SEDONA-GesaRaT: a Deep Learning Accelerated Radiative Transfer Program for 3-D Supernova Simulations

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We present SEDONA-GesaRaT, a speed-up code for supernova radiative transfer calculations based on the Monte-Carlo radiative transfer code SEDONA. We use an atomic physics neural network (APNN) (with a convolutional neural network (CNN) structure) to solve for both for local thermodynamic equilibrium (LTE) and non-LTE (NLTE) radiative transfer. SEDONA-GesaRaT is trained and validated on 119 1-dimensional (1-D) Type Ia supernova (SN Ia) radiative transfer simulation results done using SEDONA. It has been applied to the 3-dimensioal (3-D) SN Ia explosion model N100 (**?**) to perform a 3-D LTE and NLTE radiative transfer calculations for the photospheric epoch. In LTE, a speed-up factor of about ??? was obtained. In NLTE, no speed-up factor can be calculated at present since the 3-D NLTE SEDONA calculation is beyond our current resources. However, for SEDONA-GesaRaT a single NLTE radiative transfer calculation takes $\sim$ 3000 core-hours on computer ???? and a comparable SEDONA calculation would take much longer. For our most realistic NLTE calculation, spatially resolved linear polarization data cubes of the N100 model are calculated with a high signal-to-noise ratio using the integral-based technique (IBT) (**?**). The large computational speed-up factor makes SEDONA-GesaRaT promising for future large-scale simulations that systematically study the internal structures of supernovae. However, the ultimate advantages of SEDONA-GesaRaT will depend on the required computational cost of retrainings to accommodate improvements in physical realism in radiative transfer and a wider range of supernova models.

Unified Astronomy Thesaurus concepts: Ejecta (453); Monte Carlo methods (2238); Radiative transfer (1335); Radiative transfer simulations (1967); Supernovae (1668); Type Ia supernovae (1728)

1. Introduction

Radiative transfer (RT) is a critical tool in supernova (SN) research, providing the ability to synthesize observables including

light-curves, spectra, and spectropolarimetry based on the theoretical structures of SNe: i.e., SN models. Matching synthesized observables to actual observables verifies the SN models insofar as the RT is realistic. So improved realism in RT is a continuing goal and improved realism requires computational speed-ups given the large computational demands of fully adequate realism whatever that ultimately turns out to be. In this introduction, we briefly review the state of the art of radiative transfer relevant to SNe and introduce our machine learning (ML) speed-up code.

Many SN RT codes (e.g., TARDIS **?**; CMFGEN, **?**) are based on a 1-dimensional (1-D) spherically symmetric approximation. Reasonable agreement between different RT programs has been shown (**?**) and spectral and light-curve modeling based on both type Ia supernovae (SNe Ia) and core-collapse supernovae (CCSNe) models has verified these models to some degree (e.g., **???**). However, imaging of nearby SN remnants (e.g., **??**) and spectropolarimetry observations of SNe (e.g., **??**) suggest that both SNe Ia and CCSNe have complex 3-dimensional (3-D) structures which are also revealed in multidimensional hydrodynamic simulations (e.g., **???**). Therefore, 3-D radiative transfer is needed to further verify 3-D SN models.

Although several multidimensional RT codes have been developed (e.g., **??**) based on the Monte-Carlo method, 3-D time-dependent RT remains computationally challenging due to the large number of Monte-Carlo photon packets required to achieve high signal-to-noise (S/N) results and the large number of spatial grid points needed to solve for the plasma excitation and ionization state (i.e., the thermal state). In particular, very high S/N is needed to synthesize accurate polarization spectra. To reduce the Monte-Carlo noise in synthesized polarization spectra, **?** proposed a virtual packet method which increases computational efficiency, and so allows increased number of (photon) packets and increased S/N. Based on the virtual packet method, **?** developed an integral-based technique (IBT) which further increases the

computational efficiency.

Full realism in SN RT requires full non-local thermodynamic equilibrium (NLTE) requiring a detailed calculation of atomic transition rates to determine the statistical equilibrium of all the atomic levels (i.e., the full thermal state). Because such calculations are very demanding, most 3-D RT simulations adopt local thermodynamic equilibrium (LTE) or approximated NLTE to strike a balance between computational resources and physical realism. Other simplifications have been presented. For example, a level-merging method (**???**) has been developed to reduce the number of atomic levels considered in NLTE for approximate results. For another example, **?** presented a data-driven method that synthesizes 3-D NLTE RT spectra from 3-D LTE simulations and 1-D NLTE simulations using the extracted SN model along the line-of-sight.

Inspired by the progress in ML accelerated computational fluid dynamics (e.g., **?**) and several successful applications of deep neural networks on supernova spectral data analysis (e.g. **??**), we present a deep learning method to accelerate LTE and the NLTE RT for SNe. The method in embodied in the code SEDONA-GesaRaT (the Gesamtkunstwerk of Radiative Transfer). SEDONA-GesaRaT is based on SEDONA (**?**), a multi-dimensional Monte-Carlo RT code for SN spectral and light-curve simulation, and includes the IBT algorithm (**?**) developed in our previous research.

Note, the physical processes included in SEDONA are: (1) gamma-ray emission from radioactive elements; (2) gamma-ray bound-free transition, Compton scattering, and photoelectric scattering; (3) optical photon bound-bound, bound-free, free-free transitions. An NLTE solver in SEDONA can be turned on for individual elements to determine the level populations in statistical equilibrium, but the computational cost is increased by a factor of ~ 100 relative to LTE. This is a computation bottleneck for high-precision 3-D SN RT and reducing this bottleneck is a key feature of SEDONA-GesaRaT.

