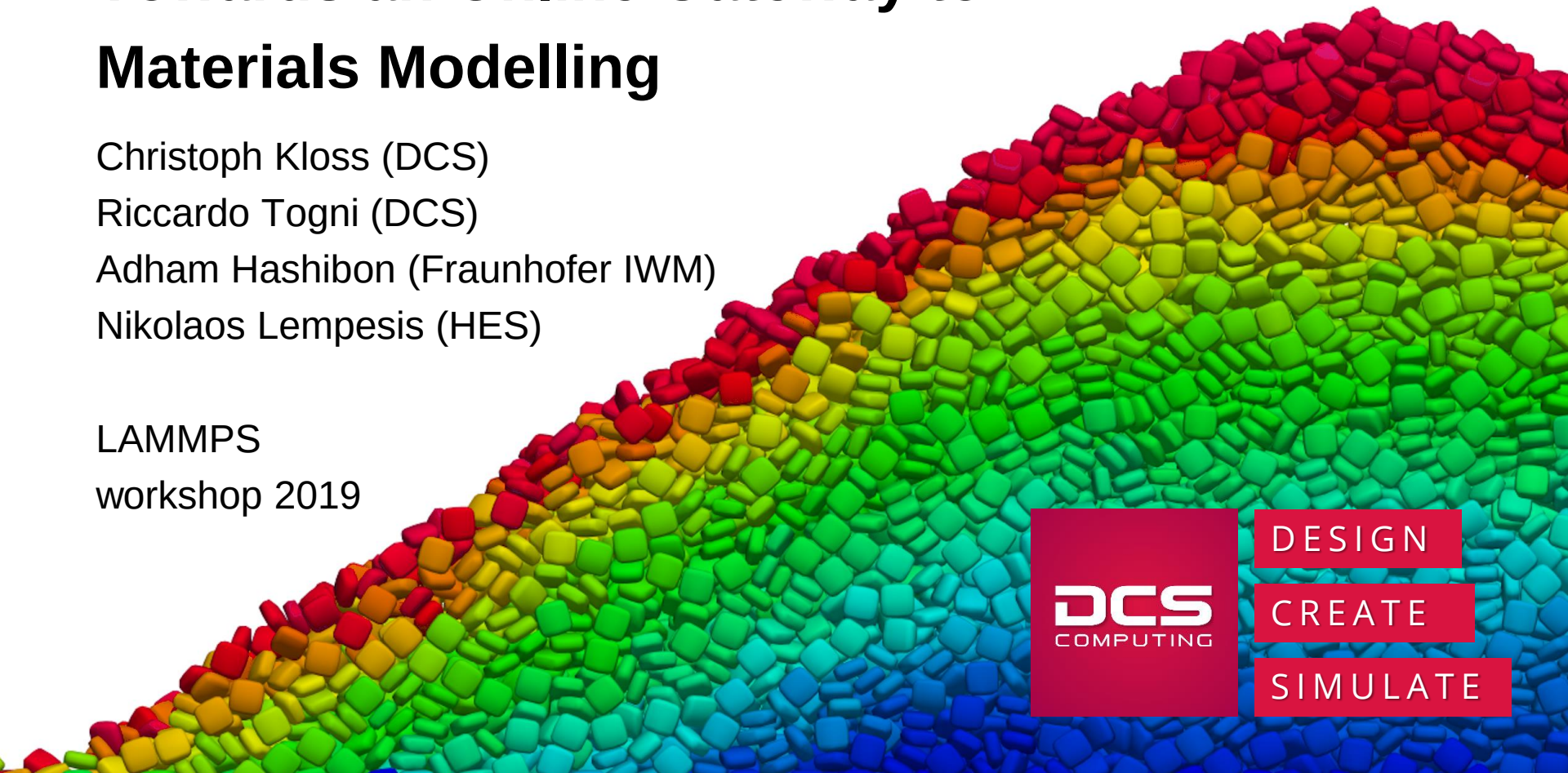
Marketplace

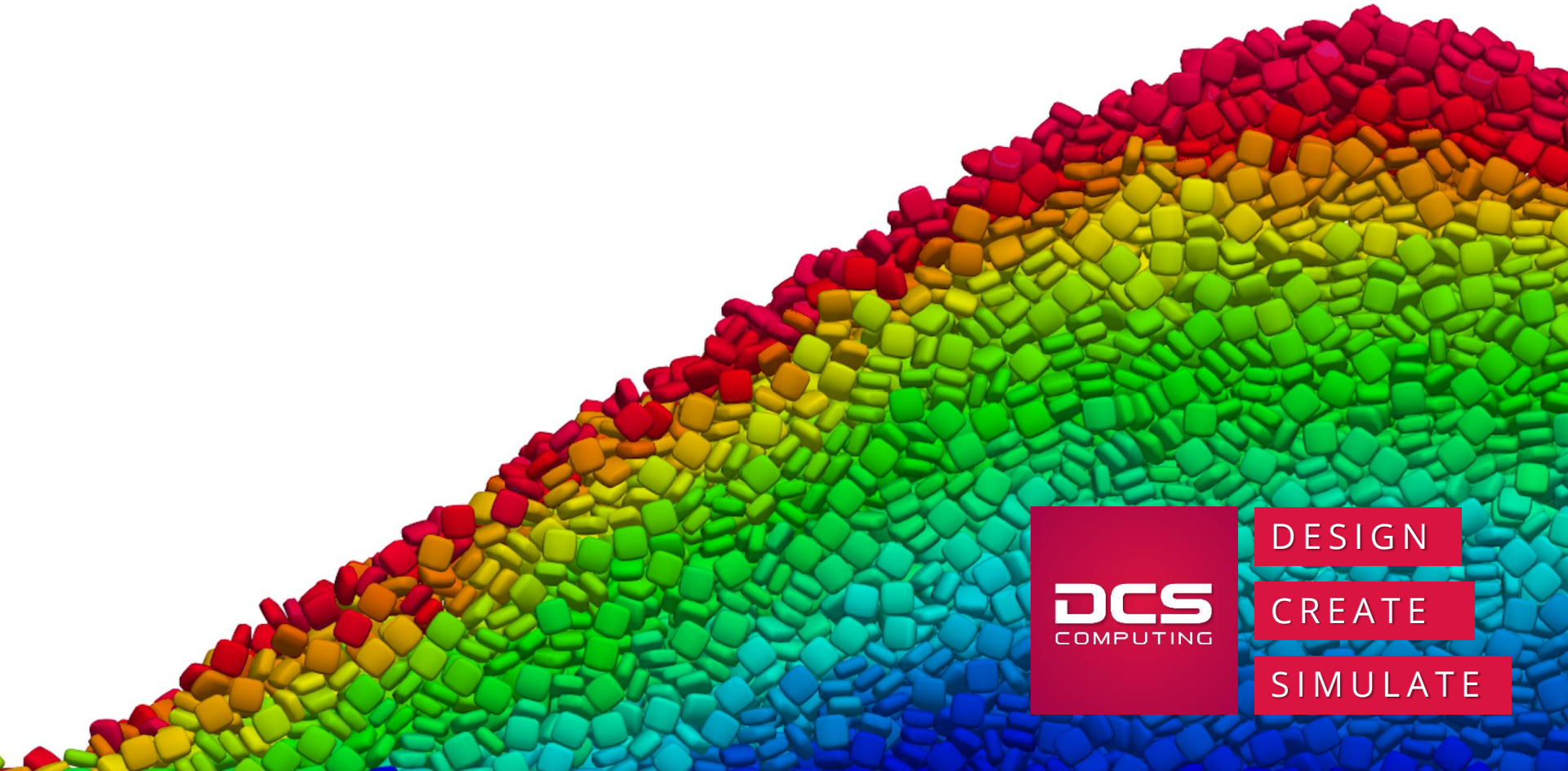
Towards an Online Gateway to Materials Modelling

Christoph Kloss (DCS)
Riccardo Togni (DCS)
Adham Hashibon (Fraunhofer IWM)
Nikolaos Lempesis (HES)

LAMMPS
workshop 2019



Background on DCS: Discrete Element Modelling



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Governing Equations for Discrete Element Method

Method – Governing equations for DEM

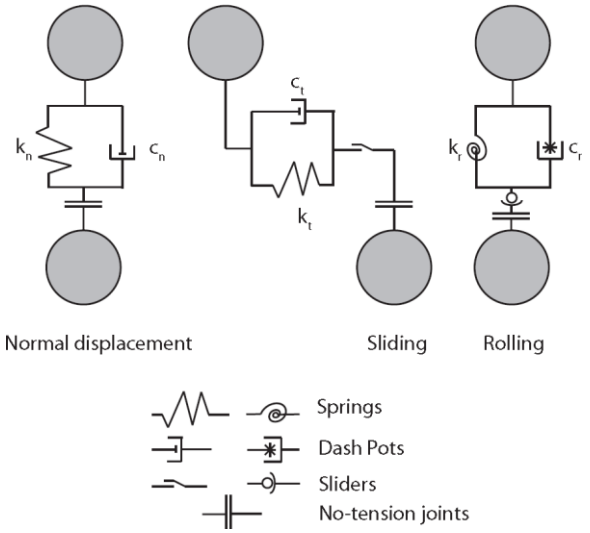
- Newton's second law for the particle phase:

$$m_p \frac{dU_p}{dt} = \sum F_{p,p} + \sum F_{p,w} + m_p g + F_p + F_f$$

$$I_p \frac{d\omega_p}{dt} = T_p$$

m… mass (kg)
$F_{p,p}$, $F_{p,w}$ … particle-particle & particle-wall interaction forces (N)
F_p … pressure force (N)
F_f … fluid forces (N)
I … momentum
ω …angular velocity
T … torque

- Soft sphere method (particles overlap during contact)
- Spring-dashpot model
- normal model (e.g. Hertz)
- tangential model (e.g. history)
- rolling friction model (e.g. epsd2)
- Other forces, e.g. lubrication force model



