Extended MARTINI Water Model for Heat Transfer Studies

Sumith Yesudasan
sumith.yesudasan@uj.edu
Department of Mechanical Engineering, University of Jamestown, Jamestown, ND

Abstract

The computationally efficient classical MARTINI model is extended to simulate heat transfer simulations of water. The current MARTINI model, variations of it and other coarse grain water models focus on reproducing the thermodynamic properties below room temperature, hence making them unsuitable for studying high temperature simulations especially evaporation at 100 °C. In this work, the MARTINI model is reparametrized using a combination of Genetic Algorithm, Artificial Neural Network and Nelder-Mead optimization technique to match the phase equilibrium properties of water. The reparametrized model (MARTINI-E) accurately reproduces density, enthalpy of vaporization and surface tension at 100°C and outperforms other leading coarse grain water models. The model is also validated using the energy conservation and enthalpy change due to latent heat in a lamellar system. This new water model can be used for simulating phase change phenomena, thin film evaporation and other energy transport mechanisms accurately.

Keywords: CGMD, water models, Molecular Dynamics, MARTINI, Optimization

1 Introduction

In the semi-conductor industry and high-concentration photovoltaics, the emergence of higher energy density calls for highly efficient and faster cooling systems. Out of many conventional cooling techniques, evaporative water cooling stands out as a best candidate due to its high specific heat capacity and high enthalpy of vaporization. Based on kinetic theory [1], an evaporative heat flux of 20,000 W/cm² can be achieved using water. However, even with the recent developments in Nano-scale fabrication techniques the maximum heat flux is limited to 500 to 1000 W/cm² [2]. This points out to our poor understanding of the nanoscale and microscale evaporation of water. Studies show that thin film evaporation has high potential to remove heat compared to bulk region [3][4]. Studying water evaporation at nanoscale using experiments is a challenging attempt. Use of molecular dynamics can become helpful in this scenario [5][6][7], however there is no single water model which can capture or simulate all of its properties [8]. Even the best performing and widely used models like SPCE [9] and TBP [8] are unsuitable to study evaporation, due to the computational cost. This shifts our focus to computationally faster models called coarse grain molecular dynamics (CGMD) models.

In a typical CGMD model, one or more water molecules are combined into a bead or a super-molecule to represent the bulk properties of the system. Most of the existing CGMD models are developed for bio-molecular studies [10][11][12][13][14][15][16][17] and is not tested for heat transfer. The existing CGMD models [12][15] mainly focus on the room temperature behavior of water or even sometimes the behavior below zero degree Celsius. While these models can capture freezing, ice formation and other properties of water [19], their applicability to high temperature applications is limited or seldom. The field of coarse graining itself is a big research area and hence the readers are advised to refer consolidated reviews found elsewhere [20][21][22]. Among various types of CGMD models, mono bead models are appealing due to its very low computational power consumption.

In this work, an extension to the existing CGMD model called MARTINI [23][10] is investigated. The mono beads represents four water molecules and interact with each other using a force field called soft Lennard-Jones (LJ) potential [24]. Using the evolutionary algorithm called genetic algorithm, the initial population (set of force field parameters) is optimized to get a local cost minima. The cost is estimated by comparing the CGMD simulation results with experimental values of density, surface tension and enthalpy...
of vaporization. A simple network of artificial neural network (ANN) is used to predict the next best population during the iteration of genetic algorithm. Local cost minimum is achieved by applying Nelder-Mead optimization to the converged solution of genetic algorithm. Such obtained parameters are able to simulate surface tension, density at constant temperature (100 °C) and pressure and enthalpy of vaporization of water with less than 1% error. This new optimized model called as MARTINI-E (MARTINI Extended) can simulate evaporation of water, heat transfer with solids, boiling and other important thermodynamics [25, 26] at nanoscale using CGMD simulation.

2 Coarse Grain Models of water

There exists a wide range of coarse grain water models in the literature, extending from single water model to analytical multi water models [20]. The present work focuses only on the CGMD models with a single bead. Figure 1a shows the coarse graining of water molecules into a bead. Figure 1b-d shows CGMD models used for simulating vapor, film and liquid phases of water.

