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Materials Modelling Software Market

AN INSIGHT INTO THE MARKET LANDSCAPE

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1. Introduction

The field of materials modelling covers a wide range of domains and sub-domains including computational chemistry[1], techniques based on quantum mechanics, continuum mechanics, statistical mechanics and thermodynamics as well as fluid dynamics. It has been described in a number of textbooks[2,3,4] and reviews[5].

We define materials modelling as any activity using physics-based models [5,6] as well as 'pre-determined' data-based models to study the behaviour of materials. A 'pre-determined' data-based model is an empirical model derived and/or parameterised from datasets ready to use for the end user in methods such as Quantitative Structure Property Relations (QSPR). It excludes machine-learning (ML) and artificial intelligence (AI) software applications which we will comment on in the Outlook section of the report.

In order to delineate materials from engineering modelling, we define materials modelling as having a 'materials focus'. Hence in materials modelling, the material itself is the subject of study and a simulation delivers new data and properties about the material as an output. In contrast, in engineering modelling, the computational representation of the material is an input in the form of materials relations required to solve a model which is targeted at the behaviour of an engineered product (e.g. a car door or aeroplane wing). Note that determining the materials relation input in engineering modelling would in itself be classified as materials modelling that takes place either as a separate activity or potentially even in an integrated (linked or coupled) simulation workflow.

Materials modelling software has been discussed in various reports and white papers[7,8,9] as well as workshops organised by the EMMC[a]. However, we are not currently aware of any market research organisation having surveyed the materials modelling field and estimated its market size.

Key traits of the field include:

- It serves a wide range of industries, including fine, intermediate, specialty and Petro-chemicals, metals and alloys, ceramics, polymers, as well as applications in many fields such as automotive, aerospace, consumer goods, electronics, energy and pharmaceutical development.
- While a lot of applications are about the design and development of the material (see Figure 1), it also plays an increasingly important role when co-developing materials with products or improving the understanding and control of manufacturing via a better understanding of existing materials behaviour.
- Due to the many time and size scales governing materials behaviour, all types of modelling entities are required, i.e. electronic, atomistic, mesoscopic and continuum volumes.
- As a result of the wide range of materials types and modelling types, the market has historically been quite fragmented with codes developed by different communities, such as quantum chemistry, electronic structure (physics), statistical thermodynamics (often the source of mesoscopic models), computational phase diagrams, phase-field models, crystal-plasticity, continuum mechanics and fluid dynamics.

[a] European Materials Modelling Council, https://emmc.eu/

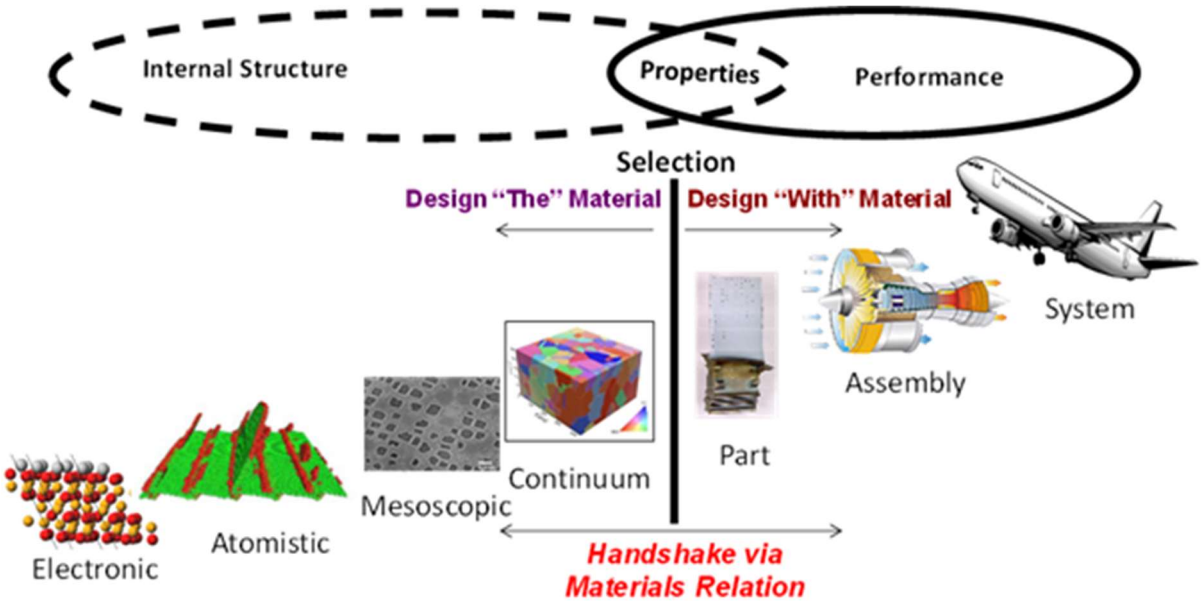

Figure 1 Segmentation of the field into Materials and Engineering Modelling, designing "the" material on the left, and the design of product "with" the material on the right (Courtesy of Granta Design).

Regarding market size, a report published in 2012[10] estimated the discrete (electronic, atomistic and mesoscopic) materials modelling software market to be about $50m. Some companies offering discrete materials modelling ("molecular modelling") software are included in Cheminformatics market reports[11]. However, the materials modelling part is typically only a fraction of the estimated $7bn market size, since cheminformatics is largely dominated by Life Sciences applications.

Most of the continuum materials modelling market would be subsumed within the Computer-Aided Engineering (CAE) market[12,13,14] which has an estimated size in the range of $5-8bn. Note that if Computer-Aided Design (CAD), Electronic Design Automation (EDA) and Architectural Engineering and Construction (AEC) software are also included, the market size increases to about $20.6bn in 2019[15].

