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**A multigrid solver for the integral equations of the theory of liquids**

by


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# A multigrid solver for the integral equations of the theory of liquids

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**Abstract**

In this article we present a new multigrid algorithm to solve the Ornstein-Zernike type integral equations of the theory of liquids. This approach is based on ideas coming from the multigrid methods for numerical solutions of integral equations (see §16 in [13]). We describe this method in a general manner as a 'template' for construction of efficient multilevel iterations for numerical solution of the integral equations in the theory of liquids. We report on several numerical experiments to illustrate the effectiveness of the method. The algorithm is tested on a model problem - a simple monoatomic fluid with a continuous short ranged potential. The tests have indicated that the method sufficiently accelerates the convergence of the numerical solution in all considered cases.

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**Key words.** Ornstein-Zernike equation, integral equations theory of liquids, multigrid methods.

## 1 Introduction

The integral equation theory of molecular liquids has been proved to be a powerful tool for the calculation of both structural and thermodynamical properties of molecular systems in fluids [17, 8, 5, 9]. However, even for the simplest case of an isotropic liquid the theory requires a non-trivial *numerical* solution of a system of integral equations of the Ornstein-Zernike (OZ) type [15]. The complexity of solution dramatically increases with the increasing number of different interacting sites of the system [17]. This is explaining the fact why the theory is still far from being 'tool of the trade' in the area of computational chemistry of condensed molecular systems, mainly, because of the lack of efficient algorithms and numerical libraries available.

The most simple algorithm to solve the OZ-type equations is the Picard algorithm[1] which is based on a successive substitution scheme. This technique is very easy to implement but it

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[1]This method is sometimes called "direct iteration method".

suffers from poor convergence [22, 17, 10]. Unfortunately, the much more efficient Newton-Raphson (NR) method cannot be applied directly to the problem because it would require the calculation and inversion of the Jacobian matrix of a size $> 10^4$ which is a tedious task. Still, there are more efficient algorithms for the OZ type equations than the plain Picard scheme. The algorithms could be roughly classified into three general domains. In the first category there are methods to improve the convergence of the Picard iterations with different techniques like vector extrapolation or iterative subspace extrapolation [18]. In the second category there are hybrid NR/Picard iteration methods [11, 25, 26, 6, 7, 10, 32] where the final solution is sought as a combination of "coarse" and "fine" components. The "coarse" component is represented as a combination of a relatively small number of basis functions while the coefficients of the expansion are found by the efficient NR algorithm. Then the obtained approximated solution is refined by the Picard iterations using the "coarse" solution as an initial guess. The coarse solution can be obtained as an expansion in the basis of roof functions [11], plane waves [25, 26, 32] or wavelets [6, 7, 10]. In the third category there are recently developed procedures for solving the OZ equation with use of matrix-free iterative Krylov or Newton-GMRES solvers [21, 2]. On a few simple examples of monoatomic liquids with short-range interaction potential there has been shown that the convergence and robustness of these methods can be improved by using multilevel iterations [22] and pseudoarc length continuation methods [28].

These days multigrid numerical methods [13, 3, 1, 33, 31] become very popular in different areas of science and engineering. The multigrid approach to complex computational problems is actively used in computational chemistry to accelerate quantum chemistry calculations [16, 20, 4, 12] as well as for the treatment of electrostatic interactions in classical molecular dynamics simulations [30, 19]. However, we are aware of only one published study on multigrid solvers for OZ equation - the work of Pettitt and Kelley [22]. In [22] a hybrid scheme have been proposed which combines multilevel nested iterations [13, 21] with Newton-GMRES algorithm for the coarse grid solver. The method has been tested on one example of a simple monoatomic liquid. The obtained results clearly indicated the superiority of the method with one-level Newton-GMRES and Picard methods.

