Equation of state for nuclear matter in core-collapse supernovae by the variational method

H. Togashi\textsuperscript{1,2}, Y. Takehara\textsuperscript{3}, S. Yamamuro\textsuperscript{3}, K. Nakazato\textsuperscript{3}, H. Suzuki\textsuperscript{3}, K. Sumiyoshi\textsuperscript{1} and M. Takano\textsuperscript{2,5}

\textsuperscript{1} Institute for Physical and Chemical Research (RIKEN), 2-1 Hirosawa, Wako, Saitama 351-0198, Japan
\textsuperscript{2} Research Institute for Science and Engineering, Waseda University, 3-4-1 Okubo Shinjuku-ku, Tokyo 169-8555, Japan
\textsuperscript{3} Department of Physics, Faculty of Science and Technology, Tokyo University of Science, Yamazaki 2641, Noda, Chiba 278-8510, Japan
\textsuperscript{4} Numazu College of Technology, Ooka 3600, Numazu, Shizuoka 410-8501, Japan
\textsuperscript{5} Department of Pure and Applied Physics, Waseda University, 3-4-1 Okubo Shinjuku-ku, Tokyo 169-8555, Japan
E-mail: hajime.togashi@riken.jp

Abstract. We construct a new nuclear equation of state (EOS) for core-collapse supernova (SN) simulations using the variational many-body theory. For uniform nuclear matter, the EOS is constructed with the cluster variational method starting from the realistic nuclear Hamiltonian composed of the Argonne v18 two-body potential and the Urbana IX three-body potential. The masses and radii of neutron stars calculated with the obtained EOS at zero temperature are consistent with recent observational data. For non-uniform nuclear matter, we construct the EOS in the Thomas-Fermi approximation. In this approximation, we assume a functional form of the density distributions of protons, neutrons, and alpha-particles, and minimize the free energy density in a Wigner-Seitz cell with respect to the parameters included in the assumed density distribution functions. The phase diagram of hot nuclear matter at a typical temperature is reasonable as compared with that of the Shen EOS.

1. Introduction
The equation of state (EOS) for hot nuclear matter is one of the crucial ingredients in the studies of core-collapse supernovae (SNe). The EOS for dense uniform matter plays important roles in the core bounce and the subsequent formation of the proto-neutron star, whereas that for non-uniform matter is indispensable for calculating various weak reactions. The EOS for nuclear matter applicable to numerical simulations of core-collapse SNe must cover an extremely wide range of baryon number densities $n_B$, proton fractions $Y_p$, and temperatures $T$. Because the construction of such EOS is laborious, the nuclear EOSs available for SN simulations are limited. A typical SN-EOS is the Lattimer-Swesty EOS [1], in which a Skyrme-type effective interaction is employed for uniform matter whereas a compressible liquid drop model is employed for non-uniform matter. The Shen EOS [2, 3], which is another typical SN-EOS, is based on the relativistic mean field theory for uniform matter and the Thomas-Fermi (TF) calculation for non-uniform matter. Recently, some new nuclear EOSs applicable to SN simulations have been proposed. However, all the SN-EOSs presently available are based on phenomenological models.
for uniform matter. It would be desirable to apply nuclear EOSs based on quantum many-body theories using bare nuclear forces to SN simulations.

Under these circumstances, we are constructing a new nuclear EOS applicable to numerical simulations of core-collapse SNe using the variational method with bare nuclear forces. We have constructed the EOS for uniform asymmetric nuclear matter for arbitrary proton fractions using the cluster variational method \([4, 5, 6]\). In the present study, we calculate the EOS for non-uniform nuclear matter in the TF approximation, and will prepare a complete EOS table available for SN numerical simulations. In this paper, we report the current status of our project.

### 2. Equation of state for uniform nuclear matter

In this section, we review the variational calculations for uniform nuclear matter reported in Refs. \([4, 5, 6]\). As in the Fermi Hypernetted Chain (FHNC) variational calculations by Akmal et al. \([7]\), we start from the nuclear Hamiltonian composed of the Argonne v18 (AV18) two-body potential and the Urbana IX (UIX) three-body potential.

At zero temperature, we express the energy per nucleon of uniform asymmetric nuclear matter \(E/N\) as the sum of the two-body energy per nucleon \(E_2/N\) and the three-body energy per nucleon \(E_3/N\). The two-body energy per nucleon \(E_2/N\) is expressed as the expectation value of the two-body Hamiltonian with the Jastrow wave function in the two-body cluster approximation. Then, \(E_2/N\) is minimized with respect to the spin-isospin-dependent central, tensor, and spin-orbit correlation functions included in the Jastrow wave function. In this minimization, we impose the extended Mayer’s condition and the healing distance condition to ensure that \(E_2/N\) of symmetric nuclear matter and neutron matter reproduce the results obtained by Akmal et al. \([7]\) using the more sophisticated FHNC variational calculations. The three-body energy per nucleon \(E_3/N\) is expressed with use of the expectation value of the three-body Hamiltonian with the Fermi-gas wave function. Four parameters included in \(E_3/N\) are determined so that the total energy per nucleon \(E/N\) reproduces the empirical saturation properties. Furthermore, they are fine-tuned so that the TF calculations of isolated atomic nuclei with the obtained \(E/N\) reproduce the gross features of experimental data \([5]\). As a result, we obtain the following values: the saturation density \(n_0 = 0.16 \text{ fm}^{-3}\), saturation energy \(E_0/N = -16.09 \text{ MeV}\), incompressibility \(K = 245 \text{ MeV}\), and symmetry energy \(E_{\text{sym}} = 30.0 \text{ MeV}\). These values are reasonable as compared with those suggested in the experimental and observational studies \([8, 9, 10]\).

