Modelling ion motion in perovskite films

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Motivation
In previous work [1], we have used an asymptotic approximation to solve the drift-diffusion equations for ion motion in perovskite films, while others have used finite difference methods. Here, we test the suitability of two different numerical methods - finite difference and spectral - for this challenging problem.

Two of the best methods available in MATLAB for solving partial differential equations, such as the time-dependent drift-diffusion equations, are the built-in function PDEPE and the open-source additional module Chebfun [2].

PDEPE is a finite-difference method that solves the equations on a user-defined mesh with adaptive time step.

Chebfun is a spectral method that solves equations with a spectrum of functions (in this case Chebyshev polynomials) and therefore does not use a mesh. Instead, the user defines the time steps.

Conclusions
1. The spectral method Chebfun can solve the problem for average ion density of up to $3.2 \times 10^{18} \text{cm}^{-3}$ using 5000 time steps
2. Finite difference method is also suitable but sub-nanometre spatial resolution is required to resolve the thin charge accumulation layers correctly
3. Unlike the asymptotic approximation, numerical methods can be used to create a fully coupled model that accounts for the electrostatic effect of electrons and holes. This is very challenging but some preliminary results have been obtained.

Motivation

<table>
<thead>
<tr>
<th>PDEPE</th>
<th>Chebfun</th>
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<tbody>
<tr>
<td>Fast (when it works)</td>
<td>When solution found, it is very accurate</td>
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<tr>
<td>Automatic time stepping</td>
<td>High spatial resolution (no mesh)</td>
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<td>Suitable for very large ion densities (~$10^{19} \text{cm}^{-3}$)</td>
<td>Can work with internal boundary conditions</td>
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<tr>
<td>Inaccurate if insufficient spatial resolution used</td>
<td>Can be slow</td>
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<tr>
<td>Cannot deal with internal boundaries</td>
<td>Careful choice of time step required</td>
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<tr>
<td>Struggles with very large ion densities (&gt;3.5x$10^{18} \text{cm}^{-3}$)</td>
<td>Struggles with very large ion densities</td>
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</tbody>
</table>

Table 1: Advantages and disadvantages of the PDEPE and Chebfun methods.

References