2. Methodology

In common with many other market size studies, our approach is based on an analysis of a range of software companies that are either exclusively active in the materials market or provide some materials modelling software products. In the latter case, we also have to distinguish between software that is specifically designed for materials modelling and software with wider applications, in particular in product and process engineering. In the latter case, we make assumptions about the share of materials modelling use.

Hence, as a basis for estimating the materials modelling market size, we assembled a list of 72 software companies and codes (see Appendix 1) which are relevant to the materials modelling field. It includes 15 large enterprises active in the field as well as 2 medium and 55 small software providers[b]. The list is surely not exhaustive due to the large and constantly evolving number of small companies.

For companies with a wide range of software products (e.g. covering CAE and various informatics applications) and covering diverse markets, we identified the materials-relevant parts or codes.

[b] Small, Medium and Large enterprises are defined by the number of employees up 50, 250, or higher, respectively, see also https://ec.europa.eu/growth/smes/business-friendly-environment/sme-definition_en

In discrete modelling, the boundary is drawn between materials applications and life science applications. Note that pharmaceutical development (i.e. from the molecule to the drug product) is included in materials modelling.

In continuum modelling, while the boundary to engineering modelling is fluid, the aim has been to identify applications that have a materials focus and estimate the related market share. Wherever possible this was done in a bottom-up way, identifying as closely as possible the relevant codes and their markets.

For example, there are continuum models designed explicitly for studying materials (Digimat[c], JMatPro[d], MatCalc[e], Material Designer[f], Micress[g], Multiscale Designer[h], Multimech[i], ThermoCalc[j], etc.). On the other hand, there are general purpose continuum mechanics and fluid dynamics codes that are typically used for CAE but are used also for materials investigations (such as Abaqus[k], NX Nastran[l], LS-Dyna[m], Fluent[n], etc.).

In electronics, a significant part of TCAD[o] is about the modelling of the semiconductor materials and their structural properties and electrical behaviour in devices and is therefore included in the materials modelling market. In fact, it is an area in which continuum and discrete materials modelling is becoming increasingly integrated as the major players offer both the traditional continuum solutions as well as electronic modelling based TCAD.

As metrics of market size, we used a combination of the following:

- Published market size data
- Published revenue data
- Historical data about acquisitions of particular codes and their estimated growth
- Number of employees involved in materials modelling times a typical FTE cost.
- Estimated materials modelling share of continuum modelling products

Key assumptions are as follows:

- FTE cost: we assumed for each employee the company requires an income of €150k to cover salary and overheads and still gain a profit.

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[c] https://www.mscsoftware.com/product/digimat

[d] https://www.sentesoftware.co.uk/jmatpro

[e] https://www.matcalc-engineering.com/index.php/matcalc-software/matcalc-6

[f] https://www.ansys.com/services/training-center/structures/ansys-material-designer

[g] https://micress.rwth-aachen.de/

[h] https://altairhyperworks.com/product/Multiscale-Designer

[i] https://www.plm.automation.siemens.com/global/en/products/simcenter/multimech.html

[j] https://www.thermocalc.com/products-services/software/thermo-calc/

[k] https://www.3ds.com/products-services/simulia/products/abaqus/

[l] https://www.plm.automation.siemens.com/global/en/products/simcenter/simcenter-nastran.html

[m] https://www.ansys.com/products/structures/ansys-ls-dyna

[n] https://www.ansys.com/products/fluids/ansys-fluent

[o] Technology computer-aided design, a branch of electronic design automation that models semiconductor fabrication and semiconductor device operation

- Materials modelling share of specific CAE products (continuum mechanics, fluid dynamics): Based on a number of private conversations, a reasonable assumption is that materials modelling accounts for between 5-10% of relevant CAE software use. In the analysis below, we use 8% to determine the materials modelling share for general purpose continuum modelling software, and 5% for the materials modelling share of company revenue based on a range of CAE codes.
- For TCAD, we used the same 8% fraction that is related to materials modelling.
- We only consider software providers (including some large distributors) but make no distinction between income based on software licenses and income from related services. Pure consulting and contract research providers are not included. Hence, also the considerable market related to industrial funding of consulting and projects at universities and research organisations is not included in this study.
- For currency conversion, we applied the mid-market rates of 31st December 2019[p].

3. Result and Analysis

As outlined above, we used a range of data about the companies and codes to estimate the market size for discrete and continuum materials modelling. The large enterprises first required segmenting to get as close as possible to the parts that are related to materials modelling.

For **Dassault Systèmes** we revisited some acquisitions they made. Discrete materials modelling was brought in via the acquisitions of Accelrys in 2014[q] and COSMOlogic in 2018[r]. We estimated revenues for Materials Studio from financial reports in 2010[s], and forecast a contribution for 2019. The revenue of COSMOlogic was based on an estimate of the number of employees. Regarding continuum modelling, Dassault Systèmes acquired ABAQUS[t] in 2005. Using ABAQUS revenue from that time[u] and annual growth of 10% (typical growth, based on CAE market reports), we forecast a revenue for 2019. The materials modelling market contribution is then obtained using the 8% share assumption outlined above. Using Dassault's share holder reports, we extracted information on Simulia, duly subtracted our value for ABAQUS, and took a 5% contribution to obtain the estimated materials modelling share. Together with our estimates for Materials Studio, COSMOlogic and ABAQUS we estimated the Dassault Systèmes contribution to the Materials Modelling Market.

