OntoTrans Open Workshop

March 15-16 2022

Application cases:
the view of the translator

Vinicius Beber, Welchy Cavalcanti, Michael Hoffmann, Michael Noeske, Peter Schiffels
Fraunhofer IFAM

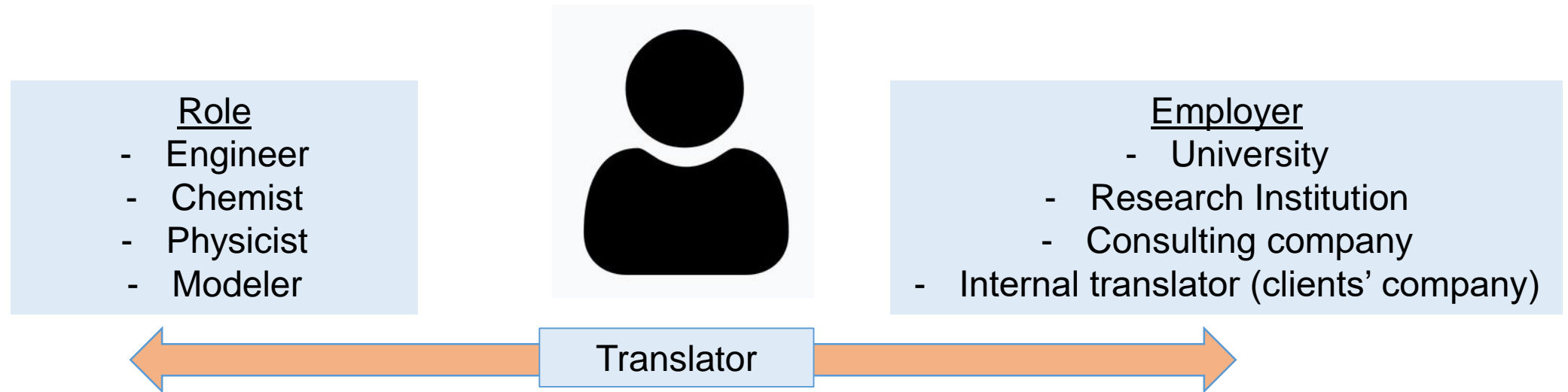Lucy Bull, Brendon Weager
Composites Evolution

Agenda

- Who is a Translator ?

- The "framework" of a Translator

- The 6 translation steps

- Application cases

- Translator's View: How OntoTrans makes my life easier

- Conclusions & Outlook
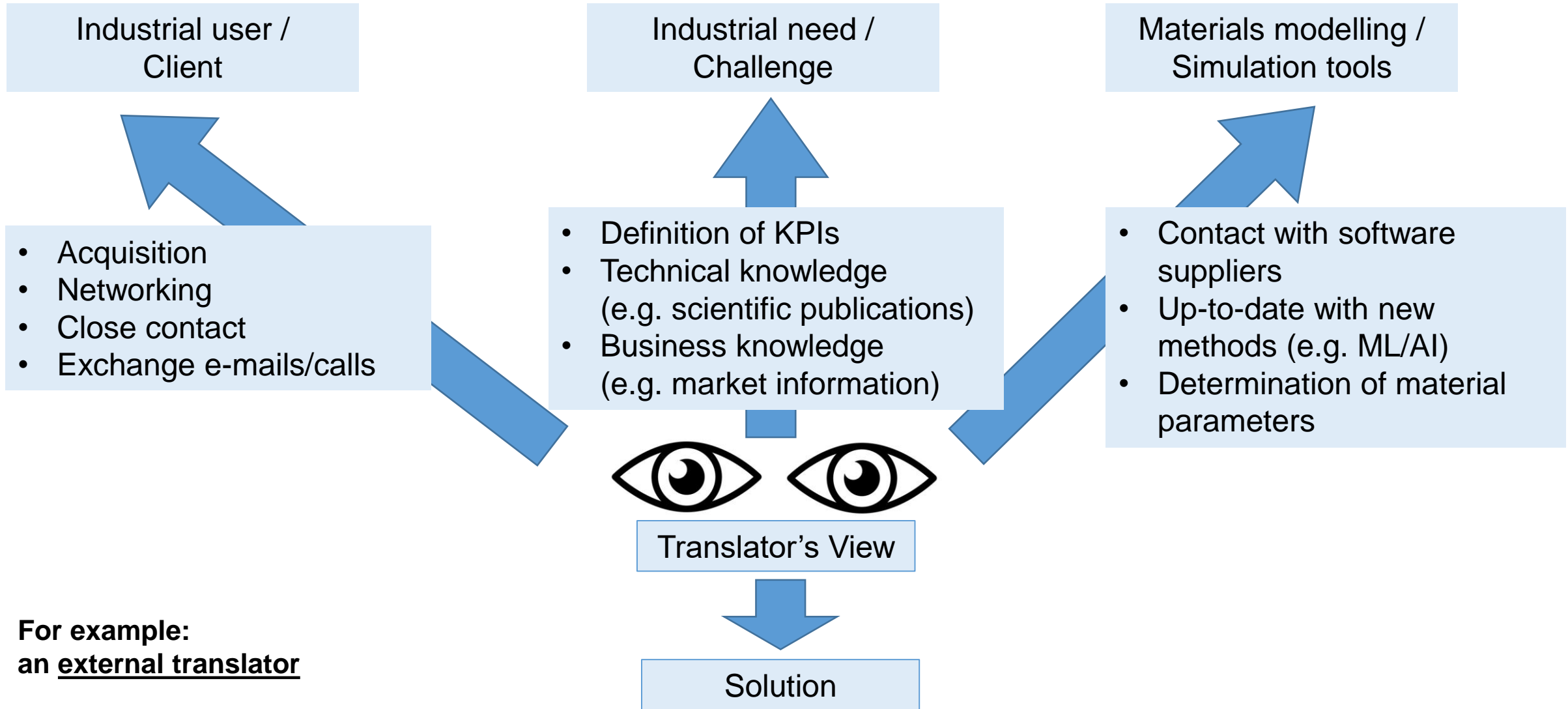
Who is a Translator ?

