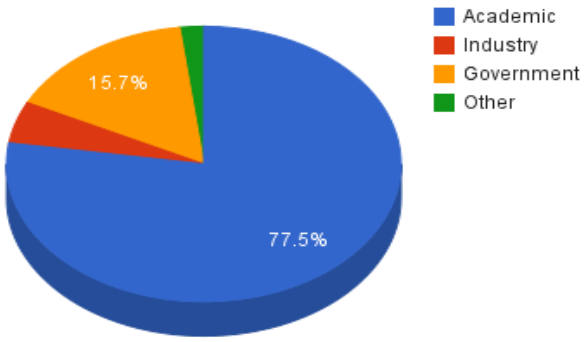
SURVEY ON STATUS AND PROSPECTS OF MULTISCALE MODELLING IN THE EUROPEAN UNION

We have conducted an online survey contacting over 2 000 researchers in industry, government and academics to gather information about the multiscale simulation research community in Europe and the world and establish a joint vision of multiscale modelling and simulation for the future. The survey comprised twenty questions (aiming at a high response rate), which addressed the background of the respondent, the present involvement in multiscale modelling and high performance computing (HPC), and its prospects for the future.

More than 200 representatives from all over the world completed the survey, most responses coming from Spain (30%), Germany (26%) and France (23%). Other European countries have also largely responded (20%) while the respondents from Japan, India and USA amount to 2%.

Background of the respondents

The majority of replies came from academic institutions (79%) and the rest from government institutions (16%) and industry (5%) (see Figure 1). Most representatives are from large institutions (>250 employees) but about 9% work for small and medium enterprises (SMEs) reflecting their interests in multiscale modelling (see Figure 2). Interestingly, only two thirds of these institutions have a modelling department relevant to their field of research, showing a high potential for growth.



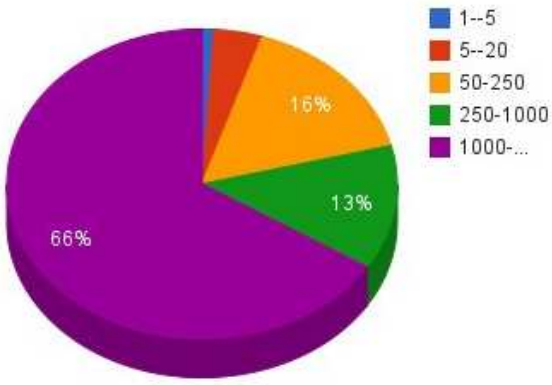


Figure 1: ***Institutional distribution of respondents*** **Figure 2:** ***Institutions size***

Nearly 75% of the respondents are developers of simulation methods and 85% have access to HPC ressources.

Responses came from many different scientific backgrounds, dominated by physics (75%), chemistry (40%) and material sciences (30%) (multiple answers were possible). Engineering and life sciences contribute to about 15% each.

The majority of responses came from respondents performing theoretical research (80%) as opposed to experimental research (see Figure 3). Quantum chemistry and atomistic molecular modelling are the most widely used simulation methods (over 50% each) that have been used in the past five years, followed by coarse grained and continuum methods (see Figure 4).

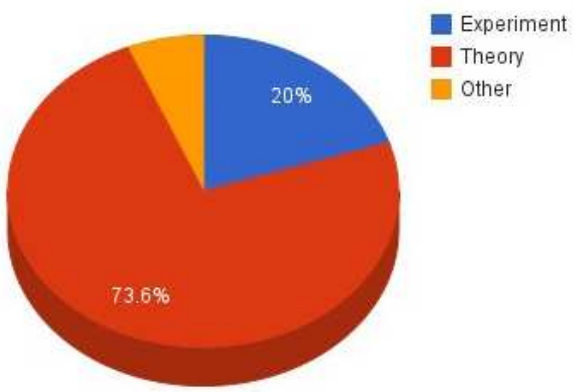


Figure 3: ***Main focus of research***

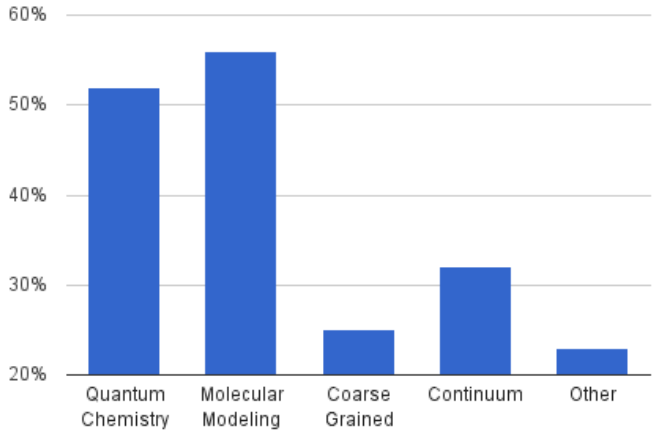


Figure 4: ***Methods presently used***

Key application areas of research are nanoelectronics, biomolecular simulations, single molecule biophysics, astrophysics and polymer dynamics.

Prospects of multiscale modelling

Most respondents believe that multiscale modelling techniques have a quite significant impact in their field of research, without reaching their optimal impact however. Nearly 75% of the respondents expect a fast growth of impact of these methods in the near future (see Figures 5).

