

Marketplace

Towards an Online Gateway to Materials Modelling

Christoph Kloss (DCS)

Riccardo Togni (DCS)

Adham Hashibon (Fraunhofer IWM)

Nikolaos Lempesis (HES)

LAMMPS

workshop 2019



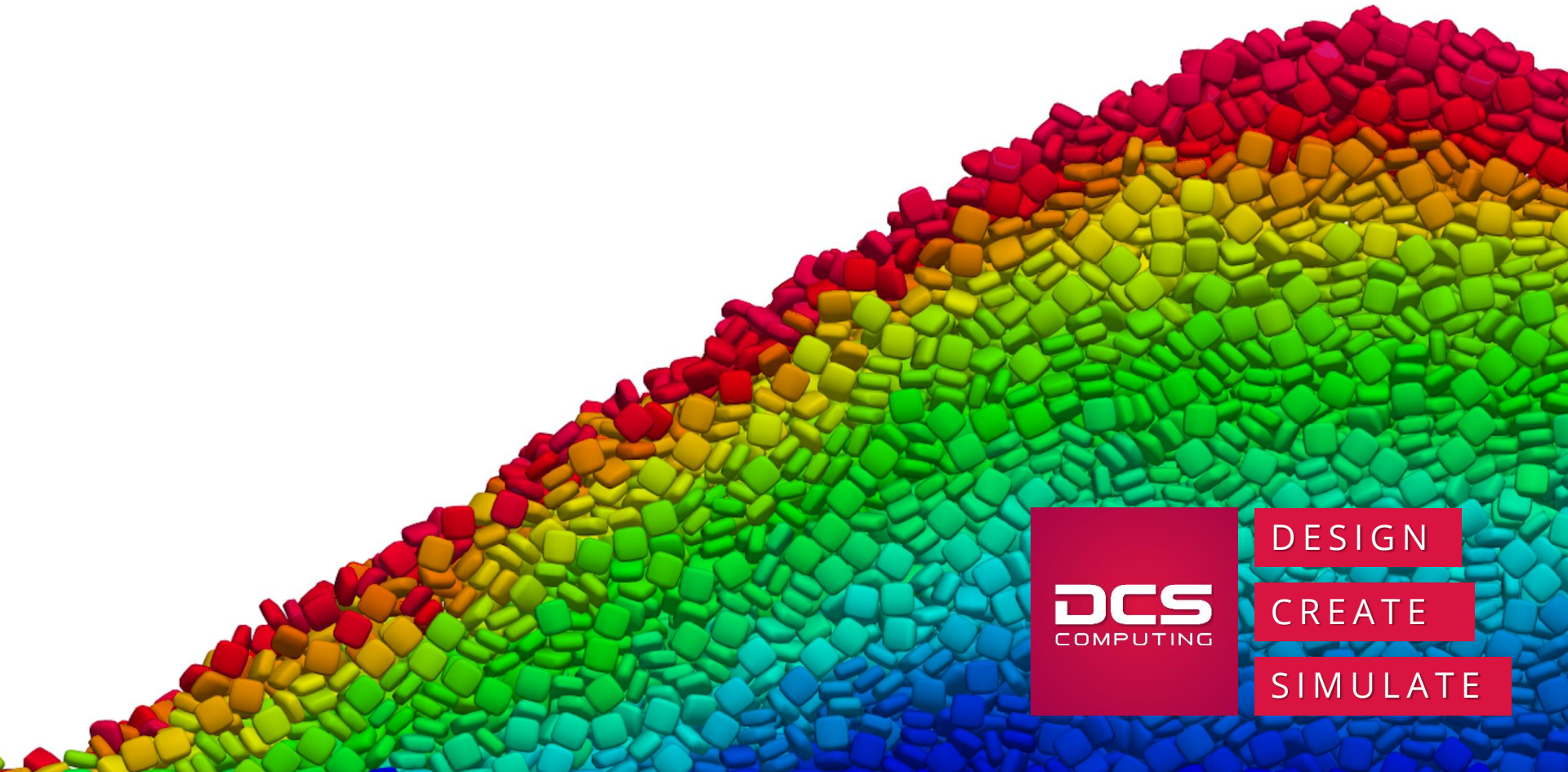
DCS
COMPUTING

DESIGN

CREATE

SIMULATE

Background on DCS: Discrete Element Modelling



DCS
COMPUTING

DESIGN

CREATE

SIMULATE

Marketplace Materials Modelling Hub

Governing Equations for Discrete Element Method

Method – Governing equations for DEM

- Newton's second law for the particle phase:

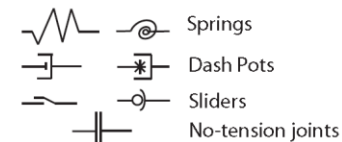
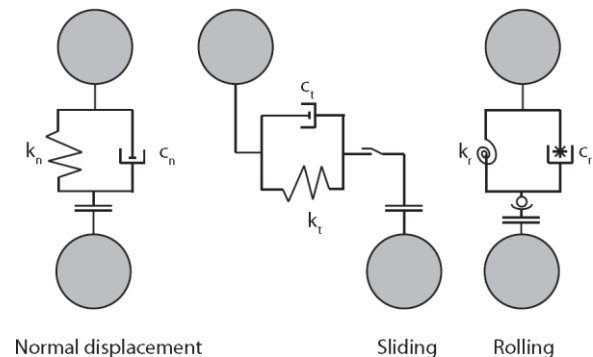
$$m_p \frac{dU_p}{dt} = \sum F_{p,p} + \sum F_{p,w} + m_p g + F_p + F_f$$

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

- 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



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 ... moment of inertia
 ω ... angular velocity
 T ... torque



Marketplace Materials Modelling Hub

Governing Equations for Discrete Element Method

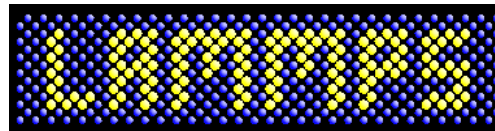
Method – Governing equations for DEM

- Newton's second law for the particle phase:

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



$= T_p$
=



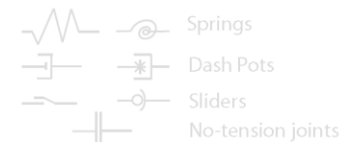
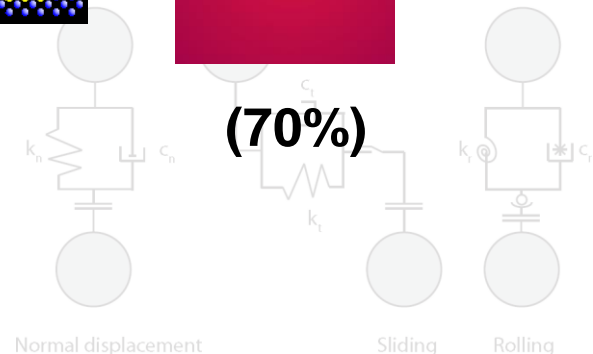
(30%)

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 ... m



(70%)

- Soft sphere (particles overlap during contact) (www.cfdem.com)
- 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

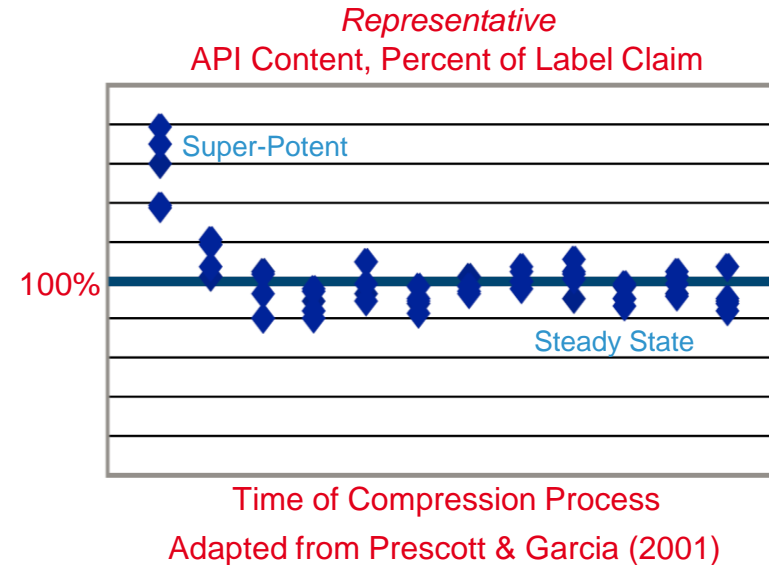
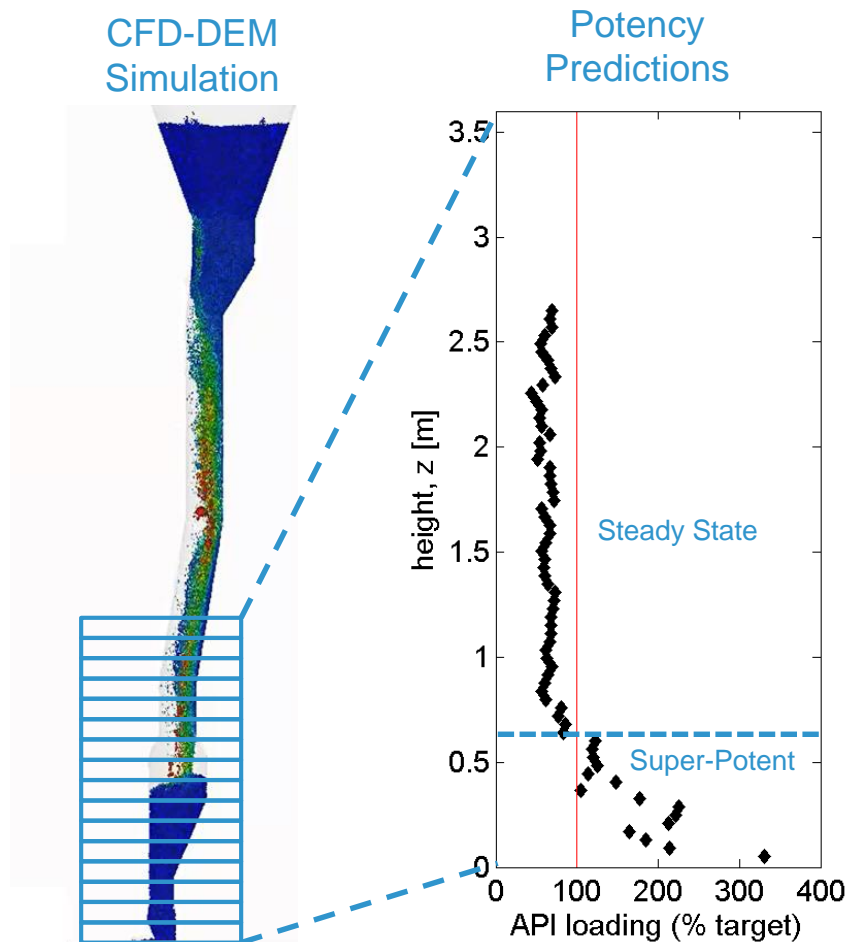