According to Klein et al.:

- Industrial users (i.e. Clients) can profit from materials modelling by…

- …translating an industrial need/challenge into …

- …a solution by means of materials modelling and simulation tools

Experts performing this process of providing a Translation service are called **Translators**
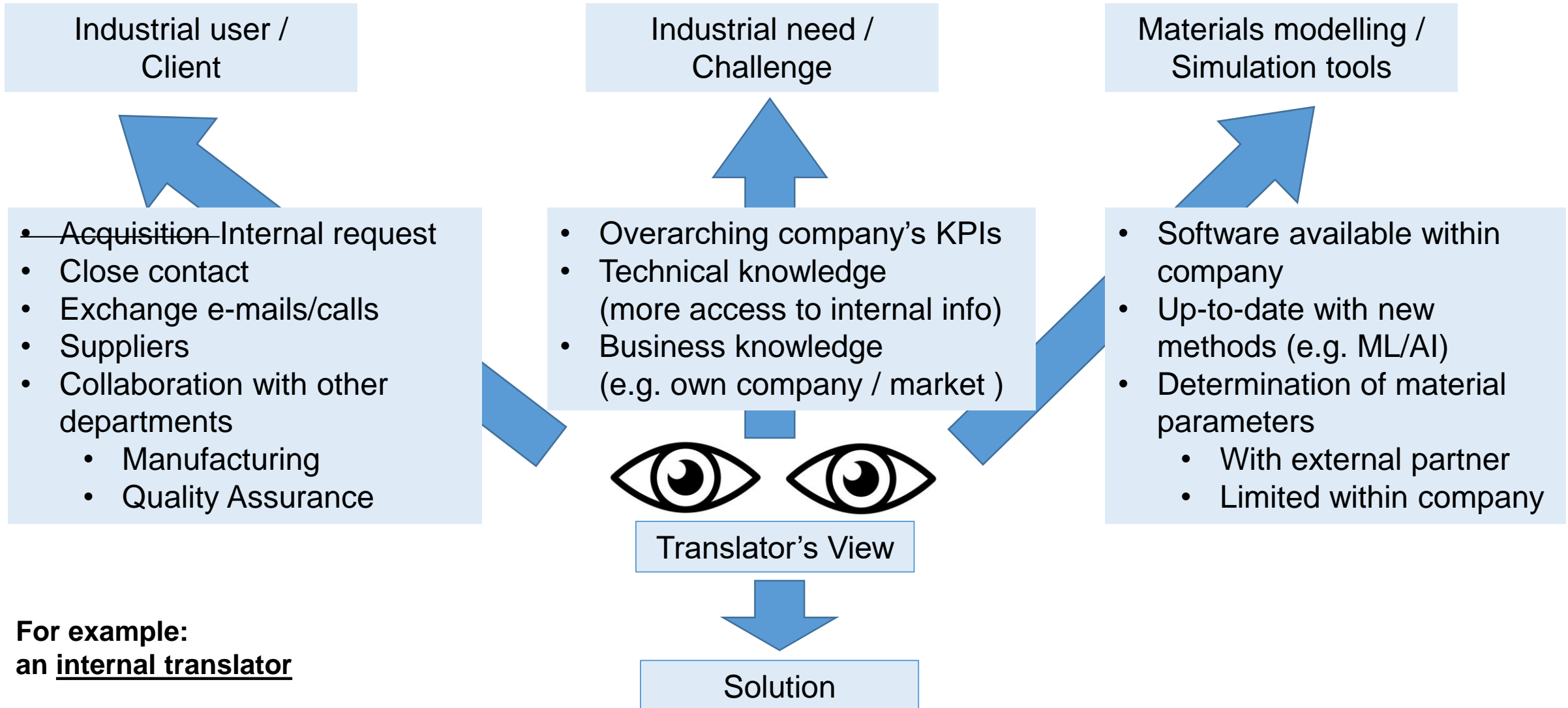
Role
- Engineer
- Chemist
- Physicist
- Modeler

Employer
- University
- Research Institution
- Consulting company
- Internal translator (clients' company)

Translator

Translation in Materials Modelling: Process and Progress (Klein et al. 2021)

Who is a Translator ?

Industrial user / Client

- Acquisition
- Networking
- Close contact
- Exchange e-mails/calls

Industrial need / Challenge

- Definition of KPIs
- Technical knowledge (e.g. scientific publications)
- Business knowledge (e.g. market information)

Materials modelling / Simulation tools

- Contact with software suppliers
- Up-to-date with new methods (e.g. ML/AI)
- Determination of material parameters

Translator's View

Solution

For example:
an external translator

Translation in Materials Modelling: Process and Progress (Klein et al. 2021)

Who is a Translator ?

Industrial user / Client

Industrial need / Challenge

Materials modelling / Simulation tools

- ~~Acquisition~~ Internal request
- Close contact
- Exchange e-mails/calls
- Suppliers
- Collaboration with other departments
  - Manufacturing
  - Quality Assurance

- Overarching company's KPIs
- Technical knowledge (more access to internal info)
- Business knowledge (e.g. own company / market)

- Software available within company
- Up-to-date with new methods (e.g. ML/AI)
- Determination of material parameters
  - With external partner
  - Limited within company

Translator's View

Solution

For example:
an <u>internal translator</u>

Translation in Materials Modelling: Process and Progress (Klein et al. 2021)

Who is a Translator ?

There are a lot of other activities that need to be done within a translation service, which require the involvement (direct or indirect) of the Translator

- Project acquisition (i.e. no project, no money, no translation)
  - Advertising (e.g. attending on trade fairs, expositions, posts on Linkedin)
  - Networking (e.g. with potential clients, potential suppliers)

- NDA / Data sharing (i.e. no contract, no money, no translation)
  - Project scope, patent, licensing agreement
  - Which data will be shared? Who owns the generated data?
  - Which platform will be used for data share?

- Procurement of equipment/consumables (i.e. no results, no money, no translation)
  - Quotation with suppliers / Purchasing
  - Maintenance of equipments

**These topics will not be covered by today's presentation,
but are nonetheless essential within the day-to-day work of a Translator**

Who is a Translator ?

Translation: the solution finding process

Translation processes may reveal missing information:

Information is **data** with meaning.

R&D project manager ← industry need / specific solution → **manufacturer**

Missing **data** (needed by manufacturer):
⇒ perform materials simulation
⇒ perform materials characterisation
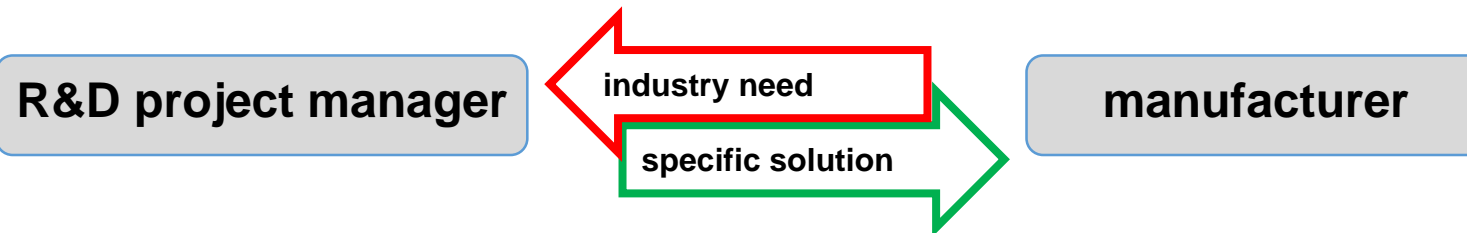
⇒ **R&D projects may help to**
  ⇒ **provide (i.e. gather or supply) missing data**
    ⇒ **connect data with concepts to provide meaning**
    ⇒ **make these data become valuable information**
      ⇒ **produce insight**

Available **data**:
• retrieved within the manufacturer
• gathered by literature or patent research

Who is a Translator?