![Figure 1: (a) Formulation of different types of CGMD models, (b) Representative vapor CGMD system, (c) Vapor-Liquid-Vapor CGMD system, (d) Liquid CGMD system](image)

2.1 Existing Coarse Grain Models

Among them, the classical MARTINI water model [23, 10], mW model [27], and the recently developed ML-mW model [19] can simulate most of the thermodynamic properties at temperatures near and below 300 K. However, their feasibility near 373.15 K (100 °C) is not tested.

2.1.1 MARTINI model

The MARTINI CGMD model maps a cluster of four water molecules to a single bead [23, 10] and interacts with each other using a standard 12-6 Lennard Jones (LJ) potential (Eq. 1).

$$E_{MARTINI} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right]$$

(1)

Here, for water, $\epsilon = 5 \text{ kJ/mol} = 1.19503 \text{ kcal/mol}$ and $\sigma = 4.7 \text{ Å}$ are standard parameters. In the computer simulations this LJ interaction potential is shifted (both potential and force smoothly goes to zero) and a cutoff distance $r_{cut} = 12 \text{ Å}$, corresponding to approximately 2.5$\sigma$ is used. These parameters and potential function corresponds to MARTINI 2.0 [10]. While MARTINI models are simple in construction, they need additional anti-freeze particles to keep water from freezing at temperatures as high as 300 K and also have poor representation of compressibility and surface tension [20].
### 2.1.2 Stillinger-Weber based models

In the mono bead category, the next leading CMGD model is called mW model [27] which is based on Stillinger-Weber (SW) potential [28]. In mW model, one water molecule is mapped onto one coarse grain bead and water is modeled as an intermediate element between carbon and silicon. The functional form of SW potential is as shown in below equations (2, 3, 4).

\[
E = \sum_i \sum_{j>i} \phi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k>j} \phi_3(r_{ij}, r_{ik}, \theta_{ijk})
\]

\[
\phi_2(r_{ij}) = A_{ij} \epsilon_{ij} \left[ B_{ij} \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] \exp \left( - \frac{\sigma_{ij}}{r_{ij} - a_{ij} \sigma_{ij}} \right)
\]

\[
\phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk} \epsilon_{ijk} \left[ \cos \theta_{ijk} - \cos \theta_{0ijk} \right]^{2} \exp \left( - \frac{\gamma_{ij} \sigma_{ij}}{r_{ij} - a_{ij} \sigma_{ij}} \right) \exp \left( - \frac{\gamma_{ik} \sigma_{ik}}{r_{ik} - a_{ik} \sigma_{ik}} \right)
\]

The parameters of mW model are further improvised recently using machine learning algorithms [19] and is called as ML-mW model. The description of the variables of SW potential and the parameters for mW and ML-mW are described elsewhere in literature [27, 19, 28]. Even though mW and ML-mW can simulate thermodynamic properties of water better than MARTINI model, the computational cost is higher due to the smaller number of water molecules mapping per bead and also the presence of three body potential functions. Moreover, the latter two models mainly focus on solidification of water and thermodynamics around 0 °C.

### 2.2 Extending the MARTINI model

The MARTINI model can represent 4 water molecules and can have larger timestep of integration (20 fs to 30 fs [29, 30]). This makes it a suitable model to investigate for its validity near 373.15 K. Instead of conventional 12-6 LJ potential, a modified form called called soft Lennard-Jones (LJ) potential [24] will be used, as shown below.

\[
E = \frac{\lambda}{N^4} \left\{ \alpha_{LJ}(1 - \lambda)^2 \left( \frac{r}{\sigma} \right)^6 \right\}^{-2} \left\{ \alpha_{LJ}(1 - \lambda)^2 + \left( \frac{r}{\sigma} \right)^6 \right\}^{-1}
\]

Here, \( \alpha_{LJ} \) is taken as 0.5 and \( n \) as 2. The remaining parameters \( \epsilon, \lambda, \) and \( \sigma \) are tunable and will be used to parametrize in this study. A simple LJ potential alone will not be sufficient to simulate the viscous nature of the water, hence a viscous force with a parameter (\( \gamma \)) scaling velocity of the beads, is added to the force field as shown below.

\[
F = -\gamma \ v
\]

### 2.2.1 Genetic algorithm phase

The coarse graining protocol used in this work is shown in the Fig. 2. It starts with a population of 50, and corresponding parameters for the model and fed into the genetic algorithm. The selection, pairing, mating and mutations are performed based on the textbook by Haupt and Ellen [31]. The selection rate is 50% and mutation rate is 20%. The mating step follows the BLX-\( \alpha \) method [32]. To create the initial population, a uniform distribution noise within interval (0, 1) is created and added to the original MARTINI parameters.

