John von Neumann Institute for Computing

Large Simulations of Shear Flow in Mixtures via the Lattice Boltzmann Equation

Kevin Stratford, Jean Christophe Desplat

published in

Parallel Computing: Architectures, Algorithms and Applications ,
C. Bischof, M. Bücker, P. Gibbon, G.R. Joubert, T. Lippert, B. Mohr, F. Peters (Eds.),
John von Neumann Institute for Computing, Jülich,
NIC Series, Vol. **38**, ISBN 978-3-9810843-4-4, pp. 593-600, 2007.
Reprinted in: Advances in Parallel Computing, Volume **15**,
ISSN 0927-5452, ISBN 978-1-58603-796-3 (IOS Press), 2008.

http://www.fz-juelich.de/nic-series/volume38

Large Simulations of Shear Flow in Mixtures via the Lattice Boltzmann Equation

Kevin Stratford[1] **and Jean Christophe Desplat**[2]

[1] Edinburgh Parallel Computing Centre, The University of Edinburgh, Edinburgh, United Kingdom
E-mail: kevin@epcc.ed.ac.uk

[2] Irish Centre for High-End Computing, Dublin, Ireland
E-mail: j-c.desplat@ichec.ie

In this paper we describe the implementation of Lees-Edwards sliding periodic boundary conditions used to perform simulations of sheared binary fluids. In conjunction with domain decomposition and parallelism using the message passing interface, we are able to perform shear simulations of significant size and duration. We discuss the scaling and performance of these large calculations on the IBM Blue Gene/L architecture.

1 Introduction

Fluid dynamics presents many computational challenges, particularly in the area of complex fluids, where microscopic/mesoscopic details of the fluid components are important in addition to the bulk properties such as the viscosity. One useful method for studying such systems is based on the lattice Boltzmann equation (LBE) for the incompressible Navier-Stokes equations (for a review see e.g., ref. 1). The LBE provides a natural way for the microscopic details — e.g., composition, liquid crystal ordering, and so on — to be coupled to the fluid flow. In addition, by relaxing the constraint of exact incompressibility the LBE allows the fluid pressure to be computed locally, and thus is extremely well suited to parallel computation.

One application where the LBE is useful is flow involving a mixture of fluids, where the fluid-fluid interface can evolve on the lattice in a natural way without the need for explicit interface tracking. One example of such a problem is *spinodal decomposition* involving two symmetric liquids. If at high temperature the liquids are miscible, a drop in temperature can cause spinodal decomposition, where the liquids separate and form domains which grow continuously in time. The growth in domain size occurs in a well-understood fashion and is ultimately limited by the container size in experiment, or the system size in simulation. However, experiments on sheared systems report saturation in the length scales after a period of (anisotropic) domain growth. The extreme elongation of the domains in the flow direction means that finite-size effects cannot be excluded as the reason for saturation even in experiments. Evidence for steady-states from simulations large enough to be uncontaminated by finite-size effects is therefore of great interest. Recently, a number of works have addressed this type of problem using simulation[5,6,12,13]; here, we describe the steps we take to implement the calculation.

In two dimensions, our recent results indicate unambiguously that non-equilibrium steady states do exist in sheared binary mixtures[6]. Such two-dimensional calculations, based typically on 1024x512 lattices run for 500,000 time steps, are tractable with relatively modest computational effort. In three dimensions, the situation is slightly more

complex as the domains can grow in the vorticity direction allowing the possibility of different physics[12]. To avoid finite-size effects here, systems of up to 1024x512x512 have been used, which must also be run for a similar length of time to probe possible steady states. These three-dimensional calculations then present a more substantial computational challenge for which parallel computing is essential.

In our LBE calculations, a shear flow is driven by block-wise introduction of Lees-Edwards sliding periodic boundary conditions (first used in molecular dynamics[2]). When using the LBE, the system is divided in the shear direction into a number of slabs which translate (conceptually) relative to each other as the simulation proceeds[10]. The translation of the slabs sets up a linear shear profile across the system. In practice, this subdivision of the system requires a refined version of the halo exchange between parallel sub-domains in the appropriate coordinate direction. We discuss two approaches to the implementation of the sliding periodic boundaries: (1) using point-to-point communication, and (2) using MPI-2 single-sided communication.

In the following section we give a brief overview of the LBE as used for binary fluids and its related performance and scalability issues. We include a number of indicative results in the final section and comment on their significance.