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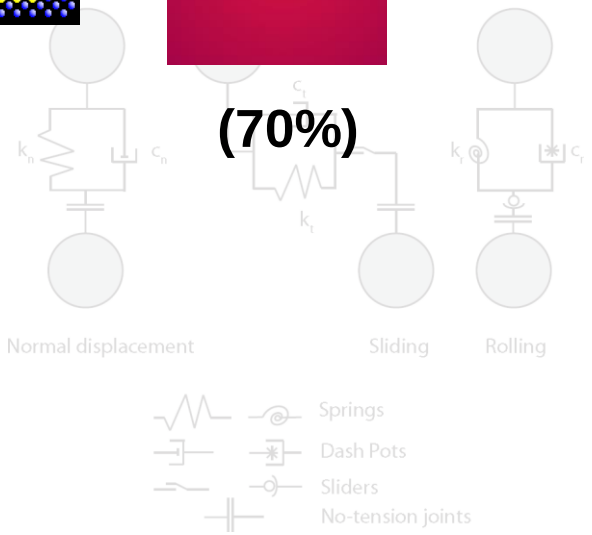
LIGGGHTS® = LAMMPS + DCS COMPUTING

(www.cfdem.com) (30%) (70%)



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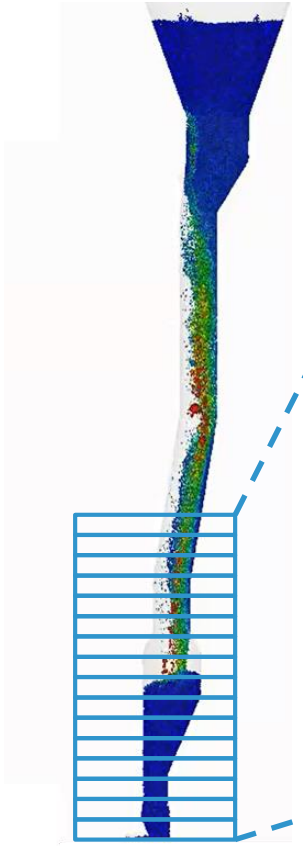
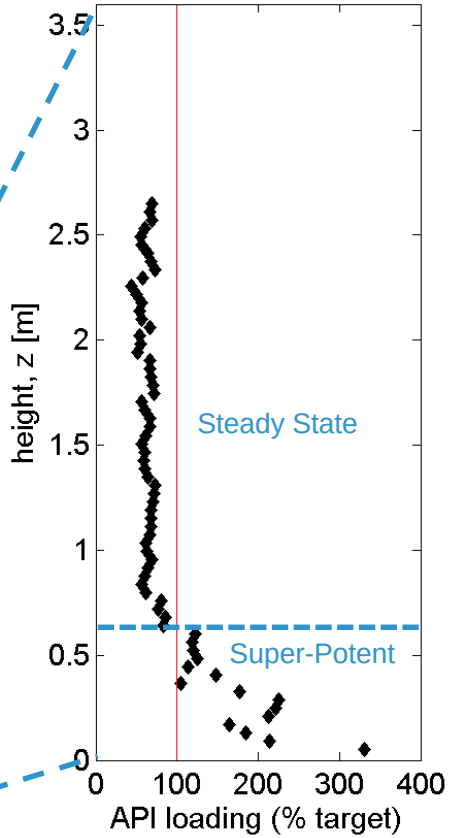
Use Case: Segregation of Pharmaceutical Powder

- **Simulation of commercial scale tablet press feed system**
- **Coupled CFD-DEM model**

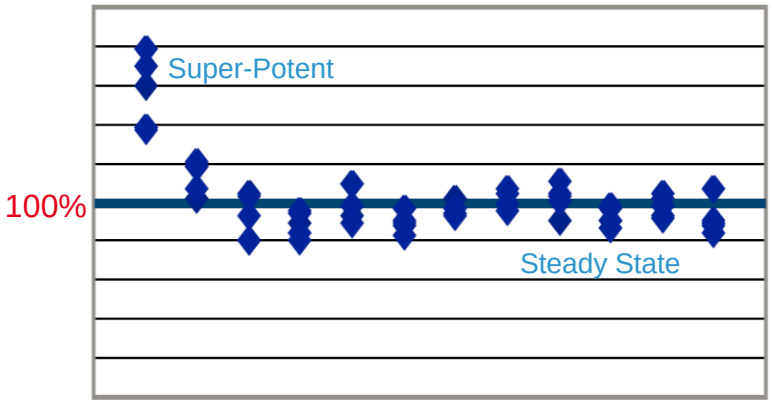
CFD-DEM Simulation



Potency Predictions



Representative
API Content, Percent of Label Claim



Time of Compression Process

Adapted from Prescott & Garcia (2001)

Ketterhagen, B. : Modeling the impact of powder segregation on pharmaceutical tablet manufacturing process, CFDEM®project user meeting 2016

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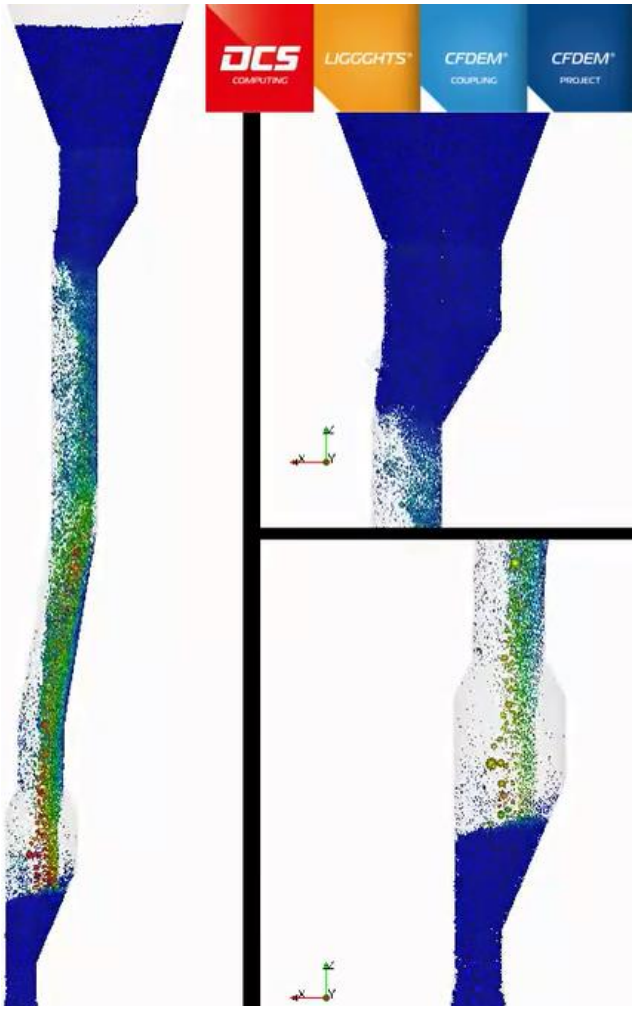
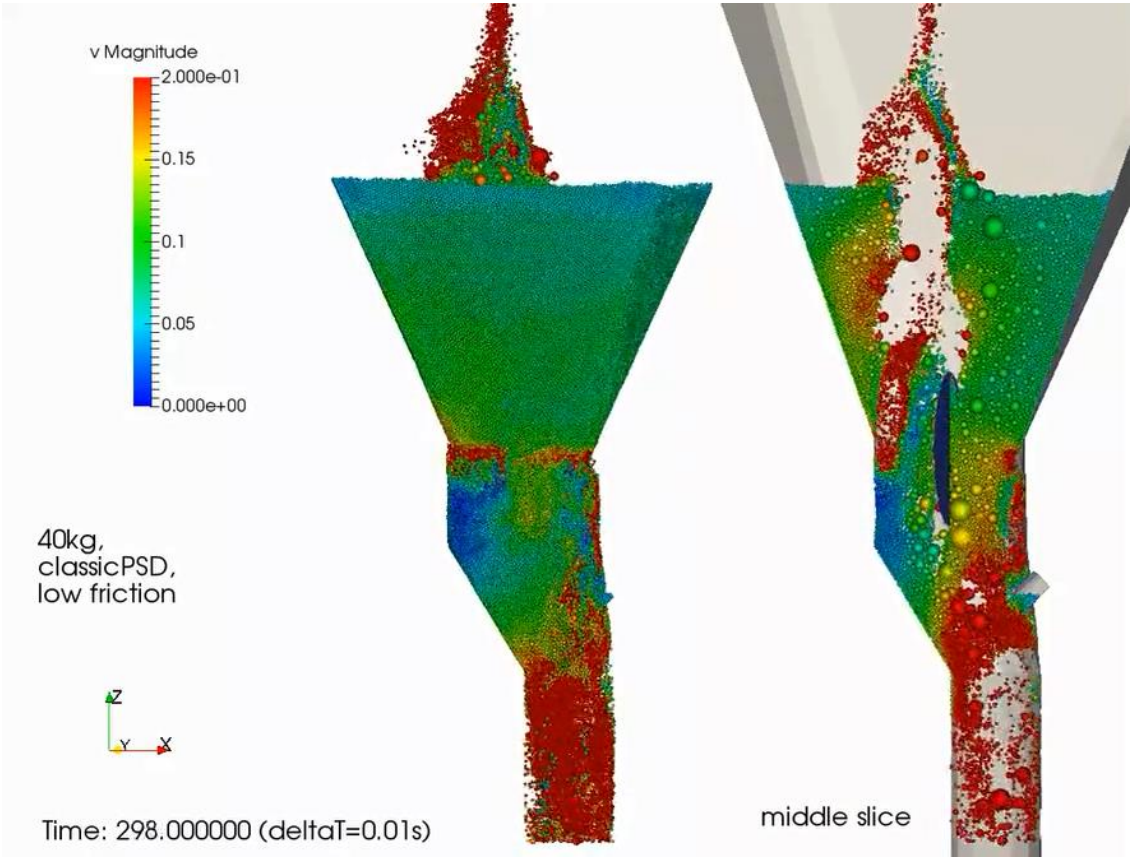
Use Case: Segregation of Pharmaceutical Powder





