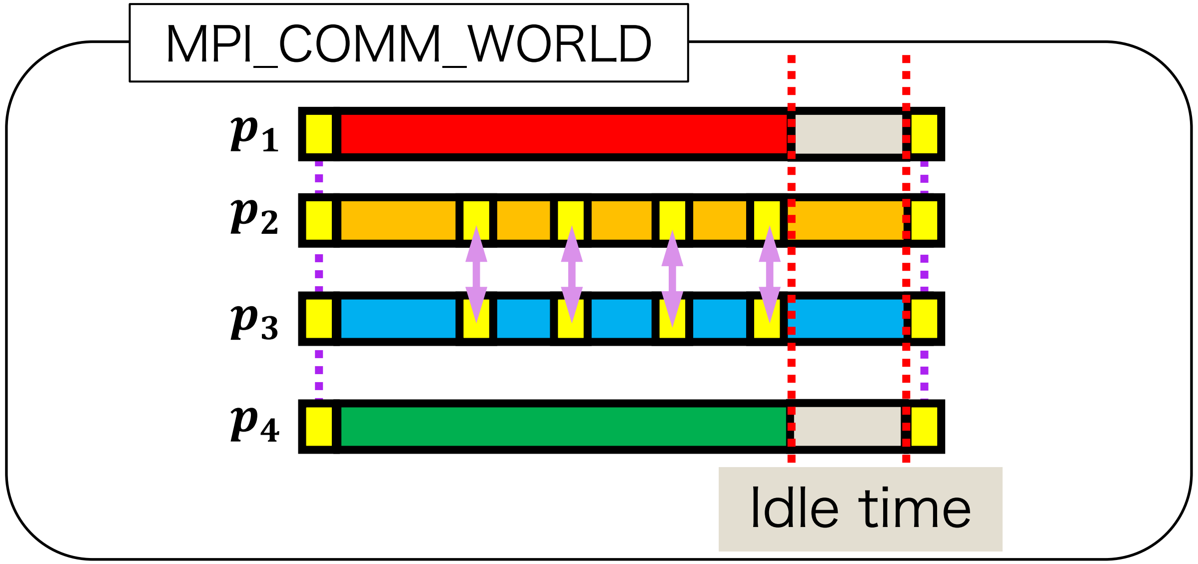
depending on the properties of the regions.

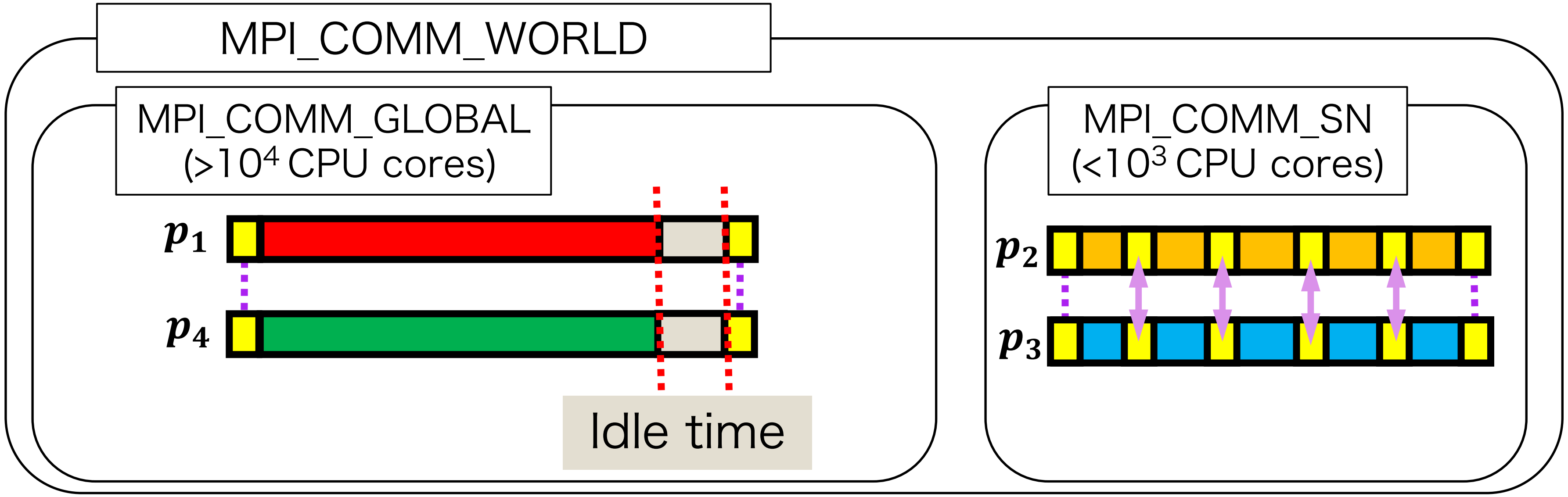
(Fujii et al. 2007; Saitoh et al. 2010; Pelupessy et al. 2012)

- Long timescale regions require the global (long) timestep.
- Short timescale regions (SNe) require short timesteps with the gravitational perturbations.

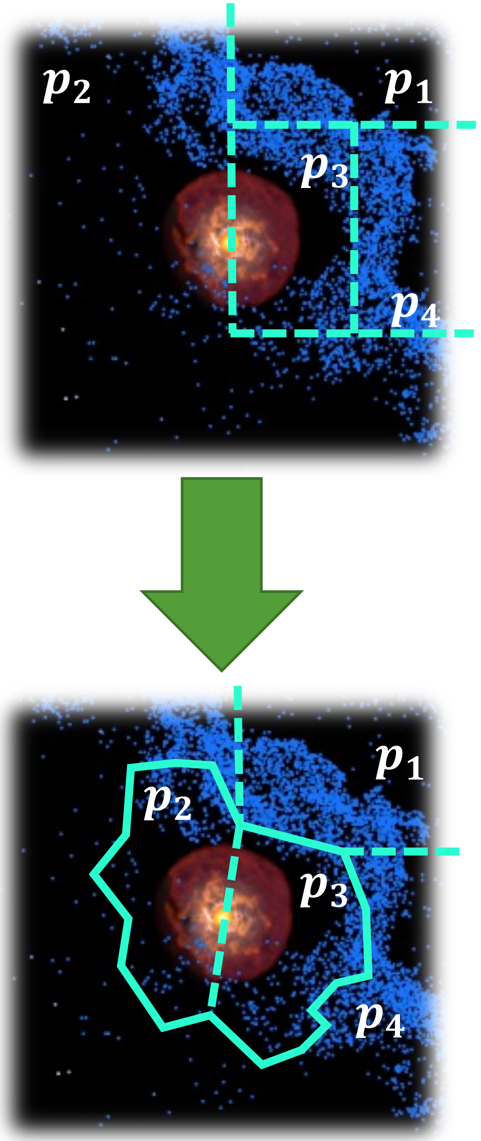
Avoid Communication Overheads



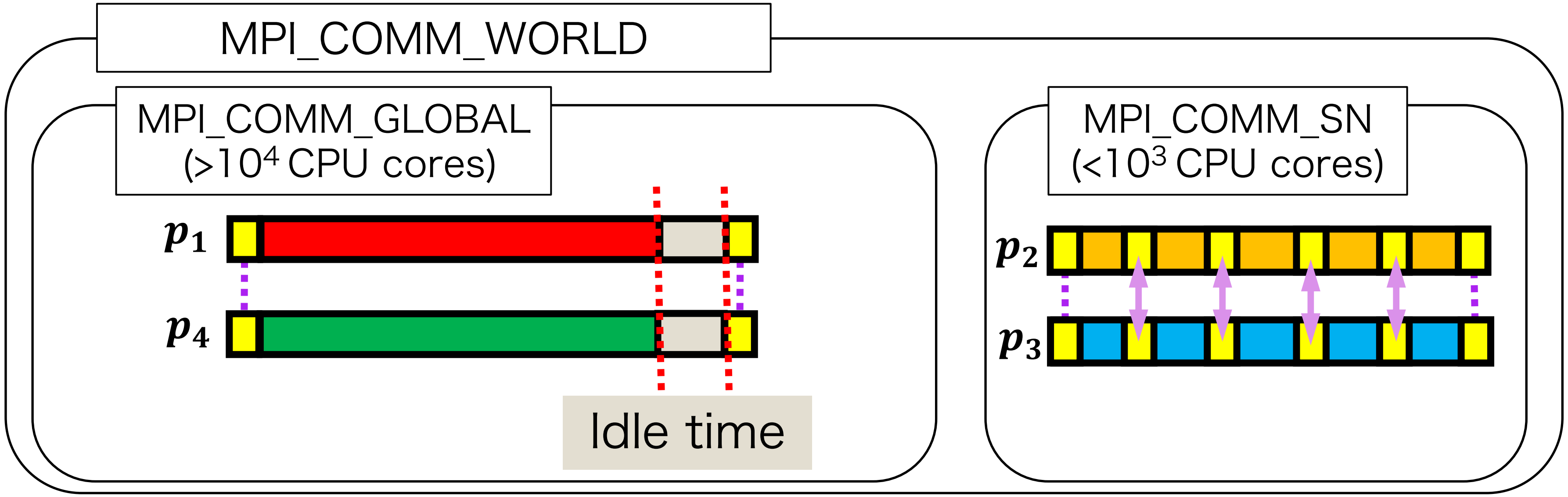




Avoid Communication Overheads



- Need to know which particles will have small timesteps in advance
- Predict the boundaries of the shells using deep learning

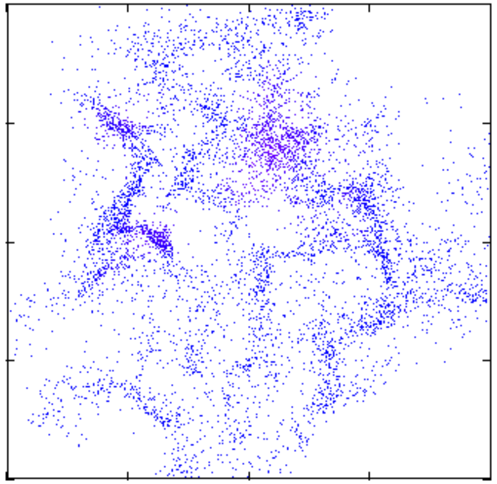


Training Data (3D cartesian grids)

SN simulations in inhomogeneous turbulent clouds

Temperature	10 [K]
Mean ambient density	40 ~ 60 [cm^{-3}]
Input energy	10^{51} [erg]
Total mass	10^{6} [$M_{\odot}$]
Mass of a gas particle	1 [$M_{\odot}$]
Softening parameter	0.5 [pc]

