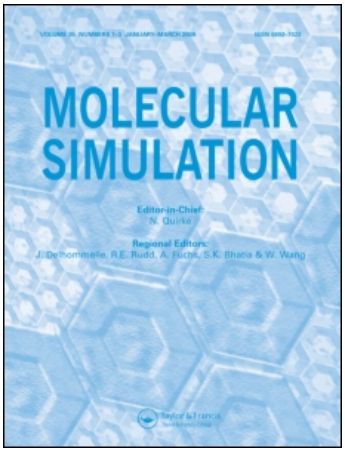

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Adaptive temperature estimation in 3D single-cell dielectrophoretic traps using the boundary element method

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We present an adaptive method for the evaluation of the temperature increase due to Joule heating in single-cell dielectrophoretic (DEP) traps. In this problem the temperature distribution in the trap can be described by a Poisson equation. The proposed algorithm produces a nearly optimal mesh for the volume integral associated with the source term, which must be calculated when using the boundary element method (BEM) to solve Poisson's equation. It is shown that this method reduces computation times by as much as an order of magnitude with respect to direct evaluation of the integral in a homogeneous mesh. The method presented is easily implemented and highly efficient in a wide variety of problems where the gradient of the source term is very high but it does not oscillate rapidly within the domain.

Keywords: Adaptive meshing; BEM; Dielectrophoresis; Single-cell trap; Poisson equation

1. Introduction

Dielectrophoresis trapping and filtering of biological cells and molecules is based on the application of strongly non-homogeneous electrical fields which polarise the cells and result in a net force that allows their manipulation [1]. Although dielectrophoretic (DEP) trapping has many advantages over other cell isolation methods, the electric field intensity within the trap can produce significant temperatures changes if the liquid buffer is highly conductive [2]. Therefore application of dielectrophoresis techniques to biological particles is limited by the temperature increase of the suspension due to Joule heating [3].

DEP traps have many inherent advantages, such as high selectivity and non-contact designs, so it is of interest to study the thermal properties of different trap designs in order to maximise trapping strength while minimizing temperature increase in the trap volume.

The temperature distribution in these traps can be obtained from a Poisson equation [4]:

$$\nabla^2 T = -\frac{\sigma |E|^2}{k} \tag{1}$$

where σ and k are the electric and thermal conductivities of the liquid buffer in the trap, and $\vec{E}$ is the electric field.

The presence of the source term on the right hand side of equation (1) introduces a volume integral in the equations of the boundary element method (BEM). Methods that transform this volume integral into a surface integral, such as the dual reciprocity method (DRM) [5,6] or the multiple reciprocity method (MRM) [7], provide an elegant solution to this problem, but are not necessarily more efficient than direct evaluation of the volume integral in all cases [8].

This work will introduce an alternative integral evaluation method that avoids this transformation and keeps the conceptual simplicity of direct evaluation, while at the same time reducing the computational time required to solve the problem. It will be shown that the proposed adaptive evaluation of the source term is straightforward to implement and highly efficient when compared to direct evaluation methods.

2. Electric field calculation

The electrical problem is solved by using the indirect formulation of the BEM [9], based on the equation for the

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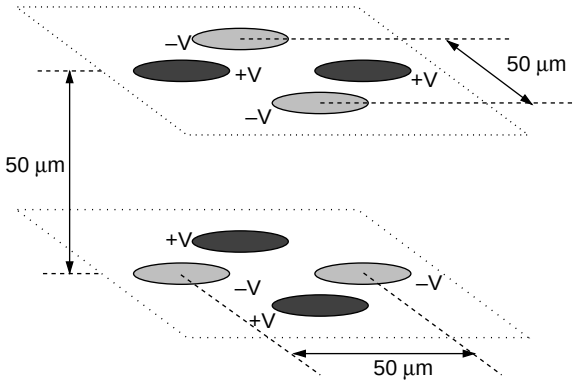

Figure 1. DEP trap geometry for electric field calculation (octupole configuration).

potential $\phi(\vec{r})$ given by:

$$\phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int_\Gamma \frac{q(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,\mathrm{d}\Gamma' \tag{2}$$

The boundary conditions used to solve this equation are given potential values at all conductors. See Ref. [10] for more details on the implementation.

To solve this equation all boundaries are discretised using quadratic isoparametric triangular elements with six nodes each. The collocation method applied to this discretization produces a set of linear equations, which are then solved using a GMRES iterative solver with Jacobi preconditioner. Once the values of the charge density $q(\vec{r})$ are known at all nodes, the electric field can be calculated at any point in space by applying $\vec{E} = -\nabla\phi$ to equation (2):

$$\vec{E}(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int_\Gamma \frac{(\vec{r}-\vec{r}\,')q(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3}\,\mathrm{d}\Gamma' \tag{3}$$

This calculation of the electric field is necessary for each point where the source term in equation (1) is evaluated.

