A Shift-and-Weight (SAW) Method for Fast Interpolation of Probe Charge Electrostatic Potentials

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INTRODUCTION: For electrostatics problems where charge distributions vary or are unknown (e.g. semiconductors, electro-mechanics), using a Green's functions (elementary solution) method, may be more efficient. The potential is a convolution of the Green's function with the charge distribution:

$$\phi(\mathbf{r}) = \int_{\Omega} \mathrm{d}\mathbf{r}' G(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}')$$

$$\begin{cases} \varepsilon_0 \nabla\left[\varepsilon(\mathbf{r})\nabla G(\mathbf{r},\mathbf{r}')\right] = -\delta(\mathbf{r}-\mathbf{r}'),\ \mathbf{r}\in\Omega \\ G(\mathbf{r},\mathbf{r}') = 0,\ \mathbf{r}\in\delta\Omega_i \end{cases}$$

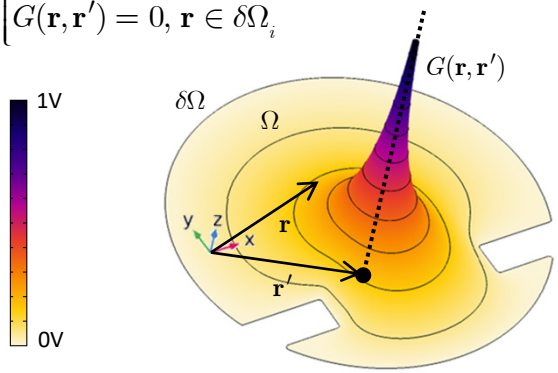

Figure 1. An elementary solution

QUESTION: Given its 6D nature is there an efficient way to compute and store $G(\mathbf{r}, \mathbf{r}')$?

COMPUTATIONAL METHODS:
The proposed **"Shift-and-Weight method" (SAW):**

1. use COMSOL Electrostatics interface (*es*) to compute and store $G(\mathbf{r}, \mathbf{r}_j)$ for a set of probe charge positions $\mathbf{r}_j \in \{\mathbf{r}_1, \mathbf{r}_2, \ldots\}$
2. to approximate elementary solution at a test charge position not in the set $\mathbf{r}' \notin \{\mathbf{r}_1, \mathbf{r}_2, \ldots\}$
   2.1. select 1-4 probe charge positions in the vicinity of the test position
   2.2. shift their elementary solutions to the test position $\mathbf{r}'$, via a displacement map $\mathbf{u}(\mathbf{r}, \mathbf{r}'\text{-}\mathbf{r}_j)$
   2.3. weight (linearly combine) the "shifted" elementary solutions based on distance to the test position $\gamma(\mathbf{r}', \mathbf{r}_j)$

$$\tilde{G}(\mathbf{u}(\mathbf{r},\mathbf{r}'-\mathbf{r}_j),\mathbf{r}') = \sum_j \gamma(\mathbf{r}',\mathbf{r}_j) G(\mathbf{r},\mathbf{r}_j)$$

The weighting functions $\gamma(\mathbf{r}', \mathbf{r}_j)$ are monotonically decreasing, partition of unity functions $\gamma(\mathbf{r}_i, \mathbf{r}_j)=\delta_{ij}$

The displacement (source) map $\mathbf{u}(\mathbf{r}, \mathbf{r}'\text{-}\mathbf{r}_j)$ is implemented as a General Extrusion, using a non-linear ramp function to get a displacement field from $G(\mathbf{r}, \mathbf{r}_j)$ itself

$$\mathbf{u}(\mathbf{r},\mathbf{r}'-\mathbf{r}_j) = \mathbf{r} + f(G(\mathbf{r},\mathbf{r}_j))\cdot(\mathbf{r}'-\mathbf{r}_j)$$

RESULTS: For a simple 2D geometry with two electrodes:

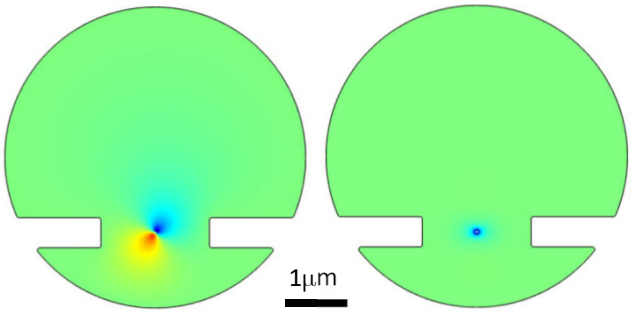

Figure 2. Spatial dependence of the SAW error within the domain with 1 probe charge (left) and 4 probe charges (right)

probe charges	max(|error|) [mV]
1	44.63
2	37.07
3	19.11
4	9.9

Table 1. Max absolute error variation with number of probe charges

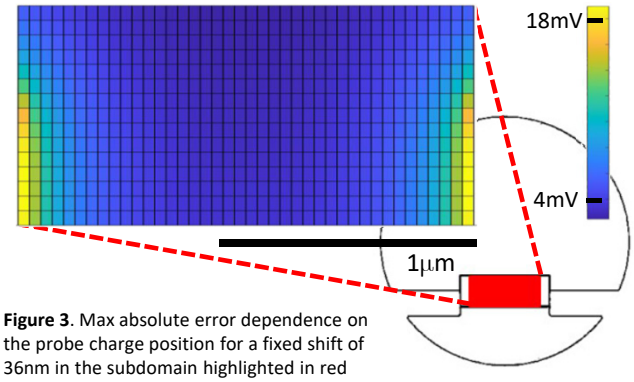

Figure 3. Max absolute error dependence on the probe charge position for a fixed shift of 36nm in the subdomain highlighted in red

dimension	T_{COMSOL} [s]	T_{SAW} [s]	speedup
2D	4.01	0.1	40×
3D	128.8	1.26	102×

Table 2. Computational time for COMSOL simulation vs. SAW method

CONCLUSIONS:

- In the center it is possible to achieve max absolute errors <10mV (1% relative) for shifts of up to 64nm (3% inter-electrode distance).
- Average speedups of 40× (2D) and 102× (3D) were demonstrated

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