Quantitative analysis and relevant features of the scientific literature related to SAXS and SANS

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Abstract. We present and discuss here numerical information derived from a systematic searching of scientific papers related to SAXS and SANS published in indexed journals - from 1945 until nowadays - recorded by the Web of Science Data Bank (WoS). We have detected interesting features regarding the time dependence of the number of papers/year, \( N(t) \), indicating the existence of three well-defined periods of historical evolution with rather well-defined boundaries. All three periods exhibit a positive and approximately linear variation of \( N(t) \) but, at the two transitions between periods, the rate of growth exhibits clear and strong increases. Differences of the historical evolutions in the numbers of papers/year related to SAXS and to SANS were established. The different behaviours regarding the numbers of papers/year related to SAXS and to SANS and the existence of three different and well defined periods for \( N(t) \) can be qualitatively understood as a consequence of the progressive and increasing availability along the last three decades of very brilliant synchrotrons, last generation commercial X-ray sources, new neutron facilities, powerful computers and novel theoretical approaches for SAS data analysis. The rates of growth in the number of papers/year published by authors from a set of different countries are approximately constant along the last two decades. For other countries we have detected a slowing down effect in the number of papers/year while a clear acceleration could be noticed for the production of SAS papers by authors from several emerging countries. These opposite trends compensate in such a way that the number of SAS (SAXS+SAXS) articles published per year all around the world maintained a vigorous linear growth - during more than 20 years - at a constant rate of 60 papers/year, without any indication of eventual saturation. The observed distribution of articles among different journals indicates that a very high fraction of the volume of SAS research is focused to the structure of soft matter.

1. Introduction
The rate of published articles in the scientific literature in most research areas is nowadays extremely high and is still increasing at a very high pace. This is also the case for the literature related to small-angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) techniques. We present here numerical results of a systematic searching of published papers related to SAXS and SANS in the Web of Science Data Bank (WoS) from Thomson Reuters. In order to establish eventually relevant features of the historical evolution, the number of published papers/year, \( N(t) \), was recorded as a function of the year of publication. The papers published from 1991 until now days recorded by us are
those that contain a predefined set of words. The search query used at WoS in the topic field was: 
((ultra*small-angle same scattering) or (gi*sans or u*sans or su*sans or gi*saxs or u*saxs or 
su*saxs) or ((small or low) same angle same scattering or saxs or sans)). In order to be retrieved an article published from 1991 until now days should contain these words in their title, key words or abstract and those published between 1945 and 1990 in their title or key words. The retrieval date was 9th April 2009. The final and total number of articles retrieved was 25791. The bibliographic data of these articles were then downloaded and analyzed using a data-mining software named VantagePoint 6.0 from Search Technology, Inc (www.thevantagepoint.com) [1]. The WoS Data Bank does not include the abstracts of papers published before 1991 so as the plot of the number of (SAXS+SANS) articles/year exhibits a sharp increase between 1990 and 1991. We have suppressed this apparent discontinuity in the annual rate $N(t)$ by multiplying the numbers of articles/year before 1991 by a factor 2.2.

The completeness of our searching procedure was estimated by checking the whole texts of all papers published by one of the authors (AFC) in indexed journals. We have verified in this particular case that 95% of the total number of published papers related to SAXS and SANS were actually recorded by the retrieval procedure applied here. This finding suggests that our retrieval procedure recorded most of the published papers related to SAXS and SANS, the fraction of articles that were missed being only a few percent.

This article aims at determining the number of papers published each year related to SAXS and SANS and their growth rate as functions of time, establishing the distributions of the number of papers/year among different countries and among different scientific journals.

2. Historical evolution of the annual number of articles related to SAXS and SANS

The number of articles related to SAS (either SAXS or SANS) published each year is displayed as a function of time, $N(t)$ in figure 1. We can clearly notice three different periods in the plot shown in figure 1, all of them with an essentially linear time dependence but with clearly different slopes, $\Delta N/\Delta t$, that indicate different growth rates. The first period ending by 1965 is featured by a low number of articles published per year and by a rather slow growth in the number of papers/year. The second period - starting by 1965 and ending by 1990 - is characterized by a moderate growth in the number of papers/year, the function $N(t)$ increasing from about 20/year in 1965 up to 300/year in 1990. Over the third period - starting in 1988 and persisting until now days - $N(t)$ exhibits an also linear time dependence but a much faster growth rate. The number of published articles increases in this period at a pace of 60 articles/year circa, from 300 articles/year in 1990 up to 1500/year in 2008.