In this article we present a universal multigrid technique for the numerical solution of the OZ type integral equations. This approach is based on ideas coming from the multigrid methods for numerical solutions of integral equations [13, 3]. Instead of the nested iteration method used in [22] we use the coarse-grid correction method which had been shown to provide better convergence than the nested iteration method [13]. The proposed approach is very flexible and allows one to combine different numerical methods to construct an effective multigrid solver for a given problem [13]. Therefore, rather than presenting an exhaustive comparison of the convergence characteristics of the proposed scheme with the other methods mentioned above, we describe this method as a general 'template' for construction of efficient multigrid iterations for numerical solution of the integral equations in the theory of liquids. We report several numerical tests proving that the method significantly accelerates the convergence of the iterations. The proposed approach is tested on a model problem - a simple fluid with continuous short ranged Lennard-Jones potential. We also investigate the robustness of the method with regard to the density of model liquid.

We will consider the problem of finding a numerical solution for the OZ equation in the simplest case of a mono-atomic isotropic liquid with spherically symmetric Lennard-Jones

interaction potential between the particles,

$$U_{LJ}(r) = 4\eta \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right], \tag{1.1}$$

where $\sigma$ and $\eta$ are the size and energy parameters, respectively, and $r$ is the interparticle distance .

In the theory of liquids the principal structural quantity of interest is the pair correlation function, $g(\mathbf{r}, \mathbf{\Theta})$, which is proportional to the probability of observing a pair of particles at a given distance $\mathbf{r}$ and mutual orientation $\mathbf{\Theta}$. For the case of a mono-atomic liquid with spherical potential between particles we can omit the $\mathbf{\Theta}$–dependence of the pair correlation function and consider it as a function $g(r)$ only, with $r = |\mathbf{r}|$.

Let us introduce the total correlation function as $h(r) := g(r) - 1$. The OZ equation relates this function with the direct correlation function $c(r)$ for an isotropic liquid with density $\rho$ by

$$h(r) = c(r) + \rho \int_{\mathbb{R}^3} c(|\mathbf{r} - \mathbf{r}'|)h(|\mathbf{r}'|)d\mathbf{r}'. \tag{1.2}$$

There are two unknowns in Eq. (1.2) and, therefore, it is still incomplete. A second equation, usually called "closure relation", is required which couples these functions with the interaction potential $U(r)$. Formally the closure relation is written as

$$h(r) = \exp[-\beta U(r) + h(r) - c(r) + b(r)] - 1, \tag{1.3}$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature, while $k_B$ is the Boltzmann constant. The closure relation introduces the bridge function $b(r)$ [27]. Given $U(r)$, $T$, $\rho$, and $b(r)$, one can find all the required correlation functions by solving the system (1.2)-(1.3) and, hence, all the thermodynamic and structural properties of the fluid can be obtained. It is common to characterise the OZ equation by the two dimensionless parameters: normalised density $\rho^* = \rho\sigma^3$ and temperature $T^* = (\beta\eta)^{-1}$ [18, 10]. We will also use these notations henceforth.

Since there is no exact expression for $b(r)$, the approximation of the bridge function is the key to contemporary IE theories. The list of such approximating closures is still expanding and includes, for example, $b(r) = 0$ for the hypernetted chain (HNC) closure, or $b(r) = \ln(1 + h(r) - c(r)) - h(r) - c(r)$ in the Percus-Yevick approximation, etc. These approximations have been studied extensively for simple liquids, and their pros and cons are well documented in the literature [14, 27]. In this work we are using the Partially Linearised Hypernetted Chain closure [23, 24] which linearises the exponent in (1.3) for the case of $b(r) = 0$ depending on the sign of the function $\Xi(r) = -\beta U(r) + h(r) - c(r)$:

$$b(r) = \begin{cases} 0 & \Xi(r) < 0 \\ \\ \ln(h(r) + 1) - h(r) & \Xi(r) > 0 \end{cases} \tag{1.4}$$

This closure has been proved to provide better convergence of the numerical iterations than the plain HNC closure [23, 24].