Marketplace Materials Modelling Hub

Use Case: Segregation of Pharmaceutical Powder



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

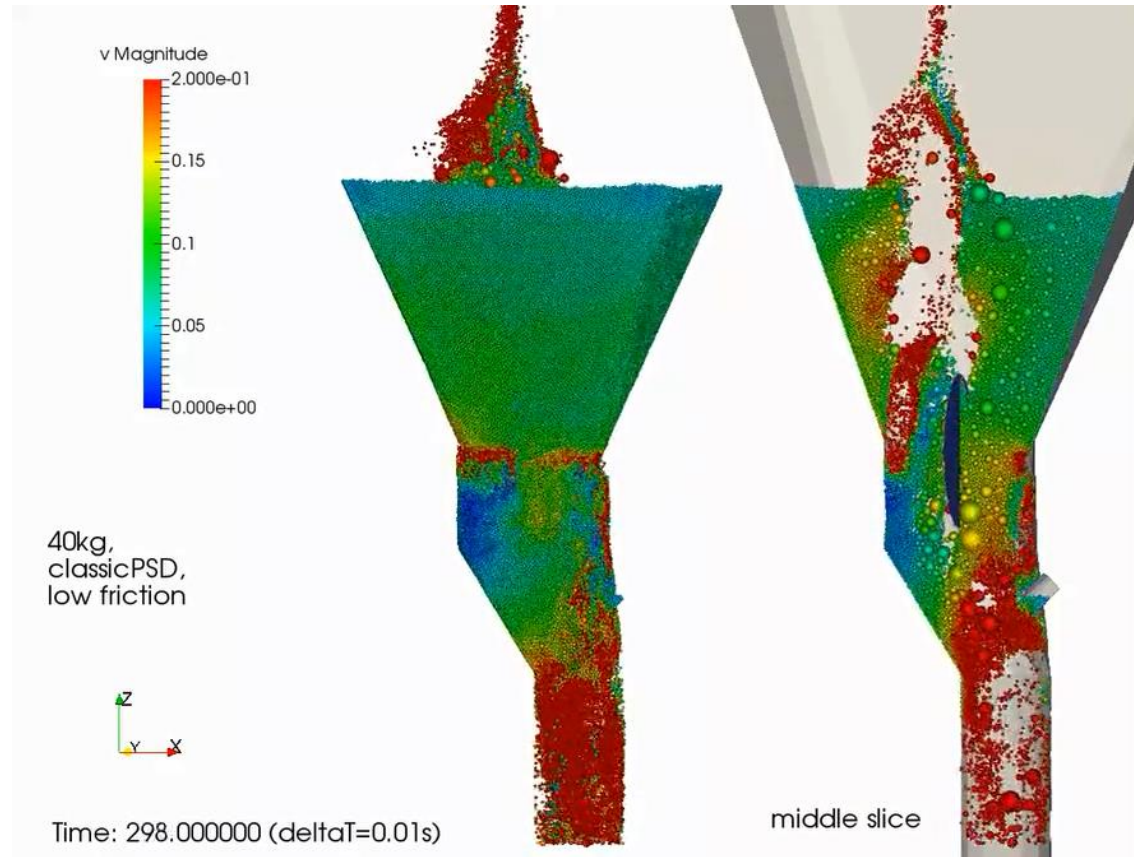
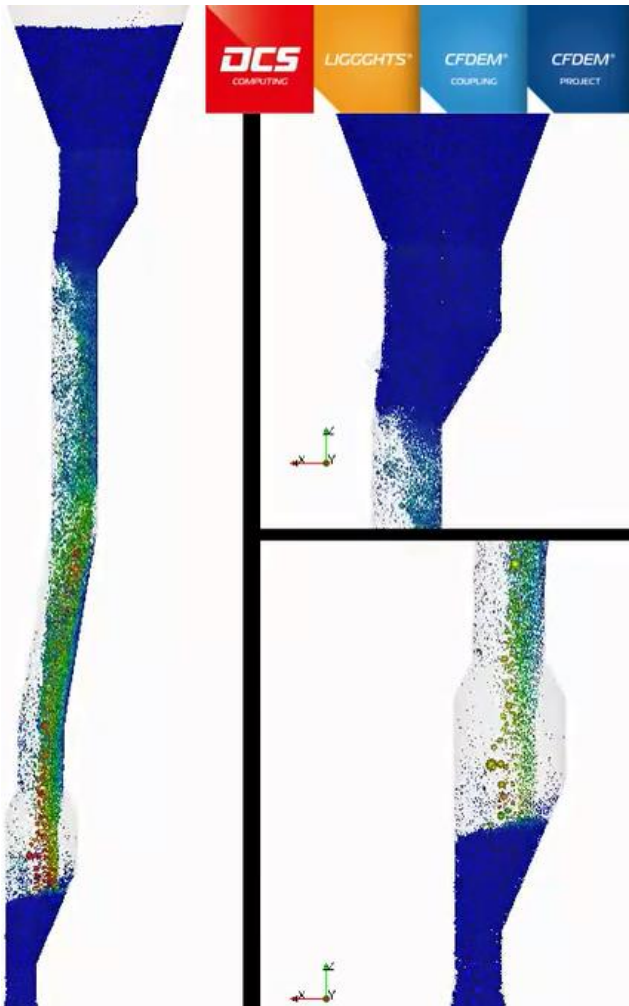


Ketterhagen, B. : Modeling the impact of powder segregation on pharmaceutical tablet manufacturing process, CFDEM®project user meeting 2016



Marketplace Materials Modelling Hub

Use Case: Segregation of Pharmaceutical Powder



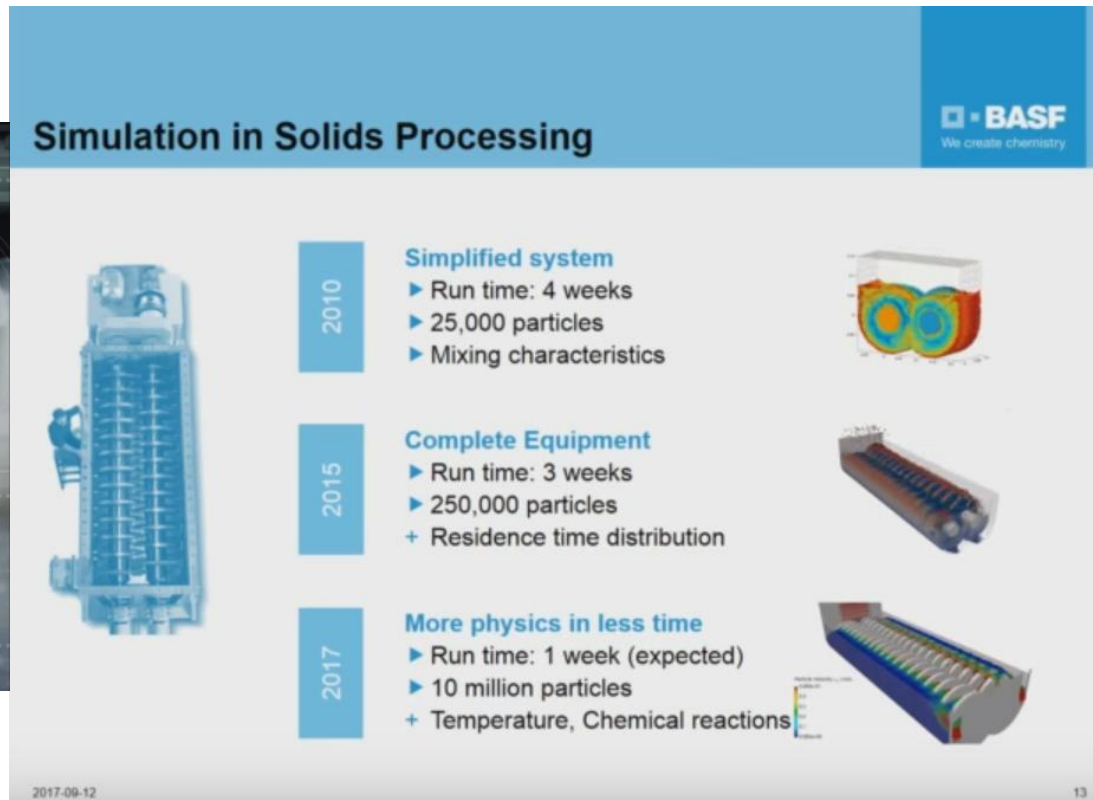
[Video: https://vimeo.com/219836723](https://vimeo.com/219836723)

