First High-Resolution Galaxy Simulations Accelerated by a 3D Surrogate Model for Supernovae

Keiya Hirashima[1,2,*] **Kana Moriwaki**[1], **Michiko S. Fujii**[1], **Yutaka Hirai**[3,4], **Takayuki R. Saitoh**[5], **Junichiro Makino**[5], **Ulrich P. Steinwandel**[2], **Shirley Ho**[2,6,7]
[1]The University of Tokyo, [2] Flatiron Institute, , [3]University of Notre Dame, [4]Tohoku University, [5]Kobe University, [6] New York University, [7] Princeton University

Abstract

We introduce new high-resolution galaxy simulations enhanced by a surrogate model that reduces the computation cost. Some stars explode at the end of their lives, known as supernovae (SNe), which play a critical role in galaxy formation. The energy released by SNe is essential for regulating star formation and driving feedback processes in the interstellar medium (ISM). However, due to insufficient mass resolution, conventional simulations have employed simple *sub-grid models*, assuming a uniform environment, which fail to capture the inhomogeneity of the shell expansion of SNe within the turbulent ISM. Our new framework integrates numerical simulations and surrogate modeling, including machine learning and Gibbs sampling. The resulting distributions of the density and temperature of the ISM in the galaxy match those obtained from direct (resolved) numerical simulation. Our new approach achieves high-resolution fidelity while reducing computational costs by approximately 75 percent, effectively bridging the physical scale gap and enabling multi-scale simulations.

1 Introduction

Supernova (SN) explosions are highly energetic events that release an immense amount of energy that heats and expels the ambient interstellar medium (ISM). SNe significantly impact galactic evolution by driving galactic outflows and turbulence and influencing star formation rates and galaxy scale heights [1, 2]. Those dynamics are consequences of the interaction among non-linear physical processes such as gravity, hydrodynamics, radiation, star formation, and chemical evolution. To investigate the interplay of those complex physical processes, numerical simulations have been employed. In recent years, the development of compute architectures, combined with improvements in algorithms, has led to a surge of galaxy formation and evolution models that can resolve detailed relevant physical processes down to the resolution of single stars in low-mass dwarf galaxy systems. Still, the current resolution of more massive galactic ecosystems such as the Milky Way (MW) is limited to $\sim 10^3$ $\mathrm{M}_\odot$[2] per resolution element due to the computational cost requirements and the lack of scalability of many approaches for feedback physics in the multiphase ISM [3, 4]. One of the bottlenecks is caused by frequent communication between nodes due to small timesteps required for resolving hot and dense events such as SNe. To skip the bottleneck, SNe have been implemented with so-called *sub-grid models* [e.g., 5], which are assuming homogeneous environments and spherical symmetries. To directly incorporate the effect of SNe, we attempt to accelerate high-resolution galaxy simulations using machine learning. This paper presents the first framework integrating our surrogate model into numerical galaxy simulations with real-time predictions, as well as the accuracy and speed-up.

*hirashima.keiya@astron.s.u-tokyo.ac.jp

[2]1 $\mathrm{M}_\odot$ (solar mass) is a unit of mass equal to that of the Sun.

Machine Learning and the Physical Sciences Workshop, NeurIPS 2024.

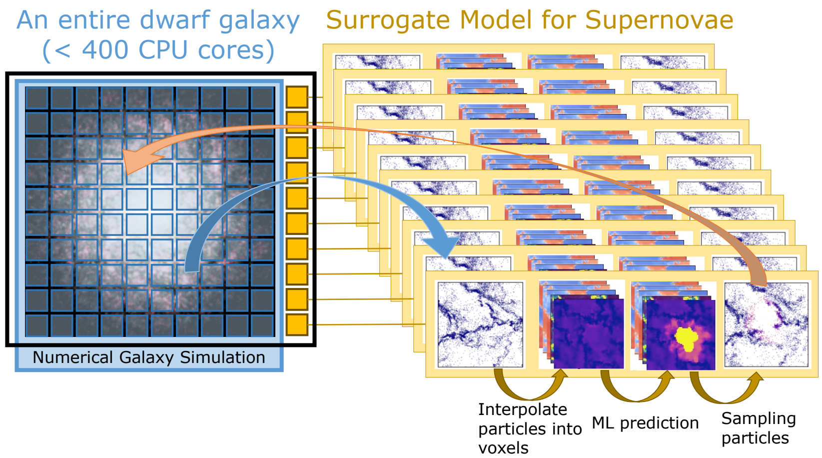

Figure 1: Schematic diagram for our new framework to skip bottlenecks of supernova feedback in galaxy simulations. Our surrogate model is 100 times faster at reconstructing the shell and distribution of thermal energy and momentum of a SN explosion in 3D.

