

The Computational Perspective

CORPORATE STRUCTURE AND COMPUTATIONAL CHEMISTRY

Large chemistry based corporations have finally come to the conclusion that they need a faster, more cost effective means for finding chemical information. Their competition is exacting a great price in terms of their research investment at a time when corporate profits are under pressure. In short, there is something approximating a crisis loose in today's research environment. In a time of crisis corporations seem more willing to accept change and, in fact, actually seek change. For their salvation they seem to be turning to computational chemistry more as a last resort than as a promising solution. The first problem which they confront is, inevitably, the question of where to fit this capability into their organization.

Today's chemical research division can often be found divided into some five subdivisions which are dictated by the now rather broadly accepted divisions of chemistry. One finds an organic division, an inorganic division, an analytic division, etc. Little thought has been given to why a research division is arranged in this manner but it becomes immediately clear that computational chemistry is somewhat different. It doesn't fit neatly into the existing picture. Nor, for that matter, is there any reason why it should.

The major divisions of chemistry are largely dictated by the research techniques that they use and the matter which is being worked on. Stated somewhat more simplistically, experimental chemists have a limited body of techniques and they do what research they can with them. In fact, the techniques available dictate how one approaches a research question. One asks the questions which one is able to ask and not always the questions which one might want to ask. Thus research organization is dictated by considerations that can certainly not be considered optimal. Computational chemistry has its own limitations but they are not the above.

A major problem for the computational chemist in the research environment is that the people to whom he must report have a somewhat limited and rather tightly focused way of structuring research projects. The computational chemist must ask his research questions in a very different manner if he is to be effective. This is of necessity the case as the computational chemist is working with information at the level of the wave function. The experimental chemist is working with information which is often many levels removed from the wave function. It might be useful to point out that what the experimentalist measures is also limited by what the wave function will permit him to measure even though he is working with information that is many levels removed. It is one of the basic ideas of Quantum Mechanics that one can obtain no information which is not contained in the wave function. I emphasize this point because it is just this difference which has some rather significant implications for organization structure.

The research director probably has no clear idea about what it is that computational people do. He simply wants them to do it and make him look good. The head of the organic division who reports to him also has no clear idea what computational people do. He simply would like to take credit for it, if things work out. The same can be said about the other division heads. With this situation in force where should one establish a computational chemistry effort?

Some corporations who have requested anonymity simply threw up their hands and established a group under a miscellaneous organizational box called "Vice President or Manager for Research Services." This is a functionality which handles the hiring of research secretaries and janitorial personnel. Dealing with the problem in this fashion will probably not guarantee failure but

it most certainly will not ensure any quick success either. The computational group will spend the next several years trying to make their case to top management for moving out of this situation. The problem which will severely limit their usefulness is one of information.

Whether or not anyone now in a research hierarchy likes the idea, it will be necessary for the computational chemistry group to tell the research director how to best use their capabilities. The head of the computational chemistry group will have to have access to the same information that the divisional research directors have access to. This person can not permit information about research goals and directions to be filtered through any other divisional head who has no clear perception about what such a group can and cannot do. To subordinate the computational chemistry head to one of the divisional directors is a guarantee that they will be ineffective. It may require a few years for this to become evident but it will happen. The computational chemistry head must sit at the same administrative level as the divisional heads. If it would satisfy ego needs of the other directors one need not call this person a director.

Another major difference in the operation of such a group is that the people within it would usually not operate as an autonomous entity as other groups tend to do. The computational head would, in reality, distribute his forces among the other groups on a project-by-project basis and pull them out when they have made their contribution. As other groups became more aware of what can be done computationally, this process would become more iterative and, in many cases, I would expect to find the other divisions developing their own personnel to carry out fairly routine calculations and to act as interfaces to the computational people. There is yet additional information in this observation.

The initial role of the computational group would change fairly early and a long term operational mode would appear. In the beginning the purpose would be to show what could be done and how it could assist in the overall research effort. As time goes on and the demand for computations increases, it would be the case that divisions that were heavy users would take on an increasing amount of the effort themselves and depend on the computational group for advice in large or especially troublesome situations, and to bring new tools into the system. One would then have a distinct role for computation and would be well advised to accept the fact that there should be a Computational Chemistry Division on the organization chart.

Resistance to such a development may certainly come from the other research directors who are interested in protecting their turf. They will undoubtedly develop arguments about proliferation of titles and organizations. These arguments will prove weak, however, in the face of the information requirement described above and the fact that the traditional director has no concept as to how to best use a computational group.

Another argument for the type of structure described above is that if the computational effort bears no fruits it will be immediately clear who is to blame and who can be released. The direct responsibility will be obvious. Certainly this option should appeal to a research director and the corporate board of directors as well.

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