The first period mentioned above was featured by a very low number of articles/year so as it can be considered a sort of “incubation” period for the current SAS literature. During the second period starting in 1965 - coincidently the year during which the first International SAS Conference was held - the rate of growth, $\Delta N/\Delta t$, became rather high. Finally during the last two decades the number of papers/year was characterized by a much stronger growth rate, which persists until nowadays without any indication of eventual saturation.

The strong growth in the number of papers/year during the third period starting by 1990 (Figure 1) can be explained by the increasing number and wider availability of (i) new synchrotron and neutron SAS setups, (ii) powerful personal computers, and (iii) newly developed theoretical approaches and fitting procedures applied to SAS data. An additional and relevant reason for the observed strong growth in the number of paper/year is the vigorous increase in the interest of materials scientists for the study of nanomaterials, which started to be widely produced during the last two decades. The growing needs of researchers for the structural characterization of newly developed nanostructured materials induced the correlated growth of the literature related to SAXS [2] and to SANS [3] and also to the more recently developed GISAXS and GISANS techniques. Another important contribution to the very high rate of growth in the number of SAS papers observed during the last two decades was the strong and increasing interest in the study of biological macromolecules in solution (proteins and
others), this contribution being enhanced by the availability of new developments of powerful simulation tools [4].

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**Figure 1.** Number of articles/year related to SAS measurements (SAXS or SANS).

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**Figure 2.** (a) Number of paper published per year containing results referring to SAXS and SANS separately. Details corresponding to 1960/1990 and 1985/2008 periods are displayed in (b) and (c), respectively.
Figure 2a exhibits separately the number of papers/year related to SAXS and those associated to SANS. Details of these curves corresponding to the periods 1960/1990 and 1990/2008 are plotted in Figure 2b and 2c, respectively. Articles published until 1973 were almost exclusively related to the SAXS technique. This happened because of the absence of a significant number of neutron facilities with SANS setups in operation until the end of the sixtieth. In 1973 the number of papers/year associated to SANS started to grow and became soon, by 1978, similar to the number related to SAXS. The equivalence of the $N(t)$ functions related to SAXS and to SANS persisted from 1978 until 2000. Nevertheless, by 2000, the number of articles/year based on SANS results exhibits a clear tendency to saturation and becomes nowadays nearly constant (about $N = 600$ papers/year). This saturation in the number of published papers related to SANS is being accompanied by a parallel acceleration in the growth rate of the number of articles/year related to SAXS, reaching nowadays a number $N = 1000$ circa. i.e. $\sim 70\%$ above those related to SANS. These positive (SAXS) and negative (SANS) deviations of $N(t)$ from a linear time dependence compensate so as the total number of (SAXS+SANS) papers/year persists in its linear growth until nowadays, as it can be seen in Figure 1.

3. Distribution among countries

Since many papers are authored by scientists from different countries, we have assigned each paper to the country in which the first author works. This seems reasonable because the order of authors is expected to be geographically distributed at random. The histogram displayed in Figure 3 exhibits the total number of papers related to SAS published from 1945 until now by first authors from different countries. The countries with the highest total numbers of published articles are USA, five European countries (France, Germany, Russia, Italy and Netherlands), and three Asiatic countries (Japan, China and India).

The numbers of articles published per year by first authors from different countries, $N(t)$, are displayed in figures 4a, b and c. These figures also show solid lines corresponding to second order polynomials, $N(t) = a_0 + a_1(t-t_0) + a_2(t-t_0)^2$, where $t_0 = 1990$, fitted to the retrieved $N(t)$ function for every country, from 1991 until 2008. The smoothed (best fitted) $N(t)$ functions were extrapolated a few years, these extrapolations expecting to yield a reasonable prediction for the near future, provided the individual trends during the last two decades are preserved.