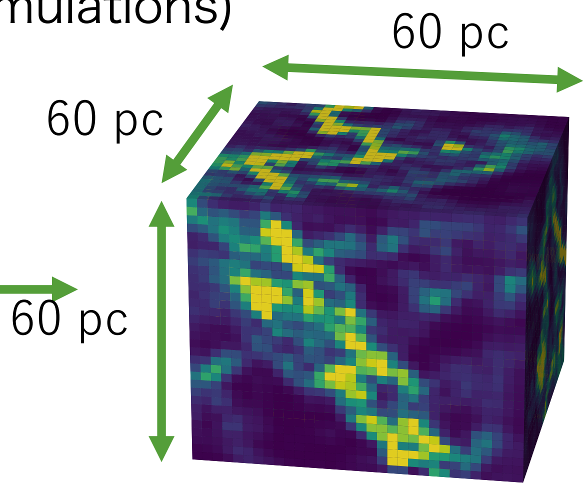
(the equivalent resolution for our galaxy simulations)



Interpolation using

SPH summation

$$\rho_i = \sum_j m_j W(r_{ij}, h_j)$$



32^3 voxels (density distribution)

Deep Learning Model

- Memory-In-Memory Network (Wang et al. 2018)
  - Generates 2D video in the future
  - Convolutional Neural Networks (CNNs)
    - Convolution is the operation like inner products.
  - Increased the dimensionality: 2D → 3D

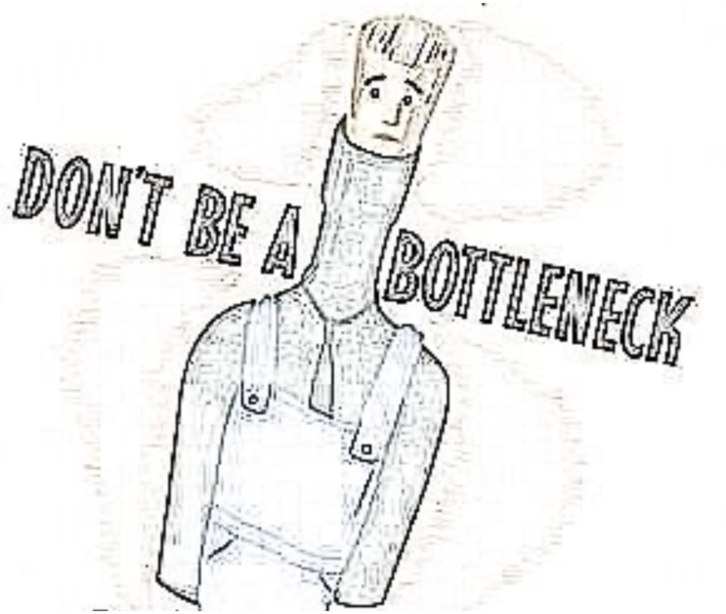
Let's learn the SN explosions with kernels!

Example. Edge detection

$\otimes$

0	1	0
1	-4	1
0	1	0

$=$

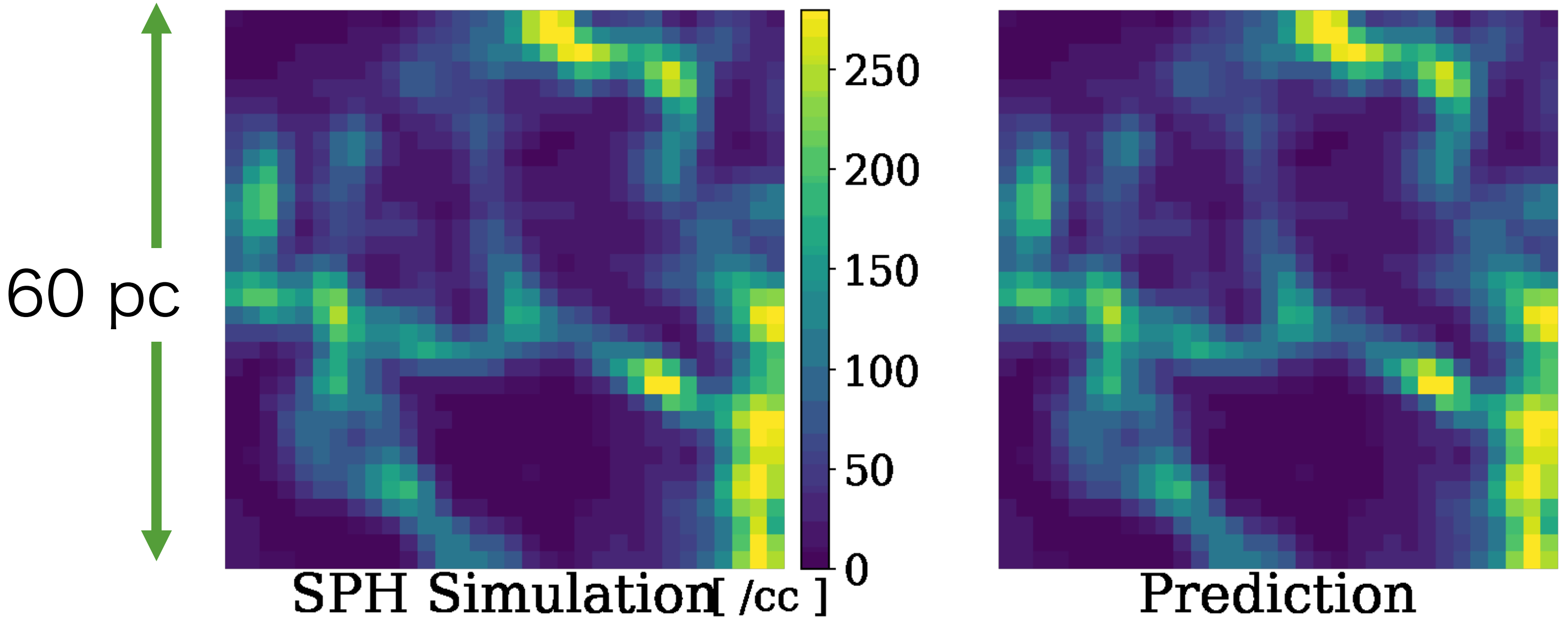


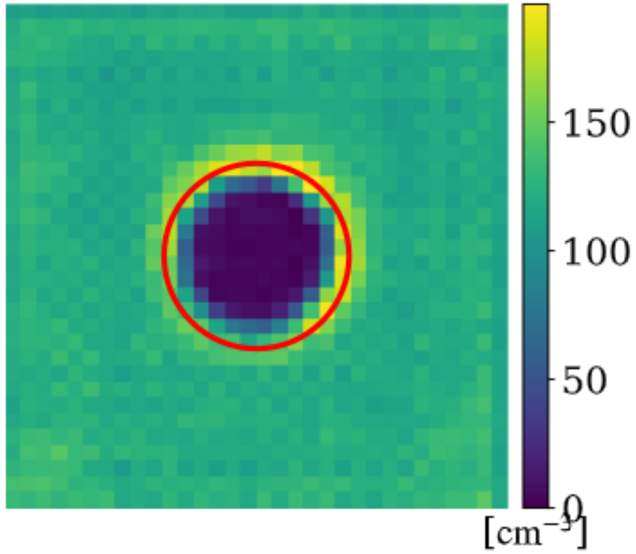
Learnable parameters
(Convolutional Neural Networks)

Forecast the Evolution of the SN Shells in Density

- Taking the initial distribution, the ML model can forecast the spatiotemporal change in density due to a SN explosion.
- Duration: 0.2 Myr

$$R(t) \propto \left(\frac{E_0}{\rho_0}\right)^{1/5} t^{2/5}$$





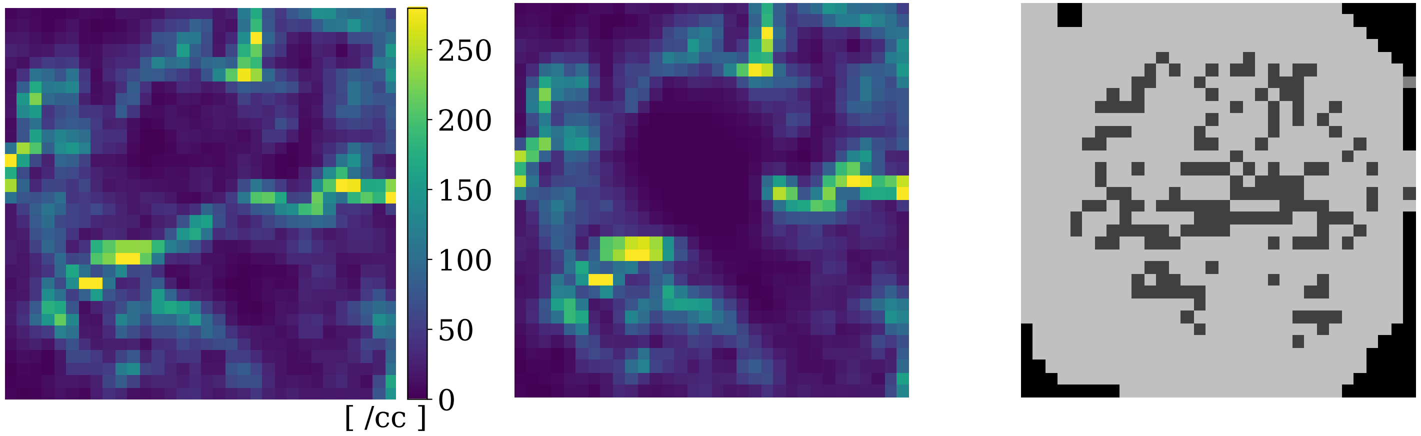
(a) Spherical

Cross section view
Left: Simulation data (ground truth)
Right: Prediction by the 3D-MIM

Hirashima et al. 2023, accepted
arXiv:2302.00026

Detect particles with small Δt

- With image processing, select (d) pale-gray region using (a) Initial Condition and (c) prediction

