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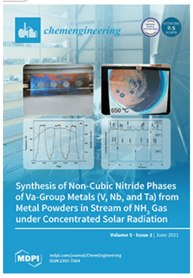

(https://www.mdpi.com/2305-7084/5/2/19)

Cover Story (**view full-size image (/files/uploaded/covers/ChemEngineering/big_cover-ChemEngineering-v5-i2.png)**): This work was performed using a solar furnace at PSA in Almeria (Spain) to synthesize higher nitride transition metals, taking advantage of the very high nitriding power of uncracked ammonia (NH3). Evidence acquired to date implies that, under solar irradiation, the temperature window for higher nitride synthesis by uncracked NH_3 gas appears to be wider compared with that realized by the corresponding reaction in the conventional electric furnace under the absence of visible light. **View this paper. (https://www.mdpi.com/2305-7084/5/2/19)**

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Scaling of Droplet Breakup in High-Pressure Homogenizer Orifices. Part II: Visualization of the Turbulent Droplet Breakup (/2305-7084/5/2/31)

by **Benedikt Mutsch (https://sciprofiles.com/profile/1027454)**, **Felix Johannes Preiss (https://sciprofiles.com/profile/1022517)**, **Teresa Dagenbach (https://sciprofiles.com/profile/author/eW1MNThFajBlRnNpMCtpakh5akdnWFBSVWpKelVOdWJ2SUEzcVpLUCtNST0=)**, **Heike Petra Karbstein (https://sciprofiles.com/profile/895419)** and **Christian J. Kähler (https://sciprofiles.com/profile/author/amNZbjZYVUs1NkN6UGJVdktuNWF3bC8ySUN0OU9iQXUxUm9OUCtRdlpabz0=)**

ChemEngineering **2021**, *5*(2), 31; **https://doi.org/10.3390/chemengineering5020031 (https://doi.org/10.3390/chemengineering5020031)** - 18 Jun 2021

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Abstract Emulsion formation is of great interest in the chemical and food industry and droplet breakup is the key process. Droplet breakup in a quiet or laminar flow is well understood, however, actual in-dustrial processes are always in the turbulent flow regime, leading to **[...] Read more.**

(This article belongs to the Special Issue **Emulsion Process Design (/journal/ChemEngineering/special_issues/Emulsion_Process)**)

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How to Modify LAMMPS: From the Prospective of a Particle Method Researcher (/2305-7084/5/2/30)

by Andrea Albano (https://sciprofiles.com/profile/888605), Eve le Guillou (https://sciprofiles.com/profile/author/OUNCWGhMdEltbHV3VXE3Mjh5SSt2N1RpQS90dlVkekFhaEUvVXJ4cjFrOWdka0VPNVRD, Antoine Danzé (https://sciprofiles.com/profile/author/U21icGZJQ2xEQUtkQ3R5ODh6NUhoSGV1am5ONTRmNlhlYUVhdXFiakNLQT0=), Irene Moulitsas (https://sciprofiles.com/profile/1335322), Iwan H. Sahputra (https://sciprofiles.com/profile/1011073), Amin Rahmat (https://sciprofiles.com/profile/790857), Carlos Alberto Duque-Daza (https://sciprofiles.com/profile/1715440), Xiaocheng Shang (https://sciprofiles.com/profile/1325492), Khai Ching Ng (https://sciprofiles.com/profile/1095777), Mostapha Ariane (https://sciprofiles.com/profile/2325920) and Alessio Alexiadis (https://sciprofiles.com/profile/author/YlYyZ0YwYUFQL0N1M1lQNTNZS2c3V0NKdWpOQmxudkY5SUZvdXF3NUFJST0=)

ChemEngineering **2021**, *5*(2), 30; https://doi.org/10.3390/chemengineering5020030 (https://doi.org/10.3390/chemengineering5020030) - 13 Jun 2021

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Abstract LAMMPS is a powerful simulator originally developed for molecular dynamics that, today, also accounts for other particle-based algorithms such as DEM, SPH, or Peridynamics. The versatility of this software is further enhanced by the fact that it is open-source and modifiable by users. [...] Read more.

(This article belongs to the Special Issue Discrete Multiphysics: Modelling Complex Systems with Particle Methods (/journal/ChemEngineering/special_issues/Particle_Methods))

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Impact of Various Feed Properties on the Performance of a Control System for a Multiple Dividing Wall Column Pilot Plant (/2305-7084/5/2/29)

by Ulrich Preißinger (https://sciprofiles.com/profile/646349), Goran Lukač (https://sciprofiles.com/profile/author/VEpJYXlkcmhCSXZ6a0RiQXYwZDR3Zz09), Igor Dejanović (https://sciprofiles.com/profile/634877) and Thomas Grützner (https://sciprofiles.com/profile/483418)

ChemEngineering **2021**, *5*(2), 29; https://doi.org/10.3390/chemengineering5020029 (https://doi.org/10.3390/chemengineering5020029) - 06 Jun 2021

Abstract Despite the attractive savings potential of multiple Dividing Wall Columns (mDWC), there are no reports in the open literature of an existing application so far. In this perspective, the control of mDWCs has been a rather little-investigated field. Pilot plants are a necessary **[...] Read more.**
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Improved Catalytic Activity of the High-Temperature Water Gas Shift Reaction on Metal-Exsolved $La_{0.9}Ni_{0.05}Fe_{0.95}O_3$ by Controlling Reduction Time (/2305-7084/5/2/28)

by **Rui Huang (https://sciprofiles.com/profile/1603166)** and **Jeong Woo Han (https://sciprofiles.com/profile/1602127)**
ChemEngineering **2021**, *5*(2), 28; **https://doi.org/10.3390/chemengineering5020028 (https://doi.org/10.3390/chemengineering5020028)** - 07 Jun 2021

Abstract The catalyst exsolved from nickel-doped perovskite oxide, $La_{0.9}Ni_{0.05}Fe_{0.95}O_3$, has been proven to be effective for gas-phase reactions. To obtain the optimum amount of exsolved nanoparticles from the parent perovskite oxide, control of the reduction treatment **[...] Read more.**
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Open Access Article **(/2305-7084/5/2/27/pdf?version=1622535053)**

Consumer Attitudes towards Microalgae Production and Microalgae-Based Agricultural Products: The Cases of Almería (Spain) and Livorno (Italy) (/2305-7084/5/2/27)

by **Tomás Lafarga (https://sciprofiles.com/profile/1326852)**, **Carlo Pieroni (https://sciprofiles.com/profile/author/Q1Rja0pxS3hJUjRoWXcyV090ZzZ0S2Z3TURleS96ZHVYUUt4Q0VMT1FNbz0=)**, **Giuliana D'Imporzano (https://sciprofiles.com/profile/2457637)**, **Lorenzo Maggioni (https://sciprofiles.com/profile/1645897)**, **Fabrizio Adani (https://sciprofiles.com/profile/1193905)** and **Gabriel Acién (https://sciprofiles.com/profile/1051237)**
ChemEngineering **2021**, *5*(2), 27; **https://doi.org/10.3390/chemengineering5020027 (https://doi.org/10.3390/chemengineering5020027)** - 28 May 2021

Abstract The production of microalgal biomass and products derived thereof for a wide variety of applications is a hot research topic, with the number of facilities being built and products and biologically active molecules launched into the market increasing every year. The aim of **[...] Read more.**
(This article belongs to the Special Issue **Industrial Cultivation of Microalgae: Technologies, Applications and Challenges (/journal/ChemEngineering/special_issues/Industrial_Cultivation_of_Microalgae)**)

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Heterogeneous Photocatalysis (/2305-7084/5/2/26)

by **Mario J. Muñoz-Batista (https://sciprofiles.com/profile/435482)** and **Rafael Luque (https://sciprofiles.com/profile/451196)**

ChemEngineering **2021**, *5*(2), 26; **https://doi.org/10.3390/chemengineering5020026 (https://doi.org/10.3390/chemengineering5020026)** - 25 May 2021

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Abstract Heterogeneous photocatalysis is a subtype of catalysis that refers to chemical processes catalysed by a semiconductor solid under proper illumination conditions [...] **Full article (/2305-7084/5/2/26)**

(This article belongs to the Special Issue **Heterogeneous Photocatalysis and Photocatalytic Nanomaterials (/journal/ChemEngineering/special_issues/photocatal_nanomaterials)**)

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Evaluation of Pulsed Electric Field Polyphenol Extraction from *Vitis vinifera*, *Sideritis scardica* and *Crocus sativus* (/2305-7084/5/2/25)

by **Achillia Lakka (https://sciprofiles.com/profile/964521)**, **Eleni Bozinou (https://sciprofiles.com/profile/2366161)**, **Dimitris P. Makris (https://sciprofiles.com/profile/469380)** and **Stavros I. Lalas (https://sciprofiles.com/profile/22177)**

ChemEngineering **2021**, *5*(2), 25; **https://doi.org/10.3390/chemengineering5020025 (https://doi.org/10.3390/chemengineering5020025)** - 13 May 2021

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Abstract This study exploited the application of pulsed electric field (PEF) on the recovery of polyphenols from aerial parts of *Sideritis scardica*, tepals of *Crocus sativus,* and fruits of *Vitis vinifera*. Short pulses of 10 μs in a period of 1 ms **[...] Read more.**

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Group Contribution Revisited: The Enthalpy of Formation of Organic Compounds with "Chemical Accuracy" (/2305-7084/5/2/24)

by **Robert J. Meier (https://sciprofiles.com/profile/661717)**

ChemEngineering **2021**, *5*(2), 24; **https://doi.org/10.3390/chemengineering5020024 (https://doi.org/10.3390/chemengineering5020024)** - 11 May 2021

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Abstract Group contribution (GC) methods to predict thermochemical properties are of eminent importance to process design. Compared to previous works, we present an improved group contribution parametrization for the heat of formation of organic molecules exhibiting chemical accuracy, i.e., a maximum 1 kcal/mol (4.2 **[...] Read more.**

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Activated Carbons for Syngas Desulfurization: Evaluating Approaches for Enhancing Low-Temperature H_2S Oxidation Rate (/2305-7084/5/2/23)

by **Christian Frilund (https://sciprofiles.com/profile/1506529)**, **Ilkka Hiltunen (https://sciprofiles.com/profile/author/all1Y0gyRWdDRUZLNTVjV1YzOThPSndVZzV0UzZ5L3VrTkNWQzBvZWtsdz0=)** and **Pekka Simell (https://sciprofiles.com/profile/1108132)**

ChemEngineering **2021**, *5*(2), 23; **https://doi.org/10.3390/chemengineering5020023 (https://doi.org/10.3390/chemengineering5020023)** - 11 May 2021

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Abstract Its relatively low cost and high surface area makes activated carbon an ideal adsorbent candidate for H_2S removal. However, physical adsorption of H_2S is not very effective; therefore, methods to facilitate reactive H_2S oxidation on carbons are **[...] Read more.**

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Simplified Approach to Predict Food Safety through the Maximum Specific Bacterial Growth Rate as Function of Extrinsic and Intrinsic Parameters (/2305-7084/5/2/22)

by Pedro D. Gaspar (https://sciprofiles.com/profile/487979), Joel Alves (https://sciprofiles.com/profile/1587317) and Pedro Pinto (https://sciprofiles.com/profile/author/cE5wTmsvM2U0MXdOYUQvaDJwenByZz09)

ChemEngineering **2021**, *5*(2), 22; https://doi.org/10.3390/chemengineering5020022 (https://doi.org/10.3390/chemengineering5020022) - 10 May 2021

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Abstract Currently, we assist the emergence of sensors and low-cost information and communication technologies applied to food products, in order to improve food safety and quality along the food chain. Thus, it is relevant to implement predictive mathematical modeling tools in order to predict [...] Read more.

(This article belongs to the Special Issue Bio-Processing and Biochemical Engineering 2021 (/journal/ChemEngineering/special_issues/Bio-Processing_and_Biochemical_Engineering_2021))

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Fortran Coarray Implementation of Semi-Lagrangian Convected Air Particles within an Atmospheric Model (/2305-7084/5/2/21)

by Soren Rasmussen (https://sciprofiles.com/profile/1441054), Ethan D. Gutmann (https://sciprofiles.com/profile/1551077), Irene Moulitsas (https://sciprofiles.com/profile/1335322) and Salvatore Filippone (https://sciprofiles.com/profile/author/WGJ0VWtNQ1Z2TmJNbTFOa0sxM0VZSHJKSGRmUEk4Ry9XUTQ4WnY2WXNIbz0=)

ChemEngineering **2021**, *5*(2), 21; https://doi.org/10.3390/chemengineering5020021 (https://doi.org/10.3390/chemengineering5020021) - 06 May 2021

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Abstract This work added semi-Lagrangian convected air particles to the Intermediate Complexity Atmospheric Research (ICAR) model. The ICAR model is a simplified atmospheric model using quasi-dynamical downscaling to gain performance over more traditional atmospheric models. The ICAR model uses Fortran coarrays to split the [...] Read more.

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ChemEngineering **2021**, *5*(2), 20; https://doi.org/10.3390/chemengineering5020020 (https://doi.org/10.3390/chemengineering5020020) - 05 May 2021

Abstract In the evaluation of gasification processes, estimating the composition of the fuel gas for different conditions is fundamental to identify the best operating conditions. In this way, modeling and simulation of gasification provide an analysis of the process performance, allowing for resource and **[...] Read more.**

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Synthesis of Non-Cubic Nitride Phases of Va-Group Metals (V, Nb, and Ta) from Metal Powders in Stream of NH_3 Gas under Concentrated Solar Radiation (/2305-7084/5/2/19)

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ChemEngineering **2021**, *5*(2), 19; https://doi.org/10.3390/chemengineering5020019 (https://doi.org/10.3390/chemengineering5020019) - 20 Apr 2021

Abstract Using a high-flux solar furnace, loosely compacted powders of Va-group transition metal (V, Nb, and Ta) were reacted with stream of NH_3 gas (uncracked NH_3 gas) being heated by concentrated solar beam to a temperature (T) range between 600 and 1000 **[...] Read more.**

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Catalin Teodoriu (https://sciprofiles.com/profile/358356) and Carl Sondergeld (https://sciprofiles.com/profile/1585983)

ChemEngineering **2021**, *5*(2), 18; https://doi.org/10.3390/chemengineering5020018 (https://doi.org/10.3390/chemengineering5020018) - 19 Apr 2021

Abstract This paper summarizes experimental studies using Nuclear Magnetic Resonance (NMR) to evaluate cement porosity, pore size distribution, and other characteristics such as Calcium Silicate Hydrate (CSH) gel structure and morphology. The first known paper on NMR experiments to investigate cement pastes was published [...] Read more.

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Heat Exchanger Network Retrofit of an Oleochemical Plant through a Cost and Energy Efficiency Approach (/2305-7084/5/2/17)

by Valli Trisha (https://sciprofiles.com/profile/author/NWNwYnpUdERQQkluUGsrYXZCSlRXcWZ5MHJpY2E0anhURnBXVGZ1QWE5VT0=), Kai Seng Koh (https://sciprofiles.com/profile/247645), Lik Yin Ng (https://sciprofiles.com/profile/1403893) and Vui Soon Chok (https://sciprofiles.com/profile/848555)

ChemEngineering **2021**, *5*(2), 17; https://doi.org/10.3390/chemengineering5020017 (https://doi.org/10.3390/chemengineering5020017) - 12 Apr 2021

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Waste and Solar Energy: An Eco-Friendly Way for Glass Melting (/2305-7084/5/2/16)

by Isabel Padilla (https://sciprofiles.com/profile/683545), Maximina Romero (https://sciprofiles.com/profile/683544), José I. Robla (https://sciprofiles.com/profile/103264) and Aurora López-Delgado (https://sciprofiles.com/profile/683543)

ChemEngineering **2021**, *5*(2), 16; https://doi.org/10.3390/chemengineering5020016 (https://doi.org/10.3390/chemengineering5020016) - 08 Apr 2021

Abstract In this work, concentrated solar energy (CSE) was applied to an energy-intensive process such as the vitrification of waste with the aim of manufacturing glasses. Different types of waste were used as raw materials: a hazardous waste from the aluminum industry as aluminum [...] Read more.

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ChemEngineering **2021**, *5*(2), 15; https://doi.org/10.3390/chemengineering5020015 (https://doi.org/10.3390/chemengineering5020015) - 06 Apr 2021

Abstract A new analytic approach is presented for determining the total volatile fatty acids (VFA_T) concentration in anaerobic digesters. The approach relies on external determination of the inorganic carbon concentration (C_T) in the analyzed solution, along with two strong-acid titration [...] Read more.

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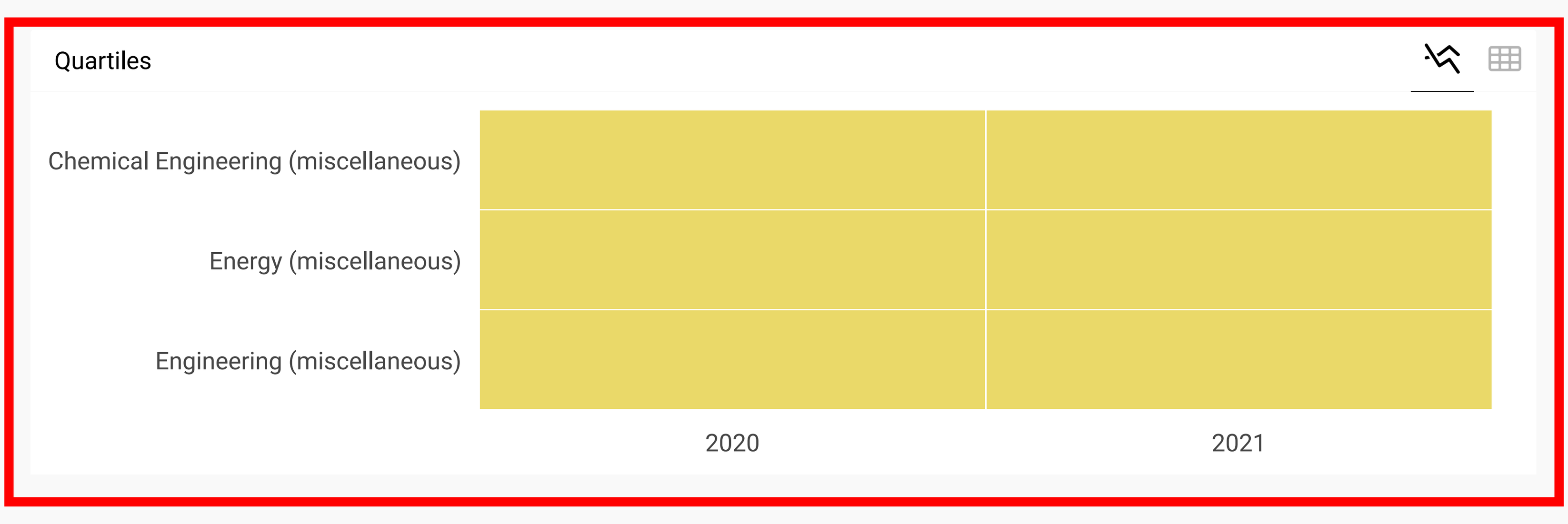