Section 2 discusses the results of SNe Ia 1-D NLTE RT simulations, which serve as the training and testing data set for the atomic physics neural network (APNN). (Note, in fact a set of APNNs are needed, but for simplicity we use the singular APNN, unless we need to specify more than one of them.) Section 3 tests the SEDONA-GesaRaT code on 3-D time-dependent RT simulations, and presents the first 3-D RT simulation result with both NLTE processes and spatially-resolved spectropolarimetry data cubes, using the SN Ia explosion model N100 (**?**). Section 4 gives the conclusions. Appendix A gives details of the APNN and its training, Appendix B details of the testing of the APNN with 1-D SN Models, and Appendix C a discussion of some details for future work. The code of SEDONA-GesaRaT is available on https://github.com/GeronimoChen/GesaRaT.

2. NLTE Radiative Transfer

2.1. Line Expansion Opacity Approximation

In SEDONA time-dependent RT calculations, the energy deposition of radioactive isotopes ^{56}Co and ^{56}Ni is calculated by transporting gamma-ray energy packets and determining the energy they deposit in the ejecta due to Compton scattering and photoionization. The radioactive energy deposited in the ejecta is re-emitted as thermal (UV/optical/infrared) photons; and the photons with similar space-time coordinates, frequencies, propagating directions are represented by an optical energy packet. When optical energy packets are propagating through a plasma cell in a time step, the packet energies and trajectories are integrated to calculate the angle-averaged specific intensity in the comoving frame ($\bar{J}_\nu$) over a given frequency grid. The plasma level population and free electron density of the plasma cell is solved under LTE or NLTE approximation with Brent's method (**?**) with the input of $\bar{J}_\nu$,

elemental abundances, and plasma density.

There are two kinds of mechanisms in SEDONA that could change the directions and the frequencies of optical energy packets, and the probability of triggering either of the mechanisms per propagating distance unit is defined as extinction coefficient. The first kind of mechanism represent the Thomson scattering process independent from the frequency, with a comoving frame extinction coefficient defined as $\bar{k}_e$:

$$\bar{k}_e = \sigma_{\rm T}\ n_e\ , \tag{1}$$

where $\sigma_{\rm T}$ is the Thomson scattering cross section, n_e is the plasma free electron number density. In the following, comoving frame quantities are denoted with a bar, whereas non-bar quantities refer to the lab frame. When an optical energy packet is triggered for Thomson scattering, the new propagating direction and the polarization state is sampled with Rayleigh scattering matrix (**?**), the comoving frame frequency and the comoving frame energy are not changed.

The second kind of mechanism represents bound-bound, bound-free, and free-free transitions, which are frequency dependent, defined as $\bar{k}$ on a given frequency grid. The emission coefficient $\bar{j}$ in the comoving frame is defined as the emitted energy per solid angle per frequency unit per volume per time unit through the isotropic emission from bound-bound, bound-free, and free-free transitions. The contribution of bound-free and free-free transitions to $\bar{k}$ follows the recipe in **?**. In the previous 1-D NLTE RT simulations using SEDONA (e.g. **?**), the bound-bound line opacity is calculated with a refined frequency grid to resolve the Voigt profile of each spectral line, and the computation resources requirements are infeasible to run ~ 100 1-D time-dependent RT simulations in this study. Therefore, the bound-bound line opacity is calculated under the Sobolev approximation and using an expansion opacity formalism (**?**). Specifically, the individual Sobolev line optical depth is calculated as

$$\tau_{\rm Sob} = \frac{h}{4\pi}\left(N_l B_{lu} - N_u B_{ul}\right) t_{\rm exp} c\ , \tag{2}$$

where h is the Planck constant, B_{lu} and B_{ul} are Einstein B coefficients, N_l and N_u are

the level population number densities of the lower level (l) and the upper level (u), $t_{\rm exp}$ is the time after the SN explosion, and c is the speed of light. The probability that a photon interacts with a line when coming into resonance with it is

$$p_{\rm int} = 1 - e^{-\tau_{\rm Sob}} \ , \tag{3}$$

where $p_{\rm int}$ is an interaction probability. In the expansion opacity formalism, the total bound-bound extinction coefficient is calculated by summing all lines within a given frequency bin

$$\bar{k}_{bb}(\bar{\nu}, \bar{\nu} + \Delta\bar{\nu}) = \frac{(\bar{\nu} + 0.5\Delta\bar{\nu}) \sum_i p_{{\rm int},i}}{\Delta\bar{\nu}\ t_{\rm exp}\ c} \ , \tag{4}$$

where $\Delta\bar{\nu}$ is the frequency bin width in the comoving frame and the summation is over all the spectral lines in the frequency bin. The bound-bound extinction coefficient is summed with the bound-free extinction coefficient and the free-free extinction coefficient, which are calculated in the same frequency bin, to form the total extinction coefficient $\bar{k}$.

The emission coefficients from bound-free, and free-free transitions are also calculated in a given frequency grid following the recipe in **?**. The bound-bound emission coefficient with line expansion opacity approximation is:

$$\bar{j}_{bb}(\bar{\nu}, \bar{\nu}+\Delta\bar{\nu}) = \frac{(\bar{\nu} + 0.5\Delta\bar{\nu})}{\Delta\bar{\nu}\ t_{\rm exp} c} \sum_i \left(\frac{p_{\rm int} A_{ul} N_u}{N_l B_{lu} - N_u B_{ul}} \right)_i \ , \tag{5}$$

where A_{ul} is the Einstein A coefficient and the summation is over all the spectral lines in the frequency bin. The bound-bound emission coefficient is summed with the bound-free and free-free emission coefficients to calculate the total emission coefficient $\bar{j}$. When the isotropic absorption and emission is triggered, the new propagating direction of the optical energy packet is sampled following isotropic emission in the comoving frame, the frequency is sampled from the total emission coefficient $\bar{j}$, the polarization state is set to zero, and the energy in the comoving frame is not changed.

Note that in the expansion opacity formalism, the individual line profiles are not resolved. This approximation should be reasonable with the bin only including optically thin lines ($\tau_{\rm sob} < 1$). If the bin includes multiple optically thick lines,

however, the angle-averaged specific intensity in the comoving frame ($\bar{J}_\nu$) in each line may be less reliable. Further NLTE studies are needed to compare the differences between resolved line transport and the expansion opacity formalism.