For every population in genetic algorithm, CGMD equilibrium simulations of vapor system, film system and bulk liquid system as shown in Fig. 1b-d is performed to estimate enthalpy of vaporization (\( dh = h_{vapor} - h_{liquid} \)), surface tension and density respectively. The vapor system (20nm × 20nm × 20nm) consists of 20 beads, film system (5nm × 5nm × 20nm) consists of 1045 beads and liquid system (7.3452nm × 7.3452nm × 7.3452nm) consists of 2000 beads. Vapor and film systems are equilibrated at 373.15 K using...
original MARTINI model parameters and NVT ensemble. The liquid system is equilibrated at 373.15 K and 1.00090 atm (saturation pressure) using NPT ensemble.

![Diagram of Coarse Graining Protocol for Extended MARTINI Model Development]

Figure 2: Coarse graining protocol for extended MARTINI model development

All CGMD simulations are performed using LAMMPS software [33] and the temperature and pressure is controlled using a Nose-Hoover thermostat and barostat [34, 35, 36] with a chain length of four. The simulations start with an energy minimization for 1000 steps, followed by equilibration runs of 50000 steps and production runs of 50000 steps. The time step of integration is chosen as 5 fs which is relatively low compared to a standard CGMD simulation. Number of steps for equilibration and production are selected based on the time required for the equilibration of energy, temperature and pressure and the standard deviations of energy and temperature is within 1%. The cut off radius for the simulations are taken as 12 Å, same as the original MARTINI model.

From the simulations, diffusion coefficient, density, surface tension and enthalpy of vaporization of the systems are estimated and compared to the experimental values from the NIST standard web book [37]. This comparison is made using a percentage error based cost function \( C \) as described in the below equation.

\[
C = 100 \frac{1}{N} \sum_{i=1}^{N} \frac{f_{XP}^i - f_{MD}^i}{f_{XP}^i}
\]  

(7)

Here, \( f \) represents the quantities density, surface tension and enthalpy of vaporization, \( N \) is the number of parameters, which is 3 in our case. A cost value closer to 0 means a very good agreement between the model and the experiments. If the score is not close enough to 0, then a new population of parameters is chosen as per
the logic given in Fig. 2. The results show that (Fig. 3) even after 50 generations, the cost value was not converging and was fluctuating near 35%.

![Figure 3: Cost function value over generations of genetic algorithm](image)

2.2.2 ANN implementation

At this point, the cut off radius of the system is increased to 18Å. This change has improved the cost function value to lower to upper twenties, but still not converging. So an Artificial Neural Network is introduced to predict the best parameters. The algorithm flowchart is shown in the Fig. 2 where the current population and cost values are fed into a neural network with 10 hidden layers and an output layer of matlab nnstart tool. Using Levenberg-Marquardt algorithm, the network is trained with a R value >0.95. Then a set of 1 million randomly generated population bank is generated with uniform distribution noise around the current best population. This bank is used to search for best parameters which have cost value less than 0.001 %. Thus selected parameters are used to replace 50% of the worst population in the original set. Still the cost function value was fluctuating near to 20%. After careful observation of the individual cost values, we decided to drop the diffusion coefficient from the cost function. This led to a quick convergence (less than 5%) of the system as shown in the Fig. 3.
2.2.3 Nelder-Mead optimization

Genetic algorithm is a metaheuristic and may not converge to its local minimum always. As this was true in our case, we decided to further optimize using downhill simplex method also known as Nelder-Mead algorithm \[38\]. There exists many variations of Nelder-Mead, of which we used the one implemented \[39\] in MATLAB software, and hence the variables and equations closely follow the notations therein. The resulting convergence of the results are shown in the Fig. \[4\]. The parameters corresponding to the best cost in genetic algorithm population is used to create initial simplex. Also, the genetic algorithm optimization leads to a $\lambda$ value of 0.995393. Hence we choose $\lambda = 1$ and avoided from further optimization. This also calls for the equivalence of both Eq. \[1\] and Eq. \[5\]. For individual steps like reflection, expansion, contraction and shrink, CGMD simulations are performed and cost values are estimated. The trend of best, worst and average cost values during the Nelder-Mead optimization is shown in the Fig. \[4\]. The iteration is stopped when worst cost converges with a tolerance value of 0.001. After 46 iterations, the Nelder-Mead converged with a best cost value of 1.287 %. The corresponding optimized parameters of the MARTINI-E model is given in Table \[1\].