Translation: the solution finding process

> translating an industrial **need** into a **solution**

=

> translating an **industrial** need into an innovation challenge

+

> case-wise translating an innovation challenge into a workflow

+

> translating a workflow into a **solution**
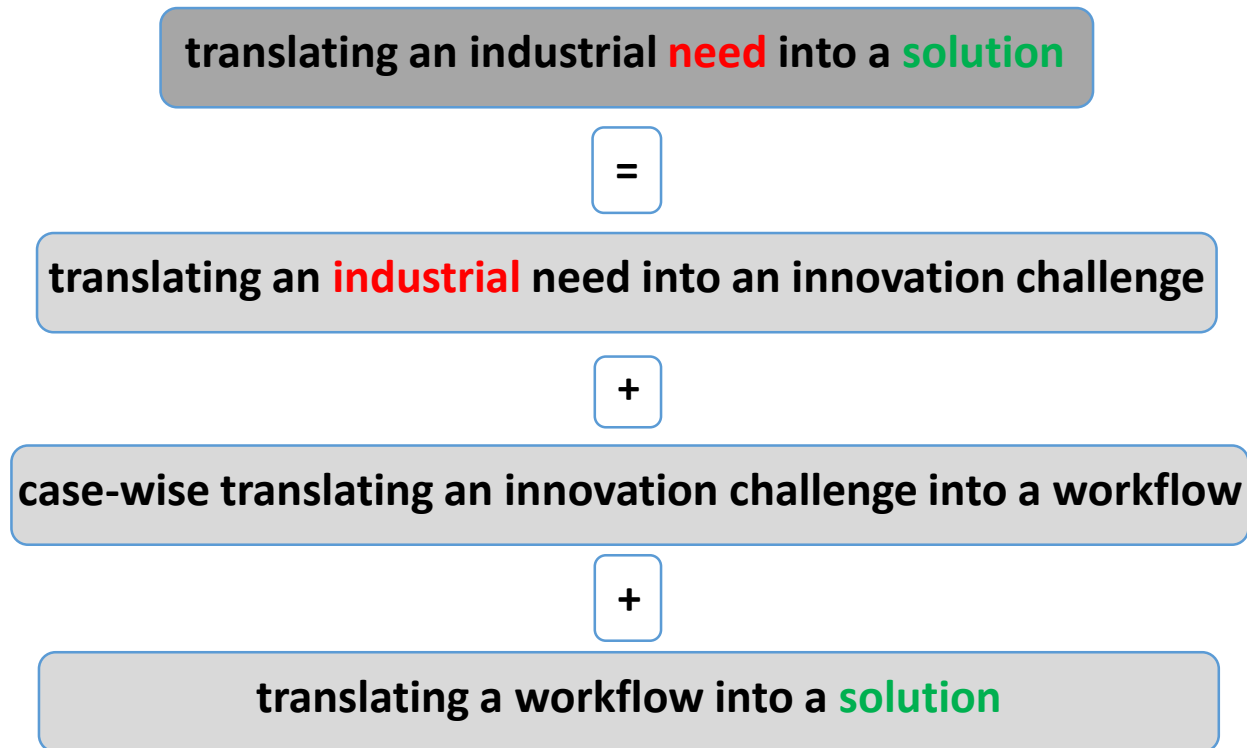
Who is a Translator?

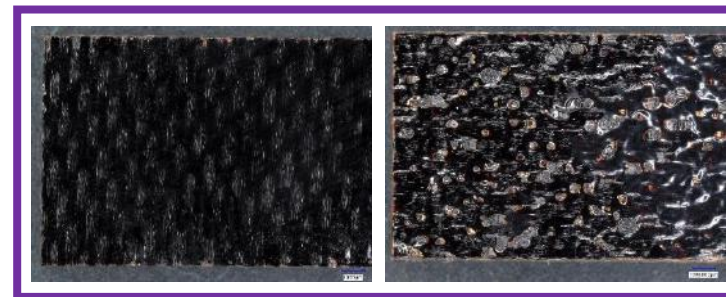**Translation processes at interfaces are at least bi-lateral and require dialogues:**

One structural brick in semiosis	One object – two observers	Two interacting bricks in translation

S … sign
I … interpretant
O … object

O … a photograph

Observer 1

experienced provider with material know-how

Observer 2

user tackling process optimisation
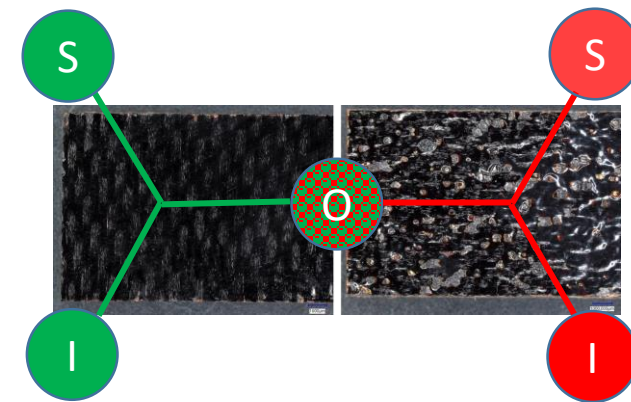
Who is a Translator?

