Journal of Solid State Electrochemistry (2024) 28:911–920
https://doi.org/10.1007/s10008-023-05457-2

FEATURE ARTICLE

While educating electrochemists, do not forget we live in a computer era

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Received: 19 January 2023 / Revised: 6 March 2023 / Accepted: 7 March 2023 / Published online: 18 March 2023

Abstract
The appearance of computers has led to considerable changes in research practices of natural sciences, including electrochemistry. The current status of the computerization in electrochemistry is briefly discussed, with the conclusion that the progress in this area is not as fast as in other natural science disciplines. Some postulates are formulated, referring to the education of young generations of electrochemists, that might bring improvements.

Keywords Theoretical electrochemistry · Computational electrochemistry · Simulation · Computational science · Education

Electrochemistry is a natural science. Any natural science requires a balanced interaction of physical experiments and theoretical modelling, as its basic operational methods. A purely "experimental" natural science does not exist. But for the last seven decades or so, a third operational method, computer experiments, has come into play as well. Apart from this, the appearance of computers has offered unprecedented possibilities for automating, intensifying, and improving the reliability of diverse research practices. This gave rise to new research areas, usually called "computational physics," "computational chemistry," etc. As a result, we witness a methodological revolution that some call "a second metamorphosis of science" [1].

The new research areas ("computational physics," "computational chemistry," etc.) are, in part, counterparts of the traditional "experimental physics," "theoretical physics," "experimental chemistry," "theoretical chemistry," etc., focused on computer experimenting, although they are not entirely separable from "theoretical physics," theoretical chemistry," etc. However, they are also perceived as interdisciplinary fields (involving physics, chemistry, etc., together with elements of mathematics and computer science), which jointly form what is now called "computational science," according to the emerging definition (see, for example, [2–4]).

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I have devoted most of the 42 years of my professional life to the efforts to introduce modern computational (and more generally computer-aided) methods to the practices of electroanalytical chemistry. My intention is to contribute to the creation of computational electrochemistry as a full-fledged area of study, understood as a part of computational science related to electrochemistry, and consistent with the aforementioned definition of computational science [2–4]. Hence, in my work, and in the present note, I perceive computational electrochemistry as an interdisciplinary field, involving not merely simple uses of computers, computer programs, and/or computational methods in electrochemistry, but also an active development of computer-aided methods, algorithms, programs, or other tools, aimed at solving diverse problems occurring in the electrochemical research [5]. I also argue [6] that computational electrochemistry should unify all kinds of computations occurring in electrochemistry: quantum computations, molecular computations, as well as those based on the assumption of continuity of matter—the latter are typical for formal electrochemical kinetics, in which I am particularly interested.

When 20 years ago I published my research program for (such understood) computational electrochemistry, with a focus on electroanalytical chemistry [5], the perspectives seemed bright. There were plenty of computer-based methods and approaches available in the non-electrochemical literature. One could be optimistic about applying them to (or adjusting them to the needs of) electroanalytical chemistry, thereby pulling out the methodology of electroanalytical chemistry from the misery of pre-computer times. One could also expect an outburst of publications dealing with an interdisciplinary development of new, computer-based approaches to studying electrochemical phenomena. Now, when the end of the first quarter of the twenty-first century is approached, one can ask if these hopes have become a reality and how the present situation in this respect might be related to the education of electrochemists.