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

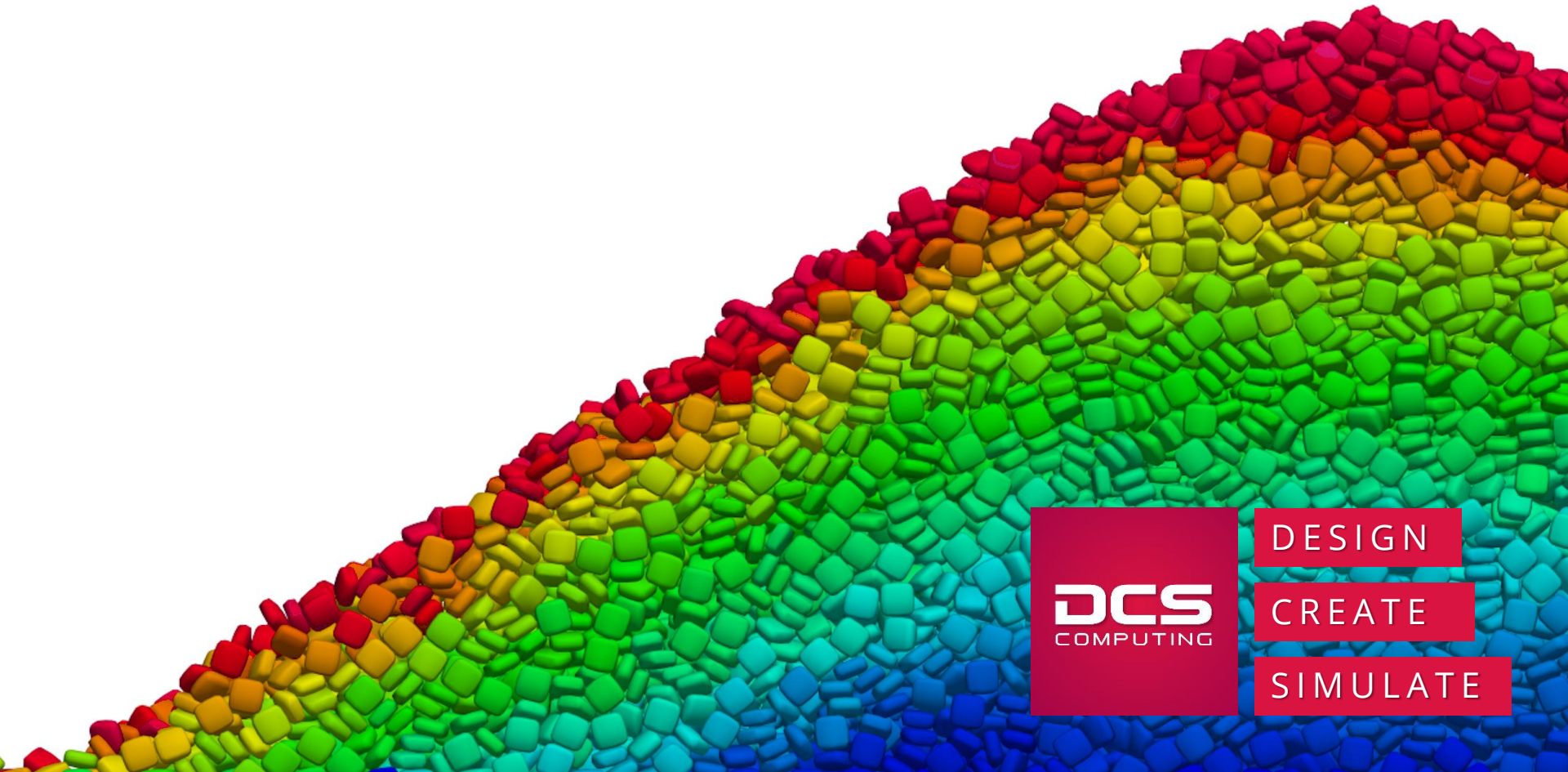
Marketplace Materials Modelling Hub

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



DCS
COMPUTING

DESIGN

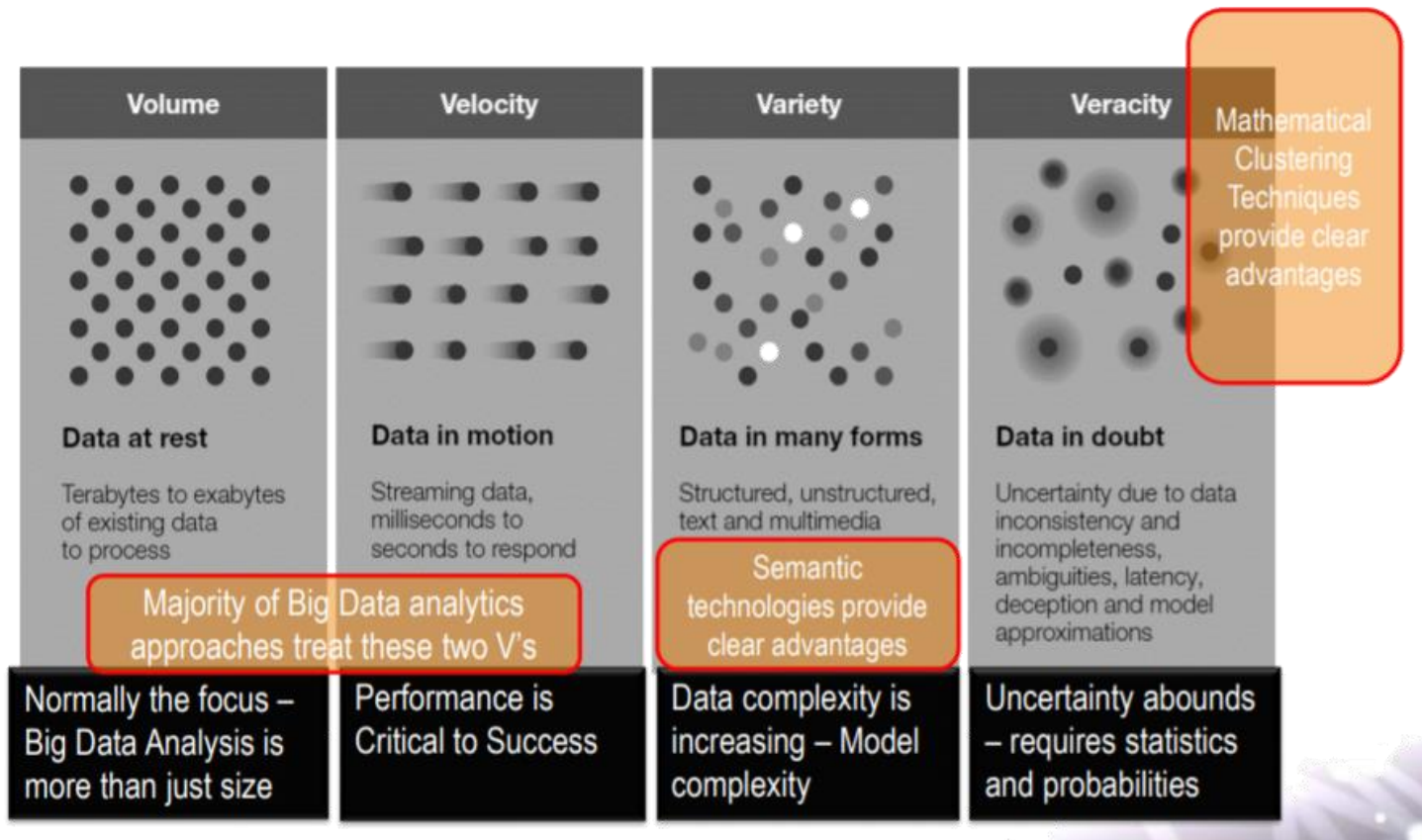
CREATE

SIMULATE

Marketplace Materials Modelling Hub

The 4 Vs of Big Data

Understanding the 4V's of Big Data



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

Marketplace Materials Modelling Hub

Interoperability of Data

Make Data **FAIR** (**F**indable, **A**ccessible, **I**nteroperable **R**eusable)

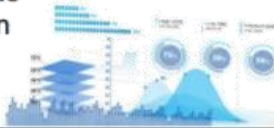
Analytics Tools

simulations
statistics
reasoning



Visualization

dashboards
exploration
search



Reporting

regulatory
internal
external



...

Data Science (machine learning, text analytics, clustering etc.)