There are only a few special cases where Eqs. (1.2) and (1.3) can be solved analytically and, therefore, numerical solutions are necessary. For numerical calculations, the Fourier

representation of the OZ equation,

$$\hat{h}(\mathbf{k}) - \hat{c}(\mathbf{k}) = \frac{\rho\hat{c}^2(\mathbf{k})}{1 - \rho\hat{c}(\mathbf{k})}, \tag{1.5}$$

is usually applied, where the hat means the three-dimensional (3D) Fourier transform (FT). This is formally a 3D equation but taking into account the spherical symmetry of the correlation functions it can be reduced to a 1D equation for the radial parts of the functions:

$$\hat{h}(k) - \hat{c}(k) = \frac{\rho\hat{c}^2(k)}{1 - \rho\hat{c}(k)}, \tag{1.6}$$

where the mapping from $k$-space to $r$-space is done by the spherical Fourier-Bessel transform which for a spherically symmetric function $f(r)$ reads as

$$\hat{f}(k) = \mathcal{T}(f(r)) = \frac{4\pi}{k}\int_0^\infty r\sin(kr)f(r)dr. \tag{1.7}$$

The inverse spherical Fourier-Bessel transform $\mathcal{T}^{-1}$ can be obtained in a similar manner:

$$f(r) = \mathcal{T}^{-1}(\hat{f}(k)) = \frac{4\pi}{r}\int_0^\infty k\sin(kr)\hat{f}(k)dk. \tag{1.8}$$

In numerical calculations, the function $f(r)$ can be assumed to be of finite support, i.e., $f(r) = 0$ for $r \geq R$. For simplicity, we approximate $f(r)$ on a regular grid $\Omega_L$ with $N_L = N_0 2^L$ points, where $N_0$ is the size of the coarsest grid, and $L$ is an integer which determines the step size $d_L$ of the grid as $d_L = 2^{-L}d_{L=0}$. Therefore, we can regard $L$ as the *resolution level*. On a regular grid, the discrete versions of the transformations (1.7) and (1.8) can be calculated with $O(N_L \log N_L)$ operations using the Fast Fourier Transform (FFT).

# 2 Multigrid iterations

## 2.1 One-level Picard iterations

For numerical treatment of the OZ equation it is common to introduce a new function $v(r) = h(r) - c(r)$ and rewrite Eqs.(1.3) and (1.5) in the following way:

$$c(r) = \exp[-\beta U(r) + v(r) + b(r)] - 1 - v(r), \tag{2.1}$$

and

$$\hat{v}(k) = \frac{\rho\hat{c}^2(k)}{1 - \rho\hat{c}(k)}. \tag{2.2}$$

One can reformulate the problem of finding a numerical solution of the system (2.1) – (2.2) with functions $v(r)$ and $c(r)$ represented on a grid $\Omega_L$ as the solution of a nonlinear equation:

$$v(r) = F(v(r)), \tag{2.3}$$

where $F(v(r))$ is given by

$$F(v(r)) = \mathcal{T}^{-1} * \frac{\rho(\mathcal{T} * c(r))^2}{1 - \rho(\mathcal{T} * c(r))}, \tag{2.4}$$

and $c(r)$ is given by Eq. (2.1). For the sake of clarity in the following we will refer on the $v(r)$ and $c(r)$ functions as $v$ and $c$.

The simplest way of finding the numerical solution of (2.3) is the Picard scheme of successive iterations [21, 29] where an $i$-iteration is given by:

$$v^i := F(v^{i-1}). \tag{2.5}$$

To facilitate the convergence the damped Picard method [29] is often used where the $i$-th iteration is given as

$$v^i := \varepsilon F(v^{i-1}) + (1 - \varepsilon)v^{i-1}, \quad 0 < \varepsilon \leq 1; \tag{2.6}$$

where $\varepsilon$ is a damping parameter. In the following we will refer on the damped Picard method applied to the problem (2.1) as Picard method and denote an $n$-steps Picard iteration for (2.1) as

$$v := \Upsilon^n(v, \varepsilon). \tag{2.7}$$

We note that the convergence of the method is not guaranteed and normally it is quite slow. Nevertheless, the method is still commonly used in the theory of liquids (often in combination with other methods) [17, 10] because it is very easy to implement.

## 2.2 Two-grid iteration

In this subsection we will briefly describe the two-grid iteration method (TGM) which is the base for the construction of multi-grid iterations [13, 3]. The proposed approach mimics the idea of the TGM method for linear problems with coarse-grid correction [13, 3].

