



Meso- and multi-scale modelling E-CAM modules III

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Executive Summary

In this report for Deliverable 4.4 of E-CAM, nine software modules in meso- and multi-scale modelling are presented.

Four of the modules have been implemented in [DL_MESO_DPD](#):

- Ewald method for the GPU version of DL_MESO_DPD
- Smooth Particle Mesh Ewald (SPME) method for the GPU version of DL_MESO_DPD
- Analysis of local tetrahedral ordering for DL_MESO_DPD
- Consistency check of input files in DL_MESO_DPD

Five of the modules concern the Grand Canonical Adaptive Resolution Scheme (GC-AdResS) and have been developed, implemented and tested in/with [GROMACS 5.1.0](#) and [GROMACS 5.1.5](#). The patches provided are for GROMACS 5.1.5. The modules provide a recipe to simplify the implementation and to allow to look into a microcanonical (i.e., NVE-like) environment. They are based on the same principles as the Abrupt AdResS modules delivered in D4.3[1]. Furthermore, we provide all the tools necessary to run and check the AdResS simulations. The modules are:

- Local Thermostat Abrupt AdResS
- Thermodynamic Force Calculator for Abrupt AdResS
- Energy (AT)/Energy(interface) ratio: Necessary condition for AdResS simulations
- Velocity-Velocity autocorrelation function for AdResS
- AdResS-Radial Distribution Function (RDF).

A short description is written for each module, followed by a link to the respective Merge-Request on the GitLab service of E-CAM. These merge requests contain detailed information about the code development, testing and documentation of the modules.

1 Introduction

Work package 4 deals with meso-scale simulations, characterized by an intermediate scale, somewhere between atomistic Molecular Dynamics (MD) and continuum mechanics, and multi-scale ones. The modules presented in this deliverable concern two methods, one in each class.

The first one is Dissipative Particle Dynamics (DPD) [2], a particle-based approach similar to MD, but where the simulated particles are fictitious ones and correspond to many microscopic degrees of freedom. This approach is a meso-scale one, is well suited to describe solvents with solutes and is commonly used in various industrial sectors.

The second method is the Grand Canonical Adaptive resolution scheme (GC-AdResS), a multi-scale method combining fine-grained (i.e., MD) and Coarse Grained (CG) resolutions. The AdResS methods can be conveniently used when the interesting dynamics is limited to a region of the system, whereas the surroundings can be treated at a lower resolution. The Grand-canonical version of the method is a rigorously derived one where the fine-grained region is an open system and the coarse-grained one acts as a reservoir [3, 4, 5].

The software modules of the present report are all built on big software packages and thus extend their applicability. The first one is DL_MESO [6, 7], a general purpose mesoscale simulation package, in particular including a DPD code. The second one is GROMACS, a widely used MD package. Both packages have previously (in deliverable 4.1 [8]) been identified as important codes for mesoscale simulations within E-CAM.

The modules that are being presented here have been developed by the E-CAM programmer Jony Castagna (Sec. 2.1 and 2.2) and the E-CAM Postdoctoral Research Associate (PDRA)s Silvia Chiacchiera (Sec. 2.3 and 2.4) and Christian Krekeler (Sec. 3). The PDRA's worked within the framework of pilot projects which implied a strong interaction with industry (S. Chiacchiera: Unilever; C. Krekeler: MODAL AG).

1.1 Overall scope of the module set

The modules presented in this report were generated within two projects.

1.1.1 Porting of electrostatics to GPUs and development of tools for DL_MESO_DPD

Concerning DL_MESO_DPD, we present four modules, two related to the GPU version of the code, two for the standard one.

The porting of DL_MESO_DPD to graphic cards (GPUs), already reported in D4.2 [9] (for a single GPU) and D4.3 [1] (for multiple GPUs), has now been extended to include electrostatics, with two alternative schemes.

Concerning the standard version of DL_MESO_DPD, a pre-processing tool for checking purposes and a post-processing tool to analyze the ordering of water-like systems are presented.

