

PAIRING INSTABILITY: INSIGHTS AND POSSIBLE REMEDIES FROM A LOCAL THERMODYNAMICS PERSPECTIVE

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I. INTRODUCTION

The *pairing* (or *clumping*) *instability* [1], [2] is a numerical issue that affects the analysis of phenomena such as turbulence and shock waves via Smoothed Particle Hydrodynamics (SPH) techniques [3], [4]. SPH algorithms are characterised by a *reordering mechanism*, by virtue of which the system typically converges towards semi-regular, glass-like structures. However, when considering turbulent flows or situations in which shocks are present, some level of particle disorder cannot be avoided. In these cases, a natural attempt to improve the convergence of SPH simulations is to increase the number of neighbours, N_H , considered in the estimation of the system local density. Nevertheless, the use of large N_H gives rise to the pairing instability, which causes particles to form closely paired, unphysical structures. Solutions to the pairing instability have been proposed where the focus is on the mathematical properties of the *smoothing kernel* appearing in the definition of the density estimator (see, e.g., [5]), or on the use of tessellation techniques [6].

In this work, we study the pairing instability from a thermodynamic perspective, in the context of the Generalised Energy-Conserving Dissipative Particle Dynamics (GenDPDE) mesoscopic approach [7]. GenDPDE is a bottom-up, Lagrangian, coarse-grain (CG) method, based on an *internal thermodynamic description* for the particles which allows us to gain insights into the driving mechanism for the pairing instability. More specifically, we observe that the local particle aggregation coincides with minimisation of the free energy associated with the particles. In the absence of thermal agitation (as is the case in SPH), this implies that the system pressure is also a minimum. Focusing our attention on liquid conditions, we find that the source of this unphysical behaviour is a poor evaluation of the local density, calculated in GenDPDE through an estimator that is formally analogous to its SPH counterpart. We therefore propose a novel solution to this numerical artefact, based on a redefinition of the density estimator that preserves modelling simplicity and computational efficiency.

II. MATERIALS AND METHODS

The GenDPDE framework describes particles as property carriers defined by a set of state variables, namely, mass m_i , position \mathbf{r}_i , momentum \mathbf{p}_i , and internal energy u_i (related to the particle temperature θ_i). The dynamics of a GenDPDE system is thus described by a set of discrete Langevin-like Equations of Motion (EoM) that express the time evolution of these variables. Moreover, each GenDPDE particle is characterised by a local volume \mathcal{V}_i , or its corresponding number density $n_i = 1/\mathcal{V}_i$ ¹, which is determined by the positions of all the neighbouring particles located no farther than a certain cut-off distance R_{cut} from particle i . Therefore, within this framework, it is possible to define a particle free energy f_i , from which the particle pressure π_i can be obtained as the derivative of f_i with respect to n_i . Similarly to SPH algorithms, π_i is directly related to the forces acting between the particles. In the present analysis, the local pressure is described by the Tait Equation of State (EoS) for weakly compressible fluids [8], which represents a traditional choice in SPH simulations:

$$\pi_i = \pi_0 + B_T \left[\left(\frac{n_i}{n_0} \right)^{\gamma_T} - 1 \right], \quad (1)$$

where γ_T is a fitting parameter, π_0 and n_0 are reference values for the pressure and density respectively, and $B_T \equiv 1/(\gamma_T \kappa_{T0})$, with κ_{T0} the isothermal compressibility of the substance at the reference state. From (1), the particle Helmholtz free energy can be derived, yielding

$$f_i = \frac{B_T - \pi_0}{n_i} + \frac{B_T}{(\gamma_T - 1)n_0} \left(\frac{n_i}{n_0} \right)^{\gamma_T - 1} + \Phi(\theta_i) \quad (2)$$

with $\Phi(\theta_i)$ a given function of the particle temperature.

The local volume in GenDPDE has traditionally been estimated through the expression [9], [10]

$$\mathcal{V}_i = \frac{1}{n_i^0} \quad \text{with} \quad n_i^0 = \sum_{j \neq i} w_{ij}, \quad (3)$$

¹Notice that this is true for homogeneous kernels, while it may not necessarily be the case for inhomogeneous kernels.