Video: https://vimeo.com/219836723

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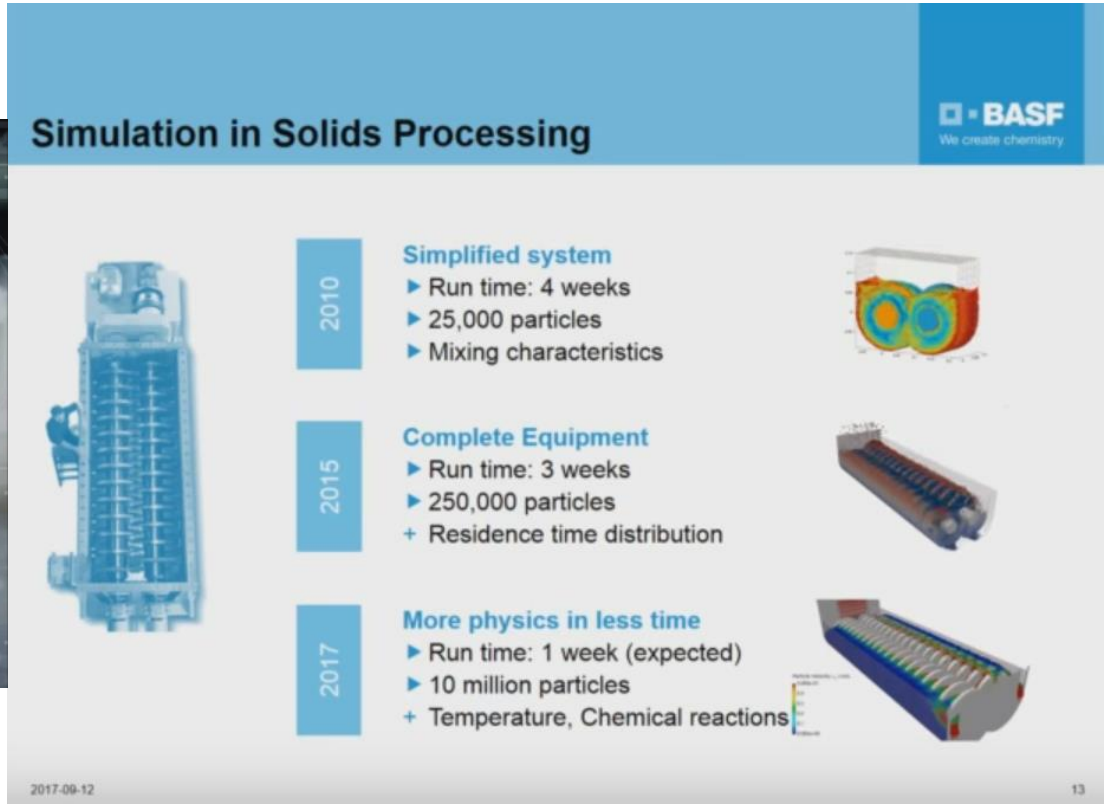
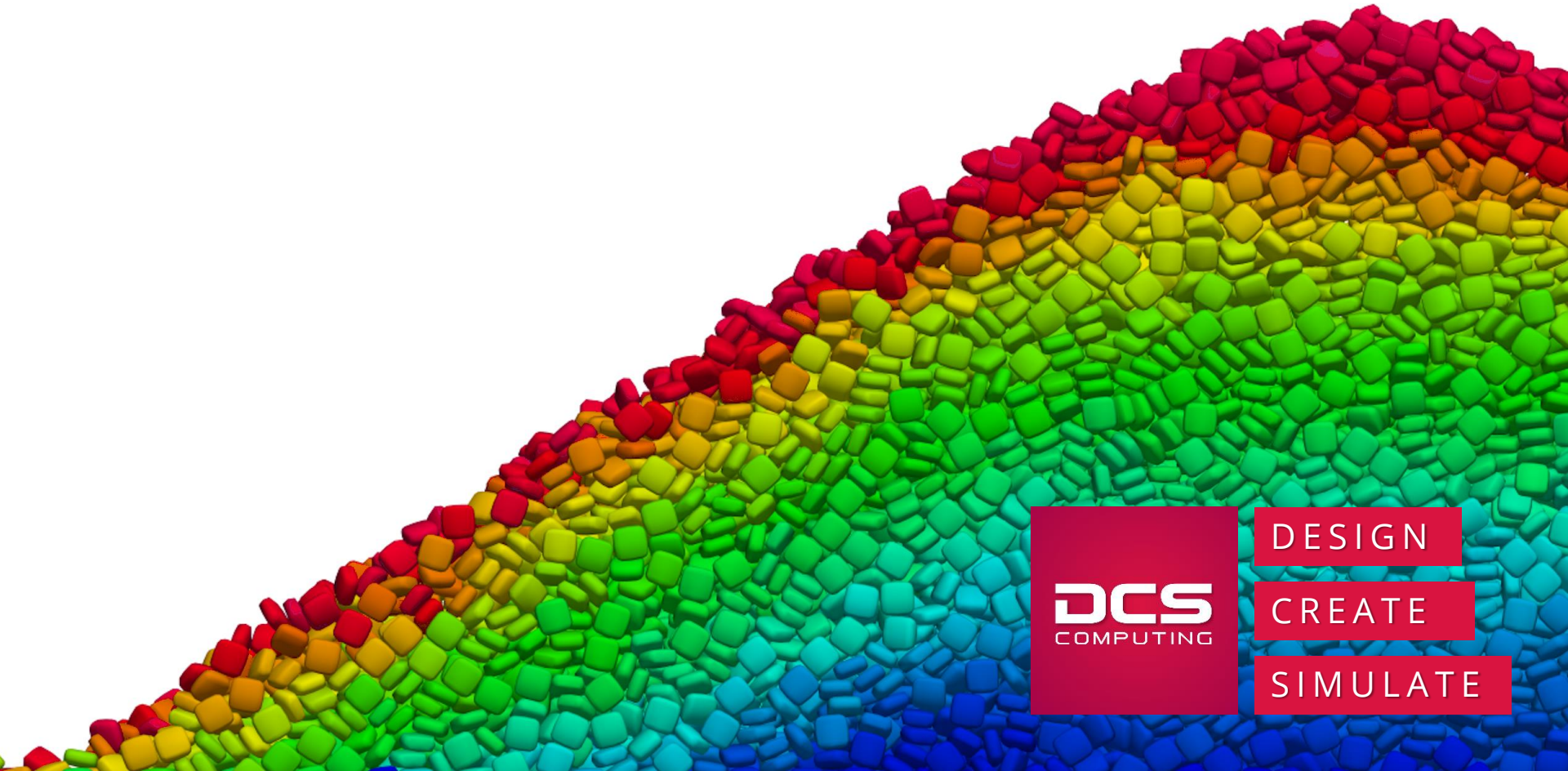
Industrial Usage of DEM Simulation – BASF Example

- **Particle based simulation in general** is on the rise, example by BASF
- Advances in Simulation of industrial solids processes
- Talk by Dr. Stephan Schenk, “Digitalization in BASF R&D”



The Challenge:
What to do with the Data



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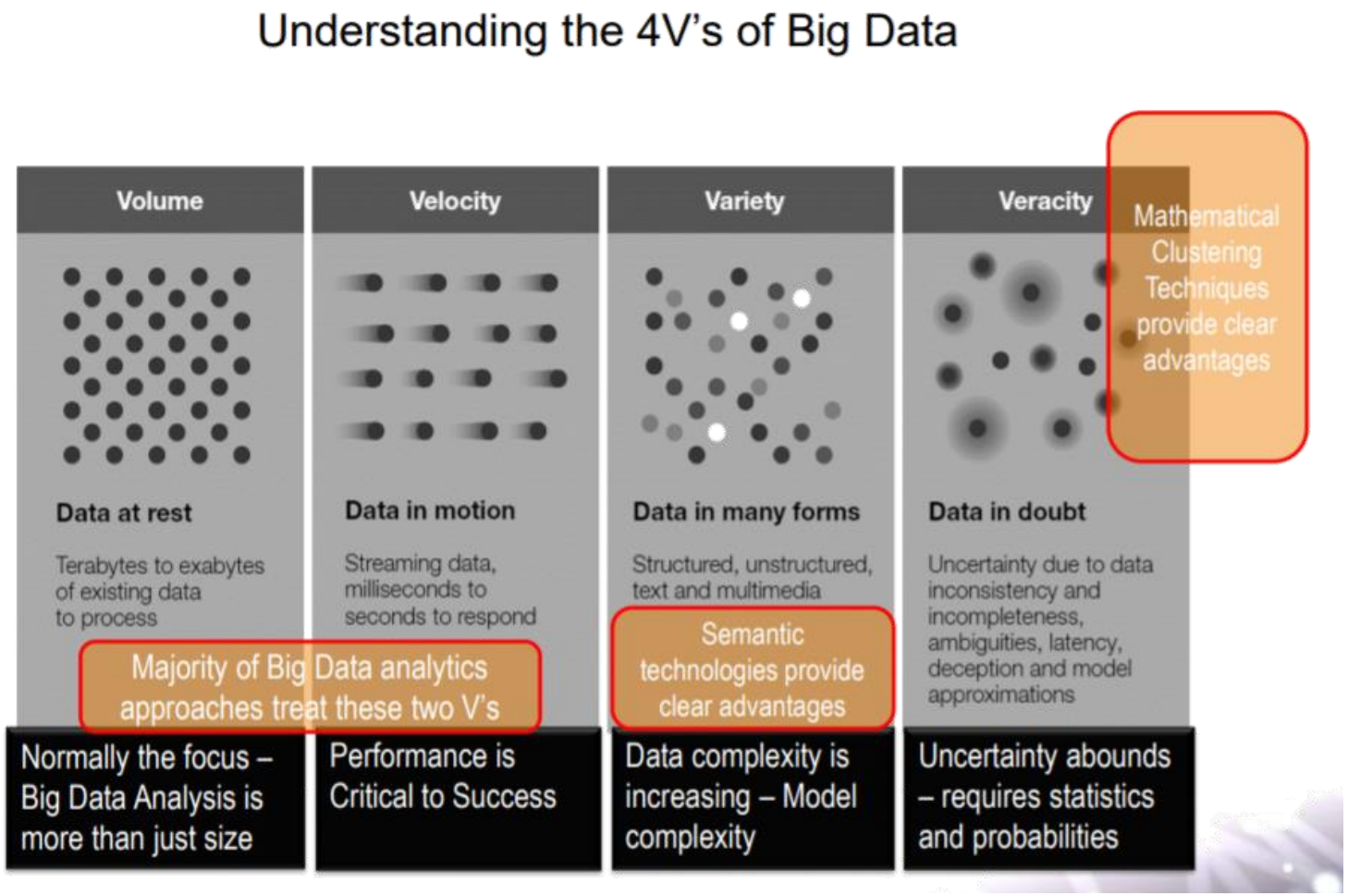
The 4 Vs of Big Data