2.2. HESMA Data Set

We downloaded the 119 SN Ia models (i.e., ejecta structure models) from the Heidelberg Supernova Model Archive (HESMA)[1] (**?**), then used SEDONA (**?**) to conduct a 1-D time-dependent RT simulation of all the models. Lists of the models are shown in Appendix A. In the 1-D time-dependent RT simulation, we use two sets of atomic data libraries: CMF_All and CMF_100. The atomic data library CMF_100 is reduced from the CMFGEN[2] (**?**) database to limit the data for each ion to no more than the 100 lowest lying levels; the total number of levels is 28,105, and the total number of transitions is 274,128. CMF_All includes all of the atomic levels and transitions from the CMFGEN database, but the Si, S, and Ca elements are kept the same as CMF_100 in order to control the NLTE atomic physics computation time; this amounts to, for all ionic species, 497,424 levels and 35,344,426 bound-bound transitions. The forbidden lines (e.g., Ca II 7291 Å, Ca II 7324 Å) are not included in the two atomic data libraries.

The HESMA SN Ia models are specified at 100 seconds after the explosion. Before the RT simulation, the model ejecta structure is remapped to day 1 after the explosion, assuming adiabatic and homologous expansion, and the energies from the decay of radioactive elements before day 1 are converted to local thermal energies, which act as the initial plasma temperatures in the following RT calculations.

We use SEDONA to perform 1-D RT simulation until 60 days after the explosion. Before 14.78 days, the simulation time step is logarithmic with $\Delta t_s/t_s = 0.02$. After 14.78 days, the simulation time step is

[1]https://hesma.h-its.org/

[2]https://sites.pitt.edu/∼hillier/web/CMFGEN.htm

Fig. 1.— The spectropolarimetry time sequence of the 3-D N100 model at the viewing direction $\mu = 0.5$, $\varphi = 3.4455$. The blue line is calculated by SEDONA which use traditional method to solve the source function, while the orange dashed line is calculated by SEDONA-GesaRaT using APNN to solve the source function, both solutions use the CMF_100 LTE recipe for atomic physics. From left to right, the first panel shows the optical wavelength flux from 2000 Å to 10000 Å, the second panel shows the infrared wavelength flux from 10000 Å to 50000 Å, the third panel shows the linear polarization percentage Q/I, the fourth panel shows the linear polarization percentage U/I. The x axes in the third and the fourth panels are in logarithmic scale for better presentation.

$\Delta t_{\rm s} = 0.2$ days. In each time step, 5×10^4 energy packets are created that are inflow to the energy packet population which also has an outflow in each time step due to energy packets escaping the SN ejecta. The frequency grid to calculate $\bar{J}_\nu$, $\bar{k}$, $\bar{j}$ is a logarithmic grid from 5×10^{13} Hz to 5×10^{15} (600 to 60000 Å) with $\Delta\nu/\nu = 0.002$; the total number of frequency grid points is 2305. After each time step and at each radial point, we record the elemental abundances, plasma density, mean intensity of the radiation field, extinction coefficients, and emissivities.

For each ejecta model, we perform four RT calculations using different atomic physics libraries and approximations:

1. Using the CMF_100 atomic library, with all elements in LTE (CMF_100 LTE).
2. Using the CMF_All atomic library, with calcium calculated in NLTE and all other elements in LTE (CMF_All Ca

NLTE).

3. Using the CMF_All atomic library, with calcium and silicon calculated in NLTE and all other elements in LTE (CMF_All Si, Ca NLTE).

4. Using the CMF_All atomic library, with calcium, sulfur, and silicon in NLTE, and all other elements in LTE (CMF_All Si, S, Ca NLTE).

We recorded the results of this calculation in every radial zone and at every time step for each of the 119 ejecta models. We used this data to train a set of atomic physics neural networks (APNNs) that were able to quickly map a given zone density and composition to the resulting vectors of the extinction coefficient and emissivity as a function of frequency. Because our training set covered the range of physical conditions relevant for SNe Ia, the APNN should be applicable for general usage for SNe Ia modeling. The details of the neural network training are discussed in Appendix A, and the testing results of APNN are illustrated in Appendix **??**.

3. Test on 3-D Models

In this section, we use the SN Ia explosion model N100 (**?**) to conduct a 3-D time-dependent RT simulation. For this purpose, we adopt the end stage of the hydrodynamic evolution of the N100 model together with the nucleosynthetic postprocessing result, and map the ejecta structure on a $50 \times 50 \times 50$ Cartesian spatial grid, and the maximum ejecta velocity is set to 28600 km/s.

SEDONA-GesaRaT uses the integral-based technique (IBT) (**?**). IBT retrieves the spectropolarimetry time sequence from a 3-D Monte Carlo RT simulation of SN at a specified viewing direction. Comparing to the default spectral retrieval method in SEDONA (direct-counting technique, DCT), IBT increases the Monte Carlo signal-to-noise ratio (S/N) by a factor of ~ 30 while only increasing the computation time by $\sim 30\%$, allowing SEDONA-GesaRaT to retrieve high S/N spectropolarimetry with limited computation time.

3.1. LTE Results Comparison

To test the performance of APNN in 3-D time-dependent RT simulations, we adopt the CMF_100 LTE atomic physics parameters to perform RT simulations on the N100 model using SEDONA and SEDONA-GesaRaT. The complete atomic physics library and the NLTE calculation are not adopted in this comparative simulation due to the excessive computation time using the traditional level population solver as shown in Table 4. Both simulations start at 1 day after the explosion, end at 60 days after the explosion, and the number of energy packets per step is 4×10^6. Before 14.78 days, the simulation time step is logarithmic with $\Delta t_s/t_s = 0.02$, after 14.78 days, the simulation time step is $\Delta t_s = 0.2$ days. The total simulation time is ~ 73.3 hours for SEDONA and ~ 56.3 hours for SEDONA-GesaRaT, measured on a 48-core computing node on TAMU HPRC Grace supercomputer[3], which is mounted with 2 chips of Intel Xeon Gold 6248R CPU.