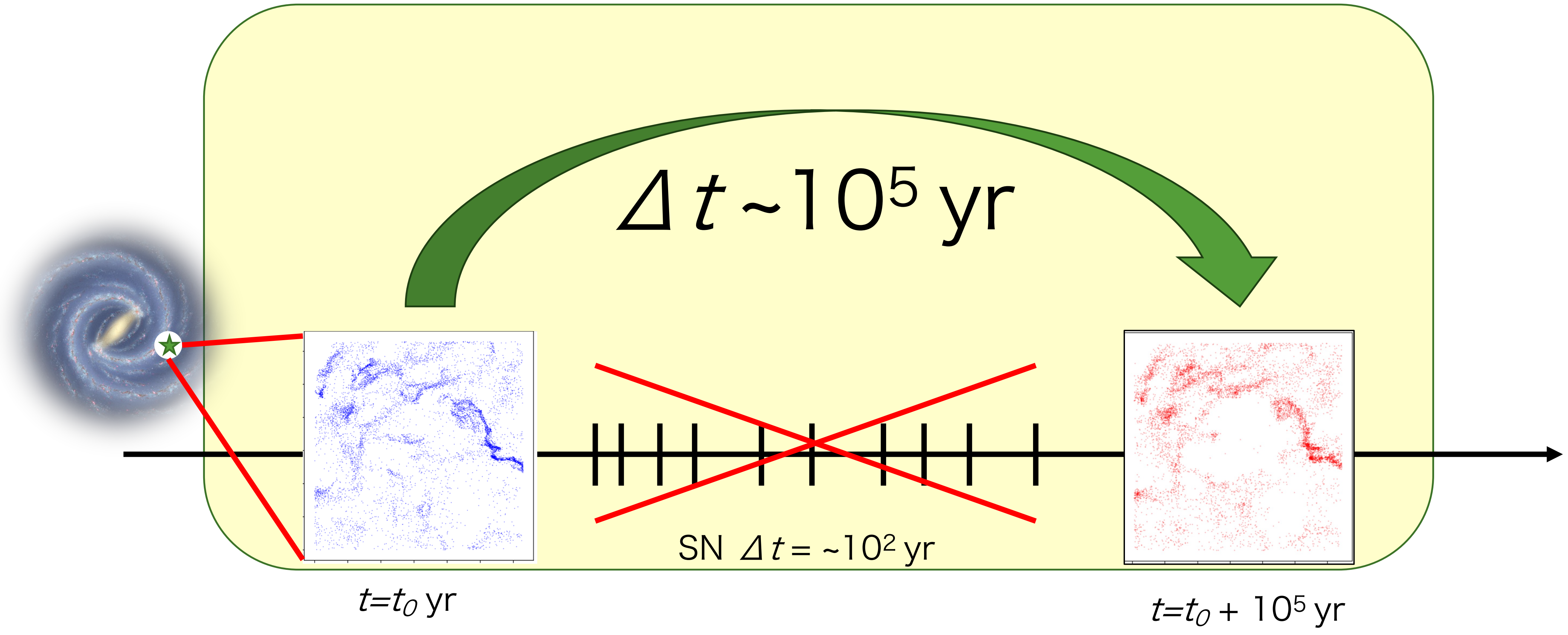


(a) Initial Distribution (t=0) (c) 3D-MIM (t=0.1 Myr) (d) Detected Particles

- The continuous region where the density becomes <90% is selected as the target region.
- Calculate the selected particles locally.

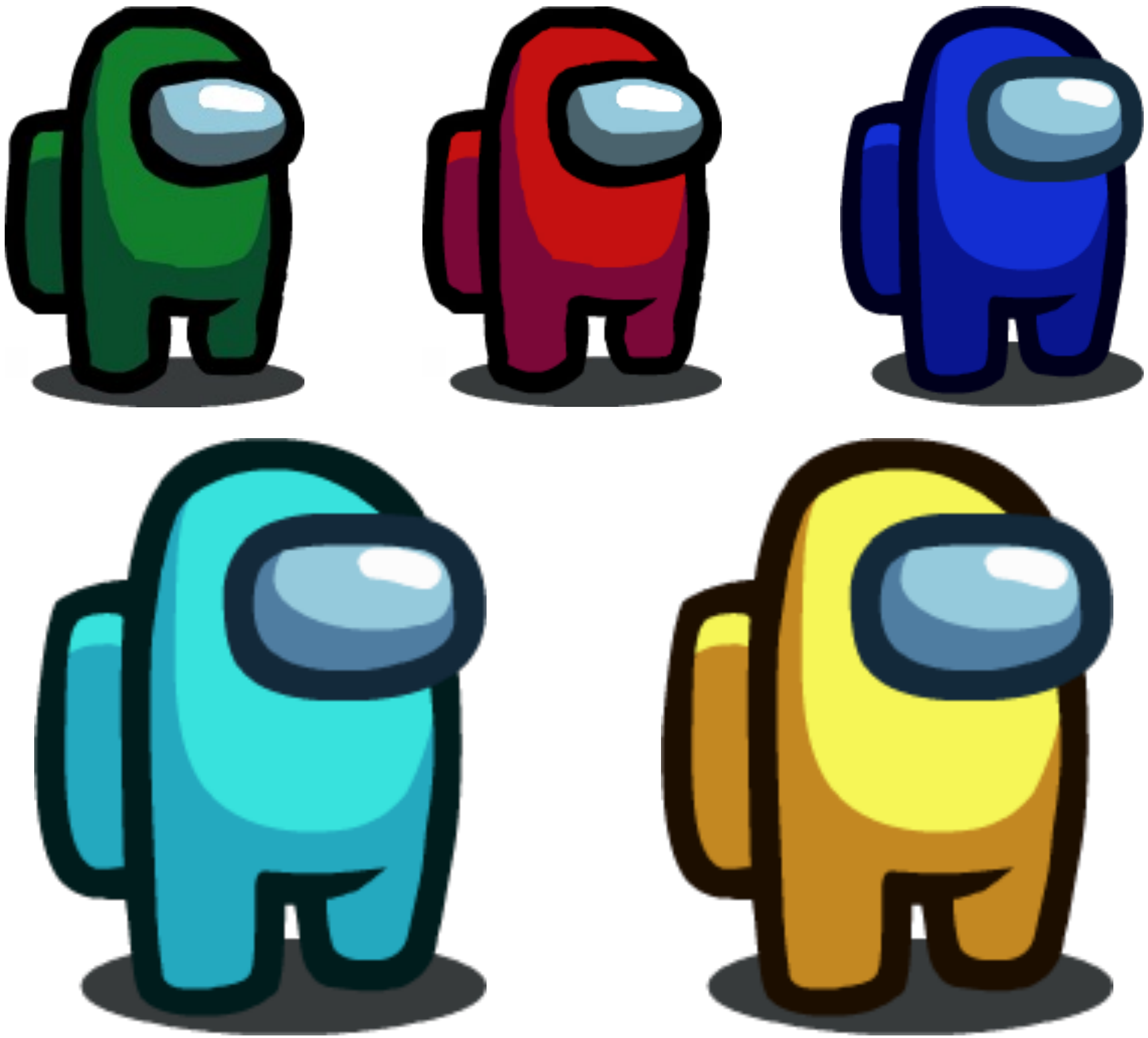
To the further speed-up

Sub-grid models



The rest of the region in the galaxy
$\Delta t \sim 10^5$ yr

We need more physics!!



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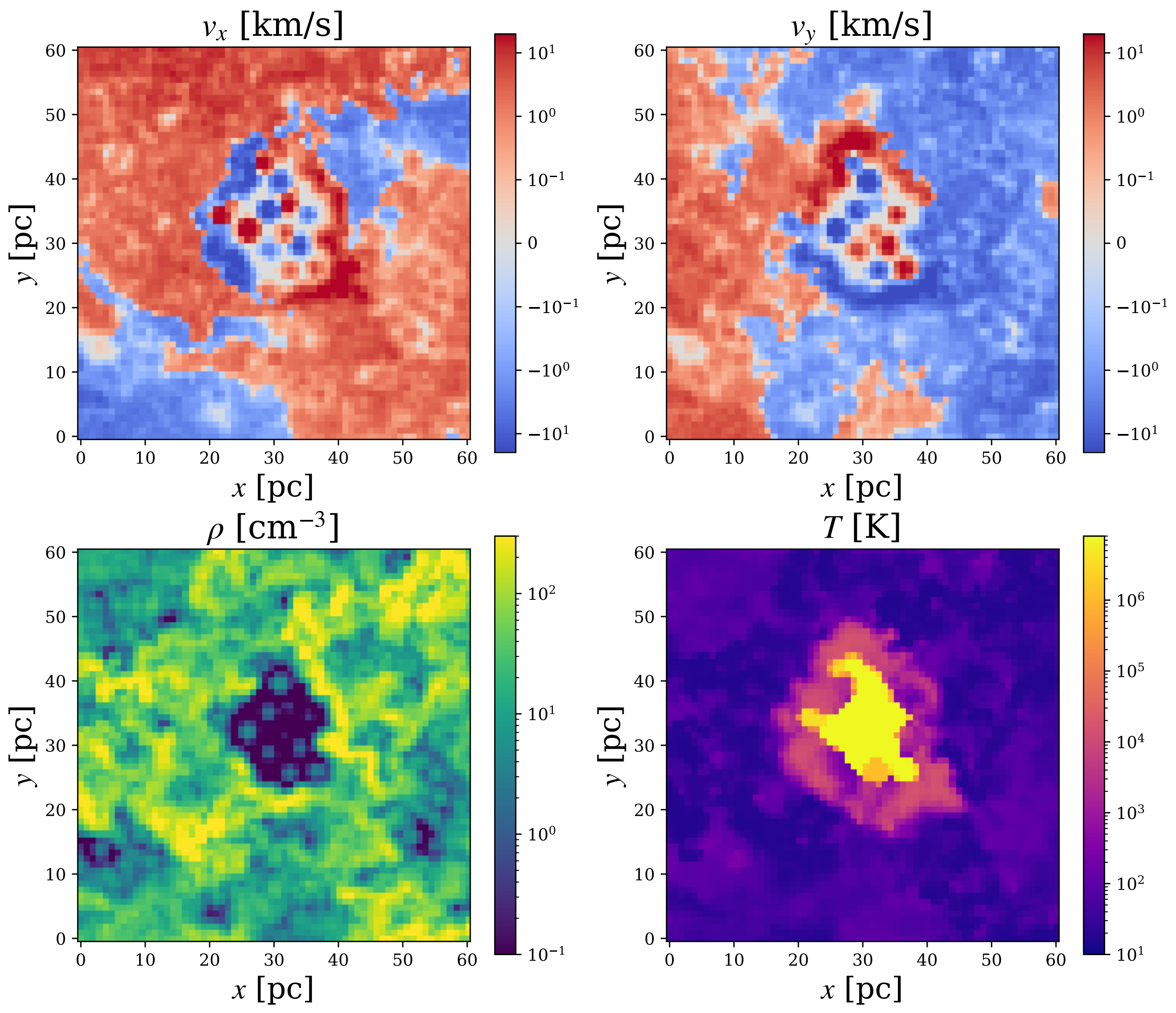
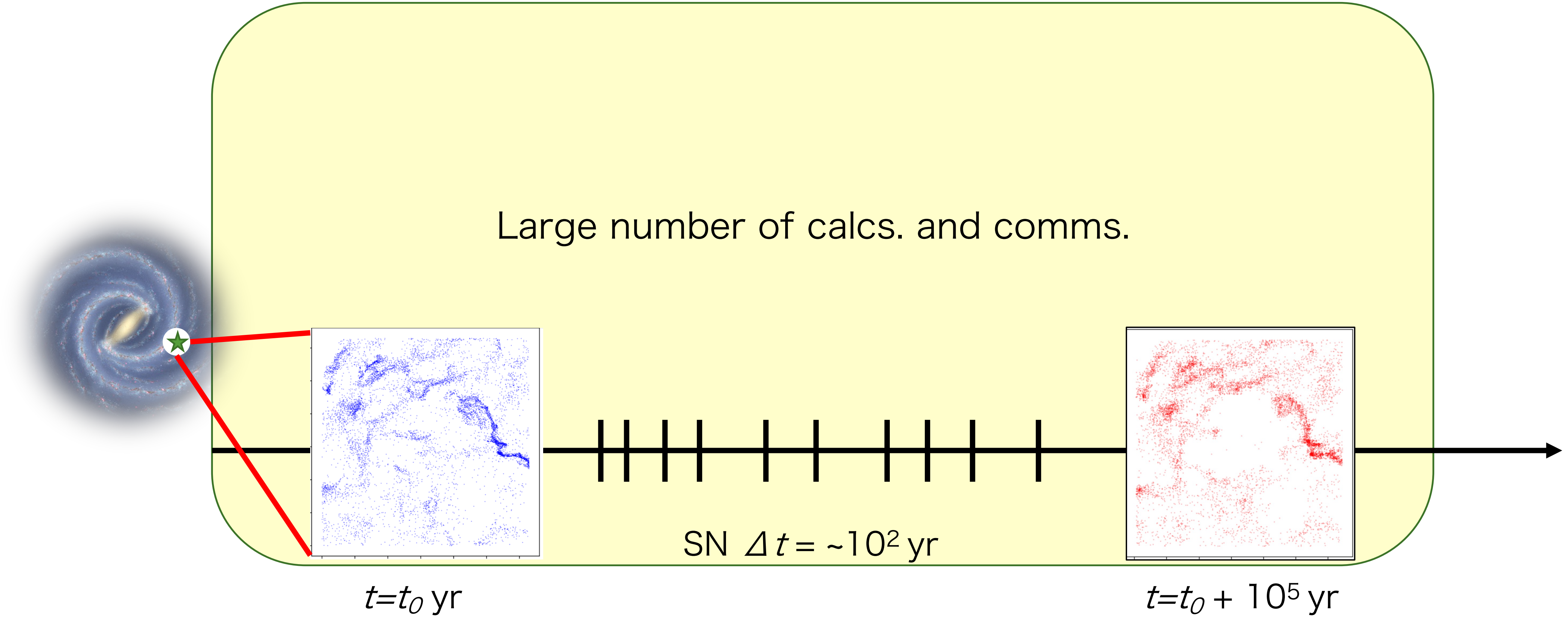
Training Data (3D cartesian grids)



