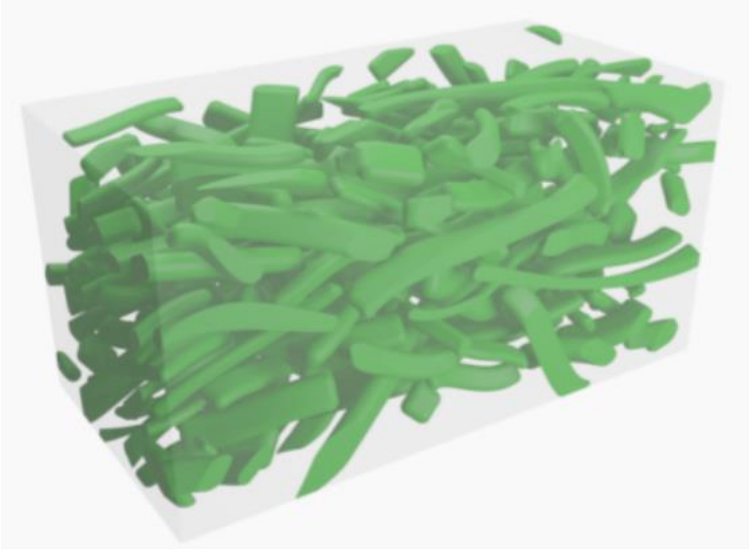
VTT webinar:
Revolutionary soft materials with VTT ProperTune® computational design

VTT – beyond the obvious

Agenda

- VTT in short – Mika Malkamäki
- Virtual design will revolutionize the development of future material solutions – Antti Puisto
- Case example – Tuukka Verho

  Development of virtual design workflows for bio-composites
- Q&A



VTT – *beyond the obvious*

VTT is a Finland based, visionary research, development and innovation partner and one of the leading research organisations in Europe.

2,093
employees

32%
a doctorate or a licentiate's degree

254 M€
turnover and other operating income

Establishment year
1942


VTT
Always aim for impact
Working together with you
VTT – beyond the obvious

Hit your material design targets faster, more accurately and cost efficiently with VTT ProperTune®

Virtual design will revolutionize the development of future materials solutions

Antti Puisto

What if you could design superior-performing biomaterials while radically shortening the time-to-market?

Introducing virtual materials design

TECHNOLOGICAL CHALLENGE

To create superior-performing materials and shorten design cycle by 50%

Fully virtual material design and testing for optimized performance

We have the capability to design fit-for-purpose materials and test their durability, sustainability, performance and even economic feasibility in advance. This is what fully virtual material design brings to the table. It spells a revolution in how industrial design and manufacturing will work in the future.

VTT ProperTune®
Performance driven material design

VTT ProperTune® optimises material design, replacing expensive, time-consuming testing and shortening time-to-market for new products by an average of 50%.

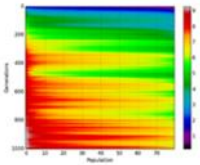
PROCESS

STRUCTURE

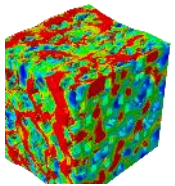
PROPERTIES

PERFORMANCE

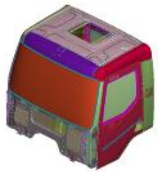
Performance driven materials design



Process models to predict microstructure



Microstructure models to predict material properties

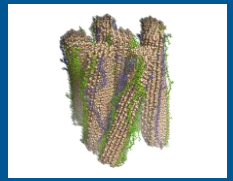


Component level models to predict performance

VTT ProperTune® is multiscale and multiphysical

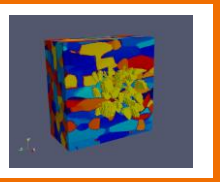
Multiscale

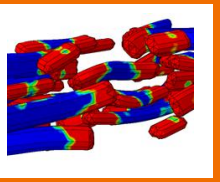
From atomistic to microstructural and to product performance and lifetime

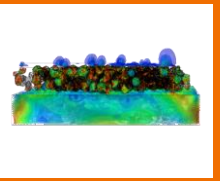


Multiphysical

- Material properties
- Manufacturing and solidification processes
- Damage and failure
- Thermodynamics and kinetics
- Chemical reactivity
- Electrochemistry
- Transport phenomena
- Electromagnetism
- Dynamics
- Process models





