Utility of super-time-stepping for electroanalytical digital simulations by explicit finite difference methods. Part 1: spatially one-dimensional models

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Utility of super-time-stepping for electroanalytical digital simulations by explicit finite difference methods. Part 1: spatially one-dimensional models

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Abstract

Super-time-stepping denotes a class of special strategies of choosing nonuniform time steps in finite-difference solutions of partial differential equations by conditionally stable explicit techniques, that allow one to effectively overcome limits of numerical stability. This is achieved by demanding the stability only at ends of certain sequences of time steps, called supersteps. The utility of one variant of the super-time-stepping is examined, for digital simulations of electroanalytical experiments described by reaction-diffusion partial differential equations in one-dimensional space geometry. The tests focus on example models of chronoamperometry and cyclic voltammetry. Reductions of computational times, and improvements of the efficiency of such simulations are observed. Implementation of the super-time-stepping requires only minor changes in computer programs for conventional explicit simulation methods. Super-time-stepping can be combined both with sequential and parallel computations, but it should be of particular interest in connection with the efforts towards parallelisation of electroanalytical simulations

Keywords: super-time-stepping, digital simulation, computational electrochemistry, chronoamperometry, cyclic voltammetry

1. Introduction

Over the past 60 years, digital simulation [1–6] has become an indispensable research tool serving for the theoretical modelling of transient electroanalytical experiments [7]. Such simulations most often consist in numerically solving systems of partial differential equations (PDEs) of the reaction-diffusion type. Among various numerical techniques, finite difference methods [8–10] are frequently employed. The application of the finite difference digital simulations

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