Lightweight Semantic Integration Layer

(semantic RMDM, APIs, semantic indexing, data annotation, catalogues, meta data and linking)



Instrument
Data



Operational DBs



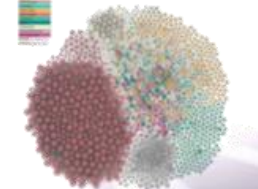
Semi-structured
Data



Unstructured
Documents



Semantic
Graph DB



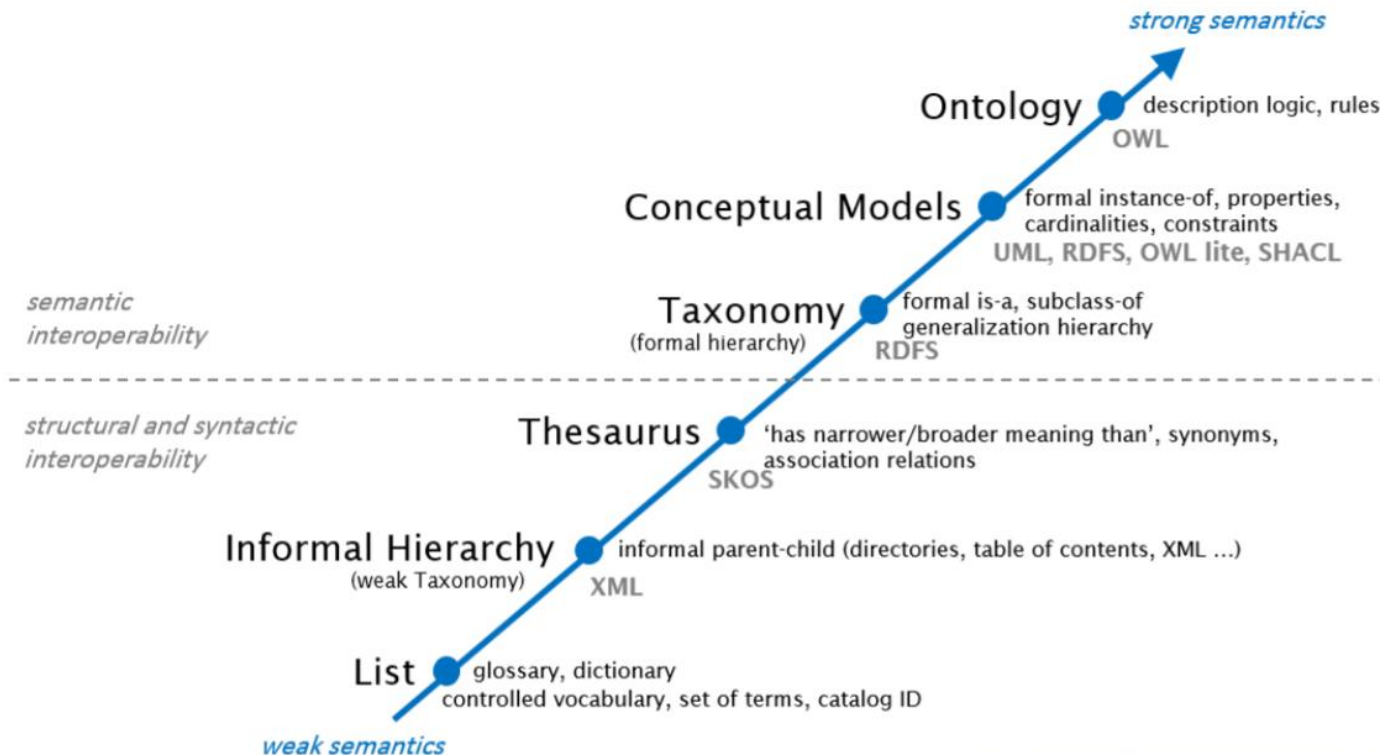
Linked Open Data
& Open APIs

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

Marketplace Materials Modelling Hub

Semantics is Key

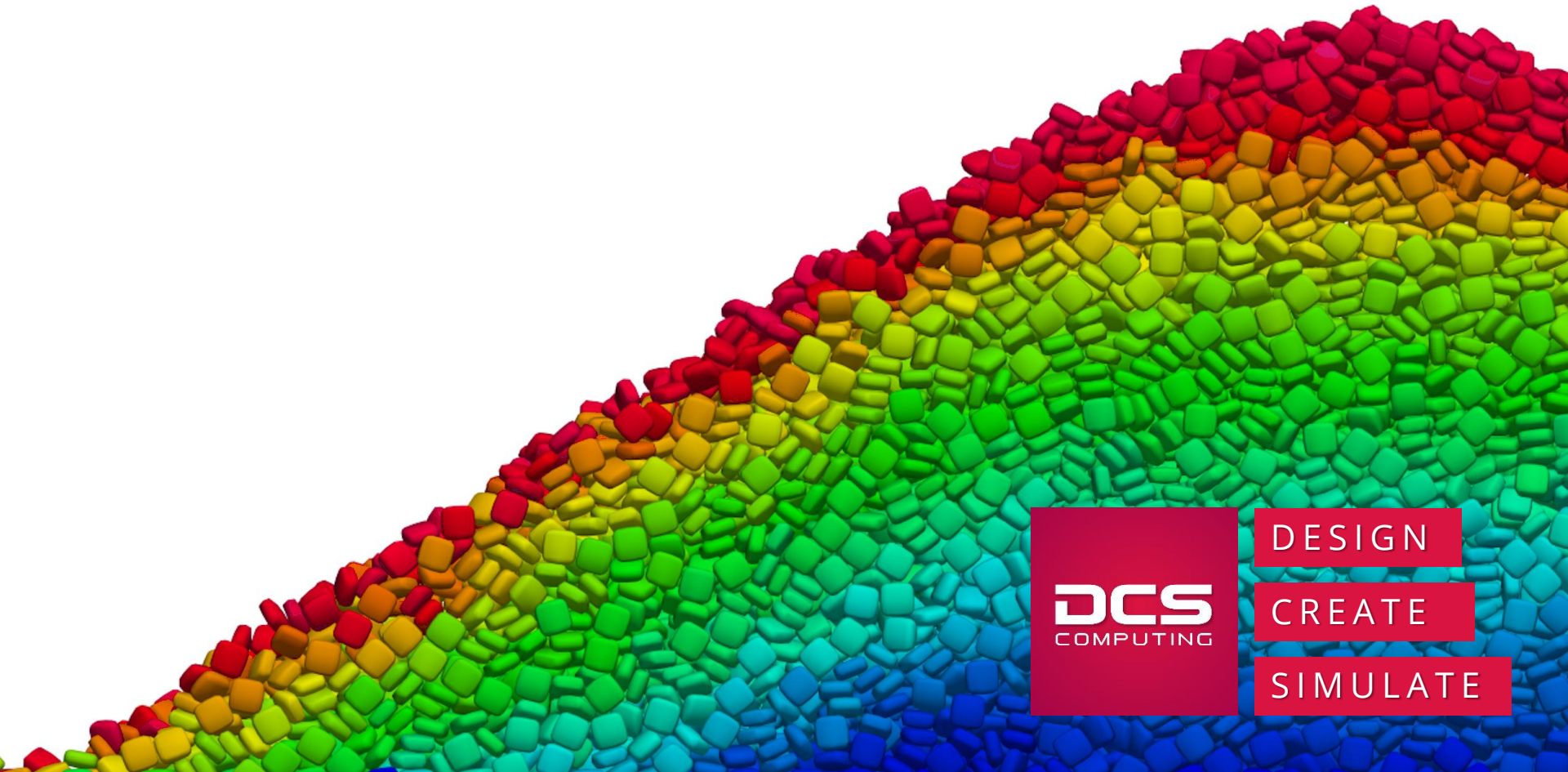
Semantic Spectrum of Knowledge Organization Systems



Deborah L. McGuinness, "Ontologies Come of Age". In Dieter Fensel, Jim Hendler, Henry Lieberman, and Wolfgang Wahlster, editors. *Spinning the Semantic Web: Bringing the World Wide Web to Its Full Potential*. MIT Press, 2003.
Michael Uschold and Michael Gruninger "Ontologies and semantics for seamless connectivity" *SIGMOD Rec.* 33, 4 (December 2004), 58-64. DOI=<http://dx.doi.org/10.1145/1041410.1041420>
Leo Obrst "The Ontology Spectrum". Book section in of Roberto Poli, Michael Healy, Achilles Kameas "Theory and Applications of Ontology: Computer Applications". Springer Netherlands, 17 Sep 2010.
Leo Obrst and Mills Davis "Semantic Wave 2008 Report: Industry Roadmap to Web 3.0 & Multibillion Dollar Market Opportunities". 2008.