![Figure 4: Cost function value variation while using Nelder-Mead algorithm](image)

| Model         | $\epsilon$ (kcal/mol) | $\sigma$ (Å) | $\lambda$ | $\gamma$ (kcal.fs.mol$^{-1}$.Å$^{-2}$) |
|---------------|------------------------|--------------|-----------|--------------------------------------|
| MARTINI       | 1.19503                | 4.7          | -         | -                                    |
| MARTINI-E     | 1.380404               | 4.815407     | 1.00      | 0.095097                             |

3 Results

After the parameterization of the model, the next step is comparing its performance with other CGMD models like original MARTINI model, mW and ML-mW models. For this purpose, a bulk liquid system, a film system and a vapor system is considered with system dimensions as shown in Table \[2\]. By varying the temperature from 350 K to 410 K, density, surface tension and enthalpy of vaporization is estimated. Note that the box dimensions of liquid system will change upon application of Nose-Hoover barostat.

After the parameterization of the model, the next step is comparing its performance with other CGMD models like original MARTINI model, mW and ML-mW models. For this purpose, a bulk liquid system, a film system and a vapor system is considered with system dimensions as shown in Table \[2\]. By varying the temperature from 350 K to 410 K, density, surface tension and enthalpy of vaporization is estimated. Note that the box dimensions of liquid system will change upon application of Nose-Hoover barostat.
Table 2: Properties of various CGMD models used for simulation

| Model   | $N_{vapor}$ | $N_{liquid}$ | $N_{film}$ | cubic $BOX_{vapor}$ | cubic $BOX_{liquid}$ | $BOX_{film}$         |
|---------|-------------|--------------|------------|---------------------|---------------------|----------------------|
| MARTINI | 2000        | 2000         | 1045       | 740.03Å             | 62.96Å              | 50Å × 50Å × 150Å     |
| MARTINI-E | 20          | 2000         | 1045       | 200Å                | 73.452Å             | 50Å × 50Å × 200Å    |
| mW      | 4005        | 4005         | 4005       | 587.63Å             | 50Å                 | 50Å × 50Å × 150Å     |
| ML-mW   | 4005        | 4005         | 4005       | 587.63Å             | 50Å                 | 50Å × 50Å × 150Å     |

Figure 5: Variation of (a) surface tension, (b) enthalpy of vaporization and (c) density with temperature for various CGMD models

The results of surface tension, enthalpy of vaporization and density variation are shown in the Fig. 5. The legends MAR, MAR-E, mW, ML-mW and EXP corresponds to original MARTINI, MARTINI-E, mW, ML-mW and Experimental values respectively. The experimental values are shown as a bold solid line. At these temperature ranges, the mW and ML-mW performs poorly and MARTINI-E turns out to be the best among all for enthalpy of vaporization Fig. 5b.

The surface tension results shows again that MARTINI-E model is closer to experimental results and is superior in comparison with other models Fig. 5a. The density simulated by MARTINI-E is slightly above the experimental values as shown in the Fig. 5c; but still within 2% error. These results show that the MARTINI-E model can be used for studies where enthalpy of vaporization, surface tension and density (compressibility) is important. Also, MARTINI-E is much accurate than other CGMD models for heat transfer.

3.1 Sensitivity due to cutoff radius

In the beginning, a cutoff radius of 12Å was used and later increased to 18Å for better results. To study the sensitivity of the cutoff radius, the liquid system (Fig. 1b) is simulated using NVT ensemble for 100,000 steps of equilibration and production.
Figure 6: Sensitivity of (a) Density and (b) Surface tension with cut off radius

The results of cutoff sensitivity study is shown in Fig. 6. The density shows variation until 18Å and surface tension also shows the same trend. Hence a minimum cutoff radius of 18Å is suggested for any CGMD simulations with MARTINI-E model.