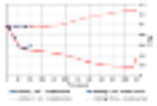


Couplings, concurrencies, interfaces and data across scales and physics

Example: VTT ProperTune® for wood

Process

Hygro-thermal and hygro-thermo-mechanical Models for wood processes

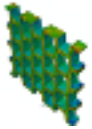


Wood moisture, temperature, pressures, strains and stresses during drying and densification processes

Properties

Structure

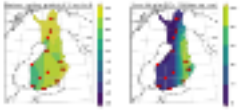
Image-Based microscale Modeling of wood and wood products



Material properties (mechanical, hygro-thermal, etc.)

Performance

Hydro-thermo-mechano-Biological models for wood components under service conditions



Wood moisture, temperature, RH, moisture-induced strains and stresses, crack risk, decay risk during product service life

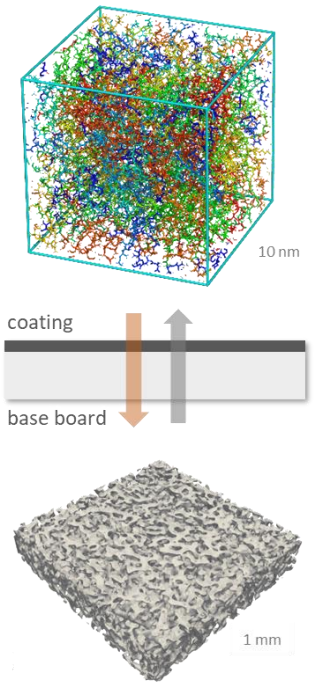
Benefits for wood product development, monitoring and maintenance (Glulam, CLT, Thermowood, veneers, LVL, new products)

- Reducing the need of experiment
- Effect of process parameters
- Process optimization
- Prediction of material properties in new products
- Sensorless monitoring
- Evaluation of moisture-induced damage
- Effect of coating and surface treatment
- Prediction of service life
- Assisting maintenance activities
- Development of user-friendly on-line tools

Example: Barrier coatings

- What if you could reduce the development time of barrier materials by half?
- Through multi-scale modelling of permeant transfer:
  - **Polymer coatings**: solubility and diffusivity from *molecular models*
  - **Cellulosic boards**: transmission rate from *empirical transport models*
  - **Nanofiber networks:** transmission rate from *finite element models*
- Enables virtual design, benchmarking and testing of a vast selection of potential barrier polymers

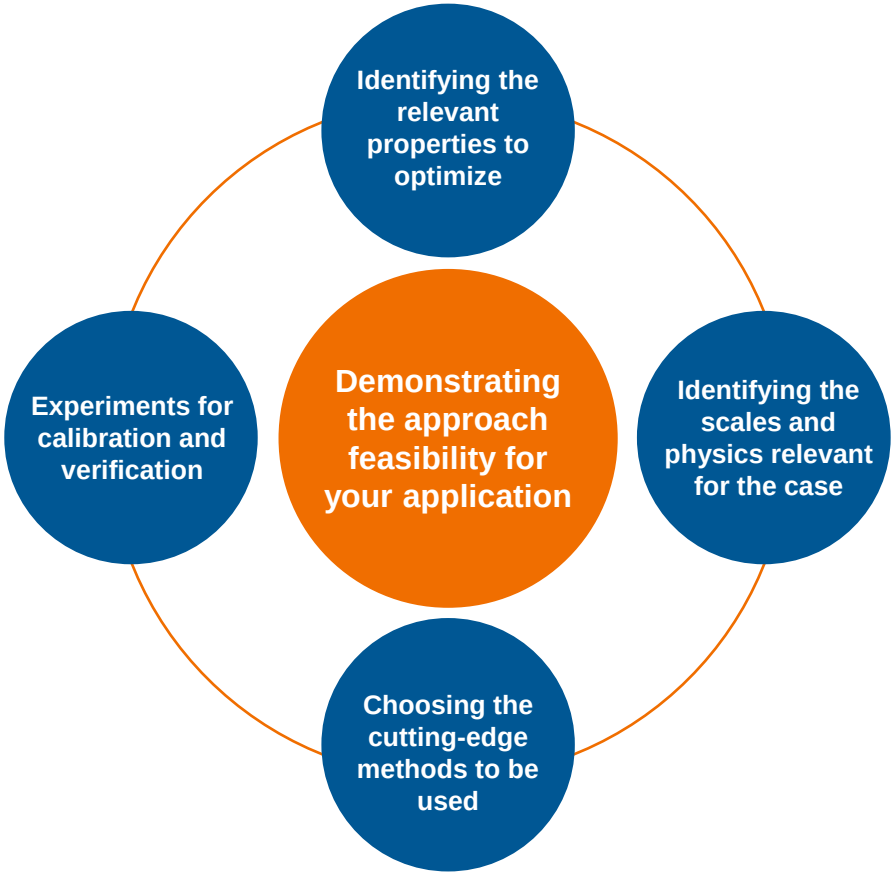
Molecular model for H_2O/O_2 permeability of a polyester film

