

"Smart Models" - a framework for adaptive multi-scale modelling

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Abstract

The business environment facing the ECPI (European Chemical & Process Industry) is changing at an ever-increasing rate, bringing with it new challenges to process engineers which the current generation of CAPE tools are ill-equipped to help them address. This paper puts forward a view of some of the challenges and offers some thoughts on a potential way forward.

Keywords: multi-scale modelling, smart models, adaptive models

1. The Business Challenge

The ECPI is now confronted with a *step-change in its global business environment.* For example, analyses by CEFIC SusChem [1], Chemicals Vision 2020 [2] and EUREKA Project 2311: CAPE-21 [3] have identified a number of major commercial, technological and societal challenges in the global marketplace. SusChem concludes that failure to address these challenges effectively will result in a dramatic decline in the ECPI's competitiveness and profitability, with a damaging impact on the EU's economy.

2. New CAPE Challenges in a Changing Business World

Process modelling and simulation have long been established as the primary weapon in the process engineer's armoury but there are a number of key areas where today's capabilities struggle to address the new business challenges:

- complex materials & mixtures, multi-phase systems, particulates;
- models of sustainable processes, including "natural" raw materials and biological species;
- more detailed unit operations models (micro- and bulk-mixing, surface interactions, turbulence, etc);
- models in manufacturing: models are typically not transferred from engineering to manufacturing;
- extended *enterprise* models typically contain only a very approximate model of the plant itself ;
- virtual organisations (VO): specialisation and collaborative working between companies, often on a world-wide basis;
- adaptive models and links to measurement systems; and,

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- performance: radically-improved performance will deliver significant benefits in both design & operations.

There seems to be an *infernal triangle* of trade-offs between model performance, quality/detail and scope. For a given technology, this triangle seems to have a constant area - we cannot "break" it in any meaningful way without a **radical change in technology**.

Charpentier and McKenna [4] also recognised the need for an integrated multidisciplinary and multi-scale approach to meet the needs of the CAPE industry today. They recommend simultaneous research in four directions:

1. total multi-scale control of the process to increase selectivity and productivity;
2. process intensification by design of novel equipment based on scientific principles and new production operating methods;
3. the synthesis of structured products, combining several functions and properties required by the customer, with special emphasis on complex fluids and solids technology; and,
4. the implementation of multi-scale and multidisciplinary computational modelling and simulation for real-life situations.

It is the latter item that we will concentrate on in this paper.

3. Modelling & Simulation Technologies

3.1. The multi-scale challenge

Many new business opportunities/high-value-added areas are inherently **multi-scale** - they involve complex micro/nano-scale materials (including bio-materials and structured/heterogeneous "natural" materials). These business activities also operate at *multiple timescales*, from reaction kinetics to supply and distribution chains.

Behaviour at each scale directly or indirectly affects that at all other scales and so it is necessary to be able to model simultaneously at all relevant scales, to integrate (or "aggregate") the modelling at the different scales and thus to predict "inter-scale interactions". For example, there is an increasing need to be able to model micro/nano-scale interactions at interfaces between phases. Catalysis, bio-activity, particle formation & growth, etc., depend on micro-mixing and interfacial effects at phase boundaries.

Hitherto, models have typically either ignored this continuum of scales in both time and space or have tackled them separately (i.e. there have been several models operating at different scales, with human intervention to interpolate and rationalise between them). Today's and tomorrow's pressures are such that this approach is no longer viable and that we now need a fundamental re-think, aimed at devising a new cohesive framework for multi-scale modelling: a single effective capability providing a flexible, consistent and systematic approach to modelling and simulation across all the scales – "from molecules to the marketplace" – and embracing the currently disparate technologies, such as MD (molecular dynamics), CFD, CAPE and business models.

3.2. A multi-scale model?

It is important to recognise that the individual scales (or levels of detail of representation) represent "slices" of a *pseudo-continuum* – from molecules to business chains – and that, for any given problem, a different combination of scales may be

required. Flexibility must therefore be maintained for users to select the most appropriate approach and to modify it as their needs evolve. For instance, depending on the purpose at hand, the following might be required:

- A reactor model may incorporate a broad variety of phenomena and sub-processes: molecules and their reactions; bio-materials and mixtures, organisms; multi-component, multi-phase fluid mixtures and their properties; particles, pellets and beds; mixing and fluid flow; phase aggregation and separation; internal equipment items (e.g. stirrers, heater/coolers); and so on. Basic information on, for example, properties, kinetics, thermodynamics, etc, may be predicted from first-principles MD or bioscience.
- Such a model might then be incorporated into a whole-flowsheet model (for example, to examine the potential impact of recycling, awkward separation issues or flexibility, dynamics and control).
- Finally, the whole may be embedded into a business model of the supply and distribution chains, for example, to optimise their dynamic capabilities to match the dynamic requirements of the marketplace and to assess the potential impact of both technical and commercial uncertainties.

Such "modelling across the scales" will enable a variety of problems to be addressed:

- Micro/surface mixing/flows will determine how catalysts behave and thus which reactions occur and how fast they occur. This will enable the prediction of, for example, hotspots and the impact of processing history on product micro-structure and properties.
- Optimised integration of kinetics, hydrodynamics and thermodynamics, for example, in the development of novel process equipment (i.e. multi-function, intensification, miniaturisation).
- Integrated development of products, processes and business chains for the global optimisation of the extended enterprise, as an integrated whole *from molecules to marketplace.*
- Improved processing of "structured" materials, such as wastes and renewables.
- "Indirect" measurement and control, including soft sensors.

