

Zhu, Wanwan; Yang, Ying; Ji, Guanghua; Lu, Benzhuo

Residual type a posteriori error estimates for the time-dependent Poisson-Nernst-Planck equations. (English) [Zbl 07444772](#)

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Summary: This paper investigates the residual type a posteriori error estimators for a fully discrete approximation to the solution of the time-dependent Poisson-Nernst-Planck equations, which are widely used to describe the electrodiffusion of ions in biomolecular solutions. The backward Euler scheme is used for the discretization in time and the continuous, piecewise linear triangular finite elements are applied to the space discretization. The main results consist in building error estimators and deriving computable upper and lower bounds on the error estimators. Some numerical experiments confirm the theoretical predictions and show the reliability and efficiency of the error estimators.

MSC:

65N15 Error bounds for boundary value problems involving PDEs

65N30 Finite element, Rayleigh-Ritz and Galerkin methods for boundary value problems involving PDEs

Keywords:

Poisson-Nernst-Planck equations; residual type a posteriori error estimators; adaptive finite element method; backward Euler scheme

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References:

- [1] Adams, RA, Sobolev Spaces (1975), New York: Academic Press, New York · [Zbl 0314.46030](#)
- [2] Ainsworth, M., Oden, J.T.: A Posteriori Error Estimation in Finite Element Analysis. Wiley (2000) · [Zbl 1008.65076](#)
- [3] Akrivis, G.; Makridakis, C.; Nochetto, R., A posteriori error estimates for the Crank-Nicolson method for parabolic equations, Math. Comput., 75, 254, 511-531 (2005) · [Zbl 1101.65094](#)
- [4] Araya, R.; Venegas, P., An a posteriori error estimator for an unsteady advection-diffusion-reaction problem, Comput. Math. Appl., 66, 12, 2456-2476 (2014) · [Zbl 1368.65186](#)
- [5] Babuška, I.; Durán, R.; Rodríguez, R., Analysis of the efficiency of an a posteriori error estimator for linear triangular finite elements, SIAM J. Numer. Anal., 29, 4, 947-964 (1992) · [Zbl 0759.65069](#)
- [6] Babuška, I.; Rheinboldt, C., Error estimates for adaptive finite element computation, SIAM J. Numer. Anal., 44, 4, 75-102 (1978) · [Zbl 0398.65069](#)
- [7] Bänsch, E.; Karakatsani, F.; Makridakis, CG, A posteriori error estimates for fully discrete schemes for the time dependent Stokes problem, Calcolo, 55, 19 (2018) · [Zbl 1395.65057](#)
- [8] Bergam, A.; Bernardi, C.; Mghazli, Z., A posteriori analysis of the finite element discretization of some parabolic equations, Math. Comput., 74, 251, 1117-1139 (2004) · [Zbl 1072.65124](#)
- [9] Bernardi, C.; Verfürth, R., A posteriori error analysis of the fully discretized time-dependent Stokes equations, SeMA J., 38, 3, 437-455 (2004) · [Zbl 1079.76042](#)
- [10] Bessemoulin-chatard, M.; Chainais-hillairet, C.; Vignal, M., Study of a fully implicit scheme for the drift-diffusion system. Asymptotic behavior in the quasi-neutral limit, SIAM J. Numer. Anal., 52, 4, 1666-1691 (2013) · [Zbl 1305.65191](#)
- [11] Bi, C.; Wang, C.; Lin, Y., A posteriori error estimates of two-grid finite element methods for nonlinear elliptic problems, J. Sci. Comput., 74, 1, 23-48 (2018) · [Zbl 1398.65270](#)
- [12] Bolintineanu, DS; Sayyed-Ahmad, A.; Davis, HT; Kaznessis, YN, Poisson-Nernst-Planck models of nonequilibrium ion electrodiffusion through a protegrin transmembrane pore, PLoS Comput. Biol., 5, 1, e1000277 (2009)
- [13] Braess, D.; Pillwein, V.; Schöberl, J., Equilibrated residual error estimates are (p) -robust, Comput. Methods Appl. Mech. Eng., 198, 1189-1197 (2009) · [Zbl 1157.65483](#)
- [14] Brenner, SC; Scott, LR, The Mathematical Theory of Finite Element Methods (1994), New York: Springer, New York · [Zbl 0804.65101](#)
- [15] Brezzi, F.; Marini, LD; Pietra, P., Numerical simulation of semiconductor devices, Comput. Methods Appl. Mech. Eng., 75, 1-3, 493-514 (1989) · [Zbl 0698.76125](#)