2 Background

Related Works Machine learning (ML) has the potential to overcome the current limitations in resolution, allowing us to extend the range of physical scales in computationally intensive simulations [e.g., 6]. In the application for astrophysical simulations, ML-based surrogate models have been used to predict the gravitational dynamics to avoid direct calculations for billions of particles, representing dark matter and stars, over billions of years [7, 8] using convolutional neural networks (CNNs). Applying CNNs to particle-based simulations is not straightforward. Nevertheless, to gain efficient computation, we have developed machine learning approaches to learn time evolution with CNNs in particle-based hydrodynamics simulations by interpolating the particles on voxels [9, 10].

Bottlenecks in Galaxy Simulations The galaxy evolution simulations in this paper were carried out using our code ASURA-FDPS [11, 12, 9] implemented with Lagrangian (particle-based) methods of N-body for dark matter and stars and smoothed particle hydrodynamics (SPH) for gas. N-body discretizes Poison equations while the SPH method discretizes Euler equations with self-gravity and radiative cooling and heating. SPH offers advantages over Eulerian methods, such as Galilean invariance for non-symmetric systems like the ISM, the avoidance of numerical diffusion, and accurate mass conservation. SPH has been widely used in computational astrophysics and fluid dynamics to solve compressible fluid problems involving multi-scale physics. There may be challenges in resolving contact discontinuity by blastwaves, such as SN shells with low mass resolution. Nevertheless, it has been verified when the mass resolution is finer than 1 $M_\odot$ [13, 14, 9].

However, simulating MW-like galaxies with 1 $M_\odot$ resolution poses computational challenges, requiring over 10^{10} gas and star particles, far beyond current capabilities. This is because achieving such high-resolution simulations necessitates small timesteps, which is critical for accurately resolving SN explosions. The timesteps are constrained due to the Courant-like hydrodynamical timestep [15] based on the signal velocity [16, 17]. The timestep of a particle i is determined as

$$\Delta t_i = C_{\rm CFL} \frac{2h_i}{\max_j [c_i + c_j - 3w_{ij}]} \tag{1}$$

where $C_{\rm CFL} = 0.3$, h_i and c_i are the SPH kernel length and sound speed of a particle i, and

$$w_{ij} = \boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij} / r_{ij}, \tag{2}$$

where $\boldsymbol{r}_{ij}$ and $\boldsymbol{v}_{ij}$ are the relative position and velocity between particles i and j, respectively. Despite gas particles typically requiring a timestep of $\sim 10^4$ years, the hot and dense regions such as SNe require $\sim 10^2$ years given $h_i \propto \rho_i^{-1/3}$ and $c_i \propto T_i^{1/2}$. This can be a bottleneck in the simulation.

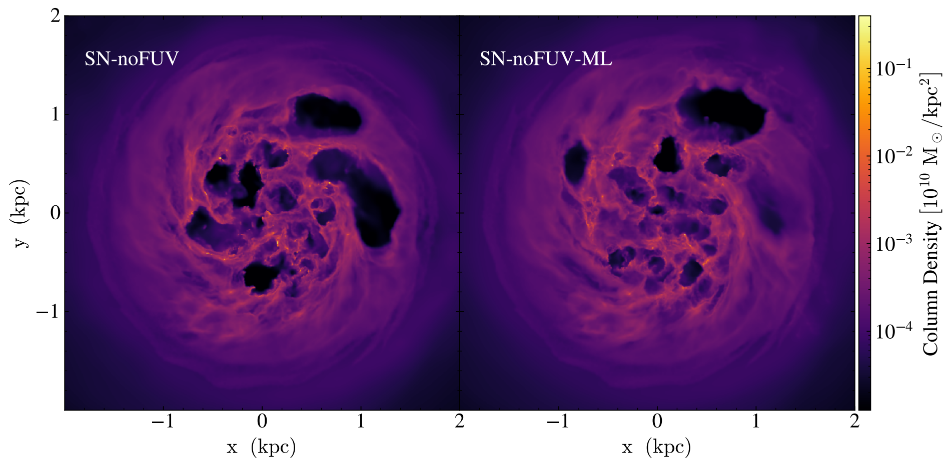

Figure 2: Face-on surface gas density at $t = 10^8$ years. The color bar represents the column density ($10^{10}\ \mathrm{M}_\odot\ \mathrm{kpc}^{-2}$). *Left*: Full numerical simulation implemented with the thermal feedback for SNe. *Right*: Our new framework with our surrogate model for SN explosions in denser environments.