where $w_{ij} \equiv w(r_{ij})$ is a smooth, monotonically decreasing, non-negative, spherically symmetric, normalised weighting function, vanishing for an interparticle distance, $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$, such that $r_{ij} \geq R_{cut}$. Nevertheless, definition (3) does not satisfy volume additivity, thus inducing an approximation on the actual system density which can negatively affect the calculation of the system properties. This is particularly true for liquids, where the potential interactions (which in GenDPDE depend on the local density) are dominant over the kinetic contributions. In this case, we find that the traditional density estimator leads the system to an equilibrium configuration that is far from the imposed nominal conditions and is characterised by an unphysical local aggregation of particles. To circumvent these issues, we propose an alternative definition of the particle volume, resulting from an approximated solution of the *partition of unity* approach [11]:

$$\mathcal{V}_i \equiv \int d\mathbf{r} \frac{w(|\mathbf{r} - \mathbf{r}_i|)}{\sum_j w(|\mathbf{r} - \mathbf{r}_j|)} \simeq \int d\Delta\mathbf{r} \frac{\tilde{w}(\Delta r)}{\tilde{w}(\Delta r) + n_i^0}, \quad (4)$$

where $\tilde{w}(\Delta r)$ is a weighting function analogous to (3), but considering a reduced cut-off distance $\tilde{R}_{cut} \equiv R_{cut}/f_{cut}$, with $f_{cut} > 1$ a tuning parameter. The explicit solution to (4) yields

$$\mathcal{V}_i = \frac{4\pi}{3} \tilde{R}_{cut}^3 - 4\pi \tilde{R}_{cut}^3 \sqrt{k_i} \left\{ (1 - k_i) \arctan\left(\frac{1}{\sqrt{k_i}}\right) + \sqrt{k_i} \left[1 - \ln\left(\frac{k_i + 1}{k_i}\right) \right] \right\}, \quad (5)$$

with $k_i = (2\pi/15)\tilde{R}_{cut}^3 n_i^0$. Equation (5) ensures proper volume estimation, provided that a suitable combination of R_{cut} and f_{cut} is chosen. Moreover, despite an apparently more complicated formula, this redefinition retains computational efficiency and avoids additional complications in the derivation of the model, unlike, e.g., a three-dimensional Voronoi tessellation approach, which would require the calculation of three-body contributions to the interparticle forces, thus breaking pairwise additivity. The beneficial effects of (5) on the behaviour of condensed phases are demonstrated by analysing the equilibrium configuration of liquid Argon in terms of both, average thermodynamic quantities and local structure, and comparing the results obtained with the two density estimators for different values of the cut-off distance R_{cut} .

III. RESULTS AND DISCUSSION

The considered thermodynamic state point and parameters of interest for the GenDPDE simulations of liquid Argon are reported in Tab. I. These correspond to the dimensionless parameters in Tab. II. The fitting parameter appearing in the Tait EoS (1) has been set to $\gamma_T = 6.0$.

The outcome of our tests considering both volume estimators, (3) and (5), are reported in Tab. III in terms of the average temperature T^* , density \bar{n}^* and pressure P^* . Here, estimator (3) is identified as V-A, and estimator (5) as V-B. It can be observed that, remarkably, V-A returns average densities that are close to the value minimising the particle free energy (2), $n_{min}^* = 0.820$, for all the considered cut-off distances. This in

TABLE I
STATE-POINT VALUES ¹

T_0 [K]	P_0 [MPa]	ρ_0 [kg/m ³]	κ_{T0} [1/Pa]	C_V [J/(kg·K)]	ν [Pa·s]	λ [W/(m·K)]
125.7	85.31	1419.7	1.49×10^{-9}	5.20×10^2	1.69×10^{-7}	0.139

¹ These values indicate, from left to right: the nominal temperature, pressure, mass density, isothermal compressibility, constant-volume heat capacity, dynamic viscosity and thermal conductivity of liquid Argon.

TABLE II
DIMENSIONLESS PARAMETERS

R_{cut}^*	T_0^*	P_0^*	n_0^*	π_0^*	C_V^*	$\gamma^*{}^2$	$\kappa^*{}^2$
1.3365	0.0111	0.127	1.000	0.1161	12.51	23.42	0.0079
1.6839	0.0111	0.127	1.000	0.1161	12.51	7.37	0.0025
2.1564	0.0111	0.127	1.000	0.1161	12.51	2.14	0.0007

² Notice that the dynamic viscosity and thermal conductivity are functions of the cut-off distance at the mesoscopic level [12].

turn implies that the particle pressure tends to vanish. Given the negligible contribution of thermal agitation, the values of P^* obtained in all V-A tests are thus close to 0. The use of the estimator V-B, on the other hand, allows us to recover the expected values for \bar{n}^* through the proper tuning of the scaling parameter, which has been set to $f_{cut} = \{1.41, 1.35, 1.33\}$ for $R_{cut}^* = \{1.3365, 1.6839, 2.1564\}$ respectively. As a result, P^* approaches P_0^* .

