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

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Abstract

Massive stars are known to explode at the end of their lives, called supernovae (SNe). SNe affect star formation and gas dynamics in galaxies. Traditional simulations have approximated this effect using so-called sub-grid models **because the simulations cannot resolve such small scales.** Our surrogate model with machine learning and Gibbs sampling better reproduces SN feedback, decreasing computational costs.

Background: Bottlenecks for Galaxy Simulations

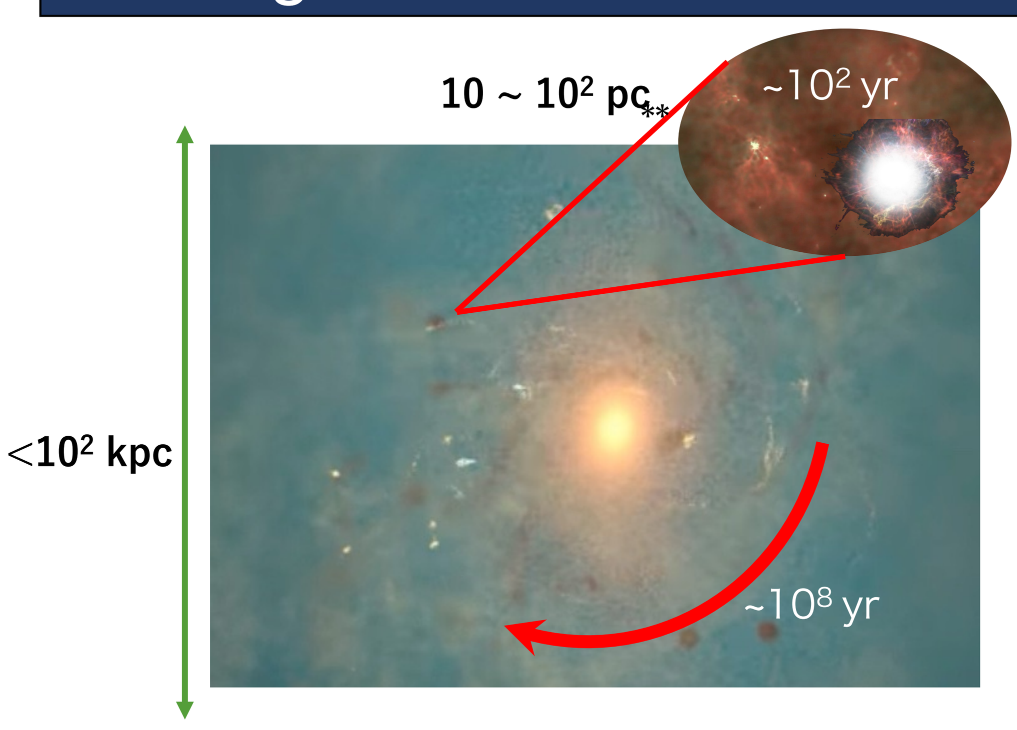

Fig.1 galaxy formation simulation using SPH*.

*SPH: Smoothed Particle Hydrodynamics
**pc: 1 pc is comparable to 3 light years.
*** $M_\odot$: a unit of mass equal to that of the Sun.
- https://www.youtube.com/watch?v=Rdd9KAUcvgQ