3.3. Can this be delivered using today's technologies?

With today's technologies, such multi-scale models might be attempted, for example, by embedding MD into kinetics/thermo/properties (K/T/P) calculations, K/T/P into CFD, CFD into CAPE and CAPE into a business modelling program (!) . A typical approach hitherto has been to select two modelling systems at two different scales and then to develop special-purpose code (typically both problem- & system-specific) to enable them to exchange information. However, a number of serious problems arise with such an approach, even on such a limited basis:

- Such an approach can only be attempted by highly-skilled modelling experts, not by the practising engineer.
- The number and nature of the "scales" would effectively be pre-defined and may be entirely inappropriate for the problem at hand (and the appropriate scales may well change as study of the problem evolves).
- Serious problems would remain regarding the adequacy of the model and its "fitness for purpose". For example, CFD has serious limitations in such areas as multi-phase flows, complex rheology and/or surface-scales [6] and MD currently struggles with simulations involving complex molecules.

- Such a deeply layered integration of pre-existing, self-contained systems will be large, difficult to solve and compute-intensive, both to develop and to use, and, more importantly, success is by no means guaranteed.

G.D. Ingram *et al.* [5] have shown that micro-scale and macro-scale models cannot be combined with complete freedom and that those that can be combined are limited and restricted. They do provide a preliminary compatibility table of frameworks. For all practical purposes, an effective multi-scale modelling capability cannot be delivered by combining today's systems. A fundamentally new approach is required, one which is designed from the outset to encompass the full range of length and time scales and to operate effectively within the context of a virtual organisation.

4. "Smart Models" - a Flexible Framework for Adaptive Multi-scale Modelling & Simulation

Performance/quality conflicts are not new! In some contexts, methods have been developed to alleviate the problem. For example, variable step-length integrators and adaptive mesh techniques and now standard in most numerical codes for solving differential equations. The key features of these techniques are typically that they are auto/adaptive, and therefore embody metrics to define the "quality" of the model and/or the solution, and that the resulting models are implicitly "mixed granularity" in that the step lengths or meshes can be on different scales in different parts of the model. The success of these methods then raises the question: *Can we apply such adaptive/granularity concepts to model complexity itself, rather than just to the solution methods?*

We are therefore developing the concept of "**smart models**", a novel hierarchical modelling architecture which incorporates "intelligence" to selectively and to adaptively manipulate the models and incorporate detail and complexity **only** in those areas of the model which are critical to providing an adequate solution and remove or approximate such detail and complexity where it is not. The concept thus reflects how an engineer might tackle such a problem by hand: *start out with some very simple models/assumptions of the individual units, get some idea of flowsheet conditions and then start digging a bit deeper where it seemed justified. This process would then be "looped" until the user felt satisfied that the quality/accuracy of the results was suitable for the purpose at hand.* The engineer thus adapts his/her approach on the basis of perceived "fitness for purpose" and uses a "mixed granularity" model, adapting and modifying the choice of granularity (i.e. of specific scales from the overall continuum) as the solution evolves. Thus, we can imagine a modelling and simulation capability within which the following hold:

- A model consists of a hierarchy of "layers" of increasing detail, complexity and sophistication, potentially spanning the entire *pseudo-continuum* of length and time scales, from molecules to business chains.
- Each layer contains a model definition of some kind and that model has a number of parameters.
- Each layer/model accepts parameters from "below" and calculates the parameters required by the layer "above".
- "Intelligence" (using e-Science capabilities, such as ontologies, languages, agents, etc) could be incorporated at any appropriate point to define and manipulate the models, parameters and solution methods, assess the quality/fitness-for-purpose of

the model and then decide how "deep" to go under any particular circumstances to satisfy the needs of the user

Such an architecture has a number of real advantages:

- It is flexible and extensible and is capable of transparent, scaleable and effective operation on different kinds of computer architecture (from single processors, through parallel architectures, clusters and to the Grid), as the scale and scope of the model and the computing power requirements evolve.[2]
- It provides a flexible, rational, consistent and transparent basis for mixed-granularity models.
- It is straightforward to incorporate "foreign modules", "legacy code", adaptive models, etc., and to integrate with laboratory or plant systems.
- Models can be distributed via the Grid and thus suitable for use in a virtual organisation.
- The performance and robustness of the simplified models could be predicted and "guaranteed", for example, for safety-critical applications
- *Fitness for purpose* can be indicated to the user.

Note that although this paper is limited to discussions on models, *knowledge based working environments* will also be required to support the complex and cross-disciplinary model-building activities, to manage the resulting models and their use across the lifecycle and to support the decision-making processes which will be based on their results.

5. Challenge to the CAPE Research Community: *Practical First Steps*

The present generation of tools has its origins more than 20 years ago. The new challenges are very much more complex than problems addressed to date and delivery of a comprehensive new CAPE-ability and its adoption into widespread industrial practice is a large and multi-disciplinary activity which will inevitably take a number of years (and the resources required are beyond the resources of even the largest centres acting individually). The challenge to the CAPE research community is, therefore, to so organise itself to undertake such initiatives in an efficient and effective manner and to avoid the duplication and fragmentation of its efforts.

As has been remarked, *"the longest journey begins with the first step"*, the objective of this paper is to stimulate discussion and debate (and, where necessary, provoke arguments!) which will lead us to some *"practical first steps"*: what is/are the best way(s) to deliver an effective solution; how can we maximise the synergistic opportunities whilst not hindering a thorough exploration of the alternatives?

References

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[2] Note that there have been some attempts to implement process simulators (today's/yesterday's generation) on high performance computers (usually SIMD). These have not been very successful (a) because SIMD is probably the wrong choice and (b) they involved the implementation of a (serial) code without any meaningful redevelopment/restructuring. What we are proposing is a new generation, *designed* for such architectures (particularly CSP/MIMD)

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