1.1.2 Further development of a new GC-AdResS scheme in GROMACS

The modules associated with this project continue the work presented in D4.2 [9] on the implementation of a recently proposed version of the GC-AdResS, namely "abrupt AdResS".

In AdResS, the simulation box is divided into three regions with different resolutions: an atomistic one (AT), a coarse-grained one (CG), and a hybrid region, which smoothly interpolates between the two via weighting functions $w(x)$ (x being the direction along which the partitioning is done). In this approach, the two resolutions coexist in the hybrid region.

In the "abrupt" AdResS, instead, the hybrid (here called Δ) region involves only the atomistic degrees of freedom, so the simulation box is divided into just two regions with different resolutions, whence the "abruptness" of the method. Still, an hybrid region is effectively there, as a domain where different forces apply: a one-body force, the so-called thermodynamic force, is present; moreover, AT and CG particles interact via the CG potential.

The first and main module presented in this deliverable implements a local thermostat, which acts on CG particles only, as opposed to the global one acting on AT particles too. The second module presents a fundamental ingredient for AdResS, the thermodynamic force (see above) calculation. Next, a set of analysis tools follows, including a check of the interface energy, a velocity-velocity autocorrelation function (for the AT region), and Radial Distribution Function (RDF) to analyze the structure of the system (for the AT region). More details about these modules are given in section 3.

1.2 General applications and possible exploitation of the codes

DPD is commonly used in the industrial context to analyze static and dynamic properties of soft-matter systems. Examples include colloidal dispersions, emulsions and other amphiphilic systems, polymer solutions, etc. Such materials are being produced or processed in industries related to oil extraction, pharmaceuticals, food, household and personal care products.

The calculation of electrostatic forces is computationally very expensive, and this is the reason why, when possible, models are designed to keep the number of charged particles low, while capturing the relevant phenomena. However for many applications it is fundamental to be able to include electrostatics and to treat it efficiently. An example of such a case are the polarisable solvent models developed within the [Unilever/E-CAM pilot project](#), where each solvent bead is augmented with at least one electric charge (for more details on the models, see the [case study](#)). The aim of that project is to describe at mesoscale level mixtures with strong dielectric contrast, as for example oil-water mixtures, which are present in biomolecular processes and in many of the soft-matter examples mentioned above [10, 11, 12]. The porting to GPUs of DL_MESO_DPD already allowed for a speed-up of calculations (see deliverable D7.4 [13]), and the inclusion of electrostatics in this version of the code is a major asset.

The other modules for DL_MESO_DPD add functionalities to the existent set of tools to pre- and post-process its results.

GC-AdResS is a very general method that, as already underlined, can conveniently be used to treat systems where the interesting dynamics takes place in a limited spatial region.

As described in D4.3[1], the implementation of the abrupt AdResS method is such to interfere as little as possible with the MD kernel for the force calculation. This removes a major performance bottleneck of the standard GC-AdResS method, and allows its integration with different MD codes.

The implementation of a local thermostat realizes a NVE-like environment for the AT part of the simulation box. When (e.g.) a thermostat is used in a NVT simulation, the dynamics of that thermostat is imposed on the system, and artificial effects may arise. In the method presented here, instead, we indirectly thermalize the AT region and thus do not impose any dynamics on it. This implies that the method can be safely used to explore time-dependent phenomena too, since then the dynamics in this region is a "real" one. For detailed information see Refs. [14, 15, 16]. This work is part of an [E-CAM pilot project focused on the development of the GC-AdResS scheme](#).

The Abrupt AdResS approach has been tested in a few systems and has proven to lead to results that have similar accuracy to the fully atomistic ones, while at the same time offering a speed-up both with respect to the fully atomistic and to the standard (i.e., smooth) AdResS approach [15].

1.3 How to read this report

For each module, we give a short overview, followed by links to the Merge-Request and the Documentation on the [GitLab service of E-CAM](#), which shows detailed information about code development, testing and documentation. The documentation shows how to use the modules in practice, while possible practical exploitation and industrial applications have been outlined above (partly, some additional remarks are added below).