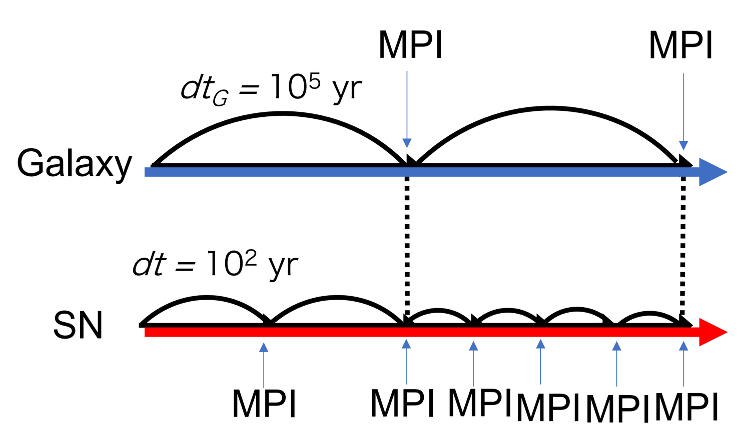

Fig.2 Integration and communication steps for each domain

- Galaxy formation involves several physical processes:
  - Gravity, hydrodynamic forces, Radiant cooling and heating, star formation, supernova (SN) explosions, and chemical evolution.
- Previous work achieved the mass resolution of $\sim 10^3 M_\odot$*** (e.g.,[1,2]):
  - This resolution means one particle in the simulation represents the mass of star clusters.
- To simulate individual stars in galaxy simulations (star-by-star sims):
  - For Milky-Way-sized galaxies, more than 10^{10} particles are needed.
  - The mass resolution of $1 M_\odot$.

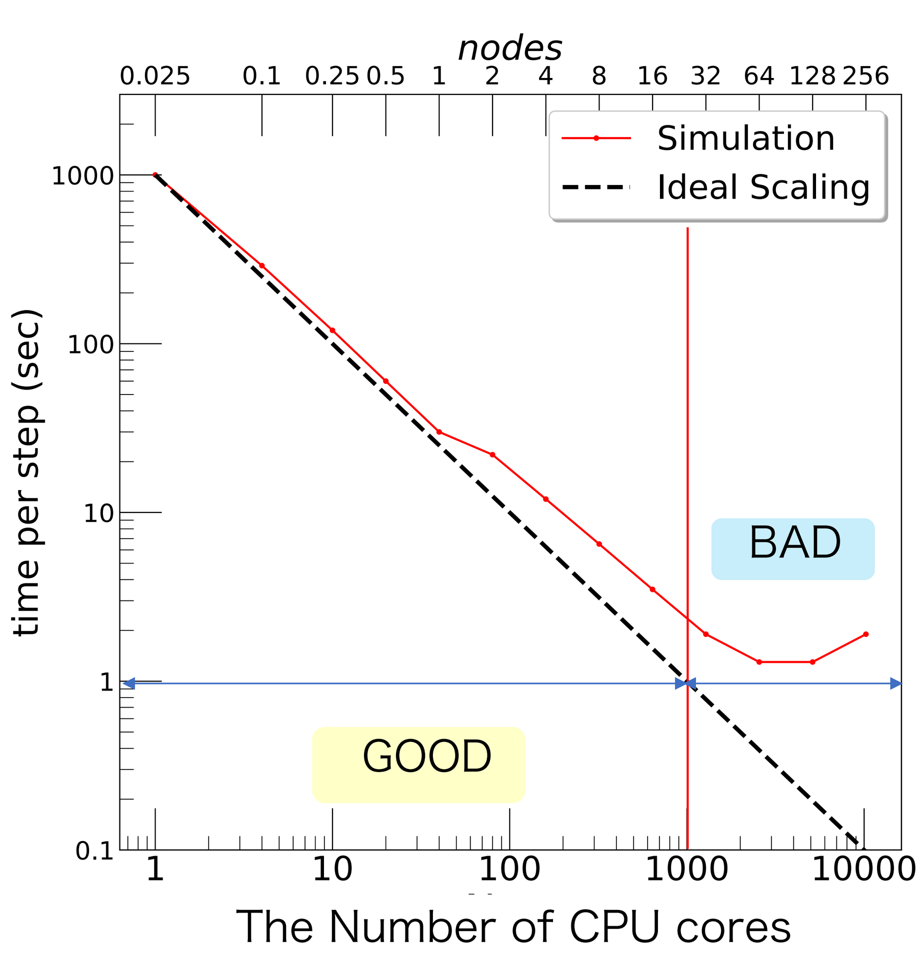

Fig.3 Strong scaling of a large galaxy simulation (Based on figure 63 in [3])

- The involvement in mass resolution depends on the scaling.
- Simulations often require smaller time steps to integrate smaller-scale phenomena (e.g., SNe) to enhance mass and spatial resolution, which increases calculation and communication costs (Fig. 2).
- However, parallelization efficiency usually **worsens** due to communication overheads (Fig. 3).
- New approaches for SN feedback are required to achieve high parallelization efficiency on 1000+ parallelization cores.