- The client…
  - Wants to solve a challenge
  - Wants to improve a process
  - Wants to make something new
  - Wants to make something faster
  - Wants to make something new faster
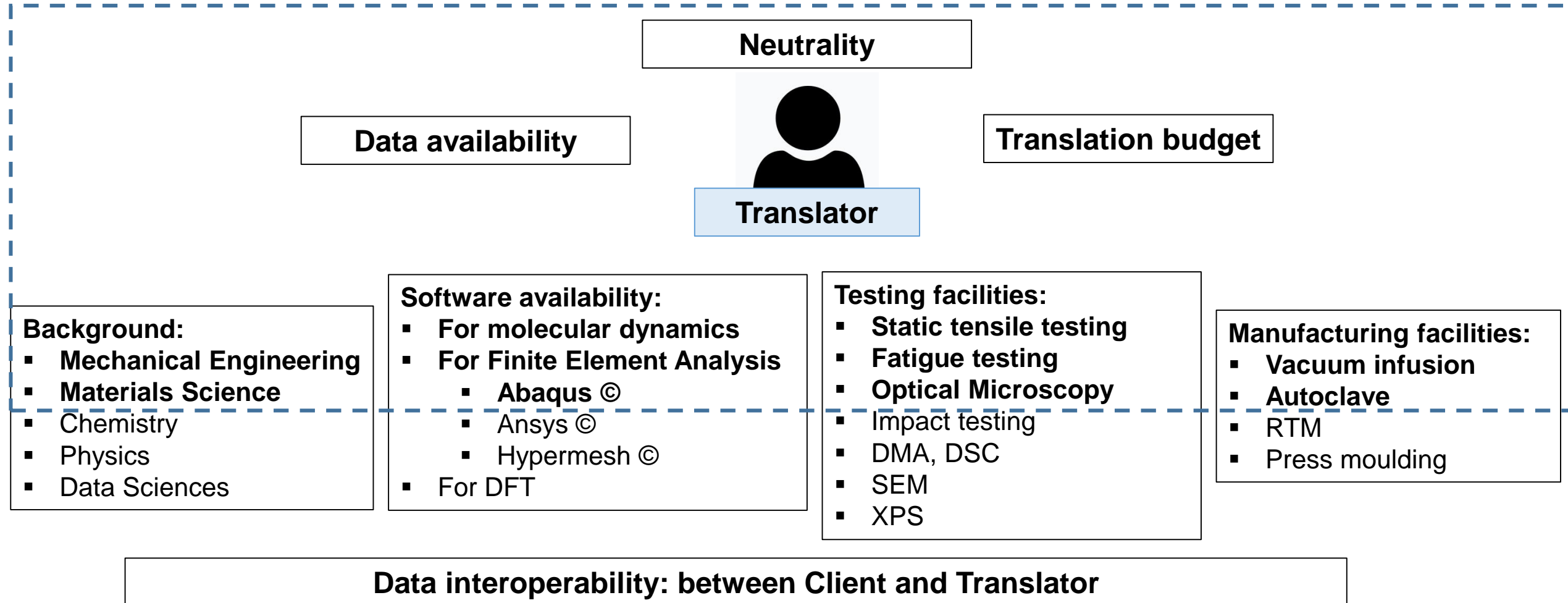
- The Translator…
  - Has to provide a solution
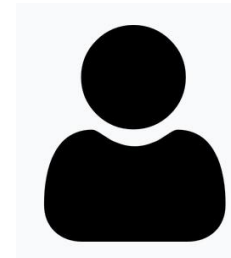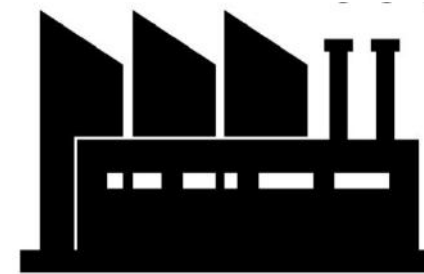
*without OntoTrans

> However, the translator by their own* is "limited" within a framework:
> - Knowledge background
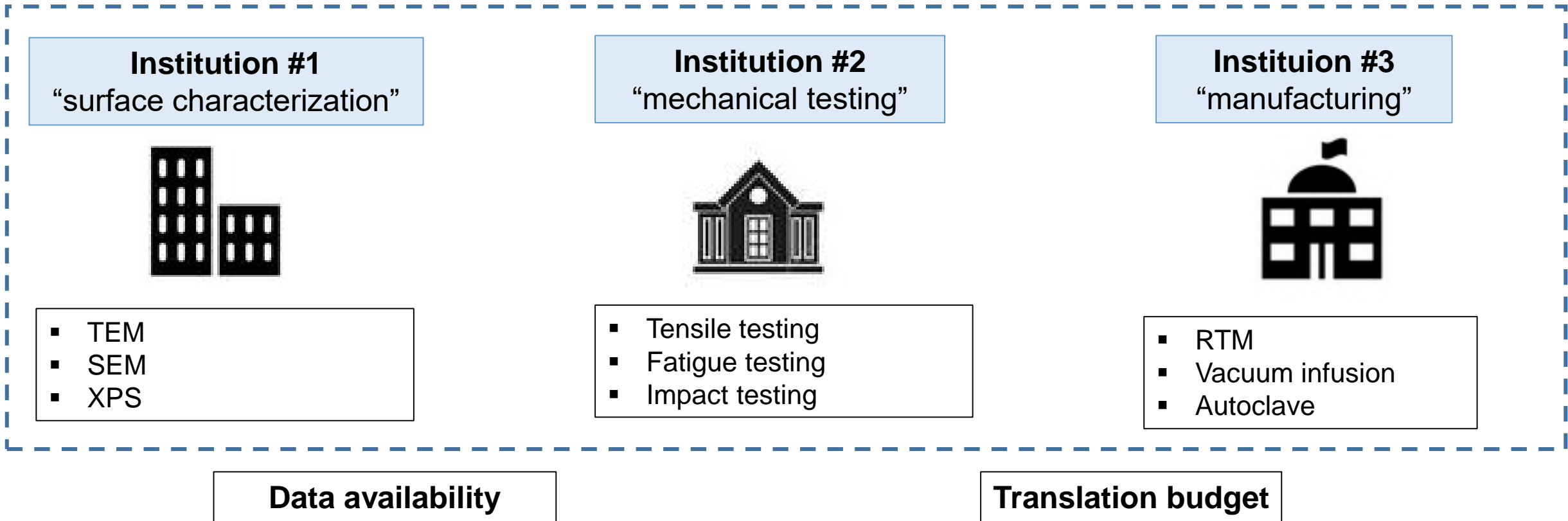> - Research facility of employer
> - Software available (license)