Some answers to this question should be obtainable by comparing the temporal changes in the numbers of publications dealing with the theories and computer simulations or other computational activities in electrochemistry and remaining natural sciences. Modern literature databases, such as Scopus [7], offer some tools that can help obtaining such information. The tools are not perfect—their main disadvantage is that they "don't understand" the intentions of their users (a true artificial intelligence still does not exist). Any database search based on the occurrences of certain keywords will obviously not find a publication that does not contain the keywords, even if the subject of the publication is closely related. Therefore, the results of such searches are likely to be incomplete or biased. Nevertheless, I have performed several Scopus searches, in the hope of obtaining at least some guidance. The searches were for the following keywords or keyword combinations: DISCIPLINE, DISCIPLINE AND THEORY, DISCIPLINE AND SIMULATION, and for the phrase "COMPUTATIONAL DISCIPLINE," where DISCIPLINE stands for PHYSICS, CHEMISTRY, BIOLOGY, or ELECTROCHEMISTRY. These keywords or phrases were searched within publication titles, abstracts, and author-declared keywords. I assumed that the papers containing the keyword DISCIPLINE form a representative sample of the papers published in a given discipline and that the number of such papers is proportional to the total number of papers in a given discipline, with a proportionality coefficient identical for all disciplines. In the further text, these two sets of papers are assumed to be equivalent, for simplicity. Additional keywords (such as THEORY or SIMULATION) then allow one to identify theoretical papers or papers dealing with simulations in a given discipline. Such assumptions might be criticized, but I often observe that research areas to which some Scopus tools automatically attribute publications are completely wrong. Of course, one has to be aware of the multiplicity of meanings the words such as THEORY or SIMULATION may have. In particular, THEORY may not necessarily mean a "hard" theory (or model) based on rigorous, mathematically formulated laws of nature; it may also mean a "soft" theory (or model) based on heuristic concepts. But such "soft" theories or models are often useful and should not be deprecated or ignored (see, for example, [8, 9]). The word SIMULATION also possesses numerous meanings and definitions (see, for example, [10, 11]).

Tables 1, 2, 3, and 4 contain absolute numbers of papers containing the above keywords or phrases, published in successive years between 1970 and 2021. As the tables reveal, all these absolute numbers of papers tend to grow from year to year (on average), because of the overall growth of the number of scientific publications. Therefore, instead of comparing absolute numbers of papers containing particular keywords, it is more informative to compare relative numbers, obtained by normalizing the absolute numbers with the total numbers of papers published in a given year in a given scientific discipline. Figures 1, 2, and 3 present such relative numbers of papers.

As can be seen in Fig. 1, the relative numbers of papers containing ELECTROCHEMISTRY AND THEORY are comparable to the relative numbers of papers containing CHEMISTRY AND THEORY and BIOLOGY AND THEORY but are about three times smaller than the relative numbers of papers containing PHYSICS AND THEORY. Furthermore, the relative numbers of theoretical electrochemical papers seem to have increased somewhat over the past 10 years or so, whereas other theoretical disciplines do not exhibit such a trend. This is surprising for me, as my subjective impression resulting from the inspection of basic electrochemical journals is that theoretical papers have been recently rather rare, at least in the domain of the theory of electroanalytical methods. But from Fig. 1, one might conclude that there is no reason to worry about theoretical electrochemistry, which performs comparably to theoretical chemistry and theoretical biology. The dominant position of theoretical physics can be attributed to the fact that this is an old and mature field, in which theorizing is of particular value with consequences for all sciences.

To a less positive conclusion leads an analogous comparison of the relative numbers of papers containing DISCIPLINE AND SIMULATION (cf. Figure 2). One can see a distinct reduction of the relative number of papers containing ELECTROCHEMISTRY AND SIMULATION over the recent decade, placing electrochemistry in the last position among the scientific disciplines considered. In all remaining disciplines an opposite, systematic growth of the relative number of simulation papers is observed. This finding agrees with my subjective impression (but again referring mostly to the modelling of electroanalytical methods) that the population of electrochemists willing to engage in the development of computer simulation approaches has decreased in recent years and currently involves only a few research groups and individuals. In addition, those who remained are often already retired or likely to retire soon.

The comparison of relative numbers of papers containing the phrase "COMPUTATIONAL DISCIPLINE," presented in Fig. 3, puts electrochemistry in an even worse position. The use of the phrase "COMPUTATIONAL ELECTROCHEMISTRY" is currently marginal, compared to "COMPUTATIONAL PHYSICS" and "COMPUTATIONAL CHEMISTRY," and

Table 1 Absolute numbers of papers containing the keywords or keyword combinations: PHYSICS, PHYSICS AND THEORY, PHYSICS AND SIMULATION, COMPUTATIONAL PHYSICS, published between 1970 and 2021