Let us firstly introduce two inter-grid conversion operators: a *restriction* or fine-to-coarse operator $R$ which maps the function $f$ from the fine grid $\Omega_L$ to the coarse grid $\Omega_{L-1}$ :

$$f_{L-1} = R * f_L, \tag{2.8}$$

and a reciprocal operator to restriction - *prolongation* or coarse-to-fine operator $P$ which interpolates the function $f$ given on the coarse grid $\Omega_{L-1}$ to the fine grid $\Omega_L$:

$$f_L = P * f_{L-1}. \tag{2.9}$$

There are many possible choices of these operators and advantages and disadvantages of some of them are well described in [13]. In our work we use the *trivial injection* [13, 3] for the restriction operator $I$ and the *cubic spline interpolation* [29] for the prolongation operator $P$.

Let us now consider the problem of finding a numerical solution of (2.3) on the fine grid $\Omega_L$ starting from an initial guess $v_L^{initial}$.

Let us assume that there is an iterative process $\Phi_0$ (e.g. (2.7) with a reasonably large $n$) which gives an accurate *numerical* solution[2] of the problem on the coarse grid $\Omega_{L-1}$ starting from $v_{L-1}^{initial} = R * v_L^{initial}$

$$v_{L-1}^{acc.} = \Phi_0(v_{L-1}^{initial}). \tag{2.10}$$

Therefore, the correction or *defect* of the solution on the level $L-1$ is given by

$$d_{L-1} = v_{L-1}^{acc.} - v_{L-1}^{initial}. \tag{2.11}$$

The main idea of the TGM iterations is to interpolate this correction to the fine level $L$ using the prolongation operator $P$ and improve the solution on this level as

$$v_L = v_L^{initial} + P * d_{L-1}. \tag{2.12}$$

The procedure then can be repeated to achieve the required accuracy of the solution on the fine grid. It has been shown in [13] that the convergence of the iterations can be sufficiently improved by additional one-level smoothing steps (2.7) before and after the coarse-grid correction (2.12). As a result we obtain the following TGM iteration loop:

**Algorithm 1** Two-grid iteration.

**procedure** $v^{out}$ :=TGM $(L, v^{in}, n_1, n_2)$

$v := \Upsilon^{n_1}(v^{in}, \varepsilon = 1)$; (pre-smoothing)
$v^r := R * v$; (restriction)
$v := v + P * (\Phi_0(v^r) - v^r)$; (coarse-grid correction)
$v^{out} := \Upsilon^{n_2}(v, \varepsilon = 1)$; (post-smoothing)

## 2.3 Multi-grid iterations

The extension of the TGM iterations to a more general multi-grid case is very straightforward: the main idea is to substitute the accurate solution on the coarse level $L-1$ by a recursive approximation of the solution with another two-grid iteration on level $L-2$, $L-3$ and so on until the coarsest level $L_0$ where the coarsest solution is found as $v_0^{acc.} = \Phi_0(v_0^{initial})$. As the general principles of the multi-grid iterations construction are well explained in [13] we will only briefly describe our algorithm below:

The parameter $\mu$ is rarely chosen bigger than 2 when the iteration is usually called W-iteration. If $\mu$ is equal to 1 it is common to call such iteration as V-iteration. In all our calculations we used $n_1 = n_2 = 1$ steps for pre- and post-smoothing.

As there is no way to find an exact solution of the problem the choice of $\Phi_0$ is quite ambiguous. It could be, e.g., the Picard process (2.7) with a sufficiently large number of iterations as well as the more efficient but more computationally expensive Newton-Raphson iterations algorithm [29, 10] or any other numerical procedure which can provide a coarse-grid solution with a reasonable accuracy (see, e.g., [21, 22]). For the sake of simplicity in our calculations we have chosen $\Phi_0(v) = \Upsilon^n(v, \varepsilon), \quad n = 10^2, \quad \varepsilon = 0.5$.

[2]Note the difference between this method for a *nonlinear* problem which uses an *accurate* solution and the TGM method for *linear* problems which uses an *exact* coarse-grid solution.