Figure 1 compares the spectropolarimetric time sequence from 2000 Å to 50000 Å between SEDONA and SEDONA-GesaRaT. We notice that the SEDONA-GesaRaT results are consistent with the SEDONA simulation results on spectral flux between 2000 Å and 50000 Å from 5 days to 50 days after the explosion. The linear polarization results from SEDONA-GesaRaT are also consistent with the results from SEDONA between 2000 Å and 10000 Å, subject to the Monte-Carlo noise. However, we notice the opacity of the S II 5640 Å spectral line is overestimated in SEDONA-GesaRaT, which causes an extra absorption feature around 17 days after the explosion. A similar issue could also be found on the Ca II infrared triplet spectral lines around 41 days after the explosion. This error indicates that the deep learning prediction performance could be further improved by refining the neural network structure and including more diverse SN Ia ejecta models in the training data set.

The tests of SEDONA-GesaRaT on 1-D time dependent simulations is performed

[3]https://hprc.tamu.edu/kb/User-Guides/Grace/

on the testing data set and an additional set of SN Ia ejecta models from (**?**), the results are discussed in the Appendix **??** Figure 7 and Figure 8. The test results shows that the current configuration of APNN is appropriate for most 3-D NLTE RT simulations and for the exploration of the NLTE effect with Si, S, or Ca elements, on the spectropolarimetry signals. Including more elements for NLTE effect in the future researches will require a larger training data set and upgraded neural network structures.

3.2. NLTE Results

In this section, we use SEDONA-GesaRaT to calculate the spectropolarimetric time series of the 3-D N100 model using Si, S, and/or Ca in NLTE. Figure 2 shows the flux and linear spectropolarimetry of the N100 model between 17 and 18 days after the explosion in the viewing direction $\mu = 0.5$, $\varphi = 3.4455$. Comparing the spectropolarimetry results under different atomic physics specifications, we notice that: (1) when treating sulfur in NLTE the emission feature of the S II 6715 Å line is enhanced, and the absorption features of S II 5454 Å and 5640 Å are enhanced; (2) when treating silicon in NLTE, the P-Cygni profile of Si II 6347 Å and 6371 Å and the absorption feature of Si II 4128 Å lines are enhanced, and the linear polarization signal at 6100 Å is suppressed.

High polarization usually occurs at the absorption feature P-Cygni lines, as seen in Figure 2 by the enhanced polarization of the Ca II H & K Lines and the Si II doublet and in Figure 3 by the enhance polarization of Ca II triplet, because unpolarized light from the photosphere is scattered out of the line-of-sight by the spectral line (**?**). We note that treating an element in NLTE may have indirect effects on the spectral features of other elements. For example, Figure 2 shows that putting silicon in NLTE modifies the spectropolarimetric feature near 4000 Å, which is primarily due to the Ca II H&K lines but is affected by blended Si II lines. The silicon also generally increases the flux between 4000 Å and 5000 Å. Moreover,

Fig. 2.— The spectropolarimetry of the N100 model between 17 and 18 days after the explosion, in the viewing direction $\mu = 0.5$, $\varphi = 3.4455$. Upper panel is the spectral flux, middle panel is the linear polarization percentage Q/I, lower panel is the linear polarization percentage U/I. The identified spectral lines are marked with vertical lines and labeled with the element names and the blueshift velocities.

the linear spectropolarimetry of the Ca II infrared triplet at 45 days after the explosion also is changed by the inclusion of Si and S elements in NLTE (Figure 3).

3.3. Resolved Image

SEDONA-GesaRaT can also simulate spatially resolved spectropolarimetry data cubes based on the IBT method (**?**). Using the N100 model, the spectropolarimetry data cube is calculated along the viewing direction $\mu = 0.5,\ \varphi = 3.4455$. The number of energy packets is 4×10^6 per time step, which is higher than that in Section 2, so as to reduce the Monte-Carlo noise in the resolved image. The total simulation time is increased to 63 hours on a 48-core computation node at the TAMU HPRC Grace supercomputer, giving a total simulation cost of 3024 core-hours. The observer image grid is defined on the SN projected image from $-32000 \times t_{\rm exp}$ km/s to $32000 \times t_{\rm exp}$ km/s, where $t_{\rm exp}$ is the time after the SN explosion, and the grid number of X and Y axes is both 20.

The linear polarization image between

Fig. 3.— Same as Figure 2, but between 45 and 46 days after the explosion and focused on 7000–9000 Å. The Ca II infrared triplet lines are marked with gray vertical lines.

17 and 18 days after the explosion at 3697 Å and at 3800 Å are shown in Figure 4. Note that the two selected wavelength values are broadly correlated with the Ca II H&K spectral lines with line-of-sight velocities 17000–20000 km/s and 10000–13000 km/s, and the Ca element density on sections of the N100 model in the corresponding velocity ranges is also shown in Figure 4. We notice that the Q and U polarization maps can be divided into four quadrants based on the positivity of signals, which is in agreement with Figure 12 of **?**. Moreover, the linear polarization intensity is broadly overlapped with the Ca element density map in the corresponding line-of-sight velocity region. Specifically, the Ca element density is zero at the center of the 17000-20000 km/s line-of-sight section, which is in agreement with the zero polarization intensity at the center of the 3697 Å polarization map; the Ca element density reaches $\sim 10^{-5.5}$ g cm^{-3} at the center of the 10000–13000 km/s line-of-sight section, which is in agreement with the non-zero polarization intensity at the center of the 3800 Å polarization map; the lower-right part of the 10000–13000 km/s line-of-sight section shows low Ca element density, which is in agreement with weak U linear polarization in the same region.