Siemens started with CAE by acquiring UGS and thus NX NASTRAN in 2005.[v] The overview graphics of a CAE market study from 2011[w] shows that Siemens share of the European market was about 50% of that of Dassault Systèmes. Assuming a similar ratio for the world market and we used the revenue of ABAQUS to

[p] https://www.xe.com/

[q] https://www.3ds.com/press-releases/single/dassault-systemes-successfully-completes-acquisition-of-accelrys/ assuming about a quarter of the business at the time from materials modelling

[r] https://www.3dsbiovia.com/micro/cosmologic/index.html

[s] https://last10k.com/sec-filings/accl/0000950130-10-000221.htm

[t] https://www.3ds.com/press-releases/single/dassault-systemes-completes-the-acquisition-of-abaqus-inc-and-introduces-the-simulia-brand/

[u] https://www.ft.com/content/087eb1c4-c6a2-11d9-a700-00000e2511c8

[v] https://www.plm.automation.siemens.com/global/en/our-story/newsroom/siemens-press-release/42392

[w] http://www.01consulting.net/02_2011_MCAE_EUROPE_Market_ES.html

estimate the NX NASTRAN one, then applying the 8% materials modelling share as above. Another product with a materials application in the Siemens suite is STAR-CCM+ which was a product by CD-adapco, which was acquired in 2016.[x] In 2019, Siemens acquired a specific materials modelling product, MultiMechanics[y] and we used a contribution based on their headcounts. In the same year, they also acquired Process Systems Enterprise [z], and, using their revenue, we allocated a share of 5% for materials modelling.

Hexagon acquired MSC in 2017[aa] and, thus, also acquired e-Xstream engineering in this process, as they were part of MSC at the time. [bb] We applied a growth rate of 10% annually on MSC's FY2017 revenue to estimate a hypothetical revenue for FY 2019 and based Hexagon's share of the materials modelling market on this. To account for the contribution of e-Xstream, we estimated their headcount and assumed the obtained figure to represent 100% contribution to the materials modelling share. This is due to the nature of their software. The "e-Xstream value" was then deducted from the MCS FY2019 forecast and the remainder underwent a 5% CAE correction.

Ansys includes a mixture of CAD and CAE products and we applied the 5% level to estimate the contribution to the materials modelling market, using their public investor reports for 2019 as a basis. Note that the 2019 revenue excludes the income of Granta Design, which was acquired in the same year.[cc] However, according to our materials modelling definition, "Materials Intelligence"[dd] would not be included in any case.

For **ESI Group**, we also took 5% of it their 2019 revenue as reported to their shareholders[ee] to be related to income due to materials modelling.

For **Altair**, we used their FY 2019 report and estimated 5% of their business to be related to materials modelling which for example includes Multiscale Designer[h]. They acquired DEM Solutions Limited[ff] in late November 2019 and we added 8% of DEM's revenue to Altair's materials modelling market share.

The estimates for **AutoForm**, **COMSOL**, **Engineering Center Steyr GmbH & Co KG** were based on headcounts and 8% were used to obtain the materials modelling share. For **Schrödinger** we used the number of employees in their materials modelling segment. The **JSOL Corporation** was split into headcount related to their discrete and continuum modelling and for the latter, we used 8% to account for materials modelling.

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[x] https://www.plm.automation.siemens.com/global/en/our-story/newsroom/siemens-press-release/43811

[y] https://www.plm.automation.siemens.com/global/en/our-story/newsroom/multimechanics-acquisition-simcenter/66874

[z] https://press.siemens.com/global/en/pressrelease/siemens-plans-acquire-process-systems-enterprise

[aa] https://www.hexagonmi.com/about-us/news/media-releases/2017/april-2017/completion-of-hexagons-acquisition-of-msc-software

[bb] https://www.e-xstream.com/about-us/about-e-xstream/company

[cc] https://www.grantadesign.com/news_articles/ansys-and-material-intelligence-leader-granta-design-sign-definitive-acquisition-agreement/

[dd] https://www.ansys.com/products/materials

[ee] https://www.esi-group.com/company/investors/key-figures/revenues

[ff] https://www.altair.com/news/altair-acquires-edem

AutoDesk have their income based mainly on CAD and their CAE is manifested in their tool Moldflow. The latter was acquired in 2008.[gg] From a previous report on the Moldflow revenue [hh] we forecast a revenue for 2019 with an annual growth of 10% and then took 8% of it to obtain the share of materials modelling.

Synopsys operates mainly in the electronics markets. Considering, as outlined above, the field of Technology CAD (TCAD) there is evidence that Synopsis has 80% of the TCAD market, **Silvaco** 15% and the rest is shared by other SMEs[ii] [jj] such as GlobalTCADSolutions, Crosslight, Cogenda Software, etc. In 2001, the TCAD market size was estimated to be $30m with an annual growth rate of 10%.[16] This means, in 2019 we can expect the market to be around $170m or €150m. Our independent research estimates the market to be slightly larger at about €173m, which means an average growth rate of 11% since 2001. Based on the latter value, we took 8% as contribution to the materials modelling market, and estimated the contributions of the individual companies pro rate to the above market shares. In addition, in 2017, Synopsys acquired QuantumWise[kk], a discrete materials modelling provider, hence we added their revenue to estimate the total for Synopsys materials market share.

For the remaining 58 companies we mostly used the number of employees related to materials modelling (developers, support, marketing, …) that we were able to gather from interviews, surveys, webpages and Linked-In. For five materials modelling companies we could use revenue as published in shareholder reports or government webpages. For companies with a business based on CAE, we allocated 8% of their estimated total revenue as a rough estimate of the share of the market which is actually due to materials focussed rather than engineering applications.

The resulting total materials modelling market size is €339.5m, with discrete modelling software taking a share of about €85m and continuum modelling about €254.5m. As can be deducted from Figure 2, the discrete modelling share of the market is about 25 % of the total.