3.2 Sensitivity due to time step

The time step of integration for classical MARTINI models in the literature is suggested to be in the range of 20 fs to 30 fs [29, 30]. Here, a sensitivity study for the time step of integration for the MARTINI-E model is conducted. To unveil the true behavior of the system under different time steps, *NVE* (microcanonical ensemble) instead of *NVT* (canonical ensemble). The liquid system (Fig. 1d) is equilibrated using *NVT* ensemble for 50,000 steps and followed by a production run of 50,000 steps in *NVE* ensemble. The Coefficient of Variation of total energy, variation of density is estimated and shown in Fig. 7. The Coefficient of Variation (CV) of energy is estimated using below equation.

\[
E_{CV} = 100 \frac{\sigma_E}{\mu_E}
\]  

Figure 7: (a) Sensitivity of density and (b) Fluctuation (Coefficient of Variation) in total energy with respect to varying time step of integration

Our results show that the coefficient of variation of the total energy of the system changes linearly with time step of integration. Also, most importantly, the system crashes due to instability after a time
step of 40 fs. Due to these reasons, even though the CV of the total energy is less than 5% until 35 fs, we recommend using time steps below 25 fs for the heat transfer simulations with MARTINI-E model.

4 Validation with a lamellar system

This section explains the validation of the new MARTINI-E model based on basics of energy balance. A CGMD model as shown in Fig. 8a with dimensions of 62.68 Å × 62.68 Å × 182.68 Å and liquid film thickness of 62.68 Å at the center with 2000 beads. This system is equilibrated for 500,000 steps at 373.15 K using a time step of 10 fs. This equilibrated system is then supplied with energy at a constant rate using a heat exchange algorithm [40]. According to energy balance of a closed system with no heat or work exchange with surroundings, the net heat input should be equal to net change in enthalpy.

As a test case, 1 kcal/mol of energy is supplied to the system in 353.6 ps representing a heat flux of 100 kW/cm² based on the film’s cross sectional base area. Figure 8b shows the system snapshot towards the end of the simulation. The time evolution of both total energy and enthalpy (h = u + pv) is shown in comparison with predicted rate (in red color) of increase in Fig. 8c,d. The results show that there is no deviation of enthalpy from the predicted rate of increase and is closely following the trend. The fluctuations seen in the Fig. 8d is due to the pressure, but the average value follows the trend. This study shows that the MARTINI-E model can conserve energy over long simulations, and most importantly the latent heat supplied is reflected as the change in enthalpy, which crucial in simulating evaporation processes.

5 Discussion

A simple extension of the original MARTINI model is developed by changing sigma and epsilon of LJ potential and adding a viscous force term to the force field. This has enabled to simulate surface tension, enthalpy of vaporization and density related to water at temperatures near 100 °C. The use of overly simplistic LJ potential limits the ability to match a larger number of parameters, say for example diffusion coefficient. This can be improvised using potential functions with more variables like Tersoff [41] or Brenner [42] potential, however with an expense in computational cost. Though the current study doesn’t focus on dielectric properties, dipole moments, radial distribution function [43], etc. it may be beneficial to match them for a more accurate version of the CGMD model.
Conclusion

The classical MARTINI model is successfully extended to use in a higher temperature range which will enable it to use for heat transfer simulations. Using a combination of genetic algorithm, artificial neural network and Nelder-Mead optimization, the original model is extended to a new model called MARTINI-E. This is validated against thermodynamic parameters including the co-existing points of temperature-pressure-density phase equilibrium, surface tension and enthalpy of vaporization. The model is validated further using the energy conservation and enthalpy change due to latent heat in a lamellar system. The new model is computationally faster like classical MARTINI model and at the same time can simulate accurately liquid-vapor co-existence and its interface. This model can be used for large scale simulations to study the heat transfer characteristics at nanoscale and evaporation of thin films which are crucial for the heat transfer research.

References

[1] WR Gambill and JH Lienhard. An upper bound for the critical boiling heat flux. ASME J. Heat Transfer, 111(3):815–818, 1989.

[2] Arvind Jaikumar, Aniket Rishi, Anju Gupta, and Satish G Kandlikar. Microscale morphology effects of copper–graphene oxide coatings on pool boiling characteristics. Journal of Heat Transfer, 139(11):111509, 2017.

[3] Sajjad Bigham, Abdolreza Fazeli, and Saeed Moghaddam. Physics of microstructures enhancement of thin film heat transfer in microchannels flow boiling. Scientific reports, 7:44745, 2017.

