

MULTI-SCALE MODELING ENVIRONMENT FOR NANOCELLULOSE APPLICATIONS

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Cellulose nanofibers show a great potential in expanding the use of sustainable raw materials in forest products industry. They will allow paper and board products to be produced with much lower consumption of raw materials, water and energy. They can also be used to develop completely new fiber-based products with characteristics that cannot be achieved with present-day raw materials. Thus, the operation space for research and development will expand considerably. This will cause a big challenge for the traditional way of development work, which is based almost solely on laboratory experiments, pilot and full-scale testing. Virtual product modeling offers a way to significantly speed up product development.

Understanding the effect of nanocelluloses and associated processes on final product properties requires multi-scale analysis. Here we introduce a set of multi-physics simulation tools that enable model-aided analysis of industrial nanocellulose applications. These tools have been developed as a joint effort of several research groups in the Re-engineering paper project of the Intelligent, resource-efficient production technologies (EffTech) research program in Forestcluster Ltd [1]. They describe structural, mechanical and optical properties of paper-like structures based on particle-level models, which cover materials and structures from nano to macro scale, i.e., from atomistic simulations to macroscopic product properties (figure 1). In addition to the detailed description of material characteristics, there is a possibility to vary physical and chemical process conditions while forming the structures.

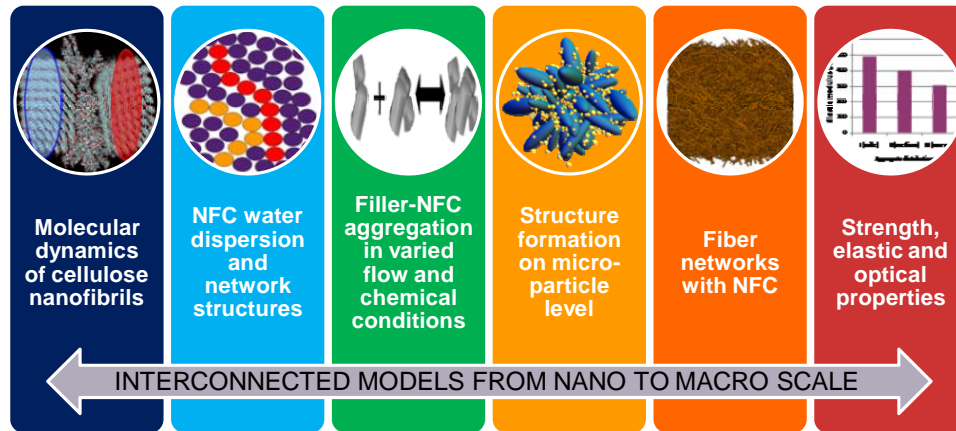


Figure 1. Combining several models enables multi-scale analysis ranging from atomistic simulations to macroscopic product properties.

The developed simulation models describe

- Cellulose nanofibers and their material interactions on an atomistic and molecular level
- Nanocellulose-water dispersion and forming of nanocellulose network structures
- Particle aggregation in varied flow and chemical conditions
- Structure formation on micro-particle level
- Fibre networks with nanocellulose reinforcement
- Strength, elastic and optical properties of sheet structures

Each simulation tool can be used independently but the maximum advantage is gained by combining several solvers together into a multi-scale and multi-physics approach. The simulation tools are integrated with the help of Simantics platform developed recently at VTT [2]. The philosophy of the Simantics is to offer an open high level application platform where different computational tools can be easily integrated to form a common environment for modelling and simulation.

As an example, we present a multi-scale simulation scenario with brief descriptions of the simulations included, and demonstrate an application case. The case includes forming of a nanocellulose composite and analysis of its properties by combining several simulations together. Although the example concentrates on nanocellulose, the adapted generic modeling approach can be applied in many other industrial areas.

The progress presented here can be seen as a first step towards the ultimate goal: Virtual product modelling environment, where different simulation solvers are united to make predictions on product properties based on materials, microscopic structure and production process. When such an environment will be combined with material data base, it will become an effective tool for product development.

[1] <http://www.forestcluster.fi>

[2] <https://www.simantics.org>



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Technical Advances and Applications in Nanotech Products



Multi-Scale Modeling Environment for Nanocellulose Applications

Erkki Hellén and Jukka Ketoja



EffTech

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2010 Intl Conf on Nanotechnology for the Forest Products Ind

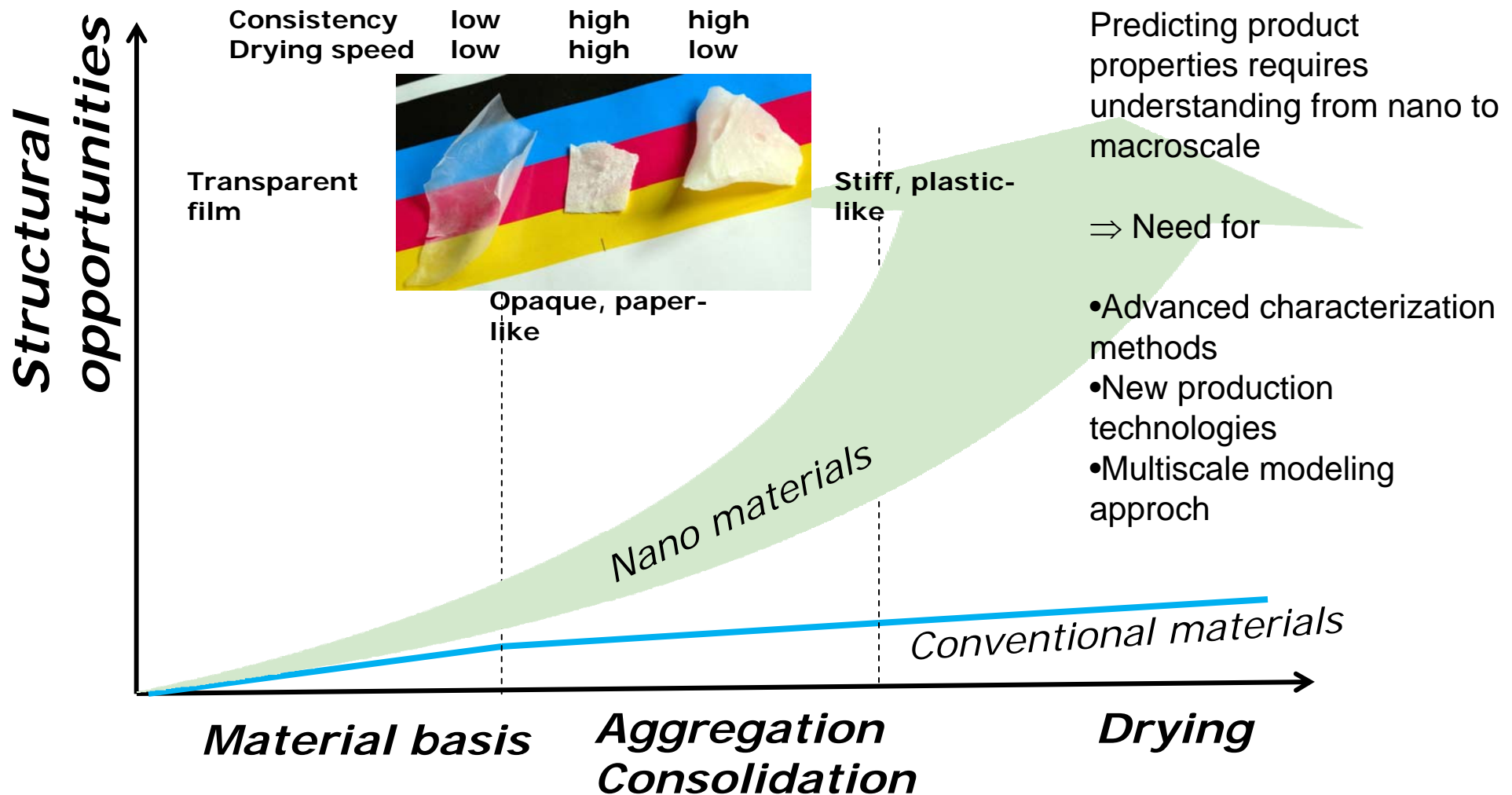
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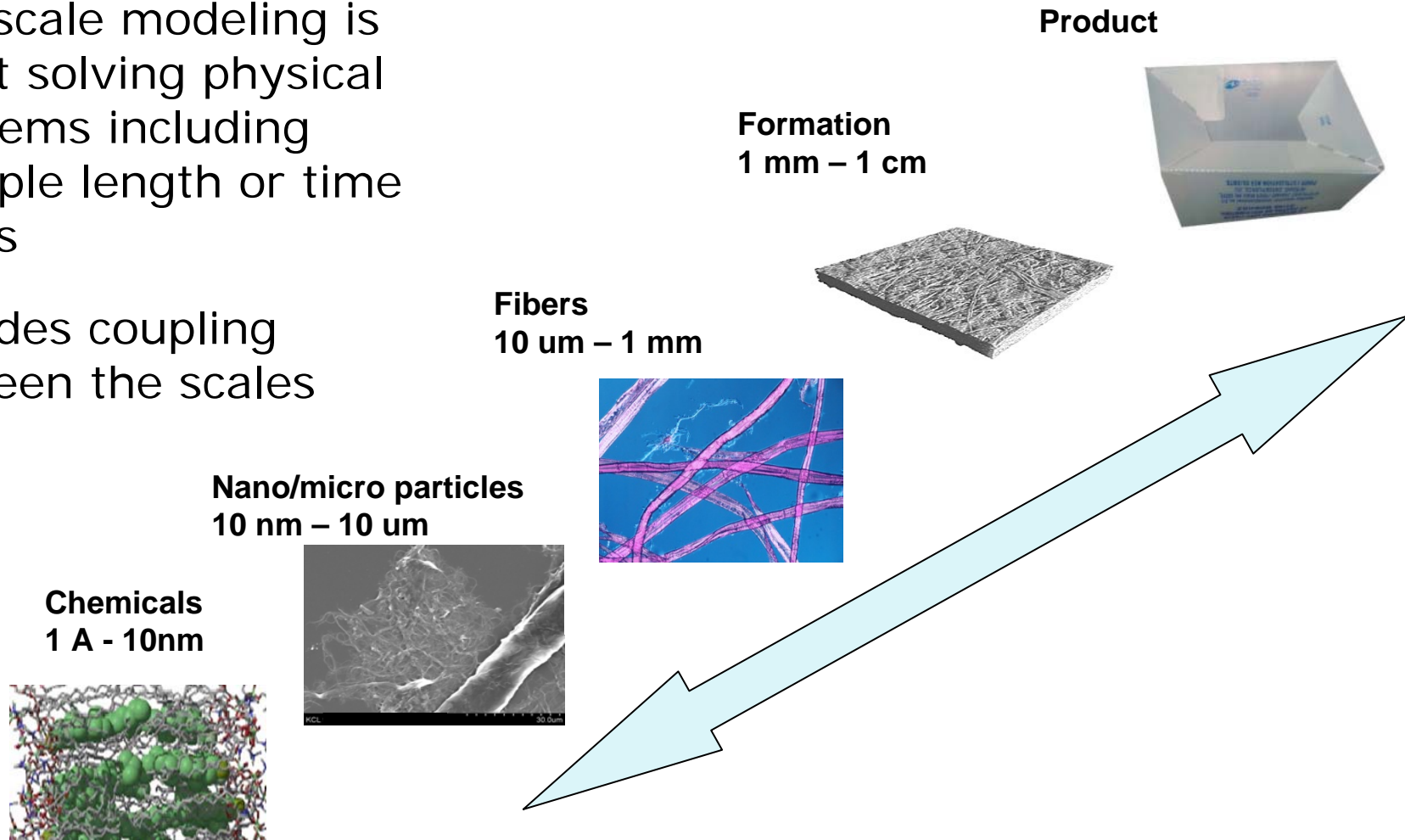
Modeling speeding up up-scaling