Problem Definition - Divide and Conquer We designed a new framework for running simulations at high speed compared to conventional numerical simulations, even when increasing the resolution. To avoid the direct computation requiring small timesteps caused by SNe, we locally replace numerical simulation for SNe with our surrogate model presented in [10]. Fig 1 shows a schematic diagram of our presenting framework. In simulations of an entire galaxy (left), our surrogate model reconstructs SNe (right), reducing the need for direct simulations. The model reconstructs a particle distribution 10^5 years after the SN explosions, while the entire galaxy is calculated with a global timestep of $2,000$ years. After the galaxy simulation progresses by 10^5 years, the surrogate model's prediction is merged into the entire galaxy simulation, indicated by the orange arrow from right to left.

3 Methods

Surrogate Model for Supernova Explosions To address computational bottlenecks in galaxy simulations with multi-scale physics, we developed a ML-based surrogate model utilizing a U-Net architecture [18] based on CNNs, presented in [10]. The loss function, mean squared error, was minimized using the ADAM optimizer [19] with a learning rate of 10^{-5}. The model is applied for SN explosions in an environment denser than a hydrogen number density of $1\ \mathrm{cm}^{-3}$ where small timesteps are especially required. The training dataset includes 300 independent SN simulations in turbulent gas clouds with a mass resolution of 1 $\mathrm{M}_\odot$ and minimum timestep of ~ 100 years calculated by equation (1). The model predicts the physical distribution at $t = 10^5$ years after a SN explosion, given the initial gas distribution. The data represents 3D scalar fields with a size of 64^3 voxels and eight channels. The first two channels receive log-transformed density and temperature to effectively learn a wide range of physical quantities due to compressible hydrodynamics. Because velocities have a bimodal distribution, the 3D velocities were allocated into the rest of the six channels as positive v_x, v_y, v_z, and negative v_x, v_y, v_z. One side of the voxels is 60 parsec.

The model can reconstruct the results of high-resolution simulations with thermal energy and momentum conservation, which are crucial for galactic evolution [e.g., 5], better than low-resolution simulations. Additionally, this inference is 100 times faster than that of direct computation. With the prediction by our ML model, we reconstruct new particle distribution by the Gibbs sampling. The total mass is always conserved by sampling the same number of particles as the input from the predicted density distribution.

Simulation set-up For direct comparison between numerical simulations and our new ML-integrated method, we use an initial condition of a dwarf galaxy originally described in [13, 20], with the initial mass of $4 \times 10^7\ \mathrm{M}_\odot$ for gas. The initial disk consists of ~ 20 million particles, setting a gas particle mass resolution of $m_{\mathrm{gas}} = 4\ \mathrm{M}_\odot$. We run two simulations, *SN-noFUV-ML* and *SN-noFUV*, which are implemented with and without the surrogate model, respectively. In *SN-noFUV*, when SNe explode, the thermal energy of 10^{51} erg is injected into 100 neighbor particles (thermal feedback). In *SN-noFUV-ML*, our surrogate model reconstructs shells and the distribution of energy and velocities of a SN. We note that our surrogate model projects high-resolution (1 $M_\odot$) predictions from the learned model onto the galaxy simulations with a mass resolution of (4 $M_\odot$). The inference is accelerated by ONNX [21] and SoftNeuro [22] for x86 and ARM architecture, respectively.

4 Results

Fidelity Fig. 2 shows the surface density for isolated galaxy simulations. SNe are implemented with the thermal feedback described in Sec. 3 in *SN-noFUV* (left) and reconstructed with our surrogate model in *SN-noFUV-ML* (right). The morphological structures of the resolved gas resemble each other. Both have distinct cavities called superbubbles, formed by some stars that formed in dense, cold regions and underwent SN explosions almost simultaneously. In general, fine mass and time resolutions are required for accurately resolving such superbubbles; otherwise, the hot gas within the bubble cools too quickly. In our new scheme (*SN-noFUV-ML*), however, despite the longer timesteps, several distinct superbubbles emerged. We note that even with the same initial condition and same implementation, the gas distributions in two different simulations do not perfectly match due to randomness in some of the physical models, such as star formation.