2 Short Description of the LBE

2.1 The LBE

The central computational object in the lattice Boltzmann approach is the distribution function $f_i(\mathbf{r};t)$, which can be thought of as representing the contributions to the density of fluid at given lattice site $\mathbf{r}$ having discrete velocity $\mathbf{c}_i$, for $i = 1,\ldots,N$. A set of N discrete velocities is chosen to ensure the appropriate symmetry properties of the Navier-Stokes equations are maintained on the lattice. In three dimensions, N is typically 15 or 19, which includes the null velocity $\mathbf{0}^3$. The non-zero $\mathbf{c}_i$ are such that $\mathbf{r}+\mathbf{c}_i\Delta t$ is a neighbouring lattice site, i.e., each element of the distribution *propagates* one lattice spacing in a different direction in a discrete time step Δt.

The N elements of the distribution function are complemented by N modes $m_i(\mathbf{r};t)$, which include the important hydrodynamic quantities of the system. In three dimensions, there are ten hydrodynamic modes: the density, three components of the momentum, and six independent components of the stress. The remaining modes are non-hydrodynamic, or "ghost" quantities, which do not have direct physical interpretation. Using Greek subscripts to denote Cartesian directions, the hydrodynamic modes may be written as moments of the distribution function: the density is $\rho(\mathbf{r};t) = \sum_i f_i(\mathbf{r};t)$; the momentum is $\rho u_\alpha(\mathbf{r};t) = \sum_i c_{i\alpha} f_i(\mathbf{r};t)$; the stress is $\Pi_{\alpha\beta}(\mathbf{r};t) = \sum_i c_{i\alpha}c_{i\beta} f_i(\mathbf{r};t)$. (In what follows we assume the repeated index is summed over.) More generally, a transformation can be made between the modes and the distributions by writing $m_i(\mathbf{r};t) = E_{ij} f_j(\mathbf{r};t)$, where E_{ij} is a known matrix of eigenvectors for a given choice of velocity set $\mathbf{c}_i$. Likewise, the inverse transformation can be used to obtain the distributions from the modes, $f_i(\mathbf{r};t) = E^{-1}_{ij} m_j(\mathbf{r};t)$.

The time evolution of the distribution is then described by a discrete Boltzmann equation, i.e., the LBE:

$$f_i(\mathbf{r}+\mathbf{c}_i\Delta t; t+\Delta t) - f_i(\mathbf{r};t) = C_{ij}\left(f_j(\mathbf{r};t) - f^{eq}_j(\mathbf{r};t)\right). \qquad (2.1)$$

The left hand side can be viewed as the propagation stage, where each element of the distribution is moved one lattice spacing in the appropriate direction. The right hand side represents a *collision* stage which introduces the appropriate physics through the collision operator C_{ij} and some choice of equilibrium distribution $f_j^{eq}(\mathbf{r};t)$. In practice, it is convenient to perform the collision stage not on the distribution function but on the modes, where the physical interpretation is clear. Both the density and the momentum are conserved by the collision, and so are unchanged. The stress is relaxed toward the equilibrium value $\Pi_{\alpha\beta}^{eq} = \rho u_\alpha u_\beta + p\delta_{\alpha\beta}$ at a rate related to the fluid viscosity, with p being the fluid pressure. Treatment of the remaining ghost modes may vary but they can, for example, be eliminated directly at each time step. As the fluid obeys an ideal gas equation of state, with $p = \rho c_s^2$ relating the pressure to the density and the speed of sound on the lattice c_s, it can be seen that the collision process is entirely local at each lattice site.

The propagation and collision stages are then performed in turn by repeated transformations between the distribution and mode representations. Computationally, the propagation stage involves essentially no floating point operations, while the collision stage requires the two matrix-vector multiplications $E_{ij}f_i$ and $E_{ij}^{-1}m_i$ needed for the transformations. This gives approximately $2N^2$ floating point operations per lattice site. The LBE (2.1) approximates the Navier-Stokes equation for incompressible flow provided a low Mach number constraint is satisfied. This means the local fluid velocity u must remain small compared with the speed of sound on the lattice c_s or, alternatively, that the density does not deviate significantly from the mean. The Mach number constraint may be thought of as analogous to the Courant-like condition in finite difference approximations to the equations of motion where information must not propagate beyond one lattice spacing in one discrete time step. In a parallel domain decomposition, one round of communication is required before the propagation stage at each step to allow neighbouring distributions to move to adjacent lattice sites. Owing to the local nature of the pressure calculation, no global communication is required.