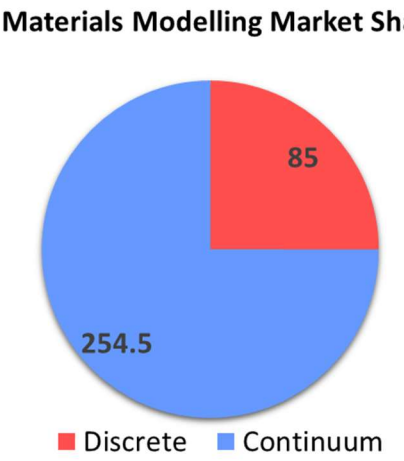

Figure 2 The materials modelling market share for discrete and continuum models

[gg] https://investors.autodesk.com/news-releases/news-release-details/autodesk-announces-intent-acquire-moldflow-leading-provider

[hh] https://www.cbronline.com/uncategorised/moldflow_reports_revenue_growth_of_46_for_fiscal_year_2001/

[ii] https://www10.edacafe.com/nbc/articles/view_article.php?articleid=216301&page_no=3

[jj] https://www.iue.tuwien.ac.at/phd/hollauer/node8.html

[kk] https://news.synopsys.com/2017-09-18-Synopsys-Strengthens-Design-Technology-Co-Optimization-Solution-with-Acquisition-of-QuantumWise

These figures were obtained by using the assumption that on average 5% or 8% of CAE software is dedicated to materials modelling. To check the sensitivity of this assumption we analysed the market also using the lower and upper range values of 3%/6% and 7%/10%, respectively. The discrete market share remains at €85m, while continuum modelling ranges from €180.3 M to €327.5m, as shown in Figure 3.

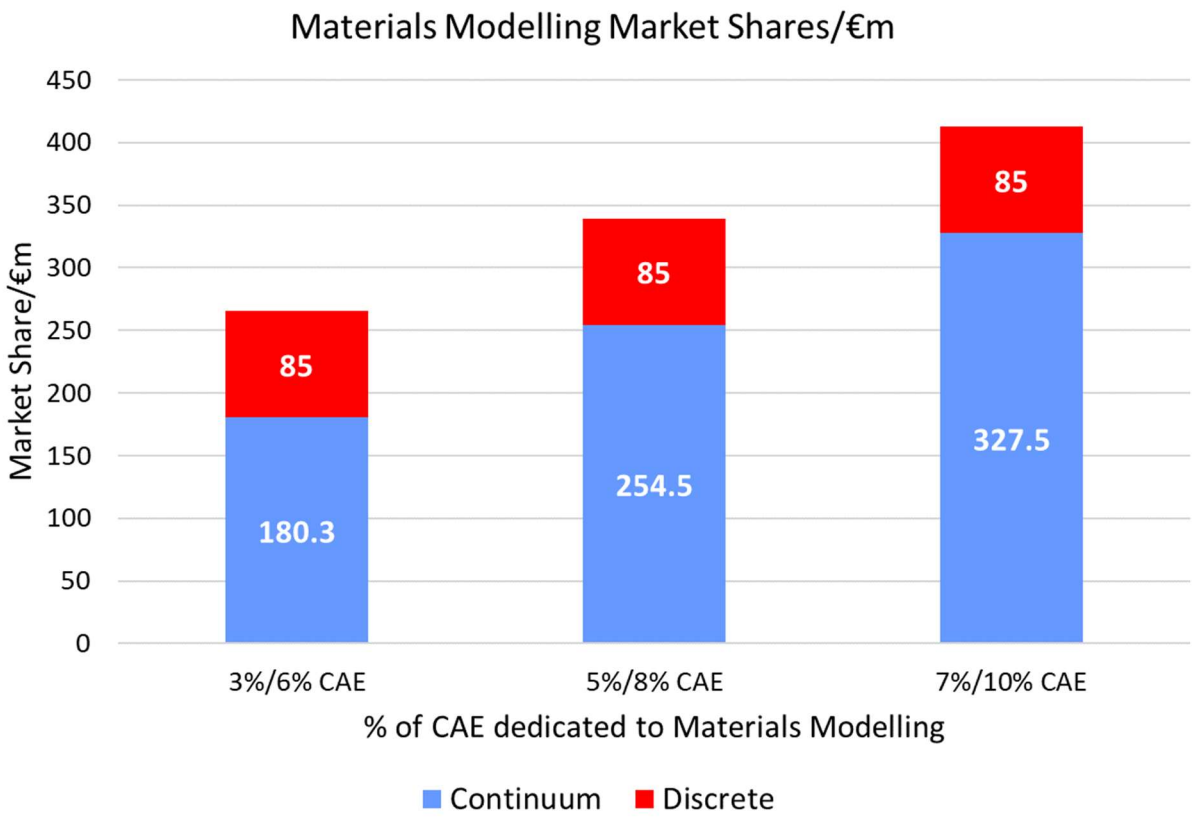

Figure 3 The materials modelling market share for discrete and continuum models, using 5% and 10% correction for CAE software

We can see in Figure 3, for the lower estimate the discrete market has a 32% share and the total market size is €265.3m, which is was 22% smaller than average. For the higher materials modelling allocation, the discrete market share is 21% of a total market of €412.5m, which is 22% larger that our average estimate. Thus, we estimate the total materials modelling market to be €339±74m and the share of the discrete market is 25±7%.

4. Distribution of market across companies

Regarding the distribution of discrete and continuum modelling across companies, we first of all note that despite some acquisitions, the market remains mostly divided into companies offering either discrete or continuum materials modelling software but not both. We included in our analysis the specific discrete materials modelling offerings of the otherwise predominantly continuum modelling providers Dassault Systemes (Materials Studio and Solvation Chemistry), Synopsys (QuantumATK) and JSOL (J-Octa). In the TCAD field, there seems to be a trend towards integrating discrete modelling, since also Silvaco now offers a so-called 'atomistic' software as part of their TCAD package[II]. On the other hand, in CAE the integration remains largely between specific materials continuum modelling and CAE software, as for example in the cases of Digimat (integrated into MSC/Hexagon), Multimech (integrated into Siemens Simcenter) and Multiscale Designer (integrated into Altair Hyperworks).