2 Modules based on DL_MESO_DPD

The base code for the following modules is DL_MESO_DPD [6, 7], the [DPD](#) code from the mesoscopic simulation package [DL_MESO](#), developed by M. Seaton at Daresbury Laboratory. This open source code is available from the Science and Technology Facilities Council ([STFC](#)) under both academic (free) and commercial (paid) licenses.

The first two modules refer to the single-GPU version of the code, following the previous work presented in deliverable D4.2 [9], and concern the inclusion of electrostatic forces. The following two are tools for the standard code, in its version 2.6.

2.1 Ewald method for the GPU version of DL_MESO_DPD

To allow DPD methods to treat systems with electrically charged particles, several approaches have been proposed in the literature, mostly based on the Ewald summation method [17]. The DL_MESO_DPD code includes standard Ewald and Smooth Particle Mesh Ewald ([SPME](#)) methods (in version 2.7, released in December 2018). Accordingly, here the same methods are implemented for the single-GPU version of the code.

The Ewald method consists in dividing the long range electrostatic forces in two parts: a short range part, solved in the real space, and a long range one, solved in the reciprocal space. An error weight function combines the two contributions.

2.1.1 Module description

The module consists of several files where the short and long ranges implementations are ported from FORTRAN to CUDA-C language. No changes in the algorithm are required to adapt the code to GPU architectures. However, the memory locality imposed by the Ewald Summation algorithm, proportional to the maximum reciprocal space vector size k_{max} , could be an issue for performance optimization and it has not been currently investigated. As the short range force subroutines are very similar to the soft potential force, a duplication of the kernel has been avoided allowing to reuse the same one, but with a different cut-off radius.

2.1.2 Motivation and exploitation

The electrostatic force calculation represents usually the main computational costs in systems where even a small amount of charged particles is present (> 1%). Being the main loop and short range force calculation offloaded to the GPU, leaving the Ewald algorithm on CPU would have a double negative impact on the performance: all data should migrate from device to host and viceversa. Porting to GPU the full short and long range interactions allowed to maintain the speedup factor of 4 when compared to the a traditional Intel 12-core.

A typical industrially relevant example for DPD which includes electrical charges would be a system with water, oil and surfactants. In this line, we considered a simulation of water with SDS (Sodium dodecyl sulfate), a surfactant used in many cleaning products². A system of 192×10^3 particles of which 1152 are charged has been simulated (using a maximum reciprocal space vector size $k_{max} = 20$ in each direction) and compared with the parallel MPI master version. The reported speedup factor is 3.5 when using a Tesla P100 card vs Intel Ivy-Bridge 12-core.

Merge Request	Merge Request for GPU Ewald method
Documentation	Meso- and Multi-Scale Modelling Software Library

2.2 SPME method for the GPU version of DL_MESO_DPD

Similarly to the above Ewald summation algorithm, the [SPME](#) [19] splits the electrostatic forces in short and long range. Again, the long range force is solved in the Fourier space, but this time the electrical charges are spread on a virtual particle mesh using an interpolation function.

²For a recent study of micelle formation in this mixture within a DPD approach see Ref. [18].

2.2.1 Module description

The module consists of several files ported from Fortran to CUDA-C language. While the implementation of the B-spline for the interpolation function requires adapting it to the GPU architecture, the Fast Fourier Transform (FFT) porting is straightforward. In fact, NVidia released the [cuFFT](#) library using the same syntax as [FFTW](#), and for its use one merely needs a change in the header file name (from *fftw.h* to *cufft.h*). As the previous module, the memory locality of the method, augmented by the order of spline interpolation, has not been optimized yet.

2.2.2 Motivation and exploitation

The Ewald summation method described above scales with $N^{1.5}$ at best, where N is the number of charged particles. The [SPME](#) allows a better scaling, $N * \log(N)$, but requires a stencil domain decomposition (i.e. decomposing the domain along one direction only) to allow the FFTW library scaling with more than 1 core. If this is not used, as in the current master version of DL_MESO_DPD, the FFTW becomes rapidly a bottleneck for scaling across several nodes. On the other side, the porting to a single GPU does not need domain decomposition and the same speedup factor (4, compared to 12-core Intel) is maintained.