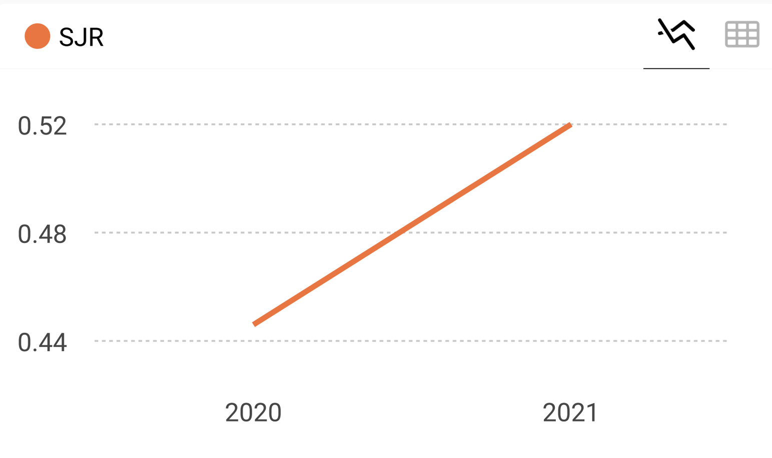

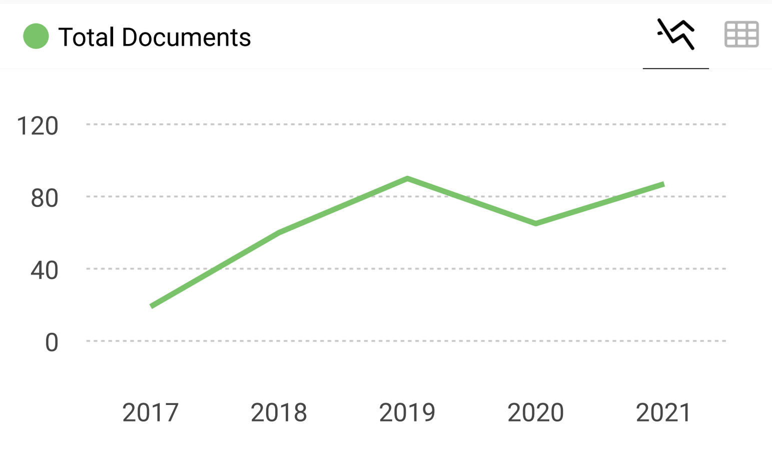

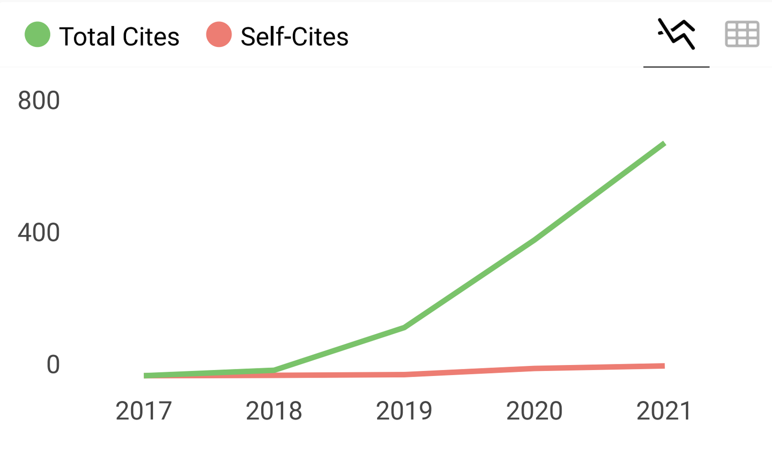

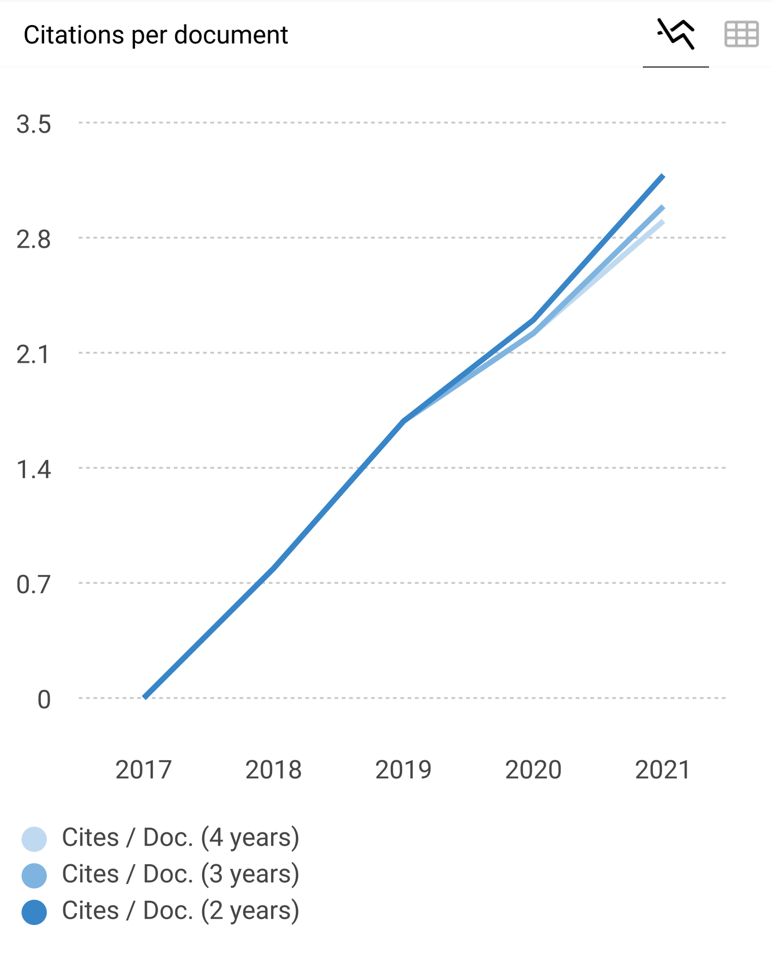

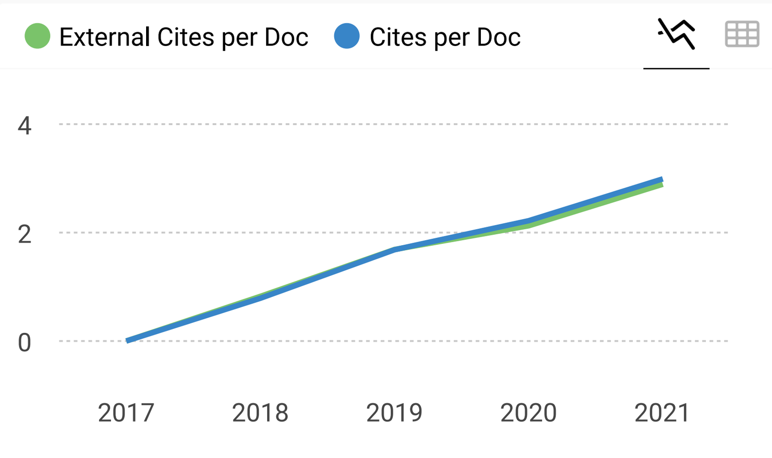

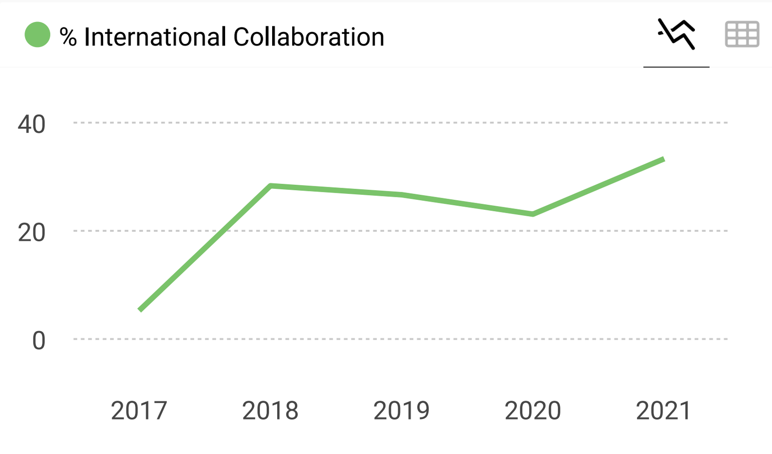

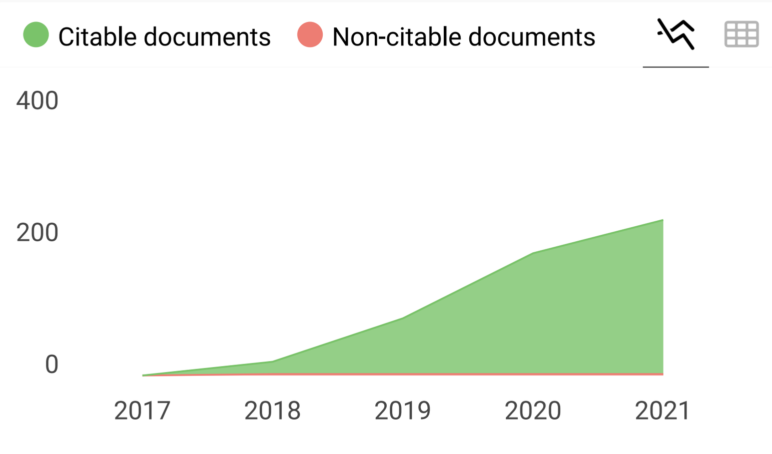

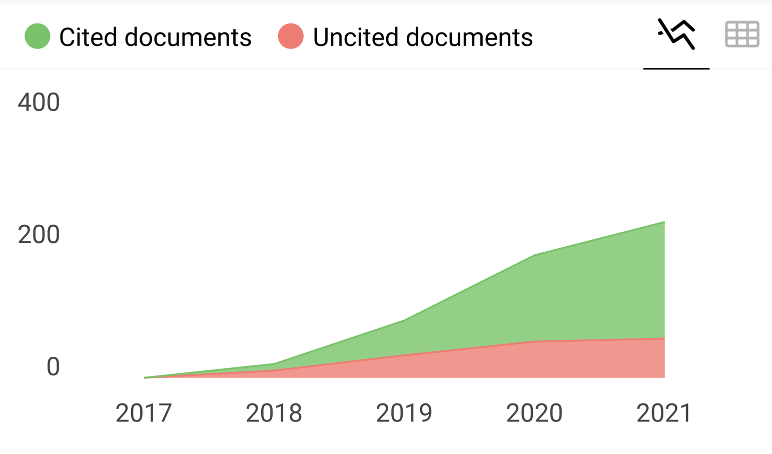

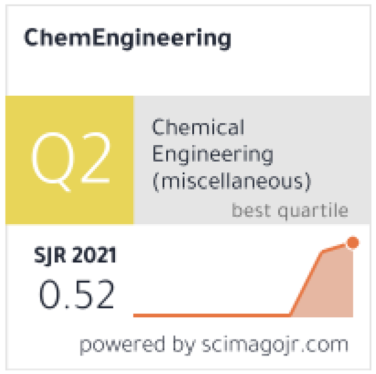

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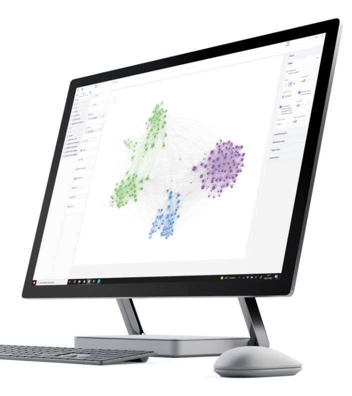

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Article

How to Modify LAMMPS: From the Prospective of a Particle Method Researcher

Andrea Albano [1,*], Eve le Guillou [2], Antoine Danzé [2], Irene Moulitsas [2], Iwan H. Sahputra [1,3], Amin Rahmat [1], Carlos Alberto Duque-Daza [1,4], Xiaocheng Shang [5], Khai Ching Ng [6], Mostapha Ariane [7] and Alessio Alexiadis [1,*]

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Academic Editors: Mark P. Heitz and Andrew S. Paluch

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Abstract: LAMMPS is a powerful simulator originally developed for molecular dynamics that, today, also accounts for other particle-based algorithms such as DEM, SPH, or Peridynamics. The versatility of this software is further enhanced by the fact that it is open-source and modifiable by users. This property suits particularly well Discrete Multiphysics and hybrid models that combine multiple particle methods in the same simulation. Modifying LAMMPS can be challenging for researchers with little coding experience. The available material explaining how to modify LAMMPS is either too basic or too advanced for the average researcher. In this work, we provide several examples, with increasing level of complexity, suitable for researchers and practitioners in physics and engineering, who are familiar with coding without been experts. For each feature, step by step instructions for implementing them in LAMMPS are shown to allow researchers to easily follow the procedure and compile a new version of the code. The aim is to fill a gap in the literature with particular reference to the scientific community that uses particle methods for (discrete) multiphysics.

Keywords: LAMMPS; particle method; discrete multiphysics

1. Introduction

LAMMPS, acronym for Large-scale Atomic/Molecular Massively Parallel Simulator, was originally written in F77 by Steve Plimpton [1] in 1993 with the goal of having a large-scale parallel classical Molecular Dynamic (MD) code. The project was a Cooperative Research and Development Agreement (CRADA) between two DOE labs (Sandia and LLNL) and three companies (Cray, Bristol Myers Squibb, and Dupont). Since the initial release LAMMPS has been improved and expanded by many researchers who implemented many mesh-free computational methods such as Perydynamics, Smoothed particle hydrodynamics (SPH), Discrete Elemet Method (DEM) and many more [2–11].

Such a large number of computational methods within the same simulator allows researchers to easily combine them for the simulation of complex phenomena. In particular, our research group has used during the years LAMMPS in a variety of settings that go from classic Molecular Dynamics [12–16], to Discrete Multiphysics simulations of cardiovascular flows [17–20], Modelling drug adsorption in human organs [21–24], Cavitation [25–27], multiphase flow containing cells or capsules [28–31], solidification/dissolution [32–34], material properties [35,36] and even epidemiology [37] and coupling particles methods with Artificial Intelligence [38–40]. An example of a Discrete Multiphysics simulation run with the basic LAMMPS's code is shown in Appendix A.

Thanks to its modular design open source nature and its large community, LAMMPS has been conceived to be modified and expanded by adding new features. In fact, about 95% of its source code is add-on file [41]. However, this can be a tough challenge for researcher with no to little knowledge of coding. The LAMMPS user manual [41] describes the internal structure and algorithms of the code with the intent of helping researcher to expand LAMMPS. However, due to the lack of examples of implementation and validation, the document can be hard to read for user who are not programmers. In fact, the available material is either very basic [41] or requires advanced programming skills [42,43].

The aim of this work is to provide several step-by-step examples with increasing level of complexity that can fill the gap in the middle to help and encourage researchers to use LAMMPS for discrete multiphysics and expand it with new adds on to the code that could fit their needs. In fact, most of the available material focuses on Molecular Dynamics (MD) and implicitly assumes that the reader's background is in MD rather than other particle methods such as SPH or DEM. On the contrary, this paper is dedicated to the particle community and highlights how LAMMPS can be used and modified for methods other than MD. This goal fits particularly well with the scope of this Special Issue on "Discrete Multiphysics: Modelling Complex Systems with Particle Methods" In particular, it relates to some of the topics of the Special Issue such by exploring the potential of LAMMPS for coupling particle methods, and by sharing some "tricks of the trade" on how to modify its code that cannot be found anywhere else in the literature.

In Section 2 LAMMPS structure and hierarchy are explained introducing the concept of style. Following the LAMMPS authors advice, to avoid writing a new style from scratch, Sections 3–6 new styles are developed using existing style are as reference. Finally, in Section 7, all the steps to write a class from scratch are shown.

2. LAMMPS Structure

After initial releases in F77 and F90, LAMMPS is now written in C++, an object oriented language that allows any programmer to exploit the class programming paradigm. The declaration of a class, including the signature of the instance variables and functions (or methods), which can be accessed and used by creating an instance of that class. The data and functions within a class are called members of the class. The definition (or implementation) of a member function can be given inside or outside the class definition.

A class has private, public, and protected sections which contain the corresponding class members.

- The private members, defined before the keyword public, cannot be accessed from outside the class. They can only be accessed by class or "friend" functions, which are declared as having access to class members, without themselves being members. All the class members are private by default.
- The public members can be accessed from outside the class anywhere within the scope of the class object.
- The protected members are similar to private members but they can be accessed by derived classes or child classes while private members cannot.

2.1. Inheritance

An important concepts in object-oriented programming is that of inheritance. Inheritance allows to define a class in terms of another class and the new class inherits the members of the existing class. This existing class is called the base (or parent) class, and the new class is referred to as a subclass, or child class, or derived class.

The idea of inheritance implements the "is a" relationship. For example, Mammal IS-A Animal, Dog IS-A Mammal hence Dog IS-A Animal as well.

The inheritance relationship between the parent and the derived classes is declared in the derived class with the following syntax:

Listing 1: C++ syntax for classes inheritance

```
class name_child_class: access_specifier name_parent_class
{ /*...*/ };
```

The type of inheritance is specified by the access-specifier, one of public, protected, or private. If the access-specifier is not used, then it is private by default, but public inheritance is commonly used: public members of the base class become public members of the derived class and protected members of the base class become protected members of the derived class. A base class's private members are never accessible directly from a derived class, but can be accessed through calls to the public and protected members of the base class.

2.2. Virtual Function

The signature of a function f must be declared with a virtual keyword in a base class C to allow its definition (implementation), or redefinition, in a derived class D. Then, when a derived class D object is used as an element of the base class C, and f is called, the derived class's implementation of the function is executed.

There is nothing wrong with putting the virtual in front of functions inside of the derived classes, but it is not required, unless it is known for sure that the class will not have any children who would need to override the functions of the base class. A class that declares or inherits a virtual function is called a polymorphic class.

2.3. LAMMPS Inheritance and Class Syntax

A schematic representation of the LAMMPS inheritance tree is shown in Figure 1: LAMMPS is the top-level class for the entire code, then all the core classes, highlighted in blue, inherit all the constructors, destructors, assignment operator members, friends and private members declared and defined in LAMMPS. The core classes perform LAMMPS fundamental actions. For instance, the Atom class collects and stores all the per-atom, or per-particle, data while Neighbor class builds the neighbor lists [41].

The style classes, highlighted in reds, inherit all the constructors, destructors, assignment operator members, friends and private members declared and defined in LAMMPS and in the corresponding core class. The style classes are also virtual parents class of many child classes that implement the interface defined by the parent class. For example, the fix style has around 100 child classes.

Each style is composed of a pair of files:

- namestyle.h
  The header of the style, where the class style is defined and all the objects, methods and constructors are declared.
- namestyle.cpp
  Where all the objects, methods and constructors declared in the class of style are defined.

When a new style is written both `namestyle.h` and `namestyle.cpp` files need to be created.

Each "family" style has its own set of methods, declared in the header and defined in the cpp file, in order to define the scope of the style. For example, the pair style are classes that set the formula(s) LAMMPS uses to compute pairwise interactions while bond style set the formula(s) to compute bond interactions between pairs of atoms [41].

Each pair style has some recurrent functions such as `compute`, `allocate` and `coeff`. Although the final scope of those functions can differ for different styles, they all share a similar role within the classes.

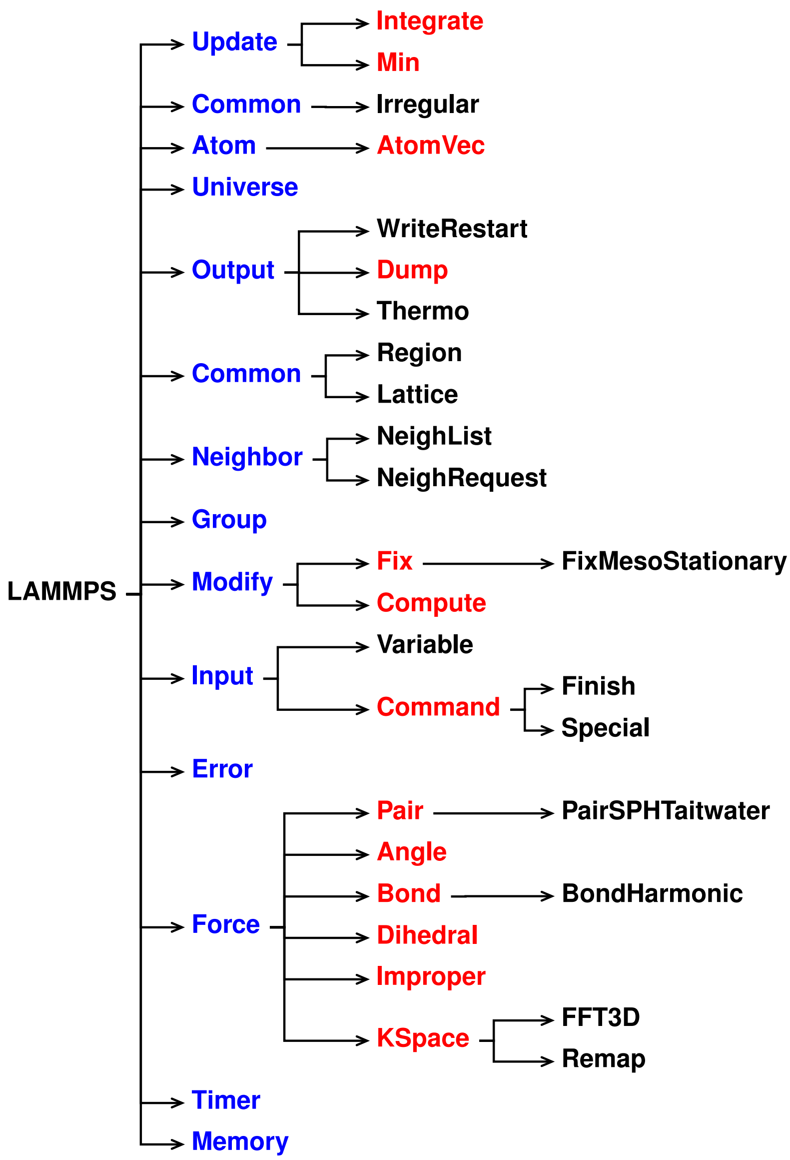


Figure 1. Class hierarchy within LAMMPS source code.

An example of a pair style, sph/taitwater, header in LAMMPS is shown in Listing 2.

Listing 2: Header file of sph/taitwater pair style (pair_sph_taitwater.h)

```
class PairSPHTaitwater: public Pair{// class definition, accessibility and Inheritance
 public:    // access specifier: public
  // public methods
  PairSPHTaitwater(class LAMMPS *); // Constructors
  virtual ~PairSPHTaitwater(); // Destructors
  virtual void compute(int, int);
  void settings(int, char **);
  void coeff(int, char **);
  virtual double init_one(int, int);
  virtual double single(int, int, int, int, double, double, double, double &);

 protected:  // access specifier: protected
  double *rho0, *soundspeed, *B;
  double **cut,**viscosity;
  int first;
// protected methods
  void allocate();
};
```

All the class members are defined in the cpp file. Taking sph/taitwater pair style as reference, each method declared in Listing 2 will be defined and commented in the next sections. Although this can be style-specific, the aim is to give an overview of how the methods are defined in the cpp in LAMMPS. Albeit different style has different methods, the understanding gained can be transferred into others style, as shown in Sections 3 and 6.