- Mass resolution: $1M_\odot$
- Summation with the SPH kernel

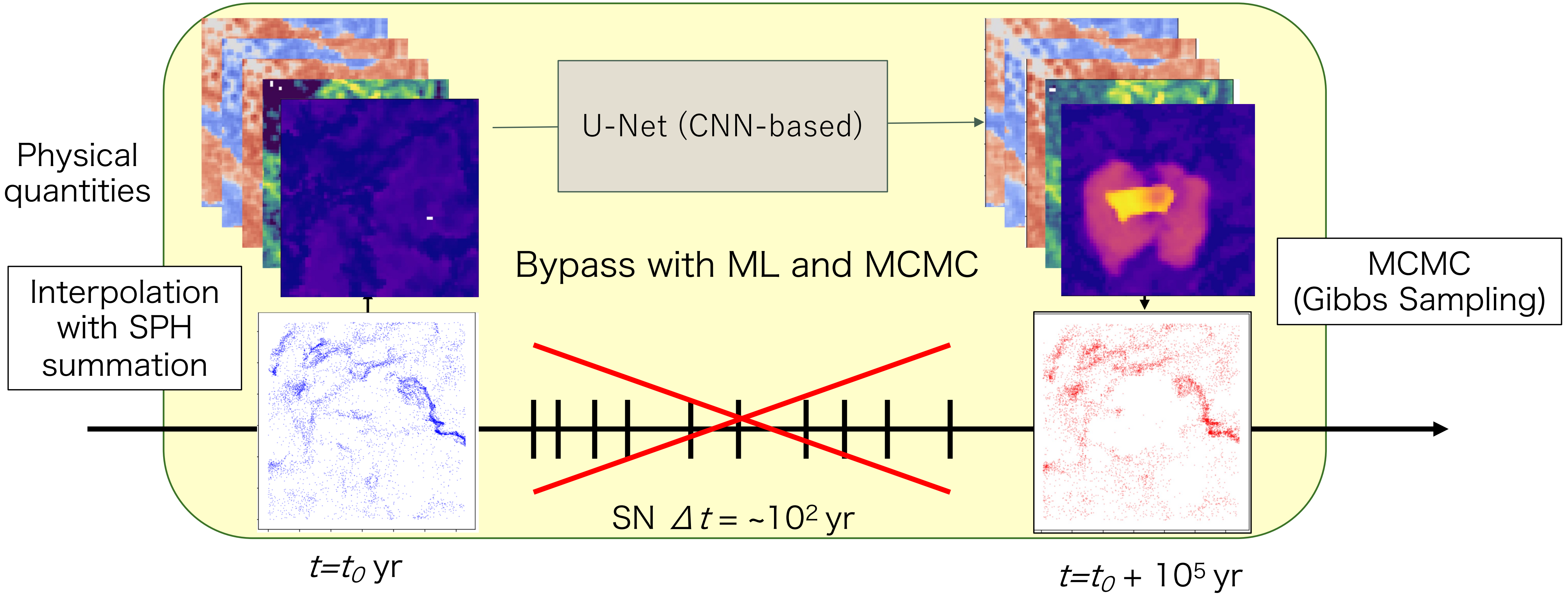
$$f_i = \sum_j m_j \frac{f_j}{\rho_j} W(r_{ij}, h).$$