Expansion of product properties

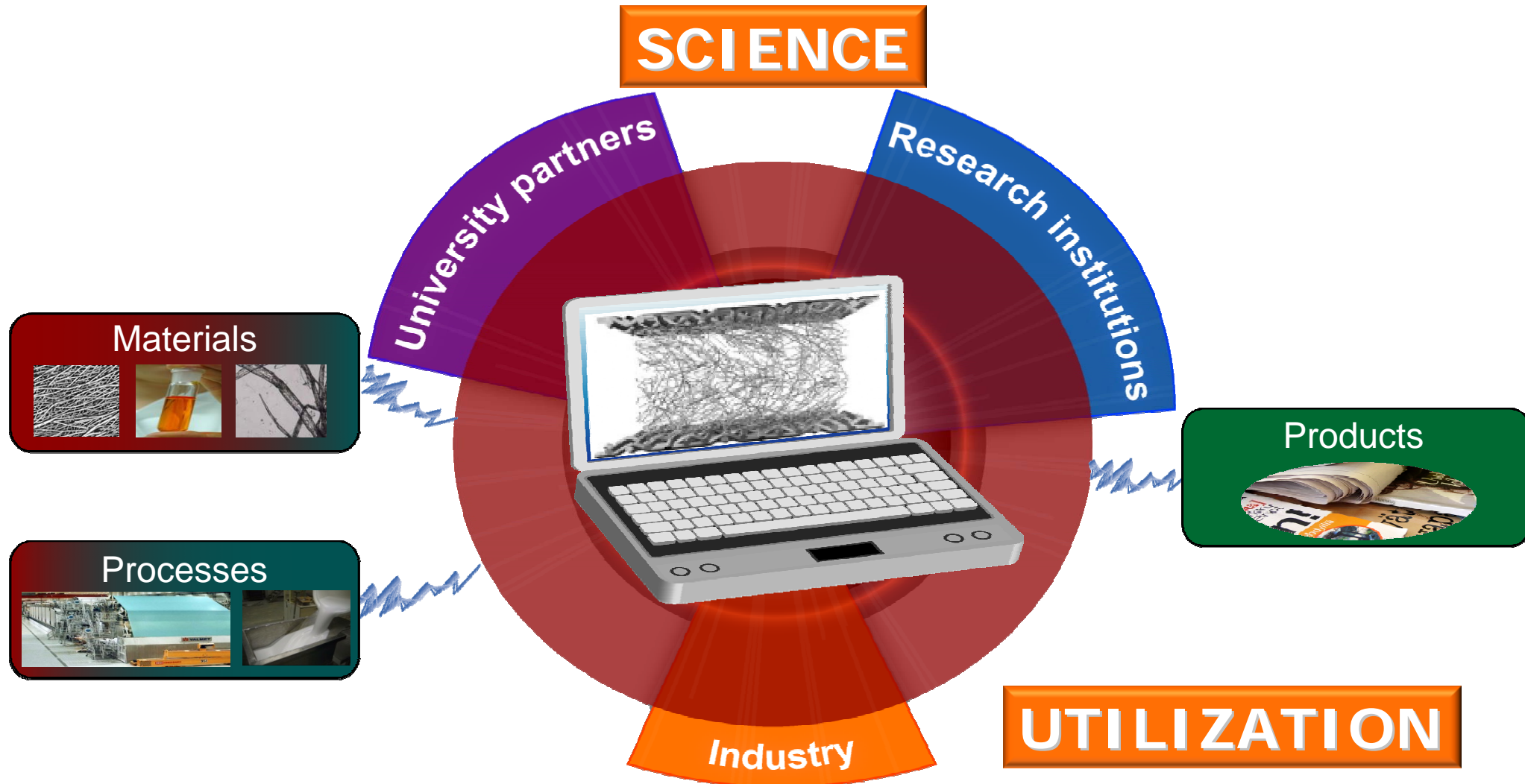


Multiscale modeling

- Multiscale modeling is about solving physical problems including multiple length or time scales
- Includes coupling between the scales



Effectiveness by combined expertise



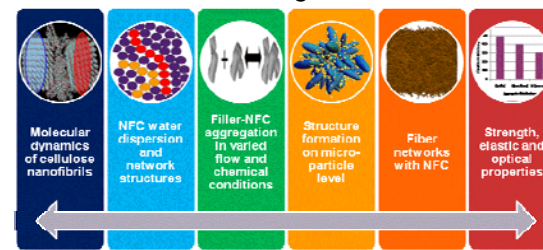
Re-engineering in a Forestcluster project

Novel raw materials (nanocellulose)