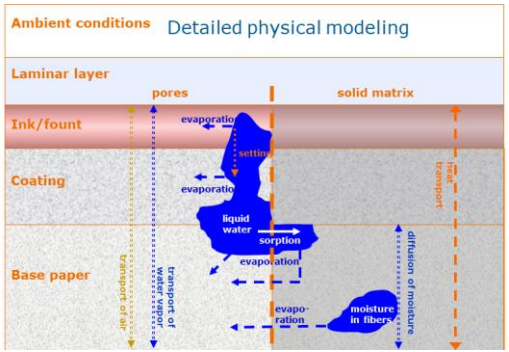


Imaging-based model for permeant transfer in a cellulose nanomaterial

Three step approach to your case using VTT ProperTune®

First step: Proof of concept





Second step:
Feature optimization of a current product

- Identify a performance critical target product feature based on the POC
- Utilize/further improve the methods established in the POC
- Add the required optimization tools (non-linear optimization, ML/AI)
- Optimize feature to obtain new properties to the target product

Third step:
Updated process, product variants etc.

Based on your needs and/or ambition level

Process development	Novel product	Other aspect

Huge impact to your business

Example cases

Examples of VTT ProperTune® use cases

Use case type:
New steel discovery

ArcelorMittal

- Discovery and design of new steel grades

Outcome: New steel performance improved ~200-250%

Use case type:
Optimize a material solution (microstructure)

Caterpillar

- Optimization of protective coatings

Outcome: coating solution performance improvement 40%

Use case type:
Capture / troubleshoot complex performance causal relations

Wärtsilä

- Design processes and methods for extreme conditions

Outcome: 3 to 5 fold design accuracy improvement, able to capture product failures

VTT ProperTune® has been developed together with our industrial partners and applied to their materials and products.

The NUMOBIO project: developing virtual design capabilities for bio-composites

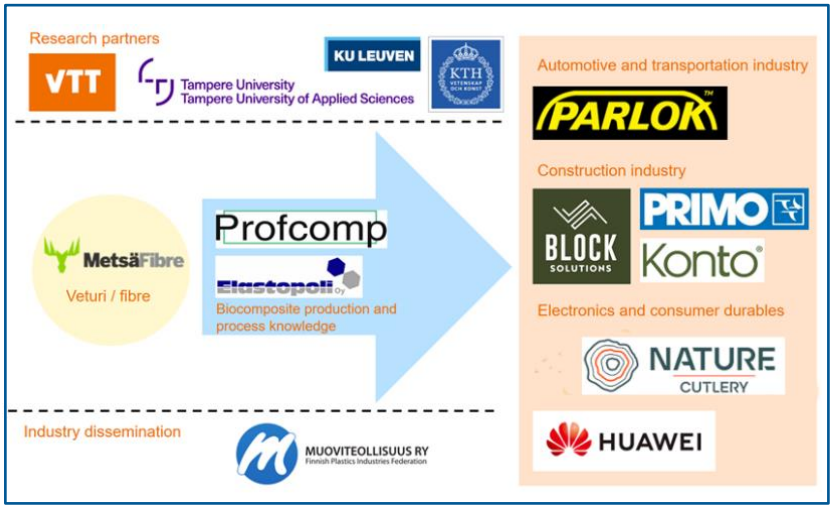
Tuukka Verho

Biocomposites: what and why?