Simulations for SN feedback



The rest of the region in the galaxy
Δt ~10^5 yr

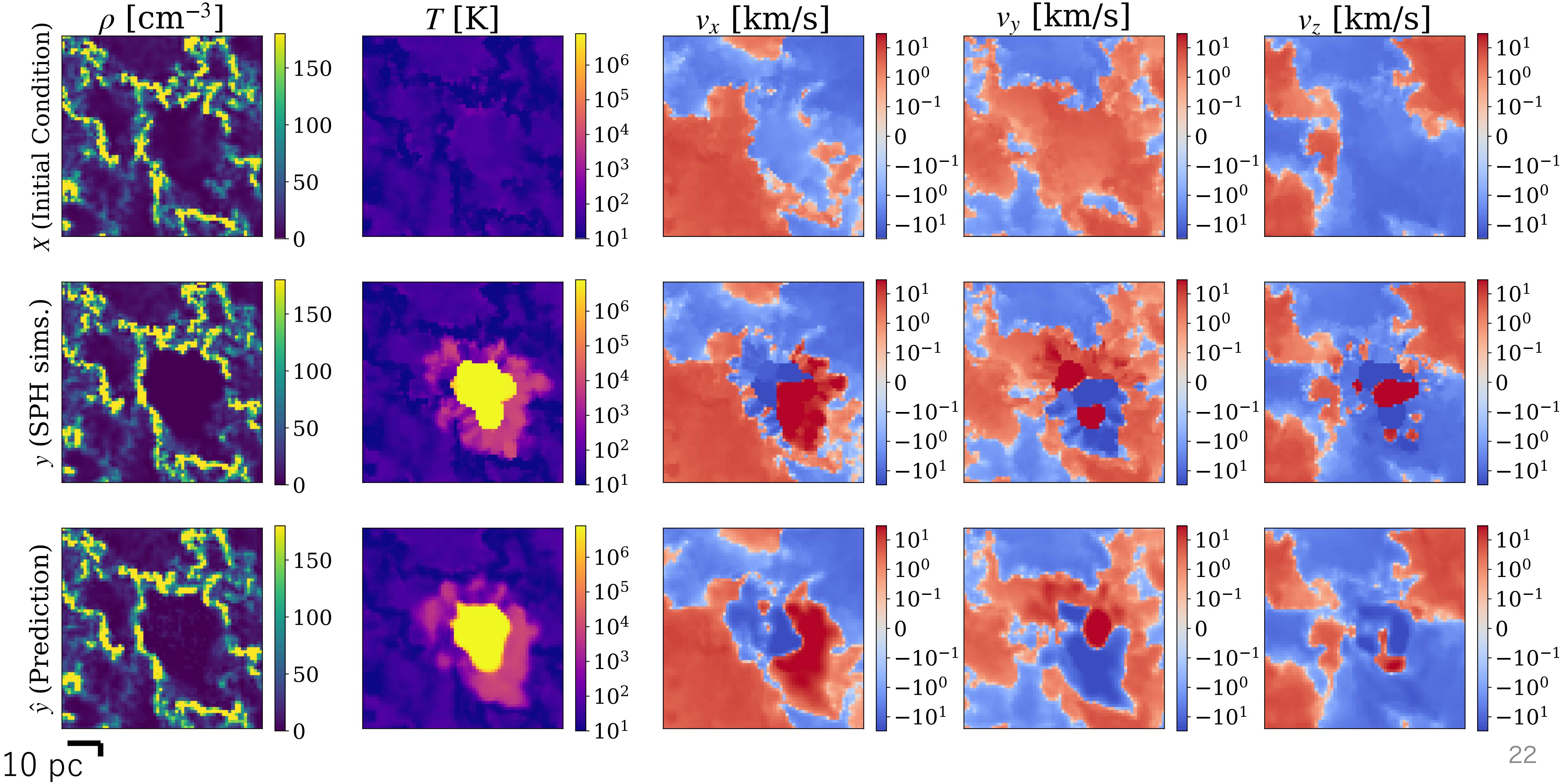
Surrogate modeling for SN feedback



The rest of the region in the galaxy
$\Delta t \sim 10^5$ yr

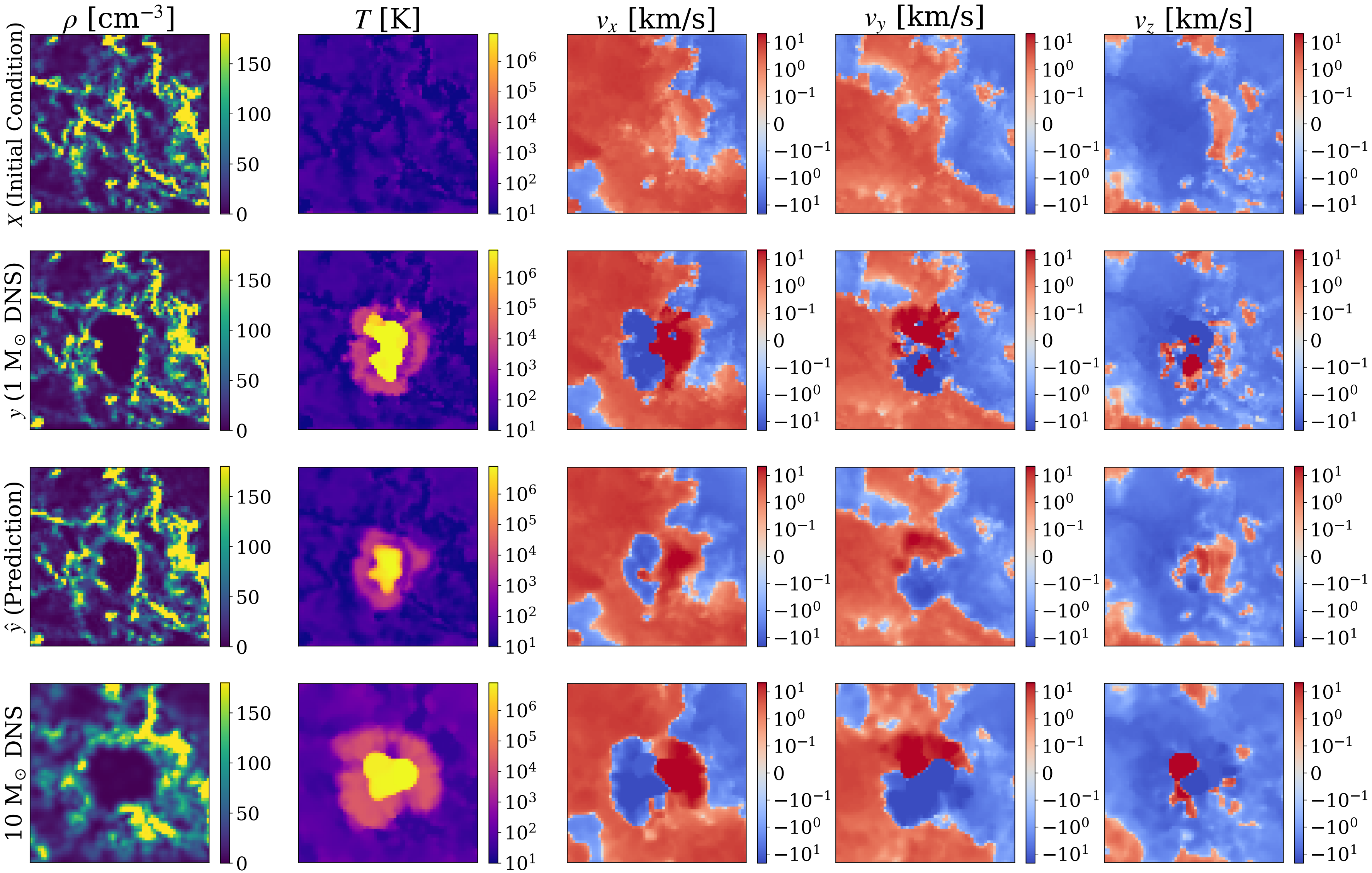
Prediction

Inhomogeneous shell emerges by the dense filament blocking.



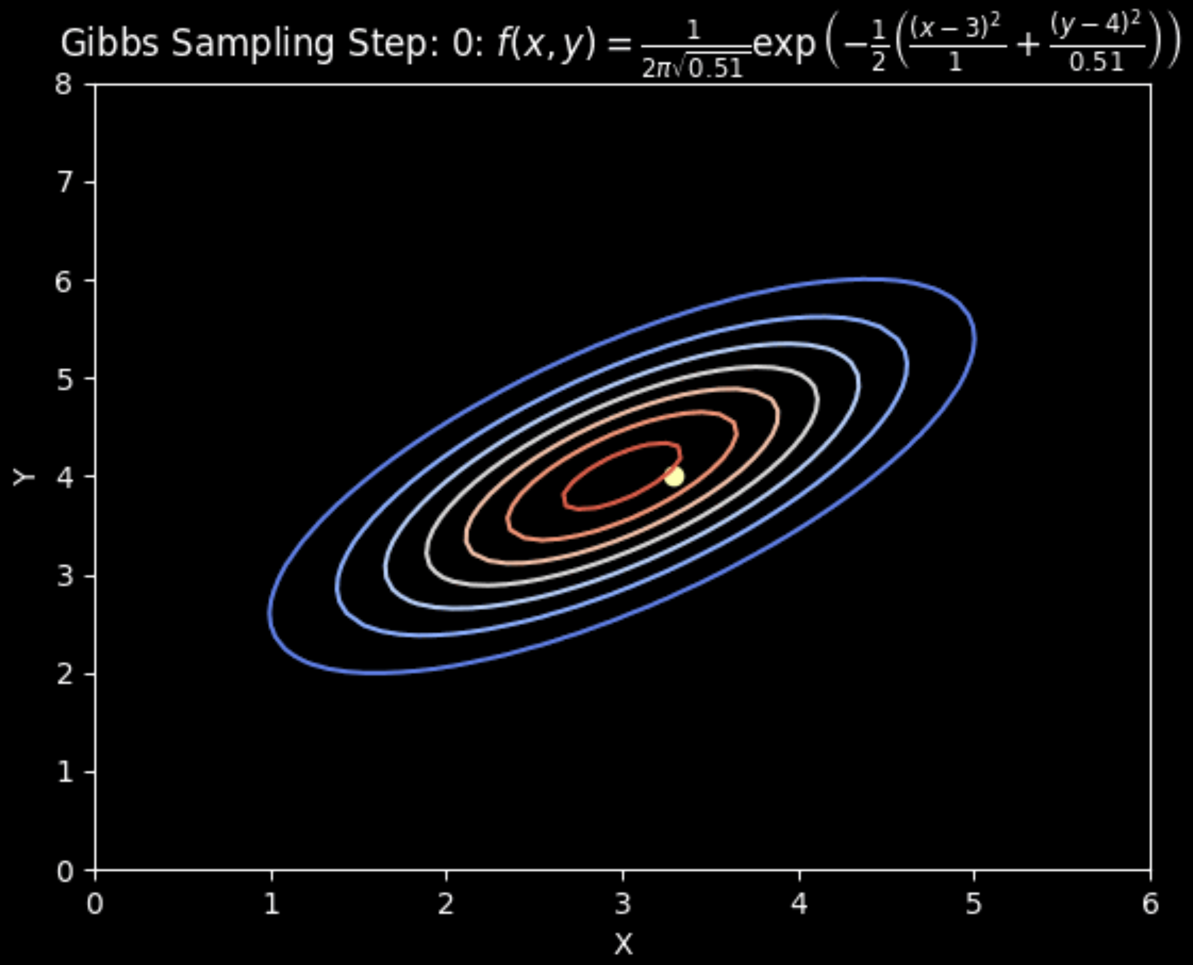
Prediction #2

Dense region：Velocities are estimated at a lower values.



Gibbs Sampling (2D)

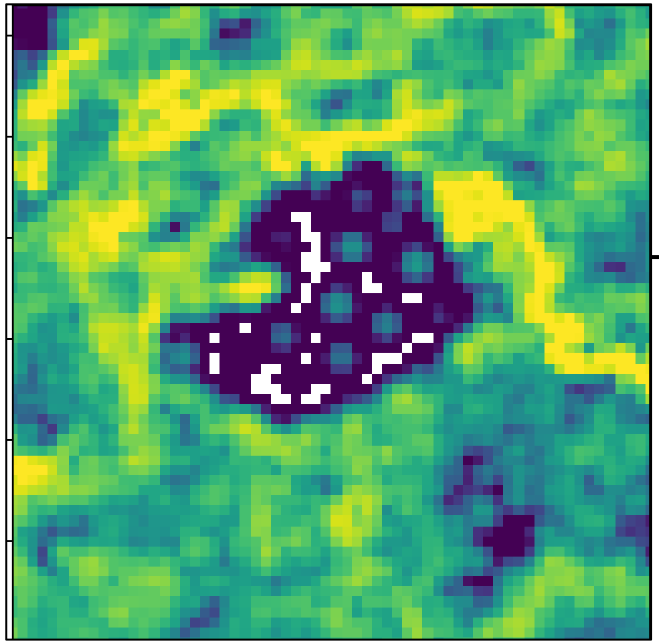
- Initialize X^0, Y^0
- for $j = 1, 2, 3, \cdots$ do
- sample $X^j \sim p(X \mid Y^{j-1})$
- sample $Y^j \sim p(Y \mid X^{j-1})$
- end for

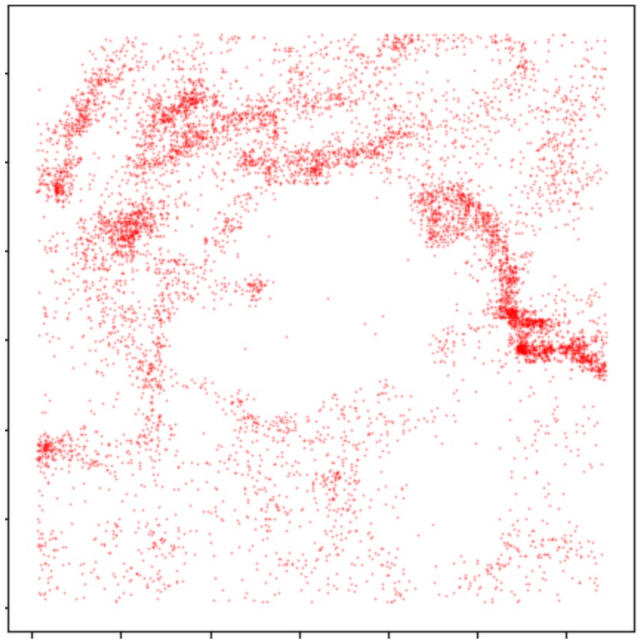


Representation by Gibbs Sampling

The particle distribution is sampled by a Markov chain Monte Carlo method.