4. Conclusions

We have presented the machine-learning-trained code SEDONA-GesaRaT, a speed-up code for supernnova radiative transfer (RT) based on and trained using the code SEDONA (**?**). The machine learning is done using an atomic physics neural network (APNN) which is a convolutional neural network (CNN). The training was done using 119 1-D SN Ia (ejecta) models. There were 4 training sets distinguished by number of atomic levels included and degree of NLTE effects included (the lowest degree being LTE) (see § 2.2 for specifications of the training sets). No forbidden lines were included in the calculations. Our calculations in this paper are restricted to the photospheric phase of SNe Ia where forbidden lines are relatively unimportant. Note, in the nebular phase, forbidden lines

absolutely necessary.

Using our most limited training set (CMF_100_LTE which is the LTE training set), SEDONA-GesaRaT was able to reproduce for a 45 day post-explosion period a sequence of SEDONA spectra and polarization spectra for the 3-D SN Ia model N100 to good accuracy (???? is there an estimate of this accuracy using mean square error MSE ????) (see § 3.1). Recall, the APNN was only trained on 1-D SN Ia models, and so the results of § 3.1 show that a 1-D training set allows the reproduction to good accuracy of the spectra and polarization spectra for 3-D SN Ia models.

Note, the utility of using SEDONA-GesaRat rather than SEDONA depends on the speed-up factor $F(n) = 1/R(n)$, where n is the number of radiative transfer calculations of comparable computation time to be done and $R(n)$ is the ratio of the computation time done using SEDONA-GesaRat to that using SEDONA. The speed-up factor is given by

$$F(n) = \begin{cases} \frac{nt(\text{SEDONA})}{nt(\text{SEDONA-GesaRat})+t(\text{training})} & \text{in general;} \\ 1 \quad \text{for} & \\ \qquad n_{\rm br} = \frac{t(\text{training})}{t(\text{SEDONA})-t(\text{SEDONA-GesaRat})} \ ; & \\ \frac{t(\text{SEDONA})}{t(\text{SEDONA-GesaRat})} & \\ \qquad \text{for } n = \infty \text{ or } t(\text{training}) = 0, & \end{cases}$$

where t(training) is the training computation time, t(SEDONA-GesaRat) and t(SEDONA) are typical radiative transfer computation times done using, respectively, SEDONA-GesaRaT and SEDONA for the same radiative transfer case, $n_{\rm br}$ is the break-even number of radiative transfer calculations, and there is an estimated computation time speed-up for using SEDONA-GesaRat rather than SEDONA for $n > n_{\rm br}$. For the CMF_100_LTE training set, we estimate $n_{\rm br}$ =?????. This estimated break-even number is promising for using SEDONA-GesaRaT for producing a large database of LTE synthetic spectra and polarization spectra for 3-D SN Ia models. Such a database would be useful in determining promising models for many particular observed SNe Ia.

In § 3.2, we use SEDONA-GesaRaT with our 3 NLTE training sets (see § 2.2) to calculate the NLTE spectrum and polarization spectrum for SN Ia model N100 for day 17.5 post-explosion. Clearly, the spectrum and polarization spectrum are sensitive to NLTE effects since they change significantly with the training set. In future work, we should include in the training set we use as a many atoms in NLTE as are needed for physical realism. Certainly, the iron-peak elements (Fe, Co, and Ni), which are very important in SN Ia spectra, should be treated in NLTE.

SNe Ia will never be resolved, but in understanding how 3-D SN Ia structures give rise to spectral and polarization spectral effects, it is necessary to study resolved images of the emission of SN Ia models. SEDONA-GesaRaT does provide such such resolved images as we demonstrate in § 3.3 where we show resolved polarization images for SN Ia model N100 for day 17.5 post-explosion. The image creation is done using the IBT spectral synthesis algorithm (**?**), which is able to reproduce spatially resolved flux and linear polarization data cubes in a specified viewing direction. For our calculation in § 3.3, the accuracy of polarization is $\sim 0.5\,\%$ and the resolution scale in the comoving frame is $\sim 3000\,\mathrm{km/s}$.????

We did not have the computer resources for a SEDONA RT calculation to compare to the SEDONA-GesaRaT RT calculation in § 3.2, and so are unable to calculate the break-even number n for our NLTE RT calculation, but it might be of order of the break-even number for our LTE calculations cited above: i.e., $n =$????. However, we note that limited tests of SEDONA-GesaRaT in 1-D radiative transfer simulations show that the APNN can reproduce the NLTE effects in SN plasma for the atoms we have considered in NLTE with speed-up factors in the range 300 to 400 (see Appendix B). This result in itself is promising for future developments of SEDONA-GesaRaT.

To conclude, SEDONA-GesaRaT is a promising code for speeding up (i.e., accelerating) the large scale production of

synthetic spectra and polarization spectra for SNe Ia, very probably all classes of supernovae, and possibly for other asymmetrical astrophysical atmospheres. However, more development and testing is needed to see how competitive it is compared to other codes.

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SEDONA (**?**), pytorch (**?**)

A. The Atomic Physics Neural Network

Using the RT simulation results discussed in Section 2, we trained an atomic physics neural network (APNN), which uses the elemental abundances $N_{\rm elem}$, plasma density $\bar{\rho}$, and angle-averaged specific intensity in the comoving frame $\bar{J}_\nu$ as input; to predict comoving frame emission coefficient $\bar{j}$, comoving frame absorption coefficient $\bar{k}$, and the comoving frame extinction coefficient due to Thomson scattering $\bar{k}_e$. Throughout the SN explosion process, the physical quantities vary across multiple orders of magnitude. We have therefore designed a normalization scheme in order to keep the calculation within the APNN dynamic range. The new APNN inputs are:

- The scalar $\rho_{\rm new}$, which is the rescaled plasma density $\rho_{\rm new} = \left(\log_{10}(\bar{\rho}) + 23\right)/4$.
- The 2305-element array $\bar{J}_{\rm nu}$, which is $\bar{J}_\nu$ divided by its maximum: $\bar{J}_{\rm nu} = \bar{J}_\nu / {\rm Max}(\bar{J}_\nu)$.
- The scalar $\bar{E}$, which is the rescaled radiation energy integrated from $\bar{J}_\nu$: $\bar{E} = \left(\log_{10}(\sum_{i=0}^{2305} \bar{J}_\nu \Delta\nu_i) - 10.5\right)/3.5$.
- The 28-element array $N_{\rm elem}$, which is the elemental abundances from hydrogen to nickel.