- Polymer reinforced with natural fibers
  - For example, softwood fibers in bio-based PLA plastic
- Advantages:
  - Renewable raw material
  - Lightweight
  - Significant reinforcement effect
  - Low cost
  - Well processable and re-processable
  - A range of fibers from different sources and different pre-processing available
- More research and development needed for full benefits

The NUMOBIO project in short

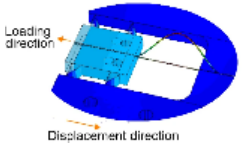
- Jointly funded project to develop industry-relevant modelling and characterization capabilities for bio-composites
- Aim: virtual design and testing of bio-composites
  - Faster development cycles, better properties
- 2 year project from 2021 to 2023
- Industry partners help to focus research and define goals



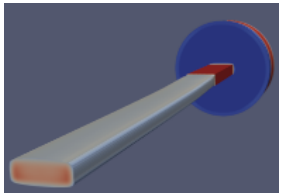
Elements of the NUMOBIO project

Fabrication, characterization and testing

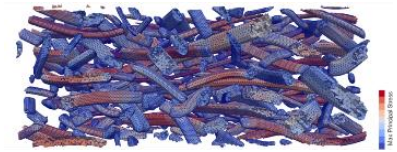
Single fiber testing (TUNI)



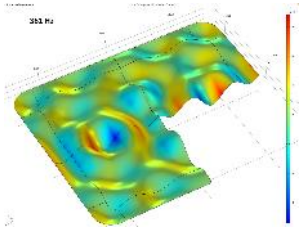
Manufacturing process models (process → structure)



Microstructure models (structure → properties)

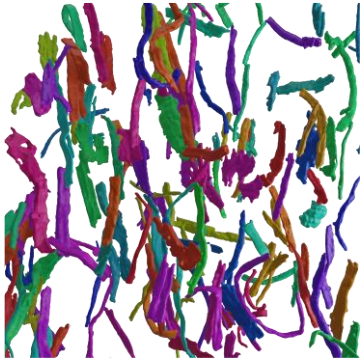


Component models (properties → performance)

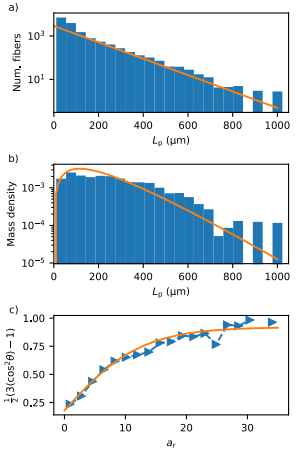


Microtomography analysis

Segmentation algorithm

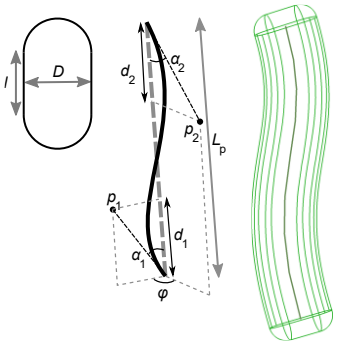


Statistical analysis

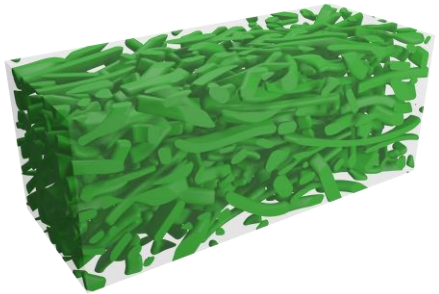


- X-ray micro/nanotomography allows identification of microstructure features
- Statistical analysis yields a set of key parameters to describe the internal structure of the material

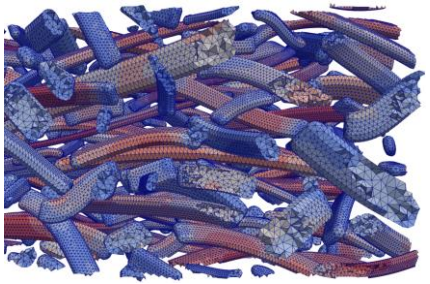
Microstructure reconstruction and model generation