Advanced multiscale modeling

coordination Jukka Ketoja, VTT

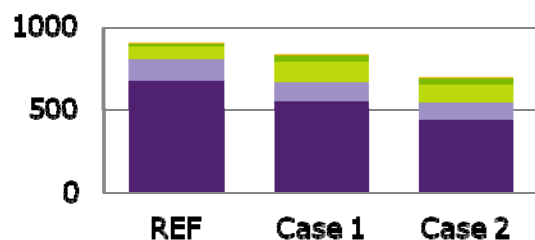


Coordination
Erkki Hellén, VTT

Sustainability, safety and feasibility



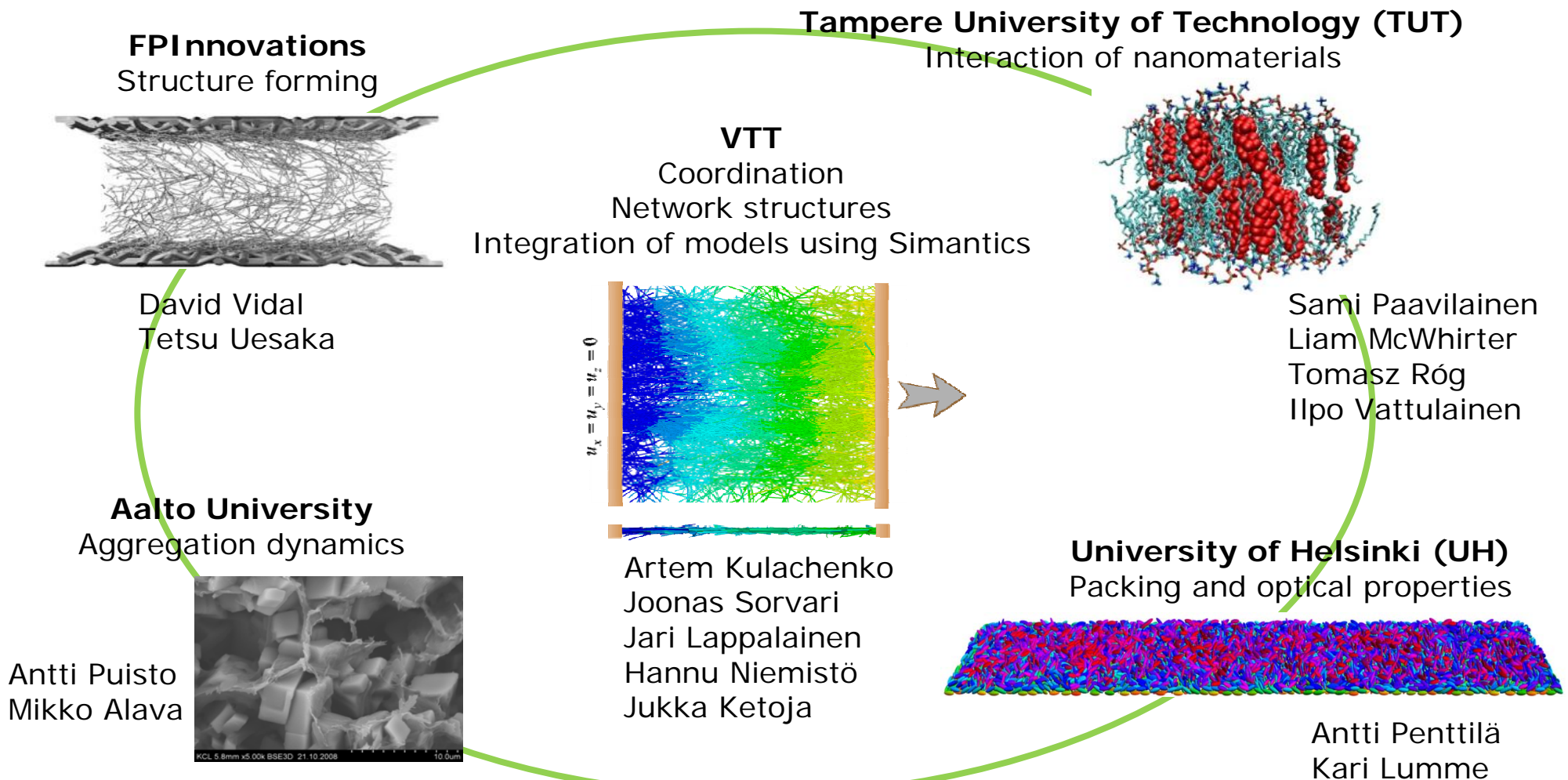
Carbon footprint



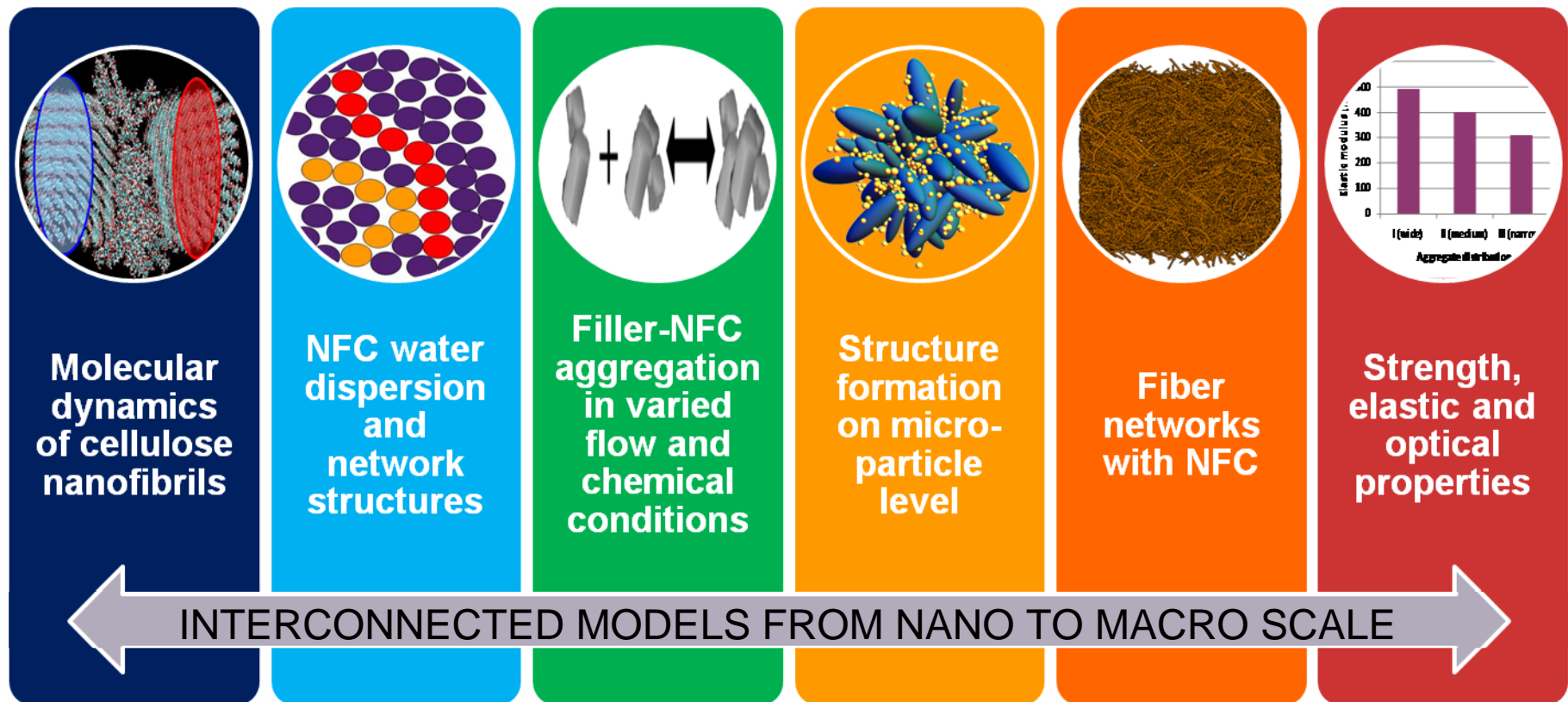
New production technologies



Modeling network



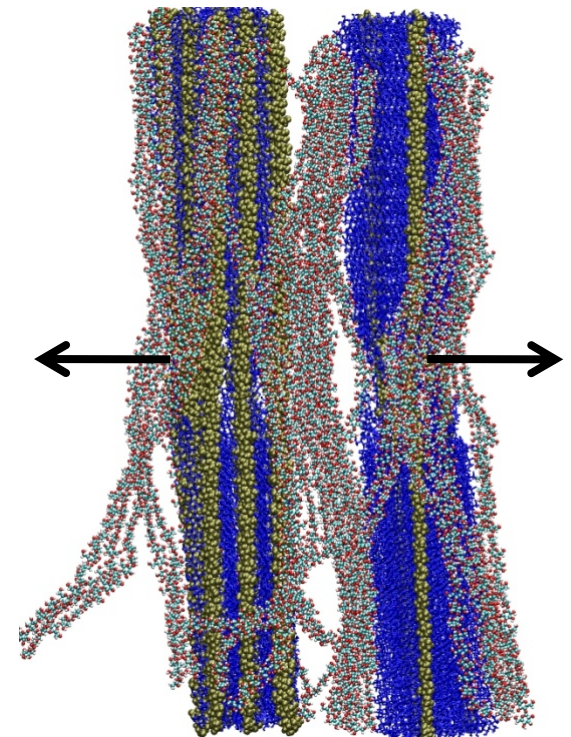
State-of-the-art simulation of materials, processes and products



NFC interactions with molecular simulations

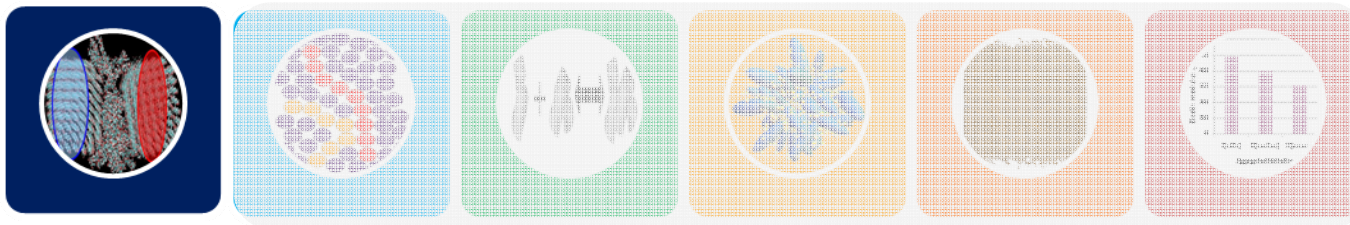
TUT: Sami Paavilainen, Tomasz Róg, Liam McWhirter, Ilpo Vattulainen

- NFC-NFC interaction and NFC bending stiffness in water suspension
- Theoretical minimum energy required for nanocellulose production is less than 2% of current energy consumption in pure mechanical grinding



Model output:

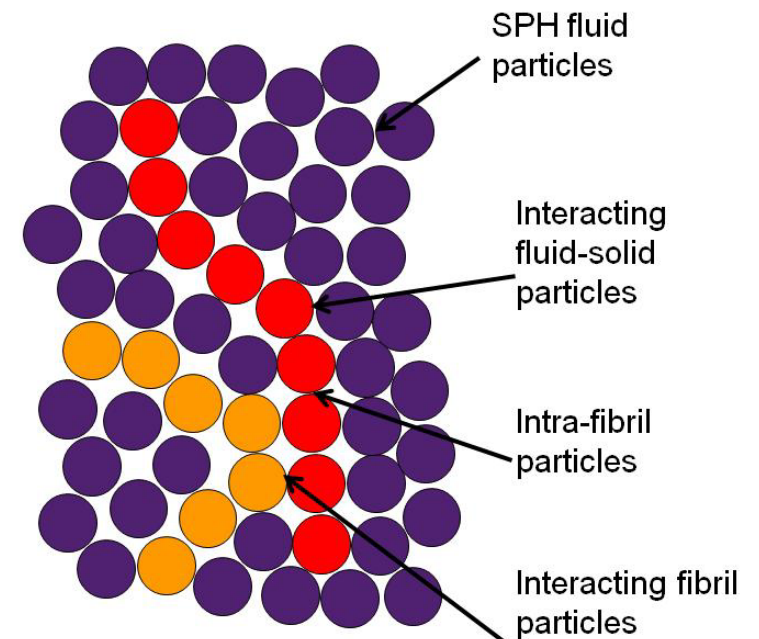
- Interaction forces
- Fibril stiffness



Simulation of NFC suspension and networks

FPIInnovations: David Vidal, Tetsu Uesaka

- NFC structures are extremely sensitive to
 - type of interactions
 - intensity and spatial distance of the interactions
 - consistency and morphology of nano-cellulose fibres



Model output:

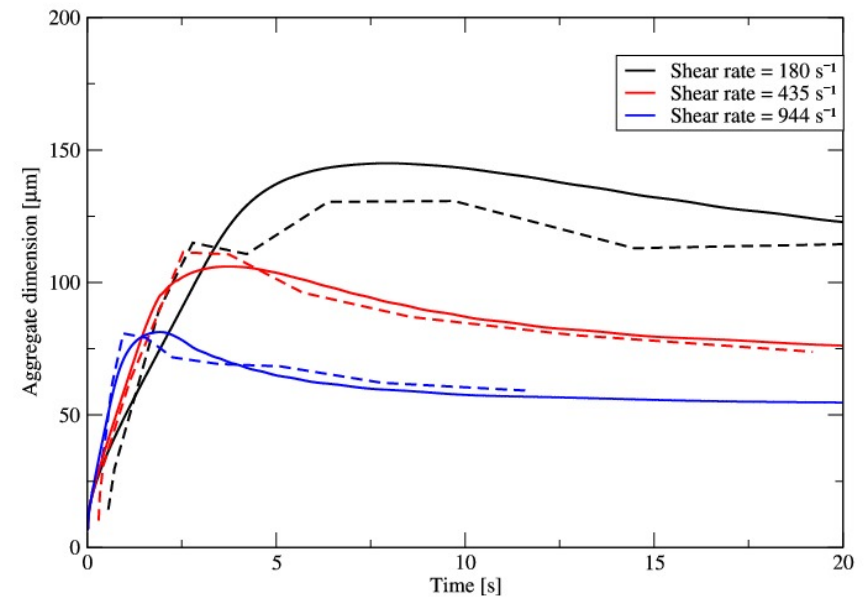
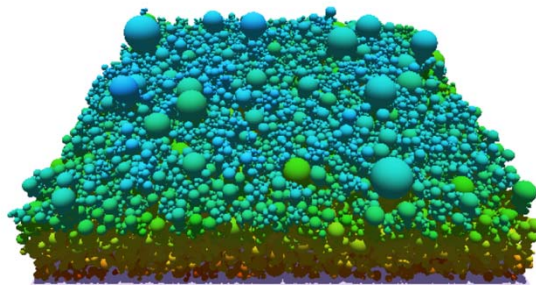
- Suspension rheology
- NFC network structure

From aggregation dynamics to sheet structures

Aalto: Antti Puisto, Mikko Alava

UH: Antti Penttilä, Kari Lumme

- Combined analysis of chemistry and flow conditions
- Verified to be adequate for several suspensions

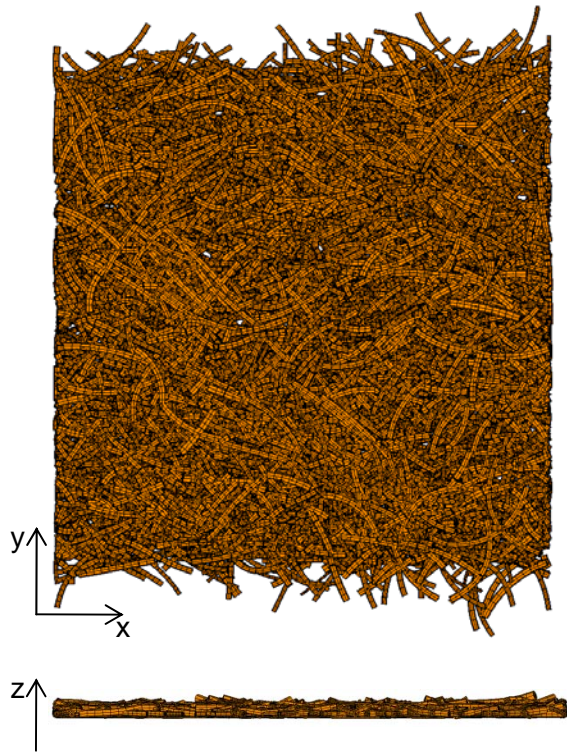


Model output:

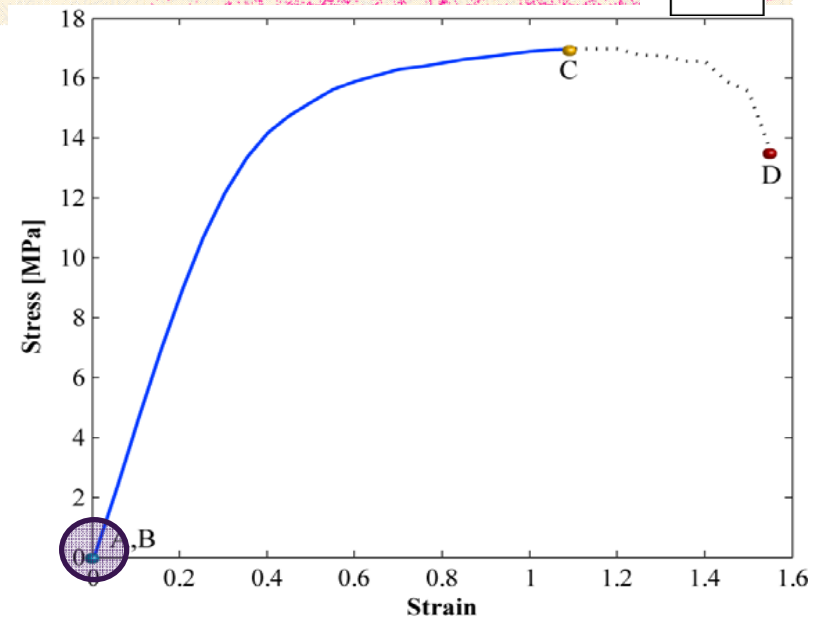
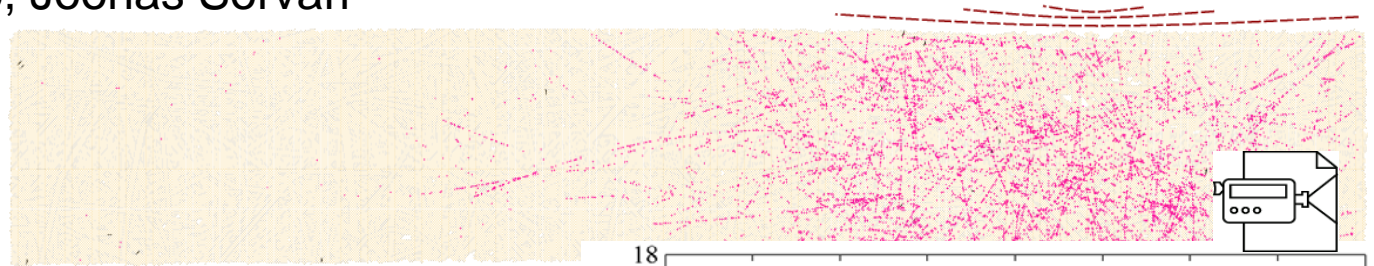
- Aggregate size distribution and its time evolution
- Sheet structures

Advanced fiber network simulations

VTT: Artem Kulachenko, Joonas Sorvari



- In typical paper samples stretch varies much more than strength



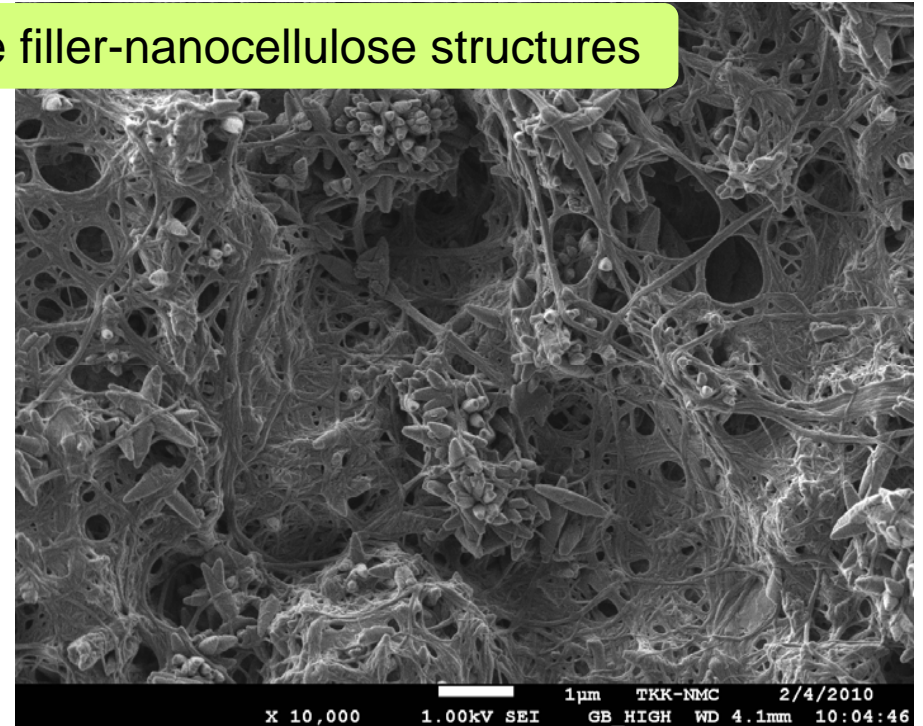
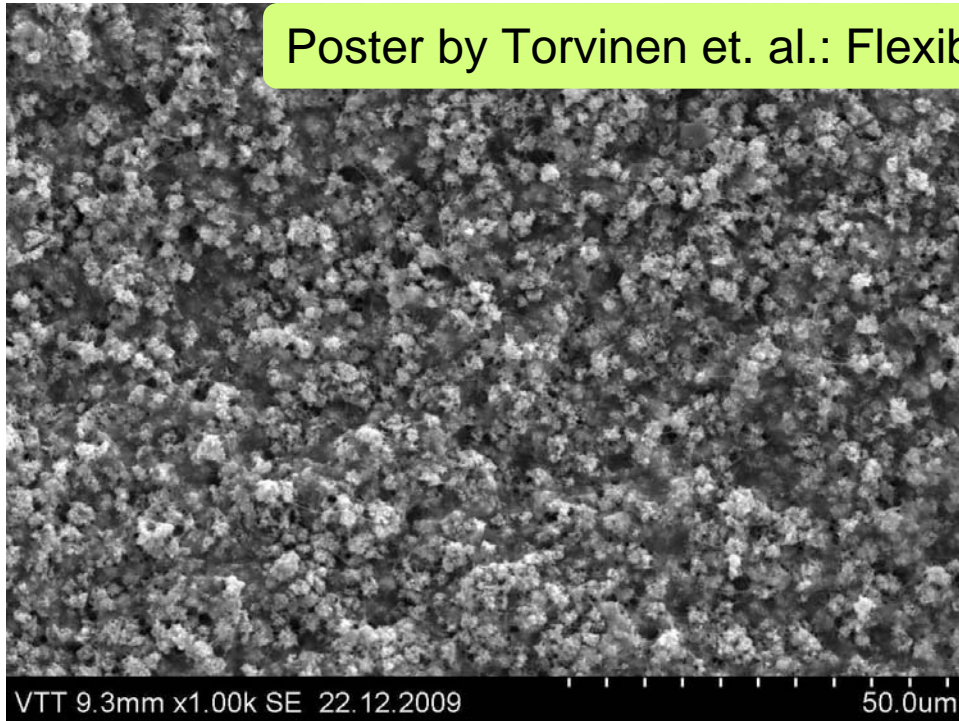
Model output:

- Sheet structure
- Mechanical properties

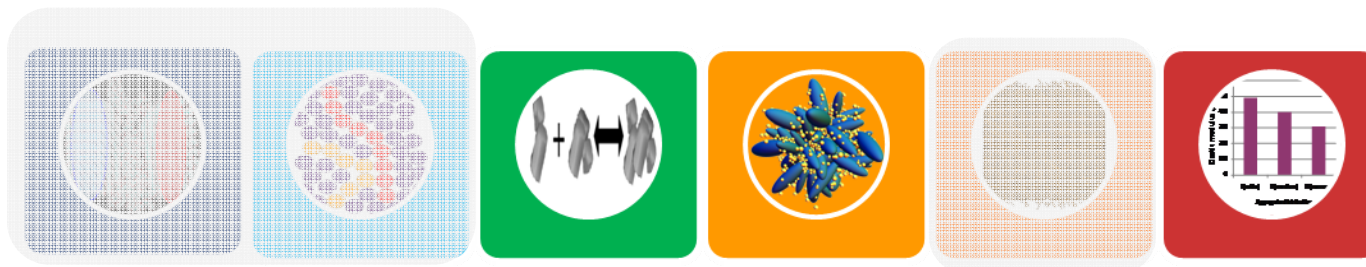
Example on combined analysis

Filler-nanocellulose composite

Poster by Torvinen et. al.: Flexible filler-nanocellulose structures



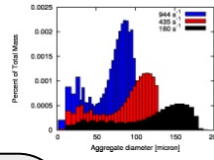
Case: effect of filler size distribution on mechanical and optical properties



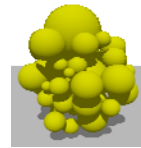
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Model connections