The new APNN outputs are:

- The scalar $k_{\rm hi}$, which is the rescaled maximum of the absorption coefficient value: $k_{\rm hi} = \left(\log_{10}({\rm Max}(\bar{k})) - 2.5\right)/2.5$.
- The scalar $k_{\rm lo}$, which is the rescaled minimum of the absorption coefficient value: $k_{\rm lo} = \left(\log_{10}({\rm Min}(\bar{k})) + 3\right)/3$.
- The 2305-element array $k_{\rm nu}$, which is the rescaled absorption coefficient $k_{\rm nu} = \frac{(\log_{10}(\bar{k}) - \log_{10}({\rm Min}(\bar{k})))}{(\log_{10}({\rm Max}(\bar{k})) - \log_{10}({\rm Min}(\bar{k})))}$.

- The scalar $j_{\rm hi}$, which is the rescaled maximum of the emission coefficient value: $j_{\rm hi} = \left(\log_{10}({\rm Max}(\bar{j})) + 13.5\right)/1.5$.
- The scalar $j_{\rm lo}$, which is the rescaled minimum of the emission coefficient value: $j_{\rm lo} = \left(\log_{10}({\rm Min}(\bar{j})) + 19\right)/3$.
- The 2305-element array $j_{\rm nu}$, which is the rescaled emission coefficient $j_{\rm nu} = \frac{(\log_{10}(\bar{j}) - \log_{10}({\rm Min}(\bar{j})))}{(\log_{10}({\rm Max}(\bar{j})) - \log_{10}({\rm Min}(\bar{j})))}$.
- The scalar K_e, which is the rescaled electron scattering opacity $K_e = (\log_{10}(\bar{k}_e) + 3)/3$.

We adopt a convolution neural network (CNN) structure in the APNN, with 33 convolution layers, 5 fully-connected layers, and 13,480,395 trainable parameters in total. In the APNN, the input $\bar{J}_{\rm nu}$ is firstly encoded with four down-sampling blocks, each block consists of four sub-blocks of convolution, layer normalization, and ReLU activation layers, and a max-pooling layer at the end of the block. The output of the fourth down-sampling block is concatenated with the input $N_{\rm elem}$, $\bar{E}$, and $\rho_{\rm new}$, then input into a stack of five fully-connected layers to predict $j_{\rm hi}$, $j_{\rm lo}$, $k_{\rm hi}$, and $k_{\rm lo}$. The output of the fourth fully-connected layer is input into a decoder network which consists of four up-sampling blocks and a convolution layer, to predict $j_{\rm nu}$ and $k_{\rm nu}$. In Figure 5, we illustrate the overall structure of the APNN. The detailed neural network structure is shown in https://geronimochen.github.io/images/APNN.png, and all the hyper-parameters can be seen in the online picture with magnification. Note that the APNN is defined on the frequency grid from 5×10^{13} Hz to 5×10^{15} Hz, adopting the APNN to other researches with different frequency grid will require extra interpolating effort.

Among the 119 SNe Ia models and the corresponding 1-D RT simulation results, 80 of them listed in Table 1 are in the training data set, 20 of them listed in Table 2 are in the validating data set, and 19 of them listed in Table 3 are in the testing data set. The

training data set is used in the APNN training process to update the trainable parameters; the validating data set is not used to update the trainable parameters, but to monitor the APNN prediction accuracy during the training process; the testing data set is only used to run 1-D RT simulation to compare the results between SEDONA-GesaRat and SEDONA radiative transfer calculations.

Model Name	Number of Shells	Model Name	Number of Shells
gcd_2021_r10_d2.6	83	gcd_2021_r10_d1.0	83
ddt_2013_n1600	95	def_2021_r60_d2.6_z	75
merger_2010_09_09	93	doubledet_2012_csdd-s	60
ddt_2013_n1600c	97	ddt_2014_rpc32_ddt8_n100	98
det_2015_one13e7	77	def_2021_r60_d2.0_z_rot1	83
doubledet_2021_m0810r_1	65	ddt_2013_n40	91
doubledet_2020_2a_21	77	def_2014_n1600def	98
def_2014_n1600cdef	92	def_2014_n20def	98
ddt_2013_n100h	91	def_2021_r57_d3.0_z	82
def_2021_r163_d2.0_z	75	def_2021_r143_d3.0_z	77
ddt_2014_c50_ddt8_n100	98	gcd_2021_r65_d2.0	83
det_2015_one15e7	73	def_2021_r60_d2.6_0.1z	80
merger_2013_09_076_z1	73	doubledet_2021_m0903_1	91
doubledet_2020_2a	77	def_2014_n150def	95
hedet_2012_hed-l	61	def_2021_r10_d3.0_z	93
def_2021_r82_d1.0_z	90	gcd_2016_gcd200	67
ddt_2013_n100	93	doubledet_2021_m0905_1	74
def_2021_r206_d1.0_z	72	doubledet_2020_1a	78
doubledet_2021_m0910_1	59	def_2021_n5_d2.6_z	88
gcd_2021_r60_d2.6	83	gcd_2021_r150_d2.6	83
def_2014_n300cdef	93	def_2014_n5def	89
ddt_2013_n100l	92	def_2014_n1def	84
ddt_2013_n150	92	def_2021_r150_d2.6_z	71
def_2014_n100def	97	det_2010_0.97	74
det_2015_co15e7	82	ddt_2013_n200	94
doubledet_2021_m1005_1	75	doubledet_2020_2a_79	76
doubledet_2020_3a	59	def_2021_r10_d6.0_z	95
def_2015_n5_hybrid	34	doubledet_2020_2b	78