In this paper, we have used a trap consisting of eight circular electrodes of radius $R = 15\,\mu\mathrm{m}$ situated at positions $(\pm 25, 0, \pm 25)\mu\mathrm{m}$ and $(0, \pm 25, \pm 25)\mu\mathrm{m}$ as shown in figure 1. The aim of this work is to introduce an effective method of evaluating the source term in the temperature calculation rather than provide highly accurate values of the DEP trap strength, so the effect of a dielectric substrate has been ignored for the sake of simplicity.

3. Temperature calculation

The temperature is obtained using the BEM as in the previous section, with an additional volume integral due to the source term in equation (1):

$$T(\vec{r}) = \int_\Gamma \frac{t(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,\mathrm{d}\Gamma' - \frac{\sigma}{k}\int_\Omega \frac{|\vec{E}(\vec{r}\,')|^2}{|\vec{r}-\vec{r}\,'|}\,\mathrm{d}\Omega' \tag{4}$$

where the electric and thermal conductivities have been taken outside of the integral because they are considered constant, and $t(\vec{r})$ is an unknown intermediate quantity proportional to the normal derivative of the temperature T at the surface. A temperature of 300 K at the domain walls is used as boundary condition. In the actual calculation the walls where the boundary condition is applied coincide with the z-planes containing the electrodes in figure 1 and extend a distance $\pm 50\,\mu\mathrm{m}$ in the x and y directions.

Discretization of the surfaces used for the temperature calculation is done, as in the electrical problem, using six noded triangular elements.

Accurate evaluation of the volume integral in equation (4) is difficult because the electric field gradient is very high in DEP traps and using Gaussian integration in a homogeneous mesh requires a very large number of evaluation cells. This in turn requires a large number of evaluations of the electric field, given by equation (3), and the whole process becomes computationally very expensive.

The following section describes the adaptive algorithm we propose for the evaluation of the volume integral in equation (4).

3.1 Adaption algorithm

The method we propose to solve the thermal problem is based on an adaptive evaluation of the volume integral. Finding an optimal mesh for each collection point in the surface, as strictly required by equation (4), is not practical as it would result in an evaluation that is even more computationally expensive than a direct evaluation in a homogeneous mesh. But for cases where the source term changes more rapidly than $1/|\vec{r}-\vec{r}\,'|$ we will assume that the optimal mesh for the source term integral provides a nearly optimal mesh for the actual system of equations.

There are two reasons for the high efficiency of the adaptive method we present:

- it does not require derivative evaluations; and
- it does not require checks for duplicated nodes.

Because we are evaluating an integral rather than a function directly, in order to obtain a highly accurate evaluation we would like to make the contribution to the integral from all the cells in which the volume is divided to be the same. Assuming that the variation of the integrand is large but smooth over the region of interest—that is, it does not fluctuate with a high frequency with respect to the domain size—, we can use as subdivision criteria for each cell the comparison of its local contribution with the average contribution from all cells in the domain. When the individual contribution from a cell to the integral is large compared to the average, the cell must be subdivided in order to refine the calculation in that region. If the contribution of the cell is small in comparison to the average then the cell is left unchanged. Once the subdivision check has been done in all cells a new evaluation of the integral is done using the refined mesh and it is compared with the previous one. If the convergence

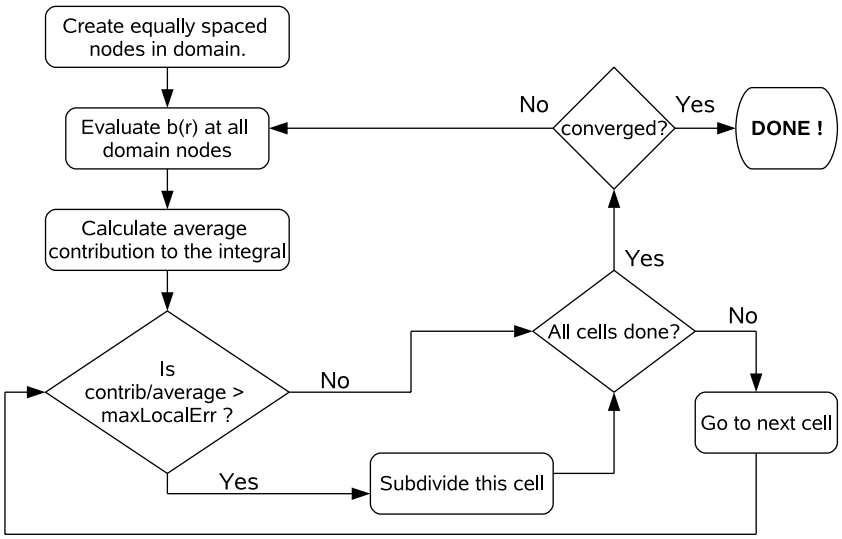

Figure 2. Adaptive meshing algorithm description. $b(r)$ stands for the source term in equation (1).