Flow/chemical conditions
Particle size distribution

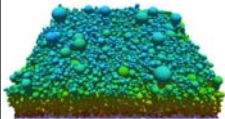


I
Aggregation
dynamics

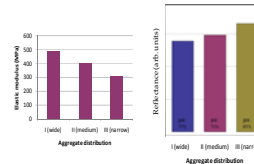


Particle size&shape

II
Packing simulations



III
Mechanical
properties

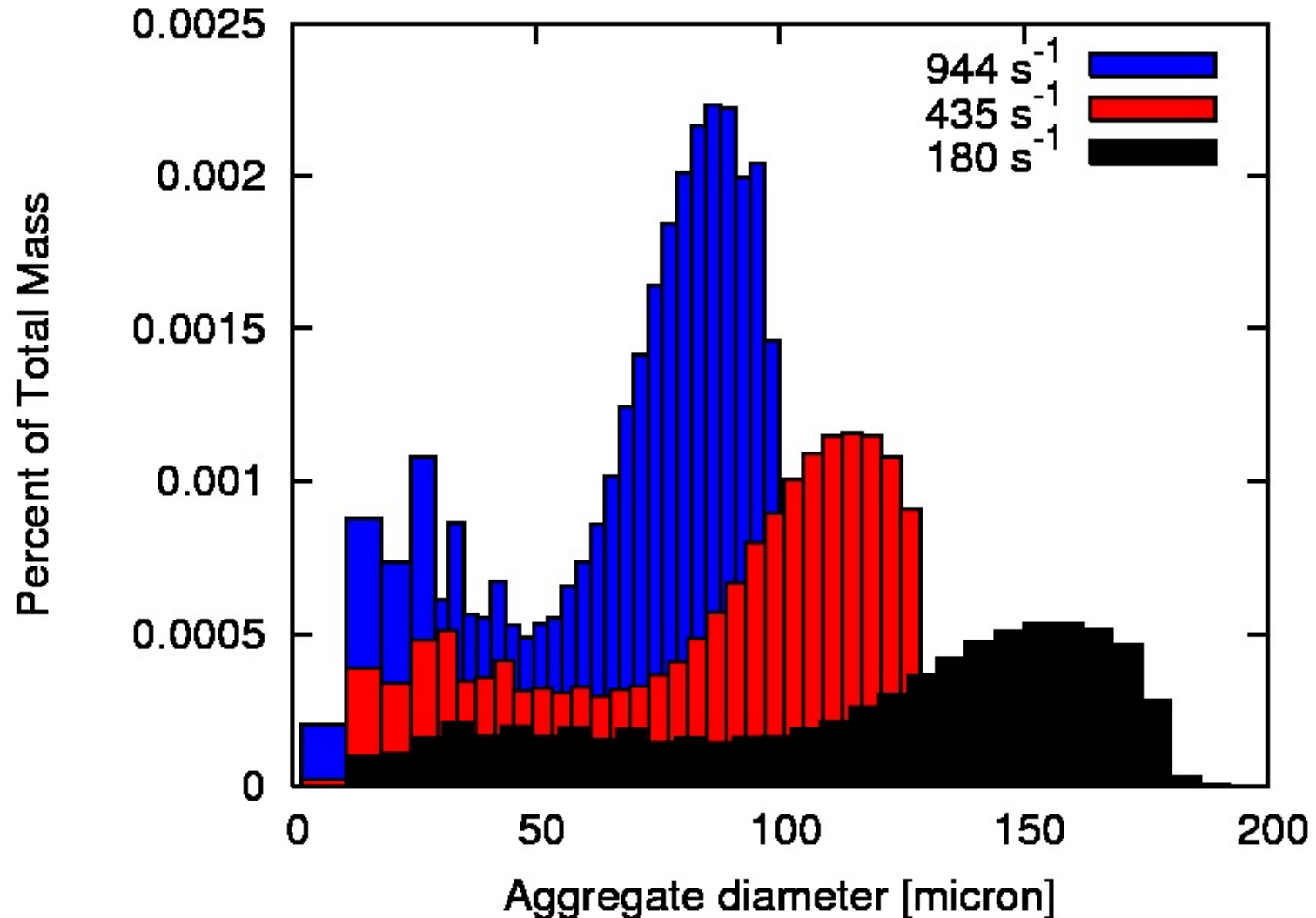


IV
Optical properties

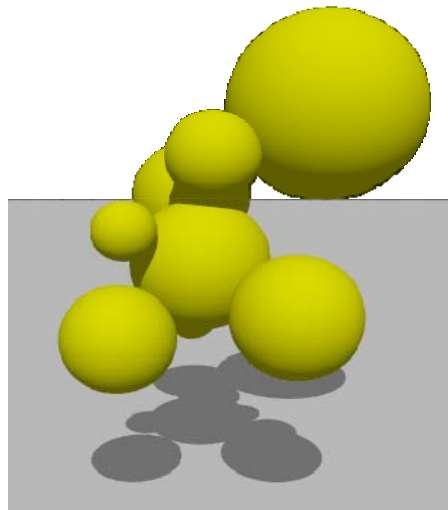
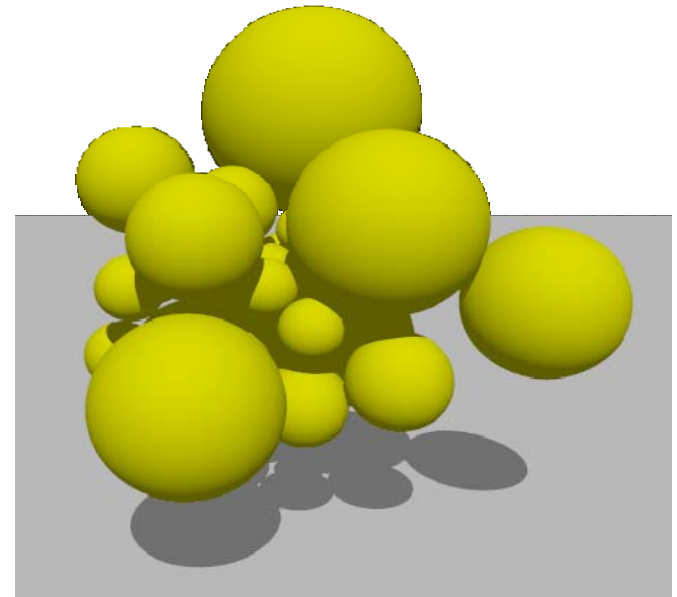
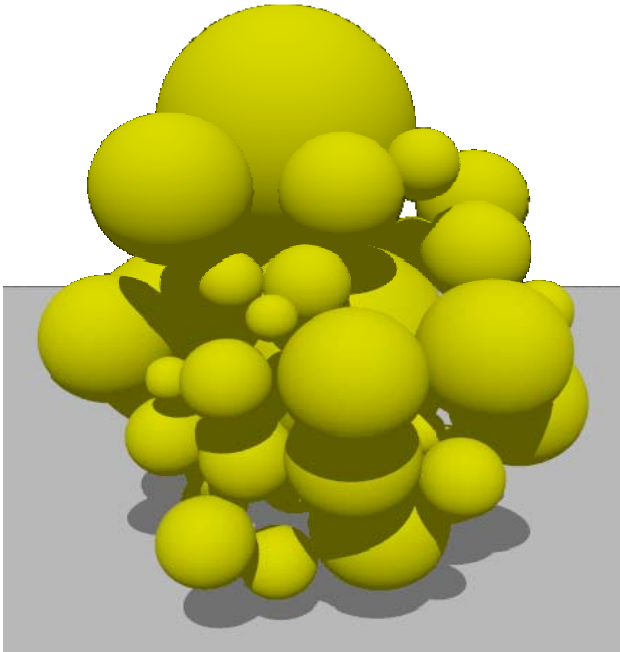
Material composition&elasticity