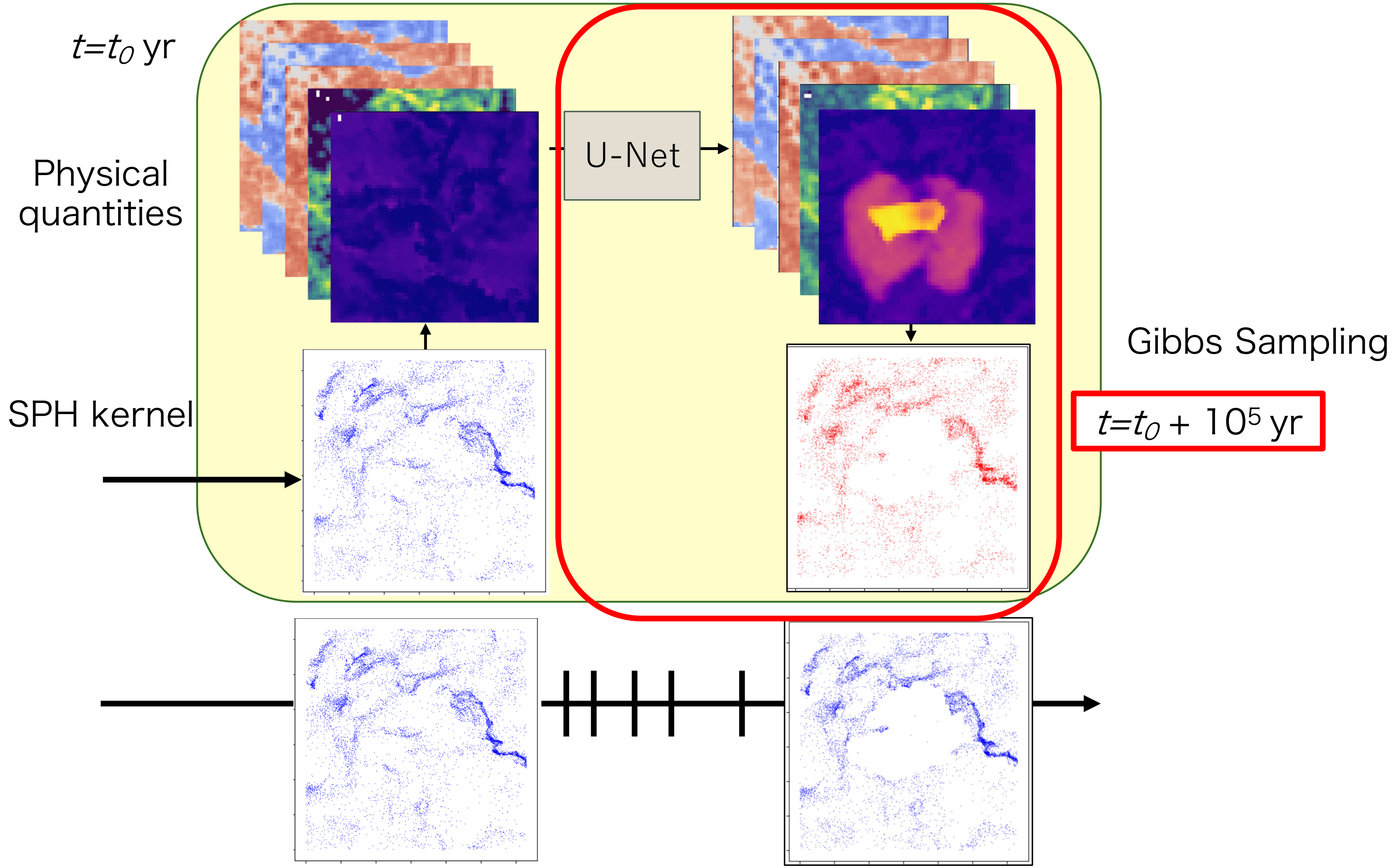
MCMC
(Gibbs Sampling)





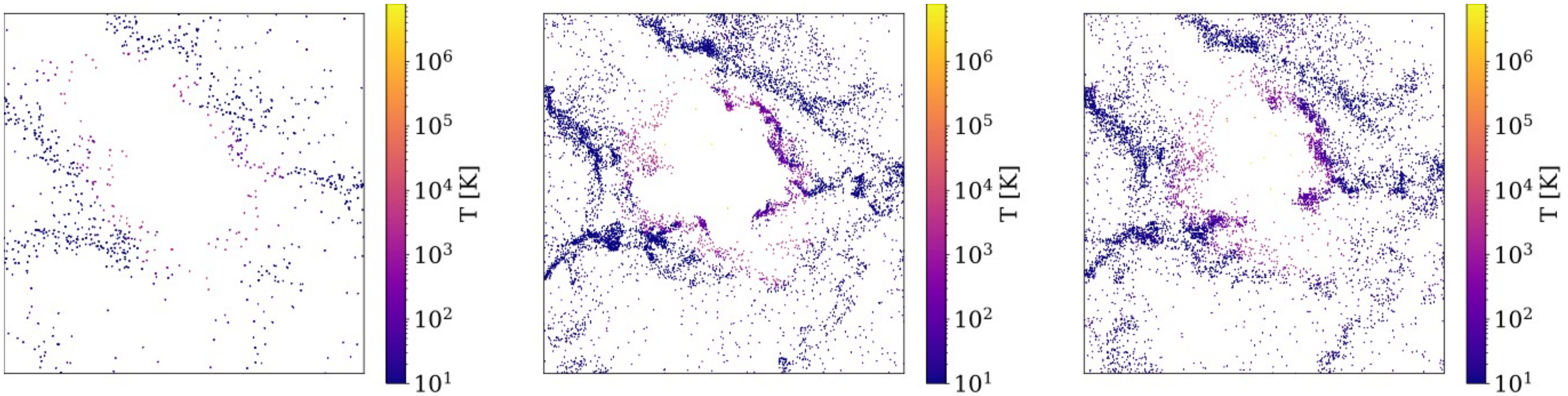
3D cartesian grids of density
~ 3D probability density function

ML + MCMC


$t=t_0$ yr
Physical quantities
SPH kernel
U-Net
Gibbs Sampling
$t=t_0 + 10^5$ yr

Validation

- Ground Truth: 1Msun sims (High-resolution)
- Baseline: 10 Msun sims (“Low”-resolution)
  - High resolution for galaxy simulations, cannot resolve supernova feedback (Hu+16, Steinwandel+20, Hirashima+23)
- Compered total thermal energy and outer momentum of hot particles ($<10^3$ K) on test data (100 results of independent simulation)



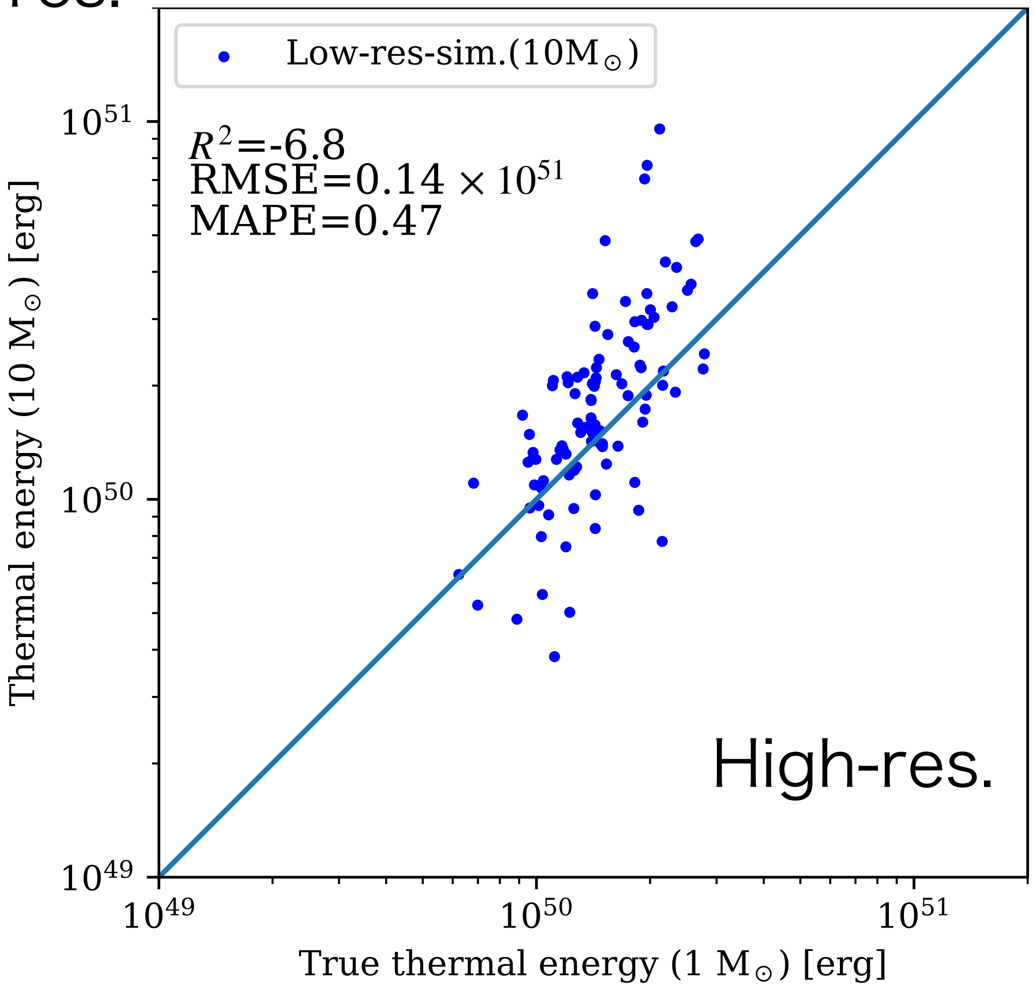
(a) 10 $M_\odot$ res-sim — (b) 1 $M_\odot$ res-sim — (c) Reconstruction

“Low”-resolution — High-resolution — Our method

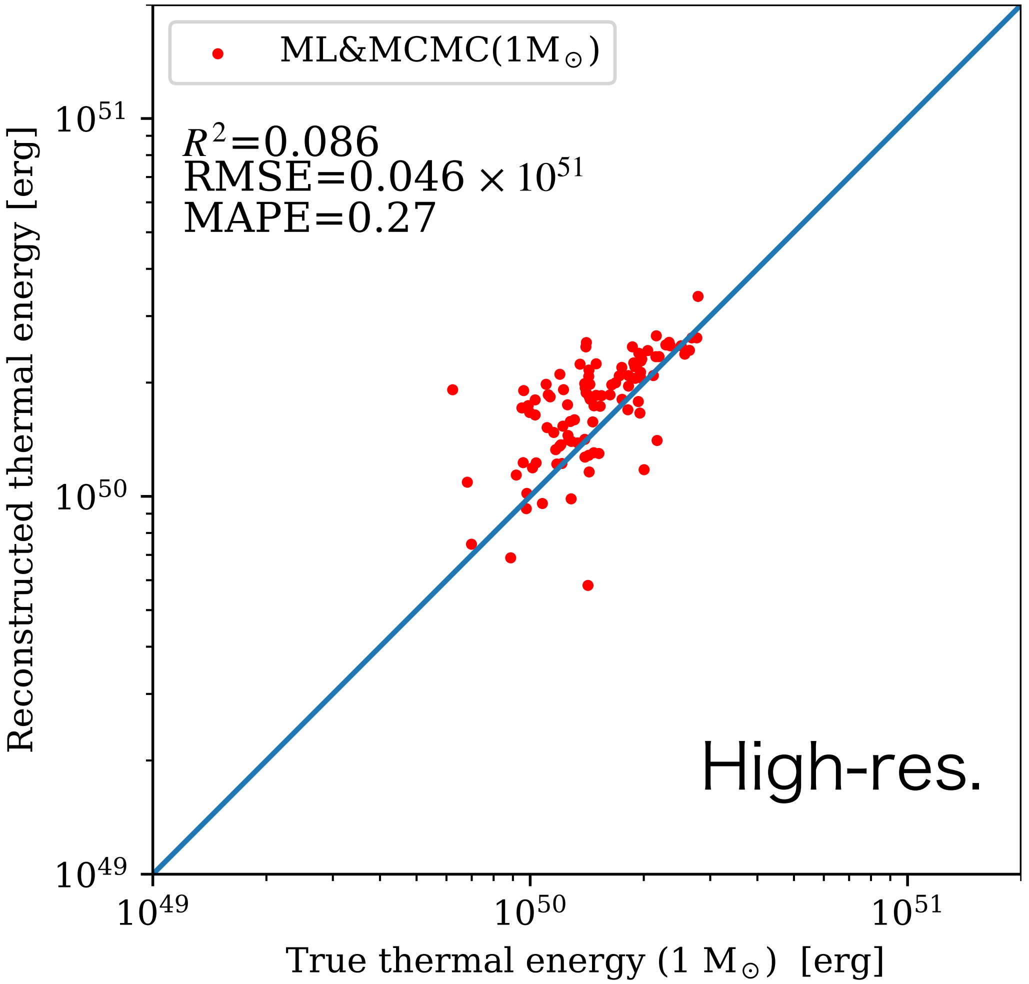
Fidelity Evaluation in Thermal Energy

- Compered to the low-res. sims., our method can duplicate the thermal energy

Low-res.