Surrogate Modeling for Supernova Feedback

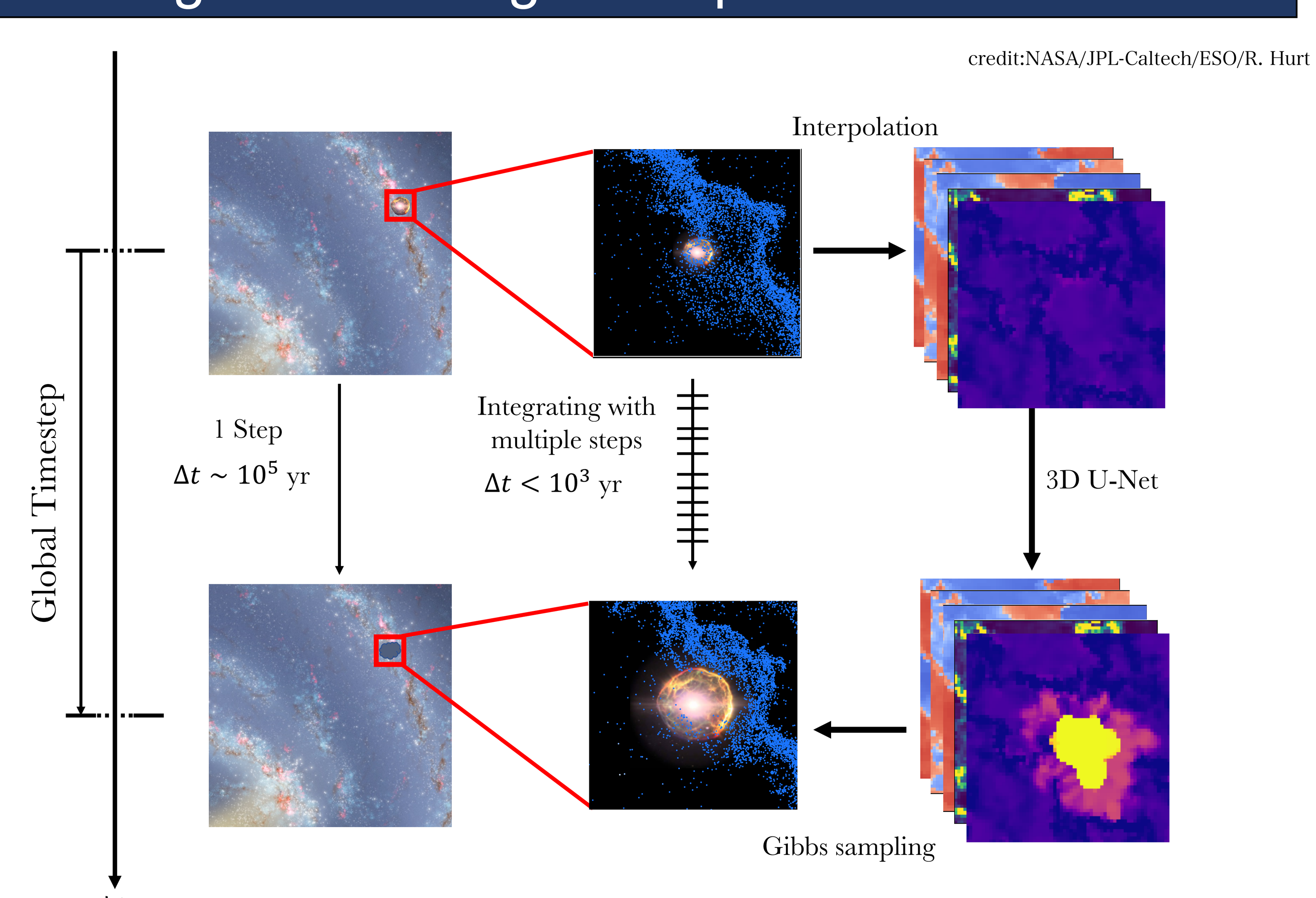

Fig.4 Surrogate modeling for computationally expensive supernova feedback

1. Interpolation
   - Physical quantities of SPH particles are interpolated in voxels with 3D Cartesian coordinates for CNN-based models.
2. 3D U-Net
   - Extended 2D U-Net [4], CNN-based model, to 3D
3. Gibbs Sampling
   - Particles are sampled using an MCMC based on predicted density distribution.