**Algorithm 2** Multi-grid iteration.

**procedure** $v^{out}$ :=MGM $(L, v^{in}, n_1, n_2, \mu)$

**if** $L = 0$ **then** $v^{out} := \Phi_0(v^{in})$ **else**
$v := \Upsilon^{n_1}(v^{in}, \varepsilon = 1)$; (pre-smoothing)
$v^r := I * v$; (restriction)
**for** $j := 1$ **step** 1 **until** $\mu$ **do** $v^{out}$ :=MGM$(L-1, v^r, n_1, n_2), \mu)$
$v := v + P * (v^{out} - v^r)$, (coarse-grid correction)
$v^{out} := \Upsilon^{n_2}(v, \varepsilon = 1)$; (post-smoothing)

# 3 Complexity analysis

## 3.1 Iterations cost

The cost of the iterations is limited by the cost of FFT which is $O(N_L log(N_L))$. So, one can estimate that the computational work $A_{o.l.}$ of one step of the one-level iteration is:

$$A_{o.l.} = CN_L log(N_L) \tag{3.1}$$

where $C$ is some constant and $N_L$ is the number of grid nodes. Some rough estimations show that the computational work $A_V$ for one step of the V-iteration is

$$A_V \leq 6CN_L log(N_L) = 6A_{o.l.}, \tag{3.2}$$

and, consequently, computational work $A_W$ for one step of the W-iteration is

$$A_W \leq 15CN_L log(N_L) = 15A_{o.l.}. \tag{3.3}$$

So, one could compare the efficiency of the iterations, normalising the computational cost to the cost of one step of the W-iteration.

## 3.2 Numerical results

In order to compare the efficiency of V- and W- multigrid iterations for different density parameters of the OZ equation we performed a series of V- and W-iteration calculations at constant value of the normalised temperature $T^* = 2$ varying the density parameter $\rho^*$ from 0.1 to 1.0. In our calculations we used 9 different grids with the size and step of the finest grid $N_8 = 2^{17}$ and $d_8 = 2^{-12}$ correspondingly. The quality of the solution was controlled by the norm of difference between the finest grid solutions at the neighbouring iterations $\Delta(i) = \|v^i - v^{i-1}\|$. For each value of $\rho^*$ the iterations started from *the same* initial guess for the both methods and continued until $\Delta(i) > 10^{-10}$ (which is close to the maximum precision in this case). The initial guess for $\rho^* = 0.1$ was calculated using the fast wavelet algorithm for finding an approximate solution of the OZ equation [10]. For all the next follow up $\rho^*$ values the initial guess was taken as the final solution for the previous $\rho^*$ value.

Figure 1 shows the dependence of the number of steps for V- and W- iterations necessary to achieve the threshold value of $\Delta = 10^{-10}$ from $\rho^*$. In accordance to (3.2) and (3.3) the

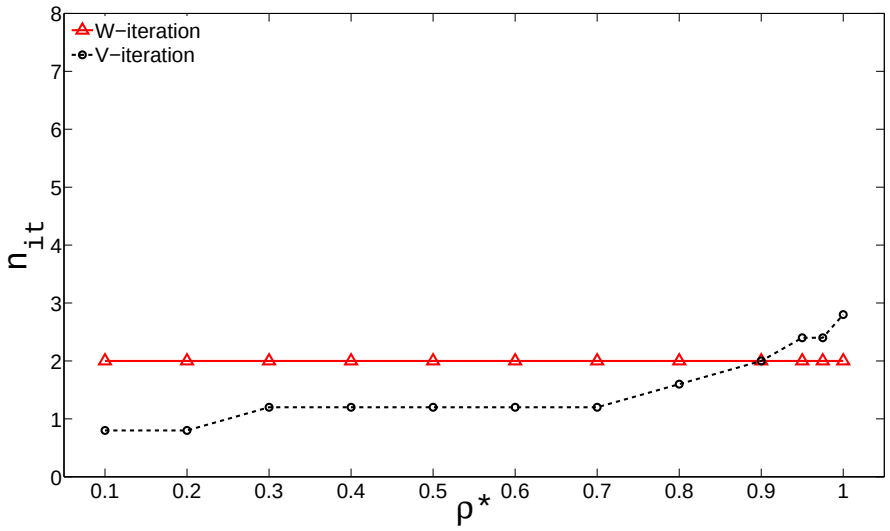


Figure 3.1: Density dependence of the computational work necessary to achieve $\Delta \leq 10^{-10}$ accuracy for two different multigrid iterations: V-iteration (circles) and W-iteration (triangles). The amount of computational work for the V-iteration was normalised per one step of the W-iteration. The points are connected by lines as a guide for the eye. For all calculations $T^* = 2.0$.

