Modelling ion motion in perovskite films

Simon E. J. O'Kane[1], Jamie M. Foster[2], James M. Cave[1], Nicola Courtier[3], Giles Richardson[3] and Alison B. Walker[1]

[1]Department of Physics, University of Bath, BA2 7AY, United Kingdom
[2]Department of Mathematics, University of Portsmouth, PO1 2UP, United Kingdom
[3]Department of Mathematical Sciences, University of Southampton, SO17 1BJ, United Kingdom

Contact: S.E.J.O'Kane@bath.ac.uk, G.Richardson@soton.ac.uk, A.B.Walker@bath.ac.uk

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.

Conclusions

1. The spectral method Chebfun can solve the problem for average ion density of up to 3.2×10^{18} 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

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.

	PDEPE	Chebfun
Advantages	• Fast (when it works) • Automatic time stepping • Suitable for very large ion densities (~10^{19} cm^{-3})	• When solution found, it is very accurate • High spatial resolution (no mesh) • Can work with internal boundary conditions
Disadvantages	• Inaccurate if insufficient spatial resolution used • Cannot deal with internal boundaries	• Can be slow • Careful choice of time step required • Struggles with very large ion densities (>3.5×10^{18} cm^{-3})

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

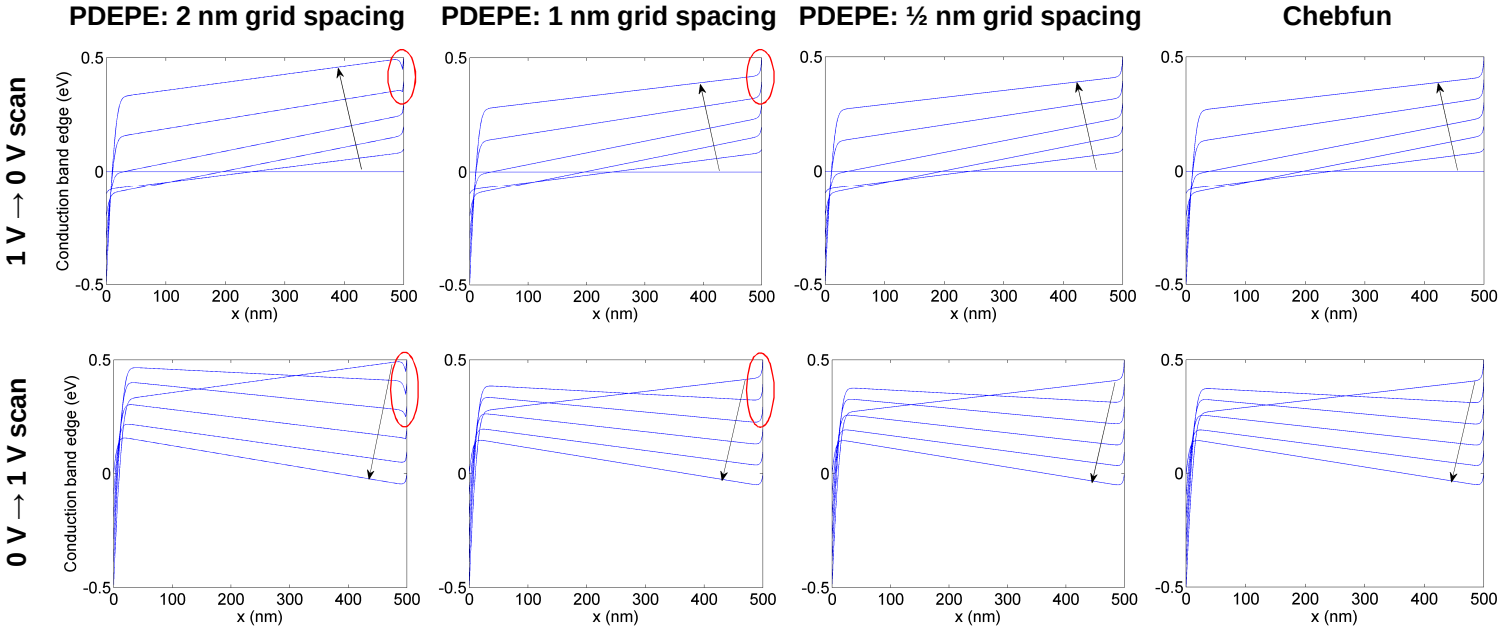

Table 2: *Variation of conduction band minimum $E_C(x)$ across a 500 nm thick perovskite film during a scan from V_{bi} = 1 V to short circuit and back, as calculated using PDEPE with three different values of grid spacing and Chebfun with 5000 time steps. An average ion density of 3.2×10^{18} cm^{-3}, close to the limit of what Chebfun can handle, was assumed. Each line represents a step of 0.2 V; the arrow indicates the direction of increasing time. The results for 1 nm grid spacing, 0.5 nm grid spacing and Chebfun show good agreement, while those for 2 nm grid spacing are different, suggesting 1 nm or smaller grid spacing is required.*

References

[1] G. Richardson, S. E. J. O'Kane, R. G. Niemann, T. A. Peltola, J. M. Foster, P. J. Cameron and A. B. Walker, "Can slow-moving ions explain hysteresis in the current-voltage curves of perovskite solar cells?", *Energy Environ. Sci.*, Vol. 9, 1476-1485, 2016.

[2] T. A. Driscoll, N. Hale and L. N. Trefethen, *Chebfun Guide*, Panufty Publications, Oxford, 2014.