The "framework" of the Translator

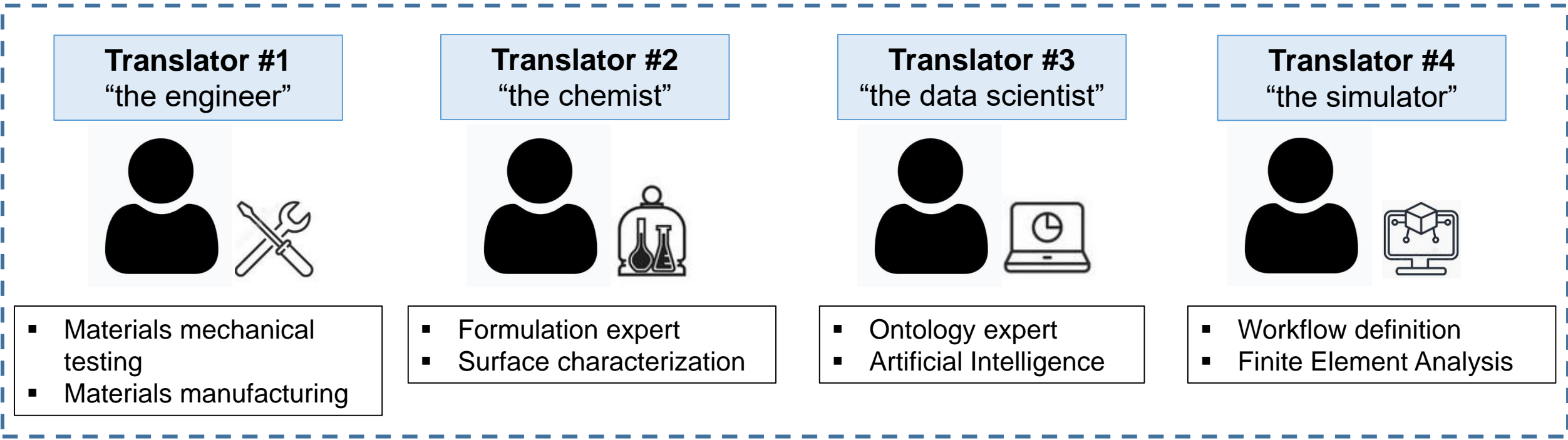**For example: a translation service dealing with composite materials**

Neutrality

Data availability

Translator

Translation budget

Background:
- **Mechanical Engineering**
- **Materials Science**
- Chemistry
- Physics
- Data Sciences

Software availability:
- **For molecular dynamics**
- **For Finite Element Analysis**
  - **Abaqus ©**
  - Ansys ©
  - Hypermesh ©
- For DFT

Testing facilities:
- **Static tensile testing**
- **Fatigue testing**
- **Optical Microscopy**
- Impact testing
- DMA, DSC
- SEM
- XPS

Manufacturing facilities:
- **Vacuum infusion**
- **Autoclave**
- RTM
- Press moulding

Data interoperability: between Client and Translator

The "framework" of the Translator

Expanding the framework: cooperation with other institutions

Institution #1 "surface characterization"	**Institution #2** "mechanical testing"	**Instituion #3** "manufacturing"

- TEM
- SEM
- XPS

- Tensile testing
- Fatigue testing
- Impact testing

- RTM
- Vacuum infusion
- Autoclave

Data availability

Translation budget

The "framework" of the Translator

Expanding the framework: a team of translators

Translator #1 "the engineer"	Translator #2 "the chemist"	Translator #3 "the data scientist"	Translator #4 "the simulator"
• Materials mechanical testing • Materials manufacturing	• Formulation expert • Surface characterization	• Ontology expert • Artificial Intelligence	• Workflow definition • Finite Element Analysis

Data availability

Translation budget

There is a guide to help translators on how to proceed with translation and benefit clients

The 6 translation steps

Translation steps according EMMC Translators Guide [1,2]

1) Good understanding of the business case

2) Good understanding of the industrial case

3) Analysis of the experimental (and modelling) data available within the client:

4) Translation to (preferably more than one) modelling workflows

5) Propose to the client modelling executor(s) and strategy for model validation

6) Translation of the modelling results to information that is understandable, reliable and usable by the client

- Iterative process

- Translation might involve a team of translators

- The translator will not necessarily be involved in all steps

- Constant communication with client

- Alignment of scope, budget and timeline/schedule

1. https://emmc.info/wp-content/uploads/2017/12/TranslatorsGuide.pdf
2. Klein, Peter; Konchakova, Natalia; Hristova-Bogaerds, Denka G.; Noeske, Michael; Simperler, Alexandra; Goldbeck, Gerhard & Höche, Daniel. (2021, April 30). Translation in Materials Modelling – Process and Progress (Version 1). Zenodo. http://doi.org/10.5281/zenodo.4729918

The 6 translation steps

According to Klein et al.:

- **Neutrality** is expressed by placing the specific interest of the Client always before the transparent interest of the Translator. Translators can be part of the modelling execution if this is of benefit of the Client

- Translators should advice the end-user/Client in the decision-making based on the modelling results using **business relevant data**

- **Confidentiality** and **trust** between Translator and Client are very significant aspects and should play a key role in the Translation practice, framed by clear-cut agreements.

Business → Translator → Modelling

Translation in Materials Modelling: Process and Progress (Klein et al. 2021)

Innovation challenges
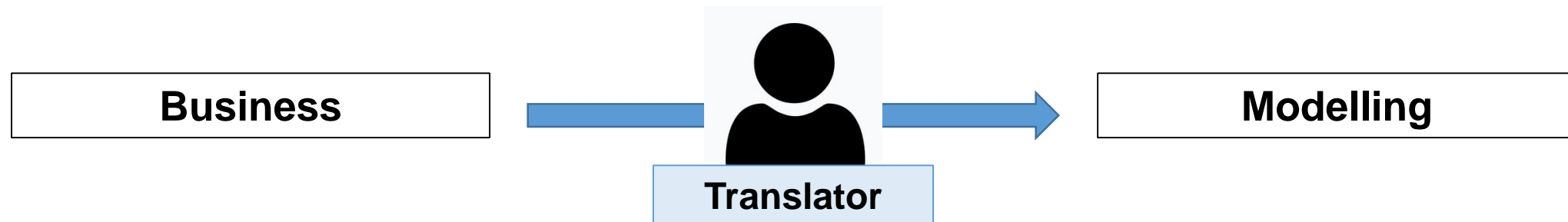
https://ontotrans.eu/project/applications/

App1: Post-launch analysis of pouch detergents

The challenge is the fast analysis of
large datasets to assess in-market initiative success

App2: Detergent Pouch Systems

The challenge is for a more integrated, digital design
and development of laundry Detergent Pouch Systems

App3: Composite prepregs
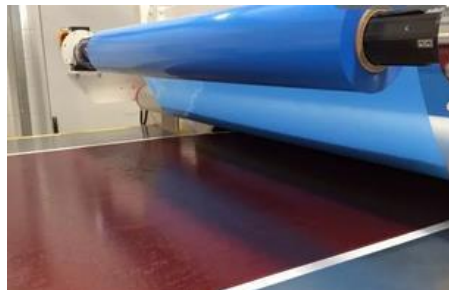
The aim is to achieve improved understanding and ultimately
control of the process to reduce time and costs in
development and manufacturing

App4: Steel Section Mill

The ultimate objective is achieving the ability of determining
process parameters given the required mechanical properties
of a target future product

Application case: Composite Prepreg

Team
OntoTrans Experts

Achieve improved understanding and ultimately control of
the process **to reduce time and costs**
in development and manufacturing

Team
Prepreg Manufacturer

External
Translator
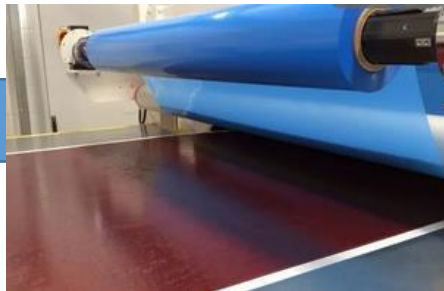
Challenge

Client

Application case: Composite Prepreg

1) Good understanding of the business case

- Market, regulatory and safety requirements drive the transition towards non-toxic, low environmental impact solutions for composite prepregs (fabrics pre-impregnated with resin).

