

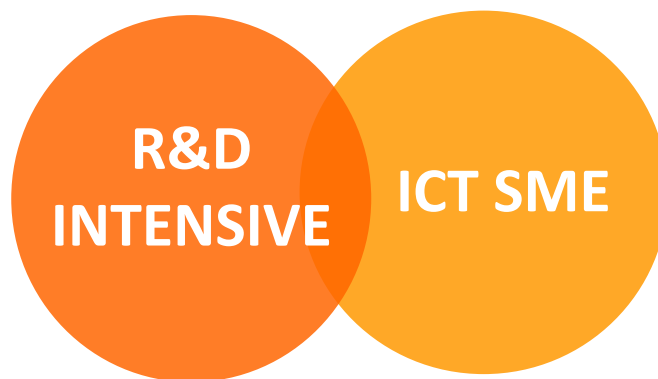


DT-NMBP-09-2018: Accelerating the uptake of materials modelling software (IA)



TREELOGIC

Big Data, Computer Vision & Analytics



R&D intensive SME that provides **ICT** technology-based solutions.

Data-driven company,

Maria Eugenia (Xenia) BELTRAN
mariaeugenia.beltran@treelogic.com



The European Materials Modelling Council

Specialisation in building scientific and technological knowledge around **data management**.



BIG DATA

MANAGEMENT OF LARGE AMOUNTS OF HETEROGENEOUS DATA IN REAL-TIME

- Hybrid computing
- Batch processing
- Stream processing
- In-memory processing
- NoSQL

COMPUTER VISION

SCENE UNDERSTANDING THROUGH VIDEO/IMAGE PROCESSING

- Adaptive techniques
- Modelling and detection
- Video analysis
- Semantic recognition

DATA SCIENCE

ADVANCED ANALYTICS TO GET VALUE FROM DATA AND FACILITATE UNDERSTANDING

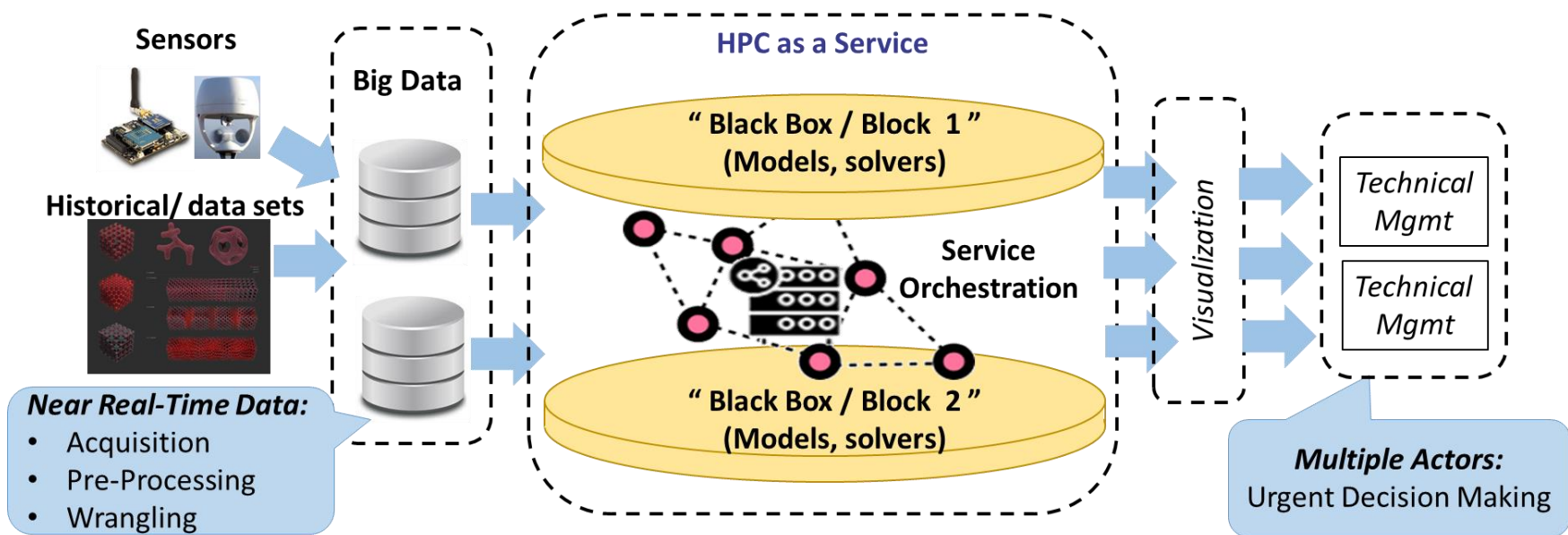
- Pattern recognition
- Behaviour modelling
- Machine learning
- Social media analysis
- Visual analytics



The European Materials Modelling Council

Coupled molecular dynamics modelling through on demand execution as a service (urgent computing paradigm)

Proposal is focus on coupling two material models (being one: molecular dyanmics) under the urgent computing → HPC as a service



Use case: industrial



Objectives & Innovative aspects

- ***Fast coupled simulation/modelling as a service → live simulations***
- ***Running a simple-to-use graphical interfaces → Human Factor***
(initial set up, sim. conditions -e.g. thermodynamic ensemble- & output)
- ***Take advantage of HPC supercomputers → scalability and upscaling***
- ***Modularity***
- ***Streamlines the data flow for fast processing***
- ***Innovative business models & market fit***

Results & Impact

- ***Flexible modelling framework → multisectoral service***
- ***Fast response (near real time) & large-scale Atomic/Molecular Parallel Sim***
- ***Cutting design costs***
- ***Easy branching out to different scenarios***



PARTICIPANTS



Looking for:

1. Existing academic/SME solvers, material models to couple w/
2. Industrial companies and manufacturers(**End-users**).