Year	PHYSICS	PHYSICS AND THEORY	PHYSICS AND SIMULATION	COMPUTATIONAL PHYSICS
2021	29,054	4909	5808	113
2020	27,653	4500	5206	102
2019	29,125	4637	5399	97
2018	26,504	4409	4915	82
2017	26,171	4569	4729	72
2016	25,463	4584	4412	73
2015	23,886	4390	4280	64
2014	27,475	4308	4453	75
2013	36,129	5294	5618	65
2012	51,510	7138	7682	61
2011	46,523	6535	7007	53
2010	45,359	5959	6760	53
2009	46,732	6292	6824	58
2008	45,188	6797	6247	29
2007	40,155	6161	5450	51
2006	40,460	6621	5024	37
2005	35,537	6320	4867	32
2004	16,826	3967	2617	23
2003	14,755	3619	1913	22
2002	19,164	3684	2076	37
2001	18,573	3415	1917	28
2000	18,942	3174	1933	16
1999	18,065	2635	1888	25
1998	17,533	2641	1827	13
1997	16,426	2550	1722	21
1996	16,198	2485	1544	21
1995	17,046	2189	1492	13
1994	11,766	2064	1385	10
1993	10,511	1599	938	13
1992	8798	1426	871	7
1991	8149	1441	729	7
1990	6869	1095	584	5
1989	7134	1007	507	18
1988	6237	916	377	4
1987	6897	1079	328	13
1986	6523	1036	322	18
1985	7649	1302	354	12
1984	6300	1063	262	4
1983	5490	862	227	1
1982	5490	891	165	2
1981	5144	895	124	2
1980	4914	841	146	2
1979	4664	766	134	3
1978	4204	738	89	3
1977	4044	774	76	2
1976	4185	777	84	2
1975	3874	669	81	2
1974	5963	873	77	2
1973	5361	740	57	1
1972	3793	439	28	3
1971	3649	438	27	3
1970	4283	602	24	1

about two orders of magnitude less frequent (in electrochemistry) than the use of the phrase "COMPUTATIONAL BIOLOGY" (in biology), which exhibits an extraordinary systematic growth of popularity from year to year. The number of papers thematically related to computational electrochemistry is surely bigger than the number of those containing the phrase "COMPUTATIONAL ELECTROCHEMISTRY." But apparently, their authors do not consider it important to label them with the phrase. This suggests that the authors do not view computational electrochemistry as a distinct area of research, with which they can identify themselves. It is also pertinent to notice that out of the electrochemical journals, only one (Electrochemistry Communications) officially declares publishing papers related to computational electrochemistry and that according to Scopus, during the entire period of existence of Electrochemistry Communications, the journal published merely 5 papers containing the phrase "COMPUTATIONAL ELECTROCHEMISTRY," between 1999 and 2007.

In my opinion, the above findings indicate that among the scientific disciplines considered, electrochemistry is the least advanced one, in the process of adopting computational and computer-aided research practices. Computational electrochemistry, in its present state, has not yet been integrated with the mainstream of computational science. The electrochemical community shows also a considerable inability, to accept changes in this respect. Even if the numbers of papers obtained by Scopus are not exact, they are surely meaningful in illustrating the "cultural" differences between electrochemistry and other natural science disciplines, in dealing with the computer revolution.

One can provide other arguments to support my opinion. As in my youth I studied physics, I always felt uncomfortable when confronted with some customary practices in electrochemistry. Every student of physics learns (usually in the first semester of the studies) that physical experiments should always be repeated many times, and their results averaged and/or subject to some other statistical analysis. Statistical methods serving for such purposes are currently available in numerous computer programs, and they were even built into some computer languages, such as Python or R. However, typical electroanalytical experiments (such as cyclic voltammetry and chronoamperometry) are rarely (if ever) repeated more than once. Furthermore, the analysis of experimental responses is often limited to selected data points on the recorded responses

Table 2 Absolute numbers of papers containing the keywords or keyword combinations: CHEMISTRY, CHEMISTRY AND THEORY, CHEMISTRY AND SIMULATION, COMPUTATIONAL CHEMISTRY, published between 1970 and 2021