Packing algorithm



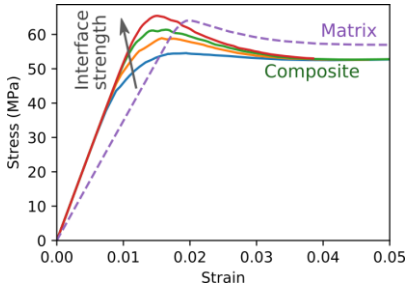
Conversion into model



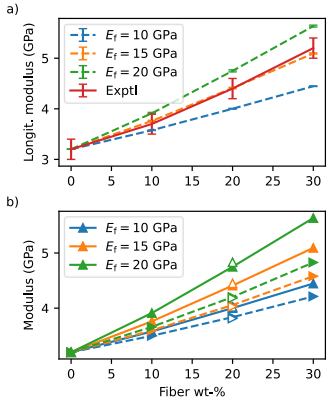
- The parametric description from statistical analysis allows defining a simplified synthetic model
- The synthetic model can be “artificially” varied to explore the parameter space

Physical properties by FEM simulation

Post-processing



Validation and results

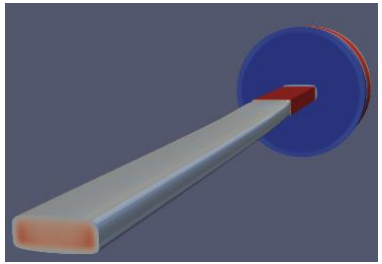


- FEM simulation allows studying e.g. mechanical properties
- Macroscopic and micromechanical testing helps define the input parameters and validate the model
- The model can predict properties and provide understanding of structure-property relationships

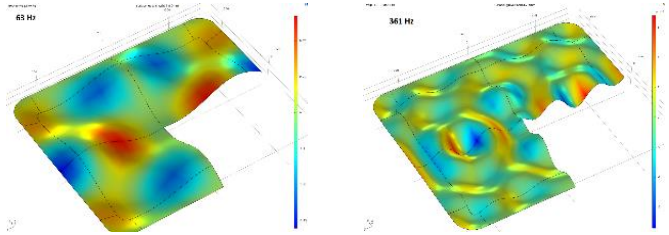
Multiscale modelling

Optimization

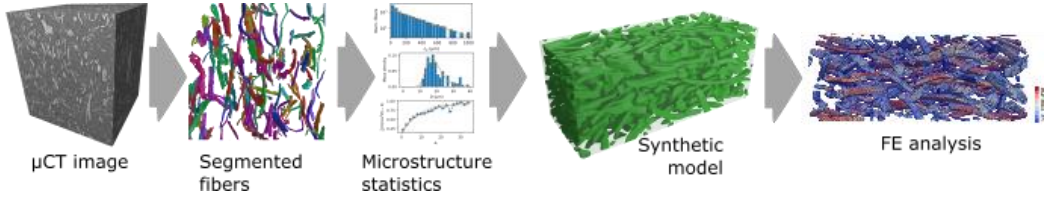
Process model



Component model



Microstructure model



Physical properties and performance

Material Properties

Stiffness
Strength
Toughness
Barrier diffusion
Oxidation
Viscoelasticity
Thermal expansion
Solubility of chemicals

Product Performance

Rigidity
Load capacity
Reliability
Lifetime
Aging
Vibroacoustic behavior
Dimensional stability
Chemical resistance

Optimal material properties with ProperTune aided design → better performance!

Summary

VTT ProperTune® is a new unique computational material design concept for **performance-driven development of soft materials,** including biomaterials, plastics and biocomposites.

It enables you to

- Reduce time-to-market of novel materials and processes by 50 %
- Achieve significant savings on overall R&D cost
- Design innovative material solutions with systematic data-driven processes
- Replace harmful, costly or poor availability materials with biobased alternatives with superior performance

What could the impact be to your business?

- To discuss your specific material development challenge, please contact: mika.malkamaki@vtt.fi

VTT

beyond

the obvious