Eric Little (OSTHUS, US) : Beyond the Models: Applying Semantic Technologies Across the Enterprise, EMMC Workshop 2018

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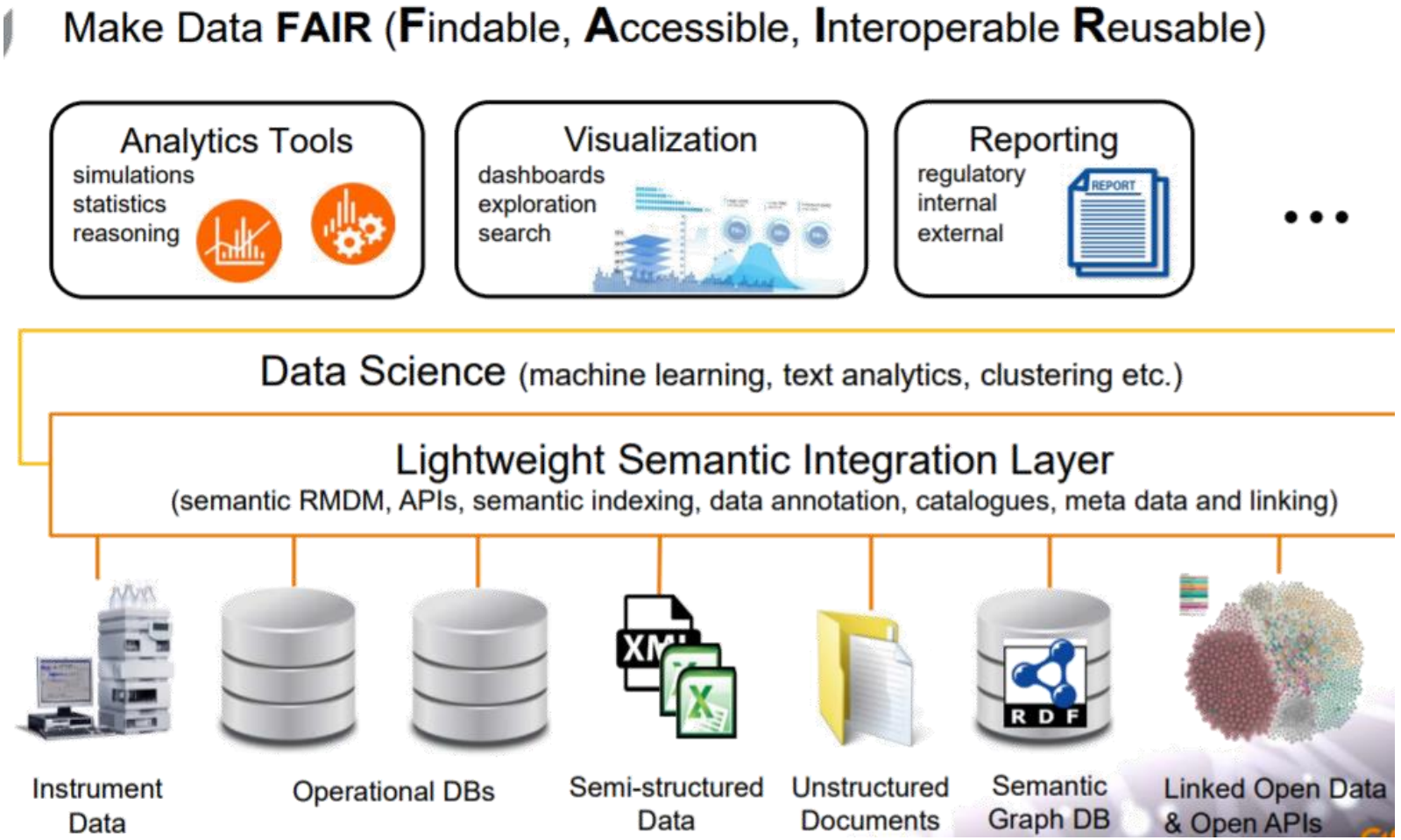
Interoperability of Data



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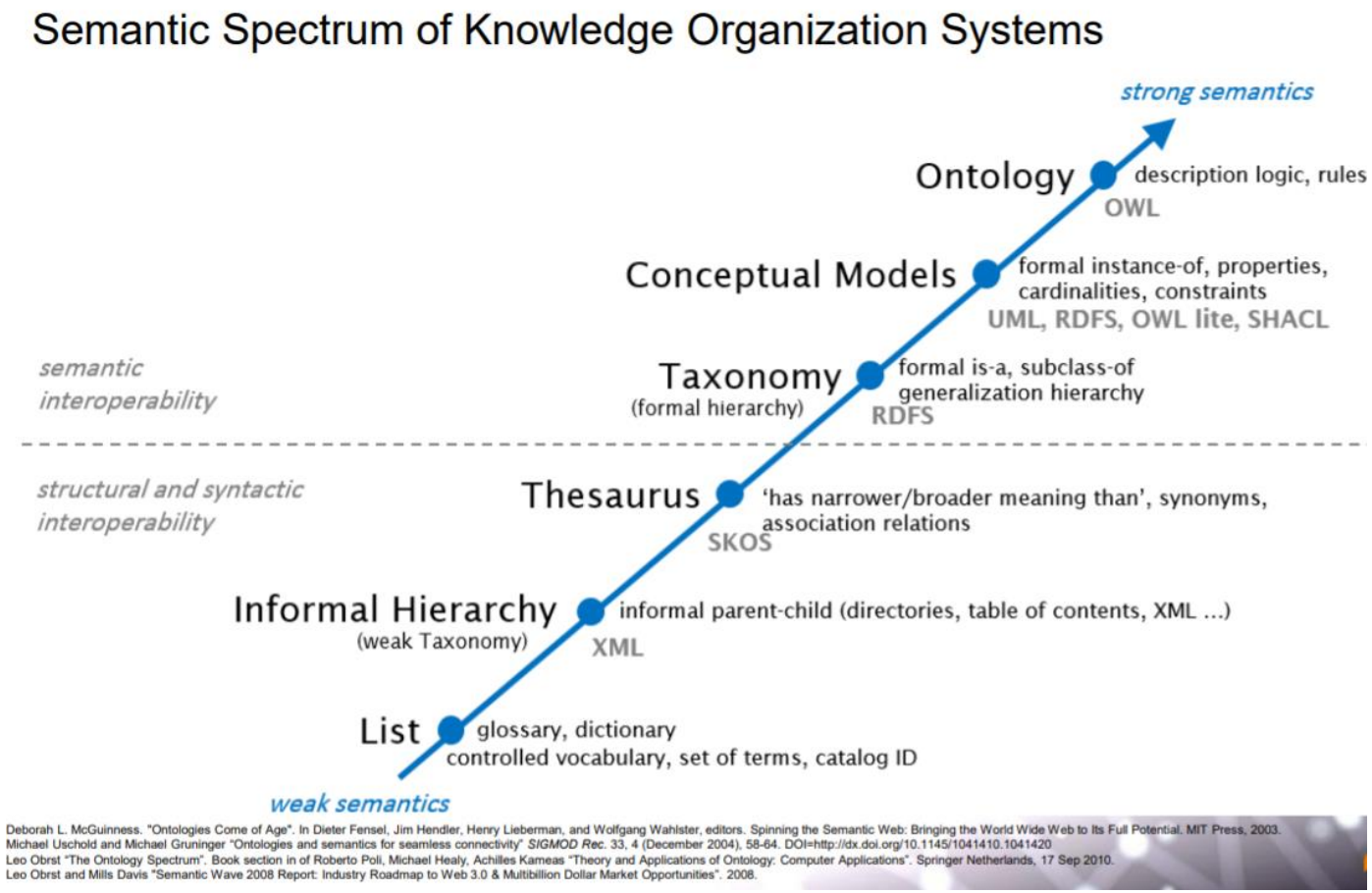
Semantics is Key