2.3.1. Constructor

Any class usually include a member function called constructors. The constructor is mechanically invoked when an object of the class is created. This allows the class to initialise members or allocate storage. Unlike the other member of the class, the constructor name must match the name of the class and it does not have a return type.

Listing 3: Constructor definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

```
PairSPHTaitwater::PairSPHTaitwater(LAMMPS *lmp) : Pair(lmp)
{
  restartinfo = 0;
  first = 1;
}
```

2.3.2. Destructor

The role of destructors is to de-allocate the allocated dynamic memory, see Section 2.3.8, being mechanically invoked just before the end of the class lifetime. Similarly to constructors, destructors does not have a return type and have the same name as the class name with a tilde ($\sim$) prefix.

Listing 4: Destructors definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

```
PairSPHTaitwater::~PairSPHTaitwater() {
  if (allocated) { /// check if the pair style uses allocate, see Section 2.8
  ///  cleanup the memory used by allocate, see Section 2.8
    memory->destroy(setflag);
    memory->destroy(cutsq);
    memory->destroy(cut);
    memory->destroy(rho0);
    memory->destroy(soundspeed);
    memory->destroy(B);
    memory->destroy(viscosity);
  }
}
```

2.3.3. `compute`

`compute` is virtual member of the pair style and is one of the most relevant functions in a number of classes in LAMMPS. For instance, in pair style classes is used to compute pairwise interaction of the specific pair style. This can seen in the commented Listing 5, where the force applied on a pair of neighboring particles is derived using the Tait equation, lines 131–151. In `compute` all the local parameters needed to compute the pairwise interaction are declared and defined within the method.

Listing 5: `compute` definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

```
1  void PairSPHTaitwater::compute(int eflag, int vflag) {
2
3  /// start variables and pointer declaration
4    int i, j, ii, jj, inum, jnum, itype, jtype;
5    double xtmp, ytmp, ztmp, delx, dely, delz, fpair;
6
7    int *ilist, *jlist, *numneigh, **firstneigh;
8    double vxtmp, vytmp, vztmp, imass, jmass, fi, fj, fvisc, h, ih, ihsq;
9    double rsq, tmp, wfd, delVdotDelR, mu, deltaE;
10 // end
11
12   if (eflag || vflag)
```

```
    ev_setup(eflag, vflag);
  else
    evflag = vflag_fdotr = 0;

/// others variables and pointers declaration and initialisation
  double **v = atom->vest; // pass the value of the pointer that points to a pointers
  // pointing to the first element of velocity vector of the particles
  double **x = atom->x; // pass the value of the pointer that points to a pointers
  // pointing to the first element of position vector of the particles
  double **f = atom->f; // pass the value of the pointer that points to a pointers
  // pointing to the first element of force vector of the particles
  double *rho = atom->rho; // pass the value of the pointer that points
  // to the density vector of the particles
  double *mass = atom->mass; // pass the value of the pointer that points
   // to the mass vector of the particles
  double *de = atom->de; // pass the value of the pointer that points
  // to the change of internal energy of the particles
  double *drho = atom->drho; // pass the value of the pointer that points
  // to the change of density of the particles
  int *type = atom->type; // pass the value of the pointer that points to the type of the particles
  int nlocal = atom->nlocal; // pass the value of the numbers of owned and ghost atoms on this proc
  int newton_pair = force->newton_pair;  // pass the value of the Newton's 3rd law settings
/// end


  // check consistency of pair coefficients

  if (first) {
    for (i = 1; i <= atom->ntypes; i++) {
      for (j = 1; i <= atom->ntypes; j++) {
        if (cutsq[i][j] > 1.e-32) {
          if (!setflag[i][i] || !setflag[j][j]) {
            if (comm->me == 0) {
              printf(
                  "SPH particle types %d and %d interact with cutoff=%g,
                  but not all of their single particle properties are set.\n",
                  i, j, sqrt(cutsq[i][j]));
            } } } } }
    first = 0;
  }


  inum = list->inum; // pass the value of number of I atoms neighbors are stored for
  ilist = list->ilist; // pass the value of the pointer pointing to the local indices of I atoms
  numneigh = list->numneigh; // pass the address of a pointer pointing to the number of J neighbors
  //  for each I atom
  firstneigh = list->firstneigh; // pass the value of a pointer that points to pointer
  // pointing to 1st J int value of each I atom




  for (ii = 0; ii < inum; ii++) { // loop for each i particles stored in inum
    i = ilist[ii]; // pass the index of the i particle
    xtmp = x[i][0]; // pass the x position of the i particle
    ytmp = x[i][1]; // pass the y position of the i particle
    ztmp = x[i][2]; // pass the z position of the i particle
    vxtmp = v[i][0]; // pass the x velocity of the i particle
    vytmp = v[i][1]; // pass the y velocity of the i particle
    vztmp = v[i][2]; // pass the z velocity of the i particle
    itype = type[i]; // pass the type of the i particle
    jlist = firstneigh[i]; // pass the 1st J int value of each I atom
    jnum = numneigh[i]; //pass number of J neighbors for each I atom

    imass = mass[itype]; // pass the mass of the i particle

```

```
    // compute force of atom i with Tait EOS
    tmp = rho[i] / rho0[itype];
    fi = tmp * tmp * tmp;
    fi = B[itype] * (fi * fi * tmp - 1.0) / (rho[i] * rho[i]);
    // end

    for (jj = 0; jj < jnum; jj++) {   // loop over neighbours list of particle i
      j = jlist[jj]; // pass the index of the j particle
      j &= NEIGHMASK;

      delx = xtmp - x[j][0]; // x distance between particles i and j
      dely = ytmp - x[j][1]; // y distance between particles i and j
      delz = ztmp - x[j][2]; // z distance between particles i and j
      rsq = delx * delx + dely * dely + delz * delz; // squared distance between particles i and j
      jtype = type[j]; // pass the type of the i particle
      jmass = mass[jtype]; // pass the mass of the j particle

      if (rsq < cutsq[itype][jtype]) { // check if i and j are neighbor

        h = cut[itype][jtype]; // pass the smoothing length
        ih = 1.0 / h; // calculate the inverse, divisions are computationally expensive
        ihsq = ih * ih; // squared inverse

        wfd = h - sqrt(rsq);

        if (domain->dimension == 3) {
          // Lucy Kernel, 3d
          wfd = -25.066903536973515383e0 * wfd * wfd * ihsq * ihsq * ihsq * ih;
        } else {
          // Lucy Kernel, 2d
          wfd = -19.098593171027440292e0 * wfd * wfd * ihsq * ihsq * ihsq;
        }

        // compute force of atom j with Tait EOS
        tmp = rho[j] / rho0[jtype];
        fj = tmp * tmp * tmp;
        fj = B[jtype] * (fj * fj * tmp - 1.0) / (rho[j] * rho[j]);
        // end

        // dot product of velocity delta and distance vector
        delVdotDelR = delx * (vxtmp - v[j][0]) + dely * (vytmp - v[j][1])
            + delz * (vztmp - v[j][2]);

        // artificial viscosity (Monaghan 1992)
        if (delVdotDelR < 0.) {
          mu = h * delVdotDelR / (rsq + 0.01 * h * h);
          fvisc = -viscosity[itype][jtype] * (soundspeed[itype]
              + soundspeed[jtype]) * mu / (rho[i] + rho[j]);
        } else {
          fvisc = 0.;
        }

        fpair = -imass * jmass * (fi + fj + fvisc) * wfd; // total pair force
        deltaE = -0.5 * fpair * delVdotDelR; // internal energy increment

   // change in force in each direction for particle i
        f[i][0] += delx * fpair;
        f[i][1] += dely * fpair;
        f[i][2] += delz * fpair;

        //change in density for particle i
        drho[i] += jmass * delVdotDelR * wfd;

        // change in internal energy for particle i
        de[i] += deltaE;

        if (newton_pair || j < nlocal) {
        // change in force in each direction for particle j
```

```
        f[j][0] -= delx * fpair;
        f[j][1] -= dely * fpair;
        f[j][2] -= delz * fpair;

        de[j] += deltaE; // change in internal energy for particle j

        drho[j] += imass * delVdotDelR * wfd; // change in density for particle j
      }

      if (evflag)
        ev_tally(i, j, nlocal, newton_pair, 0.0, 0.0, fpair, delx, dely, delz);
    }
  }
}

if (vflag_fdotr) virial_fdotr_compute();
}
```

2.3.4. `settings`

`settings` is a public void function that reads the input script checking that all the arguments of the pair style are declared. If arguments are present, `settings` stores them so they can be used by `compute`. Examples for no arguments pair style and arguments pair style input script with the corresponding `settings` are listed below:

- No arguments pair style: sph/taitwater
  As described in the SPH for LAMMPS manual [6], the command line to invoke the sph/taitwater pair style is shown in Listing 6.

  Listing 6: Command line to invoke sph/taitwater pair style

  ```
  pair_style sph/taitwater
  ```

  In this pair style there is just a string defining the pair style, `sph/taitwater`, with no arguments. For this reason in `settings`, Listing 7, when the `if` statement is true (number of arguments other than zero) an error is produced.

  Listing 7: `setting` definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

  ```
  void PairSPHTaitwater::settings(int narg, char **arg) {
    if (narg != 0)  ///  check the number of arguments
      error->all(FLERR,"Illegal number of setting arguments for pair_style sph/
       taitwater");
  }
  ```

- Arguments pair syle: sph/rhosum
  As described in the SPH for LAMMPS manual [6], the command line to invoke the sph/rhosum pair style is shown in Listing 8.

  Listing 8: Command lines to invoke sph/rhosum pair style

  ```
  pair_style sph/rhosum Nstep
  ```

  In this pair style there is a string defining the pair style, `sph/rhosum`, plus one argument, `Nstep`. For this reason in `settings`, Listing 9, when the `if` statement is true (number of arguments other than one) an error is produced. When the `if` statement is false `settings` assigns the value of `Nstep` in the variable `nstep`, line 5, by using the `inumeric` function defined in the force class.

Listing 9: `setting` definition in sph/rhosum pair style (pair_sph_rhosum.cpp)

```
1 void PairSPHRhoSum::settings(int narg, char **arg) {
2   if (narg != 1) ///  check the number of arguments
3     error->all(FLERR,
4         "Illegal number of setting arguments for pair_style sph/rhosum");
5   nstep = force->inumeric(FLERR,arg[0]); // store the variable in the position 0 (Nstep)
     into nstep
6 }
```

2.3.5. `coeff`

Similar to `setting`, `coeff` is a public void function that reads and set the coefficients used in by `compute` of the pair style. For each *i j* pair is possible to set different coefficients. The coefficients are passed in the input file with the command line pair coeff, see Listing 10. As before, examples for different pair coeff input script and the corresponding `coeff` are listed below:

- **sph/taitwater**
  As described in the SPH for LAMMPS manual [6], the command line to invoke sph/taitwater pair coeff is shown in Listing 10.

Listing 10: Command line to invoke sph/taitwater pair coeff

```
pair_coeff I J rho_0 c_0 alpha h
```

In total there are six arguments. Thus, in `coeff`, Listing 11, when `if` statement is true (number of arguments other than six) an error is produced. When the `if` statement is false `coeff` assigns the type of particles I and J plus the value of `rho_0`, `c_0`, `alpha` and `h` in from the string to the variables by using the `numeric` function defined in force class. At last, within the double `for` loop from line 19 to 32, the variables are assigned for each particles.

Listing 11: `coeff` definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

```
1  void PairSPHTaitwater::coeff(int narg, char **arg) {
2    if (narg != 6) ///  check the number of arguments
3      error->all(FLERR,
4          "Incorrect args for pair_style sph/taitwater coefficients");
5    if (!allocated) ///  check if allocate has been called
6      allocate(); ///  call allocate, see section 2.8
7
8    int ilo, ihi, jlo, jhi;
9    force->bounds(arg[0], atom->ntypes, ilo, ihi);
10   force->bounds(arg[1], atom->ntypes, jlo, jhi);
11
12  ///  store the variables in the position 2--5
13   double rho0_one = force->numeric(FLERR,arg[2]);
14   double soundspeed_one = force->numeric(FLERR,arg[3]);
15   double viscosity_one = force->numeric(FLERR,arg[4]);
16   double cut_one = force->numeric(FLERR,arg[5]);
17  /// B_one is a constant used in tait EOS inside compute, see section 2.3
18   double B_one = soundspeed_one * soundspeed_one * rho0_one / 7.0;
19
20 ///  assign the coefficient to the corresponding particle (i)
21 ///  and to the pair of particles (i,j)
22   int count = 0;
23   for (int i = ilo; i <= ihi; i++) {
24     rho0[i] = rho0_one;
25     soundspeed[i] = soundspeed_one;
26     B[i] = B_one;
27     for (int j = MAX(jlo,i); j <= jhi; j++) {
28       viscosity[i][j] = viscosity_one;
29       cut[i][j] = cut_one;
30
31       setflag[i][j] = 1;
32
33       count++;
34     }
35   }
36   if (count == 0) ///  check if the arguments have been assigned
37     error->all(FLERR,"Incorrect args for pair coefficients");
38 }
```

- **sph/rhosum**
  As described in the SPH for LAMMPS manual [6], the syntax to invoke the command is shown in Listing 12.

Listing 12: Command lines to invoke sph/rhosum pair style

```
pair_coeff I J h
```

In this case there are three arguments. Thus, in the `coeff`, Listing 13, when the `if` statement is true (number of arguments other than six) an error is produced. When the error is not produced function assigns the type of particles I and J plus the value of h in the string to the variable `cut_one`, line 11, by using `bounds` and `numeric` function defined in force class. At last, within the double `for` loop from line 14 to 20, the variables are assigned for each particles.

Listing 13: `coeff` definition in sph/rhosum pair style (pair_sph_rhosum.cpp)

```
1  void PairSPHRhoSum::coeff(int narg, char **arg) {
2    if (narg != 3) ///  check the number of arguments
3      error->all(FLERR,"Incorrect number of args for sph/rhosum coefficients");
4    if (!allocated) /// check if allocate has been called
5      allocate();  /// call allocate, see section 2.8
6
7    int ilo, ihi, jlo, jhi;
8    force->bounds(arg[0], atom->ntypes, ilo, ihi);
9    force->bounds(arg[1], atom->ntypes, jlo, jhi);
10
11   double cut_one = force->numeric(FLERR,arg[2]);
12
13 ///  assign the coefficient to the pair of particles (i,j)
14   int count = 0;
15   for (int i = ilo; i <= ihi; i++) {
16     for (int j = MAX(jlo,i); j <= jhi; j++) {
17       cut[i][j] = cut_one;
18       setflag[i][j] = 1;
19       count++;
20     }
21   }
22
23   if (count == 0) ///  check if the arguments have been assigned
24     error->all(FLERR,"Incorrect args for pair coefficients");
25 }
```

2.3.6. `init_one`

`init_one` check if all the pair coefficients for a given i j pair have been assigned. If they were assigned the methods ensure the symmetry of the matrix.

Listing 14: `init_one` definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

```
double PairSPHTaitwater::init_one(int i, int j) {
/// check if the coefficient of the pair of particles (i,j) were assigned
  if (setflag[i][j] == 0) {
    error->all(FLERR,"Not all pair sph/taitwater coeffs are set");
  }
/// ensure the matrix symmetry
  cut[j][i] = cut[i][j];
  viscosity[j][i] = viscosity[i][j];

  return cut[i][j];
}
```

2.3.7. `single`

In `single` the force and energy of a single pairwise interaction, or single bond or angle (in case of bond or angle style), between two atoms is evalutated. The method is specifically invoked by the command line compute pair/local (or compute bond/local) to calculate properties of individual pair, or bond, interactions [41].

Listing 15: `single` definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

```
double PairSPHTaitwater::single(int i, int j, int itype, int jtype,
    double rsq, double factor_coul, double factor_lj, double &fforce) {
  fforce = 0.0;

  return 0.0;
}
```

2.3.8. `allocate`

`allocate` is a protected void function that allocates dynamic memory. The dynamic memory allocation is used when the amount of memory needed depends on user input. As explained before, at the end of the lifetime of the class, the destructors will de-allocate the memory the memory used by `allocate`.

Listing 16: `allocate` definition in sph/taitwater pair style (pair_sph_taitwater.cpp)

```
void PairSPHTaitwater::allocate() {
  allocated = 1;  ///  confirm that allocated has been called
  int n = atom->ntypes;  /// assigm the value of the number of types

  memory->create(setflag, n + 1, n + 1, "pair:setflag");
  for (int i = 1; i <= n; i++)
    for (int j = i; j <= n; j++)
      setflag[i][j] = 0;

/// allocate the memory for the arguments of the pair style
  memory->create(cutsq, n + 1, n + 1, "pair:cutsq");
  memory->create(rho0, n + 1, "pair:rho0");
  memory->create(soundspeed, n + 1, "pair:soundspeed");
  memory->create(B, n + 1, "pair:B");
  memory->create(cut, n + 1, n + 1, "pair:cut");
  memory->create(viscosity, n + 1, n + 1, "pair:viscosity");
}
```

3. Kelvin–Voigt Bond Style

We can use what we learned in the previous section to generate a new dissipative bond potential that can be used to model viscoelastic materials. The Kelvin–Voigt model [44] is used to model viscoelastic material as a purely viscous damper and purely elastic spring connected in parallel as shown in Figure 2.

Since the two components of the model are arranged in parallel, the strain in each component is identical:

$$\varepsilon_{tot} = \varepsilon_{spring} = \varepsilon_{damper}. \tag{1}$$

On the other hand, the total stress σ_{tot} will be split into σ_{spring} and σ_{damper} to have $\varepsilon_{spring} = \varepsilon_{damper}$. Thus we have

$$\sigma_{tot} = \sigma_{spring} + \sigma_{damper}. \tag{2}$$

Combining Equations (1) and (2) with the constitutive relation for both the spring and the dumper, $\sigma_{spring} = k\varepsilon$ and $\sigma_{damper} = b\dot{\varepsilon}$, is possible to write that

$$\sigma = k\varepsilon(t) + b\frac{d\varepsilon(t)}{dt} = k\varepsilon(t) + b\dot{\varepsilon}, \tag{3}$$

where k is the elastic modulus and b is the coefficient of viscosity. Equation (3) relates stress to strain and strain rate for a Kelvin–Voigt material [44].

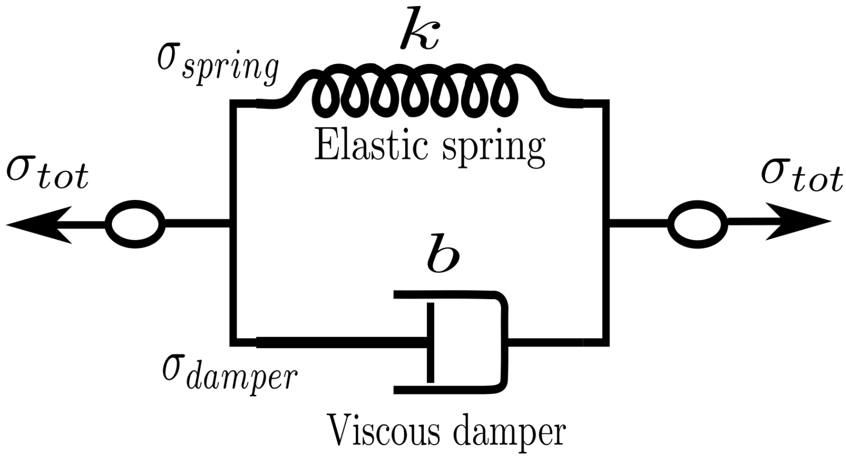


Figure 2. Schematic representation of Kelvin–Voigt model [44].

Similarly to bond test to write a new pair style called bond kv we take the bond harmonic pair style as reference. The new pair style is declared and initialised in bond_kv.h and bond_kv.cpp saved in the /src/MOLECULE directory and its hierarchy is shown in Figure 3.

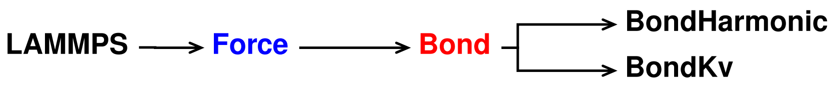


Figure 3. Class hierarchy of the new bond style.

3.1. Validation

The bond kv pair style has been validated by Sahputra et al. [45] in their Discrete Multiphysics model for encapsulate particles with a soft outer shell.

3.2. *bond_kv.cpp*

All the functions will be the same as in the reference bond harmonic. However, in our new bond kv, we need to substitute the "BondHarmonic" text by a new "BondKv" text, as can be seen in Listings 17 and 18. Form now on, when we show a side-by-side comparison between the reference and the modified file, we highlight in yellow the modified lines and in red the deleted lines.