- [16] Cárdenas, AE; Coalson, RD; Kurnikova, MG, Three-dimensional Poisson-Nernst-Planck theory studies: influence of membrane electrostatics on gramicidin a channel conductance, *Biophys. J.*, 79, 1, 80-93 (2000)
- [17] Chainais-Hillairet, C.; Peng, YJ, Finite volume approximation for degenerate drift-diffusion system in several space dimensions, *Math. Models Methods Appl. Sci.*, 14, 3, 461-481 (2004) · [Zbl 1127.65319](#)
- [18] Chen, ZM; Ji, GH, Sharp (L^1) a posteriori error analysis for nonlinear Convection-Diffusion Problems, *Math. Comput.*, 75, 253, 43-71 (2006) · [Zbl 1107.65080](#)
- [19] Chen, Z.M., Wu, H.J.: *Selected Topics in Finite Element Methods*. Science Press (2010)
- [20] Ciucci, F.; Lai, W., Derivation of micro/macro lithium battery models from homogenization, *Transp. Porous Med.*, 88, 2, 249-270 (2011)
- [21] Clément, P., Approximation by finite element functions using local regularization, *RAIRO Anal. Numer.*, 9, 7-84 (1975) · [Zbl 0368.65008](#)
- [22] Coalson, RD; Kurnikova, MG, Poisson-Nernst-Planck theory approach to the calculation of current through biological ion channels, *IEEE Trans. Nanobiosci.*, 4, 1, 81-93 (2005)
- [23] Flavell, A.; Machen, M.; Eisenberg, B.; Kabre, J.; Liu, C.; Li, X., A conservative finite difference scheme for Poisson-Nernst-Planck Equations, *J. Comput. Electron.*, 13, 1, 235-249 (2014)
- [24] Gajewski, H.; Gröger, K., On the basic equations for carrier transport in semiconductors, *J. Math. Anal. Appl.*, 113, 1, 12-35 (1986) · [Zbl 0642.35038](#)
- [25] Gao, HD; He, DD, Linearized conservative finite element methods for the Nernst-Planck-Poisson equations, *J. Sci. Comput.*, 72, 3, 1269-1289 (2017) · [Zbl 1378.65168](#)
- [26] Guignard, D.; Nobile, F.; Picasso, M., A posteriori error estimation for elliptic partial differential equations with small uncertainties, *Numer. Methods Partial Differ. Equ.*, 32, 1, 175-212 (2016) · [Zbl 1350.65007](#)
- [27] He, D.; Pan, K., An energy preserving finite difference scheme for the Poisson-Nernst-Planck system, *Appl. Math. Comput.*, 287, 214-223 (2016) · [Zbl 1410.65311](#)
- [28] Jerome, J., *Analysis of Charge Transport: A Mathematical Theory and Approximation of Semiconductor Models* (1996), New York: Springer, New York
- [29] Lakkis, O.; Makridakis, C., Elliptic reconstruction, and a posteriori error estimates, for fully discrete linear parabolic problems, *Math. Comput.*, 75, 256, 1627-1658 (2006) · [Zbl 1109.65079](#)
- [30] Liu, HL; Wang, ZM, A free energy satisfying finite difference method for Poisson-Nernst-Planck equations, *J. Comput. Phys.*, 268, 2, 363-376 (2014) · [Zbl 1349.65317](#)
- [31] Lu, BZ; Holst, MJ; McCammond, JA; Zhou, YC, Poisson-Nernst-Planck equations for simulating biomolecular diffusion-reaction processes I: finite element solutions, *J. Comput. Phys.*, 229, 19, 6979-6994 (2010) · [Zbl 1195.92004](#)
- [32] Lu, BZ; Zhou, YC; Holst, MJ; McCammon, JA, Recent progress in numerical methods for the Poisson-Boltzmann equation in biophysical applications, *Commun. Comput. Phys.*, 3, 5, 973-1009 (2008) · [Zbl 1186.92005](#)
- [33] Marcicki, J.; Conlisk, AT; Rizzoni, G., Comparison of limiting descriptions of the electrical double layer using a simplified lithium-ion battery model, *ECS Trans.*, 41, 14, 9-21 (2012)
- [34] Mathur, SR; Murthy, JY, A multigrid method for the Poisson-Nernst-Planck equations, *Int. J. Heat Mass Transf.*, 52, 17, 4031-4039 (2009) · [Zbl 1167.76343](#)
- [35] Nernst, W., The electromotive effect of the ions, *Z. Phys. Chem.*, 4, 129-181 (1889)
- [36] Nicaise, S.; Soualem, N., A posteriori error estimates for a nonconforming finite element discretization of the time-dependent Stokes problem II: Analysis of the spatial estimator, *J. Numer. Math.*, 15, 2, 137-162 (2007) · [Zbl 1123.76033](#)
- [37] Picasso, M., Adaptive finite elements for a linear parabolic problem, *Comput. Methods Appl. Mech. Eng.*, 167, 3-4, 223-237 (1998) · [Zbl 0935.65105](#)
- [38] Picasso, M.; Prachittham, V., An adaptive algorithm for the Crank-Nicolson scheme applied to a time-dependent convection-diffusion problem, *J. Comput. Appl. Math.*, 233, 1139-1154 (2009) · [Zbl 1181.65113](#)
- [39] Planck, M., On the excitation of electricity and heat in electrolyte, *Ann. Phys.*, 275, 2, 161-186 (1890)
- [40] Richardson, G.; King, JR, Time-dependent modelling and asymptotic analysis of electrochemical cells, *J. Eng. Math.*, 59, 3, 239-275 (2007) · [Zbl 1125.92066](#)
- [41] Rocchia, W.; Alexov, E.; Honig, B., Extending the applicability of the nonlinear Poisson-Boltzmann equation: multiple dielectric constants and multivalent ions, *J. Phys. Chem. B*, 105, 28, 6507-6514 (2001)
- [42] Shen, RG; Shu, S.; Yang, Y.; Lu, BZ, A decoupling two-grid method for the time-dependent Poisson-Nernst-Planck equations, *Numer. Anal.*, 83, 1613-1651 (2020) · [Zbl 1436.65189](#)
- [43] Singer, A.; Norbury, J., A Poisson-Nernst-Planck model for biological ion channels-an asymptotic analysis in a three-dimensional narrow funnel, *SIAM J. Appl. Math.*, 70, 3, 949-968 (2009) · [Zbl 1197.34080](#)
- [44] Sun, YZ; Sun, PT; Zheng, B.; Lin, G., Error analysis of finite element method for Poisson-Nernst-Planck equations, *J. Comput. Appl. Math.*, 301, 28-43 (2016) · [Zbl 1382.65326](#)
- [45] Tu, B.; Chen, M.; Xie, Y., A parallel finite element simulator for ion transport through three-dimensional ion channel systems, *J Comput. Chem.*, 34, 24, 2065-2078 (2013)
- [46] Verfürth, R., A posteriori error estimates for finite element discretizations of the heat equation, *Calcolo*, 40, 3, 195-212 (2003) · [Zbl 1168.65418](#)