- Innovative prepregs provide a potential solution.

Translator's questions:
- What are the KPIs ?
- What are the expected benefits for my client?
- What are the standards, norms and laws involved (e.g. GDPR)?

Application case: Composite Prepreg

1) Good understanding of the business case

**KPI definition: Interaction between external Translator and Client**

Key performance indicator

1. More efficient and targeted exploration

2. Deeper understanding

3. Broader exploration

4. R&D strategy development

5. Source of property data

6. Trouble shooting

7. Performance optimisation

8. Intellectual property protection

9. Value chain benefits

10. Improve communication and collaboration between R&D and production

11. Upscaling and market introduction as well as marketing benefits
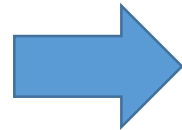
According to Client
- Improve understanding and control of process
- Improve quality of end products
- Reduce development time and costs
- Create model-based approach for future product developments

Application case: Composite Prepreg

1) Good understanding of the business case

Interaction between external Translator and Client

Case 1:

- Input: new process parameters (temperature, pressure, geometry)
- Output: expected mechanical properties

Case 2

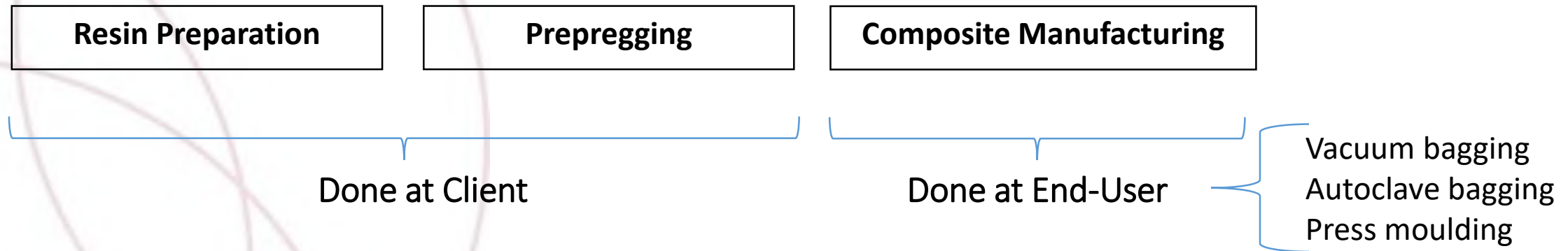- Input: required mechanical properties
- Output: suitable process parameters
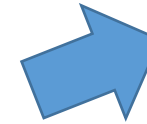
KPIs (measurable)
- Time-to-market (months)
- Number of tries (#)
- Mechanical performance
  - Interlaminar shear strength (MPa)
  - Tensile strength (MPa)

Application case: Composite Prepreg

2) Good understanding of the industrial case

Innovative Prepregs

Resin Preparation	Prepregging	Composite Manufacturing

Done at Client

Done at End-User

Vacuum bagging
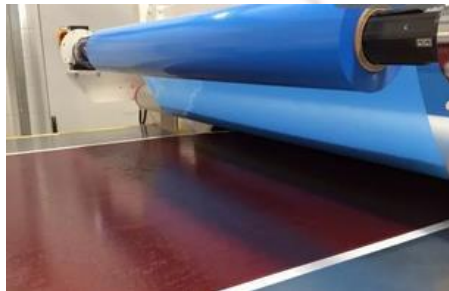Autoclave bagging
Press moulding

Translator's questions:
- How the manufacturing process is carried out ?
  - How to control it?
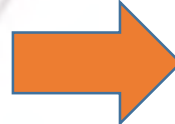- Which parameters have an influence?

Application case: Composite Prepreg
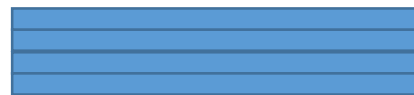
2) Good understanding of the industrial case

Resin **+** Textile Fabric **=** Prepreg

90°

0°

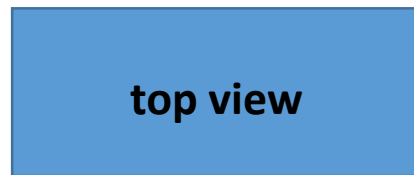One layer = 0.25 mm
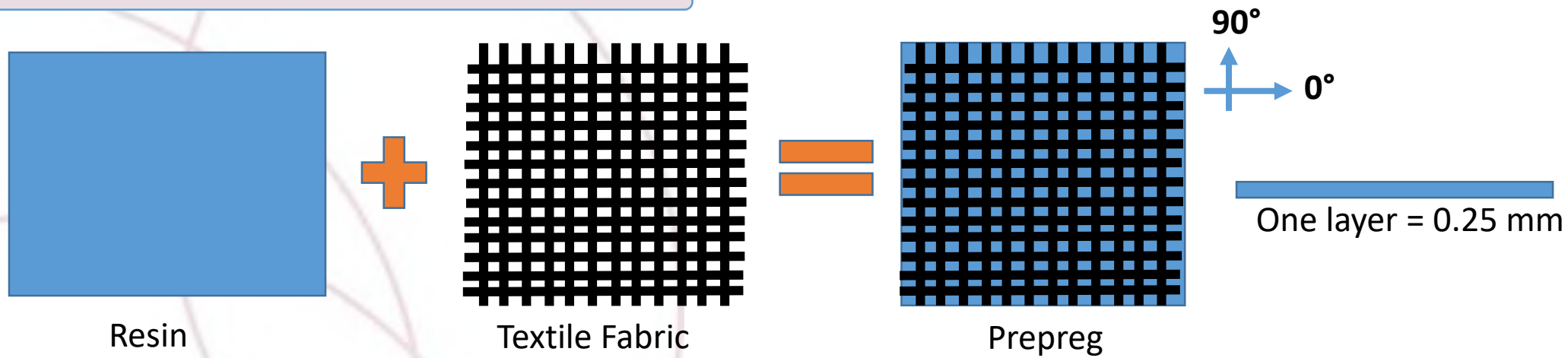
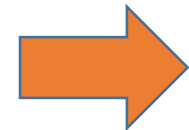**Prepreg Roll**