Listing 17: Original script (bond_harmonic.cpp)

```
#include "math.h"
#include "stdlib.h"
#include "bond_harmonic.h"
#include "atom.h"
#include "neighbor.h"
#include "domain.h"
#include "comm.h"
#include "force.h"
#include "memory.h"
#include "error.h"

using namespace LAMMPS_NS;

BondHarmonic::BondHarmonic(LAMMPS *lmp) : Bond(lmp)
 {}
BondHarmonic::~BondHarmonic()
{ ... }
void BondHarmonic::compute(int eflag, int vflag)
{ ... }
void BondHarmonic::allocate()
{ ... }
void BondHarmonic::coeff(int narg, char **arg)
```

```
{ ... }
double BondHarmonic::equilibrium_distance(int i)
{ ... }
void BondHarmonic::write_restart(FILE *fp)
{ ... }
void BondHarmonic::read_restart(FILE *fp)
{ ... }
void BondHarmonic::write_data(FILE *fp)
{ ... }
double BondHarmonic::single(int type, double rsq,
 int i, int j, double &fforce)
{ ... }
```

Listing 18: Modified script (bond_kv.cpp)

```
#include "math.h"
#include "stdlib.h"
#include "bond_kv.h"
#include "atom.h"
#include "neighbor.h"
#include "domain.h"
#include "comm.h"
#include "force.h"
#include "memory.h"
#include "error.h"

using namespace LAMMPS_NS;

BondKv::BondKv(LAMMPS *lmp) : Bond(lmp)
 {}
BondKv::~BondKv()
{ ... }
void BondKv::compute(int eflag, int vflag)
{ ... }
void BondKv::allocate()
{ ... }
void BondKv::coeff(int narg, char **arg)
{ ... }
double BondKv::equilibrium_distance(int i)
{ ... }
void BondKv::write_restart(FILE *fp)
{ ... }
void BondKv::read_restart(FILE *fp)
{ ... }
void BondKv::write_data(FILE *fp)
{ ... }
double BondKv::single(int type, double rsq,
 int i, int j, double &fforce)
{ ... }
```

Compared to the bond harmonic we are introducing a new parameter, b, from the input file. For this reason we need to modify destructor, `compute`, `allocate`, `coeff`, `write_restart` and `read_restart`. Following the order of function initialisation, see Listing 18, the destructor is modified as shown in Listing 20.

Listing 19: Original destructor (bond_harmonic.cpp)

```
BondHarmonic::~BondHarmonic()
{
  if (allocated) {
    memory->destroy(setflag);
    memory->destroy(k);
    memory->destroy(r0);
  }
}
```

Listing 20: Modified destructor (bond_kv.cpp)

```
BondKv::∼ BondKv()
{
  if (allocated) {
    memory->destroy(setflag);
    memory->destroy(k);
    memory->destroy(r0);
    memory->destroy(b);  /* dashpot/damper costant */
  }
}
```

The next function to modify is `compute`. The strain rate, $\dot{\varepsilon}$, can also be seen as the speed of deformation. To use it within the new pair style we need to declared and initialised the velocities of each particles, see Listing 22.

Listing 21: Original `compute` (bond_harmonic.cpp)

```
void BondTest::compute(int eflag, int vflag)
{
  int i1,i2,n,type;
  double delx,dely,delz,ebond,fbond;
  double rsq,r,dr,rk;

  ebond = 0.0;
  if (eflag || vflag) ev_setup(eflag,vflag);
  else evflag = 0;

  double **x = atom->x;
  double **f = atom->f;
  }
}
```

Listing 22: Modified `compute` (bond_kv.cpp)

```
void BondTest::compute(int eflag, int vflag)
{
    int i1,i2,n,type;
  double delx,dely,delz,ebond,fbond;
  double rsq,r,dr,rk

/* declaration of new variables */
  double delv_x, delv_y, delv_z;
  double dir_vx1, dir_vy1, dir_vz1, dir_vx2, dir_vy2,
   dir_vz2, dir_vx1, dir_vx1;
  double rsq_x, rsq_y, rsq_z;
/* end declaration of new variables */



  ebond = 0.0;
  if (eflag || vflag) ev_setup(eflag,vflag);
  else evflag = 0;

  double **x = atom->x;
  double **f = atom->f;
  double **v = atom->v; /* delcaration and inizalitaizon
   of a new pointer*/
  }
}
```

Moreover, inside the loop `for (n = 0; n < nbondlist; n++)` of the original `compute`, we need to add a new set of lines between the lines to calculate the spring force and the lines to calculate force and energy increment. Those lines calculate velocities and directions to compute the dashpot forces, see Listing 23.

Now is possible to write the new expression of the force applied to pair of atoms.

Listing 23: Modified compute (bond_kv.cpp)

```
/* dashpot velocities and directions */
dev_x = v[ i1 ][ 0 ] - v[ i2 ][ 0 ];
dev_y = v[ i1 ][ 1 ] - v[ i2 ][ 1 ];
dev_z = v[ i1 ][ 2 ] - v[ i2 ][ 2 ];
rsq_vx = dev_x * dev_x;
rsq_vy = dev_y * dev_y;
rsq_vz = dev_z * dev_z;
velx = sqrt( rsq_vx );
vely = sqrt( rsq_vy );
velz = sqrt( rsq_vz );

if ( v[ i1 ][ 0 ] >= 0.0 ) dir_vx1 = 1;
else dir_vx1 = -1;

if ( v[ i1 ][ 1 ] >= 0.0 ) dir_vy1 = 1;
else dir_vy1 = -1;

if ( v[ i1 ][ 2 ] >= 0.0 ) dir_vz1 = 1;
else dir_vz1 = -1;

if ( v[ i2 ][ 0 ] >= 0.0 ) dir_vx2 = 1;
else dir_vx2 = -1;

if ( v[ i2 ][ 1 ] >= 0.0 ) dir_vy2 = 1;
else dir_vy2 = -1;

if ( v[ i2 ][ 2 ] >= 0.0 ) dir_vz2 = 1;
else dir_vz2 = -1;
```

Listing 24: Original compute (bond_harmonic.cpp)

```
    if (newton_bond || i1 < nlocal) {
      f[i1][0] += delx*fbond;
      f[i1][1] += dely*fbond;
      f[i1][2] += delz*fbond;
    }

    if (newton_bond || i2 < nlocal) {
      f[i2][0] -= delx*fbond;
      f[i2][1] -= dely*fbond;
      f[i2][2] -= delz*fbond;
    }

    if (evflag) ev_tally(i1,i2,nlocal,
    newton_bond,ebond,fbond,delx,dely,delz);
  }
}
```

Listing 25: Modified compute (bond_kv.cpp)

```
/// eq 3 implementation for each force component
    if (newton_bond || i1 < nlocal) {
      f[i1][0] += (delx*fbond) - (dir_vx1*b[type]*velx);
      f[i1][1] += (dely*fbond) - (dir_vy1*b[type]*vely);
      f[i1][2] += (delz*fbond) - (dir_vy1*b[type]*velz);
    }

    if (newton_bond || i2 < nlocal) {
      f[i2][0] -= (delx*fbond) - (dir_vx2*b[type]*velx);
      f[i2][1] -= (dely*fbond) - (dir_vy2*b[type]*vely);
      f[i2][2] -= (delz*fbond) - (dir_vz2*b[type]*velz);
    }

    if (evflag) ev_tally(i1,i2,nlocal,
    newton_bond,ebond,fbond,delx,dely,delz);
  }
}
```

With the introduction of a new parameter in the pair style we need to make a new dynamic memory allocation by modifying `allocate`.

Listing 26: Original `allocate` (bond_harmonic.cpp)

```
 void BondHarmonic::allocate()
{
  allocated = 1;
  int n = atom->nbondtypes;

  memory->create(k,n+1,"bond:k");
  memory->create(r0,n+1,"bond:r0");

  memory->create(setflag,n+1,"bond:setflag");
  for (int i = 1; i <= n; i++) setflag[i] = 0;
}
```

Listing 27: Modified `allocate` (bond_kv.cpp)

```
  void BondKv::allocate()
{
  allocated = 1;
  int n = atom->nbondtypes;

  memory->create(k,n+1,"bond:k");
  memory->create(r0,n+1,"bond:r0");
  memory->create(b,n+1,"bond:b"); // new line to
 // dynamically allocate b

  memory->create(setflag,n+1,"bond:setflag");
  for (int i = 1; i <= n; i++) setflag[i] = 0;
}
```

The viscosity of the damper, b, is given by the user in the input file. For this reason, we also need to modify `coeff`.

Listing 28: Original `coeff` (bond_harmonic.cpp)

```
void BondHarmonic::coeff(int narg, char **arg)
{
  if (narg != 3) error->all(FLERR,"Incorrect args for
  bond coefficients");
  if (!allocated) allocate();

  int ilo,ihi;
  force->bounds(arg[0],atom->nbondtypes,ilo,ihi);

  double k_one = force->numeric(FLERR,arg[1]);
  double r0_one = force->numeric(FLERR,arg[2]);

  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    k[i] = k_one;
    r0[i] = r0_one;
    setflag[i] = 1;
    count++;
  }

  if (count == 0) error->all(FLERR,"Incorrect args for
   bond coefficients");
}
```

Listing 29: Modified `coeff` (bond_kv.cpp)

```
 void BondKv::coeff(int narg, char **arg)
{
  if (narg != 4) error->all(FLERR,"Incorrect args for
  bond coefficients");
  if (!allocated) allocate();

  int ilo,ihi;
  force->bounds(arg[0],atom->nbondtypes,ilo,ihi);

  double k_one = force->numeric(FLERR,arg[1]);
  double r0_one = force->numeric(FLERR,arg[2]);
  double b_one = force->numeric(FLERR,arg[3]);
// to allocate in b_one the 3rd argument of bond_coeff
  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    k[i] = k_one;
    r0[i] = r0_one;
    b[i] = b_one;
// to allocate the value stored in b_one used in compute
    setflag[i] = 1;
    count++;
  }

  if (count == 0) error->all(FLERR,"Incorrect args for
  bond coefficients");
}
```

This pair style also has the `write_restart` and `read_restart` functions that have to be modified. They basically, write and read geometry file that can be used as a support file in the input file.

Listing 30: Original `write_restart` and `read_restart` (bond_harmonic.cpp)

```
void BondHarmonic::write_restart(FILE *fp)
{
  fwrite(&k[1],sizeof(double),atom->nbondtypes,fp);
  fwrite(&r0[1],sizeof(double),atom->nbondtypes,fp);
}
/*------------*/
void BondHarmonic::read_restart(FILE *fp)
{
  allocate();

  if (comm->me == 0) {
    fread(&k[1],sizeof(double),atom->nbondtypes,fp);
    fread(&r0[1],sizeof(double),atom->nbondtypes,fp);
  }
  MPI_Bcast(&k[1],atom->nbondtypes,MPI_DOUBLE,0,world);
  MPI_Bcast(&r0[1],atom->nbondtypes,MPI_DOUBLE,0,world);

  for (int i = 1; i <= atom->nbondtypes; i++)
  setflag[i] = 1;
}
```

Listing 31: Modified `write_restart` and `read_restart` (bond_kv.cpp)

```
void BondKv::write_restart(FILE *fp)
{
  fwrite(&k[1],sizeof(double),atom->nbondtypes,fp);
  fwrite(&r0[1],sizeof(double),atom->nbondtypes,fp);
  fwrite(&b[1],sizeof(double),atom->nbondtypes,fp);
}
/*------------*/
void BondKv::read_restart(FILE *fp)
{
  allocate();

```

```
  if (comm->me == 0) {
    fread(&k[1],sizeof(double),atom->nbondtypes,fp);
    fread(&r0[1],sizeof(double),atom->nbondtypes,fp);
    fread(&b[1],sizeof(double),atom->nbondtypes,fp);
  }
  MPI_Bcast(&k[1],atom->nbondtypes,MPI_DOUBLE,0,world);
  MPI_Bcast(&r0[1],atom->nbondtypes,MPI_DOUBLE,0,world);
  MPI_Bcast(&n[1],atom->nbondtypes,MPI_DOUBLE,0,world);


  for (int i = 1; i <= atom->nbondtypes; i++)
  setflag[i] = 1;
}
```

3.3. *bond_kv.h*

In the header of the new pair style we need to substitute the "BondHarmonic" text by a new "BondKv" text as well as declare a new protected member in the class, the pointer to *b*.

Listing 32: Original header (bond_harmonic.h)

```
#ifdef BOND_CLASS

BondStyle(harmonic,BondHarmonic)

#else

#ifndef LMP_BOND_HARMONIC_H
#define LMP_BOND_HARMONIC_H

#include "stdio.h"
#include "bond.h"

namespace LAMMPS_NS {

class BondHarmonic : public Bond {
 public:
  BondHarmonic(class LAMMPS *);
  virtual ~BondHarmonic();
  virtual void compute(int, int);
  void coeff(int, char **);
  double equilibrium_distance(int);
  void write_restart(FILE *);
  void read_restart(FILE *);
  void write_data(FILE *);
  double single(int, double, int, int, double &);

 protected:
  double *k,*r0;

  void allocate();
};
}
#endif
#endif
```

Listing 33: Modified header (bond_kv.h)

```
#ifdef BOND_CLASS

BondStyle(kv,BondKv)

#else

#ifndef LMP_BOND_KV_H
#define LMP_BOND_KV_H

#include "stdio.h"
```

```
#include "bond.h"

namespace LAMMPS_NS {

class BondKv : public Bond {
 public:
  BondKv(class LAMMPS *);
  virtual ~BondKv();
  virtual void compute(int, int);
  void coeff(int, char **);
  double equilibrium_distance(int);
  void write_restart(FILE *);
  void read_restart(FILE *);
  void write_data(FILE *);
  double single(int, double, int, int, double &);

 protected:
 double *k,*r0, *b; // new pointer

  void allocate();
};
}
#endif
#endif
```

3.4. Invoking kv Pair Style

Now the new pair style is completed. To run LAMMPS with the new style we need to compile it and then invoke it by writing the command lines in shown in Listing 34 in the input file.

Listing 34: Command lines to invoke the kv pair style

```
bond_style kv
bond_coeff K r0 b
```

4. Noble–Abel Stiffened-Gas Pair Style

In the SPH framework is possible to determine all the particles properties by solving the particle form of the continuity equation [6,26]

$$\frac{d\rho_i}{dt} = \sum_j m_j \mathbf{v}_{ij} \nabla_j W_{ij}; \tag{4}$$

the momentum equation [6,26]

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j m_i m_j \left(\frac{P_i}{\rho_i} + \frac{P_i}{\rho_i} + \Pi_{ij} \right) \nabla_j W_{ij}; \tag{5}$$

and the energy conservation equation [6,26]

$$m_i \frac{de_i}{dt} = \frac{1}{2} \sum_j m_i m_j \left(\frac{P_i}{\rho_i} + \frac{P_i}{\rho_i} + \Pi_{ij} \right) : \mathbf{v}_{ij} \nabla_j W_{ij} - \sum_j \frac{m_i m_j}{\rho_i \rho_j} \frac{(\kappa_i + \kappa_j)(T_i - T_j)}{r_{ij}^2} \mathbf{r_{ij}} \cdot \nabla_j W_{ij}. \tag{6}$$

However, to be able to solve this set of equations an Equation of State (EOS) linking the pressure P and the density ρ is needed [46]. In the user-SPH package of LAMMPS one EOS is used for the liquid (Tait's EOS) and one for gas phase (ideal gas EOS). In this section we will implement a new EOS for the liquid phase. Note that with similar steps is also possible to implement a new gas EOS.

Le Métayer and Saurel [47] combined the "Noble–Abel" and the "Stiffened-Gas" EOS proposing a new EOS called Noble–Abel Stiffened-Gas (NASG), suitable for multiphase flow. The expression of the EOS does not change with the phase considered. For each phases, the pressure and temperature are calculated as function of density and specific internal energy, e.g.,

$$P(\rho, e) = (\gamma - 1)\frac{(e-q)}{\left(\frac{1}{\rho} - b\right)} - \gamma P_\infty, \tag{7}$$

and temperature-wise

$$T(\rho, e) = \frac{e-q}{C_v} - \left(\frac{1}{\rho} - b\right)\frac{P_\infty}{C_v}, \tag{8}$$

where P, ρ, e, and q are, respectively, the pressure, the density, the specific internal energy, and the heat bond of the corresponding phase. γ, P_∞, q, and b are constant coefficients that defines the thermodynamic properties of the fluid.

For this new pair style, called sph/nasgliquid, we take as a reference the sph/taitwater pair style declared and initialised in pair_sph_taitwater.h and pair_sph_taitwater.cpp files in the directory /src/USER-SPH. All the files regarding sph/nasgliquid must be saved in the /src/USER-SPH directory and its hierarchy is shown in Figure 4..

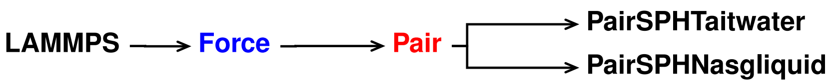


Figure 4. Class hierarchy of the new bond style.

4.1. *Validation*

The sph/nasgliquid pair style has validated by Albano and Alexiadis [26] to study the Rayleigh collapse of an empty cavity.

4.2. *pair_sph_nasgliquid.cpp*

All the functions will be the same as in the reference sph/taitwater. However, in our new sph/nasgliquid, we need to substitute the "PairSPHTaitwater" text in "PairSPHNasgliquid", as can be seen in Listings 35 and 36.

Listing 35: Original script (pair_sph_taitwater.cpp)

```
#include <cmath>
#include <cstdlib>
#include "pair_sph_taitwater.h"
#include "atom.h"
#include "force.h"
#include "comm.h"
#include "neigh_list.h"
#include "memory.h"
#include "error.h"
#include "domain.h"

using namespace LAMMPS_NS;

PairSPHTaitwater::PairSPHTaitwater(LAMMPS *lmp) :
Pair(lmp)
{...}
PairSPHTaitwater::∼PairSPHTaitwater()
{...}
void PairSPHTaitwater::compute(int eflag, int vflag)
{...}
void PairSPHTaitwater::allocate()
```

```
{...}
void PairSPHTaitwater::settings(int narg, char **/*arg*/)
{...}
void PairSPHTaitwater::coeff(int narg, char **arg)
{...}
double PairSPHTaitwater::init_one(int i, int j)
{...}
```

Listing 36: Modified script (pair_sph_nasgliquid.cpp)

```
#include <cmath>
#include <cstdlib>
#include "pair_sph_nasgliquid.h"
#include "atom.h"
#include "force.h"
#include "comm.h"
#include "neigh_list.h"
#include "memory.h"
#include "error.h"
#include "domain.h"

using namespace LAMMPS_NS;

PairSPHNasgliquid:: PairSPHNasgliquid(LAMMPS *lmp) :
Pair(lmp)
{...}
PairSPHNasgliquid::~ PairSPHNasgliquid()
{...}
void PairSPHNasgliquid::compute(int eflag, int vflag)
{...}
void PairSPHNasgliquid::allocate()
{...}
void PairSPHNasgliquid::settings(int narg, char **/*arg*/)
{...}
void PairSPHNasgliquid::coeff(int narg, char **arg)
{...}
double PairSPHNasgliquid::init_one(int i, int j)
{...}
```

For the sph/nasgliquid we need to pass a total of 12 arguments from the input file, while they were only six for sph/taitwater. For this reason we need to modify destructor, `compute`, `allocate`, `settings` and `coeff`. Following the order of function initialisation, see Listing 36, the destructor is modified as shown in Listing 38.

Listing 37: Original destructor (pair_sph_taitwater.cpp)

```
PairSPHTaitwater::~PairSPHTaitwater() {
  if (allocated) {
    memory->destroy(setflag);
    memory->destroy(cutsq);
    memory->destroy(cut);
    memory->destroy(rho0);
    memory->destroy(soundspeed);
    memory->destroy(B);
    memory->destroy(viscosity);
  }
}
```

Listing 38: Modified destructor (pair_sph_nasgliquid.cpp)

```
PairSPHNasgliquid::~PairSPHNasgliquid() {
  if (allocated) {
    memory->destroy(setflag);
    memory->destroy(cutsq);
    memory->destroy(cut);
    memory->destroy(soundspeed);
    memory->destroy(B);
    memory->destroy(CP);
```

```
    memory->destroy(CV);
    memory->destroy(gamma);
    memory->destroy(P00);
    memory->destroy(b);
    memory->destroy(q);
    memory->destroy(q1);
    memory->destroy(viscosity);
  }
}
```

In the NASG EOS the pressure is function of both density, ρ, and internal energy, e. For this reason, we need to declare more pointers and variables in `compute` compared to the reference pair style, see line 6 and 20 in Listing 40.