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

The Marketplace Project



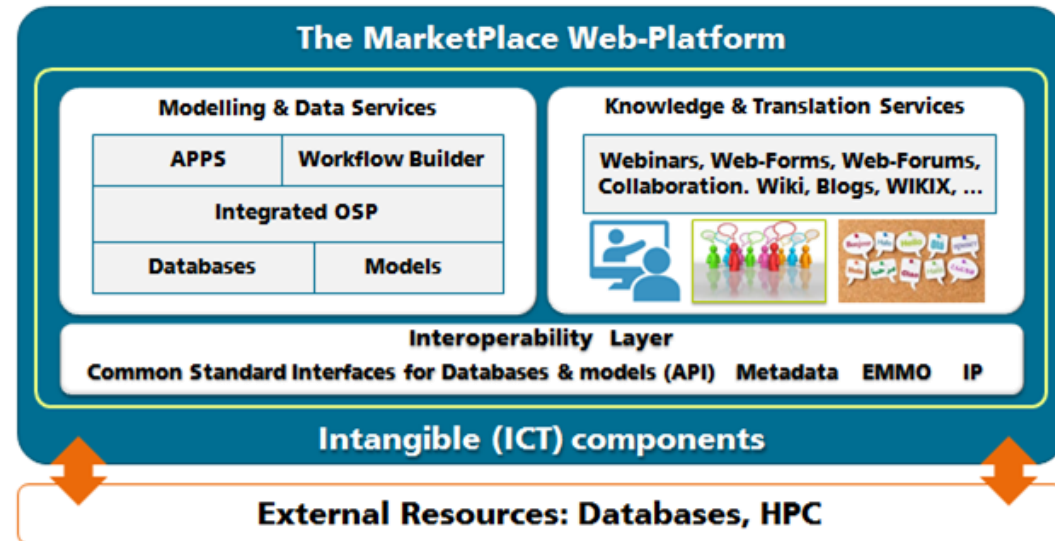
DCS
COMPUTING

DESIGN

CREATE

SIMULATE

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.**



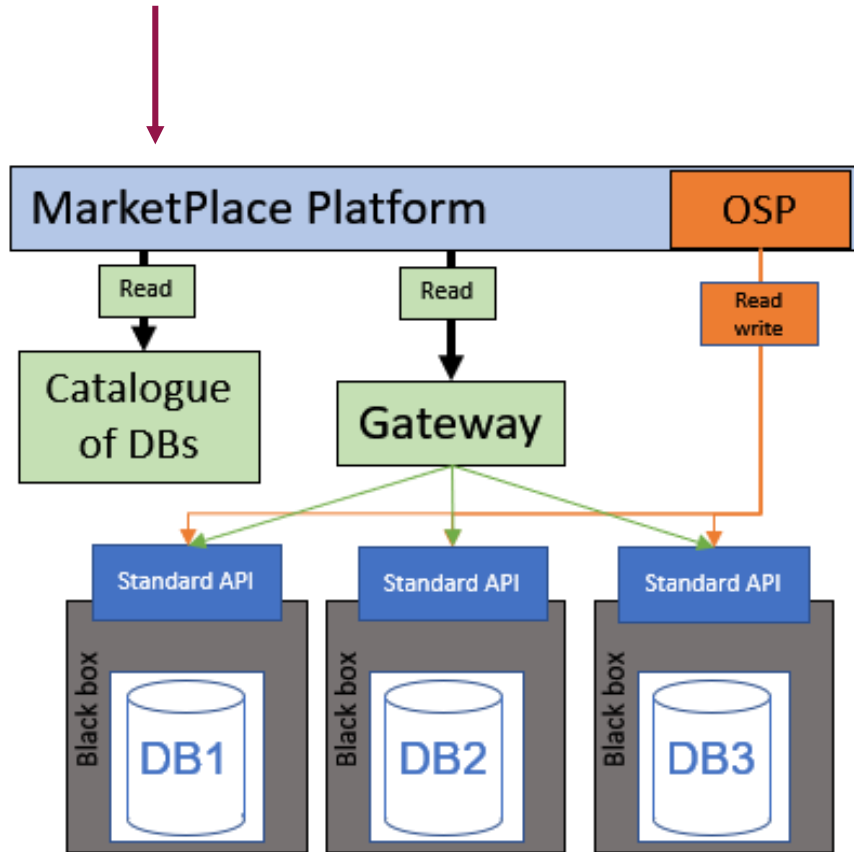
www.the-marketplace-project.eu



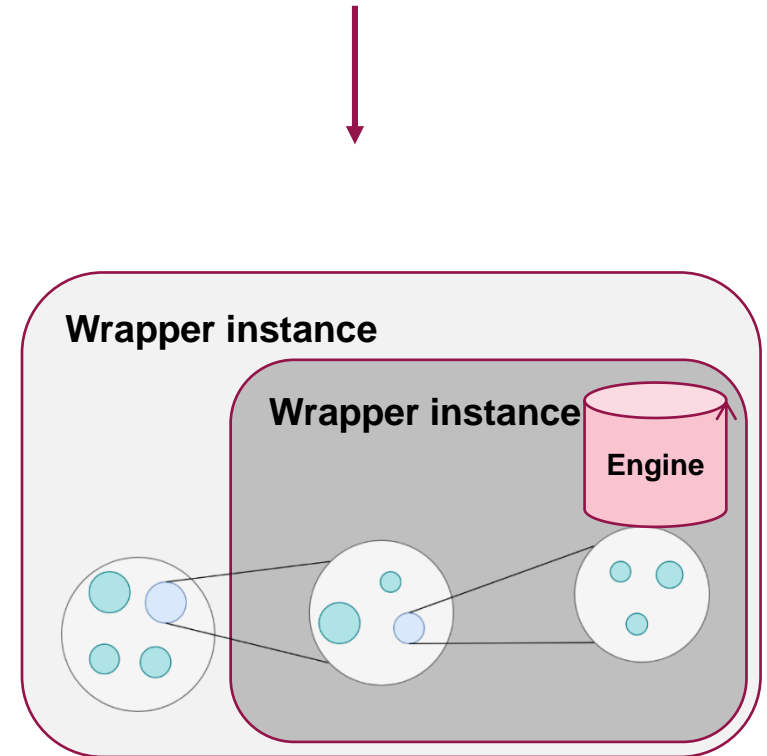
Marketplace Materials Modelling Hub

Marketplace EU Project

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



Integrated database services



Ontology- and wrapper-based interoperability

Marketplace Materials Modelling Hub

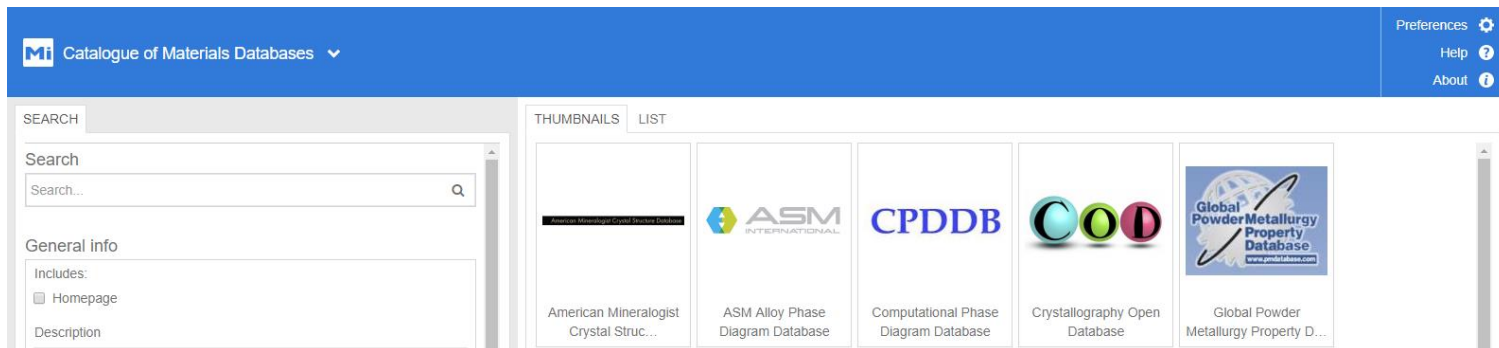
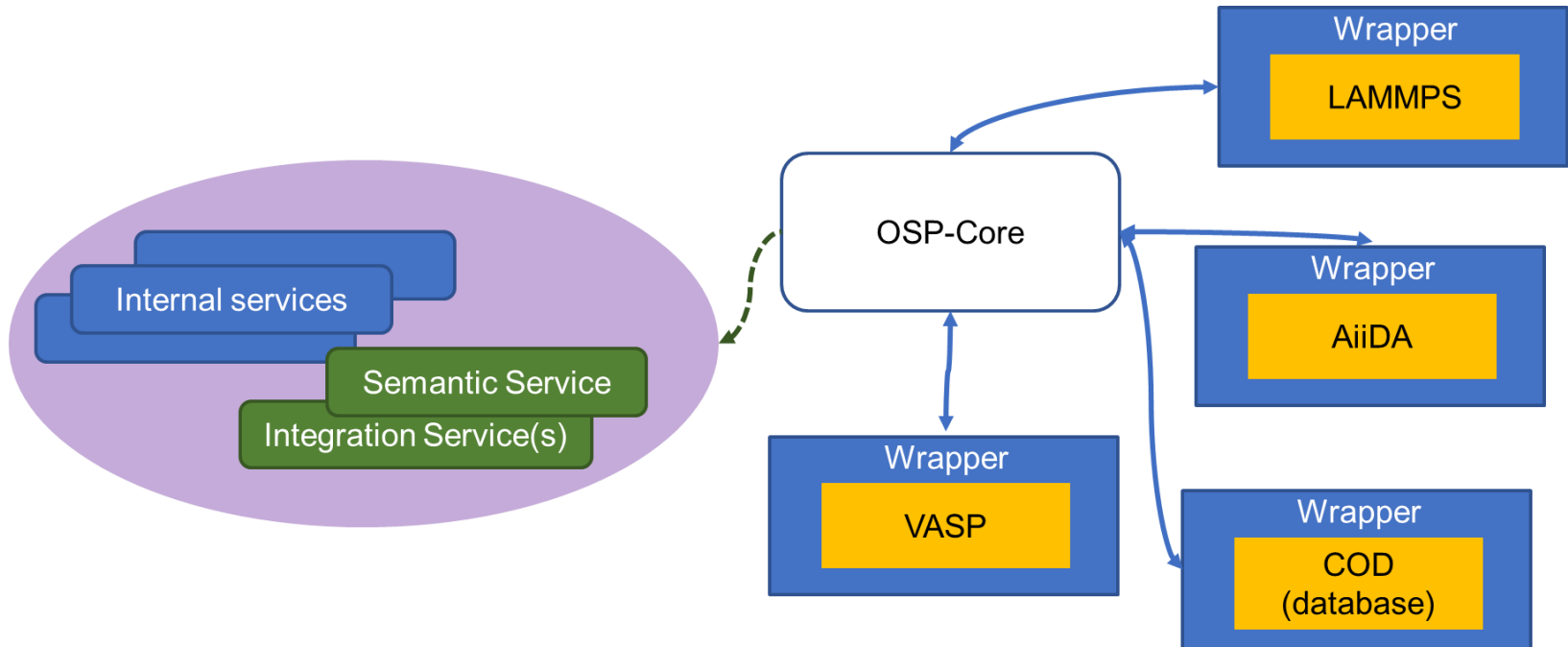
Intangible and Tangible Components