Model Name	Number of Shells	Model Name	Number of Shells
def_2021_r60_d2.0_z_rot2	74	ddt_2014_rpc40_ddt8_n100	98
def_2021_r48_d5.0_z	78	ddt_2013_n300c	49
gcd_2021_r48_d5.0	82	def_2021_r10_d2.0_z	92
doubledet_2021_m1002_1	85	det_2010_1.06_0.075ne	78
doubledet_2021_m1105_1	85	gcd_2021_r51_d4.0	80
doubledet_2021_m0910r_1	64	def_2021_r120_d5.0_z	65
def_2021_r10_d5.0_z	85	def_2014_n10def	90
ddt_2013_n5	86	gcd_2021_r57_d3.0	84
def_2014_n3def	90	det_2015_one17e7	80
def_2014_n200def	95	def_2021_r60_d2.6_0.0001z	77

Table 2: The SN Ia models used in the validating data set.

Model Name	Number of Shells	Model Name	Number of Shells
det_2010_0.81	71	det_2015_one10e7	84
doubledet_2012_eldd-s	66	def_2021_r60_d2.6_0.001z	81
doubledet_2021_m0803_1	88	doubledet_2021_m1003_1	82
ddt_2013_n100_z0.01	93	doubledet_2020_2a_i55	76
doubledet_2020_2a_13	63	def_2021_r60_d2.6_0.01z	80
def_2014_n100hdef	97	def_2021_r60_d2.6_z_co0.28	69
doubledet_2021_m1010_1	86	gcd_2021_r82_d1.0	86
def_2021_r10_d1.0_z	78	def_2021_r10_d2.6_z	82
def_2021_r114_d6.0_z	49	gcd_2021_r10_d2.0	81
doubledet_2012_csdd-l	60		

Table 3: The SN Ia models used in the testing data set.

Fig. 5.— The illustrative neural network structure for the APNN.

We use the `adam` (**?**) optimization algorithm to train the APNN, and we use the mean square error (MSE) as a loss function. The training batch size is 64, and the learning rate is 0.0001. The neural network is trained with 200 epochs. After each epoch, the neural network uses the validating data set to measure the MSE. The neural network is programmed with the `pytorch` framework (**?**), and the training time is ~ 2 days using a NVIDIA-A100 GPU.

Four APNNs are trained to account for the four atomic physics approximation specifications discussed in Section 2. The left panel of Figure 6 shows the MSE in the validating data set of the APNN trained in the data sets with different atomic physics

approximations. With an increase in the size of the atomic data library and the inclusion of more elements for the NLTE calculation, the final MSE also increases. This phenomenon suggests that the increased complexity in atomic physics calculation also increases the fitting difficulty for the APNN.

In the middle and right panels of Figure 6, two examples of the APNN predicted absorption and emission coefficients in the validating data set are shown and compared to the truth. Note that the large fluctuations and the spikes in the absorption and emission coefficients are directly related to the spectral lines instead of the Monte-Carlo noise. We notice the APNN predictions on all the atomic physics approximation specifications are consistent with the results from the traditional method. In the most complex recipe (using CMF_All atomic data library and Si, S, Ca elements considered for the NTLE effect), the performance does not decrease compared to the other three simpler specifications.

B. Test on 1-D Models

The APNN is integrated into SEDONA-GesaRaT to replace the traditional atomic physics calculation module. The APNN is translated into the C++ language using the LibTorch[4] module to adapt the SEDONA code. Thereafter, we run SEDONA-GesaRaT on the testing data set for the 1-D time-dependent RT calculations.

Figure 7 shows several examples of comparing the SEDONA-GesaRaT spectra and the original SEDONA spectra using the SNe Ia models in the testing data set (see Table 3). The SEDONA-GesaRaT spectra have successfully reproduced the spectral time sequence of the original SEDONA from early to late phase, and the spectral features are captured with high accuracy. The agreement is typically ???? in MSE.

[4]https://pytorch.org/cppdocs/index.html

Fig. 6.— Left Panel: The MSE value on the validating data set of the APNNs trained on different atomic physics libraries and approximations. Middle and Right Panel: A comparison of the absorption and emission coefficients calculated from APNN (orange thin line) and from traditional methods (blue thick line). Note, the orange thin line and the blue thick line overlapped badly in the panels and, in fact, they agree to within ??? in MSE. Middle panel uses CMF_All atomic library and the Ca element only is in NLTE. Right panel uses CMF_All atomic library and the Si, S, Ca elements are all in NLTE. The two examples are randomly drawn from the validating data set.

All the SN Ia models in the training, validating, and testing data set are obtained from HESMA (**?**). The hydrodynamic simulations are performed with LEAFS program (**?**); the merging process in the violent merger scenario are performed with GADGET program (**?**); the nucleosynthesis simulations are preformed on 384-isotope using tracing particle method (**?**). Due to the same nucleosynthesis and hydrodynamic simulation programs, the SN Ia models could share potential similarities and reduce the generalization ability of the APNN when applied to new SN Ia models. Moreover, some SN Ia models in the training and the testing sets have high similarities due to the similar nucleosynthesis and hydrodynamic simulation conditions, which could also result in an overestimation of the APNN performances when it is applied to new SN Ia models. For example, ddt_2013_n100_z0.01 in the testing data set shares the same hydrodynamic simulation process with ddt_2013_n100 in the training data set, with different isotope abundances during the nucleosynthesis simulation. Therefore, we have used new SN Ia models from **?** (which use FLASH (**?**) program for hydrodynamic simulations, and use the JINA RECALIB(**?**) program with a 205-isotope network for nucleosynthesis simulation) in order to test the generalization ability of the APNN. Figure 8 shows some example radiative transfer simulation results with the new SN Ia models. We notice that SEDONA-GesaRaT has successfully reproduced the spectral time sequence under LTE approximation with typical MSE ???, while the APNN trained on CMF_All atomic library with the NLTE process on Si, S, and Ca elements shows worse accuracy with typical MSE ??? on this new testing data set than on the HESMA testing SN Ia models, but we deem the accuracy still probably acceptable for many applicatons????. We conclude that APNNs trained with the NLTE process of no more than 3 elements are probably not severely impacted by the size and dimensionality limitation of the current training data set based on the HESMA SN Ia models. On the other hand, with the inclusion of more elements for NLTE process, a more inclusive data set will probably be required.