Listing 39: Original `compute` (pair_sph_taitwater.cpp)

```
void PairSPHTaitwater::compute(int eflag, int vflag) {
  int i, j, ii, jj, inum, jnum, itype, jtype;
  double xtmp, ytmp, ztmp, delx, dely, delz, fpair;

  int *ilist, *jlist, *numneigh, **firstneigh;
  double vxtmp, vytmp, vztmp, imass, jmass,
  fi, fj, fvisc, h, ih, ihsq;
  double rsq, tmp, wfd, delVdotDelR, mu, deltaE;

  if (eflag || vflag)
    ev_setup(eflag, vflag);
  else
    evflag = vflag_fdotr = 0;

  double **v = atom->vest;
  double **x = atom->x;
  double **f = atom->f;
  double *rho = atom->rho;
  double *mass = atom->mass;
  double *de = atom->de;
  double *drho = atom->drho;
  int *type = atom->type;
  int nlocal = atom->nlocal;
  int newton_pair = force->newton_pair;
```

Listing 40: Modified `compute` (pair_sph_nasgliquid.cpp)

```
1  void PairSPHNasgliquid::compute(int eflag, int vflag) {
2    int i, j, ii, jj, inum, jnum, itype, jtype;
3    double xtmp, ytmp, ztmp, delx, dely, delz, fpair;
4
5    int *ilist, *jlist, *numneigh, **firstneigh;
6    double vxtmp, vytmp, vztmp, imass, jmass,
7    fi, fj, fvisc, h, ih, ihsq, iirho, ijrho;
8    double rsq, tmp, wfd, delVdotDelR, mu, deltaE;
9
10   if (eflag || vflag)
11     ev_setup(eflag, vflag);
12   else
13     evflag = vflag_fdotr = 0;
14
15   double **v = atom->vest;
16   double **x = atom->x;
17   double **f = atom->f;
18   double *rho = atom->rho;
19   double *mass = atom->mass;
20   double *de = atom->de;
21   double *e = atom->e;
22   double *drho = atom->drho;
23   int *type = atom->type;
24   int nlocal = atom->nlocal;
25   int newton_pair = force->newton_pair;
```

Another modification for `compute` regards the expression of the force applied to the *i*-th, see Listing 42, and *j*-th, see Listing 44, particle.

Listing 41: Original `compute` (pair_sph_taitwater.cpp)

```
// compute pressure of atom i with Tait EOS
tmp = rho[i]/rho0[itype];
fi = tmp * tmp * tmp;
fi = B[itype] * (fi * fi * tmp - 1.0)/ (rho[i] * rho[i]);
```

Listing 42: Modified `compute` (pair_sph_nasgliquid.cpp)

```
// compute pressure of atom i with NASG EOS
tmp = e[i] / imass;
iirho= 1.0/rho[i];
iirho= iirho - b[itype];
fi = (( tmp - q[itype]) * B[itype] / iirho);
fi = fi - gamma[itype] * P00[itype];
fi = fi / (rho[i] * rho[i]);
```

Listing 43: Original `compute` (pair_sph_taitwater.cpp)

```
// compute pressure  of atom j with Tait EOS
tmp = rho[j] / rho0[jtype];
fj = tmp * tmp * tmp;
fj = B[jtype] * (fj * fj * tmp - 1.0) / (rho[j] * rho[j]);
```

Listing 44: Modified `compute` (pair_sph_nasgliquid.cpp)

```
// compute pressure  of atom j with NASG EOS
tmp = e[j] / jmass;
ijrho= 1/rho[j];
ijrho= ijrho - b[jtype];
fj = ((tmp - q[jtype])* B[jtype]/ijrho);
fj = fj - gamma[jtype]*P00[jtype];
fj = fj / (rho[j] * rho[j]);
```

With the introduction of a new parameter in the pair style we need to make a new dynamic memory allocation by modifying `allocate`.

Listing 45: Original allocate (pair_sph_taitwater.pp)

```
void PairSPHTaitwater::allocate() {
  allocated = 1;
  int n = atom->ntypes;

  memory->create(setflag, n + 1, n + 1, "pair:setflag");
  for (int i = 1; i <= n; i++)
    for (int j = i; j <= n; j++)
      setflag[i][j] = 0;

  memory->create(cutsq, n + 1, n + 1, "pair:cutsq");
  memory->create(rho0, n + 1, "pair:rho0");
  memory->create(soundspeed, n + 1, "pair:soundspeed");
  memory->create(B, n + 1, "pair:B");
  memory->create(cut, n + 1, n + 1, "pair:cut");
  memory->create(viscosity,n + 1,n + 1,"pair:viscosity");
}
```

Listing 46: Modified allocate (pair_sph_nasgliquid.cpp)

```
void PairSPHNasgliquid::allocate() {
  allocated = 1;
  int n = atom->ntypes;

  memory->create(setflag, n + 1, n + 1, "pair:setflag");
  for (int i = 1; i <= n; i++)
    for (int j = i; j <= n; j++)
      setflag[i][j] = 0;
```

```
  memory->create(cutsq, n + 1, n + 1, "pair:cutsq");
  memory->create(soundspeed, n + 1, "pair:soundspeed");
  memory->create(B, n + 1, "pair:B");
  memory->create(CP, n + 1, "pair:CP");
  memory->create(CV, n + 1, "pair:CV");
  memory->create(gamma, n + 1, "pair:gamma");
  memory->create(P00, n + 1, "pair:P00");
  memory->create(b, n + 1, "pair:b");
  memory->create(q, n + 1, "pair:q");
  memory->create(q1, n + 1, "pair:q1");
  memory->create(cut, n + 1, n + 1, "pair:cut");
  memory->create(viscosity,n + 1,n + 1,"pair:viscosity");
}
```

The 12 arguments used in the pair style are passed by the used in the input file. For this reason, we also have to modify `coeff`.

Listing 47: Original `coeff` (pair_sph_taitwater.cpp)

```
void PairSPHTaitwater::coeff(int narg, char **arg) {
  if (narg != 6)
    error->all(FLERR,
        "Incorrect args for pair_style sph/taitwater
        coefficients");
  if (!allocated)
    allocate();
  int ilo, ihi, jlo, jhi;
  force->bounds(FLERR,arg[0], atom->ntypes, ilo, ihi);
  force->bounds(FLERR,arg[1], atom->ntypes, jlo, jhi);
  double rho0_one = force->numeric(FLERR,arg[2]);
  double soundspeed_one = force->numeric(FLERR,arg[3]);
  double viscosity_one = force->numeric(FLERR,arg[4]);
  double cut_one = force->numeric(FLERR,arg[5]);
  double B_one=soundspeed_one*soundspeed_one*rho0_one/7.0;
  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    rho0[i] = rho0_one;
    soundspeed[i] = soundspeed_one;
    B[i] = B_one;
    for (int j = MAX(jlo,i); j <= jhi; j++) {
      viscosity[i][j] = viscosity_one;
      cut[i][j] = cut_one;
      setflag[i][j] = 1;
      count++; } }
```

Listing 48: Modified `coeff` (pair_sph_nasgliquid.cpp)

```
void PairSPHNasgliquid::coeff(int narg, char **arg) {
  if (narg != 12)
    error->all(FLERR,
        "Incorrect args for pair_style sph/nasgliquid
         coefficients");
  if (!allocated)
    allocate();
  int ilo, ihi, jlo, jhi;
  force->bounds(FLERR,arg[0], atom->ntypes, ilo, ihi);
  force->bounds(FLERR,arg[1], atom->ntypes, jlo, jhi);
  double soundspeed_one = force->numeric(FLERR,arg[2]);
  double viscosity_one = force->numeric(FLERR,arg[3]);
  double cut_one = force->numeric(FLERR,arg[4]);
  double CP_one = force->numeric(FLERR,arg[5]);
  double CV_one = force->numeric(FLERR,arg[6]);
  double gamma_one = force->numeric(FLERR,arg[7]);
  double P00_one = force->numeric(FLERR,arg[8]);
  double b_one = force->numeric(FLERR,arg[9]);
  double q_one = force->numeric(FLERR,arg[10]);
  double q1_one = force->numeric(FLERR,arg[11]);
  double B_one = (gamma_one - 1);
```

```
  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    soundspeed[i] = soundspeed_one;
    B[i] = B_one;
    CP[i] = CP_one;
    CV[i] = CV_one;
    gamma[i] = gamma_one;
    P00[i] = P00_one;
    b[i] = b_one;
    q[i] = q_one;
    q1[i] = q1_one;
    for (int j = MAX(jlo,i); j <= jhi; j++) {
      viscosity[i][j] = viscosity_one;
      cut[i][j] = cut_one;
      setflag[i][j] = 1;
      count++;  }  }
```

4.3. *pair_sph_nasgliquid.h*

In the header of the new pair style we need to substitute the "PairSPHTaitwater" text in "PairSPHNasgliquid" as well as declare new protected members in the class, the pointers to the new arguments.

Listing 49: Original header (pair_sph_taitwater.h)

```
#ifdef PAIR_CLASS

PairStyle(sph/taitwater,PairSPHTaitwater)

#else

#ifndef LMP_PAIR_TAITWATER_H
#define LMP_PAIR_TAITWATER_H

#include "pair.h"

namespace LAMMPS_NS {

class PairSPHTaitwater : public Pair {
 public:
  PairSPHTaitwater(class LAMMPS *);
  virtual ~PairSPHTaitwater();
  virtual void compute(int, int);
  void settings(int, char **);
  void coeff(int, char **);
  virtual double init_one(int, int);

 protected:
  double *rho0, *soundspeed, *B;
  double **cut,**viscosity;
  int first;
  void allocate();
};
}
#endif
#endif
```

Listing 50: Modified header (pair_sph_nasgliquid.h)

```
#ifdef PAIR_CLASS

PairStyle(sph/nasgliquid,PairSPHNasgliquid)

#else

#ifndef LMP_PAIR_NASGLIQUID_H
#define LMP_PAIR_NASGLIQUID_H

```

```
#include "pair.h"

namespace LAMMPS_NS {

class PairSPHNasgliquid : public Pair {
 public:
  PairSPHNasgliquid(class LAMMPS *);
  virtual ~PairSPHNasgliquid();
  virtual void compute(int, int);
  void settings(int, char **);
  void coeff(int, char **);
  virtual double init_one(int, int);

 protected:
  double *soundspeed, *B, *CP, *CV, *gamma, *P00,
  *b, *q, *q1;
  double **cut,**viscosity;
  int first;
  void allocate();
};
}
#endif
#endif
```

4.4. Invoking Sph/Nasgliquid Pair Style

Now the new pair style is completed. To run LAMMPS with the new style we need to compile it and then invoke it by writing the command lines shown in Listing 51 in the input file.

Listing 51: Command lines to invoke the NASG pair style for liquid

```
pair_style sph/nasgliquid
pair_coeff  I J c_0 alpha h Cv Cp gamma P00 b q q'
```

5. Multiphase (Liquid–Gas) Heat Exchange Pair Style

In LAMMPS thermal conductivity between SPH particles is enabled using the sph/heatconduction pair style inside the user-SPH package. However, the pair style is designed only for mono phase fluid where the thermal conductivities is constant ($\kappa_i = \kappa$). When more than one phase is present, the heat conduction at the interface can be implemented by using [6,26]

$$m_i \frac{de_i}{dt} = \sum_j \frac{m_i m_j}{\rho_i \rho_j} \frac{(\kappa_i + \kappa_j)(T_i - T_j)}{r_{ij}^2} \mathbf{r_{ij}} \cdot \nabla_j W_{ij}. \tag{9}$$

In the new pair style, called sph/heatgasliquid, one phase is assumed to be liquid with an initial temperature of $T_{l,0}$ and the other is assumed to be and ideal gas. Each time-step the temperature of the fluid is updated as [26].

$$T_l = T_{l,0} + \frac{E_l - E_{l,0}}{C_{p,l}}, \tag{10}$$

where $T_{l,0}$ is the reference temperature, E_0 the internal energy in [J], E_l internal energy [J] at the current time step and $C_{p,l}$ is heat capacity of the fluid in [J K^{-1}]. The temperature of the gas is updated following the ideal EOS [26].

$$T_g = MM \frac{(\gamma - 1)e_g}{R}, \tag{11}$$

where MM is the molar mass [kg kmol^{-1}], e_g is the specific internal energy in [J kg^{-1}], γ is the heat capacity ratio and R is the ideal gas constant in [J K^{-1} kmol^{-1}]. Generally the choice of the reference states $E_{l,0}$ is arbitrary, but if the Equation of State (EOS) used for the phase is function of both density and internal energy of the reference state will be determined by the EOS.

In the sph/heatgasliquid pair style is important to check if the i-th and j-th particles are liquid or gas phase to apply either Equation (10) or Equation (11). This "phase check" is explained in Section 5.2 `compute` function is modified.

For the energy balance the new pair style needs $T_{l,0}$, $E_{l,0}$, $C_{p,l}$ and κ_l for the liquid phase and κ_g for the gas phase. Moreover, for the phase check, the particle types of each phases must be specified. All this informations is passed by the user in the in the input file.

The reference pair style is sph/heatconduction. It is declared and initialised in the pair_sph_heatconduction.cpp pair_sph_heatconduction.cpp files in the directory /src/USER-SPH. All the files regarding sph/heatgasliquid must be saved in the /src/USER-SPH directory and its hierarchy is shown in Figure 5.

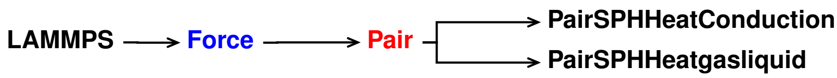


Figure 5. Class hierarchy of the new pair style.

5.1. Validation

The sph/heatgasliquid pair style has validated by Albano and Alexiadis [26] to study the role of the heat diffusion in for a gas filled Rayleigh collapse in water.

5.2. pair_sph_heatgasliquid.cpp

All the functions will be the same as in the reference sph/heatconduction. However, in our new sph/heatgasliquid, we need to substitute the "PairSPHHeatConduction" text in "PairSPHHeatgasliquid", as can be seen in Listings 52 and 53.

Listing 52: Original script (pair_sph_heatconduction.cpp)

```
#include "math.h"
#include "stdlib.h"
#include "pair_sph_heatconduction.h"
#include "atom.h"
#include "force.h"
#include "comm.h"
#include "memory.h"
#include "error.h"
#include "neigh_list.h"
#include "domain.h"

using namespace LAMMPS_NS;

PairSPHHeatConduction::PairSPHHeatConduction(LAMMPS *lmp)
: Pair(lmp)
{ ... }
PairSPHHeatConduction::~PairSPHHeatConduction()
{ ... }
void PairSPHHeatConduction::compute(int eflag, int vflag)
{ ... }
void PairSPHHeatConduction::allocate()
{ ... }
void PairSPHHeatConduction::settings(int narg, char **arg)
{ ... }
void PairSPHHeatConduction::coeff(int narg, char **arg)
{ ... }
double PairSPHHeatConduction::init_one(int i, int j)
{ ... }
double PairSPHHeatConduction::single(int i, int j,
 int itype, int jtype, double rsq, double factor_coul,
 double factor_lj, double &fforce)
{ ... }
```

Listing 53: Modified script (pair_sph_heatgasliquid.cpp)

```
#include <cmath>
#include <cstdlib>
#include "pair_sph_heatgasliquid.h"
#include "atom.h"
#include "force.h"
#include "comm.h"
#include "memory.h"
#include "error.h"
#include "neigh_list.h"
#include "domain.h"

using namespace LAMMPS_NS;

PairSPHHeatgasliquid::PairSPHHeatgasliquid(LAMMPS *lmp)
: Pair(lmp)
{ ... }
PairSPHHeatgasliquid::~PairSPHHeatgasliquid()
{ ... }
void PairSPHHeatgasliquid::compute(int eflag, int vflag)
{ ... }
void PairSPHHeatgasliquid::allocate()
{ ... }
void PairSPHHeatgasliquid::settings(int narg, char **arg)
{ ... }
void PairSPHHeatgasliquid::coeff(int narg, char **arg)
{ ...
double PairSPHHeatgasliquid::init_one(int i, int j)
{ ... }
double PairSPHHeatgasliquid::single(int i, int j,
int itype, int jtype, double rsq, double factor_coul,
double factor_lj, double &fforce)
{ ... }
```

For the sph/heatgasliquid we need to pass a total of nine arguments from the input file, while they were only seven for sph/heatconduction. For this reason we need to modify destructor, `compute`, `allocate`, `settings` and `coeff`. Following the order of function initialisation, see Listing 53, the destructor is modified by removing the heat diffusion coefficient, line 6 in Listing 54.

Listing 54: Original destructor (pair_sph_heatconduction.cpp)

```
1 PairSPHHeatConduction::~PairSPHHeatConduction() {
2   if (allocated) {
3     memory->destroy(setflag);
4     memory->destroy(cutsq);
5     memory->destroy(cut);
6     memory->destroy(alpha);
7   }
8 }
```

Listing 55: Modified destructor (pair_sph_heatgasliquid.cpp)

```
PairSPHHeatgasliquid::~PairSPHHeatgasliquid() {
  if (allocated) {
    memory->destroy(setflag);
    memory->destroy(cutsq);
    memory->destroy(cut);
  }
}
```

To compute Equation (6) we need to declare more variables in `compute` compared to the reference pair style, see line 4 in Listing 57.

Listing 56: Original `compute` (pair_sph_heatconduction.cpp)

```
void PairSPHHeatConduction::compute(int eflag, int vflag){
  int i, j, ii, jj, inum, jnum, itype, jtype;
  double xtmp, ytmp, ztmp, delx, dely, delz;
```

Listing 57: Modified `compute` (pair_sph_heatgasliquid.cpp)

```
void PairSPHHeatgasliquid::compute(int eflag, int vflag){
  int i, j, ii, jj, inum, jnum, itype, jtype;
  double xtmp, ytmp, ztmp, delx, dely, delz;
  double Ti, Tj, ki, kj;  /// new parameters
```

Another important modification is to add the phase check inside `compute`. The phase check has to be implemented for both the *i*-th particle and the *j*-th particle inside the loop over neighbours, `for (ii = 0; ii < inum; ii++)` in the reference pair style. The phase check for the *i*-th particle starts after the assignment of `imass`, line 3 of Listing 58.

Listing 58: Modified `compute` (pair_sph_heatgasliquid.cpp)

```
1  imass = mass[itype];
2
3  if (itype == liquidtype)
4       {
5          Ti= e[i] - el0;
6          Ti= Ti/CPl;
7          Ti= T0l + Ti;
8          ki=kl;
9        }
10 else {
11         Ti=0.40*e[i]*18;
12         Ti= Ti/imass;
13         Ti= Ti/8314.33;
14         ki=kg;
15       }
```

Similarly, for the *j*-th the phase check start at line 3 of Listing 59.

Listing 59: Modified `compute` (pair_sph_heatgasliquid.cpp)

```
1       jmass = mass[jtype];
2
3     if (jtype == liquidtype)
4       {
5          Tj= e[j] - el0;
6          Tj= Tj/CPl;
7          Tj= T0l + Tj;
8          kj=kl;
9     }
10    else {
11         Tj=0.40*e[j]*18;
12         Tj= Tj/jmass;
13         Tj= Tj/8314.33;
14         kj=kg;
15    }
16
```

The last change in `compute` is to implement the change in internal energy as shown in Equation (9).

Listing 60: Original `compute` (pair_sph_heatconduction.cpp)

```
      D = alpha[itype][jtype]; // diffusion coefficient

       deltaE = 2.0 * imass * jmass / (imass+jmass);
       deltaE *= (rho[i] + rho[j]) / (rho[i] * rho[j]);
       deltaE *= D * (e[i] - e[j]) * wfd;

       de[i] += deltaE;
       if (newton_pair || j < nlocal) {
         de[j] -= deltaE;
       }
```

Listing 61: Modified `compute` (pair_sph_heatgasliquid.cpp)

```
       deltaE = imass * jmass / (rho[i] * rho[j]);  ///
       deltaE *= (ki + kj) * (Ti - Tj) * wfd;   ///
       ///  implementation of eq 3.4
       de[i] += deltaE;
       if (newton_pair || j < nlocal) {
         de[j] -= deltaE;
       }
```

With the introduction of new arguments in the pair style we need to make a new dynamic memory allocation by modifying `allocate`.

Listing 62: Original allocate (pair_sph_heatconduction.cpp)

```
void PairSPHHeatConduction::allocate() {
  allocated = 1;
  int n = atom->ntypes;

  memory->create(setflag, n + 1, n + 1, "pair:setflag");
  for (int i = 1; i <= n; i++)
    for (int j = i; j <= n; j++)
      setflag[i][j] = 0;

  memory->create(cutsq, n + 1, n + 1, "pair:cutsq");
  memory->create(cut, n + 1, n + 1, "pair:cut");
  memory->create(alpha, n + 1, n + 1, "pair:alpha");
}
```

Listing 63: Modified allocate (pair_sph_heatgasliquid.cpp)

```
void PairSPHHeatgasliquid::allocate() {
  allocated = 1;
  int n = atom->ntypes;

  memory->create(setflag, n + 1, n + 1, "pair:setflag");
  for (int i = 1; i <= n; i++)
    for (int j = i; j <= n; j++)
      setflag[i][j] = 0;

  memory->create(cutsq, n + 1, n + 1, "pair:cutsq");
  memory->create(cut, n + 1, n + 1, "pair:cut");
}
```

The nine arguments used in the pair style are passed by the user in the input file. For this reason, we also have to modify `coeff`.