Fig. 3 shows the density and temperature distribution in the galaxy. The histograms are averaged between 10^8 years with an interval of 10^7 years. *SN-noFUV-ML* replicates the bimodal distribution in density and temperature for *SN-noFUV*.

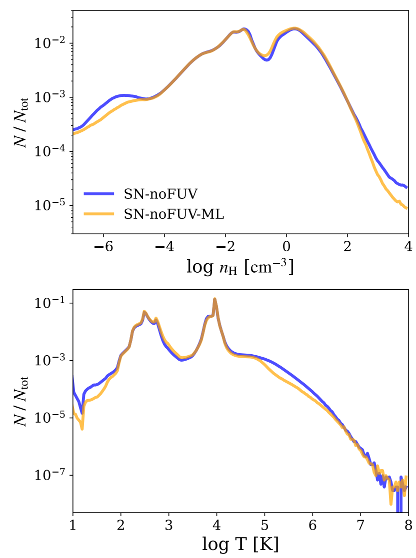

Figure 3: Density and temperature of gas in the galaxy. The particles are averaged using snapshots for 10^8 years.

Speed-up Fig. 4 compares calculation steps between full numerical simulations (*SN-noFUV*) and simulations accelerated by the surrogate model for SN feedback (*SN-noFUV-ML*). This type of galaxy simulation usually requires a few months to years. Thus, our surrogate model's reduction of the calculation steps may help run these simulations within a practical time and resources. As a practical example for a total simulation period of 10^9 years using $\sim$500 Cascade Lake CPUs, our framework can be completed within two months, reducing the runtime by approximately six months.

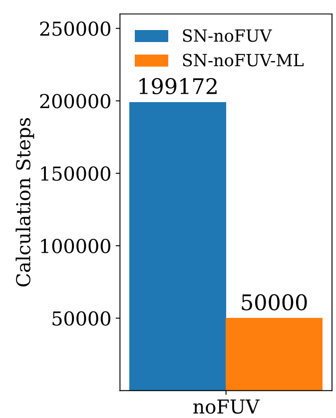

Figure 4: The comparison of calculation steps between direct simulations and our new framework accelerated by the surrogate model for 10^8 years.

5 Conclusions

We have implemented a surrogate model, incorporating a CNN-based machine learning model, into our galaxy simulation code. Our surrogate model projects high-resolution predictions of SN explosions from the learned model onto galaxy simulations. Our results show that this new framework can accurately replicate superbubbles, which typically require fine mass and time resolution, even with a fourfold speedup. Additionally, our simulation code with the surrogate model for SNe can reconstruct gas density and temperature structures. We plan to run high-resolution simulations for LMC-like and WM-like galaxies, which are ten and one hundred times larger than the galaxy studied in this paper and have been challenging to simulate fully numerically. Our new framework may enable these high-resolution and more massive galaxy simulations, allowing us to study the evolution of structures in galaxies such as the MW in much more detail than ever.

References

[1] Naab, T., J. P. Ostriker. Theoretical Challenges in Galaxy Formation. *ARA&A*, 55(1):59–109, 2017.

[2] Somerville, R. S., R. Davé. Physical Models of Galaxy Formation in a Cosmological Framework. *ARA&A*, 53:51–113, 2015.

[3] Hopkins, P. F., A. Wetzel, D. Kereš, et al. FIRE-2 simulations: physics versus numerics in galaxy formation. *MNRAS*, 480(1):800–863, 2018.

[4] Applebaum, E., A. M. Brooks, C. R. Christensen, et al. Ultrafaint Dwarfs in a Milky Way Context: Introducing the Mint Condition DC Justice League Simulations. *ApJ*, 906(2):96, 2021.

[5] Kim, C.-G., E. C. Ostriker. Momentum Injection by Supernovae in the Interstellar Medium. *ApJ*, 802(2):99, 2015.

[6] Kochkov, D., J. A. Smith, A. Alieva, et al. Machine learning-accelerated computational fluid dynamics. *Proceedings of the National Academy of Science*, 118(21):e2101784118, 2021.

[7] He, S., Y. Li, Y. Feng, et al. Learning to predict the cosmological structure formation. *Proceedings of the National Academy of Science*, 116(28):13825–13832, 2019.

[8] Jamieson, D., Y. Li, R. A. de Oliveira, et al. Field-level Neural Network Emulator for Cosmological N-body Simulations. *ApJ*, 952(2):145, 2023.

[9] Hirashima, K., K. Moriwaki, M. S. Fujii, et al. 3D-Spatiotemporal forecasting the expansion of supernova shells using deep learning towards high-resolution galaxy simulations. *MNRAS*, 526(3):4054–4066, 2023.