Year	CHEMISTRY	CHEMISTRY AND THEORY	CHEMISTRY AND SIMULATION	COMPUTATIONAL CHEMISTRY
2021	127,512	6636	11,784	1230
2020	146,963	6417	12,256	1179
2019	156,690	5871	12,043	1014
2018	151,105	5892	10,958	994
2017	147,085	5712	10,429	910
2016	148,862	7167	11,192	879
2015	161,413	6724	9612	664
2014	142,717	6543	6979	708
2013	113,489	6119	5968	643
2012	104,043	5934	5691	702
2011	97,423	5045	5481	490
2010	93,357	4667	5130	378
2009	83,079	4432	6019	291
2008	76,970	3232	3491	271
2007	63,963	2944	3467	222
2006	60,222	3223	3164	270
2005	55,829	2610	2352	178
2004	46,796	1890	1721	175
2003	41,698	1694	1705	140
2002	45,361	1279	1099	108
2001	35,705	1067	979	112
2000	28,196	714	808	97
1999	23,240	545	750	89
1998	20,927	567	645	72
1997	19,399	578	640	85
1996	18,172	448	507	62
1995	19,124	436	418	34
1994	18,430	474	374	50
1993	17,921	435	309	30
1992	17,639	384	313	28
1991	16,594	291	209	20
1990	14,016	249	178	15
1989	10,903	237	129	8
1988	9869	220	103	12
1987	9383	220	119	4
1986	10,155	278	103	6
1985	11,904	299	100	3
1984	12,271	240	61	0
1983	11,348	222	69	2
1982	10,484	181	34	0
1981	8845	169	43	2
1980	9232	197	40	1
1979	8947	172	34	0
1978	8152	162	23	0
1977	8072	136	33	1
1976	7338	150	21	0
1975	6725	137	18	1
1974	6945	129	15	0
1973	6882	133	13	0
1972	7261	110	16	0

Table 2 (continued)

Year	CHEMISTRY	CHEMISTRY AND THEORY	CHEMISTRY AND SIMULATION	COMPUTATIONAL CHEMISTRY
1971	8213	153	10	0
1970	8944	120	9	0

(for example, one only analyzes a cyclic voltammetric peak height or potential), the rest of the collected data, together with its information content, being ignored. Ironically, such a practice seems to be considered by some electrochemical experts as a standard or most desirable way of analyzing the experimental data. Reviewers of my papers dealing with the theory and computational aspects of electroanalytical experiments regularly urge me to provide "diagnostic criteria" serving for theoretical model discriminations or parameter determinations. But the concept of the "diagnostic criteria" dates back to the pre-computer era, when the storage and analysis of experimental results were technically difficult, and some "quick and dirty" methods of obtaining conclusions were needed. For example, plotting a voltammetric peak height as a function of the potential sweep rate was a diagnostic criterion enabling an identification of reversible charge transfers. Today, using such "quick and dirty" data analysis methods makes little sense, as the experimental data is normally obtained in digital form, and a plethora of robust computer-aided data analysis methods applicable to digital data are available, such as (for example) multiparameter/multiresponse fitting, possibly supported by sensitivity analysis [12–14], Bayesian inference [14], bootstrap resampling [15], or (recently extremely fashionable in the computer science world) model identification based on machine learning [14, 16]. Although such modern techniques are addressed sometimes in the electrochemical literature, as the above references prove, their use is still rather sporadic.

In the nineties of the past century, there were some efforts to create simulation environments for electroanalytical chemistry, some of which were supplied with data analysis algorithms. I would mention here, in particular, EASIEST [17], ELSIM [18], and DigiSim [19]. There were a few more, but out of all these programs, only DigiSim (currently called DigiElch) remained at the battlefield until today, having a fairly large number of users, and it has also been used for teaching [20]. The users of DigiSim/DigiElch benefit from automatic parameter estimation routines. However, one may not be so sure whether the users understand these routines [21]. A worrying aspect also is that in spite of the enormous progress in the scientific software technology, that occurred since those times, the present activity in the area of the development of this type of programs appears rather minor. This situation contrasts with the fact that the development of "problem-solving environments for computational science" is formulated to be a crucial research goal for computational science [22].

In addition, there exist spectacular computer-based research technologies, invented outside electrochemistry, and apparently not ever applied in electrochemistry. One of them are "robot scientists" [23] capable of automatically proposing research hypotheses and performing relevant experiments. The robot scientists have proven effective in drug design investigations, which in some aspects resemble typical electrochemical investigations. In both scientific areas, there often occurs a recursive sequence of experiments and theoretical model adjustments, which may well be dedicated to a robot, thereby releasing human investigators from tedious routine actions.