2.2 Binary Mixtures

A number of different methods are available to represent mixtures which use a lattice kinetic equation analogous to the LBE[7,8]. Here, we use a method which employs a compositional order parameter to represent the relative concentration of the two fluids, along with the appropriate dynamics near the interface. The coupling between the fluids introduces a force in the Navier-Stokes equations from the bending of the interface, while the order parameter is advected at the local fluid velocity. The order parameter introduces a new distribution to represent the composition of the fluid. This distribution undergoes the same propagation stage to the density distribution $f_i(\mathbf{r};t)$, and a similar collision process to introduce the required interfacial physics. In what follows, we only refer specifically to the density distribution; an analogous description holds for the distribution representing the composition.

2.3 Lees Edwards Sliding Periodic Boundaries

There are a number of different ways in which shear can be introduced into a system in the LBE picture. For example, it is particularly easy to represent solid walls with the LBE

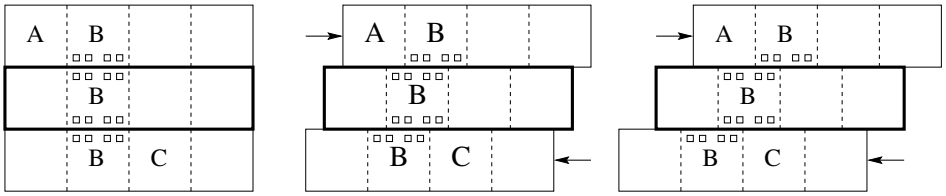

Figure 1. Schematic diagram showing the blockwise decomposition of the system with different slabs translating relative to each other at a constant velocity $\pm u_{LE}$ in the horizontal direction. Here, the sliding boundaries are represented by the horizontal lines, and four processor subdomains (A, B, C, D) by the vertical dashed lines. Elements of the distribution f_i which cross the sliding boundaries (i.e., those at adjacent lattice sites, small squares) undergo a transformation to account for the relative change in velocity. As adjacent blocks translate, communication is required between different subdomains to obtain the neighbouring lattice sites as a function of the displacement $u_{LE}t$. For example, subdomain B requires no direction communication at $t = 0$ (left), but communication with A at the upper edge and C at the lower edge at the later times (middle, right).

by using reflection boundary conditions for the distributions ("bounce-back on links"). Two side walls, or planes, moving in opposite directions at velocity u_w and separated by the length of the system in the shear direction L can then impart shear to fluid with rate $\dot{\gamma} = 2u_w/L$. While straightforward, this approach does not allow high shear rates to be achieved when the distance between the walls becomes large. Owing to the low Mach number constraint, the maximum fluid velocity near the walls is c_s, and hence the overall shear rate is limited to no more than $2c_s/L$. Likewise, using a body force on the bulk of the fluid to drive, for example, a Couette flow, is subject to the same sort of limitation.

To overcome this constraint, block-wise Lees-Edwards sliding periodic boundary conditions have been introduced[10]. Here, the system is decomposed into two or more slabs which translate relative to each other at a fixed velocity $\pm u_{LE}$. While the value of u_{LE} is subject to the same Mach number constraint as for the solid walls, a large number of slabs N_{LE} may be used to increase the maximum available shear rate to $2N_{LE}c_s/L$. In no block does the flow locally exceed approximately u_{LE} relative to the lattice, so the Mach number constraint is always obeyed. The situation is represented schematically in Fig. 1. Three horizontal slabs are shown, the central one of which can be considered at rest (only relative motion of the blocks is important). At its upper boundary the central block sees the neighbouring block translate to the right at speed u_{LE}, while the block at its lower boundary translates in the opposite direction. Conventional periodic boundary conditions are applied at the limits of the system in all dimensions. The resulting fluid flow is represented in Fig. 2. The velocity or flow direction is parallel to the sliding boundaries, while a velocity gradient is set up in the direction normal to the boundaries.