Diffraction indices

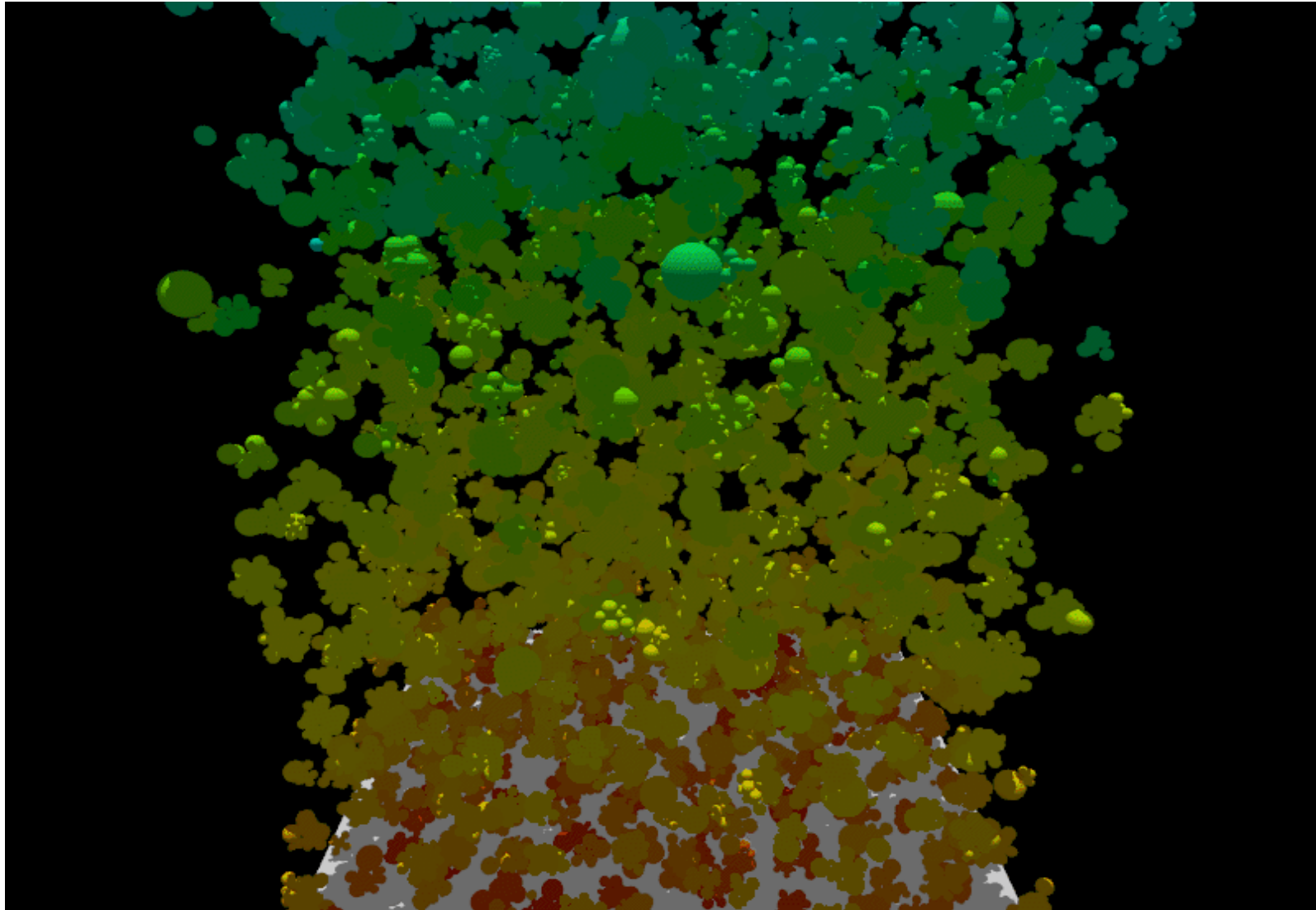
Aggregate size distributions



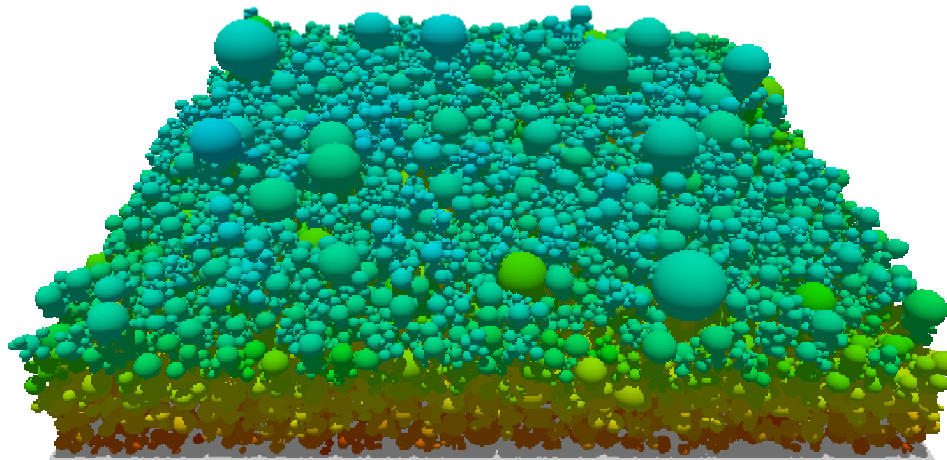
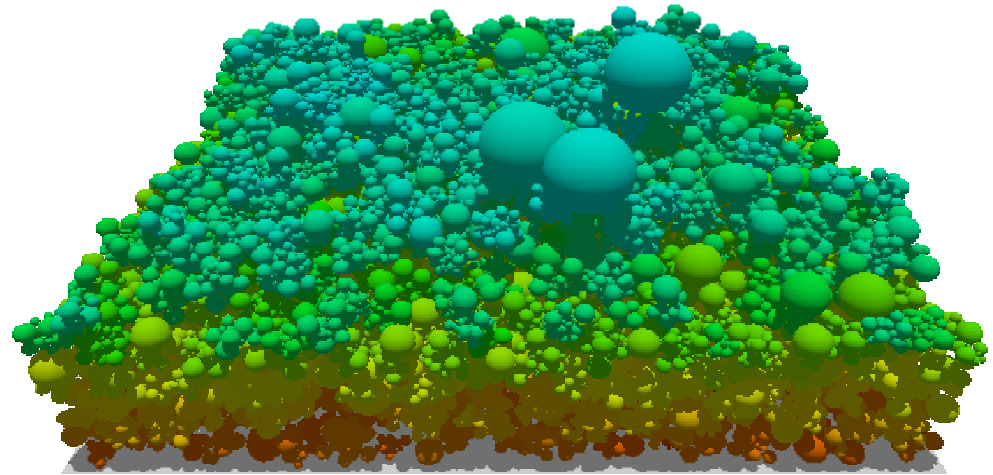
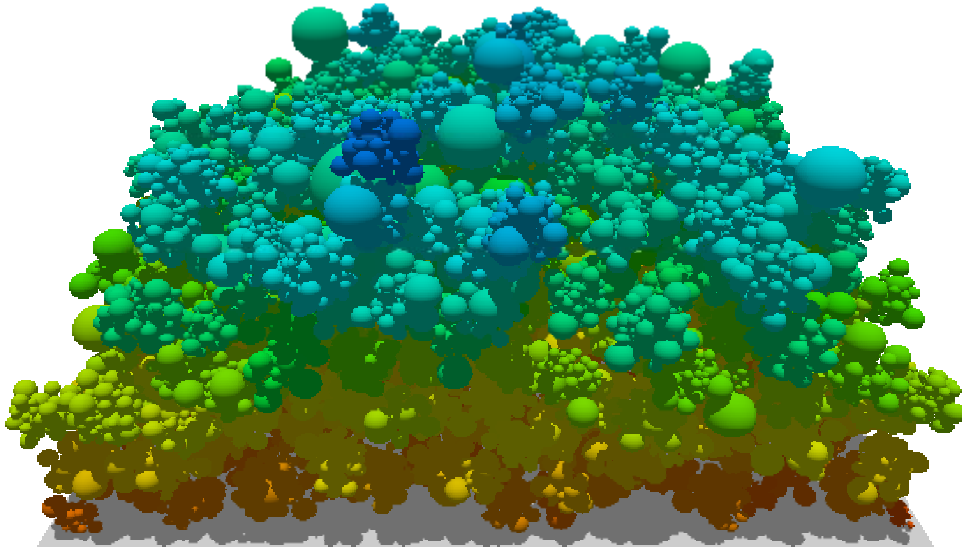
Model aggregates