The obtained \(E/N\) for neutron matter and symmetric nuclear matter are in good agreement with the results of the FHNC calculations by Akmal et al. \([7]\). Furthermore, we have applied the obtained \(E/N\) to neutron stars. The masses and radii of neutron stars with the present EOS are consistent with recent observational data \([11, 12, 13]\).

For uniform nuclear matter at finite temperatures, the free energies per nucleon \(F/N\) are calculated with an extension of the variational method by Schmidt and Pandharipande \([14, 15]\). In this method, \(F/N\) is expressed with use of the averaged occupation probabilities of single particle states for protons \(f_p(k, m^*_p)\) and for neutrons \(f_n(k, m^*_n)\), respectively. Here, \(m^*_i (i = p, n)\) are the effective masses. Then, \(F/N\) is minimized with respect to \(m^*_p\) and \(m^*_n\).

The obtained \(F/N\) for neutron matter and symmetric nuclear matter are in good agreement with the results of the FHNC calculations by Mukherjee \([16]\), which are extensions of the results by Akmal et al. Other thermodynamic quantities derived from \(F/N\), such as the internal energies, entropies, and pressures are also reasonable.

Using this nuclear EOS for uniform matter, we have performed general-relativistic spherically-symmetric numerical simulations of core-collapse SNe \([17]\). For the EOS of non-uniform matter, the low-density part of the Shen EOS is adopted. In the simulation with neutrino transfers, the stellar explosion is not successful because of the energy loss by neutrino emissions. This result is consistent with other modern spherical SN simulations. Furthermore, the stellar core with the variational EOS at the bounce is more compact than that with the Shen EOS. This implies
that the variational EOS is softer than the Shen EOS. This relative softness of the variational
EOS is consistent with the fact that the incompressibility of the variational EOS is smaller than
that of the Shen EOS, \( K = 281 \text{ MeV} \).

The EOS for uniform nuclear matter obtained in this way with our variational method is
reasonable over a wide range of \( n_B, Y_p, \) and \( T \). At extremely low densities, however, \( F/N \) tends
to be slightly lower than expected because of the formation of deuteron clusters. This deuteron
clustering is an interesting phenomenon because it is caused by many-body calculations with
realistic nuclear forces. However, this clustering is inappropriate for a systematic description
of the non-uniform phase of SN matter. In fact, we will treat non-uniform matter by the TF
method, in which \( F/N \) for uniform matter is necessary. Therefore, in this study, we slightly
modify the healing distance condition employed in the calculation of \( E_2/N \) to remove the
deuteron clustering. Details of this treatment will be reported elsewhere [18].

### 3. Equation of state for non-uniform nuclear matter

In this section, we construct an EOS for non-uniform nuclear matter that is consistent with
the EOS for uniform nuclear matter reported above. For this purpose, we adopt the TF
approximation as is conducted by Shen et al. [2, 3], or originally by Oyamatsu in a study
of neutron star crusts [19]. In this approximation, non-uniform matter is regarded as a mixture
of free neutrons, free protons, alpha-particles, and a single heavy nucleus that is located at
the center of a Wigner-Seitz (WS) cell in a body-centered cubic (BCC) lattice. The nucleus
is assumed to be spherical, and the number densities of nucleons \( n_i(r) \) (\( i = n \) for neutron and
\( i = p \) for proton) in the WS cell are parameterized as follows:

\[
n_i(r) = \begin{cases} 
(n_i^{\text{in}} - n_i^{\text{out}})[1 - (r/R_i)^3] + n_i^{\text{out}} & (0 \leq r < R_i), \\
\quad (R_i \leq r < R_{\text{cell}}).
\end{cases}
\]

\( R_{\text{cell}} \) is the radius of the WS cell. The number density of alpha-particles \( n_\alpha(r) \) is given by

\[
n_\alpha(r) = \begin{cases} 
-n_\alpha^{\text{out}}[1 - (r/R_p)^3] + n_\alpha^{\text{out}} & (0 \leq r < R_p), \\
\quad (R_p \leq r < R_{\text{cell}}).
\end{cases}
\]