[10] —. Surrogate Modeling for Computationally Expensive Simulations of Supernovae in High-Resolution Galaxy Simulations. *arXiv e-prints*, arXiv:2311.08460, 2023.

[11] Saitoh, T. R., H. Daisaka, E. Kokubo, et al. Toward First-Principle Simulations of Galaxy Formation: I. How Should We Choose Star-Formation Criteria in High-Resolution Simulations of Disk Galaxies? *PASJ*, 60(4):667–681, 2008.

[12] Iwasawa, M., A. Tanikawa, N. Hosono, et al. Implementation and performance of FDPS: a framework for developing parallel particle simulation codes. *PASJ*, 68(4):54, 2016.

[13] Hu, C.-Y., T. Naab, S. Walch, et al. Star formation and molecular hydrogen in dwarf galaxies: a non-equilibrium view. *MNRAS*, 458(4):3528–3553, 2016.

[14] Steinwandel, U. P., B. P. Moster, T. Naab, et al. Hot phase generation by supernovae in ISM simulations: resolution, chemistry, and thermal conduction. *MNRAS*, 495(1):1035–1060, 2020.

[15] Courant, R., K. Friedrichs, H. Lewy. Über die partiellen Differenzengleichungen der mathematischen Physik. *Mathematische Annalen*, 100:32–74, 1928.

[16] Monaghan, J. J. SPH and Riemann Solvers. *Journal of Computational Physics*, 136(2):298–307, 1997.

[17] Springel, V. The cosmological simulation code GADGET-2. *MNRAS*, 364(4):1105–1134, 2005.

[18] Ronneberger, O., P. Fischer, T. Brox. U-Net: Convolutional Networks for Biomedical Image Segmentation. *arXiv e-prints*, arXiv:1505.04597, 2015.

[19] Kingma, D. P., J. Ba. Adam: A method for stochastic optimization. In Y. Bengio, Y. LeCun, eds., *3rd International Conference on Learning Representations, ICLR 2015, San Diego, CA, USA, May 7-9, 2015, Conference Track Proceedings*. 2015.

[20] Hu, C.-Y., T. Naab, S. C. O. Glover, et al. Variable interstellar radiation fields in simulated dwarf galaxies: supernovae versus photoelectric heating. *MNRAS*, 471(2):2151–2173, 2017.

[21] ONNX Runtime developers. Onnx runtime. `https://onnxruntime.ai/`, 2021. Version: 1.17.1.

[22] Hilaga, M., Y. Kuroda, H. Matsuo, et al. SoftNeuro: Fast Deep Inference using Multi-platform Optimization. *arXiv e-prints*, arXiv:2110.06037, 2021.

Acknowledgement

The authors thank Carolina Cuesta-Lazaro for fruitful discussions. This research used computational resources of the supercomputer Fugaku provided by the RIKEN Center for Computational Science. The computations reported in this paper were, in part, performed using CfCA XC50 system (National Astronomical Observatory of Japan) and resources made available by the Flatiron Institute. The model was trained using Wisteria/BDEC-01 at the Information Technology Center at the University of Tokyo. This research was supported by MEXT as "Program for Promoting Research on the Supercomputer Fugaku" (Structure and Evolution of the Universe Unraveled by Fusion of Simulation and AI; Grant Number JPMXP1020230406; Project ID: hp230204, hp240219). This work was also supported by JSPS KAKENHI Grant Numbers 22H01259, 22KJ0157, 21H04499, 21K03614, and 23K03446. KH is supported by JSPS Research Fellowship for Young Scientists and accompanying Grants-in-Aid for JSPS Fellows (22J23077 and 22KJ1153), JEES · Mistubishi corporation science technology student scholarship in 2022, and The University of Tokyo doctoral fellowship with the IIW program, and thanks CCA at the Flatiron Institute for hospitality and the National Science Foundation under Cooperative Agreement PHY-2019786 (The NSF AI Institute for Artificial Intelligence and Fundamental Interactions, `http://iaifi.org/`) for support while a portion of this research was carried out. YH is supported by the grant OISE-1927130: The International Research Network for Nuclear Astrophysics (IReNA), awarded by the US National Science Foundation (NSF). UPS is supported by a Flatiron Research Fellowship (FRF) at the Flatiron Institutes Center for Computational Astrophysics (CCA). The Flatiron Institute is supported by the Simons Foundation.