Listing 64: Original `coeff` (pair_sph_heatconduction.cpp)

```
void PairSPHHeatConduction::coeff(int narg, char **arg) {
  if (narg != 4)
    error->all(FLERR,"Incorrect number of args for
    pair_style sph/heatconduction coefficients");
  if (!allocated)
    allocate();

```

```
  int ilo, ihi, jlo, jhi;
  force->bounds(arg[0], atom->ntypes, ilo, ihi);
  force->bounds(arg[1], atom->ntypes, jlo, jhi);

  double alpha_one = force->numeric(FLERR,arg[2]);
  double cut_one   = force->numeric(FLERR,arg[3]);

  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    for (int j = MAX(jlo,i); j <= jhi; j++) {
//printf("setting cut[%d][%d] = %f\n", i, j, cut_one);
      cut[i][j] = cut_one;
      alpha[i][j] = alpha_one;
      setflag[i][j] = 1;
      count++;
    }
  }

  if (count == 0)
    error->all(FLERR,"Incorrect args for pair
    coefficients");
}
```

Listing 65: Modified `coeff` (pair_sph_heatgasliquid.cpp)

```
void PairSPHHeatgasliquid::coeff(int narg, char **arg) {
  if (narg != 9)
    error->all(FLERR,"Incorrect number of args for
     pair_style sph/heatgasliquid coefficients");
  if (!allocated)
    allocate();

  int ilo, ihi, jlo, jhi;
  force->bounds(FLERR,arg[0], atom->ntypes, ilo, ihi);
  force->bounds(FLERR,arg[1], atom->ntypes, jlo, jhi);

  el0 = force->numeric(FLERR,arg[2]);
  kl = force->numeric(FLERR,arg[3]);
  kg = force->numeric(FLERR,arg[4]);
  T0l = force->numeric(FLERR,arg[5]);
  double cut_one = force->numeric(FLERR,arg[6]);
  CPl = force->numeric(FLERR,arg[7]);
  liquidtype = force->numeric(FLERR,arg[8]);

  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    for (int j = MAX(jlo,i); j <= jhi; j++) {
//printf("setting cut[%d][%d] = %f\n", i, j, cut_one);
      cut[i][j] = cut_one;
      setflag[i][j] = 1;
      count++;
    }
  }
  if (count == 0)
    error->all(FLERR,"Incorrect args for pair
     coefficients");
}
```

5.3. *pair_sph_heatgasliquid.h*

In the header of the new pair style we need to substitute the "PairSPHHeatConduction" text in "PairSPHHeatgasliquid" and declare new protected members in the class.

Listing 66: Original header (pair_sph_heatconduction.h)

```
#ifdef PAIR_CLASS

PairStyle(sph/heatconduction,PairSPHHeatConduction)

#else

#ifndef LMP_PAIR_SPH_HEATCONDUCTION_H
#define LMP_PAIR_SPH_HEATCONDUCTION_H

#include "pair.h"

namespace LAMMPS_NS {

class PairSPHHeatConduction : public Pair {
 public:
  PairSPHHeatConduction(class LAMMPS *);
  virtual ~PairSPHHeatConduction();
  virtual void compute(int, int);
  void settings(int, char **);
  void coeff(int, char **);
  virtual double init_one(int, int);
  virtual double single(int, int, int, int, double,
  double, double, double &);

 protected:
  double **cut, **alpha;
  void allocate();
};
}
#endif
#endif
```

Listing 67: Modified header (pair_sph_heatgasliquid.h)

```
#ifdef PAIR_CLASS

PairStyle(sph/heatgasliquid,PairSPHHeatgasliquid)

#else

#ifndef LMP_PAIR_SPH_HEATGASLIQUID_H
#define LMP_PAIR_SPH_HEATGASLIQUID_H

#include "pair.h"

namespace LAMMPS_NS {

class PairSPHHeatgasliquid : public Pair {
 public:
  PairSPHHeatgasliquid(class LAMMPS *);
  virtual ~PairSPHHeatgasliquid();
  virtual void compute(int, int);
  void settings(int, char **);
  void coeff(int, char **);
  virtual double init_one(int, int);
  virtual double single(int, int, int, int, double,
  double, double, double &);

 protected:
  int liquidtype;
  double el0, kg, kl, T0l, CPl;
  double **cut;
  void allocate();
};
}
#endif
#endif
```

5.4. Invoking Sph/Heatgasliquid Pair Style

Now the new pair style is completed. To run LAMMPS with the new style we need to compile it and then invoke it by writing the command lines shown in Listing 68 in the input file.

Listing 68: Command lines to invoke the sph/heatgasliquid pair style

```
pair_style    sph/heatgasliquid
pair_coeff     i j el0 kl kg T10 h Cpl liquidtype
```

6. Full Stationary Fix Style

In LAMMPS a `fix` style is any operation that is applied to the system, usually to a group of particles, during time stepping or minimisation used to alter some property of the sytem [41]. There are hundreds of fixes defined in LAMMPS and new ones can be added. Usually fixes are used for time integration, force constraints, boundary conditions and diagnostics.

In the user-sph package in LAMMPS there is the so called meso/stationary fix used to set boundary condition. With meso/stationary is possible to fix position and velocity for a group of particles, walls as example, but internal energy and density will be updated. In some cases, it is useful to have a fully stationary conditions that maintains constant also the energy and the density. For this new fix, called meso/fullstationary, we take as a reference the meso/stationary fix declared and initialised in fix_meso_stationary.h and fix_meso_stationary.cpp files in the directory /src/USER-SPH. All the files regarding meso/fullstationary must be saved in the /src/USER-SPH directory and its hierarchy is shown in Figure 6.

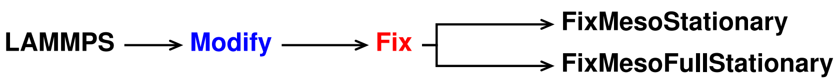


Figure 6. Class hierarchy of the new fix style.

6.1. Validation

The meso/fullstationary has been used in the validation of the new viscosity class to set the boundary condition of a constant asymmetric heated walls, see Section 7.2.

6.2. *fix_meso_fullstationary.cpp*

All the functions will be the same as in the reference meso/stationary. However, in our new fullstationary, we need to substitute the "FixMesoStationary" text in "FixMesoFullStationary", as can be seen in Listings 69 and 70.

Listing 69: Original script (fix_meso_stationary.cpp)

```
#include <cstdio>
#include <cstring>
#include <cmath>
#include <cstdlib>
#include "fix_meso_stationary.h"
#include "atom.h"
#include "comm.h"
#include "force.h"
#include "neighbor.h"
#include "neigh_list.h"
#include "neigh_request.h"
#include "update.h"
#include "integrate.h"
#include "respa.h"
#include "memory.h"
#include "error.h"
#include "pair.h"

```

```
using namespace LAMMPS_NS;
using namespace FixConst;

FixMesoStationary:: FixMesoStationary(LAMMPS *lmp,
int narg, char **arg) : Fix(lmp, narg, arg)
{...}
int FixMesoStationary::setmask()
{...}
void FixMesoStationary::init()
{...}
void FixMesoStationary::initial_integrate(int /*vflag*/)
{...}
void FixMesoStationary::final_integrate()
{...}
void FixMesoStationary::reset_dt()
{...}
```

Listing 70: Modified script (fix_meso_fullstationary.cpp)

```
#include <cstdio>
#include <cstring>
#include <cmath>
#include <cstdlib>
#include "fix_meso_fullstationary.h"
#include "atom.h"
#include "comm.h"
#include "force.h"
#include "neighbor.h"
#include "neigh_list.h"
#include "neigh_request.h"
#include "update.h"
#include "integrate.h"
#include "respa.h"
#include "memory.h"
#include "error.h"
#include "pair.h"

using namespace LAMMPS_NS;
using namespace FixConst;

FixMesoFullStationary::FixMesoFullStationary(LAMMPS *lmp,
 int narg, char **arg) : Fix(lmp, narg, arg)
{...}
int FixMesoFullStationary::setmask()
{...}
void FixMesoFullStationary::init()
{...}
void FixMesoFullStationary::initial_integrate
(int /*vflag*/)
{...}
void FixMesoFullStationary::final_integrate()
{...}
void FixMesoFullStationary::reset_dt()
{...}
```

For the meso/fullstationary we need to modify two function: `initial_integrate`, see Listing 72 line 16 and 17, and `final_integrate`, see Listing 74 line 14 and 15.

Listing 71: Original initial_integrate (fix_meso_stationary.cpp)

```
void FixMesoStationary::initial_integrate(int vflag) {

  double *rho = atom->rho;
  double *drho = atom->drho;
  double *e = atom->e;
  double *de = atom->de;
  int *type = atom->type;
  int *mask = atom->mask;
  int nlocal = atom->nlocal;
  int i;

  if (igroup == atom->firstgroup)
    nlocal = atom->nfirst;

  for (i = 0; i < nlocal; i++) {
    if (mask[i] & groupbit) {
      e[i] += dtf * de[i];
// with this line is possible to update internal energy
      rho[i] += dtf * drho[i];
// ... and density every half-step
    }}}
```

Listing 72: Modified initial_integrate (fix_meso_fullstationary.cpp)

```
void FixMesoFullStationary::initial_integrate(int vflag) {

  double *rho = atom->rho;
  double *drho = atom->drho;
  double *e = atom->e;
  double *de = atom->de;
  int *mask = atom->mask;
  int nlocal = atom->nlocal;
  int i;

  if (igroup == atom->firstgroup)
    nlocal = atom->nfirst;

  for (i = 0; i < nlocal; i++) {
    if (mask[i] & groupbit) {
      e[i] +=0; // with this line internal energy
      rho[i] += 0; // ... and density are constant
    }}}
```

Listing 73: Original final_integrate (fix_meso_stationary.cpp)

```
void FixMesoStationary::final_integrate() {

  double *e = atom->e;
  double *de = atom->de;
  double *rho = atom->rho;
  double *drho = atom->drho;
  int *type = atom->type;
  int *mask = atom->mask;
  double *mass = atom->mass;
  int nlocal = atom->nlocal;
  if (igroup == atom->firstgroup)
    nlocal = atom->nfirst;

  for (int i = 0; i < nlocal; i++) {
    if (mask[i] & groupbit) {
      e[i] += dtf * de[i];
      rho[i] += dtf * drho[i];
    }}}
```

Listing 74: Modified final_integrate (fix_meso_fullstationary.cpp)

```
vvoid FixMesoFullStationary::final_integrate() {

  double *e = atom->e;
  double *de = atom->de;
  double *rho = atom->rho;
  double *drho = atom->drho;
  int *mask = atom->mask;
  int nlocal = atom->nlocal;
  if (igroup == atom->firstgroup)
    nlocal = atom->nfirst;

  for (int i = 0; i < nlocal; i++) {
    if (mask[i] & groupbit) {
      e[i] += 0; //  with this line internal energy
      rho[i] += 0; //... and density are constant
    }}}
```

6.3. *fix_mes_fullstationary.h*

In the header of the new fix we need to substitute the "FixMesoStationary" text in "FixMesoFullStationary".

Listing 75: Original header (pair_sph_heatconduction.h)

```
#ifdef FIX_CLASS

FixStyle(meso/stationary,FixMesoStationary)

#else

#ifndef LMP_FIX_MESO_STATIONARY_H
#define LMP_FIX_MESO_STATIONARY_H

#include "fix.h"

namespace LAMMPS_NS {

class FixMesoStationary : public Fix {
 public:
  FixMesoStationary(class LAMMPS *, int, char **);
  int setmask();
  virtual void init();
  virtual void initial_integrate(int);
  virtual void final_integrate();
  void reset_dt();

 private:
  class NeighList *list;
 protected:
  double dtv,dtf;
  double *step_respa;
  int mass_require;

  class Pair *pair;
};
}
#endif
#endif
```

Listing 76: Modified header (pair_sph_heatgasliquid.h)

```
#ifdef FIX_CLASS

FixStyle(meso/fullstationary,FixMesoFullStationary)

#else

```

```
#ifndef LMP_FIX_MESO_FULLSTATIONARY_H
#define LMP_FIX_MESO_FULLSTATIONARY_H

#include "fix.h"

namespace LAMMPS_NS {

class FixMesoFullStationary: public Fix {
 public:
  FixMesoFullStationary(class LAMMPS *, int, char **);
  int setmask();
  virtual void init();
  virtual void initial_integrate(int);
  virtual void final_integrate();
  void reset_dt();

 private:
  class NeighList *list;
 protected:
  double dtv,dtf;
  double *step_respa;
  int mass_require;

  class Pair *pair;
};
}
#endif
#endif
```

6.4. Invoking Meso/Fullstationary Fix

Now the new fix is completed. To run LAMMPS with the new style we need to compile it and then invoke it by writing the command lines shown in Listing 77 in the input file.

Listing 77: Command lines to invoke the new pair style

```
fix ID group-ID meso/fullstationary
```

7. Viscosity Class

Viscosity in the SPH method has been addressed with different solutions [46]. Shock waves, for example, have been a challenge to model due to the arise of numerical oscillations around the shocked region. Monaghan solved this problem with the introduction of the so-called Monaghan artificial viscosity [48]. Artificial viscosity is still used nowadays for energy dissipation and to prevent unphysical penetration for particles approaching each other [25,49]. The SPH package of LAMMPS uses the following artificial viscosity expression [6], within the sph/idealgas and sph/taitwater pair style.

$$\Pi_{ij} = -\alpha h \frac{c_i + c_j}{\rho_i + \rho_j} \frac{\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}}{r_{ij}^2 + \epsilon h^2}, \tag{12}$$

where α is the dimensionless dissipation factor, c_i and c_j are the speed of sound of particle i and j. The dissipation factor, α, can be linked with the real viscosity in term of [6]

$$\alpha = 8 \frac{\mu}{ch\rho}, \tag{13}$$

where c is the speed of sound, ρ the density, μ the dynamic viscosity and h the smoothing length.

The artificial viscosity approach performs well at a high Reynolds number but better solutions are available for laminar flow: Morris et al. [50] approximated and implemented the viscosity momentum term for SPH. The same solution can be found in the sph/taitwater/morris pair style with the expression [6].

$$\sum_j \frac{m_i m_j (\mu_i + \mu_j)\mathbf{v}_{ij}}{\rho_i \rho_j} \left(\frac{1}{r_{ij}} \frac{\partial W_{ij}}{\partial r_i} \right), \tag{14}$$

where μ is the real dynamic viscosity.

In LAMMPS both the dissipation factor and the dynamic viscosity are treated as a constant between a pair of particles when they interact within the smoothing length. In this section we want to make the viscosity a per atom property instead of a pair property only existing within a pair style. Moreover, five temperature dependent viscosity models are added. For this example, no reference file is used; a new class, Viscosity, is implemented in LAMMPS from scratch and its hierarchy is shown in Figure 7.

Figure 7. Class hierarchy of the new class.

7.1. Temperature Dependant Viscosity

In literature multiples empirical models that correlate viscosity with temperature are available [51–53]. In the new viscosity class five different viscosity models have been implemented:

1. Andrade's equation [54]

$$\mu = Aexp\left(\frac{B}{T} + CT + DT^2 \right), \tag{15}$$

where μ is the viscosity in [Kg m^{-1} s^{-1}], T is the static temperature in Kelvin, A, B, C and D are fluid-dependent dimensional coefficients available in literature.

2. Arrhenius viscosity by Raman [55,56]

$$\mu = C_1 exp(C_2/T), \tag{16}$$

where μ is the dynamic viscosity in [Kg m^{-1} s^{-1}], T is the temperature in Kelvin, C_1 and C_2 are fluid-dependent dimensional coefficients available in literature.

3. Sutherland's viscosity [57,58] for gas phase
Sutherland's law can be expressed as:

$$\mu = \frac{C_1 T^{3/2}}{T + C_2}, \tag{17}$$

where μ is the viscosity in [Kg m^{-1} s^{-1}], T is the static temperature in Kelvin, C_1 and C_2 are dimensional coefficients.

4. Power-Law viscosity law [57] for gas phase
A power-law viscosity law with two coefficients has the form :

$$\mu = BT^n, \tag{18}$$

where μ is the viscosity in [Kg m^{-1} s^{-1}], T is the static temperature in Kelvin, and B is a dimensional coefficient.

5. Constant viscosity

With constant viscosity both dissipation factor and dynamic viscosity will be constant during the simulation.

When the artificial viscosity is used the dissipation factor of Equation (12) is defined as the arithmetic mean of the dissipation factors of i-th particle and j-th particle.

$$\alpha_{ij} = -\frac{4}{h}\left(\frac{\mu_i}{c_i\rho_i} + \frac{\mu_j}{c_j\rho_j}\right), \tag{19}$$

where α_{ij} is the dissipation factor of the particles pair i and j.

7.2. Validation

In order to validate the new Viscosity class, we will study the effect of asymmetrically heating walls in a channel flow, and more specifically the effect on the velocity field of the fluid. The data obtained with our model will be compared with the analytical solution obtained by Sameen and Govindarajan [59].

The water flows between two walls in the x-direction with periodic conditions. The walls are set at different temperatures T_{cold} and T_{hot} , see Figure 8. Both water and walls are modelled as fluid following the tait EOS. The physical properties of the walls are set constant throughout the simulation using the full stationary conditions described in Section 6.

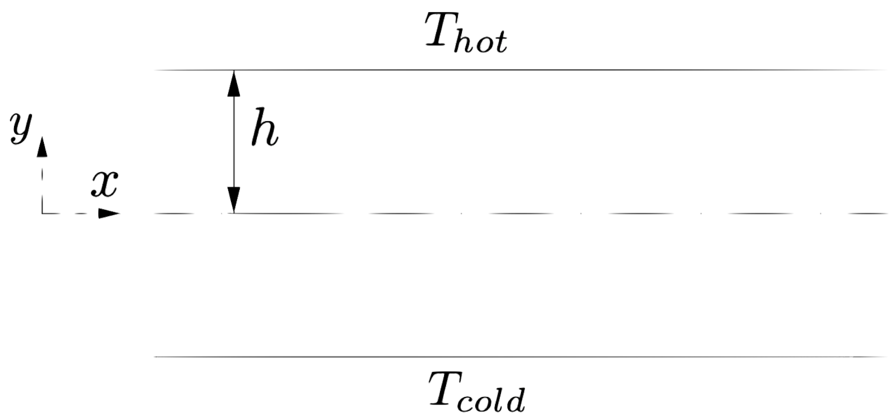


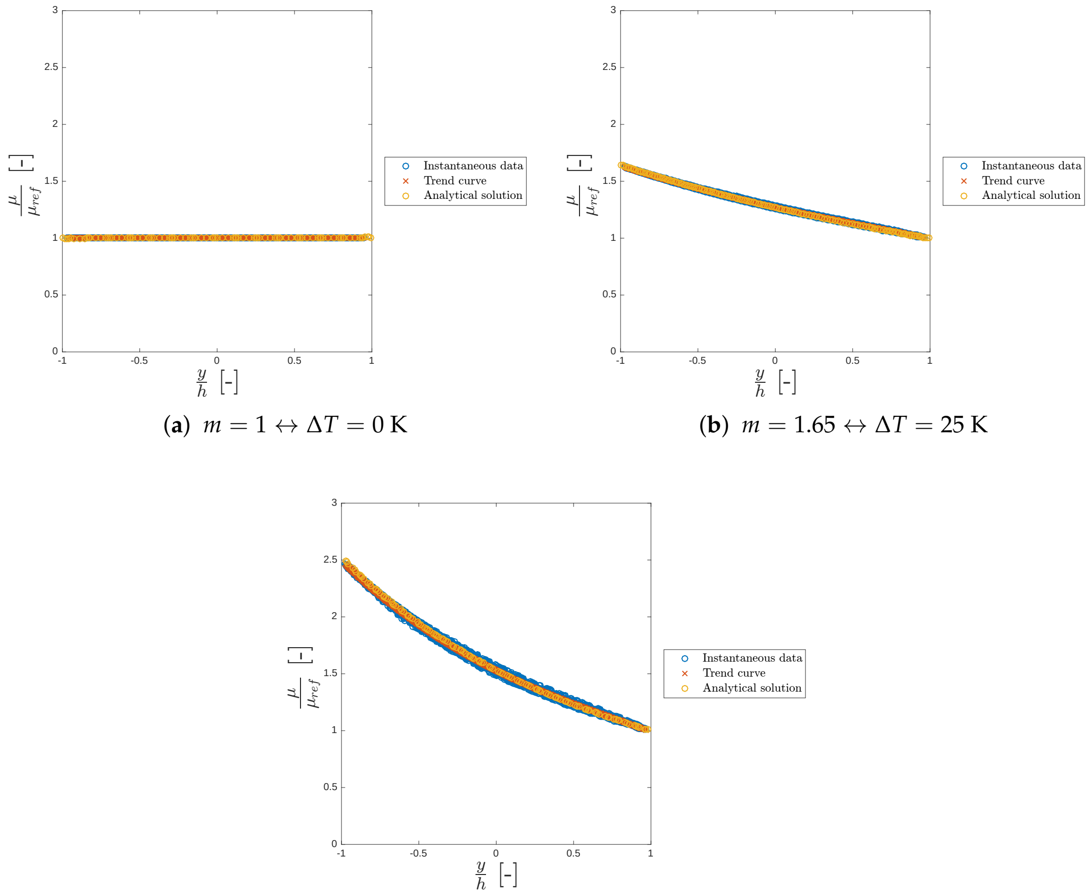
Figure 8. Geometry of the simulation.