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



Marketplace Materials Modelling Hub

Integration of Software & Databases via Wrappers



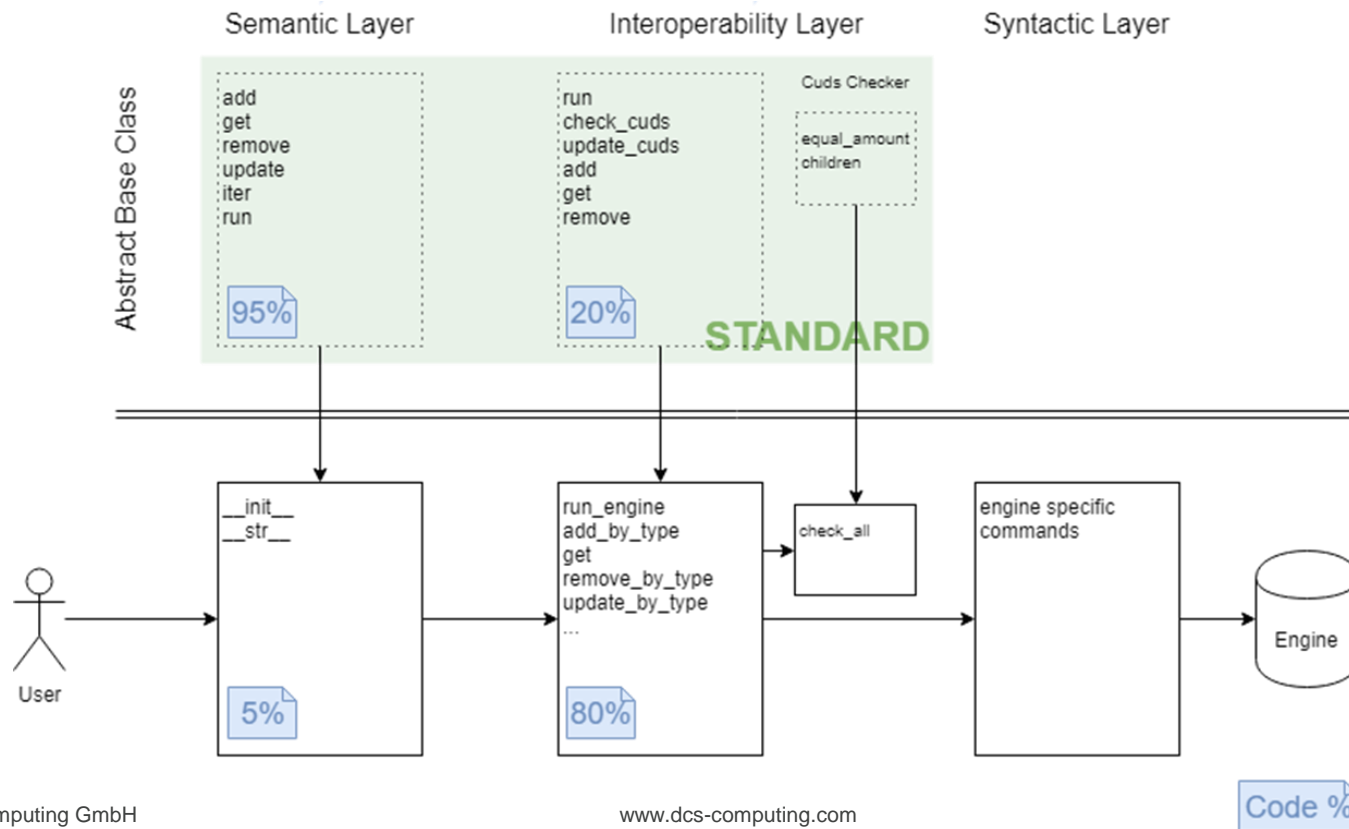
Marketplace Materials Modelling Hub

Interoperability based on Open Standard / Ontology

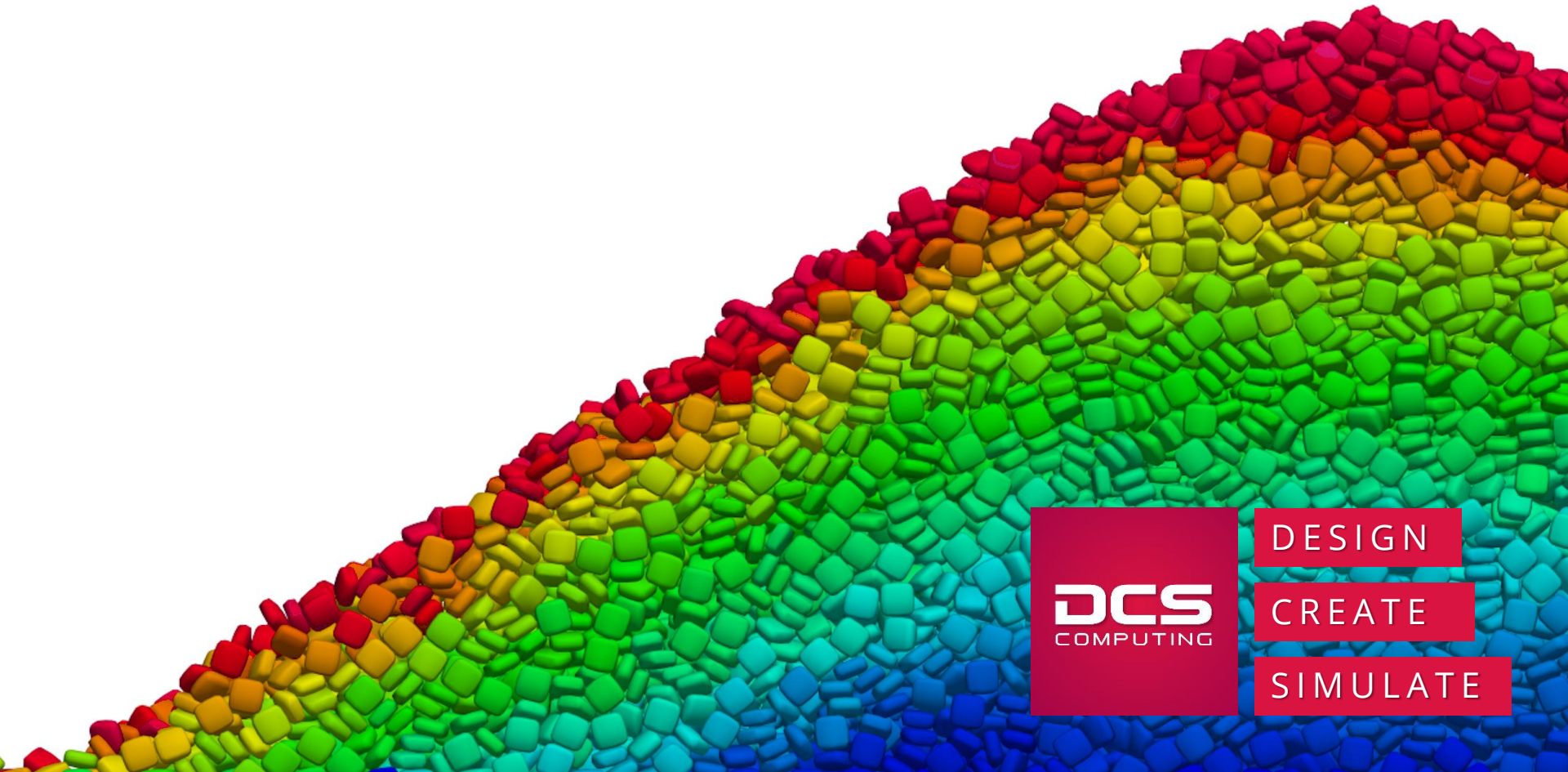
CUDS = Common Universal Data Structure based on EMMO (European Materials Modelling Ontology)