[II] https://silvaco.com/webinar/tcad-of-innovative-nanodevices-with-victory-atomistic/

The contributions to the market from the different companies, allocated to discrete and continuum modelling, is shown in Figure 4. Note that these are not directly related to company sizes, since in a number of cases, materials modelling is just a part (and sometimes a small part) of their business.

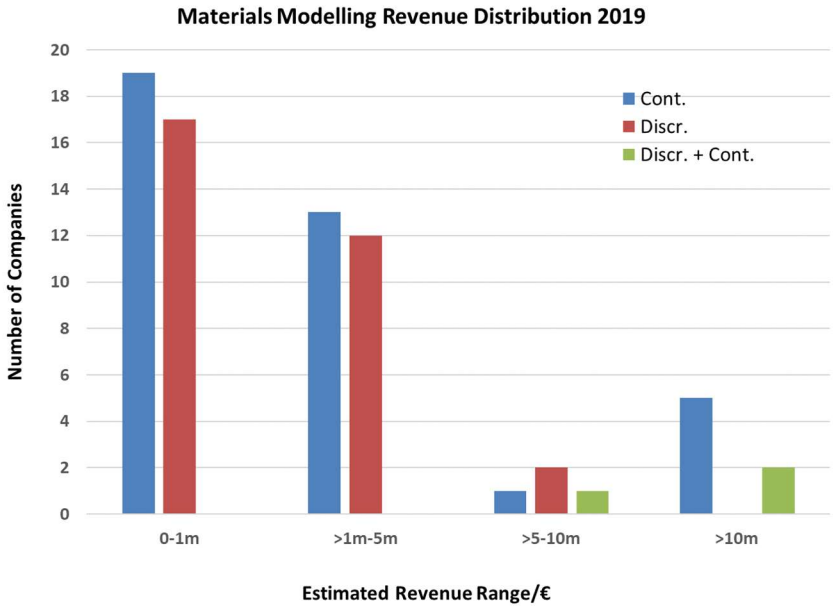

Figure 4 Materials modelling revenue distribution for providers of continuum (Cont.), discrete (Discr.) or both types (Discr. + Cont.) of modelling software.

About 80% of all considered companies had estimated revenue of up to €5m related to materials modelling. The pure discrete materials modelling software market is distributed across a wide range of players mostly up to €5m revenue with only 6% in the €5-10m bracket. Typically, these are pure discrete modelling providers. The picture is very different for the continuum modelling market, where providers feature in all revenue brackets. All providers of both materials modelling types are large enterprises.

5. Size of companies involved in materials modelling

As noted above, the market is served by small, medium and large enterprises. According to these categories, we included in our study 76.4% small, 2.8% medium and 20.8% large enterprises. (Figure 5)

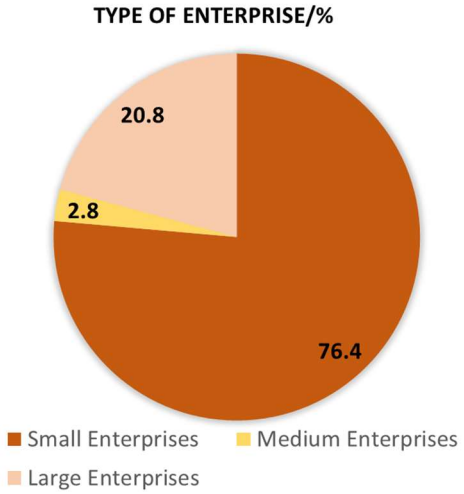

Figure 5 Type of enterprises on the materials modelling software market

In Figure 6 Market shares for the discrete and the continuum market we can see that while large enterprises dominate market share of continuum modelling (98 %), they capture only a bit more than half of the discrete modelling market (52 %).

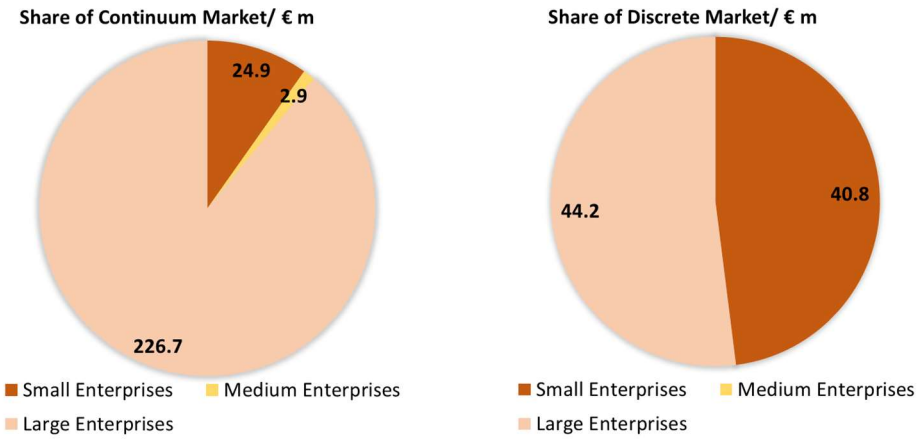

Figure 6 Market shares for the discrete and the continuum market

The continuum materials modelling market of the large enterprises is €226.7m and that of small and medium enterprises is €24.9m and €2.9m, respectively. For discrete modelling the market of the large enterprises is €44.2m, while the smaller companies take a share of €40.8m.

In Figure 7 Enterprises offering continuum software, shown in number of companies and Figure 8 Enterprises offering discrete software, shown in number of companies, we show the distribution by number of companies relative to their size, separately for discrete and continuum modelling providers. Note that here the (few) companies selling both software types are counted in both categories.

