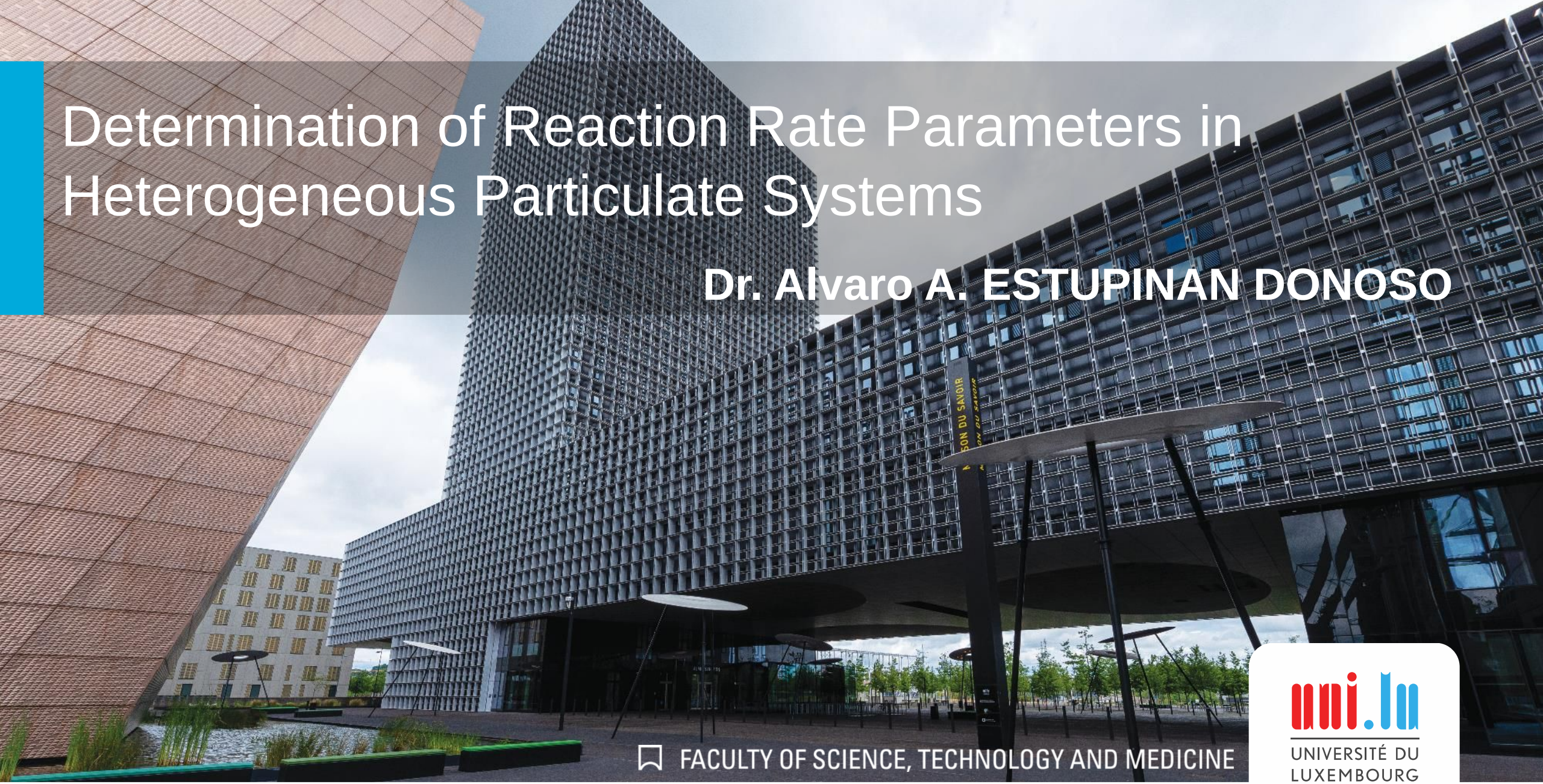
Determination of Reaction Rate Parameters in Heterogeneous Particulate Systems

Dr. Alvaro A. ESTUPINAN DONOSO



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Luxembourg National Research Fund
Supported by the Luxembourg National Research Fund (FNR) Grant: 13564670

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High Performance Computing in Luxembourg

Where is Luxembourg?