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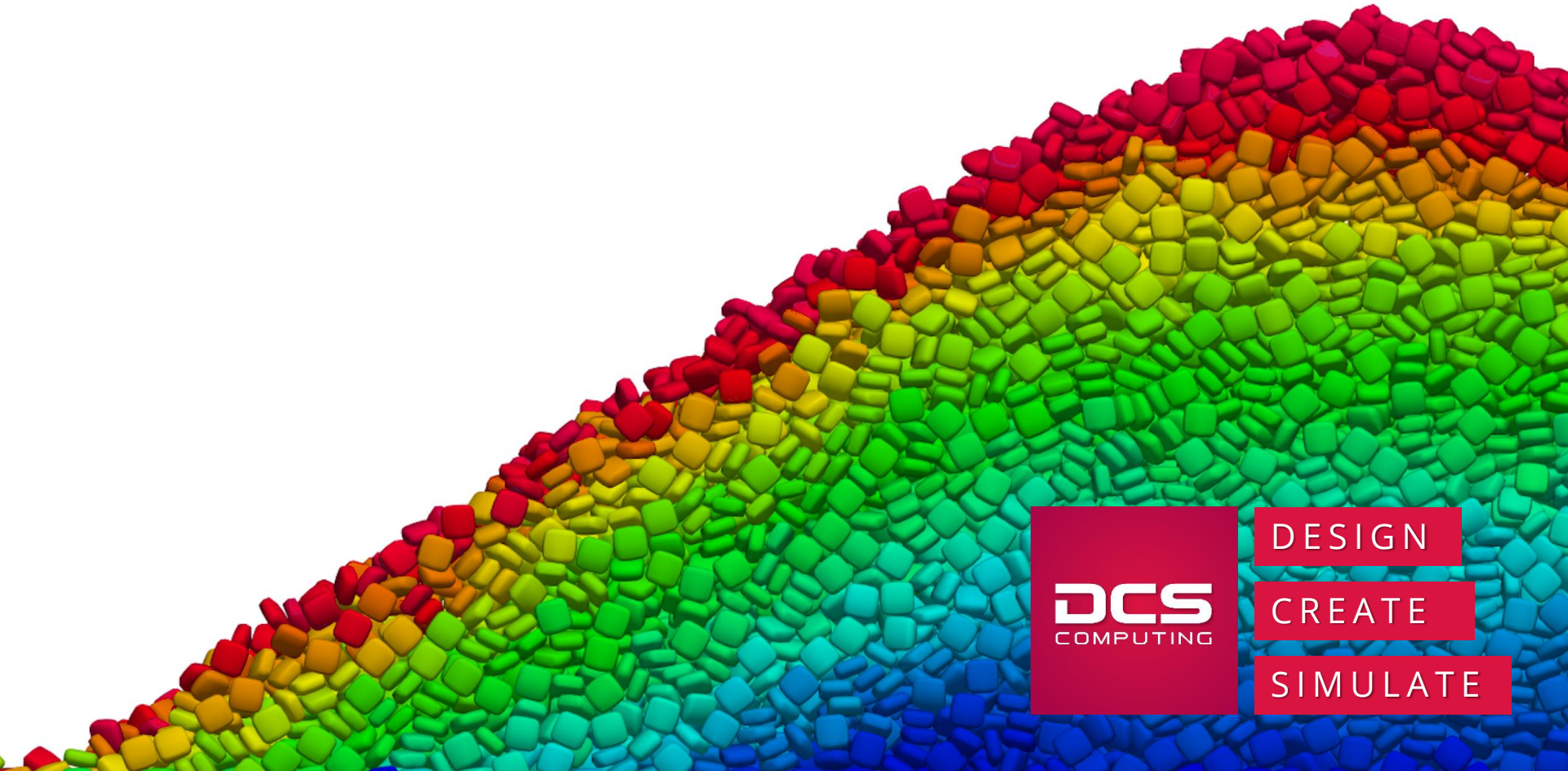
The Marketplace Project



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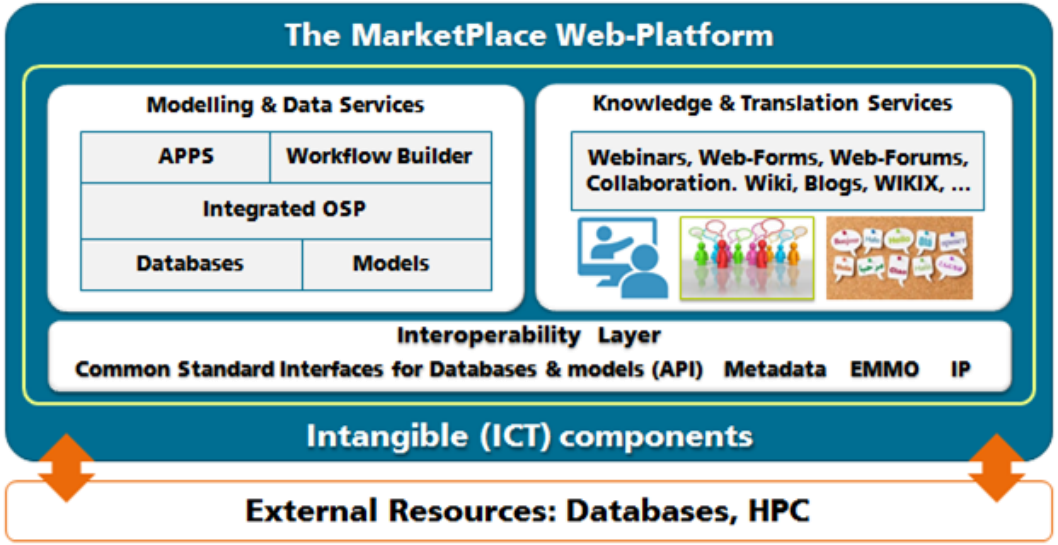
Slide title

MARKETPLACE is to leverage recent software engineering and ICT advances to collect, adapt and integrate all scattered modelling components from all fragmented materials modelling and industrial communities and provide **a single point of access - an on-line gateway - to all materials modelling activities in Europe**.



www.the-marketplace-project.eu

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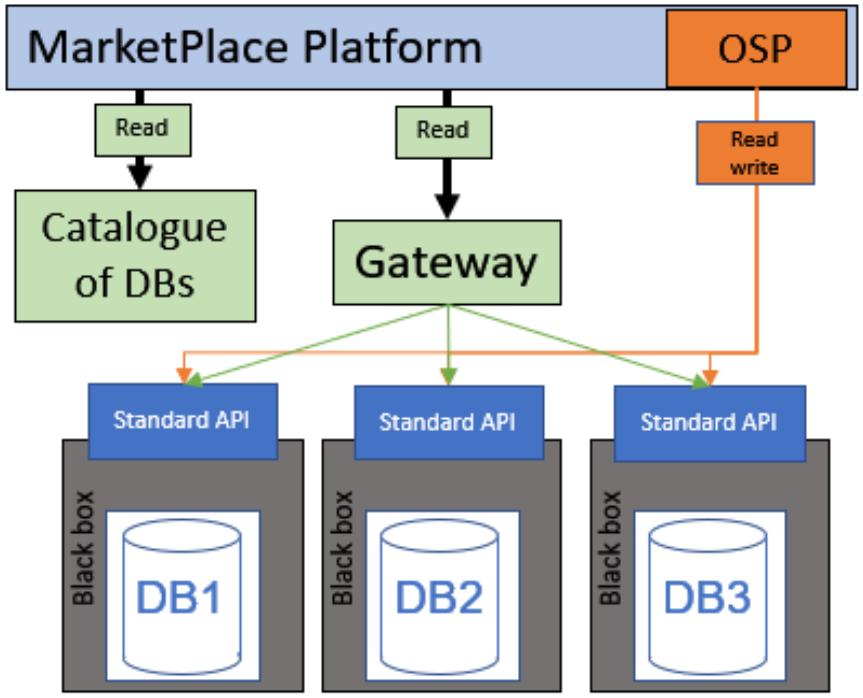
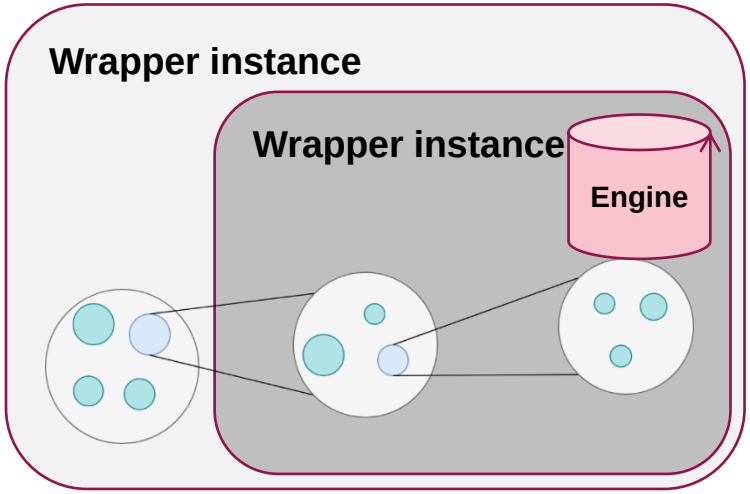
Marketplace EU Project

Databases // Translation // Catalogues // Training // Apps // Workflow Builders



Integrated database services



Ontology- and wrapper-based interoperability

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Intangible and Tangible Components

Infrastructure (intangible components) vs Populated Marketplace (w/ tangible components)