criteria set by the user is met the subdivision ends, otherwise a new subdivision check is done again, and so on until the convergence criteria is met. This process is shown in figure 2.

It is important to notice that in cases where the source term oscillates rapidly within the domain this approximated method will not provide accurate results unless it is complemented by a consistency check. One can easily imagine a case where, due to thelack of a criteria involving local derivatives, the contribution from a cell where the integrand is highly oscillating is underestimated if the evaluation point falls on a local minimum of the oscillation. A simple test would consist on a second evaluation of the source term with a slightly displaced mesh to verify that the original mesh is adequate and it is not missing regions of particularly fast spatial change. For many physical problems, as the one shown in this paper, this is not relevant, and the adaptive evaluation is both accurate and efficient.

The choice of insertion points at each subdivision level is such that there is no need to keep track of the nearest neighbors of each point or to double check in order to avoid repeated nodes. This advantage is gained because the subdivision is done in terms of evaluation cells. At each subdivision level if the contribution of a cell to the total value of the integral exceeds the average contribution from all cells by a relative amount set by the user, the cell is divided in eight identical cells. For subdivision purposes the original cell ceases to exist—it is flagged as an inactive cell in the code—and it is substituted by its eight children as shown in figure 3. When the integral is calculated in the refined mesh at the next subdivision level theintegrand is evaluated at the centre of each of the new eight cells besides the original point marking the centre of the parent cell. In this way there is never the risk of introducing a new evaluation point on a position currently occupied by another, and the implementation of the algorithm becomes very efficient.

4. Results

In order to test the efficiency of the adaptive algorithm we have studied the temperature distribution in a single-cell DEP trap consistent on eight electrodes with alternating potentials of intensity ± 7.5 V. The electrodes are circles or radius $R = 15\,\mu$m, and the electric and thermal conductivities of the buffer liquid were set to $\sigma = 0.75$ S/m and $k = 0.6$ W/mK, respectively. As a baseline for comparison we calculated the volume integral both using the adaptive evaluation method and a standard Gaussian integration scheme.

For the Gaussian integration case the volume of integration was divided in an equal number of cells in the three spatial directions and then either one or eight points schemes were used to calculate the source term. The total number of evaluation points ranged from 10^3 to 10^7. In all cases once the required spatial division was done the source term was calculated as the sum of the contributions from all cells, weighted by the cell volume and evaluated at the cell centre:

$$\int_{\Omega} b(\vec{r})\,\mathrm{d}\Omega \approx \sum_{i=1}^{n} b(\vec{r}_i)\Delta V_i \tag{5}$$

Figure 4 shows the refined mesh for the case under study. The initial mesh was a set of $10 \times 10 \times 10$ points and

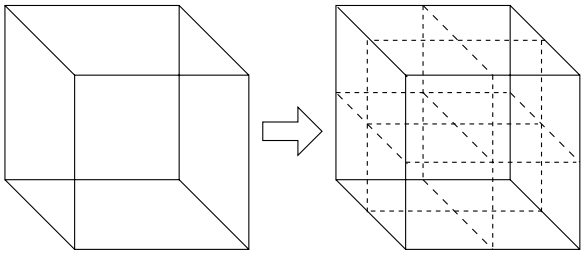

Figure 3. Cell division.

