

Industrial Workshop and Model Reduction for Metallurgy

Friday 22nd August, College Court, Leicester, 14:30 – 18:00

In this session we aim to develop links between academic mathematicians and industry. There are three objectives:

- To improve understanding of what facilitates and what limits interactions with industry;
- To scope a set of grant applications related to the IMPaCT Centre for Doctoral Training (CDT) (<http://www2.le.ac.uk/study/research/funding/impact>) of which the University of Leicester is a partner. IMPaCT's focus is on metallurgic engineering;
- To develop an international network of model reduction experts who will be able to visit the UK to collaborate in solving mathematical challenges identified through IMPaCT.

In this session Peter Elkington from Weatherford International (<http://www.weatherford.com/>) will talk about the challenges and opportunities of working with universities, using examples from the geoscience domain. Peter is Weatherford's Chief R&D Geoscientist, responsible for managing projects focussed on advanced processing and data integration, and has over 33 years industry experience in operational, commercial and research posts.

We will also have Jean-Christophe Gebelin, from Doncasters (<http://www.doncasters.com/>), a key partner in the IMPaCT CDT, who will discuss the mathematical challenges facing Doncasters and broader industry. We will also have Nick Green from Doncasters who is the main contact in the development of the IMPaCT CDT.

Professor Jeff Brooks, the Director of PRISM (<http://www.prism2.org/>) at the University of Birmingham will also attend. Jeff has many years of experience in developing algorithms for modelling of materials. Jeff is particularly interested in GPU FGPA programming, and how do we make software implementation more adaptable and reusable on future computational platforms. He would also like to explore techniques for visualisation of multidimensional datasets so that complex systems and interrelationships can be interpreted and demonstrated to "non-experts".

Finally, colleagues from Engineering and Computer Science at Leicester will attend in order to ensure a wide range of expertise in understanding the challenges, and the state of the art in methods of solution, and computational technology available.

We will have a case study presented by Alexander Gorban illustrating high value projects that mathematician can have with external partners. He developed a diagnostic tool for a veterinary company, and this became a REF impact case study.

MintWeld

Here we will describe a recent project in which mathematicians worked with engineers and demonstrates the range of mathematical challenges that arise in the metallurgy industry.

MintWeld was an FP7 project comprising of 11 academic and industrial partners across UK/EU with the goal of developing an integrated modelling framework of the welding and post-welding processes across the whole multiscale/multiphysics range. While the achievements of the project, which finished in September 2013, were very significant with respect to the improvement of models of welding at all scales (electronic, atomistic, mesoscale, continuum), the task of model integration and linking between modelling and industrial processes has proved very challenging.

scale
(time/length)

models

quantum

(10^{-12} s / 10^{-10} to 10^{-9} m)

ab-initio
quantum
mechanical

*thermodynamic data;
force fields, including
Hydrogen-alloy interaction;
interfacial properties
Inter-atomic potentials*

*atomic arrangement at
interfaces*

classical

(10^{-7} s / 10^{-9} to 10^{-8} m)

molecular
dynamics

*interface structure/
thermodynamic
properties of solid-
liquid & solid-solid
interfaces*

*chemistry;
crystal orientation;
stress*

*diffusion of
hydrogen,*

*cohesive zone
model*

structural
integrity,

hot cracking
+
hydrogen
embrittlement

nano-micro

(10^{-3} s / 10^{-9} to 10^{-3} m)

phase field crystal
phase field

*dendrite kinetics;
solidification interface;
microscopic
morphology*

*latent heat; enthalpy
change; grain structure;
local chemistry; thermal
field and local gradients*

*microstructure &
chemistry,
thermodynamics of
fracture/ defect growth,
residual stress,*

calculation of
phase equilibria
and diagrams

grain

(10^{-3} to 10^1 s /
 10^{-4} to 10^{-2} m)