Interoperability based on Open Standard

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



Use Case: Injection Molding



DCS
COMPUTING

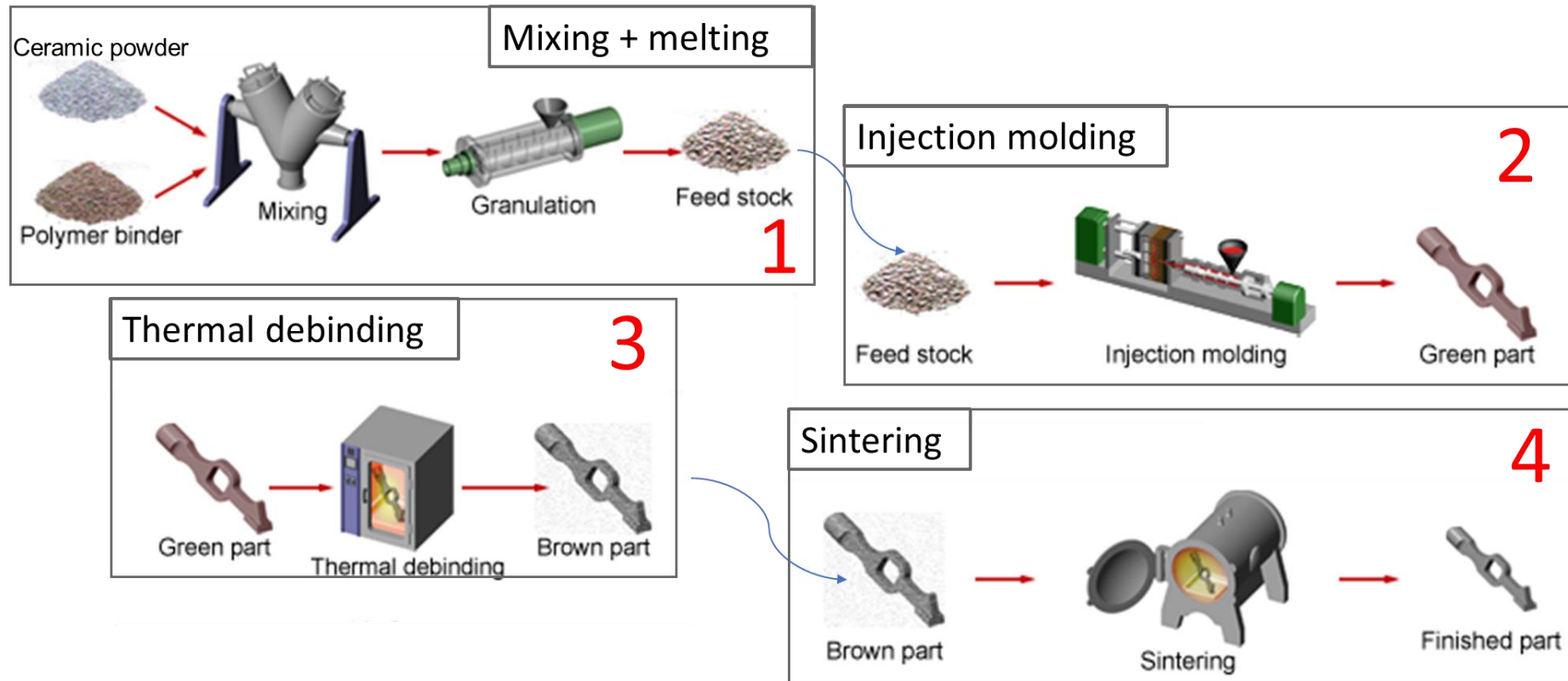
DESIGN

CREATE

SIMULATE

Marketplace Materials Modelling Hub

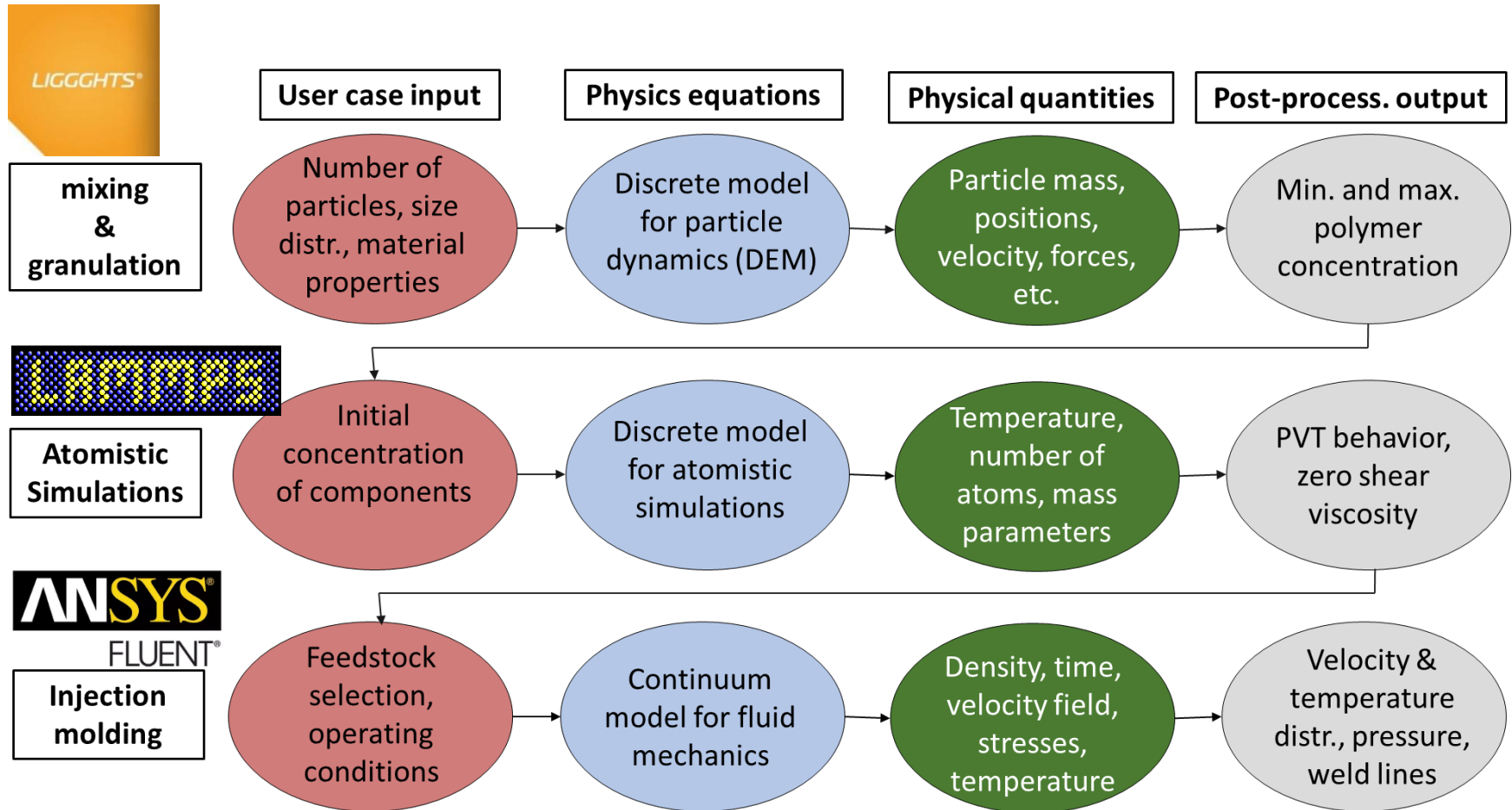
Use Case: Ceramic Injection Molding



(used for dental implant)