Figure 7 Enterprises offering continuum software, shown in number of companies shows that of the companies offering continuum modelling, 26 (63.4%) are small enterprises, 2 (4.9%) are medium and 13 (31.7%) are large enterprises.

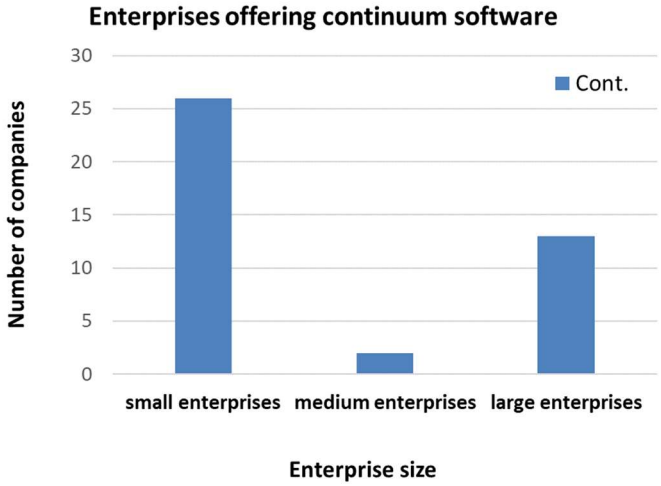

Figure 7 Enterprises offering continuum software, shown in number of companies

Figure 8 Enterprises offering discrete software, shown in number of companies shows that for companies selling discrete modelling software, the percentage of small enterprises is 29, which is about 85.3 %.

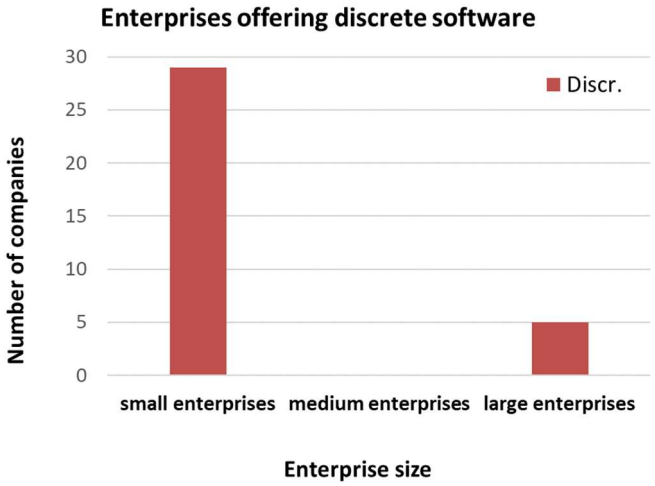

Figure 8 Enterprises offering discrete software, shown in number of companies

We can tentatively conclude from these figures that the discrete modelling market is far less consolidated than the continuum modelling market, which is also supported by the above observation that not many large CAE companies have integrated discrete modelling, while several have acquired pure-play continuum materials modelling companies. Of course, the proviso is that we may have missed new and emerging materials modelling companies at the lower end of the market and of course have also not included many small CAE companies for which a fraction of business could be allocated to materials.

6. Free and Open Source Software (FOSS)

In addition to the commercial software market, there is what could be called a "hidden" market served by free and open source software. In order to estimate a monetary value (which by no means can provide a full estimate of economic value) we look into the amount of investment required to cover staff costs including overheads. Budgets to cover these are mostly provided by grant bodies in the case of FOSS. To keep things straightforward, we took the same amount of € 150 k per FTE as in the company revenue estimates. Numbers of staff were typically based on the number of developers of the codes which can be obtained from websites and/or activity on public repositories such as GitHub.

Since FOSS software is often limited to highly skilled users, industrial use may require substantial additional investment in expertise and training which is not included in our estimates.

Only major codes that we are aware of have been included below. In addition, there is a very large number of smaller developments, in some cases for research and also educational purposes. A good source for tools in the nanoscale (and particular, nano-electronics) field is Nanohub[mm].

The FOSS electronic modelling market

Table 1 Electronic FOSS software and its licensing lists the electronic software on the FOSS market:

Table 1 Electronic FOSS software and its licensing

Code	License	Info
AbInit	GPL	https://www.abinit.org/
CASTEP	Proprietary	http://www.castep.org/Main/HomePage

[mm] https://nanohub.org/

	Academic free and commercials are charged	
CONQUEST	MIT	http://www.order-n.org/
CP2K	GPL	https://www.cp2k.org/
DALTON	LGPL v2	https://daltonprogram.org/
deMon2k	Proprietary Academic free and commercials are charged	http://www.demon-software.com/public_html/index.html
Fleur	MIT	http://www.flapw.de/MaX-4.0/
NEMO-3D	LGPL v2	https://engineering.purdue.edu/gekcogrp/software-projects/nemo3D/
NWChem	Educational Community License 2.0 like Apache	https://nwchemgit.github.io/
OpenMX	GPL v3	http://www.openmx-square.org/
QuantumEspresso	GPL	https://www.quantum-espresso.org/
Siesta	GPL	https://departments.icmab.es/leem/siesta/
The Elk Code	GPL	http://elk.sourceforge.net/
Yambo	GPL	http://www.yambo-code.org/

These codes are supported by an estimated investment of €14.9m.