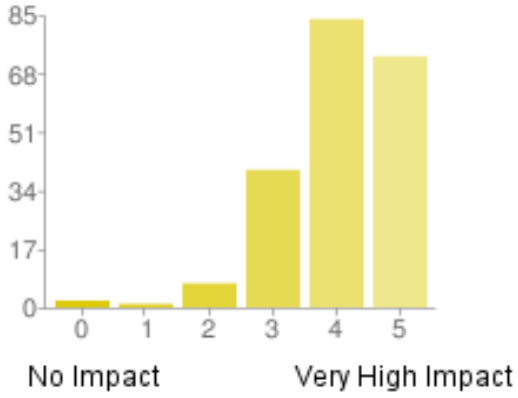


Figure 5(a): ***Present overall impact of modelling and simulations in the respondent's field***

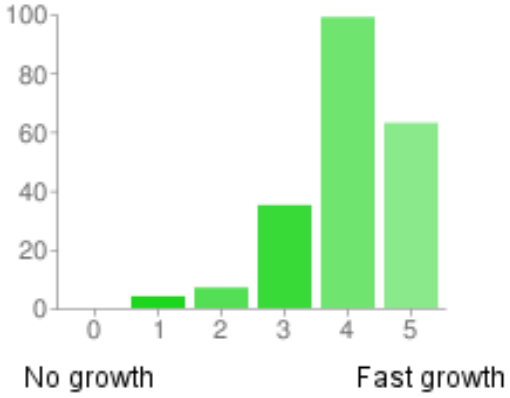


Figure 5(b): ***Expectations of growth of impact of modelling and simulations in the respondent's field***

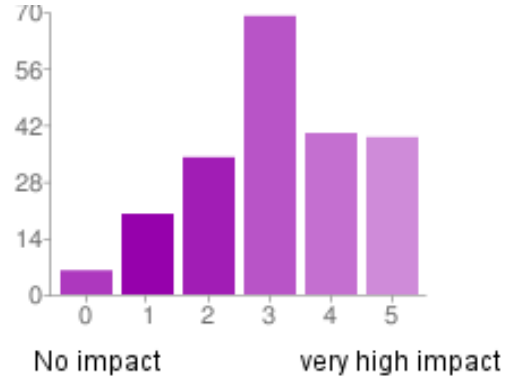


Figure 5(c): ***Present overall impact of multiscale modelling in the respondent's field***

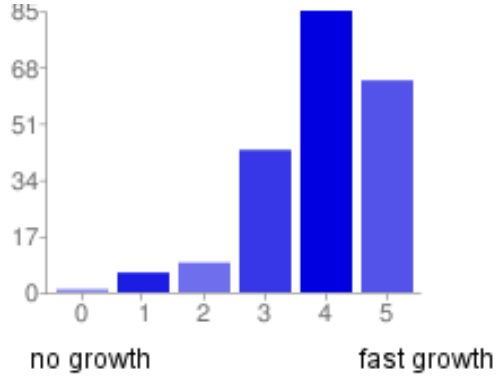


Figure5(d): ***Expectations of growth of impact of multiscale modelling in the respondent's field***

The fastest growth of impact of multiscale modelling methods is expected in the field of biomolecular simulations for large complex bio-systems (including membranes), drug development and functional genomics; and interfaces between different materials in nanoelectronics, energy storage systems, electronics, nanotechnologies and material science.

Over 50% of the respondents esteem the funding in the area of multiscale modelling to be not presently sufficient to fully realize this potential (see Figure 6). The respondents are also mainly neutral in assessing the competitiveness of the funding levels within the EU in comparison with other regions (see Figure 7). The majority believe nonetheless that EU funding schemes would be very suitable to realize the impact of multiscale modelling (see Figure 8).

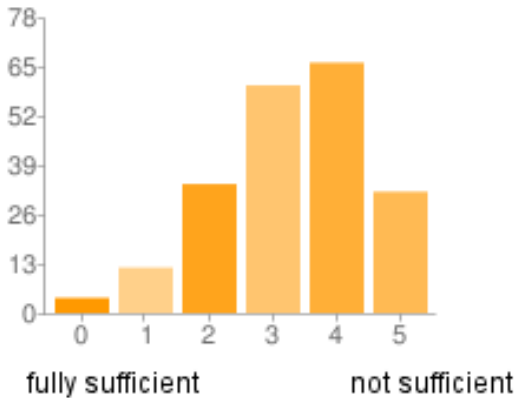


Figure 6: ***Adequacy of present funding levels***

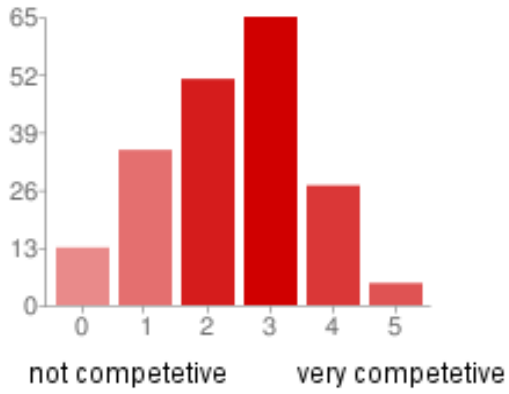


Figure 7: ***Competitiveness of present funding within the EU in comparison to other regions***

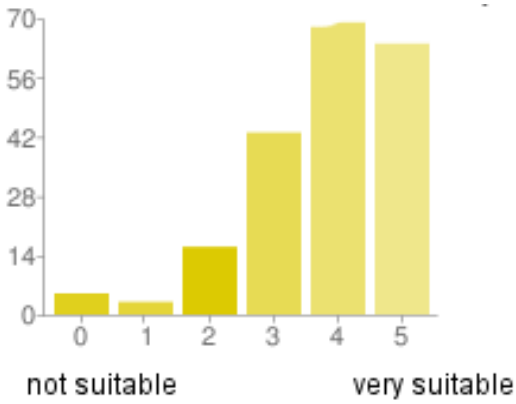


Figure 8: ***Suitability of EU funding schemes to realize the impact of multiscale modelling***