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Optimal control of a class of PDE and state constrained bio-mass transport problems

There is a critical need for optimal protocols for the equilibration of chemical additives necessary for the cryopreservation of cells and tissues. Cells must be equilibrated with high concentrations of permeating chemicals (CPAs) before the cooling process, and this must be reversed after warming. This problem is well suited for mathematical optimization because the concomitant osmotically induced volume fluxes contribute to potential sources of cell damage that define state constraints, there is a time-dependent toxicity to these high concentrations that defines a cost functional, and the transport of water and solutes across cell membranes is well described by a nonlinear system of ordinary differential equations. If we view extracellular concentrations of these additives as controls, these pieces of the problem can be combined to formulate a state constrained optimal control problem. We have previously defined analytical time optimal controls for a two-solute system that governs transport across single-cell membranes that has driven exciting new applications in the field of cryopreservation. Here we develop new theory to extend the optimization to an arbitrary number of solutes. Next, we note that these optimal controls cannot, in application, be achieved at the cell membrane. In light of this, we present a theory of how to extend optimal controls away from the cell membrane by using inverse-problem techniques to solve the associated PDE constrained nonlinear optimal control problem with state constraints. Finally, we provide several real-world examples.