The SDS-water system (192×10^3 particles) has been simulated and compared with the parallel MPI master version for 3 different maximum reciprocal space vector sizes: 20, 40 and 100 (uniform in each direction). A spline of 8th order has been used. The speedup factor reported is 5 when using a Tesla P100 card vs Intel Ivy-Bridge 12-core. The most important advancement to note is that this speedup would be the same even if more cores were used with the master version. This is due to the missing stencil domain decomposition mentioned above.

Merge Request	Merge Request for GPU SPME method
Documentation	Meso- and Multi-Scale Modelling Software Library

2.3 Analysis of local tetrahedral ordering for DL_MESO_DPD

2.3.1 Module description

The module `tetrahedral.f90` is a post-processing utility for DL_MESO_DPD, to be used with version 2.6 (dating November 2015). It processes the trajectory (HISTORY) files and analyzes the local tetrahedral ordering, a feature that is relevant, for example, in water-like systems.

The local ordering in liquid water can be assessed considering the coordinates of oxygen atoms [20]. In particular, for each oxygen, its four nearest neighbouring oxygens are considered, whereas the hydrogens are disregarded. At the mesoscale level, the user will select one (appropriate) bead species and analyze its local ordering.

In particular, given a particle j , we first find its four nearest neighbours (n.n.). Then, an *orientational* tetrahedral order parameter is build using $q = 1 - \frac{3}{8} \sum_{i=1}^3 \sum_{k=i+1}^4 (\cos \psi_{ik} + \frac{1}{3})^2$, where i, k are n.n. of j and $\psi_{ik} = \theta_{ijk}$ is the angle between the particles i, j and k . Of course, the quantity is then averaged over the central particle and over time. A *translational* tetrahedral order parameter, S_k , is defined too, as $S_k = 1 - \frac{1}{3} \sum_{i=1}^4 \frac{(r_i - \bar{r})^2}{4\bar{r}^2}$, where i is a n.n. of j and $\bar{r} = \frac{1}{4} \sum_{i=1}^4 r_i$. For a discussion of both quantities, please see Ref. [20].

2.3.2 Motivation and exploitation

This module was developed in the context of the [pilot project 1 of WP 4](#), which concerns the derivation of a realistic polarizable model of water to be used in DPD simulations.

Tetrahedral ordering is a feature that water has due to hydrogen bonding, and that can be captured at mesoscale level by SPC-like trimer models $(+q, -2q, +q)$, where q are partial electric charges and SPC stays for Simple Point Charge.

Merge Request	Merge Request for tetrahedral.f90
Documentation	Meso- and Multi-Scale Modelling Software Library

2.4 Consistency check of input files in DL_MESO_DPD

2.4.1 Module description

The module `check_config.f90` is a pre-processing utility for DL_MESO_DPD, to be used with version 2.6 (dating November 2015). It checks that the content of the optional configuration (CONFIG) file is consistent with that of the necessary input files (CONTROL and FIELD). In particular, it checks: the system dimensions, its composition and the bead content of all the molecules. In addition, in case hard walls are present, it checks that none of the stretching bonds between beads crosses a hard wall.

When running `check_config.f90`, the outcome of the different checks is sent to the standard output. The most important messages are: warnings, error messages and hints to fix them. For completeness, some information about the system size and composition is printed too.

2.4.2 Motivation and exploitation

The DL_MESO_DPD input files (CONTROL, FIELD and CONFIG) can be written by hand (doable for small systems) or generated using some tool (DL_MESO_DPD utilities and GUI, or GUIs from related projects, as DL_POLY [21] or Aten [22]). For hand-written files, it is useful to check for consistency between the files before running a simulation: this allows to detect certain mistakes which would not prevent DL_MESO_DPD from running, but would lead to wrong results. Automatically generated input files will in principle be individually correct, but it is still a good idea to check that their combination does not lead to conflicts.