Summing up, I would argue that the present status of computational electrochemistry is far from satisfactory. There is a question what could be done to improve this situation. In my opinion, young generations of electrochemists should be more comprehensively (than thus far) educated in this area. They should also be prepared for (and encouraged in) undertaking interdisciplinary investigations between electrochemistry and widely understood computational science. It is illusory to expect (as some may do) that experts from other scientific disciplines (such as mathematics or computer science) will produce relevant algorithms and tools to be used by electrochemists. From my experience, such externals experts are uninterested in electrochemistry and its problems. Even scientific journals devoted to mathematics, numerical methods, computational science, and computer science are not willing to consider and publish papers related to electrochemical applications, as they perceive such papers as too specialized or incorrectly classify them as related to engineering areas. However, mathematical problems pertinent to electroanalytical chemistry are unique in many aspects; for example, they often involve reaction–diffusion systems with complicated boundary conditions not encountered in any other areas of science. Hence, they should be of interest to mathematicians and computational scientists, who need challenging examples for their studies of various methods and algorithms. But the currently marginal intellectual transfer between electrochemistry, mathematics, and computational science leaves such problems largely unknown outside electrochemistry, so that mathematicians keep using old and much less interesting examples from the more commonly known areas, such as e.g. heat transfer studies.

Hence, I believe a considerable effort must be undertaken by the electrochemical community, and this calls for adequate educational curricula. All those who intend to work in the area of traditional electrochemical experiments and investigations should be better educated about the existing computer-aided methods and techniques and about benefits of computer experiments or simulations. This postulate is consistent with the earlier observation [24] of shortcomings in these aspects of the education of electrochemists. But in the first place, I would suggest creating new kinds of interdisciplinary studies, with the aim of

Table 3 Absolute numbers of papers containing the keywords or keyword combinations: BIOLOGY, BIOLOGY AND THEORY, BIOLOGY AND SIMULATION, COMPUTATIONAL BIOLOGY, published between 1970 and 2021

Year	BIOLOGY	BIOLOGY AND THEORY	BIOLOGY AND SIMULATION	COMPUTATIONAL BIOLOGY
2021	46,835	1559	2295	7505
2020	42,721	1714	2418	6702
2019	42,156	1616	2363	6804
2018	40,170	1681	2236	6003
2017	39,529	1634	2126	5828
2016	38,830	1651	2175	5617
2015	37,972	1607	2194	5449
2014	40,171	1651	2093	5139
2013	41,483	1579	1997	4333
2012	40,431	1663	2038	4403
2011	38,657	1708	2037	4005
2010	36,589	1716	1757	3925
2009	33,452	1913	1576	4016
2008	30,382	1294	1494	3039
2007	28,570	1245	1279	2788
2006	28,070	1105	1147	2657
2005	26,566	801	820	2547
2004	18,418	724	587	2098
2003	16,558	577	464	1247
2002	14,322	447	313	1011
2001	11,611	407	269	660
2000	9611	333	242	407
1999	8822	273	192	234
1998	7443	242	126	152
1997	6662	227	131	56
1996	6767	226	139	34
1995	6498	208	102	19
1994	6037	175	80	13
1993	5958	175	96	13
1992	5747	158	57	4
1991	4944	137	32	0
1990	3740	122	24	2
1989	3407	106	36	3
1988	3069	77	28	1
1987	2699	81	26	0
1986	2415	87	21	0
1985	2540	91	21	0
1984	2453	86	26	0
1983	2320	71	15	0
1982	2022	66	17	0
1981	1934	70	9	0
1980	1804	82	17	0
1979	1879	62	16	0
1978	1596	76	12	0
1977	1707	65	35	0
1976	1838	66	16	0
1975	1759	86	19	0
1974	2408	85	18	0
1973	2061	26	6	0
1972	1387	42	8	0
1971	1435	31	3	0
1970	1446	37	2	0

Table 4 Absolute numbers of papers containing the keywords or keyword combinations: ELECTROCHEMISTRY, ELECTROCHEMISTRY AND THEORY, ELECTROCHEMISTRY AND SIMULATION, COMPUTATIONAL ELECTROCHEMISTRY, published between 1970 and 2021