absolute numbers of the V-iteration steps were normalised by the factor 2.5 to allow one to make the direct comparison of the computational work.

As one can see from the picture, for the W-iteration method the amount of computational work necessary to achieve the required accuracy remains *constant* for the whole range of densities. In contrast, the computational work of V-iteration increases with $\rho^*$. At the low densities, the V-iteration is somewhat more efficient than the W-iteration but this method looses its advantage when $\rho^*$ becomes bigger than 0.9 (see also inset on Figure 2). The results clearly indicate the good *robustness* of the W-cycle iteration.

We note that, despite of the different behaviour at different $\rho^*$, both multigrid methods provide very high efficiency compared to the one-level Picard iteration method. As an illustrative example we will consider the problem of finding a numerical solution of the OZ equation with $T^* = 2.0$ and $\rho^* = 1.0$ by different methods. Figure 2 shows the direct comparison of the computational work necessary to achieve an accuracy $\Delta$ by different methods: W- and V- multigrid iteration and the one-level plain Picard method. The inset shows the detailed comparison between the convergence of W- and V- multigrid iteration methods. The computational work was normalised to the amount of computational work per one step of the W-cycle (see Eqs.(3.1)-(3.3)).

The parameters of the finest grid were the same as in the previous example. As one can see from the picture, the multigrid iterations provide much better convergence rate than the one-grid Picard one. The W-iteration has the best convergence rate among the all three methods and is $\geq 10^2$ times more efficient than the one-level iteration method.

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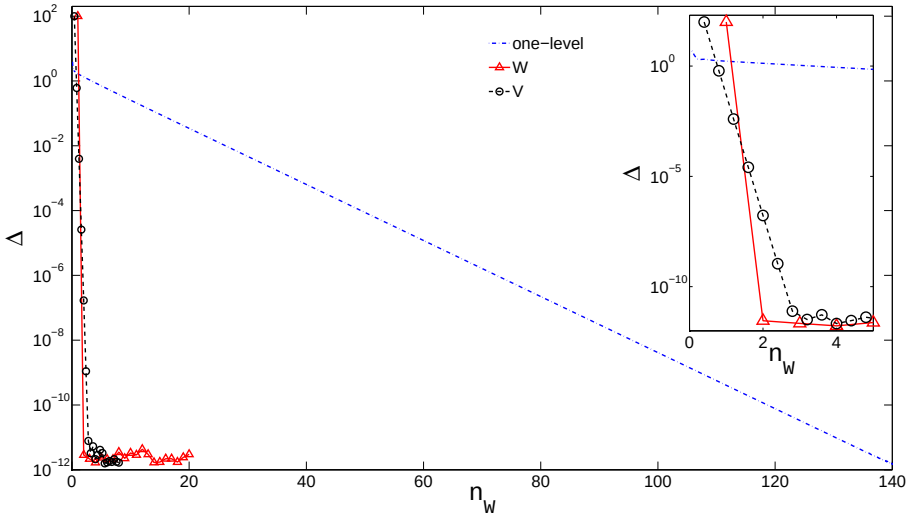


Figure 3.2: Dependence of $\Delta$ from the computational work for three different numerical methods: V-iteration (circles) and W-iteration (triangles) and one-level Picard iteration (dash-dotted line). The amount of computational work for all methods was normalised per one step of the W-iteration. For all calculations $T^* = 2.0$ and $\rho^* = 1.0$ .The inset shows the detailed comparison between the convergence rate of the W- and V- multigrid iteration methods.

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