The plasma level population solver in SEDONA (**?**) uses the Brent's method (**?**), which is an iterative algorithm. With this solver, the atomic physics data library and the LTE/NLTE approximations have a direct effect on the computing time in an iteration and the number of iterations depends on the convergence criteria and the plasma status. The computation time of absorption and emission coefficients from a known level population is small ??? compared to the plasma level population calculation. In an example 1-D RT simulation using the ddt_2013_n100 model, we notice that the convergence is reached between 6 and 22 iterations for all the plasma states and ~ 70 of the plasma states are converged between 7 and 9 iterations. We list the typical computation times in core seconds for convergence (where the number of iterations is typically 10) for a level population calculation using different atomic physics specifications (see § 2) using the SEDONA solver and the APNN (which has the same typical computation time for all atomic physics specifications????) in Table 4. To emphasize, the computation time for level population calculation using the APNN only depends on the neural network structure and has no iterative algorithm.

From Table 4, note that the APNN can reproduce the NLTE effects in SN plasma for the atoms we have considered in NLTE with speed-up factors in the range 300 to 400.

C. Discussion of Future Work

A minor inaccuracy of APNN is observed on the S II 5640 Å spectral line in 3-D LTE simulations (see § LTE Results Comparison). This inaccuracy could be alleviated by including the 1-D RT simulation results with different numbers of Monte-Carlo quanta during the generation of the training and validating data, and refining the neural network structures. Although the 1-D RT simulated spectral time sequence accuracy is not reduced, the mean squared error (MSE) loss measured on the validating data set increases with

Fig. 7.— A comparison between the SEDONA spectral time series (blue line) and SEDONA-GesaRaT spectral time series (orange dashed line) for a sample of the 1-D SN Ia explosion models used in testing the APNN. See Table 3 for the complete set of models. The 1-D SN Ia explosion model names are shown in the title of each panel. The time after the explosion is labeled on the left of each spectrum in the figure.

Fig. 8.— A comparison between the SEDONA spectral time series (blue line) and SEDONA-GesaRaT spectral time series (orange dashed line). The 1-D SN Ia models are from (**?**) and not from the training set of SN Ia models from HESMA. The model names in the title of each panel are encoded with the total mass and progenitor C/O elemental ratio, for example, "M1.0_30/70" means the progenitor mass is 1.0 solar mass, the progenitor C/O elemental ratio is 30% and 70%. The time after the explosion is labeled on the left of each spectrum in the figure.

Atomic physics specifications	Typical computation time (core-seconds)
CMF_100 LTE	1.19
CMF_All Ca NLTE	57.92
CMF_All Si, Ca NLTE	65.86
CMF_All Si, S, Ca NLTE	72.09
APNN	**0.17**

Table 4: The computation time for solving the level population and calculating absorption and emission coefficients in one zone using four different atomic physics specifications (see § 2) using the SEDONA solver Note, the SEDONA requires an iterative algorithm to reach convergence. Typcially 10 ??? iterations required for this table. The APNN solves all atomic physics specifications with with typically the same time: i.e., ~ 0.17 ???? as shown in the table.

the inclusion of more elements for the NLTE processes in APNN training. We also notice that the inclusion of more elements (e.g., Si, S) in NLTE could result in the change of other elements' (e.g., Ca) spectopolarimetric line shapes. These phenomena suggest that the further upgrade of SEDONA-GesaRaT will require a more physically complete NLTE solution, which depends on both the accuracy of atomic physics data and the stability of the NLTE solver. A further comparison of atomic physics data libraries (e.g., **??**) and NLTE solvers (e.g., **??**) is necessary. Furthermore, with the current APNN being trained on 1-D SN Ia ejecta models, the application of SEDONA-GesaRaT to core-collapse SNe will require new training data with the necessary elemental abundances (e.g., hydrogen and helium elements).

The NLTE effect of the Fe-group elements (Fe, Co, and Ni), is crucial to accurately model SNe Ia. However, we notice that the computation time and the numerical instability are significantly increased with the inclusion of the Fe-group elements for NLTE calculations,

which is probably due to the large number of atomic levels and spectral lines. Moreover, we notice that the inclusion of more elements for NLTE calculation could reduce the APNN performance on 1-D testing SN Ia ejecta models, and this phenomenon is more obvious on the new testing data set from outside of the HESMA data base (as shown in Figure 8). Therefore, to accurately perform radiative transfer simulation with the NLTE effect of the Fe-group elements using SEDONA-GesaRaT, an upgraded neural network structure (e.g. vision transformer structure, **?**) will be necessary, and a larger data set of SN Ia radiative transfer simulations will be required. Apart from increasing the computing speed and numerical stability on the current SEDONA program, the new data set could also be collected from existing radiative transfer simulation results using other programs (e.g. CMFGEN **?**; ARTIS **?**).

Our previous researches have proposed an artificial-intelligence assisted inversion (AIAI) method to estimate the SN Ia ejecta structure from the observed spectra, which has been successfully applied to $\sim$ 100 observed SNe Ia **??**. While the AIAI method relies on a large-scale RT simulation to create an SN Ia model and spectral libraries, the previous researches are limited to $\sim 10^5$ spectra calculated from simple 1-D time-dependent RT simulations due to computational resources. The newly-developed SEDONA-GesaRaT provides an efficient solution for the complex 3-D NLTE RT simulations, making it ideal for the further investigation of SN Ia models in 3-D, and the modeling of SN Ia spectropolarimetry observations (e.g., **?**).