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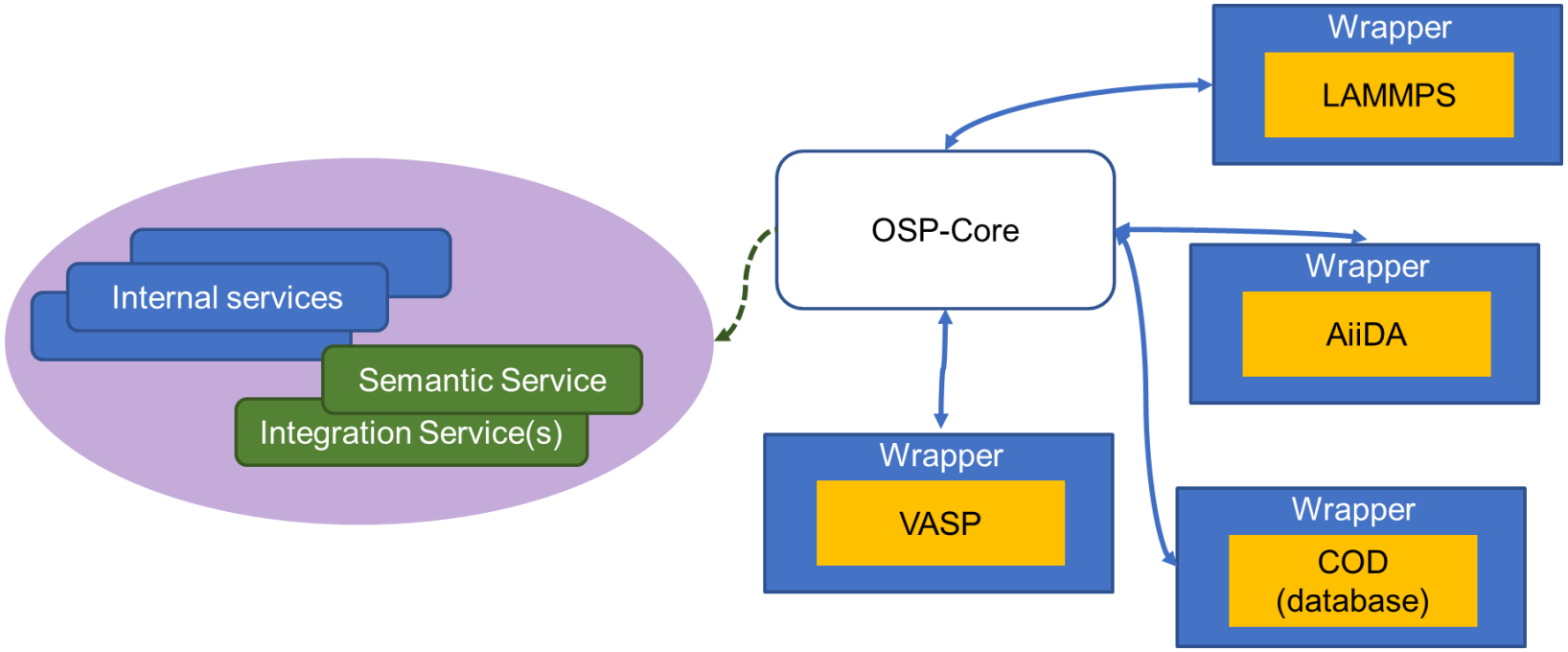
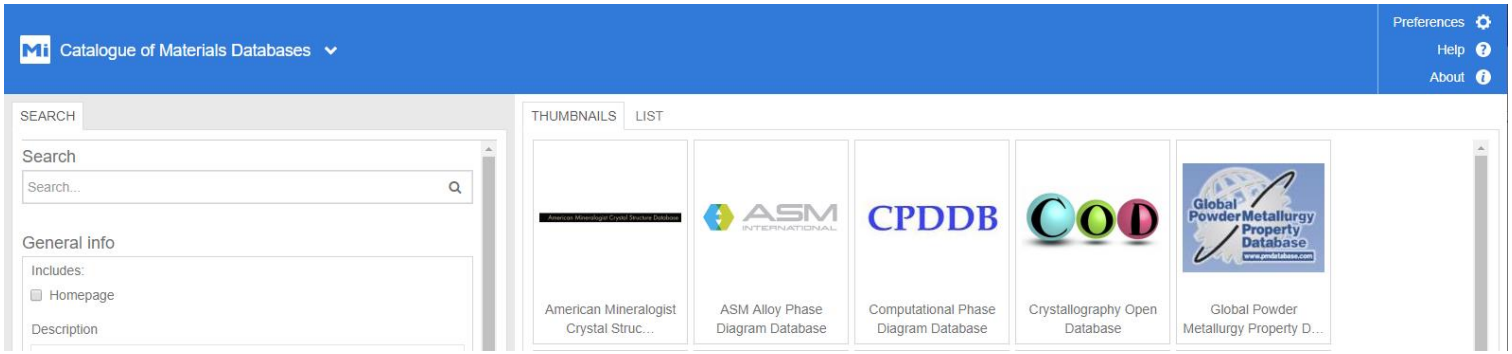
Integration of Software & Databases via Wrappers





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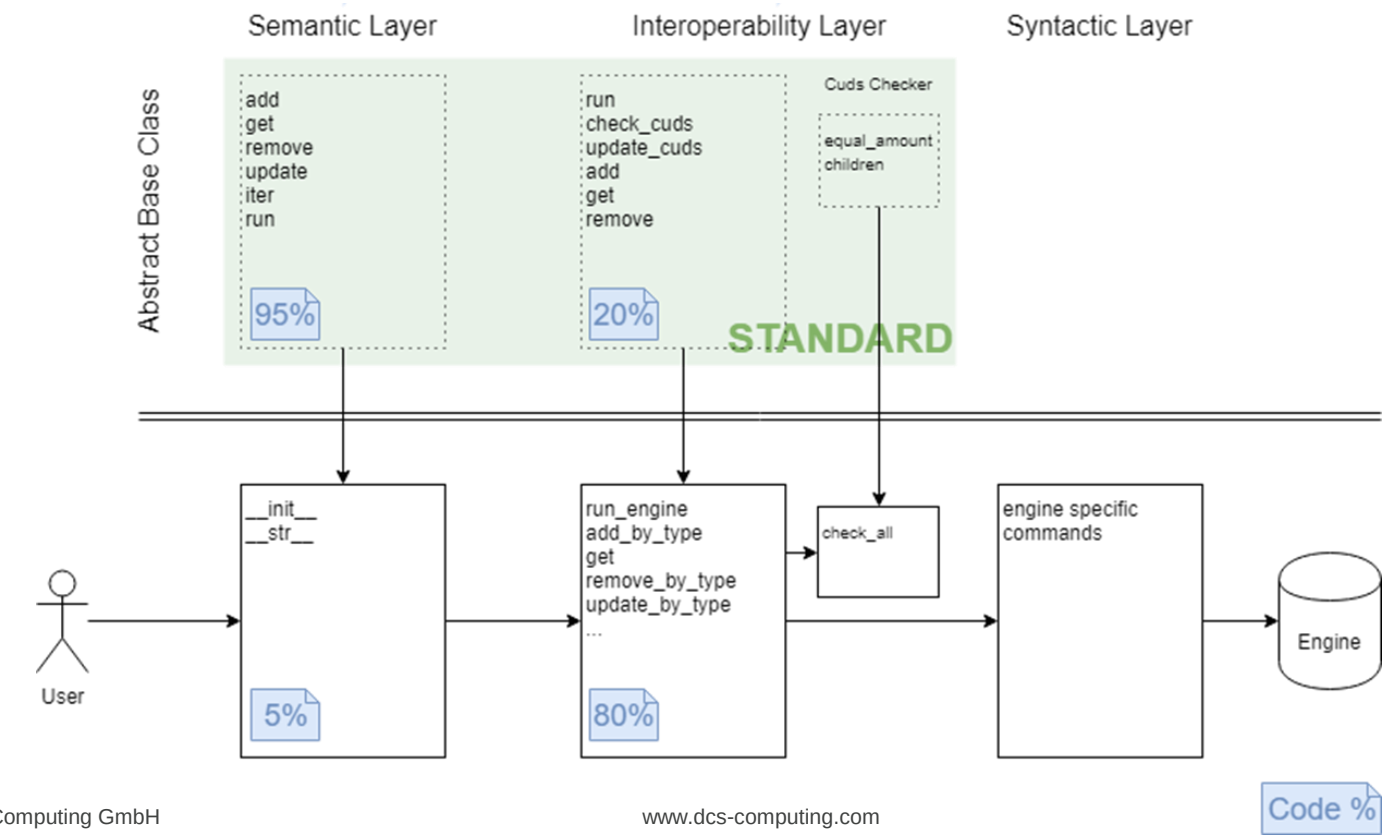
Interoperability based on Open Standard / Ontology

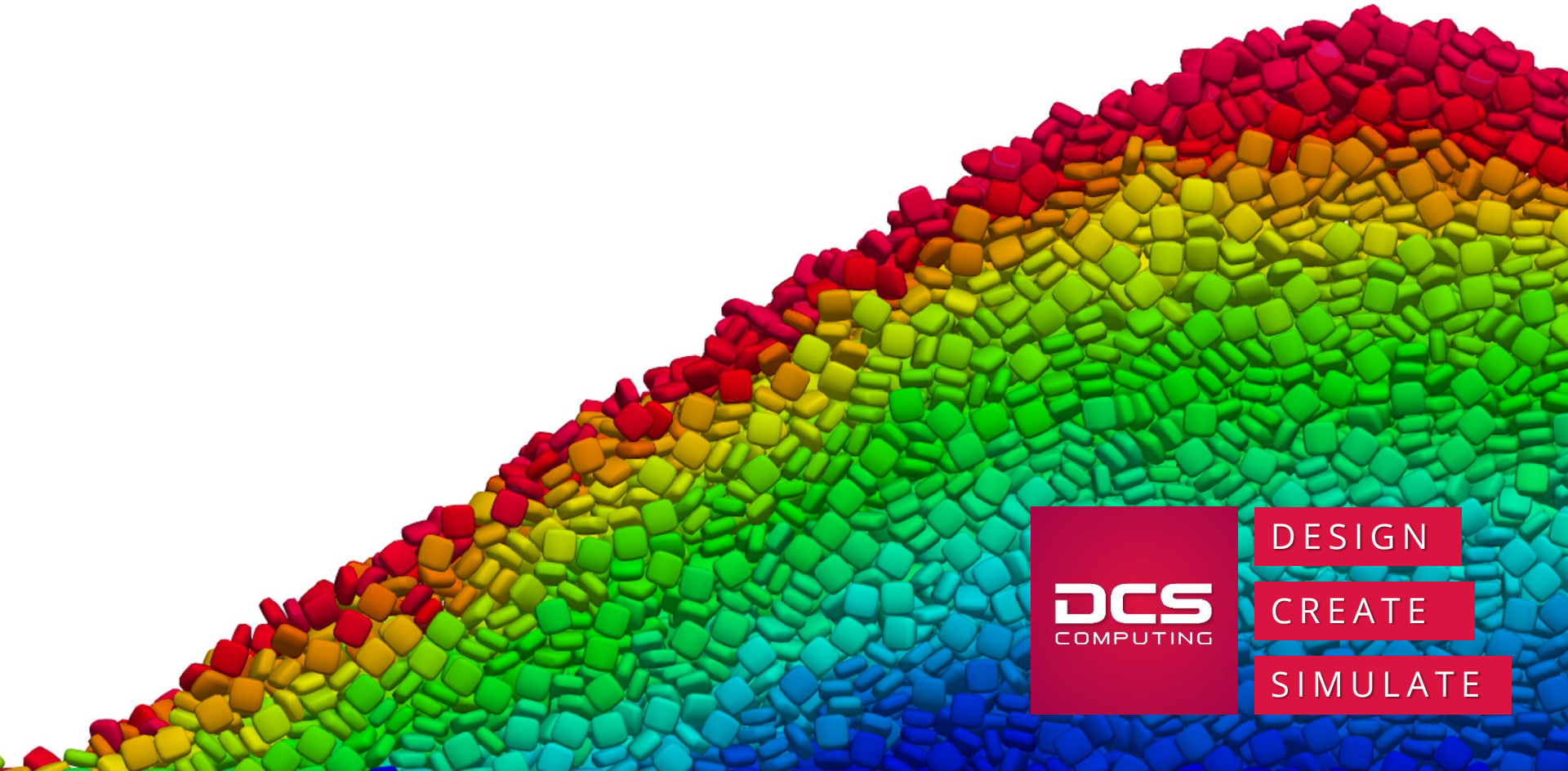
CUDS = Common Universal Data Structure based on EMMO (European Materials Modelling Otology)