Morphological Evaluation

Fig 5 shows the (a) initial condition, (b) simulation elapsed 10^5 years, (c) reconstruction by sampling particles from the predicted 3D physical quantities, and (d) simulation elapsed 10^5 years with a low resolution. The color represents the temperature. We find that reconstruction (c) can resolve the detailed SN shell better than (d). Although (c) is globally similar to the high-resolution simulation (high-res. sims.), it is more fuzzy due to the limitation of spatial resolution. Comparing (b) and (d), the low-resolution simulation (low-res. sims), which has been employed in recent galaxy simulations, even has the challenge of resolving the thin, dense shell of the SN.

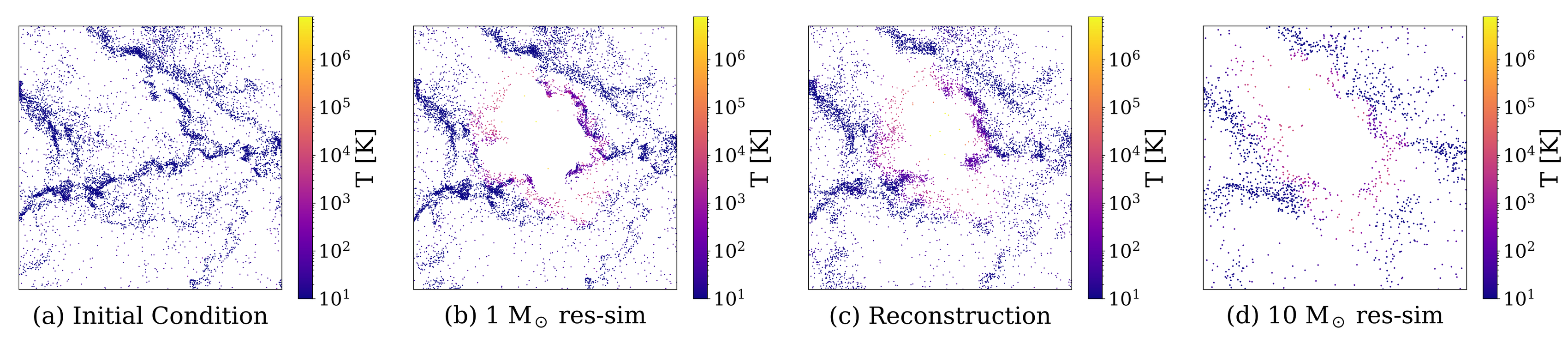

Fig.5 (a) The initial condition just before a SN explodes. **(b)** The result of high-resolution ($1\ M_\odot$) simulation 10^5 years after the explosion. **(c)** The reconstruction 10^5 years after the explosion by our approach. **(d)** The result of low-resolution ($10\ M_\odot$) simulation 10^5 years after the explosion. The color bar represents the temperature T of each particle.

Fidelity Evaluation

Settings:

- Evaluate the discrepancy between the low-res. ($10\ M_\odot$) to high-res. ($1\ M_\odot$) sims. (left), and our surrogate model to the high-res. sims. (right).
- Low-res. sims. use the same initial turbulence field as high-res. ones.

Performance of Our Surrogate Model:

- Successfully reconstructs the thermal energy of high-res. sims.
- Both show some bias in outer radial momentum.