![Figure 3. Geographical distribution of the total number of papers related to SAS (SAXS or SANS).](image-url)
The numbers of papers/year related to SAS (SAS+SANS) published from 1991 exhibit different overall features for three different groups of countries, as it can be seen in Figure 4a, b and c. For the first group composed of France, Russia, Italy and Austria (Figure 4a) the number of papers/year grows linearly, i.e. \( N(t) = a_0 + a_1(t - t_0) \). For all these countries, the second order coefficient of the fitted polynomials, \( a_2 \), is smaller than the corresponding statistical error bar, so as the number of papers from these countries exhibit the same linear and growing behavior as that observed for the total number of SAS papers/year published by authors from all countries (Figure 1). On the other hand, USA, Germany, Japan, England, Netherlands, Denmark, Sweden and Belgium (Figure 4b) belong to a second group of countries for which the second order polynomial coefficient is negative, \( a_2 < 0 \), so indicating a slowing down in the growth rate of the number of articles/year. On the contrary, for a third group of countries, composed of China, India, South Korea, Brazil, Spain, Australia, Switzerland and Canada, the second order polynomial coefficient is positive, \( a_2 > 0 \), thus evidencing an acceleration in the growth rate of the number of papers/year (Figure 4c). The acceleration noticed for the third group of countries compensates the slowing down observed for countries of the second group, so as the total number of paper published per year by authors from all countries preserves its linear growth over the whole 20 year period, from 1988 until nowadays, as previously verified in the plot displayed in Figure 1.

Not surprisingly, all countries that exhibit the highest numbers of published papers (USA, France, Germany, Japan, UK, Italy and Russia) and also all of those that showed a positive acceleration in the growth rate of published papers (China, India, South Korea, Brazil, Switzerland, Australia, Canada, Switzerland and Spain) possess one or several synchrotron radiation sources in operation and/or under construction.

The histogram displayed in figure 5 indicates the number of paper/year published 10 years ago (red) and nowadays (green), and the expected values within 10 year provided the parabolic trend observed during the past 20 years is preserved along the forthcoming decade (blue). We can notice that the distribution among countries within 10 years is expected to be more homogeneous than nowadays, i.e. the differences between the number of papers published per year by developed countries such as USA, Germany and France, and those published by emerging countries tend to decrease. Emerging countries such as China and India exhibit a particularly strong increase in the growth rate of

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**Figure 4.** Annual numbers of papers published by first authors from different countries. The curves were vertically shifted for clarity. (a) Countries with an annual number of published papers exhibiting a linear growth over the whole period. (b) Countries that exhibit a slowing down in the growth rate of the number of papers/year. (c) Countries that exhibit a positive acceleration in the growth rate. The distances between horizontal lines correspond to 50 articles. The numbers of papers published in 2008 corresponding to all countries are indicated.
the number of published papers/year so as one can guess that in the forthcoming years and provided the trends prevailing during the past 20 years persist, these countries will reach a number of papers/year comparable to most of the developed countries.

**Figure 5.** Histogram of the number of articles published per year in 1998 (red) and 2008 (green) by authors from different countries. The blue bars correspond to the expected annual numbers under the assumption that the trends observed during the last 20 years will be preserved during the forthcoming decade.

4. Distribution among journals
The number of articles/year based on SAXS and SANS techniques in the eight journals that have published until now the highest total number of articles related to SAXS and SANS are displayed in figure 6a, in which the different curves were vertically displaced for clarity. The numbers of SAXS or SANS papers published per year in each journal exhibit many oscillations over time but an approximately linear overall trend prevails. The numbers of articles/year published by the Journal of Applied Crystallography and Physica B exhibit particularly strong oscillations and nearly periodic and narrow peaks. The peaks corresponding to Journal of Applied Crystallography occur at years during which the Proceedings of the International SAS Conferences appeared [5]. Similarly, the peaks associated to Physica B occur at years during which Proceedings of International SANS Conferences were published.

Figure 6b exhibits the straight lines, without vertical displacements, that best fitted to the data plotted in Figure 6a. Three journals with the highest number of papers/year in 2008 (Macromolecules, Langmuir and Polymers) publish results of investigations dealing with proteins, thin organic films, polymeric materials and other “soft” materials. On the other hand, the next journals in the ranking – Journal of Physical Chemistry B, Journal of Applied Crystallography and Physica B - publish papers focusing to all types of materials. This obviously indicates that SAXS and SANS techniques are more widely applied to the investigation of soft matter, the highest number of papers being published by Macromolecules, followed by Langmuir and Polymers. The results plotted in Figure 6b qualitatively suggest that the observed difference between the number of articles/year related to structural
characterization of soft matter (organic films, polymers and protein in solution) and those related to inorganic materials still nowadays tends to increase.

5. Most cited articles
We have also retrieved from WoS Data Bank the articles most cited in the literature related to SAXS and SANS. Ten articles received more than 400 citations and two of them, both related to SAXS, received more than 1000 citations. The references corresponding to the two most cited articles are:

- “CdSe/ZnS core-shell quantum dots: Synthesis and characterization of a size series of highly luminescent nanocrystallites” [6] (1206 citations).
- “Buildup of ultra thin multilayer films by a self-assembly process. Consecutively alternating adsorption of anionic and cationic polyelectrolytes on charged surfaces” [7] (1136 citations).