Interoperability based on Open Standard

Connecting new Tool to Platform automagically connects to all other tools onboarded (no N^2 effort)



Use Case: Injection Molding



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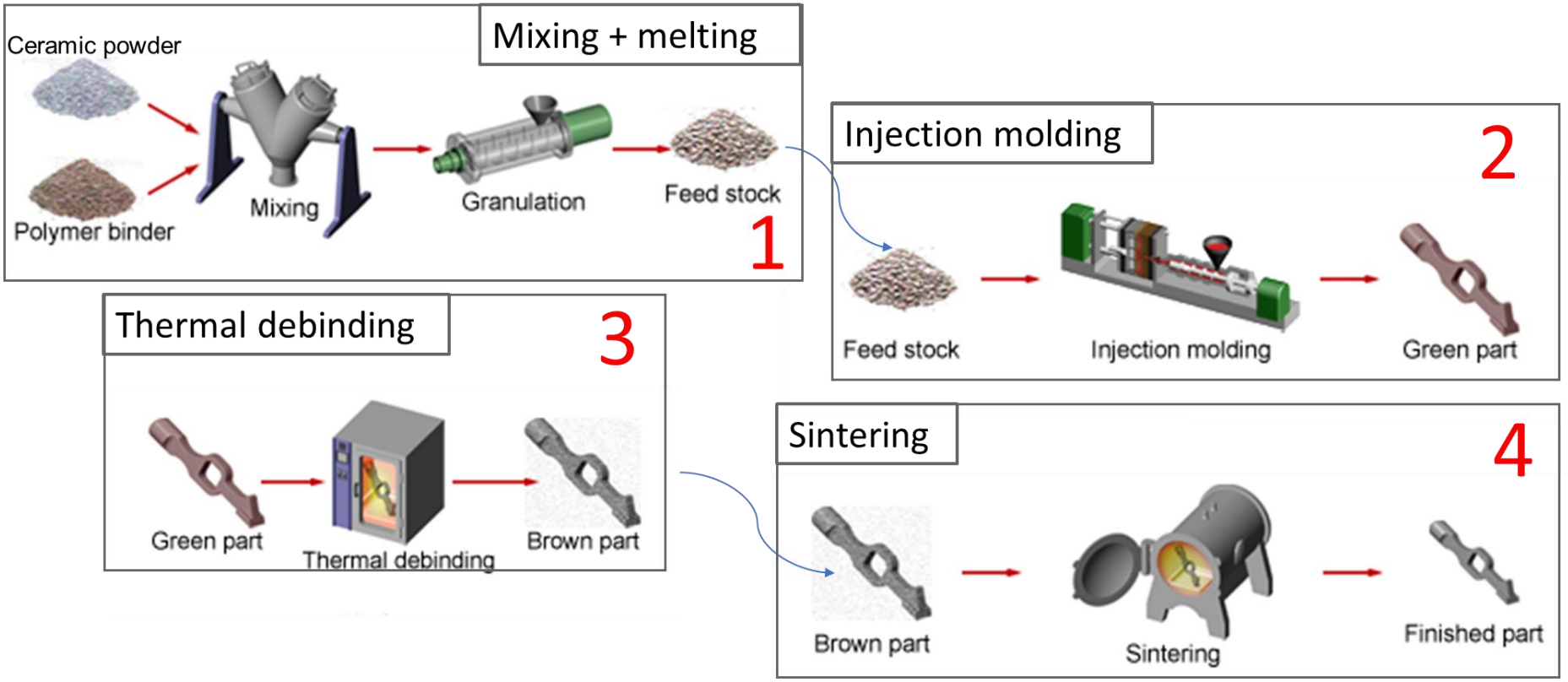
Use Case: Ceramic Injection Molding



(used for dental implant)

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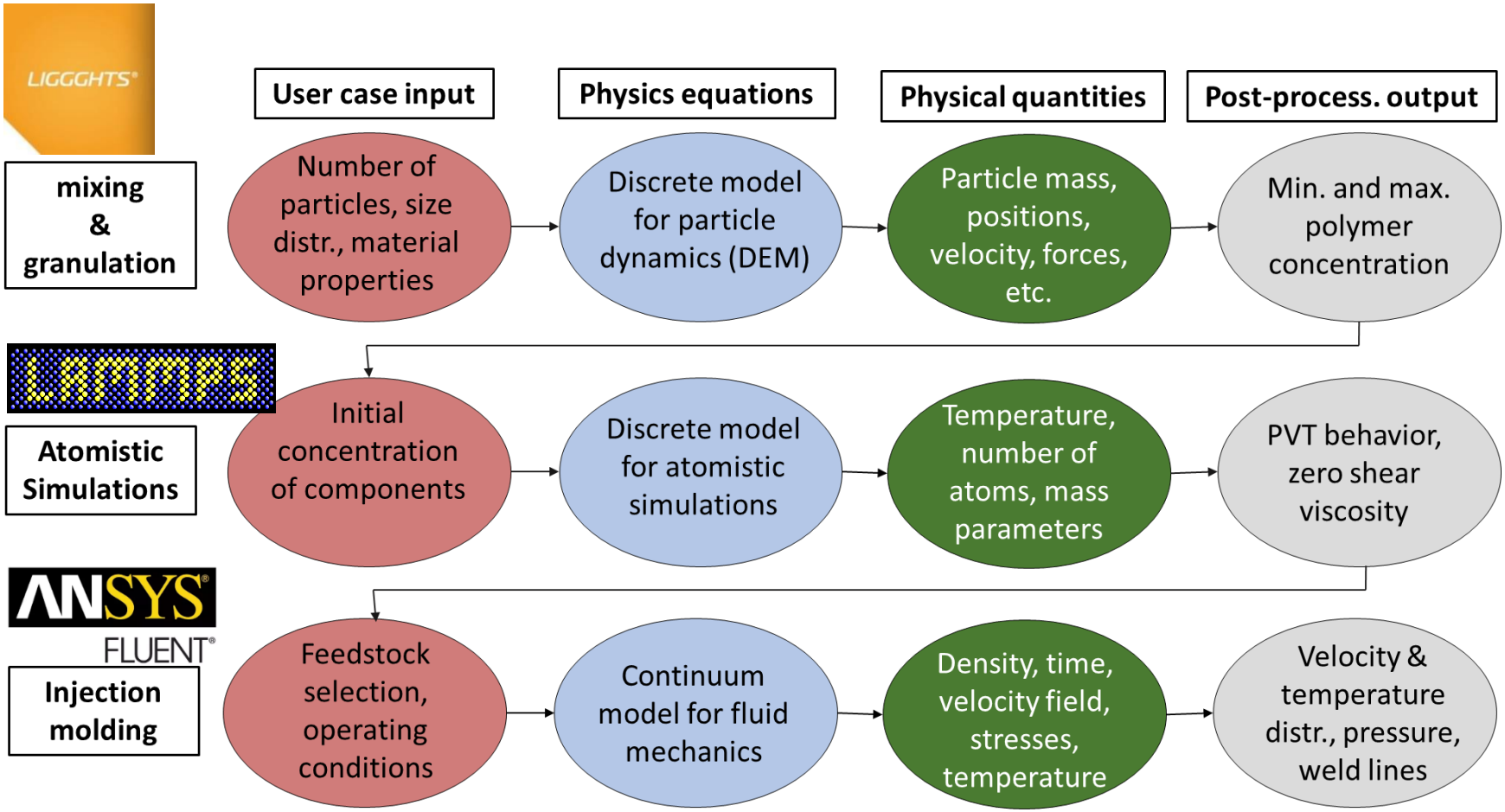
MODA = Use Case Description