Year	ELECTROCHEMISTRY	ELECTROCHEMISTRY AND THEORY	ELECTROCHEMISTRY AND SIMULATION	COMPUTATIONAL ELECTROCHEMISTRY
2021	5819	426	290	8
2020	6012	393	214	8
2019	5664	369	231	7
2018	5717	342	205	9
2017	5568	365	198	6
2016	5143	300	183	7
2015	5009	274	184	4
2014	4615	276	196	4
2013	4629	263	151	8
2012	4100	225	173	10
2011	5140	266	214	11
2010	4831	238	225	11
2009	5985	254	339	5
2008	6299	303	416	10
2007	6882	286	384	13
2006	7406	334	334	8
2005	8208	423	405	8
2004	8198	454	387	7
2003	6234	248	242	5
2002	5546	240	216	9
2001	4565	198	145	3
2000	3707	116	109	4
1999	2946	104	91	1
1998	2613	106	57	1
1997	2710	116	91	0
1996	2685	134	84	0
1995	2315	80	55	0
1994	2460	83	75	0
1993	2232	91	56	0
1992	1870	95	48	0
1991	1825	70	45	0
1990	1779	80	48	0
1989	1575	53	32	0
1988	1317	36	18	0
1987	1671	55	26	0
1986	1512	55	17	0
1985	1990	95	25	0
1984	2270	139	32	0
1983	1575	88	15	0
1982	804	27	3	0
1981	692	28	9	0
1980	617	28	6	0
1979	600	30	7	0
1978	510	27	6	0
1977	441	25	3	0
1976	427	22	5	0
1975	421	19	4	0
1974	361	19	2	0
1973	393	23	6	0
1972	299	15	2	0
1971	215	6	1	0
1970	336	15	1	0

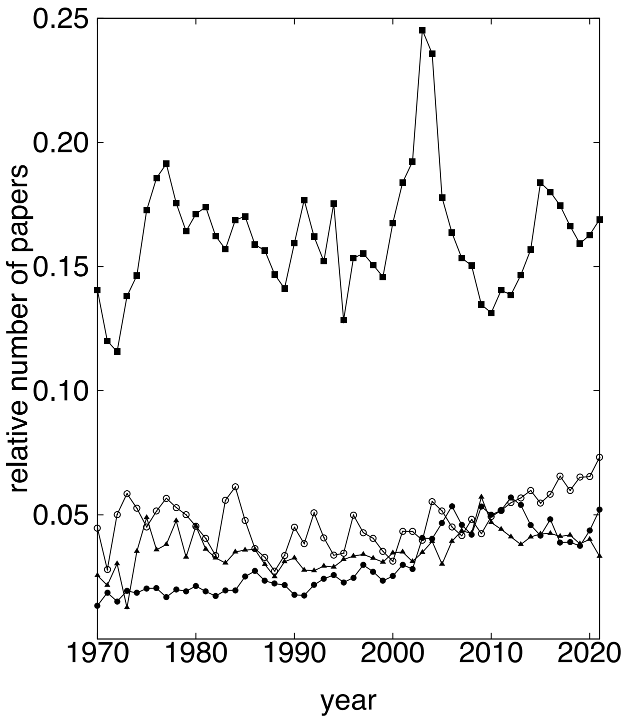

Fig. 1 Relative numbers of papers containing the keyword combinations: PHYSICS AND THEORY (black squares), CHEMISTRY AND THEORY (black circles), BIOLOGY AND THEORY (black triangles), and ELECTROCHEMISTRY AND THEORY (white circles), published between 1970 and 2021