To match the condition used by Sameen and Govindarajan we set the cold wall temperature to $T_{cold} = 295$ K and the temperature dependence of the dynamic viscosity described by the Arrhenius model, Equation (16), with $C_1 = 0.000183$ [Ns m^{-2}] and $C_2 = 1879.9$ K [59]. To describe the asymmetric heating Sameen and Govindarajan introduced the parameter m, defined as:

$$m = \frac{\mu_{cold}}{\mu_{ref}} \tag{20}$$

where $\mu_{ref} = \mu_{hot}$ is the viscosity at the hot wall in the case of asymmetric heating and μ_{cold} is the viscosity at the cold wall. By combining (16) and (20), with the given T_{cold}, is possible to express the temperature difference of the walls ΔT as function of m.

Figure 9 shows the viscosity trend for different values of m and the corresponding ΔT. Sometimes, in particle methods, instantaneous data can be noisy (scattered) as can be seen from the blue circles of both Figures 9 and 10.



(**a**) $m = 1 \leftrightarrow \Delta T = 0$ K (**b**) $m = 1.65 \leftrightarrow \Delta T = 25$ K

(**c**) $m = 2.5 \leftrightarrow \Delta T = 50$ K

Figure 9. Dimensionless viscosity profile for different $m = \mu_{cold}/\mu_{ref}$. Blue circles are the instantaneous data in the x direction, the orange curve is the trend curve extrapolated from the instantaneous data, yellow circles are obtained form the analytical solution from Sameen and Govindarajan [59].

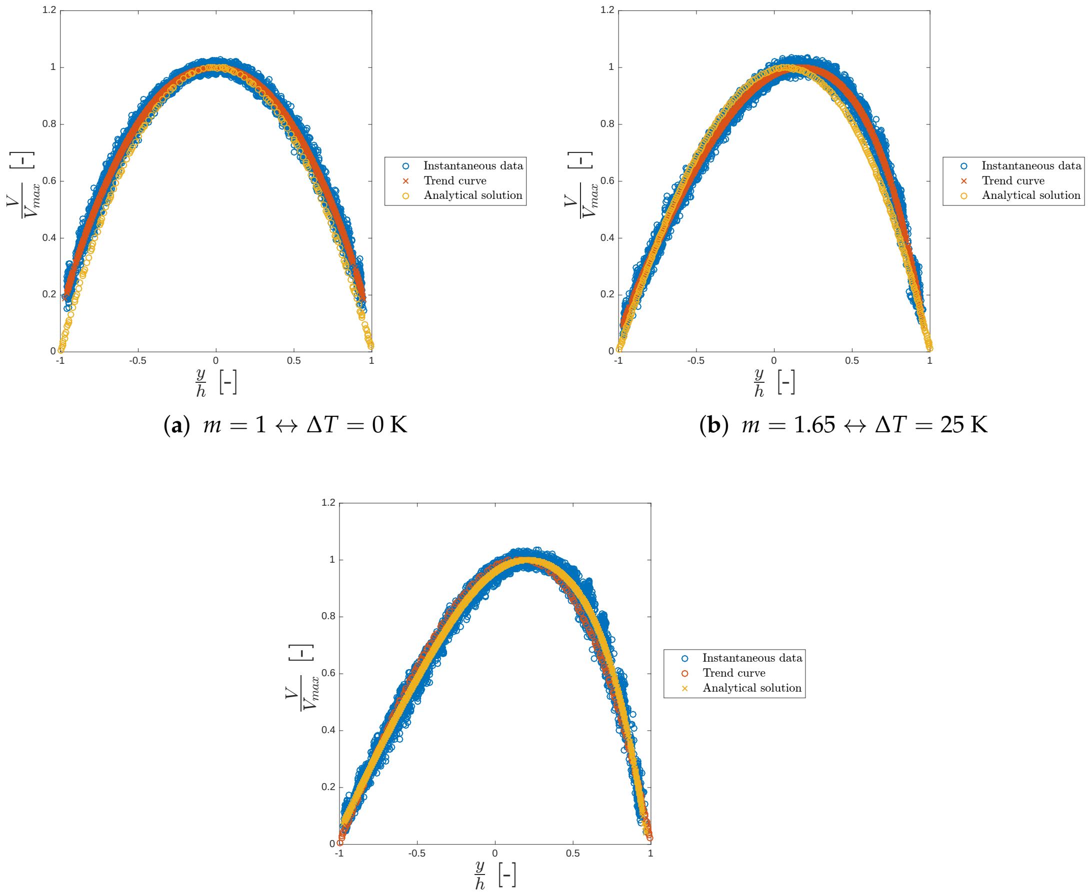
In all the cases considered, the model is in good agreement with the work of Sameen and Govindarajan.

Figure 10 shows the dimensionless velocity trend for different values of m.

Again, the model is in good agreement with the analytical solution of Sameen and Govindarajan always laying within the velocity scattered points. In both our model and in the analytical solution the maximum of the velocity shifts to the right as m increases. We can conclude that our model is in good agreement with the literature, showing the typical viscosity and velocity profiles for asymmetric heating confirming the correct functionality of the new viscosity class.

7.3. New Abstract Class: Viscosity

To implement the new viscosity model a new abstract class has been created, called Viscosity. The class has no attribute, and one virtual method: `compute_visc`, that is used to compute the viscosity using one of the Equations (15)–(18). As usual, the Viscosity class is divided in two files, see Listings 78 and 79. As it is an abstract class, it cannot be instantiated. It is used as a base, a mold, to implement the viscosity models. All implemented viscosity classes, such as the ones implementing the Arrhenius viscosity or the Sutherland viscosity, will inherit from this class.



(**a**) $m = 1 \leftrightarrow \Delta T = 0$ K (**b**) $m = 1.65 \leftrightarrow \Delta T = 25$ K

(**c**) $m = 2.5 \leftrightarrow \Delta T = 50$ K

Figure 10. Dimensionless velocity profile for different $m = \mu_{cold}/\mu_{ref}$. Blue circles are the instantaneous data in the x direction, the orange curve is the trend curve extrapolated from the instantaneous data, yellow circles are obtained form the analytical solution from Sameen and Govindarajan [59].

Listing 78: viscosity.cpp

```
#include "viscosity.h"

using namespace LAMMPS_NS;

Viscosity::Viscosity() {};
```

Listing 79: viscosity.h

```
#ifndef LAMMPS_VISCOSITY_H
#define LAMMPS_VISCOSITY_H

namespace LAMMPS_NS {
    class Viscosity {
        /**
         * Abstract base class for the viscosity attribute.
         * All viscosity types should inherit from this class.
         */
    public:
        Viscosity();
        /**
         * Virtual function.
         * Returns the viscosity, given the temperature.
         */
        virtual double compute_visc(double temperature) = 0;
```

```
    };
}
#endif //LAMMPS_VISCOSITY_H
```

This type of base class is called an interface, though as the code is written in C++, there is no actual difference in the implementation. The difference is only in concepts.

This structure allows for a very simple procedure to add a new viscosity type to LAMMPS, as one doesn't have to go through all of the code everytime a new viscosity type is implemented. All that is required is to implement a new viscosity class inheriting from the Viscosity abstract class and modify the `add_viscosity` function. The details of the changes required for those two actions are detailed later in this section.

Another structure one might think of to implement the viscosity abstract base class would be a template. Indeed, templates are more efficient than inherited classes as inherited classes create additional virtual calls when calling the class's methods. However, the choice of which viscosity should be called is made at runtime, and not at compile time, which means the abstract base class would be a better fit. When runtime polymorphism is needed, the structure preferred is an abstract base class.

The abstract class is not the most efficient implementation, but it allows for simplicity of use, which is important considering most of LAMMPS users are not programmers. In this work, we have chosen to sacrifice a bit of efficiency to gain ease of use.

7.4. Implementing a New Viscosity Class

In this section the steps to implement one of Equations (15)–(18) are shown, using the four parameter exponential viscosity as an example.

A new class is created that inherits from the Viscosity abstract class. The new class have as much attributes as the viscosity type has parameters. In this example that means four, as shown in the header in Listing 80.

Listing 80: viscosity_four_parameter_exp.h

```
#ifndef LAMMPS_VISCOSITY_FOURPARAMETEREXP_H
#define LAMMPS_VISCOSITY_FOURPARAMETEREXP_H

#include "math.h"
#include "viscosity.h"
namespace LAMMPS_NS{

class ViscosityFourParameterExp  : public Viscosity{
    /**
     * Implementation of the four parameter exponential viscosity.
     * This viscosity has four attributes.
     */
private:
    double A;
    double B;
    double C;
    double D;
public:
    ViscosityFourParameterExp(double A, double B, double C, double D);

    double compute_visc(double temperature) override final;

};
};
#endif //LAMMPS_VISCOSITY_FOURPARAMETEREXP_H
```

The constructor therefore should take as arguments the four parameters of the Andrade's equation and initialise the class's attributes with those values. The last step is to implement the `compute_visc` method so it returns the value of the viscosity at the given temperature. The implementation of both those functions is shown in Listing 81.

Listing 81: viscosity_four_parameter_exp.cpp

```
#include "viscosity_four_parameter_exp.h"

using namespace LAMMPS_NS;

ViscosityFourParameterExp::ViscosityFourParameterExp(double A, double B, double C,
     double D) {
    this->A = A;
    this->B = B;
    this->C = C;
    this->D = D;
}

double ViscosityFourParameterExp::compute_visc(double temperature) {
    return  A*exp(B/temperature +C*temperature + D *temperature*temperature);
}
```

Similar steps have to be taken to implement the classes corresponding to the other viscosity models, see the Supplementary material.

7.5. Processing the Viscosity in the Atom Class

In the header of the Atom class we need to include the new viscosity class and declare a new set of public members.

Listing 82: Original header (atom.h)

```
#include "pointers.h"
#include <map>
#include <string>
```

Listing 83: Modified header (atom.h)

```
#include "pointers.h"
#include "viscosity.h"
#include <map>
#include <string>
```

We add two new attributes in the USER-SPH section of the Atom attribute lists: `viscosity`, a pointer to a Viscosity object and `viscosities`, a pointer to an array containing the values of dynamic viscosities for all atoms at the current time step.

Listing 84: Original header (atom.h)

```
 // USER-SPH package
  double *rho,*drho,*e,*de,*cv;
  double **vest;
```

Listing 85: Modified header (atom.h)

```
 // USER-SPH package
  double *rho,*drho,*e,*de,*cv;
  double **vest;
  Viscosity *viscosity;
  double *viscosities;

```

We want to be able to choose which type of viscosity is being used in the simulation from the input file, using a new command called `viscosity`. Let's discuss the implementation of this feature. First we need to define the `viscosity` command. This is done by modifying the `execute_command` method of the Input class. We then define a new function called `add_viscosity`, whose declaration is shown in Listing 86 and definition in Listing 87. This function will have to be modified each time one wants to create a new viscosity class. In `add_viscosity`, the element arg[0] is the string representing the type of viscosity. For each viscosity class, the method performs the following procedure:

- It checks which type of viscosity is asked to be created using the function strcmp on arg[0] (for Andrade's viscosity it corresponds to line 3 of Listing 87)
- It checks if the number of arguments is coherent with the number of parameter of the viscosity type (line 4–5)
- It scans the coefficients of that viscosity type (line 6–10)
- It creates the appropriate viscosity and initializes the Viscosity attribute (line 11).

This process should be followed for any new implementation.

Listing 86: Modified header (atom.h)

```
1 void add_viscosity(int narg, char **arg);
```

Listing 87: New add_viscosity function (atom.cpp)

```
1 void Atom::add_viscosity(int narg, char **arg) {
2     if (narg < 1) error->all(FLERR, "Too few arguments for creation of viscosity");
3     if (!strcmp(arg[0], "FourParameterExp")) {
4         if (narg != 5)
5           error->all(FLERR, "Wrong number of arguments for creation of four
6           parameter exponential viscosity");
7         double A, B, C, D;
8         sscanf(arg[1], "%lg", &A);
9         sscanf(arg[2], "%lg", &B);
10        sscanf(arg[3], "%lg", &C);
11        sscanf(arg[4], "%lg", &D);
12        this->viscosity = new ViscosityFourParameterExp(A, B, C, D);
13        std::cout <<"Viscosity created" <<std::endl;
14    } else {
15        if (!strcmp(arg[0], "SutherlandViscosityLaw")) {
16            if (narg != 3)
17                error->all(FLERR, "Wrong number of arguments for creation of Sutherland
    viscosity");
18            double A, B;
19            sscanf(arg[1], "%lg", &A);
20            sscanf(arg[2], "%lg", &B);
21            this->viscosity = new SutherlandViscosityLaw(A, B);
22            std::cout <<"Viscosity created" <<std::endl;
23        } else {
24            if (!strcmp(arg[0], "PowerLawGas")) {
25                if (narg != 2)
26                  error->all(FLERR, "Wrong number of arguments for creation of power law
    gas viscosity");
27                double B;
28                sscanf(arg[1], "%lg", &B);
29                this->viscosity = new PowerLawGas(B);
30                std::cout <<"Viscosity created" <<std::endl;
31            } else {
32                if (!strcmp(arg[0], "Arrhenius")) {
33                    if (narg != 3)
34                      error->all(FLERR, "Wrong number of arguments for creation of
    Arrhenius viscosity");
35                    double A;
36                    double B;
37                    sscanf(arg[1], "%lg", &A);
38                    sscanf(arg[2], "%lg", &B);
39                    this->viscosity = new ViscosityArrhenius(A, B);
40                    std::cout <<"Viscosity created" <<std::endl;
41                } else {
42                    if (!strcmp(arg[0], "Constant")) {
43                        if (narg != 2)
44                            error->all(FLERR, "Wrong number of arguments for creation
45                            of Constant viscosity");
46                        double A;
47                        sscanf(arg[1], "%lg", &A);
48                        this->viscosity = new ViscosityConstant(A);
49                        std::cout <<"Viscosity created" <<std::endl;
50                    } else {
51                        std::cout <<"Nothing implemented for " << arg[0]<< std::endl;
```

```
                }
            }
        }
    }
}
}
```

All headers of the new viscosity types implemented in the `add_viscosity` function need to be included in the Atom class, see Listing 88.

Listing 88: New include (atom.cpp)

```
#include <string.h>
#include <iostream>
#include "viscosity_four_parameter_exp.h"
#include "viscosity_sutherland_law.h"
#include "viscosity_power_law_gas.h"
#include "viscosity_arrhenius.h"
#include "viscosity_constant.h"
```

The viscosity attribute is initialised to NULL in the constructor, see Listing 89.

Listing 89: Inside Atom::Atom(LAMMPS *lmp) : Pointers(lmp) (atom.cpp)

```
 viscosity = NULL;
```

In the destructor of the Atom class, we add a line to delete the viscosity attribute, see Listing 90.

Listing 90: Inside Atom:: Atom() (atom.cpp)

```
  memory->destroy(viscosity);
```

The `extract` function is modified to process the viscosity attribute, see Listing 91.

Listing 91: Modified extract function (atom.cpp)

```
  if (strcmp(name, "viscosity") == 0) return (void *) viscosity;
```

7.6. Using compute_Visc in SPH Pair Styles: Tait Water Implementation

The dynamic viscosity is used to compute the artificial viscosity force, that is used in the compute function of the following SPH pair style: sph/idealgas, sph/lj, sph/taitwater and sph/taitwater/morris. In this section the steps to implement compute_visc in sph/taitwater are shown, the others required a similar procedure.

The first function to modify is the destructor, as we don't have to allocate the viscosity parameter anymore.

Listing 92: Original file (pair_sph_taitwater.cpp)

```
PairSPHTaitwater::~PairSPHTaitwater() {
  if (allocated) {
    memory->destroy(setflag);
    memory->destroy(cutsq);
    memory->destroy(cut);
    memory->destroy(rho0);
    memory->destroy(soundspeed);
    memory->destroy(B);
    memory->destroy(viscosity);
  }
}
```

Listing 93: Modified file (pair_sph_taitwater.cpp)

```
PairSPHTaitwater::~PairSPHTaitwater() {
  if (allocated) {
    memory->destroy(setflag);
    memory->destroy(cutsq);
```

```
    memory->destroy(cut);
    memory->destroy(rho0);
    memory->destroy(soundspeed);
    memory->destroy(B);
  }
}
```

For the same reason as the destructor we need to modify allocate.

Listing 94: Original file (pair_sph_taitwater.cpp)

```
void PairSPHTaitwater::allocate() {
  allocated = 1;
  int n = atom->ntypes;
  memory->create(setflag, n + 1, n + 1, "pair:setflag");
  for (int i = 1; i <= n; i++)
    for (int j = i; j <= n; j++)
      setflag[i][j] = 0;
  memory->create(cutsq, n + 1, n + 1, "pair:cutsq");
  memory->create(rho0, n + 1, "pair:rho0");
  memory->create(soundspeed, n + 1, "pair:soundspeed");
  memory->create(B, n + 1, "pair:B");
  memory->create(cut, n + 1, n + 1, "pair:cut");
  memory->create(viscosity, n + 1,n + 1,"pair:viscosity");
}
```

Listing 95: Modified file (pair_sph_taitwater.cpp)

```
void PairSPHTaitwater::allocate() {
  allocated = 1;
  int n = atom->ntypes;
 memory->create(setflag, n + 1, n + 1, "pair:setflag");
  for (int i = 1; i <= n; i++)
    for (int j = i; j <= n; j++)
      setflag[i][j] = 0;
  memory->create(cutsq, n + 1, n + 1, "pair:cutsq");
  memory->create(rho0, n + 1, "pair:rho0");
  memory->create(soundspeed, n + 1, "pair:soundspeed");
  memory->create(B, n + 1, "pair:B");
  memory->create(cut, n + 1, n + 1, "pair:cut");
}
```

Inside the compute function of the sph/taitwater pair style we need to declare a new set of variables. Where e is the energy and cv the heat capacity, now needed to calculate the temperature and thus the viscosity.

Listing 96: Original file (pair_sph_taitwater.cpp)

```
int *type = atom->type;
int nlocal = atom->nlocal;
int newton_pair = force->newton_pair;
```

```
         [linebackgroundcolor={\listyellow{4,5,6,7}},
         label=820, caption={\small Modified file (pair\textunderscore sph\textunderscore
    taitwater.cpp)}\label{32}]  % Start your code-block

int *type = atom->type;
int nlocal = atom->nlocal;
int newton_pair = force->newton_pair;
double *e = atom->e;
double *cv = atom->cv;
Viscosity* viscosity = atom->viscosity;
double* viscosities = atom->viscosities;
```

The next modification is inside the loop over the j-th atom when the force induced by the artificial viscosity is calculated inside the pair's `compute` function.

The dynamic viscosities μ_i and μ_j are calculated for each atoms, using the formula implemented in the `compute_visc` method. The temperature for the i-th atom is obtained using $T_i = e_i/cv_i$. It is important to note that using such expression for the energy balance prevents the reference state of the internal energy to be set at 0.

The constant viscosity matrix element is replaced by the formula defined in Equation (19), see Listings 97 and 98.

Listing 97: Original file (pair_sph_taitwater.cpp)

```
// artificial viscosity (Monaghan 1992)
if (delVdotDelR < 0.) {
    mu = h * delVdotDelR / (rsq + 0.01 * h * h);
    fvisc = -viscosity[itype][jtype] * (soundspeed[itype]
     + soundspeed[jtype]) * mu / (rho[i] + rho[j]);
} else {
    fvisc = 0.;
}
```

Listing 98: Modified file (pair_sph_taitwater.cpp)

```
viscosities[i] = viscosity->compute_visc(e[i]/cv[i]);
viscosities[j] = viscosity->compute_visc(e[j]/cv[j]);
// artificial viscosity (Monaghan 1992)
if (delVdotDelR < 0.) {
    mu = h * delVdotDelR / (rsq + 0.01 * h * h);
    fvisc =-4/h*(viscosities[i]/(soundspeed[itype]*rho[i])
    +viscosities[j]/(soundspeed[jtype]*rho[j]))
    *(soundspeed[itype]+ soundspeed[jtype])
    * mu / (rho[i] + rho[j]);
} else {
    fvisc = 0.;
}
```

Viscosity is now a per atom property, this means that we don't have to pass its value then the pair style is invoked. For this reason we need to delete the viscosity related lines inside coeff.