Merge Request	Merge Request for check_config.f90
Documentation	Meso- and Multi-Scale Modelling Software Library

3 Modules based on the Grand Canonical Adaptive Resolution Scheme

Grand Canonical Adaptive resolution scheme is an advanced method, which in its essence combines two different scales, atomistic and coarse grained. The old version couples those two regions together via a smooth coupling of forces in a transition region. That means that in the old smooth coupling scheme we have three regions, namely the atomistic (AT), the transition or Δ , and the coarse grained (CG) region. The theory and the methodology of that is given in Refs. [3, 4, 5]. GC-AdResS has been implemented in several MD packages in some form (GROMACS [23, 24], ESPResSo++ [25, 26], and LAMMPS [27]).

Our new approach, the Abrupt AdResS, is a significant step into using the same principle, but leaving the necessary complicated technical constructs to make AdResS work behind. As described in the various papers regarding GC-AdResS (smooth coupling) there are certain technical restrictions regarding the Δ region and the CG potential. The smooth coupling in the Δ region had to be [3, 4, 5]:

$$F_i = \sum_j w_i(x) w_j(x) F_{ij}^{at} + \sum_j (1 - w_i(x) w_j(x)) F_{ij}^{cg} + F_{th}.$$

In our new implementation, the Abrupt coupling scheme divides the simulation box into:

- AT region - atomistic degrees of freedom
- CG region - coarse grained degrees of freedom
- Δ region - equals the region where the thermodynamic force is applied

The comparison between the old smooth coupling (which still has its advantages) and the new Abrupt coupling is shown in Fig. 1.

As reported previously (Deliverable 4.3 [1]) the speedup with the smooth coupling technique, due to GC-AdResS, was only up to a factor of 2, independently of the studied systems. There are several reasons. The force interpolation is working on the two body forces directly, which means it has to be included in the most central force kernel, which of course slows the code down. Then another problem is the parallelization of the AdResS code and the load balancing.

Our main project goal is to find a way to implement GC-AdResS in other codes. It is very unlikely that developers take the most optimized part of their codes apart to put in some interpolation, which in turn slows the code down. Abrupt AdResS does not have this problem. It utilizes the optimized internal code structures which lead to a better

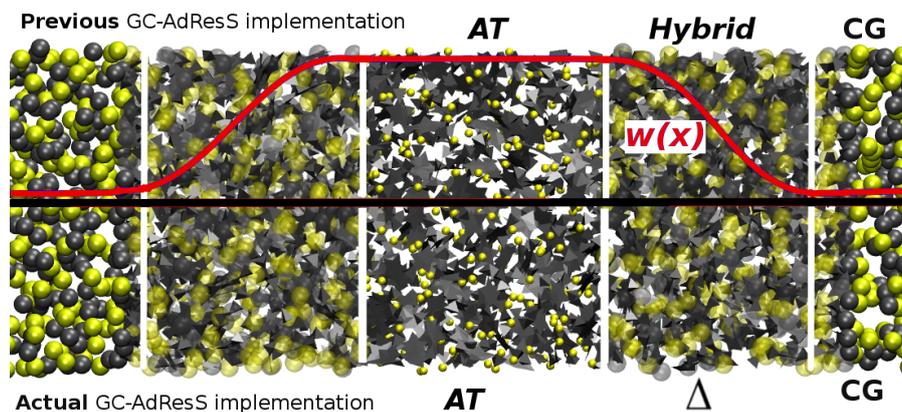


Figure 1: Schematic comparison between the previous GC-AdResS implementation and the actual one presented here, based on 1,3-Dimethylimidazolium chloride simulations. The old scheme requires a weighting function in the hybrid region $w(x)$. In this way the atomistic degrees of freedom are slowly switched on in a controlled way. The new scheme (lower half) still requires a transition region Δ , but here the switching function is implicitly included in the interactions and the thermodynamic force.

performance and is now independent of the hardware architecture. And all the necessary theoretical conditions to couple two systems are kept and still valid. In our case we do not even have to change our input files. With this ansatz we introduced a new way to implement AdResS in all MD based codes.