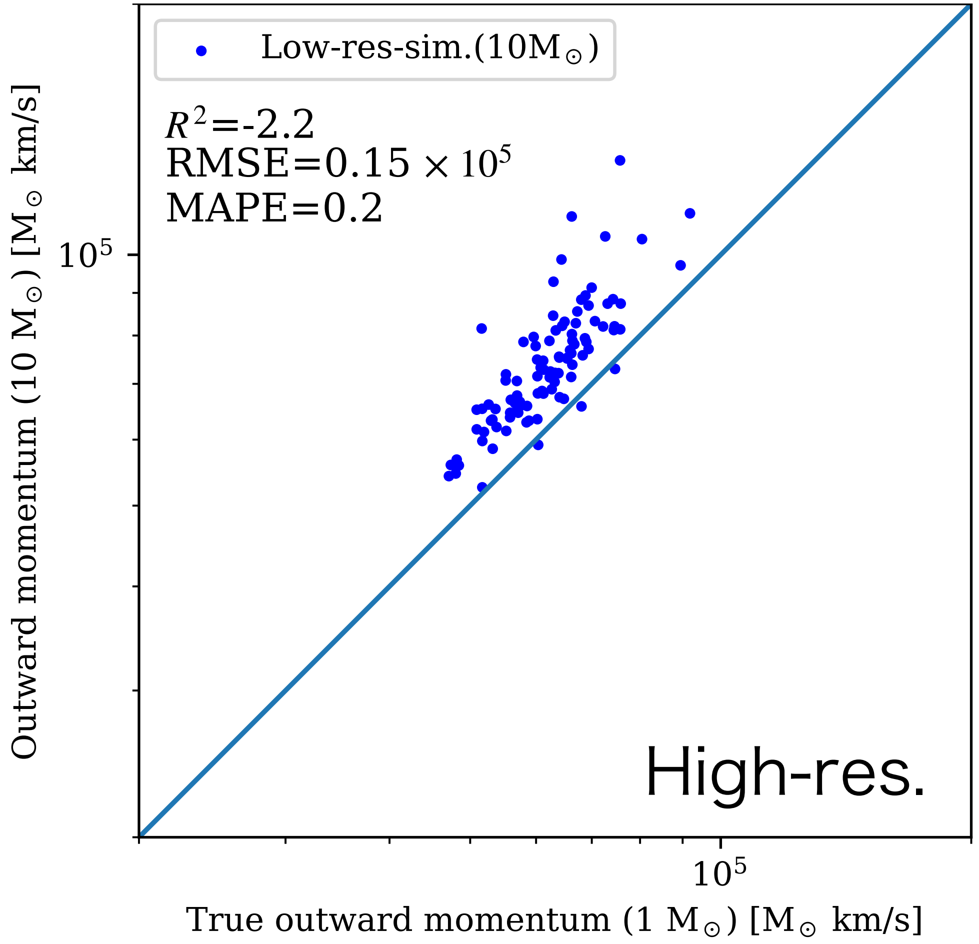
Ours



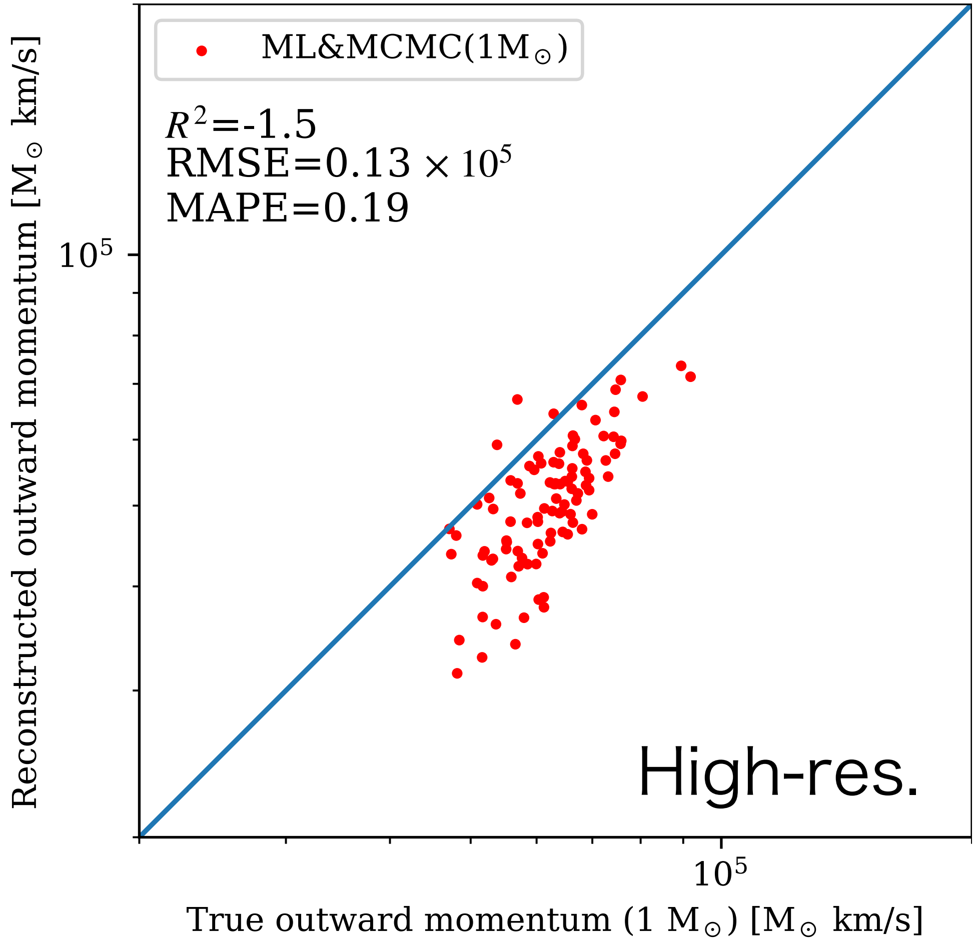
Fidelity Evaluation in Outer Momentum

- Almost similar to the low-res. sims.
- Need to get the bias removed

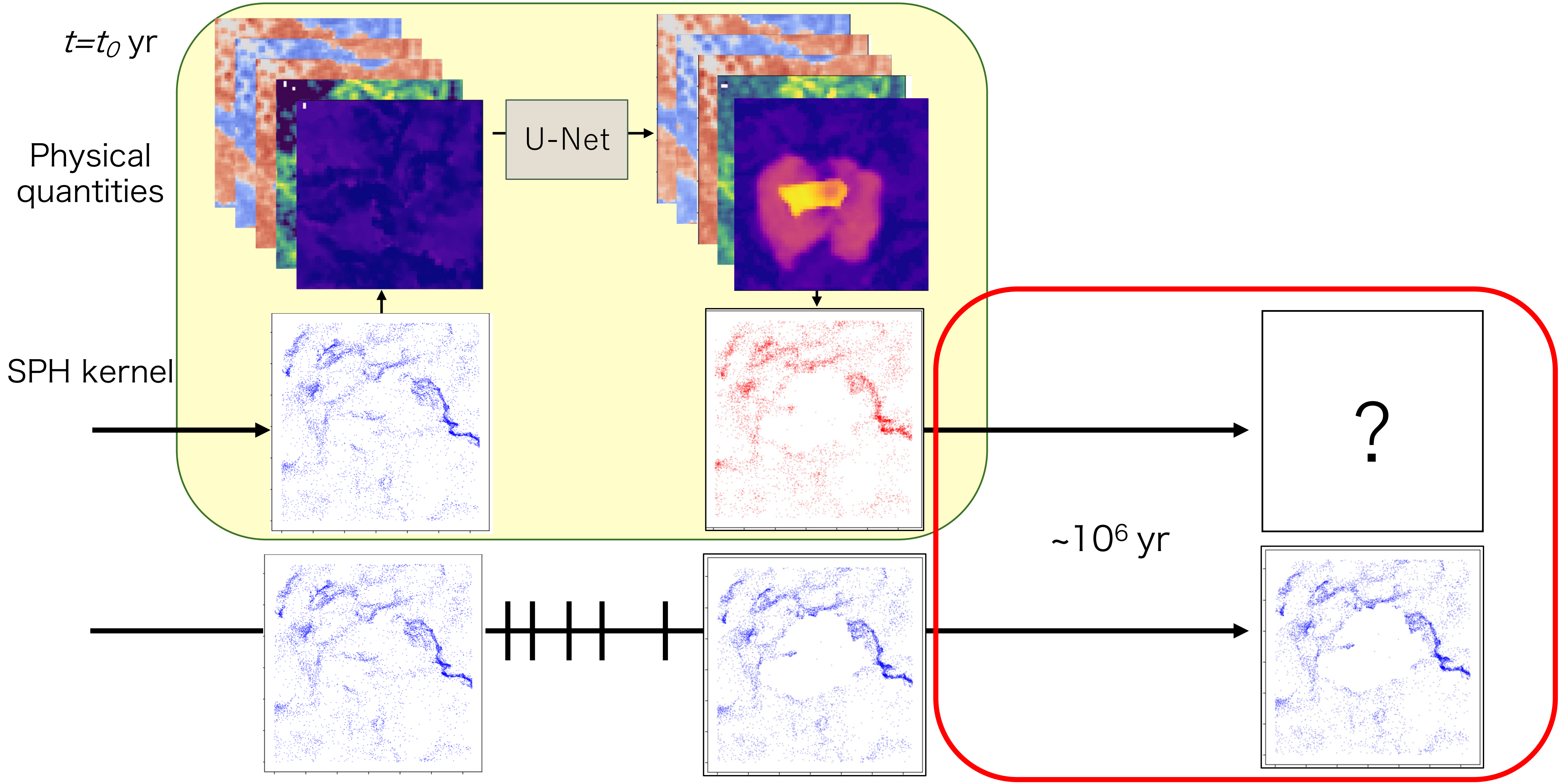
Low-res.