Sheet structures from aggregates

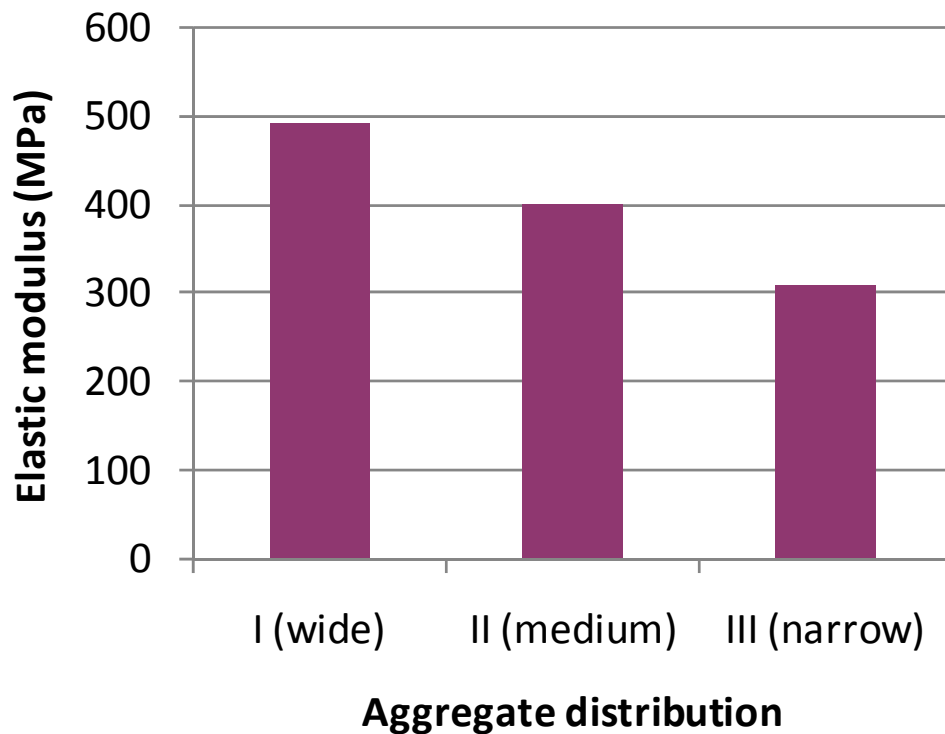


Resulting structures

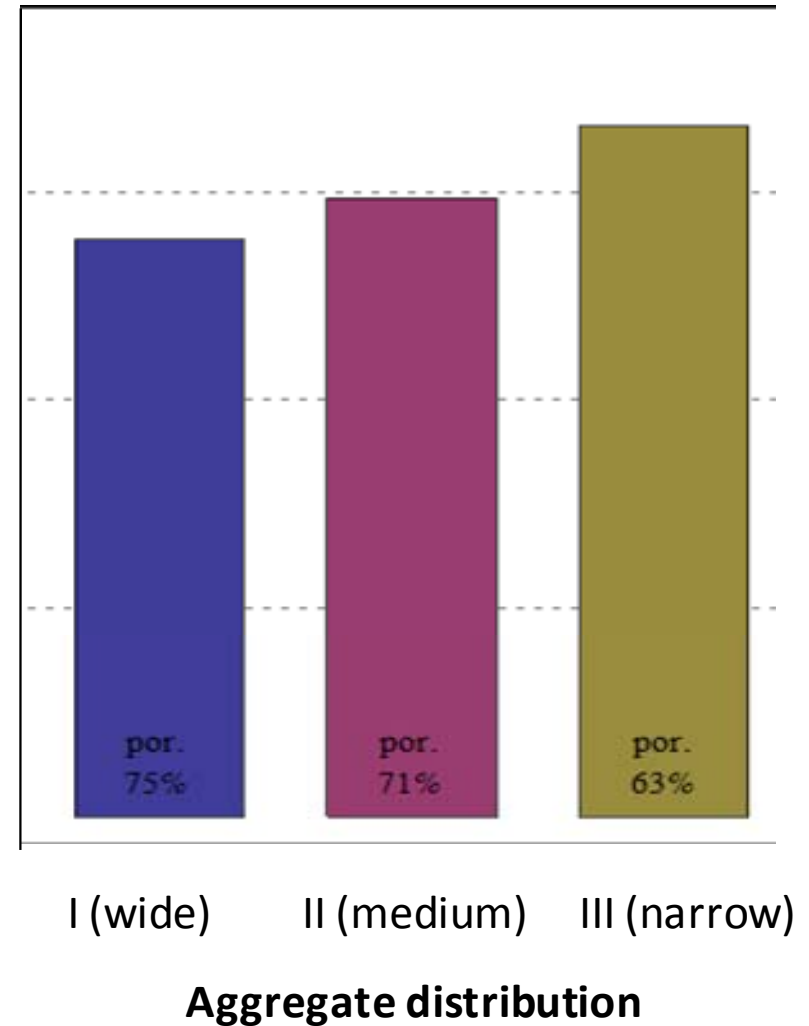


Mechanical and optical properties

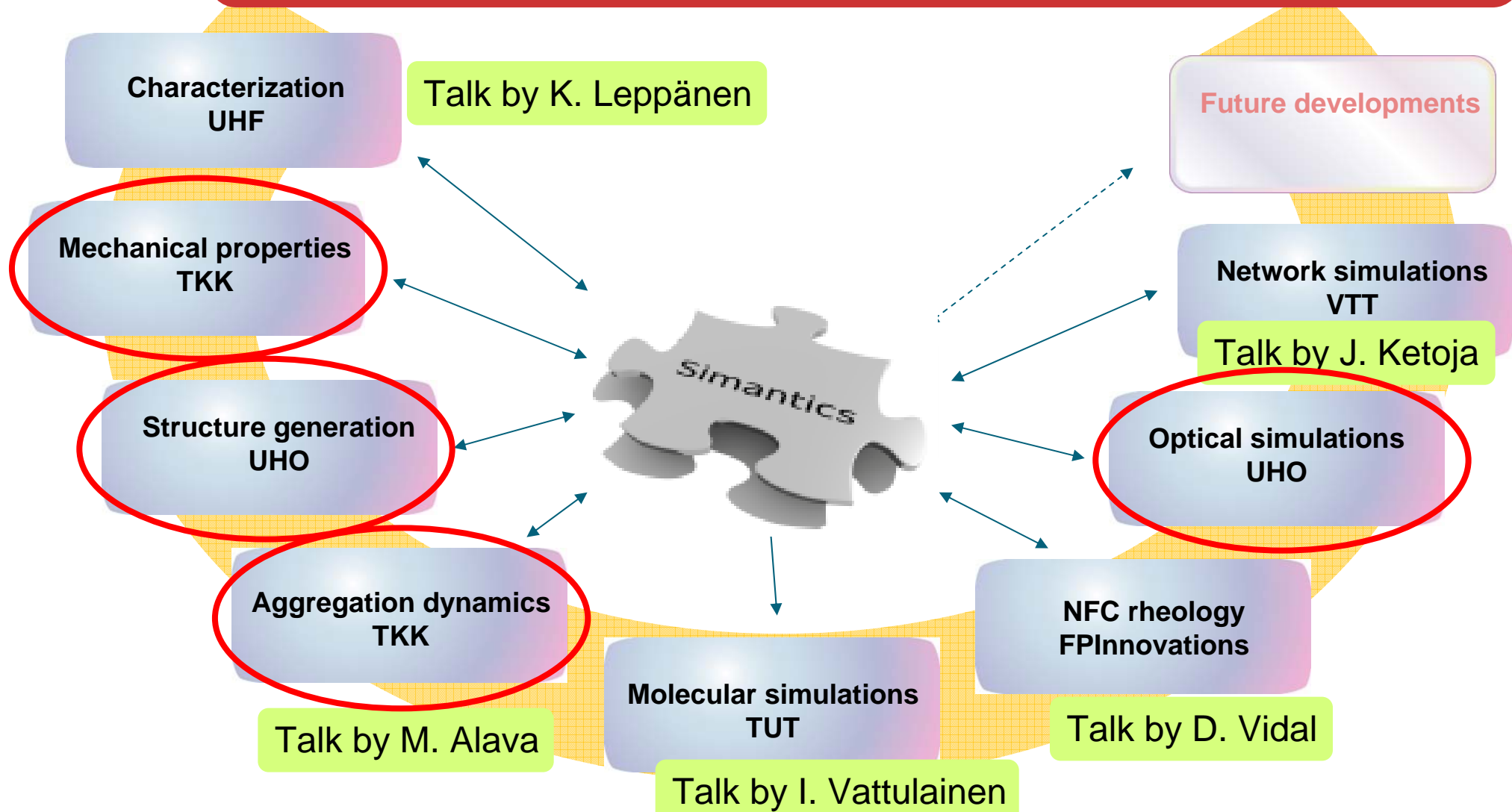
Considerable increase of stiffness by control of flocculation dynamics



Reflectance (arb. units)