Using the above density distribution functions, the free energy of a WS cell is expressed as

\[
F = \int \text{d}r f(n_p(r), n_n(r), n_\alpha(r)) + F_0 \int \text{d}r |\nabla (n_p(r) + n_n(r))|^2 + \frac{c_2}{2} \int \text{d}r \int \text{d}r' \frac{|n_p(r) + 2n_n(r) - n_e|[n_p(r') + 2n_n(r') - n_e]}{|r - r'|} + c_{\text{bcc}} \frac{(Z_{\text{non}}e)^2}{a}.
\]

The first term on the right-hand side of Eq. (3) is the bulk term, where \( f(n_p(r), n_n(r), n_\alpha(r)) \)
is the local free energy density expressed as the sum of the contribution from nucleons and
that from alpha-particles. The former contribution is obtained in the previous section, whereas, in
the calculations of the latter, the alpha-particle is treated as a classical particle with a fixed
volume. The second term on the right-hand side of Eq. (3) is the gradient term. \( F_0 \) is chosen to
be 68.00 MeV fm\(^{-3}\) so that the TF calculation for isolated atomic nuclei reproduces the gross
features of their empirical masses and radii [5]. The third term represents the Coulomb energy.
Here, the uniform density distribution of electrons is assumed and their number density is given
by \( n_e = n_B Y_p \). The last term on the right-hand side of Eq. (3) is the correction term for the BCC
lattice. Here \( a \) is the lattice constant defined as \( a^3 = V_{\text{cell}} = 4\pi R_{\text{cell}}^3/3 \), \( Z_{\text{non}} \) is the non-uniform
part of the charge number per cell, and \( c_{\text{bcc}} = 0.006562 \) [19]. Then, the average free energy
density of the WS cell \( F/V_{\text{cell}} \) is minimized with respect to the parameters \( \alpha, n_n^{\text{in}}, n_n^{\text{out}}, R_n, t_n, n_p^{\text{in}}, n_p^{\text{out}}, R_p, t_p, \) and \( n_\alpha^{\text{out}} \) with \( n_B, Y_p, \) and \( T \) being fixed.
Figure 1. Free energies per nucleon $F/N$ at $T = 1$ MeV for various proton fractions $Y_p$ as functions of the nucleon number density $n_B$. $F/N$ for uniform matter are also shown.

Figure 2. Phase diagram of hot nuclear matter at $T = 1$ MeV. The shaded region represents the non-uniform phase where the mass fraction of heavy nuclei is given as $X_A$. The dashed line is the boundary where the mass fraction of alpha-particles $X_\alpha = 10^{-4}$.

The obtained $F/N$ is shown in Figure 1, together with the results for uniform matter. It is seen that $F/N$ of non-uniform matter becomes lower than $F/N$ for uniform matter in the region $10^{-7} \text{fm}^{-3} \lesssim n_B \lesssim 10^{-1} \text{fm}^{-3}$, and the critical density at which the non-uniform phase disappears is about $10^{-4} \text{fm}^{-3}$ regardless of $Y_p$.

Figure 2 shows the obtained phase diagram of hot nuclear matter at $T = 1$ MeV. The shaded region represents the non-uniform phase and the dashed line shows the boundary where the mass fraction of alpha-particles $X_\alpha = 10^{-4}$. It is seen that, at $n_B \lesssim 10^{-9} \text{fm}^{-3}$, $X_\alpha$ is negligibly small. As $n_B$ increases, alpha-particles and heavy nuclei appear in nuclear matter. The non-uniform phase appears at a density of $10^{-6} - 10^{-5} \text{fm}^{-3}$, which is higher than the value of $n_B \sim 10^{-7} \text{fm}^{-3}$ found in Fig. 1. This discrepancy is due to the mixing of alpha-
particles in the uniform phase. In Fig. 1, when we consider the alpha-mixing in uniform matter, the corresponding \( F/N \) becomes lower, and the density range for non-uniform matter becomes smaller. The critical density between uniform and non-uniform phases is about \( 10^{-1} \, \text{fm}^{-3} \), which is largely independent of \( Y_p \), as indicated above. It is also confirmed that the present phase diagram based on the variational EOS is close to that based on the Shen EOS [3]. Here we note that the mass numbers and the proton numbers of heavy nuclei appearing in the non-uniform phase are larger than those in the Shen EOS, though the corresponding data are not explicitly shown in this paper. This difference may be related to the fact that the symmetry energy of the present EOS is smaller than that of the Shen EOS.

4. Summary and concluding remarks

In this paper, we reported the current status of our project to construct a new SN-EOS based on realistic nuclear forces. We first constructed the EOS for uniform asymmetric nuclear matter based on the AV18 and UIX potentials using the cluster variational method. Furthermore, the present variational EOS was found to be softer than the Shen EOS in core-collapse SN simulations. Using the free energies for uniform matter, we constructed the EOS for non-uniform matter in the TF approximation. The obtained phase diagram at \( T = 1 \, \text{MeV} \) is reasonable as compared with that of the Shen EOS. A more systematic study of the EOS for non-uniform matter over a wide range of \( n_B, Y_p, \) and \( T \), including the chemical composition in nuclear matter, is now in progress, and will be reported elsewhere in the near future [18].

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