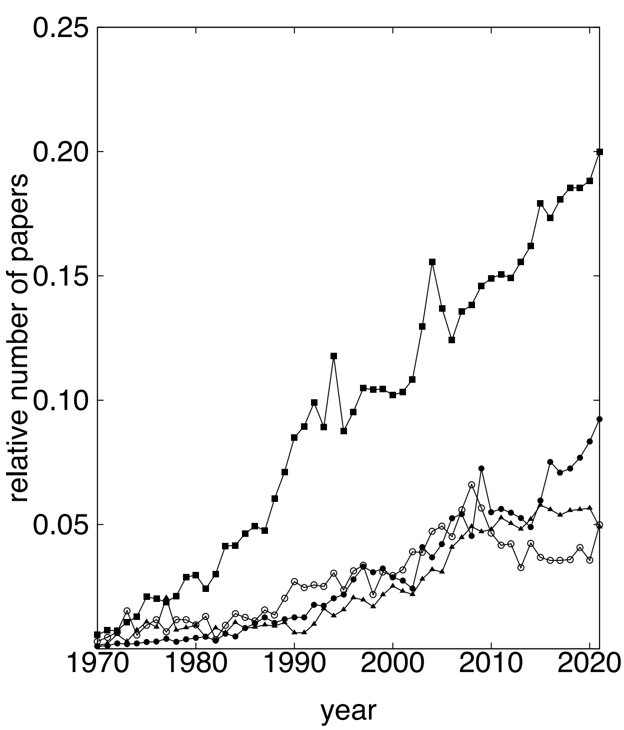

Fig. 2 Relative numbers of papers containing the keyword combinations: PHYSICS AND SIMULATION (black squares), CHEMISTRY AND SIMULATION (black circles), BIOLOGY AND SIMULATION (black triangles), and ELECTROCHEMISTRY AND SIMULATION (white circles), published between 1970 and 2021

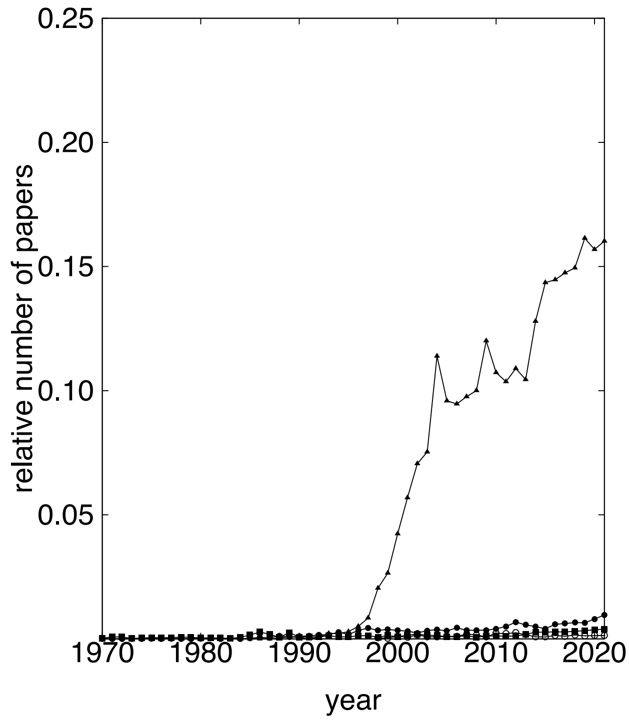

Fig. 3 Relative numbers of papers containing the phrase: "COMPUTATIONAL PHYSICS" (black squares), "COMPUTATIONAL CHEMISTRY" (black circles), "COMPUTATIONAL BIOLOGY" (black triangles), and "COMPUTATIONAL ELECTROCHEMISTRY" (white circles), published between 1970 and 2021

educating interdisciplinary specialists. It should be noted that interdisciplinary university studies combining a number of traditional natural sciences and computer science have been advocated for a long time and have become quite frequent in recent decades (see, for example, [25, 26]). Sadly, I am not aware of similar studies combining electrochemistry and computer science, but there is no reason for not opening such studies. This might even be a useful trick attracting young people to electrochemistry, as nowadays most of the ambitious youngsters think it is only computer science that offers the most attractive careers for them, which deprives traditional natural science disciplines of new talented adepts.

Of course, education of young electrochemists is not the only issue that awaits improvements. Another painful problem is the deficiency of quality journals in which interdisciplinary computational electrochemists can publish. Yet another problem is the deficiency of initiatives aimed at creating publicly available databases of electrochemical experimental results. Databases of this sort exist in other scientific areas (for example, in biomedicine), and they are fundamental for stimulating the development of data analysis algorithms (cf., for example, [27]). But these, and other problems, are probably topics for a different *Special Volume*.

Acknowledgements The access to Scopus was provided by the library of the Cracow University of Technology.

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