cutting

stacking

e.g. 4 layers = 1 mm

top view

Moulding & Curing

*Composite laminate: Anisotropic properties

Application case: Composite Prepreg

3) Analysis of the experimental (and modelling) data available within the client

Clients' Proprietary Data	Clients' Publicly Available Data	Additional Data
▪ Internal measurements 　▪ Viscosity ▪ Resin formulation ▪ Tools geometry ▪ Manufacturing price	▪ Product data sheet 　▪ Mechanical properties 　▪ Fibre content 　▪ Density ▪ Product sell price	▪ Benchmark values ▪ Reference values of mechanical properties 　▪ Tensile strength 　▪ Interlaminar shear strength

Data, data format, metadata

Translator's questions:
- Is the available data FAIR (findable, accessible, interoperable, reusable)?
- Will I need extra experiments/characterisation for additional simulation parameters?
- Can I get more data from an external repository?

Application case: Composite Prepreg

3) Analysis of the experimental (and modelling) data available within the client

Data interoperability

- It is very common that the Client creates parts (geometry) with a specific software that has proprietary file format (e.g. Ansys©, Pro-Engineering©, CATIA©)

- Afterwards, the Translator needs the geometry of the part as an input for a Finite Element Analysis (e.g. Hypermesh ©, Abaqus ©), which does not necessarily "communicates", i.e. is interoperable, with the original CAE software

- There are "open file formats" (e.g. STEP-file) which are common to most software, but usually many features are "lost in translation"

- In the worst case scenario, the translator has to build the geometry representation from scratch

Application case: Composite Prepreg

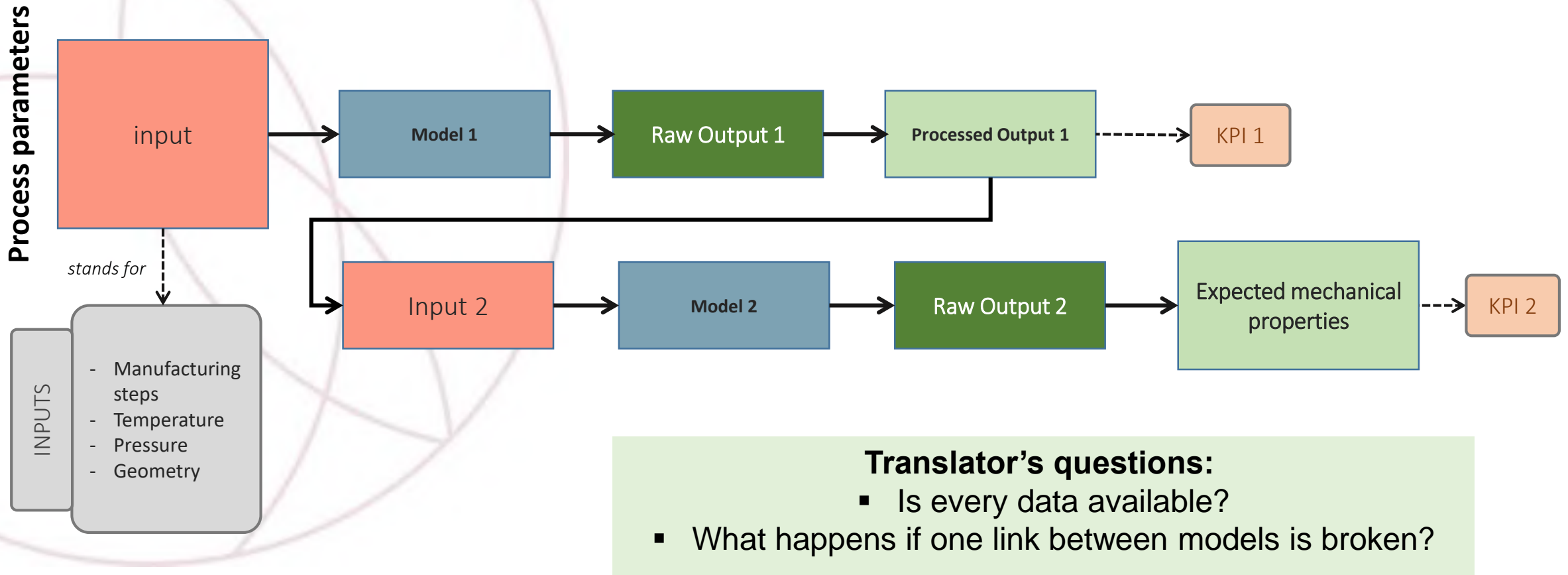**3) Analysis of the experimental (and modelling) data available within the client**

Missing data (information)

- During the translation process, it is usual that in order to carry out a workflow, some properties (or parameters) required for the simulation (i.e. materials modelling) are not necessarily available

- Potential solutions:

- Carry out experiments (by the translator or external provider) to obtain the missing data
  - Use materials modelling to obtain the missing data
    - Use molecular dynamics to determine the Young's modulus for a Finite Element Analysis
  - Find the missing parameter on industrial dataspace (or parameter repository)
  - Guess (or assume) the value of the missing parameter based on reference values
    - This could lead to a reduced confidence interval (statistical)

Application case: Composite Prepreg

4) Translation to (preferably more than one) modelling workflows

MODA Representation of Workflow Case 1: After agreement between Client and External translator

Process parameters

input → Model 1 → Raw Output 1 → Processed Output 1 ⇢ KPI 1

stands for

INPUTS
- Manufacturing steps
- Temperature
- Pressure
- Geometry

Input 2 → Model 2 → Raw Output 2 → Expected mechanical properties ⇢ KPI 2

Translator's questions:
- Is every data available?
- What happens if one link between models is broken?