We continued looking into this direction, and made further progress in understanding what is essential for the Abrupt coupling scheme. We found out that the thermodynamic force F_{th} , already an important part of the smooth coupling AdResS, is much more important in the new coupling. This force ensures that the densities in the coupled regions are the same. In the abrupt coupling case, together with the force capping, it removes any possible interfaces which would hinder proper particle transfer. The F_{th} and the force capping are acting only on single particles, thus they do not significantly slow the code.

In this document we present 5 modules which show an advancement in Abrupt AdResS (follow up of the modules already reported in deliverable D4.3: Meso- and Multi-scale Modelling E-CAM modules II[1]); a more flexible thermodynamic force calculator and some tools to analyze the results. Currently 3 PhD students are working at the Free University (FU) of Berlin with Abrupt AdResS and the modules presented here. Two students will use the modules we developed and implement them into a MD code which was developed by Felix Höfling at the FU Berlin as part of a DFG (Deutsche Forschungsgemeinschaft, the German Research Foundation) project (CRC 1114). While another student will use this setup and the Path-Integral MD (PI-MD) codes to apply the method to different water models.

3.1 Local Thermostat Abrupt AdResS

3.1.1 Module Purpose

The purpose of this module is to expand the application of Abrupt AdResS by an additional function. Now with this setup we can study NVE like systems.

3.1.2 Module Motivation

With Abrupt AdresS we implemented a new partitioning scheme to bypass the performance problems in the smooth coupling GC-AdResS implementation. We switched to the general interaction kernel and simplified the neighboring list search. This module takes this new ansatz and combines it with a local thermostat approach (see Ref.[15]).

The advantages of this modules are: we can thermalize the transition and the coarse grained region, the atomistic region is thermalized indirectly. Furthermore, we still have a method which is decoupled from the core of any MD code.

3.1.3 Module Description

This module combines two different approaches.

The first part is the Abrupt coupling scheme already presented in D4.3 [1]. In any AdResS simulations the simulation box is partitioned into different regions. The Abrupt coupling scheme has one atomistic and one coarse grained region, coupled via a transition (Δ) region, where only an additional force is acting on the molecules. The forces are calculated via the standard GROMACS kernels, which increase the performance.

The second part is using the idea of a local thermostat, which was introduced in previous work by Agarwal et al. [14]. Since in AdResS the simulation box is partitioned into different regions the next logical step is to adapt the thermalization of the box and apply the thermostat only in the hybrid and coarse grained region, since the hybrid region is an artificial region and the coarse grained region represents a reservoir. Thus the atomistic region is thermalized only indirectly.

3.1.4 Module Usage

Here is also a short manual on how to run the test and set up the local thermostat simulation within this Abrupt AdResS simulations in GROMACS:

- a. mandatory requirement: a working full atomistic simulation (molecular configuration, force fields and optimal MD input parameter)
- b. You need a very well converged NVT run, which can be used as starting point for the coarse grained (CG) and then later the AdResS simulations.
- c. You have to generate a coarse grained (CG) potential. We use, for convenience, the inverse Boltzmann iteration provided in the VOTCA package [28]. The resulting tabulated CG potentials are used in the AdResS simulation. Alternatively you can use WCA potentials or standard Lennard-Jones potentials. The main requirement for the AdResS simulation is that the density in the CG region is the same as in the atomistic (AT) region.
- d. The next step is to create a double resolution configuration and adjust the dependencies (force field, topology, index file, GROMACS input file).

The local thermostat simulations are significantly different from the Abrupt coupling AdResS simulations. The atomistic region is indirectly thermalized by the hybrid/coarse grained, which leads to a NVE-like environment. To make sure the simulations run smoothly, a tabulated potential for shifted Lennard-Jones potentials is needed. Furthermore, GROMACS has to be compiled with double precision. It is easy to see when the simulation didn't work, as the atomistic region is evacuated by all molecules and the resulting density has an error of around 50% and higher.