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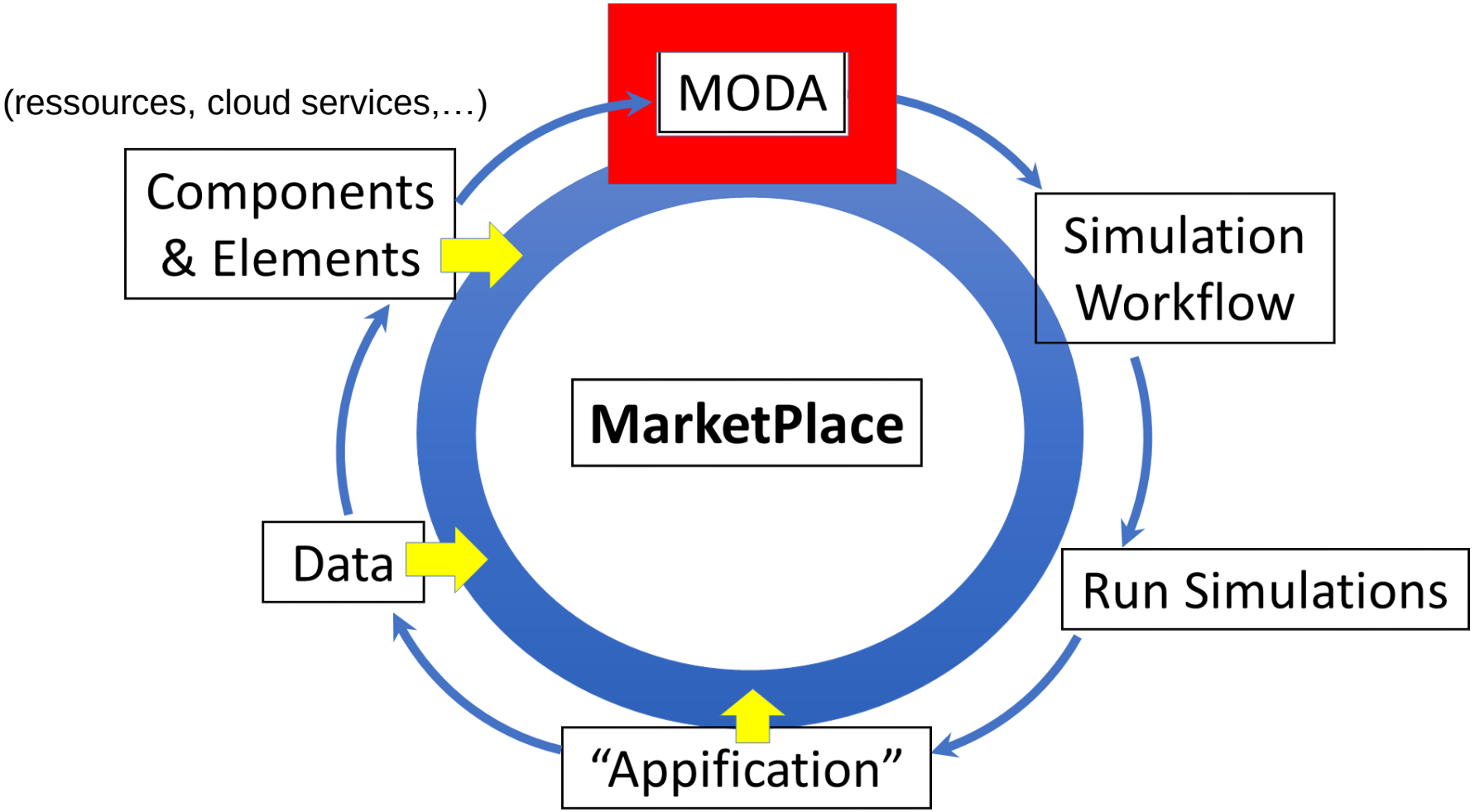
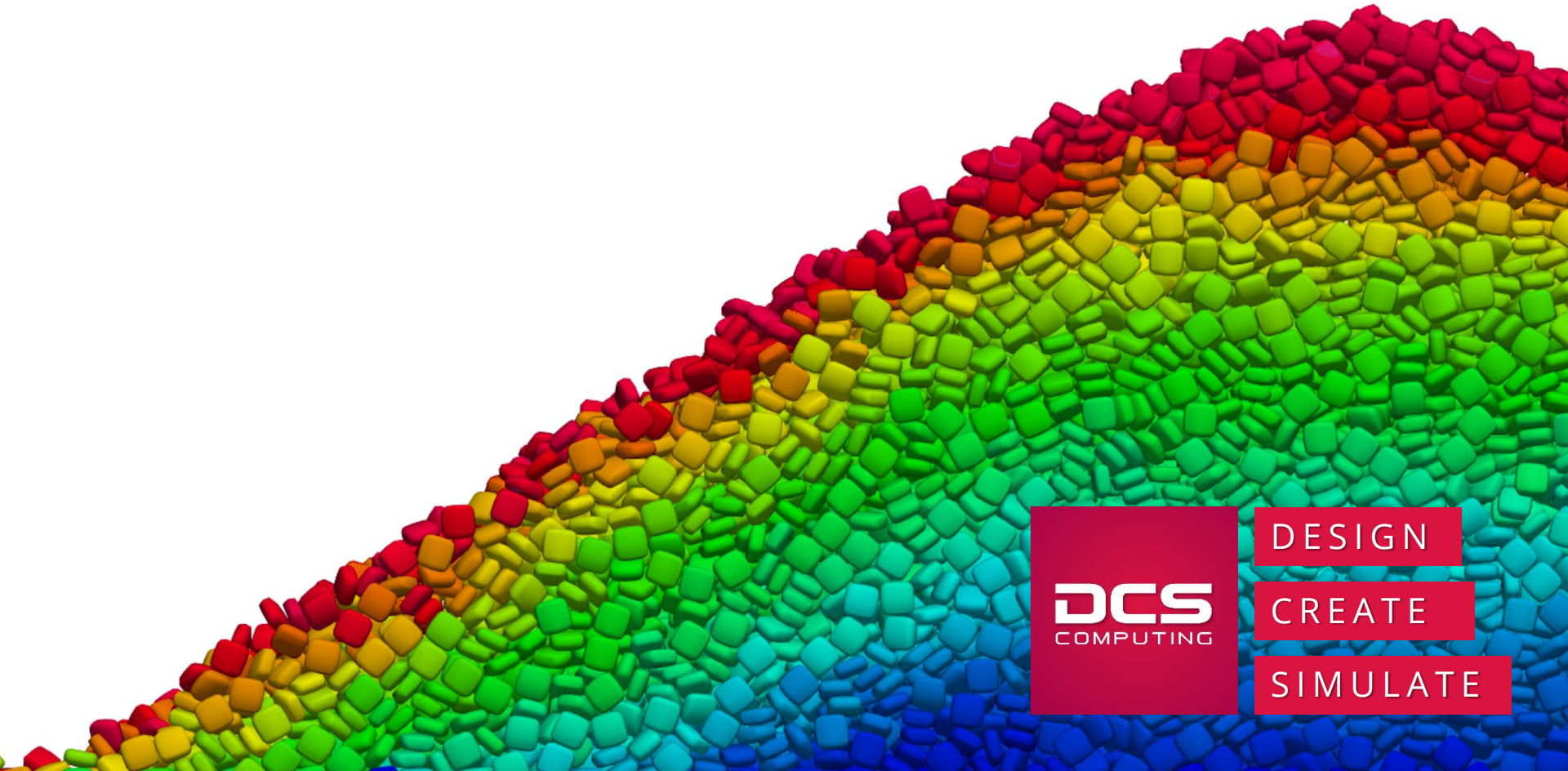
Development Cycle Around Use Case Description



Conclusions



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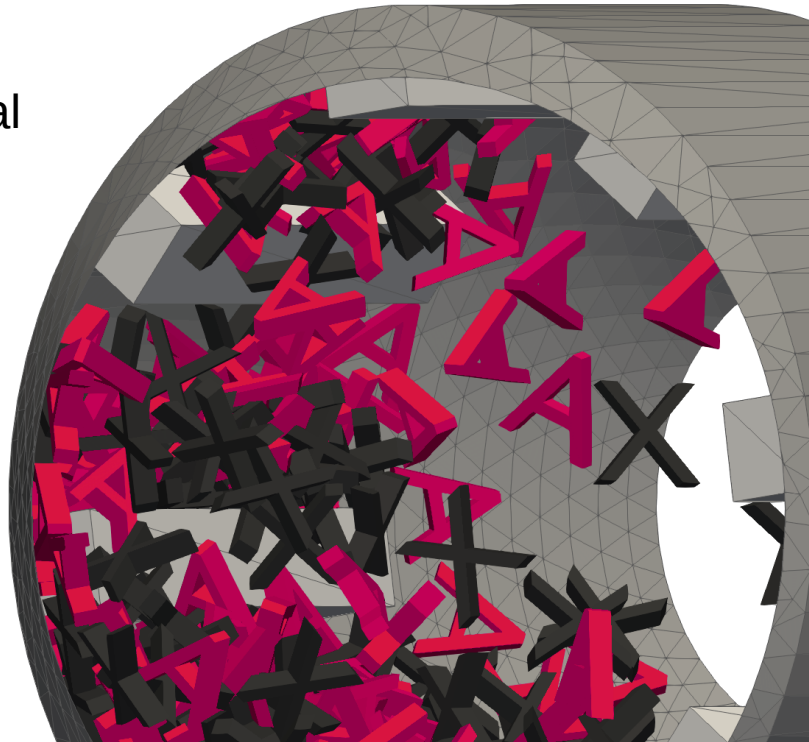
Conclusions

What will the future bring?

- Increased availability of resources leads to more data being generated
- **FAIR** data will be of highest value
- **Interoperability of data** is needed
- **Ontology-** and **Open Standards** based interoperability is needed
- Standards on use case description is beneficial for multi-scale modelling



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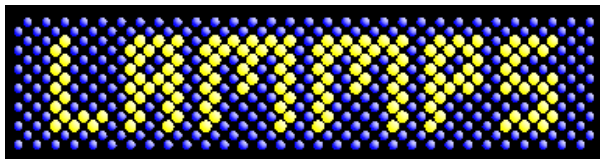
Acknowledgement



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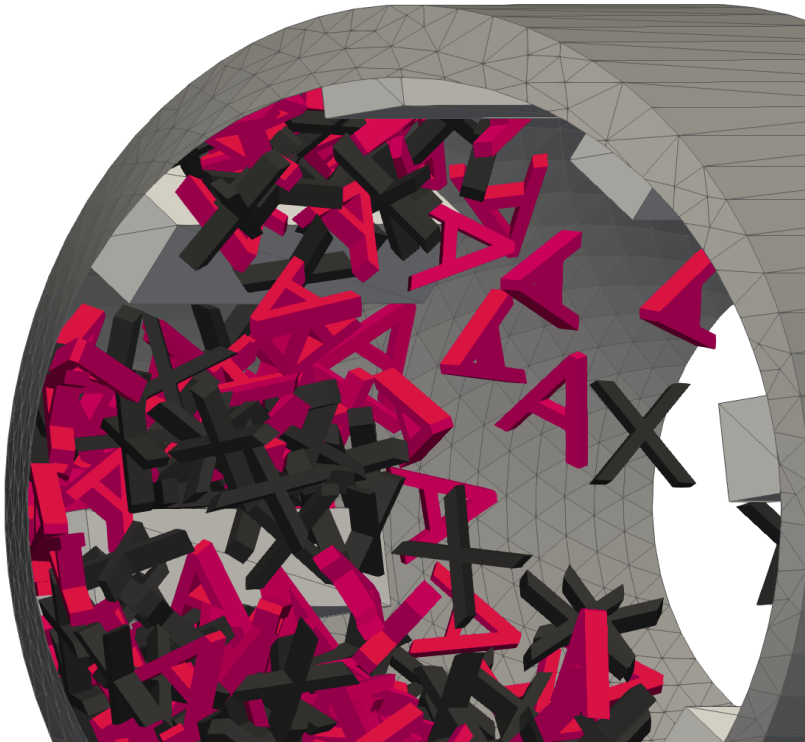
This project has received funding from the European Union's H2020 research and innovation programme under grant agreement No 760173

Questions?



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