As shown in Fig. 1, the sliding boundaries separate lattice sites in adjacent planes of the system but do not coincide. This means the collision stage can take place locally at each lattice site unaffected by the presence of the sliding boundaries. However, at the propagation stage, elements of the distribution associated with velocities $\mathbf{c}_i$ which have a component crossing the boundary must undergo a Galilean transformation to take account of the velocity difference between the slabs. As the relative velocity u_{LE} is not a lattice vector $\mathbf{c}_i$, the transformation required is best understood in terms of the modes rather than the distributions[9]. We denote the hydrodynamic quantities in the upper slab with a star. In

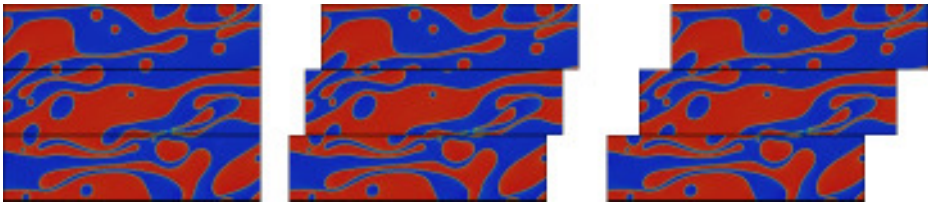

Figure 2. A schematic representation of the result from a binary mixture undergoing shear as a function of time. As the simulation proceeds, the shear causes domains of the two fluids (here shaded differently) to stretch and elongate in the flow direction. As the slabs translate relative to each other, the fluid motion remains continuous across the sliding boundaries. A coherent picture can be obtained by displacing the slabs $u_{LE}t$ and using the periodic boundary conditions in the horizontal direction. The shear direction is in the vertical; the flow direction is horizontal; in three dimensions the vorticity direction is perpendicular to the page.

crossing the boundary from the central block to the upper block the density is unchanged $\rho^\star = \rho$, the momentum is incremented $\rho u^\star_\alpha = \rho u_\alpha + \rho u_{LE\alpha}$, and the stress $\Pi^\star_{\alpha\beta} = \Pi_{\alpha\beta} + \rho u^\star_\alpha u_{LE\beta} + \rho u^\star_\beta u_{LE\alpha} + \rho u_{LE\alpha} u_{LE\beta}$. There is no change in the ghost modes if they are constrained to zero at each step. Having the appropriate modes $m^\star_i$ allows the corresponding transformed distributions $f^\star_i = E^{-1}_{ij} m^\star_j$ to be computed.

In the case of a binary mixture, the interfacial force in the Navier-Stokes equations requires information on the spatial gradient of the order parameter. The method used for the exchange of information required for gradients normal to the sliding boundaries is the same as that for the distributions.

2.4 Implementation

The starting point for the implementation of the sliding periodic boundary conditions in parallel is a regular three-dimensional domain decomposition. While sliding boundaries are required at regular intervals in the shear direction to drive the flow, their placement should not constrain the processor decomposition and so affect the parallel scaling of a large calculation. However, to avoid unnecessary complication, it is convenient to ensure the sliding boundaries coincide with neither the processor subdomain boundaries nor the true periodic boundary in the shear direction. This does not, in practice, place any serious constraint on the number of slabs which can be used, as the slab boundaries and the processor subdomain boundaries can be interleaved. This means that the halo exchange of distribution values required at the processor boundaries (and the actual periodic boundaries) is unchanged in the presence of shear. In practice, the slabs are typically 8–32 lattice sites in thickness; smaller slabs increase the communication requirement and open the possibility of artifacts at the boundaries.

While the blocks translate conceptually in relation to one another, there is clearly no movement of memory associated with the blocks. For lattice sites at the edge of a slab, the neighbouring locations *in memory* are fixed at time $t = 0$. As time proceeds, the location in memory associated with a neighbouring physical lattice site moves in the opposite direction to the translating slab (see Fig. 3). At times $t > 0$, an extra communication is therefore required in the along-boundary direction to make neighbouring information available; potentially two different processor subdomains are involved at each boundary