The FOSS atomistic modelling market

Table 2 lists the atomistic software on the FOSS market:

Table 2 Atomistic FOSS software and its licensing

Code	License	
DL AKMC	LGPL	http://www.ccp5.ac.uk/DL_AKMC/
DL Monte	BSD	https://www.ccp5.ac.uk/DL_MONTE
DL Poly	Proprietary Academic free and commercials are charged	https://www.scd.stfc.ac.uk/Pages/DL_POLY.aspx
GROMACS	GPL/LGPL	http://www.gromacs.org/
GULP	Proprietary Academic free and commercials are charged	https://gulp.curtin.edu.au/gulp/news.cfm
LAMMPS	GPL	https://lammps.sandia.gov/
NAMD	Proprietary Academic free and commercials are charged	https://www.ks.uiuc.edu/Research/namd/
Py-ChemShell	LGPL 3	https://www.chemshell.org/documentation
Tinker	Proprietary Academic free and commercials are charged	https://dasher.wustl.edu/tinker/
Vampire	GPL	https://vampire.york.ac.uk/

These codes are supported by an estimated investment of €6.9m.

The FOSS mesoscopic modelling market

Table 3 Mesoscopic FOSS software and its licensing lists the mesoscale software on the FOSS market:

Table 3 Mesoscopic FOSS software and its licensing

Code	License	
DL Meso	Proprietary Academic free and commercials are charged	https://www.scd.stfc.ac.uk/Pages/DL_MESO.aspx
ESPResSo-Extensible Simulation Package for RESearch on Soft Matter	GPL v3	http://espressomd.org/wordpress/
HOOMD-blue	BSD	http://glotzerlab.engin.umich.edu/hoomd-blue/
LIGGGHTS	GPL v2	https://www.cfdem.com/liggghts-open-source-discrete-element-method-particle-simulation-code
OCTA	Proprietary free Commercialised version via J-OCTA	http://octa.jp/#intro
ParaDis	LGPL	http://paradis.stanford.edu/
Quasicontinuum	GPL v2	http://qcmethod.org/

These codes are supported by an estimated investment of €4m.

The FOSS continuum modelling market

Table 4 Continuum FOSS software and its licensing lists the continuum software on the FOSS market:

Table 4 Continuum FOSS software and its licensing

Code	License	
Calculix	LGPL	http://www.dhondt.de/
Cantera	Proprietary free	https://cantera.org/
CatalyticFoam	GPL v3	http://www.catalyticfoam.polimi.it/
Code Aster	GPL	https://code-aster.org/spip.php?rubrique2
Code Saturne	GPL v2	https://www.code-saturne.org/cms/
Damask	GPL v3	https://damask.mpie.de/bin/view/Home/WebHome
Elmer FEM	LGPL	http://www.elmerfem.org/blog/
Goma	GPL	https://www.gomafem.com/
OpenFoam	GPL	https://www.openfoam.com/
OpenPhase Core	GPL v3	https://openphase-solutions.com/
Peridigm	BSD	https://peridigm.sandia.gov/
SALOME	LGPL	https://www.salome-platform.org/

These codes are supported by an estimated minimum investment of €3.6m.

Thus, the total “hidden” market we uncovered would contribute € 29.3m.

7. Conclusions and Outlook

The total market size for materials modelling software is estimated to be in the range of €339.5m, based on an analysis including the major companies active in the field as well as a relatively large number of small companies (total of 72). The share of discrete modelling is in the range of €85m, i.e. about 25% of continuum materials modelling. As the focus of the big enterprises is more on engineering modelling, PLM etc., the materials modelling market is dominated by a large number of small enterprises (up to 50 employees) making up about 76.4 % of the players, and most business located in the €1m to €5m range, both for discrete and continuum modelling.

Regarding Market growth, there are hardly any data available on past market sizes. An estimate of the discrete materials modelling market published in a previous Goldbeck Consulting report[10] was €45m ($50m) in 2011, which means a 4-5% annual growth rate. That has also likely been the long-term average growth rate since the early days of materials modelling, when according to unpublished reports the market size in 1990 was about $20m. In contrast, the continuum materials modelling market has likely grown at a similar rate to the CAE market overall, which is in the range of 10-12% per annum. Circumstantial evidence for that include the growing use of continuum models for materials applications and the strong growth of software companies based specifically on continuum materials modelling (for example e-Xstream) and the closer integration of continuum materials modelling with the much larger CAE field. Due to the stronger ("multiscale") integration, evidenced also by the continued acquisitions of materials modelling companies by CAE/PLM players, a stronger pull-through demand for materials modelling overall, hence also discrete materials modelling is expected.

The current report did not include the market for materials data nor the emerging materials modelling solutions based on data-based models, ML and AI. We can expect to see a confluence of materials modelling and data technologies into a broader materials informatics market, where physics-based models together with experiments provide a source of data as well as insights, while data-based models, ML and AI greatly enhance the capability to utilise our heterogeneous knowledge sources for maximum benefit.

Traditional players in the materials data field include CCDC[nn] and ICSD[oo] (Crystallographic Data) in terms of atomistic representations, as well as Granta Design[pp] (now part of Ansys) regarding macroscale properties. In the field of ML and AI there are of course generic technologies offered by big players such as IBM and Google, open source solutions such as Tensorflow[qq] and more engineering focussed companies such as Mathworks[rr]. A more dedicated materials offering is developed by Citrine[ss] and Intellegens[tt].

[nn] https://ccdc.cam.ac.uk/

[oo] https://www.psds.ac.uk/icsd

[pp] https://www.ansys.com/products/materials/ansys-granta-materials-data-for-simulation

[qq] https://www.tensorflow.org/

[rr] https://www.mathworks.com/

[ss] https://citrine.io/

[tt] https://intellegens.ai/

Finally, there is a nascent market in quantum-computing solutions for computational chemistry. There is a wide interest in this potential breakthrough technology, with chemistry and materials science covered by some large enterprises with hardware interests (IBM, Google) as well as dedicated quantum computing software providers such as Cambridge Quantum Computing[uu], Phasecraft[vv], Riverlane[ww], HQS Quantum Simulations[xx] and SaaS provider Qu&Co[yy].