[4] Qingyang Wang and Renkun Chen. Ultra high flux thin film boiling heat transfer through nanoporous membranes. Nano letters, 18(5):3096–3103, 2018.

[5] Yigit Akkus and Ali Beskok. Molecular diffusion replaces capillary pumping in phase-change-driven nanopumps. Microfluidics and Nanofluidics, 23(2):14, 2019.

[6] Yigit Akkus, Anil Koklu, and Ali Beskok. Atomic scale interfacial transport at an extended evaporating meniscus. Langmuir, 35(13):4491–4497, 2019.

[7] Sumith YD and Shalabh C Maroo. Surface-heating algorithm for water at nanoscale. The Journal of Physical Chemistry Letters, 6(18):3765–3769, 2015.

[8] William L Jorgensen, Jayaraman Chandrasekhar, Jeffry D Madura, Roger W Impey, and Michael L Klein. Comparison of simple potential functions for simulating liquid water. The Journal of chemical physics, 79(2):926–935, 1983.

[9] HJC Berendsen, JR Grigera, and TP Straatsma. The missing term in effective pair potentials. Journal of Physical Chemistry, 91(24):6269–6271, 1987.

[10] Siewert J Marrink, H Jelger Risselada, Serge Yefimov, D Peter Tieleman, and Alex H De Vries. The martini force field: coarse grained model for biomolecular simulations. The journal of physical chemistry B, 111(27):7812–7824, 2007.

[11] Teemu Murtola, Emma Falek, Michael Patra, Mikko Karttunen, and Ilpo Vattulainen. Coarse-grained model for phospholipid/cholesterol bilayer. The Journal of chemical physics, 121(18):9156–9165, 2004.

[12] Aleksey Vishnyakov, Runfeng Mao, Ming-Tsung Lee, and Alexander V Neimark. Coarse-grained model of nanoscale segregation, water diffusion, and proton transport in nafion membranes. The Journal of chemical physics, 148(2):024108, 2018.
[13] Sumith Yesudasan, Xianqiao Wang, and Rodney D Averett. Molecular dynamics simulations indicate that deoxyhemoglobin, oxyhemoglobin, carboxyhemoglobin, and glycated hemoglobin under compression and shear exhibit an anisotropic mechanical behavior. *Journal of Biomolecular Structure and Dynamics*, 36(6):1417–1429, 2018.

[14] Sumith Yesudasan and Rodney D Averett. Coarse grain molecular dynamics simulation of fibrin polymerization. *arXiv preprint arXiv:1710.00123*, 2017.

[15] Sumith Yesudasan, Xianqiao Wang, and Rodney D Averett. Coarse-grained molecular dynamics simulations of fibrin polymerization: effects of thrombin concentration on fibrin clot structure. *Journal of molecular modeling*, 24(5):109, 2018.

[16] Sumith Yesudasan, Xianqiao Wang, and Rodney D Averett. Fibrin polymerization simulation using a reactive dissipative particle dynamics method. *Biomechanics and modeling in mechanobiology*, 17(5):1389–1403, 2018.

[17] Sumith Yesudasan and Rodney D Averett. Multiscale network model for fibrin fibers and fibrin clot with protofibril binding mechanics. *arXiv preprint arXiv:1808.04036*, 2018.

[18] Bryan Raubenolt, Gaurav Gyawali, Wenwen Tang, Katy Wong, and Steven Rick. Coarse-grained simulations of aqueous thermoresponsive polyethers. *Polymers*, 10(5):475, 2018.

[19] Henry Chan, Mathew J Cherukara, Badri Narayanan, Troy D Loeffler, Chris Benmore, Stephen K Gray, and Subramanian KRS Sankaranarayanan. Machine learning coarse grained models for water. *Nature communications*, 10(1):379, 2019.

[20] Kevin R Hadley and Clare McCabe. Coarse-grained molecular models of water: a review. *Molecular simulation*, 38(8-9):671–681, 2012.

[21] Sereina Riniker, Jane R Allison, and Wilfred F van Gunsteren. On developing coarse-grained models for biomolecular simulation: a review. *Physical Chemistry Chemical Physics*, 14(36):12423–12430, 2012.