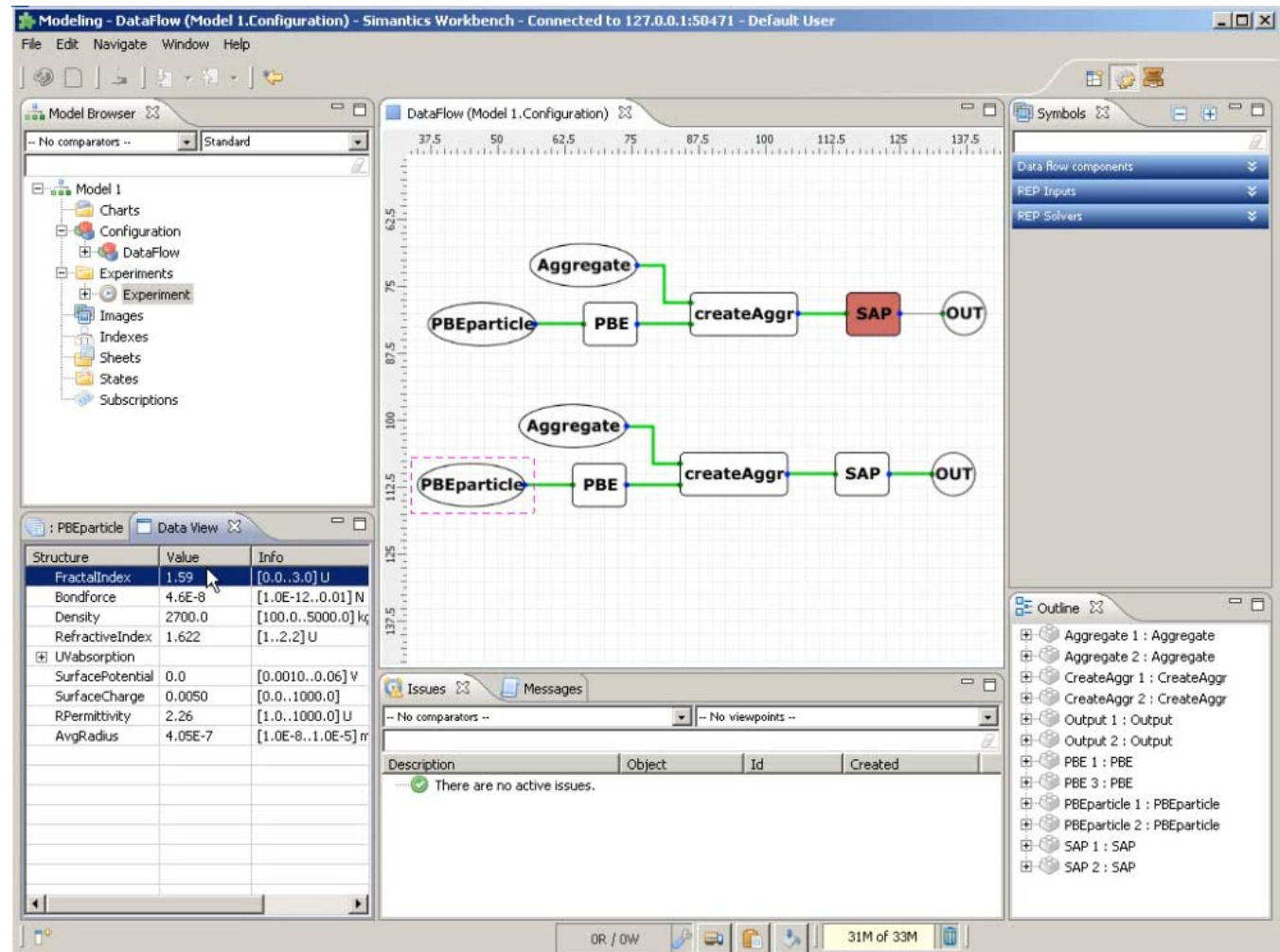


Synergy from joint analysis

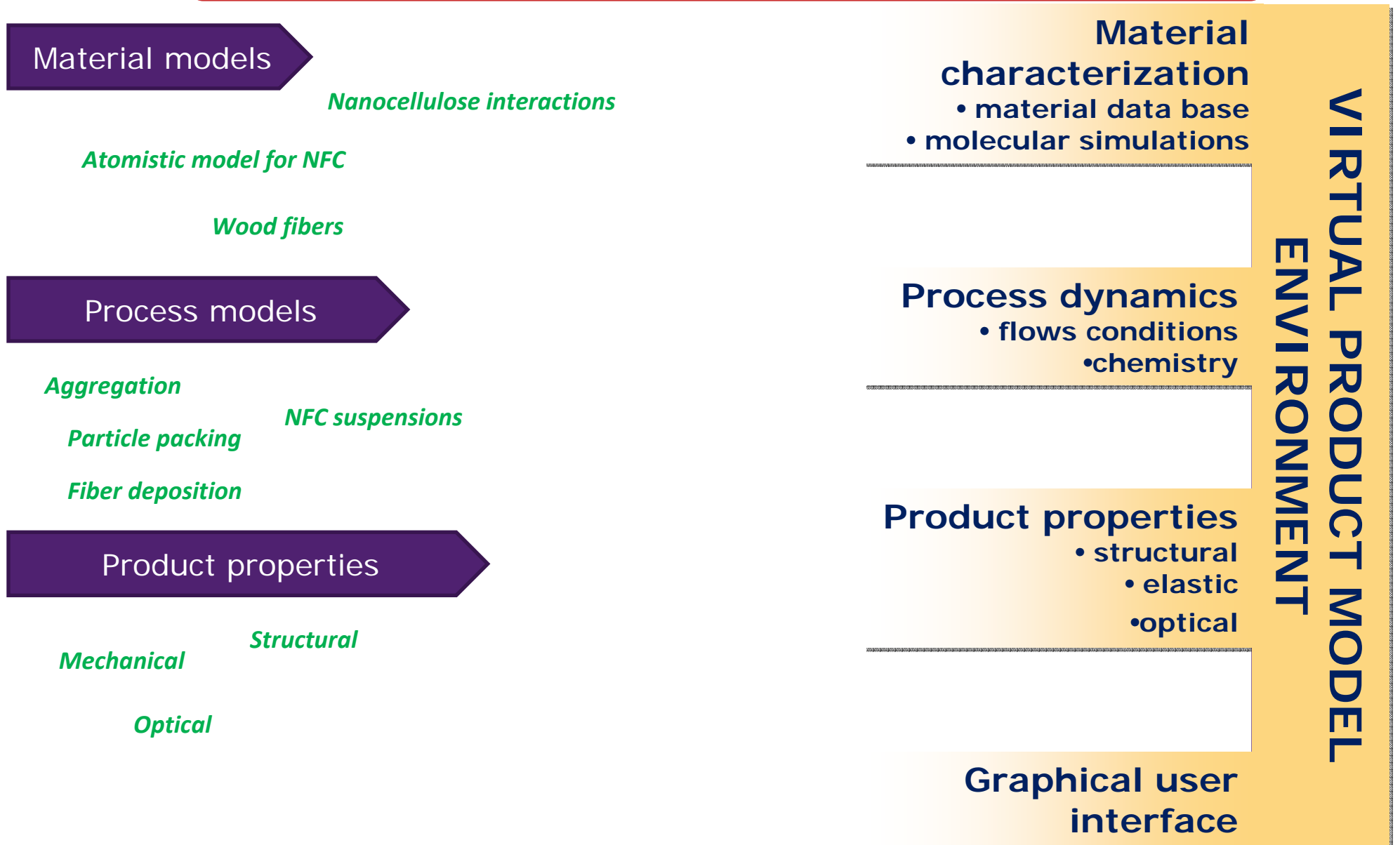


Integration of models using Simantics environment

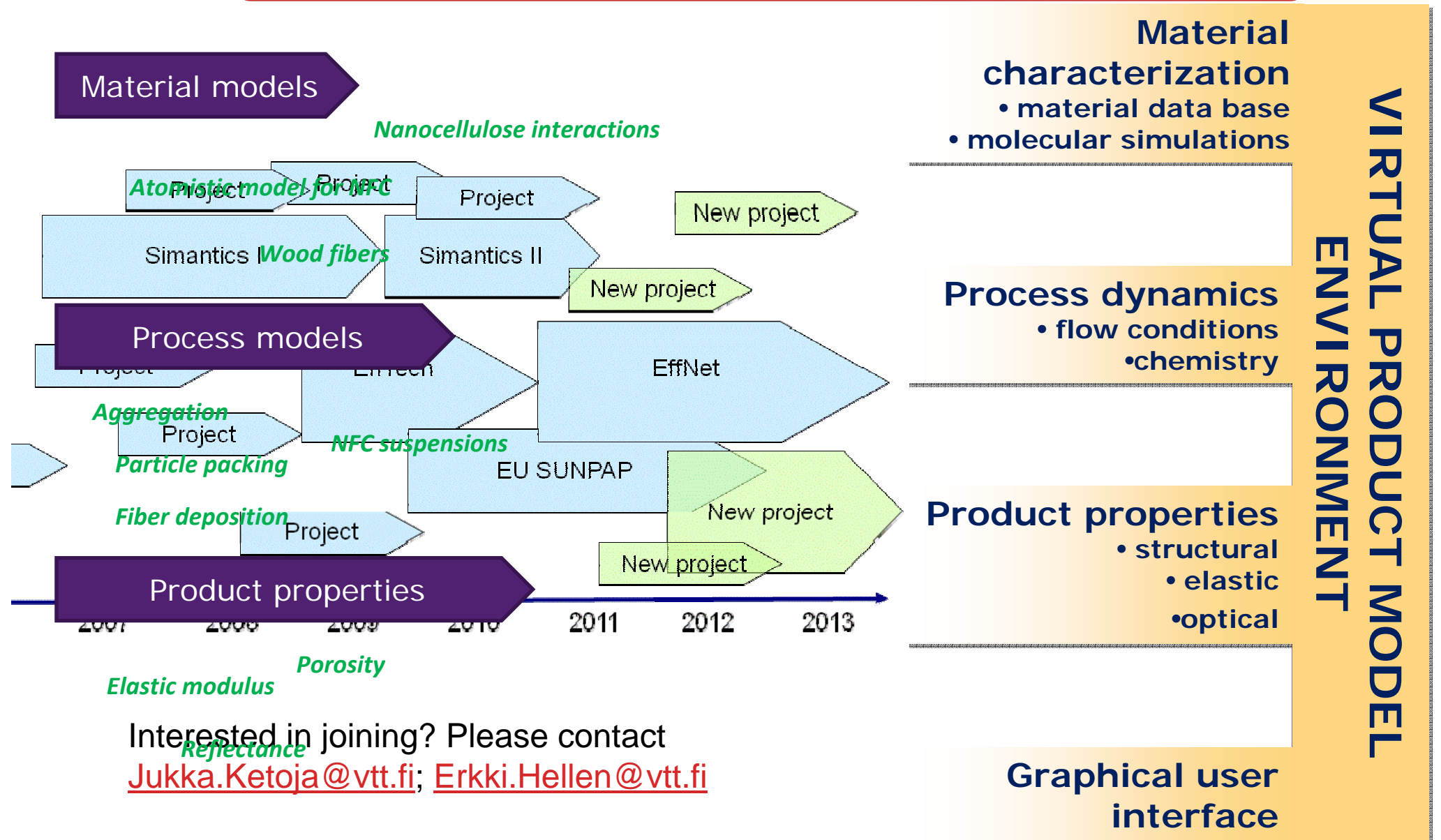
- Open software platform for modelling and simulation
- Offers configuration of multiple simulation solvers & remote use from the simulation servers
- Utilizes powerful semantic modelling language
- Developed at VTT by avg. 8 pers. since 1/2008
- Several other simulator projects in progress: Apros, Balas, OpenModelica, VTT Talo, OpenFOAM, ..
- Organised future maintenance and development by THTH Association/Simantics division
- www.simantics.org



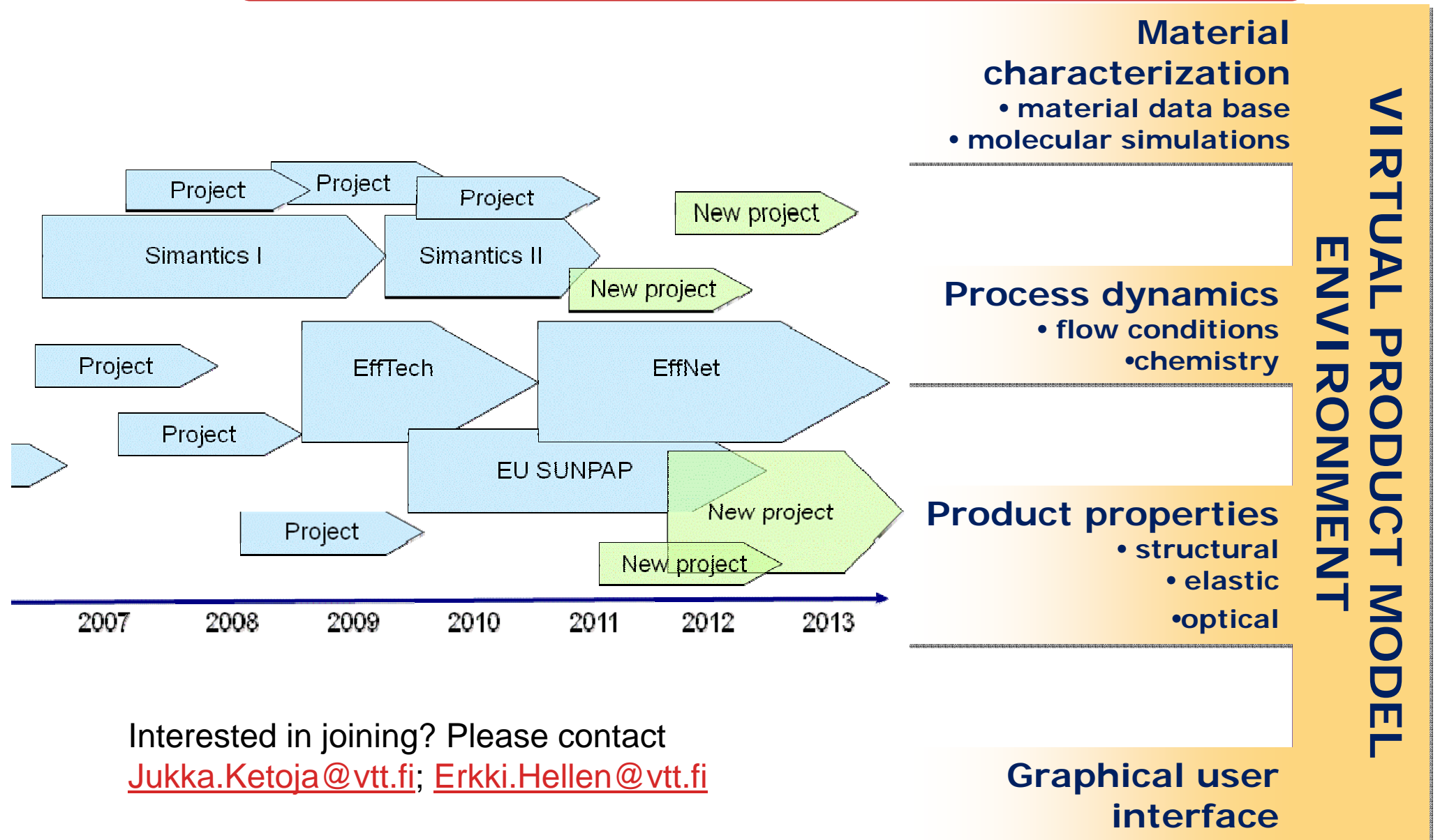
First steps towards virtual product modeling



Together towards virtual product modeling

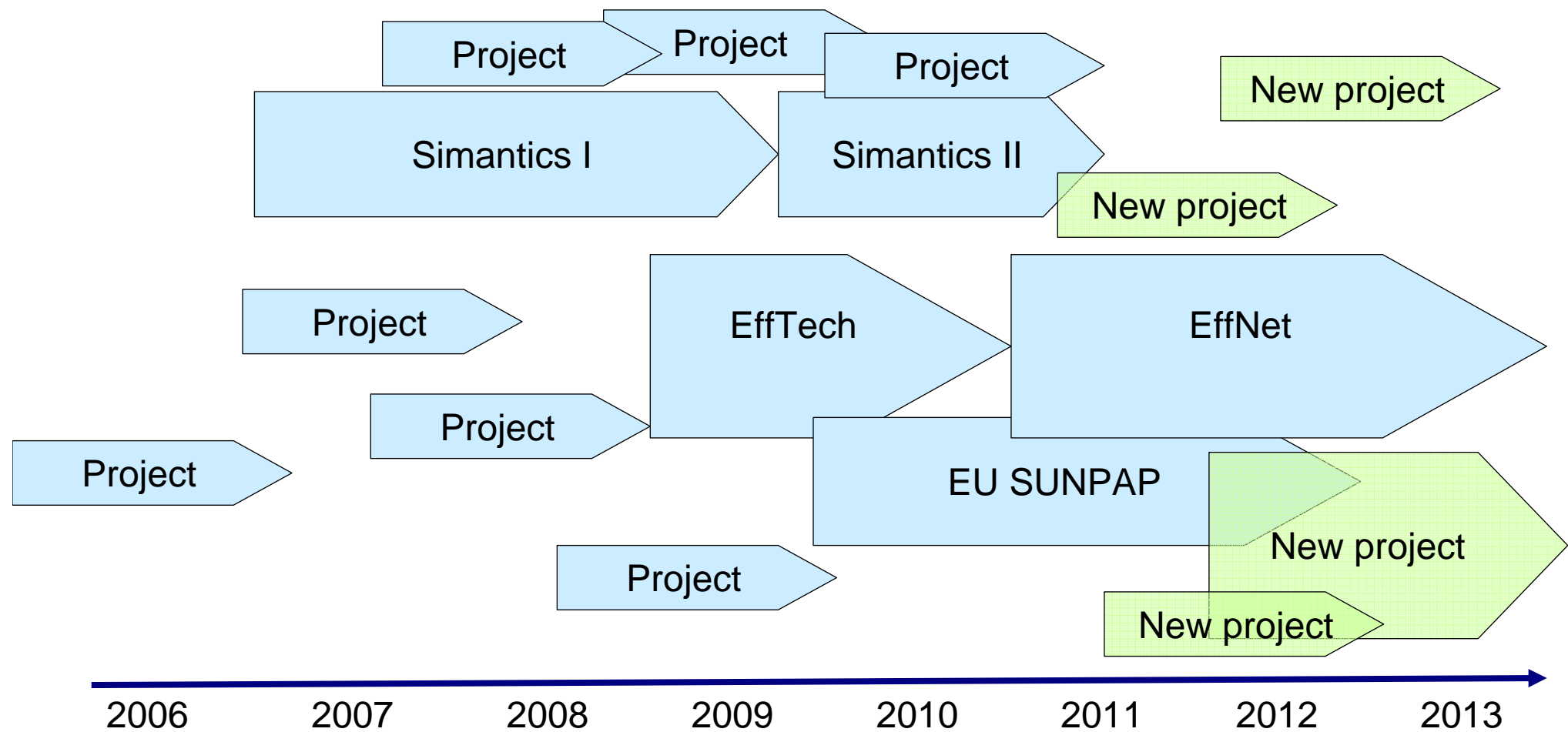


Together towards virtual product modeling



Interested in joining? Please contact
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Project portfolio



Acknowledgments

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Links: www.forestcluster.fi/ and portal.forestcluster.fi/

EffTech