Application case: Composite Prepreg

5) Propose to the client modelling executor(s) and strategy for model validation

Model validation

- Translator executes workflow (e.g. using materials modelling)

- Client provides prepreg for manufacturing

- Translator act as a "surrogate" of a Client's end user

- Translator manufacturers composite laminate with Client's prepreg

- Translator test the composite laminate
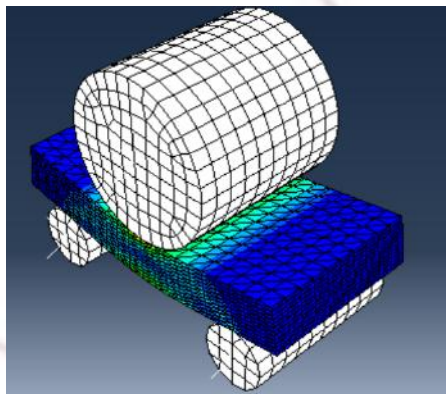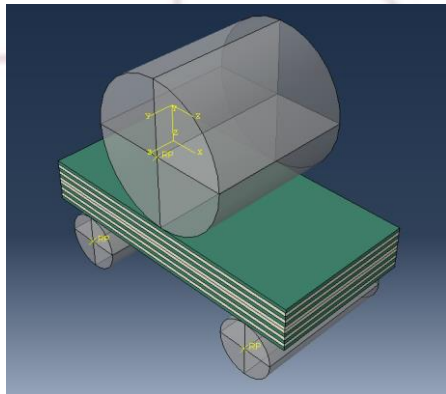
- Translator and Client discuss KPIs

Translator's questions:
- Is there an alternative model validation method ?
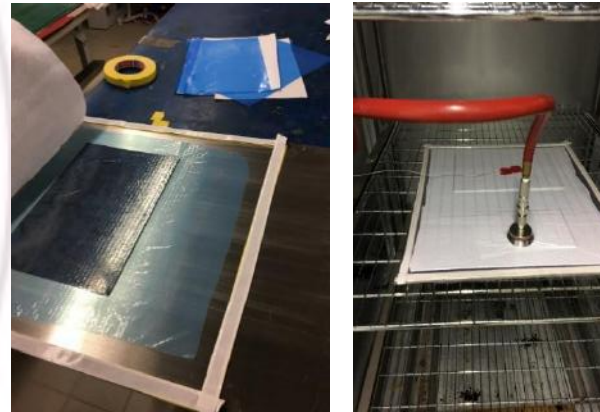- Is the validation broad enough to cover all aspects ?

Application case: Composite Prepreg

6) Translation of the modelling results to information that is understandable, reliable and usable to client
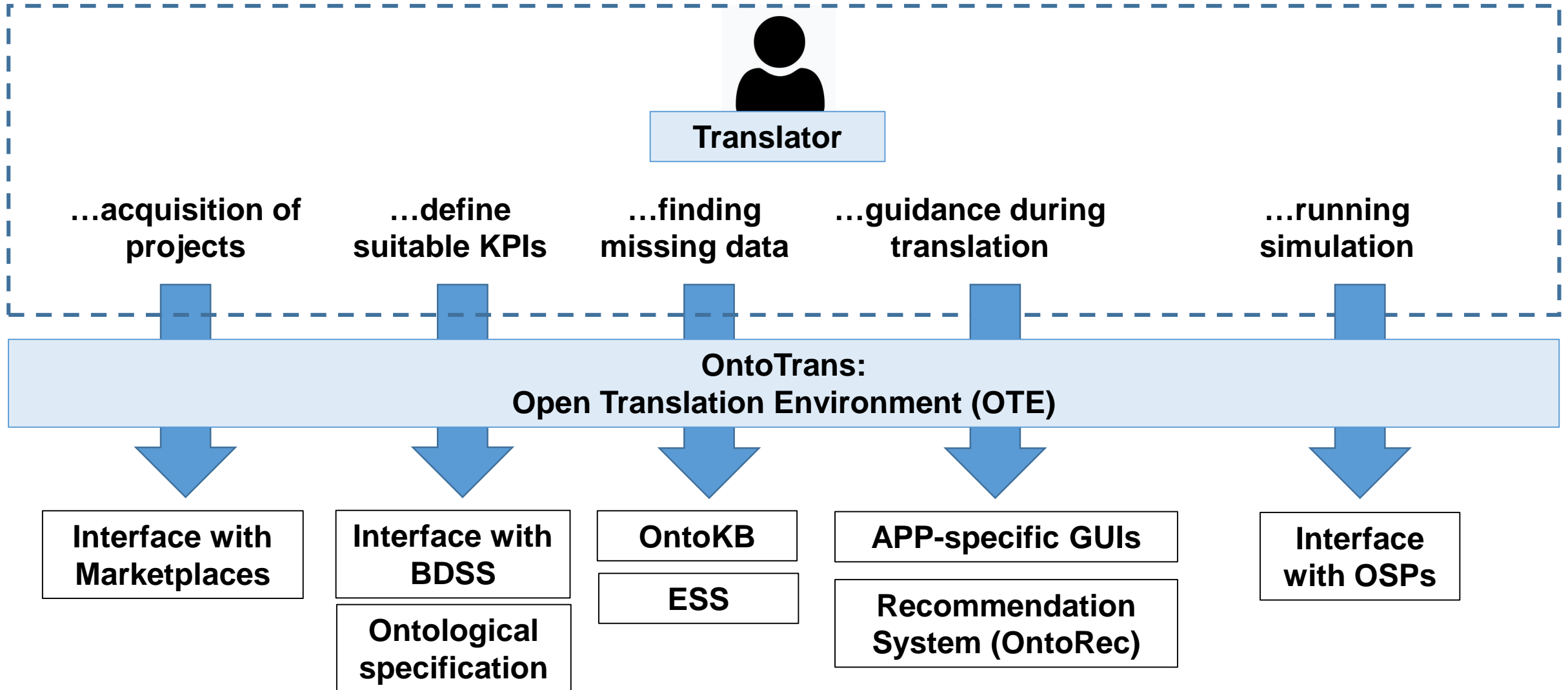
Simulation

Manufacturing

Testing

Validation

Translator's questions:
- How to present the results?
- How to make the results (re) usable to my client?

Translator's View: How OntoTrans makes life easier

Translator

…acquisition of projects

…define suitable KPIs

…finding missing data

…guidance during translation

…running simulation

OntoTrans: Open Translation Environment (OTE)

Interface with Marketplaces

Interface with BDSS

Ontological specification

OntoKB

ESS

APP-specific GUIs

Recommendation System (OntoRec)

Interface with OSPs

Conclusions & Outlook

- Translator (or team of) provides service of translating an industrial challenge into a solution by means of materials modelling and simulation tools
  - Translation involves activities covering NDA signing on data sharing to simulation
  - Translator can be internal or external

- The translator is "limited" by a framework, since it is not possible to provide all available simulation, characterization, and manufacturing services

- The EMMC six translation steps provide a structured pathway for the translation process
  - Within OntoTrans the six steps are being followed for 4 Application Cases

- OntoTrans provides an environment that can "expand" the translator's framework
  - Support through acquisition of projects, definition of KPIs, finding missing data, running of workflows

Thank you!