[22] Emiliano Brini, Elena A Algaer, Pritam Ganguly, Chunli Li, Francisco Rodríguez-Ropero, and Nico FA van der Vegt. Systematic coarse-graining methods for soft matter simulations–a review. *Soft Matter*, 9(7):2108–2119, 2013.

[23] Siewert J Marrink, Alex H De Vries, and Alan E Mark. Coarse grained model for semiquantitative lipid simulations. *The Journal of Physical Chemistry B*, 108(2):750–760, 2004.

[24] Thomas C Beutler, Alan E Mark, René C van Schaik, Paul R Gerber, and Wilfred F Van Gunsteren. Avoiding singularities and numerical instabilities in free energy calculations based on molecular simulations. *Chemical physics letters*, 222(6):529–539, 1994.

[25] Sumith YD and Shalabh C Maroo. Origin of surface-driven passive liquid flows. *Langmuir*, 2016.

[26] Sumith Yesudasan Daisy. *Molecular dynamics study of solid-liquid heat transfer and passive liquid flow*. PhD thesis, Syracuse University, 2016.

[27] Valeria Molinero and Emily B Moore. Water modeled as an intermediate element between carbon and silicon. *The Journal of Physical Chemistry B*, 113(13):4008–4016, 2008.

[28] Frank H Stillinger and Thomas A Weber. Computer simulation of local order in condensed phases of silicon. *Physical review B*, 31(8):5262, 1985.
[29] Moritz Winger, Daniel Trzesniak, Riccardo Baron, and Wilfred F van Gunsteren. On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models. *Physical Chemistry Chemical Physics*, 11(12):1934–1941, 2009.

[30] Siewert J Marrink, Xavier Periole, D Peter Tieleman, and Alex H de Vries. Comment on “On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models” by M. Winger, D. Trzesniak, R. Baron and W.F. van Gunsteren, *Phys. Chem. Chem. Phys.*, 2009, 11, 1934. *Physical Chemistry Chemical Physics*, 12(9):2254–2256, 2010.

[31] Randy L Haupt and Sue Ellen Haupt. *Practical genetic algorithms*. Wiley Online Library, 2004.

[32] Larry J Eshelman and J David Schaffer. Real-coded genetic algorithms and interval-schemata. In *Foundations of genetic algorithms*, volume 2, pages 187–202. Elsevier, 1993.

[33] Steve Plimpton. Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, 117(1):1–19, 1995.

[34] Glenn J Martyna, Mark E Tuckerman, Douglas J Tobias, and Michael L Klein. Explicit reversible integrators for extended systems dynamics. *Molecular Physics*, 87(5):1117–1157, 1996.

[35] Glenn J Martyna, Douglas J Tobias, and Michael L Klein. Constant pressure molecular dynamics algorithms. *The Journal of chemical physics*, 101(5):4177–4189, 1994.

[36] Wataru Shinoda, Motoyuki Shiga, and Masuhiro Mikami. Rapid estimation of elastic constants by molecular dynamics simulation under constant stress. *Physical Review B*, 69(13):134103, 2004.

[37] EW Lemmon, ML Huber, and MO McLinden. Nist standard reference database 23: Reference fluid thermodynamic and transport properties-refprop, version 9.1, standard reference data program. *National Institute of Standards and Technology: Gaithersburg, MD*, 2013.

[38] John A Nelder and Roger Mead. A simplex method for function minimization. *The computer journal*, 7(4):308–313, 1965.

[39] Jeffrey C Lagarias, James A Reeds, Margaret H Wright, and Paul E Wright. Convergence properties of the nelder–mead simplex method in low dimensions. *SIAM Journal on optimization*, 9(1):112–147, 1998.

[40] Tamio Ikeshoji and Bjørn Hafskjold. Non-equilibrium molecular dynamics calculation of heat conduction in liquid and through liquid-gas interface. *Molecular Physics*, 81(2):251–261, 1994.

[41] Jerry Tersoff. New empirical approach for the structure and energy of covalent systems. *Physical Review B*, 37(12):6991, 1988.

[42] Donald W Brenner, Olga A Shenderova, Judith A Harrison, Steven J Stuart, Boris Ni, and Susan B Sinnott. A second-generation reactive empirical bond order (rebo) potential energy expression for hydrocarbons. *Journal of Physics: Condensed Matter*, 14(4):783, 2002.

[43] Roger W Hockney and James W Eastwood. *Computer simulation using particles*. crc Press, 1988.