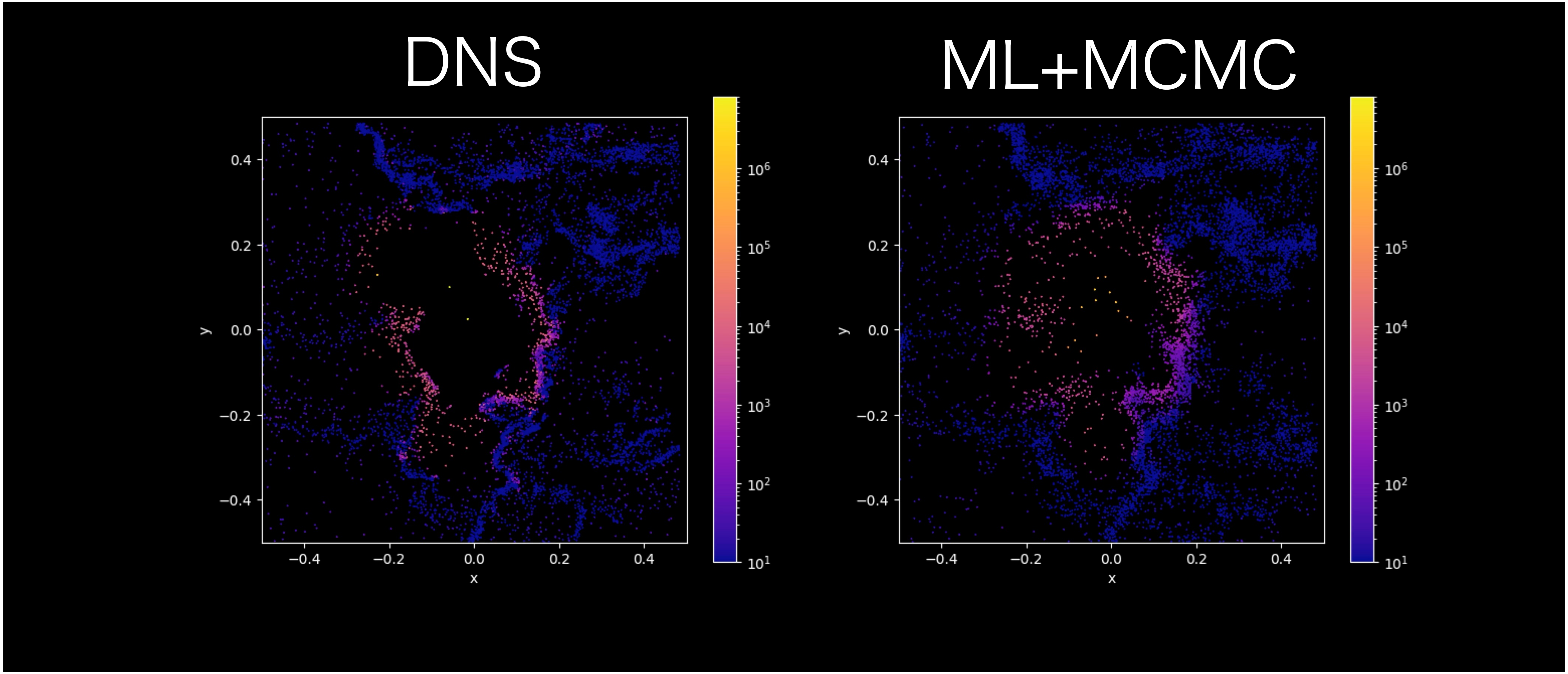
Ours



Experiment | Rerun the simulation



Preliminary Restart Run from 0.1 Myr



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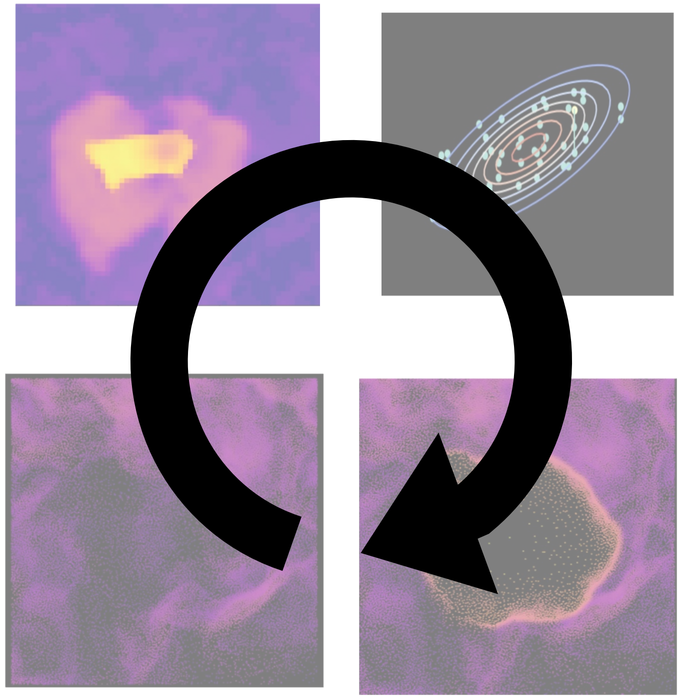
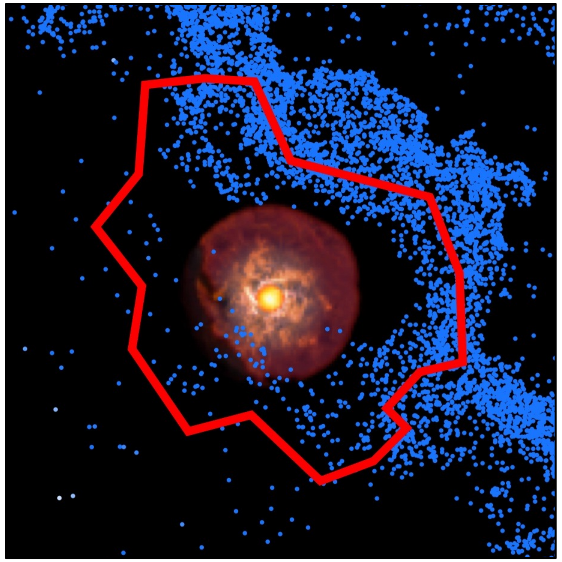
To conclude

Surrogate modeling

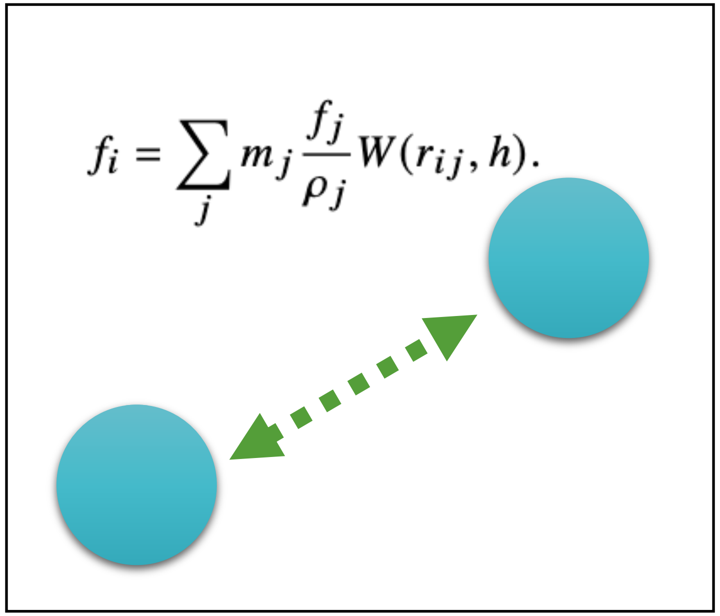


Hamiltonian Splitting

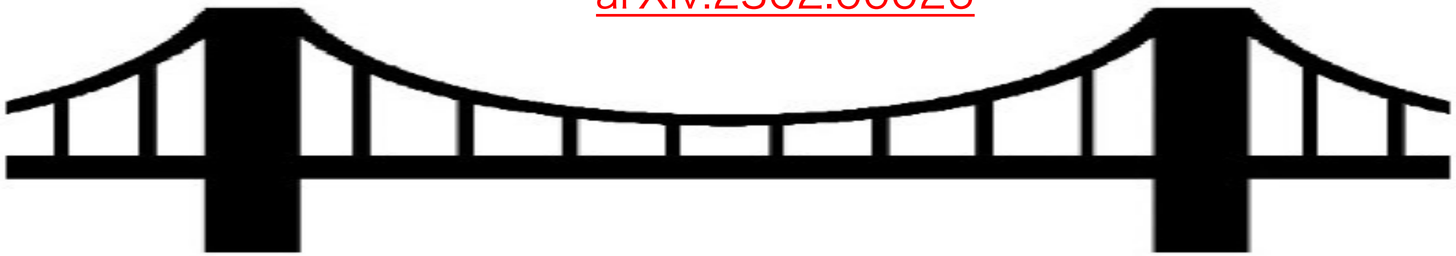


Hirashima et al. 2023, accepted for MNRAS
arXiv:2302.00026

Direct Numerical Simulations



- Stochastic
- Fast



- Deterministic
- Expensive

Accelerates 3D CNN Inference

SoftNeuro® [1] optimized 3D Unet for Fugaku!

	TF (Desktop, OneDNN) (16 cores / 32 threads)	TF (Fugaku) (1 node / 48 cores)	Softneuro (Fugaku) (1 node / 48 cores)
Elapsed time	710 [ms]	2820 [ms]	147 [ms]
CPU usage	36%	3.5%	68%

x19 FASTER!

Morpho's "SoftNeuro" Enables 19x Faster Inference of 3D Simulation on Fugaku

Press 2023/02/08

Tokyo, Japan – February 8th, 2023– Morpho, Inc. (hereinafter, "Morpho"), a global leader in image processing and imaging AI solutions, announced today that it has provided deep learning inference engine "SoftNeuro®" to a project

1. https://arxiv.org/abs/2110.06037
2. https://www.morphoinc.com/

Summary and Future Work

- An approach for surrogating SN simulations with ML and MCMC
- Need more accurate predictions
  - try generative models?
- Need higher-res simulations
  - Preparing for higher resolution (0.1 Msun) simulations
- Try particle-based models (e.g. Graph Neural Networks)

Thank You!!!!