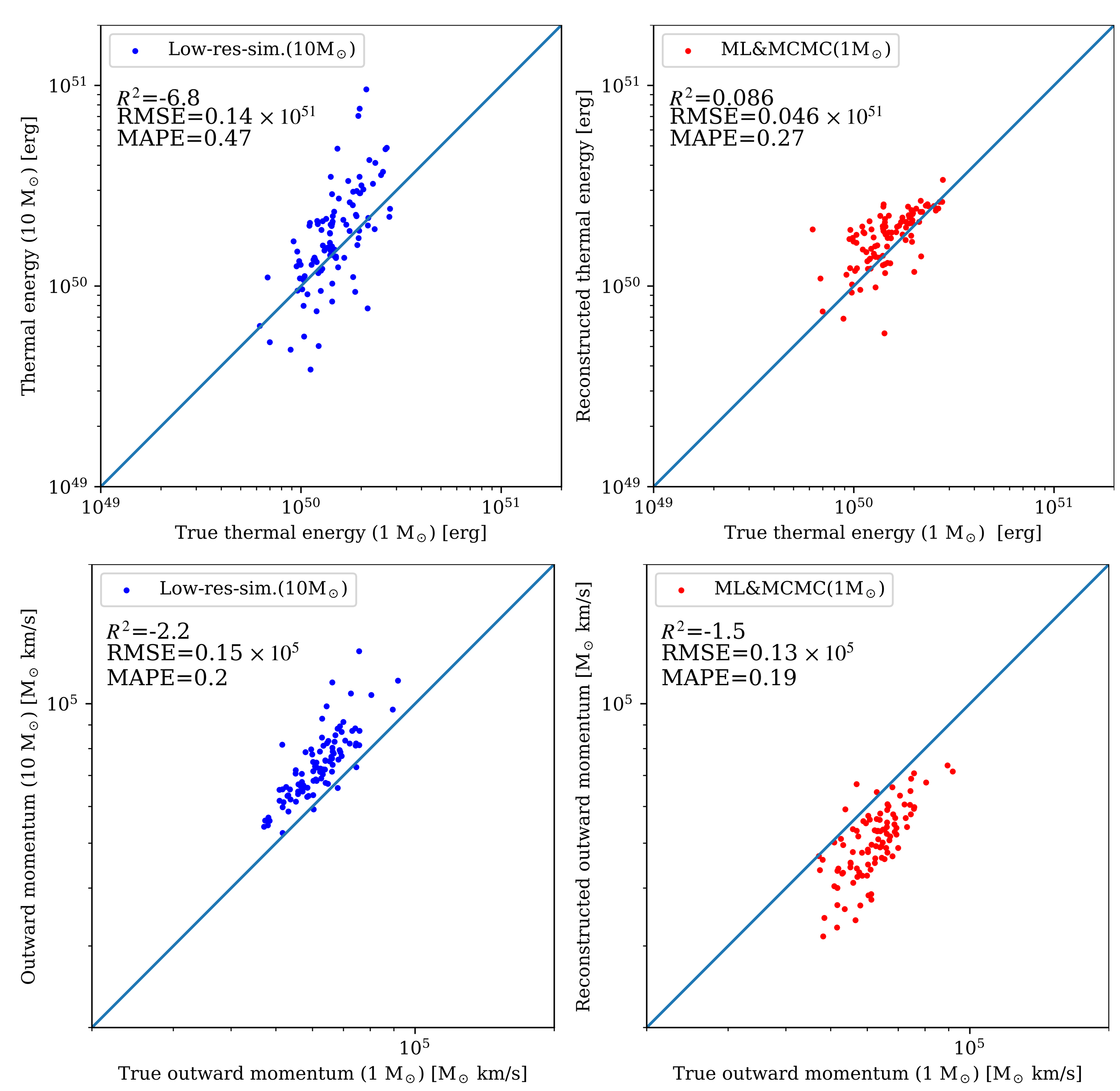

Fig.6 Fidelity evaluation in thermal energy (**top**) and outer radial momentum (**bottom**). Using the high-resolution simulation ($1\ M_\odot$ resolution; x-axis) results as a baseline, we compared our method (y-axis, **right**) with the corresponding low-resolution simulation ($10\ M_\odot$ resolution; y-axis, **left**). We evaluate 100 test data by the determination coefficient R^2, root mean squared error (RMSE), and mean absolute percentage error (MAPE).

Takeaways & Future Direction

- Developed the first surrogate model for SN feedback toward high-resolution galaxy formation simulations.
- Our approach can produce results that are more consistent than low-resolution simulations ($10\ M_\odot$), which is sufficiently high compared to the mass resolution of current galaxy formation simulations.
- Will study the method to project the prediction of the model learning high-resolution calculations onto low-resolution simulations.

References

[1] Applebaum et al. (2021) [2] Grand et al. (2021) [3] Springel et al. (2021) [4] Ronneberger et al. (2015)