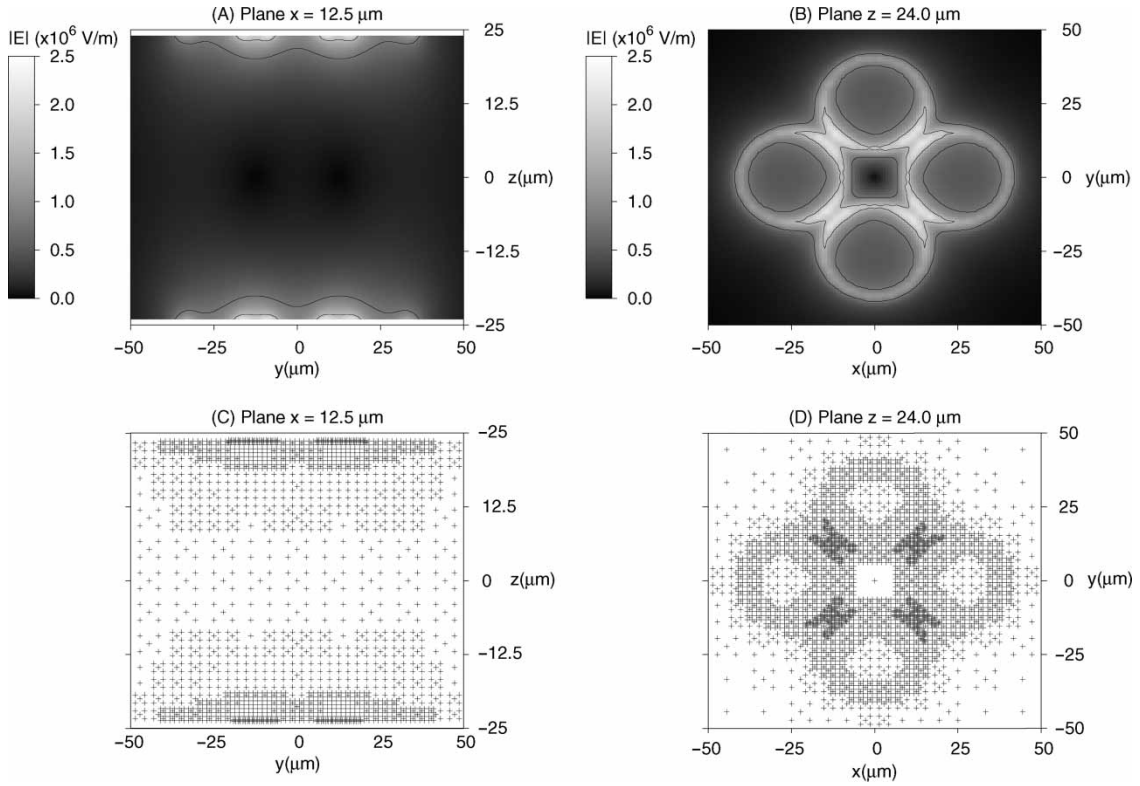

Figure 4. Refined mesh compared to values of the electric field. Notice the refinement in regions of very high field intensity.

after five subdivisions the maximum error, defined as the difference between the contribution of each cell and the average contribution divided by the average contribution, was reduced to 0.5% and a refined mesh containing 96,160 evaluation points was obtained. The clustering of the points reflects the successive levels of refinement.

Notice how the mesh was automatically refined in the areas where the electric field intensity is highest, such as the regions surrounding the electrodes edges. Even with a rough initial mesh and without providing any extra information about the source term the algorithm produces a refined mesh that follows the source term variation across the domain accurately.

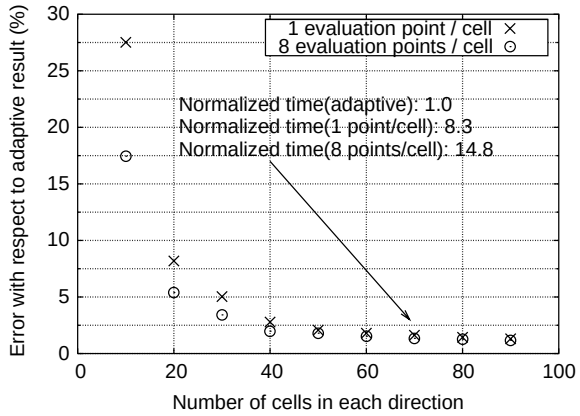

Figure 5. Error in homogeneous mesh integration compared to adaptive case. Results for the homogeneous mesh approach the adaptive result as the mesh is progressively refined.

Figure 5 shows the difference between the results obtained using direct evaluation in homogeneous meshes of increasing sizes and the result from the adaptive version. Notice that a reduction of one order of magnitude in running time can be obtained when the adaptive method is used.

Actual running times for the adaptive integration and the direct evaluations with 1 and 8 nodes per cell were 9 m 35 s, 1 h 15 m 6 s and 2 h 13 m 19 s respectively. Calculations were done on a single 2.4 GHz Opteron processor in a cluster node with 32 Gb of RAM.

The presented method provides a fast and easily implementable method of solving Poisson equations with strongly non-homogeneous source terms in the BEM formulation. There is potential for improvement in the implementation of the adaption algorithm, as cells could be fused together to form larger cells in areas of very small contribution to the integral, reducing the number of evaluation nodes while keeping the quality of the result.

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