We have tried to establish the common features of highly cited articles related to SAXS and SANS. In most of these articles, several experimental techniques for materials characterization are applied, so as attracting the attention of a spectrum of readers wider than in case of the application of a single technique. Another common feature of many highly cited articles is that they include results of SAXS or SANS - and eventually of other techniques – for structural characterization, this structural information being also applied to understand different properties of the studied materials.

6. Contribution of SAS to the general scientific literature
We have already pointed out that the rate of growth of the scientific literature during the last decades is very high. The same can be said about the volume of the literature related to SAS (SAXS+SANS), which increased from about 20 published papers per year in the sixties of last century up to 1500 papers/year circa in 2008. We have determined the fraction of the annual number of papers related to SAS with respect to the total annual number of papers published in the literature, and established the trend of this fraction as a function of time. In order to perform this analysis, eight journals were selected, in which papers related to SAS are more commonly published. These journals were those also selected in section 4 for the plots displayed in figure 6. We have then determined the annual number of articles related to SAS, \( N_{SAS} \), and the annual number of all articles, \( N_{Total} \), published in these journals, from 1980 until 2008. The fraction of the number of papers related to SAS with respect to the total number of published articles, \( N_{SAS}/N_{Total} \), is displayed as a function of time in figure 7.
This function exhibits a set of nearly periodic peaks that, again, are clear effects coming from the contribution of the periodic proceedings of the International SAS Conference series.

![Figure 7. Number fraction of articles related to SAS with respect to the total number of articles published in eight selected journals. The dashed straight line is a guide for the eyes.](image)

The results plotted in figure 7 demonstrate that the fraction of the number of papers related to SAS with respect to those of the whole literature published in the selected journals, exhibits a significant increase, from less than 2.0% in 1980 up to 4.5% circa in 2008. This trend indicates that beside the strongly increasing volume of published research related to SAXS and SANS during the last three decades, these experimental techniques also exhibit a clearly increasing relevance with respect to the general scientific literature.

7. Main conclusions
The presented results of our searching over the SAXS/SANS literature obviously do not yield an evaluation of the quality of the research performed but they allowed us to infer some interesting insights into historical trends, geographical distribution and other features of the published articles related to these experimental techniques.

The time dependence of the number of papers published per year from 1945 until 2008 clearly indicate the existence of three periods of the historical evolution of the SAXS/SANS literature (1945/1965, 1965/1990 and 1990/2008), each of them with different and successively increasing growth rates. The relevant features of these three periods of growing activity seem to be well correlated to the parallel and increasing availability of brighter (synchrotron and commercial) X-ray sources, new neutron facilities and more powerful personal computers and also to the development of new theoretical approaches for SAS analysis. Another relevant reasons for the observed strong growth in the number of SAXS/SANS paper/year during the last two decades are (i) the vigorous increase in the interest of materials scientists for new nanomaterial development and characterization and (ii) the significant increase in the number of biology oriented researchers doing SAS studies of macromolecules in solution taking benefit from the availability of new powerful simulation tools for data analysis.

The results regarding the distribution of papers among authors from various countries during the last two decades showed three different groups of countries with different historical trends. A first group exhibits a linear growth in the number of papers/year, a second group composed of developed countries shows a slowing down in the growth rate and, inversely, a third group of emerging countries exhibit a clear positive acceleration. The opposite trends of the second and third groups tend to
compensate in such a way that the linear growth and high slope in the number of SAS (SAXS+SAXS) articles/year produced all around the world are preserved over two decades, starting in 1990 and up to now without any apparent saturation effect.

References
[1] Zhu D and Porter A L 2002 Technological Forecasting and Social Change 69 495
[2] Peterlik H and Fratzl P 2006 Monatshifte fur Chemie 137 529-543
[3] Meinichenko Y B and Wignall G D 2007 J. Appl Phys 102 02101
[4] Petoukhov M V and Svergun D I 2007 Curr. Opin Struct. Biol. 17 562
[5] Craievich A 2003 J. Appl. Cryst. Proc. of the XII International SAS Conference. Foreword.
[6] Dabbousi B O, Rodriguez-Viejo J et al. 1997 J Phys Chem B 101 9463-9475
[7] Decher G, Hong J D et al. 1992 Thin Solid Films 210 831-835