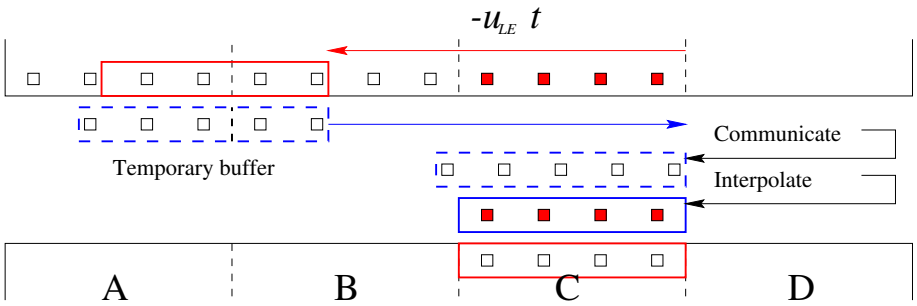

Figure 3. Schematic diagram showing the pattern of communication and interpolation required in the fixed frame of reference of memory to compute appropriate boundary-crossing distribution values for the propagation stage. For the given displacement $u_{LE}t$, the values required by processor subdomain C in the lower slab are found split between processor subdomains A and B in the upper slab. Communication of transformed distributions $f_i^\star$ takes place to a temporary buffer, where linear interpolation to the final values (shaded lattice sites) required by C can also take place. An analogous exchange takes place in the opposite direction for values required in the upper slab.

as a function of time. The processor subdomains involved are determined by the current displacement $u_{LE}t$; periodic boundaries mean this displacement is modulo the system size in the direction of the sliding boundaries.

Further, as the displacement $\pm u_{LE}t$ is not necessarily a whole number of lattice spacings, an interpolation between neighbouring memory locations is required to get the appropriate cross-boundary distribution values $f_i^\star$ so that the propagation stage can take place as normal. To do this, communication of all values required for a linear interpolation are received by a temporary buffer. The interpolation, determined by the displacement modulo the lattice spacing takes place in the temporary buffer. The boundary-crossing distributions are finally copied to the memory locations neighbouring the destination lattice sites.

2.5 MPI Communications

Two different implementations of the along-boundary communication have been used. The first uses MPI point-to-point communication[14] via `MPI_Send` and `MPI_Recv` between the relevant subdomains. The second uses MPI 2[15] single-sided communication via `MPI_Get`. This requires that appropriate memory allocations are made with `MPI_Alloc_mem` and appropriate remote memory access windows are identified with `MPI_Win_create`. In both cases, the source process for the exchanged data can be computed as a function of time from the slab displacement $u_{LE}t$ modulo the system size in the along-boundary direction.

Where MPI-2 implementations are available, for example on the IBM p690+, we have found that both implementations give very similar results in terms of performance. The results described use the point-to-point implementation. MPI-2 implementation of single-sided communication is not universally available at the time of writing.

3 Results

A recent work[12] has examined the characteristics of shear flow in three-dimensional binary fluids using the methods described here. The requirement that finite size effects be

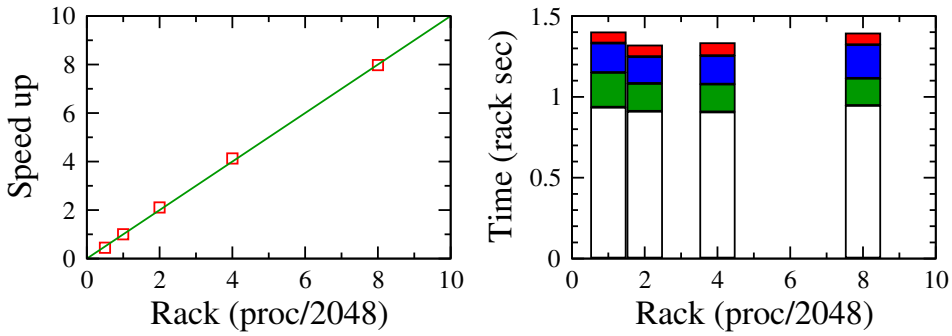

Figure 4. Benchmark results for a 1024x512x512 lattice with shear driven by 32 equally spaced Lees-Edwards sliding boundaries, performed on the IBM Blue Gene/L system at Thomas J. Watson Research Center. The left panel shows the scaling of the calculation as a function of the number of racks (2048 processors, all virtual node mode) normalised to one rack. The right panel shows rack number multiplied by time in seconds for various parts of the calculation: from the bottom, collision, propagation, lattice halo swaps, and Lees-Edwards transformation (including along-boundary communication).

excluded means that large system sizes of up to 1024x512x512 lattice sites have been used. Shear was generated by 32 equally spaced slabs in one of the shorter directions. The calculations were performed using the IBM Blue Gene/L machine at the University of Edinburgh, where a single rack is available (2048 MPI tasks in virtual node mode — all computations take place in this mode). To investigate the scaling of this type of calculation on larger machines, we have also run the same 1024x512x512 problem on the BG/L system at IBM Thomas J. Watson Research Center on up to 8 racks (16,384 MPI tasks). The scaling of the calculation and breakdown of the LBE algorithm are illustrated in Fig. 4. The scaling of the calculation is extremely good, while the absolute performance is is in the range of 5–10% of theoretical peak performance.