- [47] Verfürth, R.: A Posteriori Error Estimation Techniques for Finite Element Methods. Oxford University Press (2013) · [Zbl 1279.65127](#)
- [48] Xie, Y.; Cheng, J.; Lu, BZ, Parallel adaptive finite element algorithms for solving the coupled electro-diffusion equations, *Mol. Based Math. Biol.*, 1, 90-108 (2013) · [Zbl 1276.35143](#)
- [49] Yang, Y.; Lu, BZ, An error analysis for the finite element approximation to the steady-state Poisson-Nernst-Planck equations, *Adv. Appl. Math. Mech.*, 5, 1, 113-130 (2013) · [Zbl 1262.65182](#)
- [50] Yang, Y.; Tang, M.; Liu, C.; Zhou, LQ, Superconvergent gradient recovery for nonlinear Poisson-Nernst-Planck equations with applications to the ion channel problem, *Adv. Comput. Math.* (2020) · [Zbl 1465.65148](#) · [doi:10.1007/s10444-020-09819-6](#)
- [51] Yang, Y.; Zhou, AH, Local averaging based a posteriori finite element error control for quasilinear elliptic problems with application to electrical potential computation, *Comput. Methods Appl. Mech. Eng.*, 196, 1-3, 452-465 (2006) · [Zbl 1121.65367](#)
- [52] Yan, NN; Zhou, AH, Gradient recovery type a posteriori error estimates for finite element approximations on irregular meshes, *Comput. Methods Appl. Mech. Eng.*, 190, 32-33, 4289-4299 (2001) · [Zbl 0986.65098](#)
- [53] Yan, NN; Zhou, ZJ, A posteriori error estimates of constrained optimal control problem governed by convection diffusion equations, *Front. Math. China*, 3, 3, 415-442 (2008) · [Zbl 1158.65046](#)
- [54] Ye, X., A posteriori error estimate for finite volume methods of the second order elliptic problem, *Numer. Methods Partial Differ. Equ.*, 27, 1165-1178 (2011) · [Zbl 1227.65104](#)

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