Adaptive temperature estimation in 3D single-cell dielectrophoretic traps using the Boundary Element Method

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ABSTRACT

We present an adaptive method for the evaluation of the temperature increase due to Joule heating in single-cell dielectrophoretic 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 to solve Poisson’s equation. It is shown that this method reduces computation times by as much as an order of magnitude compared to direct evaluation methods and is straightforward to implement.

Keywords: Adaptive meshing, BEM, dielectrophoresis, single-cell trap, Poisson equation

1 Introduction

Application of dielectrophoresis techniques [1] to biological particles is limited by the temperature increase of the suspension due to Joule heating [2]. The temperature distribution in these traps can be obtained from a Poisson equation [3]:

\[ \nabla^2 T = -\frac{\sigma |E|^2}{k} \] (1)

where \( \sigma \) 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 Eq. 1 introduces a volume integral in the equations of the Boundary Element Method (BEM). Methods that transform this volume integral into a surface integral are typically more expensive and less accurate than its direct evaluation [4], but even direct integration becomes expensive when the source term is highly non-homogeneous.

This paper presents a adaptive evaluation of the source term which is highly efficient when compared to direct evaluation methods and is straightforward to implement.

2 ELECTRIC FIELD CALCULATION

The electrical problem is solved by using the indirect formulation of the boundary element method [5], based on the equation for the potential \( \phi(\vec{r}) \) given by:

\[ \phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \int_{\Gamma} \frac{q(\vec{r}')}{|\vec{r} - \vec{r}'|} d\Gamma' \] (2)

The boundary conditions used to solve this equation are given potential values at all conductors and continuity of the potential and the normal component of the electric displacement at all dielectric interfaces. See reference [6] for more details on the implementation.

To solve this equation all boundaries are discretized 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 Eq. (2):

\[ \vec{E}(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \int_{\Gamma} \frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|^3} d\Gamma' \] (3)

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

3 TEMPERATURE CALCULATION

The temperature is obtained using the boundary element method as in the previous section, with an additional volume integral due to the source term in Eq. (1):

\[ T(\vec{r}) = \int_{\Gamma} t(\vec{r}') d\Gamma' - \frac{\sigma}{k} \int_{\Omega} \frac{|\vec{E}(\vec{r})|^2}{|\vec{r} - \vec{r}'|^3} d\Omega' \] (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.

Accurate evaluation of the volume integral in Eq. (4) is difficult because the electric field gradient is very high.
in dielectrophoretic 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 Eq. (3), and the whole process becomes computationally very expensive.

### 3.1 Adaption algorithm

The method we propose to solve this 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 Eq. (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 \(1/|\mathbf{r} - \mathbf{r}'|\) 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
- 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 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 1.

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 the lack 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 2. When the integral is calculated in the refined mesh at the next subdivision level the integrand is evaluated at the centers of each of the new eight cells besides the original point marking the center 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 dielectrophoretic 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 center:

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

Figure 3 shows the refined mesh for the case under study. The initial mesh was a set of $10 \times 10 \times 10$ points and after 5 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 96160 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 4: 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 4 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.

The presented method provides a fast and easily implementable method of solving Poisson equations with strongly non-homogeneous source terms in the Boundary Element Method 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.

REFERENCES