4 Summary

We have described the implementation of Lees-Edwards sliding periodic boundary conditions in parallel to allow simulations of large systems under shear. In conjunction with high performance computing this method, based on the LBE, provides an excellent way to investigate the properties of complex fluids.

Acknowledgements

We thank IBM Thomas J. Watson Research Center for the chance to use their Blue Gene/L system, along with Ronojoy Adhikari, Mike Cates and Paul Stansell for many useful discussions. KS acknowledges support from the UK EPSRC Grant EP/C536452 (RealityGrid). JCD is grateful to the Irish Centre for High-End Computing for access to its facilities.

References

1. S. Succi, *The Lattice Boltzmann Equation and Beyond*, (Clarendon Press, Oxford 2000).
2. A. W. Lees and S. F. Edwards, *The computer study of transport processes under extreme conditions*, J. Phys. C: Solid State Phys., **5**, 1921, (1972).
3. Y. H. Qian, D. d'Humières and P. Lallemand, *Lattice BGK models for Navier-Stokes Equation*, Europhys. Lett., **17**, 479, (1992).
4. M. E. Cates, V. M. Kendon, P. Bladon and J.-C. Desplat, *Inertia, coarsening and fluid motion in binary mixtures*, Faraday Disc., **112**, 1, (1999).
5. F. Corberi, G. Gonnella and A. Lamura, *Spinodal decomposition of binary mixtures in uniform shear flow*, Phys. Rev. Lett., **81**, 3852, (1998); *Two-scale competition in phase separation with shear*, Phys. Rev. Lett., **83**, 4057, (1999).
6. P. Stansell, K. Stratford, J.-C. Desplat, R. Adhikari and M. E. Cates, *Nonequilibrium steady states in sheared binary fluids*, Phys. Rev. Lett., **96**, 085701, (2006).
7. M. R. Swift, W. R. Osborn and J. M. Yeomans, *Lattice Boltzmann simulation of non-ideal fluids*, Phys. Rev. Lett., **75**, 830, (1995); M. R. Swift, E. Orlandini, W. R. Osborn, and J. M. Yeomans, *Lattice Boltzmann simulations of liquid-gas and binary fluid systems*, Phys. Rev. E, **54**, 5041, (1996).
8. A. K. Gunstensen, D. H. Rothman, S. Zaleski and G. Zanetti, *Lattice Boltzmann model of immiscible fluids*, Phys. Rev. A, **43**, 4320, (1991); X. Shan and H. Chen, *Lattice Boltzmann model for simulating flows with multiple phases and components*, Phys. Rev. E, **47**, 1815, (1993); L.-S. Luo and S. S. Girimaji, *Theory of the lattice Boltzmann method: Two-fluid model for binary mixtures*, Phys. Rev. E, **67**, 036302, (2003).
9. R. Adhikari, J.-C. Desplat and K. Stratford, *Sliding periodic boundary conditions for the lattice Boltzmann and lattice kinetic equations*, cond-mat/0503175, (2005).
10. A. J. Wagner and I. Pagonabarraga, *Lees-Edwards boundary conditions for lattice Boltzmann*, J. Stat. Phys., **107**, 521, (2002).
11. K. Stratford, R. Adhikari, I. Pagonabarraga and J.-C. Desplat, *Lattice Boltzmann for binary fluids with suspended colloids*, J. Stat. Phys., **121**, 163, (2005).
12. K. Stratford, J.-C. Desplat, P. Stansell and M. E. Cates, *Binary fluids under shear in three dimensions*, Phys. Rev. E, **76**, 030501(R), (2007).
13. J. Harting, G. Giupponi and P. V. Coveney, *Structural transitions and arrest of domain growth in sheared binary immiscible fluids and microemulsions*, Phys. Rev. E, **75**, 041504, (2007).
14. Message Passing Interface Forum (1995), *A message passing interface standard*. http://www.mpi-forum.org/
15. Message Passing Interface Forum (1997). *MPI-2: Extensions to the message passing interface*. http://www.mpi-forum.org/