As advances in materials are at the core of providing solutions to many societal issues and our need increases to integrate materials more closely into a future digital tapestry of designing, developing, manufacturing, using and re-cycling products, the current materials modelling and emerging materials informatics market will remain dynamic and is likely to grow strongly.

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Disclaimer

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[uu] https://cambridgequantum.com/

[vv] https://www.phasecraft.io/

[ww] https://www.riverlane.com/

[xx] https://quantumsimulations.de/

[yy] https://quandco.com/

Acronyms

AEC - Architectural Engineering and Construction

AI - artificial intelligence

BSD - Berkeley Software Distribution

CAD - Computer Aided Design

CAE - Computer Aided Engineering

EDA - Electronic Design Automation

EMMC - European Materials Modelling Consortium

FOSS – Free and Open Source Software

FTE - Fulltime Employee

FY - Financial Year

GPL - GNU General Public License

LGPL - GNU Lesser General Public License

MIT - MIT License is a permissive free software license originating at the Massachusetts Institute of Technology (MIT)

ML - machine learning

PLM - product lifecycle management

QSPR - Quantitative Structure Property Relations

TCAD - Technology computer-aided design

Appendix 1: Enterprises included

Small Enterprises

Alphastar Coorporation	Continuum	8% CAE correction based on number of FTEs
Asimptote	Continuum	8% CAE correction based on number of FTEs
BEASY	Continuum	Number of FTEs
CCDC	Discrete	Number of FTEs
Computherm	Continuum	Number of FTEs
COSMOS	Discrete	Number of FTEs
Crystal	Discrete	Number of FTEs
CrystalMaker Software Ltd	Discrete	Financial Report
Culgi	Discrete	Number of FTEs
DANTE	Continuum	8% CAE correction based on number of FTEs
DCS Computing	Continuum	Number of FTEs
ESRD	Continuum	8% CAE correction based on Number of FTEs
Electricant	Continuum	Number of FTEs
Espeem	Discrete	Number of FTEs
Exabyte	Discrete	Number of FTEs
FaccTs	Discrete	Number of FTEs
Gaussian Inc	Discrete	Number of FTEs
GTT	Continuum	Number of FTEs
HyperSizer	Continuum	8% CAE correction based on number of FTEs
MatCalc-Engineering	Continuum	Number of FTEs
Materials Design	Discrete	Number of FTEs
MATFEM Partnership	Continuum	8% CAE correction based on number of FTEs
Math2Market GmbH	Continuum	Financial Report
MicroMagus	Continuum	Number of FTEs
Molcas	Discrete	Number of FTEs
Molpro	Discrete	Number of FTEs
MOLSIS Inc.	Discrete	Number of FTEs
Nanomatch	Discrete	Number of FTEs
Petachem	Discrete	Number of FTEs
ProSim	Continuum	8% CAE correction based on financial report
Q-Chem	Discrete	Number of FTEs
QM Simulations Inc.	Discrete	Number of FTEs
Quantemol	Continuum	Number of FTEs
QWED	Continuum	Number of FTEs
RDMChem	Discrete	Number of FTEs
Scienomics	Discrete	Number of FTEs
SCM	Discrete	Number of FTEs
Semichem Inc.	Discrete	Number of FTE
Sente Software Ltd	Continuum	Based on financial report
Simune	Discrete	Number of FTEs

SSA	Continuum	8% CAE correction based on financial report
SuessCo Simulations	Continuum	Number of FTEs
SunergoLab Inc	Continuum	Number of FTEs
TCAD others (GlobalTCAD solutions, Crosslight, Cogenda Software, …)	Continuum	8% CAE correction based on share of TCAD market
ThermoCalc	Continuum	Number of FTEs
Third Wave Systems	Continuum	8% CAE correction based on number of FTEs
TIBERLAB	Discrete	Number of FTEs
Turbomole GmbH	Discrete	Number of FTEs
VASP Software GmbH	Discrete	Number of FTEs
Vextec	Continuum	8% CAE correction based on number of FTEs
Virtual Lab	Discrete	Number of FTEs
Wavefunction	Discrete	Number of FTEs
Wien2k	Discrete	Number of FTEs
X-Ability	Discrete	Number of FTEs
Zacros	Discrete	Number of FTEs

Medium Enterprises

Access e.V.	Continuum	Number of FTEs in their Software Department
Transvalor	Continuum	8% CAE correction based on Number of FTEs

Large Enterprises

Altair	Continuum	5% CAE correction on financial report 8% CAE correction on DEM Solutions Ltd financial report
Ansys	Continuum	5% CAE correction on financial report
AutoDesk	Continuum	8% CAE correction for Moldflow revenue
AutoForm	Continuum	8% CAE correction based on number of FTEs
COMSOL	Continuum	8% CAE correction based on number of FTEs
Dassault Systèmes	Both	8% CAE correction for ABAQUS revenue 5% CAE correction for SIMULIA revenue Financial Report for Materials Studio Number of FTEs for Cosmologics
Engineering Center Steyr GmbH & Co KG	Continuum	8% CAE correction based on number of FTEs
ESI Group	Continuum	5% CAE correction on financial report
Fujitsu	Discrete	Number of FTEs based in FQS Poland
Hexagon	Continuum	5% CAE correction based MSC's financial report Number of FTEs for e-Xstream
JSol Corporation	Both	Number of FTEs in materials science 8% CAE correction on number of FTEs in CAE
Schrödinger	Discrete	Number of FTEs in Materials Science
Siemens	Continuum	8% CAE correction for NASTRAN and STAR-CCM+ revenues

		5% CAE correction based on PSE's financial report Number of FTEs for MultiMechanics
Silvaco	Discrete	8% CAE correction based on share of TCAD market
Synopsys	Both	8% CAE correction based on share of TCAD market Financial Report for QuantumWise

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