The consequences of the use of (3) and the beneficial effects of the redefinition (5) are also visible in terms of the local structure of the system, as displayed in Fig. 1. Here, the radial distribution function (RDF) is shown for all the considered cut-off distances, comparing the curves obtained using V-A and V-B. Notably, simulations with V-A return structures that are characterised by unexpected *secondary shoulders*, indicative of a spurious local aggregation of particles at distances smaller than R_{cut}^* . This unphysical behaviour, which is particularly evident for $R_{cut}^* = 1.3365$, reflects the tendency of the system to reorder in a way that favours minimisation of the particle free energy over equilibration at the desired thermodynamic state point. Contrarily, the volume estimation in V-B eliminates this artefact, allowing us to obtain typical liquid phase RDFs, consistent with the dimension of the lowest length scale, namely $(1/n_0^*)^{1/3}$.

Finally, by comparing the total simulation times for V-A and V-B in all tests, Tab. IV proves that the redefinition (5) does not

TABLE III
AVERAGE THERMODYNAMIC QUANTITIES

R_{cut}^*	T^*		\bar{n}^*		P^*	
	V-A	V-B	V-A	V-B	V-A	V-B
1.3365	0.0115 ± 0.0001	0.0112 ± 0.0001	0.799 ± 0.001	0.997 ± 0.001	0.008 ± 0.001	0.136 ± 0.001
1.6839	0.0112 ± 0.0001	0.0112 ± 0.0001	0.811 ± 0.001	1.000 ± 0.001	0.011 ± 0.001	0.128 ± 0.001
2.1564	0.0111 ± 0.0001	0.0111 ± 0.0001	0.870 ± 0.001	1.000 ± 0.001	0.041 ± 0.001	0.127 ± 0.001

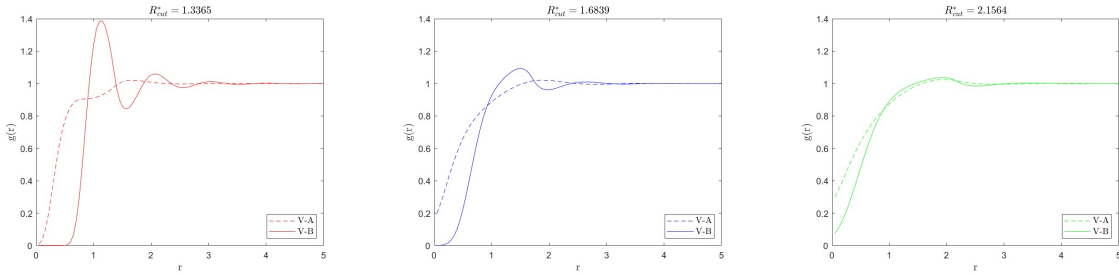


Fig. 1. RDFs for $R_{cut}^* = 1.3365$ (left), $R_{cut}^* = 1.6839$ (centre), $R_{cut}^* = 2.1564$ (right). In all diagrams, the dashed line refers to the curves obtained with the density estimator V-A, while the continuous line refers to estimator V-B. The different local structures obtained by considering (3) and (5) can be observed.

TABLE IV
TOTAL SIMULATION TIME ³

R_{cut}^*	Total simulation time [hours]	
	V-A	V-B
1.3365	25.11	26.84
1.6839	12.71	15.46
2.1564	15.84	16.34

³ All simulations have been performed using a homemade parallel Fortran code and exploiting the same computational resources and number of CPUs.

affect significantly the numerical performance of the algorithm.

IV. CONCLUSIONS

In this work, we have exploited the local thermodynamic framework of GenDPDE to investigate the pairing instability, a relevant numerical issue that occurs in SPH simulations. We have shown that the cause of this artefact is the poor evaluation of the local density obtained by use of a traditional expression for the volume estimator. More specifically, we have observed that the non-negligible error in the density calculation leads to an unphysical behaviour of the particles, which tend to clump and move collectively, altering the local structure of the system to favour energy minimisation over equilibration at the imposed nominal conditions. We have demonstrated that these numerical issues can be overcome if an alternative definition of the volume estimator is considered instead, which yields a significantly better density calculation while also maintaining modelling simplicity and computational efficiency.

ACKNOWLEDGMENTS

GC acknowledges funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 945413 and from the Universitat Rovira i Virgili (URV). GC and JBA also acknowledge support from the grant PID2021-122187NB-C33, funded by MCIN/AEI/10.13039/501100011033 and “ERDF A way of making Europe”. Research performed by JBA was sponsored by the Army Research Office, and was accomplished under Cooperative Agreement Number W911NF-20-2-0227. JPL acknowledges support in part for a grant of computer time from the DoD High Performance Computing Modernization Program

at the Army, Navy, and Air Force Supercomputing Resource Centers.

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