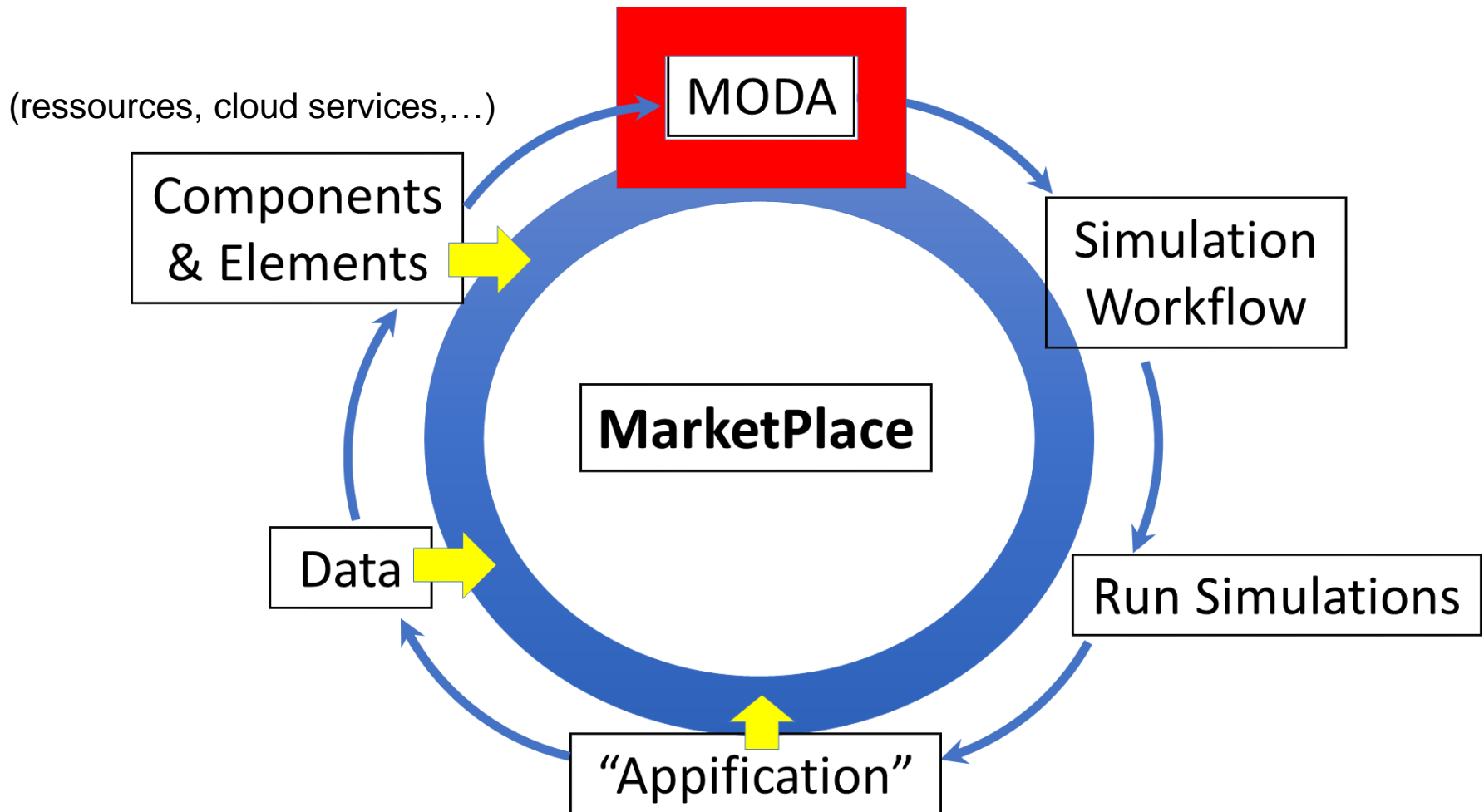
Marketplace Materials Modelling Hub

MODA = Use Case Description

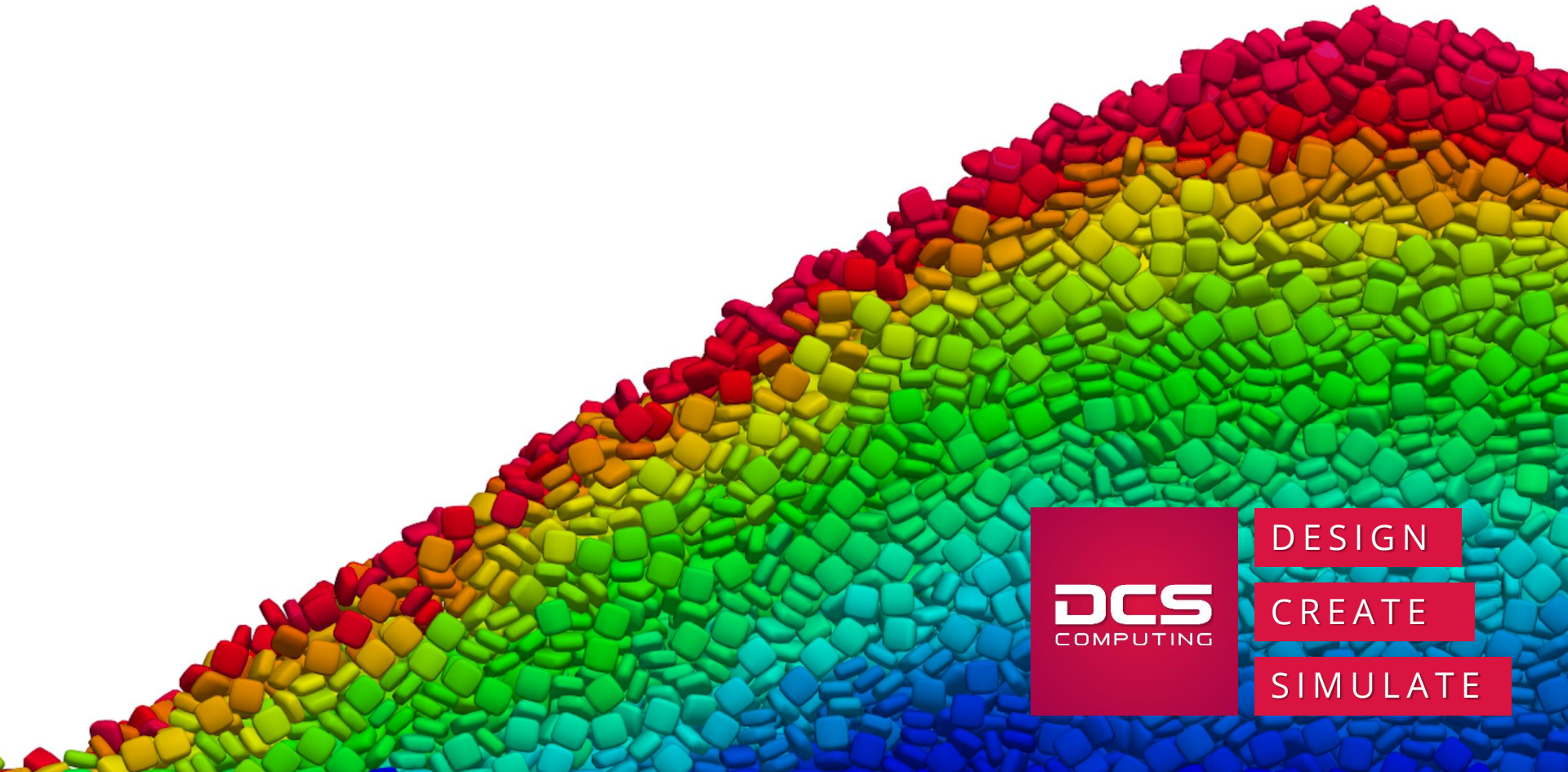


Marketplace Materials Modelling Hub

Development Cycle Around Use Case Description



Conclusions



DCS
COMPUTING

DESIGN

CREATE

SIMULATE

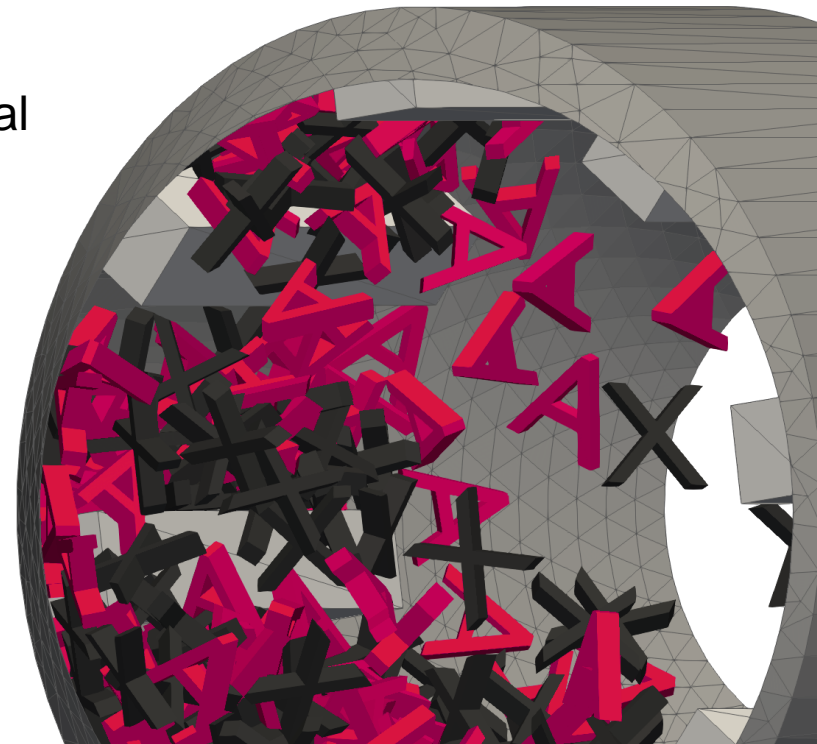
Marketplace Materials Modelling Hub

Conclusions

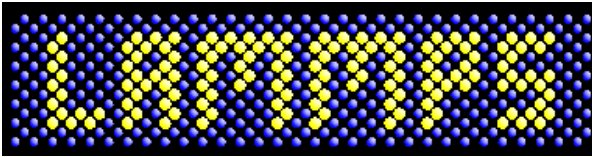


What will the future bring?

- 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



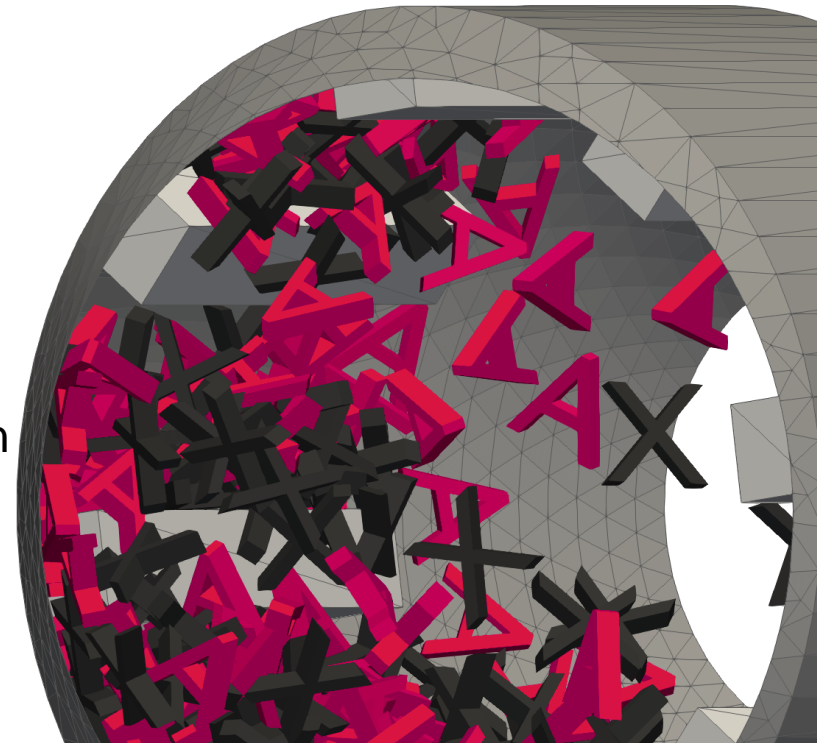
Marketplace Materials Modelling Hub Acknowledgement



www.the-marketplace-project.eu

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

Questions?



Marketplace Materials Modelling Hub

Want to become Part of the Story?

Linz, Austria



Open PhD position
www.dcs-computing.com/open-jobs

ESPCI  PARIS
EDUCATION SCIENCE INNOVATION



UNIVERSITY OF TWENTE.



BOSCH
Invented for life



SACMI