front
tracking

*boundary conditions;
solidification fronts;
mushy zone
permeability*

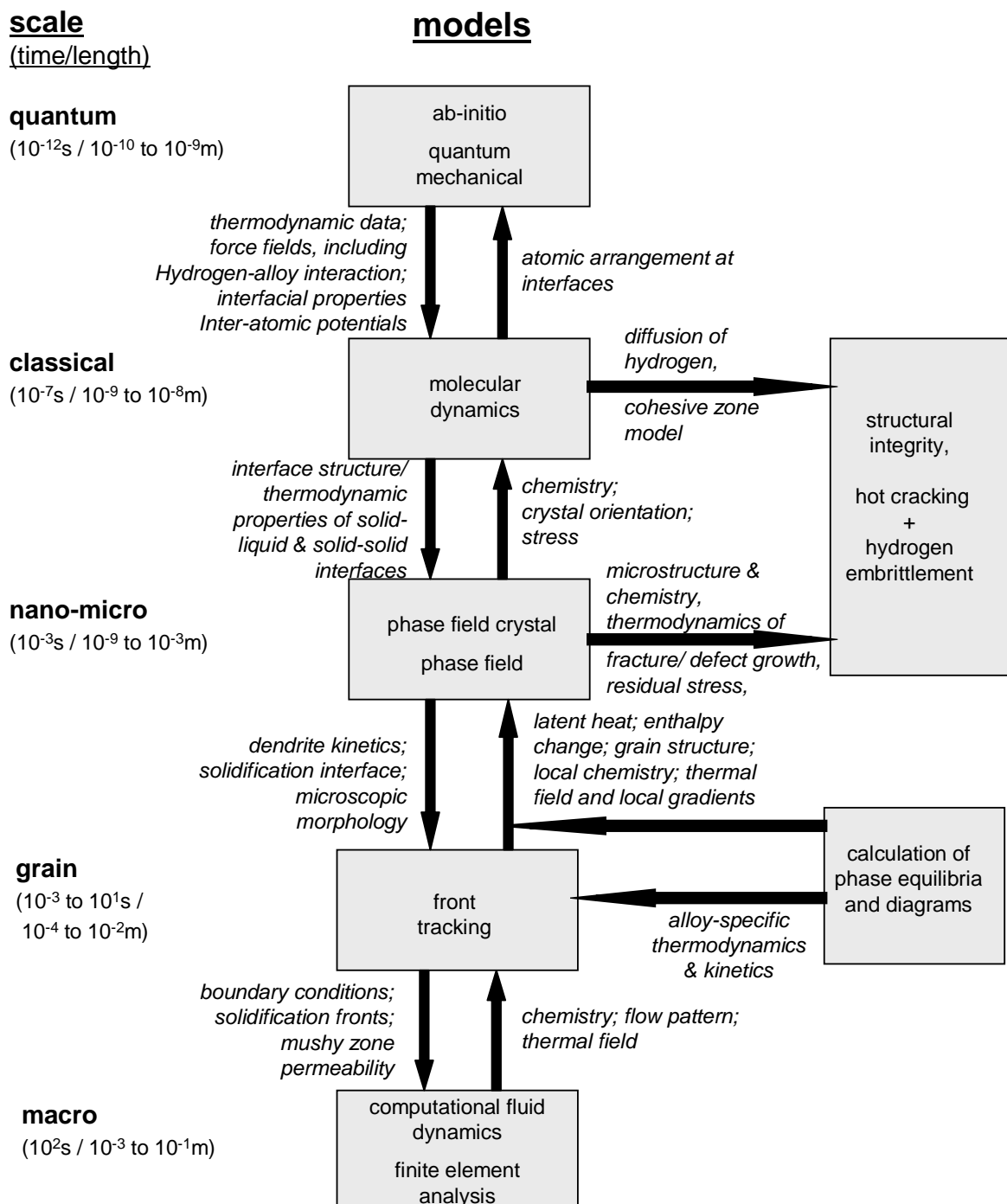
*chemistry; flow pattern;
thermal field*

*alloy-specific
thermodynamics
& kinetics*

macro

(10^2 s / 10^{-3} to 10^{-1} m)

computational fluid
dynamics
finite element
analysis



The above diagram demonstrates the vast range of scales and modelling approaches required for a comprehensive description of welding processes. The project achieved well established data flow and integration between the neighbouring scales (as indicated by the arrows). However, proper integration would require a more holistic approach, probably with the use of mathematical tools within the fields data mining and model reduction, integrated databases of modelling and experimental/validation data, etc.

In a wider context of advanced materials & nanotechnology (AM&N) modelling, many mathematical challenges were identified in a meeting dedicated to the development of the policy for AM&N modelling, simulation and design within the EU Horizon 2020 programmes. For details, see

http://ec.europa.eu/research/industrial_technologies/pdf/leit-materials-modelling-policy_en.pdf

Programme

13:15-14:30	Lunch
14:30-15:00	Weatherford interaction with Universities, Peter Elkington
15:00-15:30	IMPACT DTC and mathematical challenges for Doncasters – Jean-Christophe Gebelin
15:30-16:15	Round table discussion on problems of industrial importance
16:15-16:45	Coffee
16:45-17:10	Feedback from round table
17:10-17:25	Case Study in Data Mining – Alexander Gorban
17:25-17:55	Making a plan for collaboration
17:55-18:00	Close industrial session