Another problem with the simulation can be: an "artificial" interface is introduced and checks for the diffusion, the RDFs, etc (full list see below) ensure that those regions mix and that you have proper particle transfer.

When the MD run finished normally, we have several mandatory checks to see if the simulation was successful or not:

- a. Easiest check: load the conf.gro and the trajectory file and check if you see particle diffusion or depleted areas.
- b. we check the density along the X-direction or along the radius. If you have no thermodynamic force you have rather pronounced spikes in the density at the interfaces. If you have a converged thermodynamic force the density has to be quite flat.
- c. static properties: crucial RDFs (e.g. for water the oxygen-oxygen RDF)
- d. $p(N)$: The fluctuation of the particle number in an AT subsystem has to be the same, regardless if the system is simulated fully atomistically or with GC-AdResS.
- e. The density diffusion for each region (via a helpful expansion for VMD [29], namely the density profile tool, see Ref. [30]).
- f. If we only thermalize the transition region, the AT region is NVE-like, which means it is even possible to determine the dynamics of the system.

3.1.5 Exploitation

The patch provided in this modules couples these two approaches. The application to water, as well as an overview over the theory, can be found in Ref.[15]. A more recent work has been submitted for publications [16], where we use the Abrupt AdResS technique together with the local thermostat approach and replace the reservoir with ideal non-interacting particles, thus building a mean-field reservoir.

Merge Request	Local thermostat Abrupt AdResS
Documentation	Meso- and Multi-Scale Modelling Software Library

3.2 Thermodynamic Force Calculator for Abrupt AdResS

3.2.1 Module Purpose

We introduced with the Abrupt AdResS method a new way of coupling the different simulation regions together. Now a new code to calculate the thermodynamic force is needed, since VOTCA [28], the previous tool, is not designed for this.

3.2.2 Module Motivation

Abrupt AdResS presents a very straightforward way to implement a new partitioning scheme. The drawback is that the particles mix in a very narrow region in space. The distance of the molecules at that interface can be too small, which has to be compensated via a force capping. However the flux of particles at that interface is fast, which leads to a rather localized discrepancy in the density. The thermodynamic force calculator in VOTCA (implemented up to version 1.3 [28]) is designed for the smooth coupling over a larger region in space. Thus this code cannot be used for the small area of disturbance in this new scheme and a new code to calculate the thermodynamic force was needed.

3.2.3 Module Description

Here we present a very flexible thermodynamic force calculator for the abrupt coupling scheme. It is a mix between bash and Python scripts and can be applied even to the older smooth coupling scheme. The thermodynamic force is calculated by calculating the gradient of the density in a specific region in space. Thus any code taking this into account can be used.

The code provided is designed to be easy adjustable and can be used on different computer architectures (knowledge of bash is an advantage).

3.2.4 Exploitation

For the detailed discussion of the role and the basic principles behind this force, see Ref. [15]. It has also been used in a more recent work, which has been submitted for publications [16].

Merge Request	Thermodynamic force calc
Documentation	Meso- and Multi-Scale Modelling Software Library

3.3 Energy (AT)/Energy(interface) ratio: Necessary condition for AdResS simulations

3.3.1 Module Purpose

This module provides the code to check one very important quantity, the interaction energy in the atomistic region compared with the interaction energy in the comparable subregion in a full atomistic simulation.

3.3.2 Module Motivation

The difference between those energies is the interaction energy at the interface. There is a mathematically derived condition for AdResS simulations: a simulation is valid only if the interface energy is much smaller than the interaction energy in the atomistic region. That means that the interface energy does not influence the full atomistic region or that the influence is negligible.

3.3.3 Module Description

The theory is described in Ref. [14]. This code is based on that theory and has been developed to check the energy of the local thermostat GC-AdResS simulations presented in the paper cited above.

3.3.4 Exploitation

This module will be used in the C01 Project of the SFB CRC 1114.