Listing 99: Original coeff (pair_sph_taitwater.cpp)

```
void PairSPHTaitwater::coeff(int narg, char **arg) {
  if (narg != 6)
    error->all(FLERR,
        "Incorrect args for pair_style sph/taitwater
         coefficients");
  if (!allocated)
    allocate();

  int ilo, ihi, jlo, jhi;
  force->bounds(FLERR,arg[0], atom->ntypes, ilo, ihi);
  force->bounds(FLERR,arg[1], atom->ntypes, jlo, jhi);

  double rho0_one = force->numeric(FLERR,arg[2]);
  double soundspeed_one = force->numeric(FLERR,arg[3]);
  double viscosity_one = force->numeric(FLERR,arg[4]);
  double cut_one = force->numeric(FLERR,arg[5]);
  double B_one = soundspeed_one*soundspeed_one*rho0_one/7;

  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    rho0[i] = rho0_one;
    soundspeed[i] = soundspeed_one;
    B[i] = B_one;
    for (int j = MAX(jlo,i); j <= jhi; j++) {
      viscosity[i][j] = viscosity_one;
      cut[i][j] = cut_one;
      setflag[i][j] = 1;
      count++;
    }
  }
  if (count == 0)
    error->all(FLERR,"Incorrect args for pair
```

```
    coefficients");
}
```

Listing 100: Modified coeff (pair_sph_taitwater.cpp)

```
void PairSPHTaitwater::coeff(int narg, char **arg) {
  if (narg != 5)
    error->all(FLERR,
        "Incorrect args for pair_style sph/taitwater
         coefficients");
  if (!allocated)
    allocate();

  int ilo, ihi, jlo, jhi;
  force->bounds(FLERR,arg[0], atom->ntypes, ilo, ihi);
  force->bounds(FLERR,arg[1], atom->ntypes, jlo, jhi);

  double rho0_one = force->numeric(FLERR,arg[2]);
  double soundspeed_one = force->numeric(FLERR,arg[3]);
  double cut_one = force->numeric(FLERR,arg[4]);
  double B_one = soundspeed_one*soundspeed_one*rho0_one/7;

  int count = 0;
  for (int i = ilo; i <= ihi; i++) {
    rho0[i] = rho0_one;
    soundspeed[i] = soundspeed_one;
    B[i] = B_one;
    for (int j = MAX(jlo,i); j <= jhi; j++) {
      cut[i][j] = cut_one;
     setflag[i][j] = 1;
      count++;
    }
  }
  if (count == 0)
    error->all(FLERR,"Incorrect args for pair
     coefficients");
}
```

The last modification is in init_one. Again, we delete lines related to the former viscosity attribute.

Listing 101: Original file (pair_sph_taitwater.cpp)

```
double PairSPHTaitwater::init_one(int i, int j) {
  if (setflag[i][j] == 0) {
    error->all(FLERR,"All pair sph/taitwater coeffs
     are set");
  }
  cut[j][i] = cut[i][j];
  viscosity[j][i] = viscosity[i][j];
  return cut[i][j];
}
```

Listing 102: Modified file (pair_sph_taitwater.cpp)

```
double PairSPHTaitwater::init_one(int i, int j) {
  if (setflag[i][j] == 0) {
    error->all(FLERR,"All pair sph/taitwater coeffs
     are set");
  }
  cut[j][i] = cut[i][j];
  return cut[i][j];
}
```

7.7. Running the New Software with Mpirun

At this stage, the software is designed to only run in serial. Changes need to be made to make it run with Message Passing Interface (MPI). This will allow the software to run in parallel: some computations being independent from each other, they can be performed at the same time. Instead of using one processor for a long time, we will use multiple processors for a shorter period. The simulation will therefore take more computing resources but will take a lot shorter to compute. The original SPH module can already be run with MPI however as we have modified the code that is no longer true. We need to make additional changes to the software. All those changes are located in the Atom Vec Meso class of the SPH module.

In LAMMPS, the different MPI processes have to communicate with each other as the computations they perform are not completely independent from each other. They need data from other processes in order to perform their own calculations. They communicate with each other using a buffer that will contain all the necessary data. The buffer is simply an array that we will fill with the data. The different methods for packing and unpacking this buffer are defined in the Atom Vec Meso class. We need to add a new data to transmit: the calculated viscosity.

The first thing to do is to increase the size of the buffers in their initialisation so they can accept the viscosity value, an example is shown in Listings 103 and 104.

Listing 103: Original constructor (atom_vec_meso.cpp)

```
AtomVecMeso::AtomVecMeso(LAMMPS *lmp) : AtomVec(lmp)
{
  molecular = 0;
  mass_type = 1;
  forceclearflag = 1;

// we communicate not only x forward but also vest ..
  comm_x_only = 0; .
// we also communicate de and drho in reverse direction
  comm_f_only = 0;
// 3 + rho + e + vest[3], that means we may
// only communicate 5 in hybrid
  size_forward = 8;
  size_reverse = 5; // 3 + drho + de
  size_border = 12; // 6 + rho + e + vest[3] + cv
  size_velocity = 3;
  size_data_atom = 8;
  size_data_vel = 4;
  xcol_data = 6;

  atom->e_flag = 1;
  atom->rho_flag = 1;
  atom->cv_flag = 1;
  atom->vest_flag = 1;
}
```

Listing 104: Modified constructor (atom_vec_meso.cpp)

```
AtomVecMeso::AtomVecMeso(LAMMPS *lmp) : AtomVec(lmp)
{
  molecular = 0;
  mass_type = 1;
  forceclearflag = 1;

// we communicate not only x forward but also vest ...
  comm_x_only = 0;
// we also communicate de and drho in reverse direction
  comm_f_only = 0;
// 3 + rho + e + vest[3] + viscosities, that means we may
// only communicate 6 in hybrid
  size_forward = 9;
  size_reverse = 5; // 3 + drho + de
// 6 + rho + e + vest[3] + cv + viscosities
  size_border = 13;
  size_velocity = 3;
  size_data_atom = 8;
  size_data_vel = 4;
```

```
  xcol_data = 6;

  atom->e_flag = 1;
  atom->rho_flag = 1;
  atom->cv_flag = 1;
  atom->vest_flag = 1;
}
```

Then, we added the relevant elements of the attribute `viscosities` to the buffer in all the methods handling buffers, an example is shown in Listings 105 and 106.

Listing 105: Original `pack_vec_hybrid` (atom_vec_meso.cpp)

```
int AtomVecMeso::pack_comm_hybrid(int n, int *list,
 double *buf) {
  //printf("in AtomVecMeso::pack_comm_hybrid\n");
  int i, j, m;

  m = 0;
  for (i = 0; i < n; i++) {
    j = list[i];
    buf[m++] = rho[j];
    buf[m++] = e[j];
    buf[m++] = vest[j][0];
    buf[m++] = vest[j][1];
    buf[m++] = vest[j][2];
  }
  return m;
}
```

Listing 106: Modified `pack_vec_hybrid` (atom_vec_meso.cpp)

```
int AtomVecMeso::pack_comm_hybrid(int n, int *list,
 double *buf) {
  //printf("in AtomVecMeso::pack_comm_hybrid\n");
  int i, j, m;

  m = 0;
  for (i = 0; i < n; i++) {
    j = list[i];
    buf[m++] = rho[j];
    buf[m++] = e[j];
    buf[m++] = vest[j][0];
    buf[m++] = vest[j][1];
    buf[m++] = vest[j][2];
    buf[m++] = viscosities[j];
  }
  return m;
}
```

After making those changes for all the methods in the class, the software can be run using mpirun.

7.8. Invoking, Selecting and Computing a Viscosity Object

To compute the new viscosity a new argument was added to the `compute` command: `viscosities`. This allows the user to use the `compute` command to output the dynamic viscosity to the dump file. This can be done by the following command:

```
compute            viscosities_peratom all meso/viscosities/atom
```

The implementation of this feature is simple, as it is very similar to other `compute` argument implementation. All that needs to be done is to modify another `compute`'s implementation, such as `compute_meso_rho_atom` so it processes the variable `viscosities` instead of `rho`.

The viscosity used in the simulation can be invoked in the input file, using the following command:

```
viscosity     [type of viscosity]     [parameters of the viscosity]
```

The type of viscosity can be chosen from the following list:

- FourParameterExp: the four parameter exponential viscosity law.
- SutherlandViscosityLaw: the Sutherland viscosity law.
- PowerLawGas: the power viscosity law for gases.
- Arrhenius: the Arrhenius viscosity law.
- Constant: a constant viscosity.

For example, to invoke the four parameter exponential viscosity, we can write in the input file:

```
viscosity      FourParameterExp C1 C2 C3 C4
```

As stated earlier, this list can easily be extended by the user by modifying the `add_viscosity` function defined earlier.

8. Conclusions

Particle methods are very versatile and can be applied in a variety of applications, ranging from modelling of molecules to the simulation of galaxies. Their power is even amplified when they are coupled together within a discrete multiphysics framework. This versatility matches well with LAMMPS, which is a particle simulator, whose open-source code can be extended with new functionalities. However, modifying LAMMPS can be challenging for researchers with little coding experience and the available support material on how to modify LAMMPS is either too basic or too advanced for the average researcher. Moreover, most of the available material focuses on MD; while the aim of this paper is to support researchers that use other particle methods such as SPH or DEM.

In this work, we present several examples, explained step-by-step and with increasing level of complexity. We begin with simple cases and concluding with more complex ones: Section 3 shows the implementation of the Kelvin–Voigt bond style used to model encapsulate particles with a soft outer shell and validated validated by simulating spherical homogeneous linear elastic and viscoelastic particles [45]; Section 7 show how to implement a new per-atom temperature dependant viscosity property and is validated finding the same viscosity and velocity trend shown by Sameen and Govindarajan [59] in their analytical solution for a channel flow in a asymmetrical heating walls.

The work perfectly fits in the "Discrete Multiphysics: Modelling Complex Systems with Particle Methods" special issue by sharing some in dept know-how and "trick and trades" developed by our group in years of use of LAMMPS. In fact, the aim is to support, in several ways, researchers that use computational particle methods. Often researchers tend to write their own code. The advantage of this approach is that the code is well understood by the researcher and, therefore, easily extendible. However, this sometimes implies reinventing the wheel and countless hours of debugging. Familiarity with a code like LAMMPS, which has an active community of practice and is periodically enriched with new features would be beneficial to this type of researchers allowing them to save considerable time. In the long term, there is another advantage. Modules written for in-house code are hardly sharable. At the moment, the largest portion of the LAMMPS community is dedicated to MD. While this article was under review, for instance, a new book dedicated to modifying LAMMPS came out [60]. However, it focuses only on MD and it does not mention other discrete methods like SPH or DEM. Instead, the aim of this paper is to make LAMMPS more accessible for the Discrete Multiphysics community facilitating sharing reusable code among practitioners in this field.

Supplementary Materials: The codes used in this work are freely available under the GNU General Public License v3 and can be downloaded from the University of Birmingham repository (http://edata.bham.ac.uk/560/).

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Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

MS	Molecular Dynamics
DMP	Discrete MultiPhysics
SPH	Smoothed Particle Hydrodynamics
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
EOS	Equation Of State
LSM	Lattice Spring Model

Appendix A. An Example of Discrete Multiphysics Simulation in LAMMPS

In this section we present a simple case of DMP simulation with LAMMPS. It is an explanatory example deliberately simple for illustrative purposes. It involves only a small number of particles. Sensitivity analysis of the results with the model resolution or other numerical parameters are beyond the scope of this example and not carried out.

The geometry is a 2D tube with an elastic membrane at one end (Figure A1). The tube contains a liquid simulated with the SPH model, Tait EOS and Morris viscosity. The wall is simulated with stationary particles and the membrane with the LSM using Hookean springs. In Figure A1, the liquid particles are red, the wall particles blue and the membrane particles yellow. During the simulation, the fluid is subjected to a force in the x-direction that pushed the particles against the membrane. Because the membrane is elastic, it stretches inflating the right end of the tube like a balloon. The resolution of the membrane is ten times higher than the fluid. This ensures that, as the membrane stretches, fluid particles do not 'leak' in the gaps formed between two consecutive membrane particles. The Lennard Jones potential, truncated to consider only the repulsive part, is used to avoid compenetration between solid and liquid particles. A weaker Lennard Jones potential is used as 'artificial pressure' to avoid excessive compression of the fluid particles.

The initial data file (data.initial) for the geometry was create according to LAMMPS' rules for formatting the Data File [41] and is shared as additional material. In Data File, the fluid particles are called `type 1`, the wall particles `type 2` and the membrane particles `type 3`. Here we focus on the input file (membrane.lmp), which is also shared in its entirety as additional material. We do not discuss LAMMPS syntax (the reader can refer to LAMMPS User's Guide for this [41]), but only on specific parts of the input file that concern the DMP implementation.

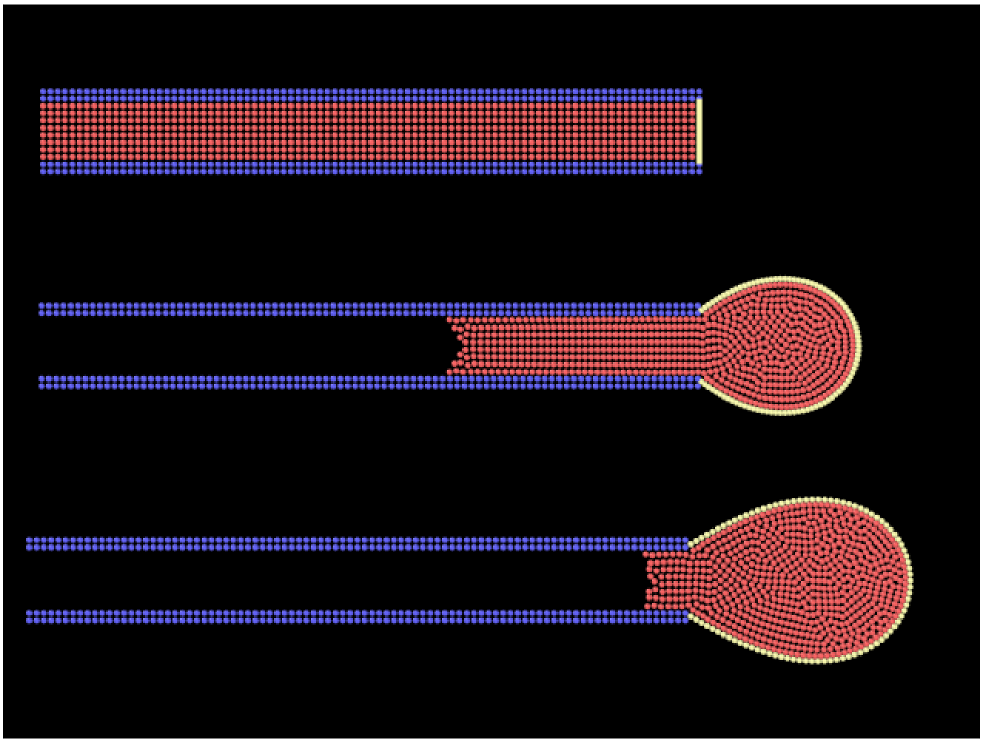

Figure A1. The inflating balloon simulation.

The first section of the input file determines the dimensionality of the problem (2D), the boundary conditions (periodic), the units used (SI), the type of potential used in the simulation (`atom_style`) and the input file that contains the initial position of all the particles

```
dimension         2
boundary       p p p
units              si
atom_style  hybrid meso bond angle
read_data      data.initial
```

The crucial line for DMP simulations is the `hybrid` keyword of the `atom_style`, which allows for combining different particle models. The keyword `meso` refers to the SPH model and `bond`, in the case under consideration, to the LSM. The `angle` keyword corresponds to angular springs, but, as it will be clear later, it is not used in this simulation.

The following section contains several variables that are going to be used later on. In particular, the initial particle distance is `dL` and their mass `m`. The resolution of the membrane is `Nt` times higher than the fluid. The initial distance between membrane particle is therefore `db=dL/Nt` and their mass `mM=m/Nt`.

```
variable    dL       equal  0.000111111
variable    m     equal  1.23457e-05
variable    Nt       equal 10
variable    dB       equal ${dL}/${Nt}
variable    mM       equal  ${m}/${Nt}
variable    h     equal 1.5*${dL}
variable    h2       equal ${dL}/${Nt}
variable    c     equal 0.1
variable    mu       equal 1.0e-3
variable    rho      equal 1000
variable    kA       equal 1.e-8
variable    kB       equal 100
variable    skin     equal 0.3*${h}
variable    epsL     equal 1.e-12
variable    epsS     equal 1.e-10
variable    sgmL  equal ${dL}
```

```
variable    sgmS  equal 0.5*${sgmL}/${Nt}
variable    fmax     equal 0.00005
variable    ft    equal ramp(0.,${fmax})
```

The section below identifies particles `type 1` as a group called `fluid`, particles `type 2` as a group called `wall` and particles `type 3` as a group called `membrane`. The mass of `type 3` particles is assigned (the mass of `type 1`, 2 was assigned in the data.initial file). The density of all particle is also assigned based on the value `rho` defined previously.

```
group           fluid      type 1
group           wall    type 2
group           membrane   type 3
mass 3 ${mM}
set group all meso/rho ${rho}
```

The next section defines the pair potentials for non-bonded particles. In this simulation, we use different styles together (keyword `hybrid/overlay`). The `sph/taitwater/morris` pair style, which is used for all pair interactions except 2-2 (i.e., wall particles with themselves); and the Lennard Jones potential `lj/cut`, which, as explained above, is used both as 'artificial pressure' and to avoid compenetration of solid and fluid particles.

```
pair_style hybrid/overlay sph/taitwater/morris lj/cut ${sgmL}
pair_coeff 1 * sph/taitwater/morris ${rho} ${c} ${mu} ${h}
pair_coeff 2 3 sph/taitwater/morris ${rho} ${c} ${mu} ${h2}
pair_coeff 3 3 sph/taitwater/morris ${rho} ${c} ${mu} ${h2}

pair_coeff 1 * lj/cut ${epsL} ${sgmL}
pair_coeff 2 * lj/cut ${epsL} ${sgmL}
pair_coeff 1 3 lj/cut ${epsS} ${sgmL}
pair_coeff 3 3 lj/cut ${epsS} ${sgmS}
```

After the non-bonded potentials, the script assigns the `harmonic` potential, with Hook constant `kB` and equilibrium distance `dB`, to the bonded particles (i.e., the membrane). All pairs of bonded particles are assigned in the data.initial file.

```
bond_style  harmonic
bond_coeff  1 ${kB} ${dB}
angle_style none
```

The next section assigns several parameters that determine how the Newton equation of motion is solved numerically. The force `fmax` is added to all fluid particle in the x-direction, and an artificial viscosity is added for stability reasons.

```
fix 2 fluid addforce ${fmax} 0.0 0.0
fix 5 fluid meso
fix 6 membrane meso
fix 8 wall meso/stationary
fix 9 all viscous 0.01
```

The last commands determine the value and the number of timesteps used in the simulation plus a variety of computations for output and other purposes that are not discussed here (the reader can refer to the User's Guide).

```
compute rho_peratom all meso/rho/atom
compute rho_ave all reduce ave c_rho_peratom
compute vmax fluid reduce max vx
thermo            10000
thermo_style custom step c_rho_ave c_vmax
thermo_modify      norm no
neighbor       ${skin} bin
dump   dump_id all custom 10000 dump.lammpstrj id type x y z vx vy
timestep           1.e-6
run                2500000
```

Appendix B. How to Compile LAMMPS

LAMMPS is build as a library and executable [41] either by using GNU make [61] or a build environment with CMake [62]. In this appendix LAMMPS will be compiled only using make and it is compiled in BlueBEAR. For more details of the compiling process in LAMMPS refer to the user manual [41].

To compile LAMMPS in your own directory you can follow those steps

1. Download the file from here. Select the code you want, click the "Download Now" button, and your browser should download a gzipped tar file. Save the file in your directory on BlueBEAR
2. Unpack the file with the following command line command prompt:

Listing A1: Command to open the tar file on BlueBEAR

```
tar -xvf lammps-stable.tar.gz
```

3. Before compiling is important to set up the environment, with BlueBEAR

Listing A2: Commands to set the environment for compile LAMMPS on BlueBEAR

```
module purge

module load bluebear

module load Eigen/3.3.4-foss-2019a
```

4. Enter in the /src directory in your new LAMMPS directory. The src directory directory contains the C++ source and header files for LAMMPS. It also contains a top-level Makefile and a MAKE sub-directory with low-level Makefile.* files for many systems and machines.
5. Type the following command to compile a serial version of LAMMPS:

Listing A3: Command to compile LAMMPS on BlueBEAR

```
make serial
```

or a multi-threaded (parallel) version of LAMMPS:

Listing A4: Command to compile LAMMPS on BlueBEAR

```
make mpi
```

If you get no errors and an executable file lmp_mpi is produced.

6. Depending on the features you need, you will have to install same packages in your compiled LAMMPS. Is possible to check which packages is installed in your compiled LAMMPS by typing

Listing A5: Command to check the list of installed packages (you must be inside the /src directory)

```
make ps
```

It is possible to install the packages you need with the command line

Listing A6: Command to install a specific package

```
make yes-NAMEPACK
```

or un-install them with

Listing A7: Command to un-install a specific package

```
make no-NAMEPACK
```

More `make` commands are explained in LAMMPS user manual [41]. After the installation of the desired packages you need to compile it again (step 5).

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