Merge Request	Analyse energy
Documentation	Meso- and Multi-Scale Modelling Software Library

3.4 Velocity-Velocity autocorrelation function for AdResS

3.4.1 Module Purpose

This module provides the code to run a velocity-velocity autocorrelation function to compare the dynamics in the AT region with a full atomistic NVE simulation.

3.4.2 Module Motivation

This module provides the velocity-velocity autocorrelation functions for full atomistic and AdResS simulations.

3.4.3 Module Description

The full atomistic velocity-velocity autocorrelation is normally straightforward. In case of AdResS only the atomistic region has to be included in the calculation of the autocorrelation function.

The paper Ref. [14] describes the correlation functions and why they can be used in AdResS. This code is based on that theory and has been developed to check the dynamics of the local thermostat GC-AdResS simulations presented in the paper cited above.

Necessary for this code to work is a trajectory which contains the velocities of the particles. These files are rather large, from our experience short simulations are sufficient if the velocities are printed out every few steps.

3.4.4 Exploitation

This module can be used to generally calculate velocity-velocity autocorrelation functions in MD simulations.

Merge Request	Analyse vacf
Documentation	Meso- and Multi-Scale Modelling Software Library

3.5 AdResS-RDF

3.5.1 Module Purpose

This module should provide a general scheme to obtain radial distribution functions using existing programs.

3.5.2 Module Motivation

In GC- AdResS simulations we introduce artificial interfaces, from atomistic to hybrid and hybrid to coarse grained. To make sure that we indeed have an open system we have to check several properties, from structural to dynamic properties. Radial distribution functions (RDFs) are the easiest way to check the structural properties of the simulation.

3.5.3 Module Description

This module is dedicated to describe a straightforward and easy way to generate them for the atomistic regions in the GC-AdResS simulations. In the current implementation in GROMACS we have two geometric setups. One is radial and the other is a slab like structure. Our tool of choice to calculate the RDFs is VMD ([VMD: Main page](#)), a widely spread and helpful tool for analyzing molecular dynamics simulations.

3.5.4 Exploitation

This is a general scheme to obtain radial distribution functions.

Merge Request	RDF for GC-AdResS
Documentation	Meso- and Multi-Scale Modelling Software Library

4 Outlook

The deliverable contains nine modules that are integrated in two big software packages: DL_MESO_DPD, and GRO-MACS, that focus on meso- and multi-scale modelling.

The latest Ewald and SPME modules have significantly increased the capability of the DL_MESO_DPD on GPUs allowing system with electrically charged particles to be simulated. The code shows very good performance when compared to the parallel MPI version, mainly due to its missing domain decomposition of the long force range term, not required in the GPU version.

The development of additional pre- and post-processing tools for DL_MESO_DPD increases its usability. Work is in progress to analyze the response to spatially-modulated electric fields.

We recently presented a new general version of the GC-AdResS scheme and provided related tools to check the simulation. We have tested the abrupt ADResS ansatz on various systems (water, tetrahedral, and ionic liquids) and found a much better performance than with the old implementation. This new set of modules is based on the same principle and expands it to a NVE-like environment. This is a significant step towards a better understanding of multi-resolution procedures and ultimately new standards in multi-scale simulations. Also it will show us what degrees of freedom are important in a simulation.

Concerning future plans, new features will be added to the DL_MESO GPU version, like the smearing approximation of the charge distribution for the SPME method and, about the AdResS method, a new version which involves a further simplification has been very recently submitted for publication. This newest method will be implemented in a (Berlin developed) MD code within the DFG / CRC1114 Project.

All of the modules have been accepted into the E-CAM software library or were under final review at the time of submission.

References

Acronyms Used

FFT	Fast Fourier Transform
MD	Molecular Dynamics
DPD	Dissipative Particle Dynamics
STFC	Science and Technology Facilities Council
GC-AdResS	Grand Canonical Adaptive resolution scheme
PDRA	Postdoctoral Research Associate
AT	Atomistic
CG	Coarse Grained
SPME	Smooth Particle Mesh Ewald
FFT	Fast Fourier Transform
RDF	Radial Distribution Function

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