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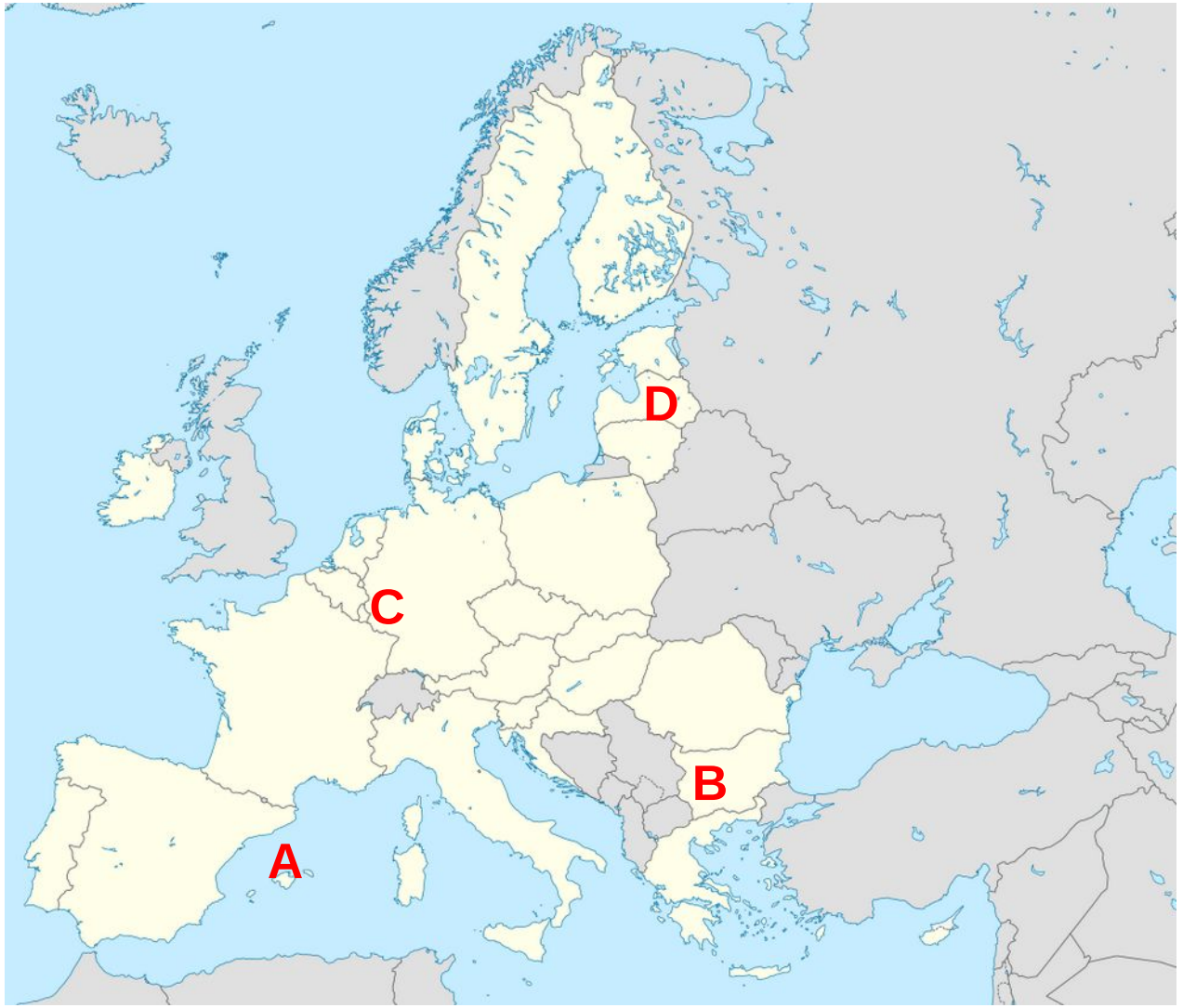
Where is Luxembourg?

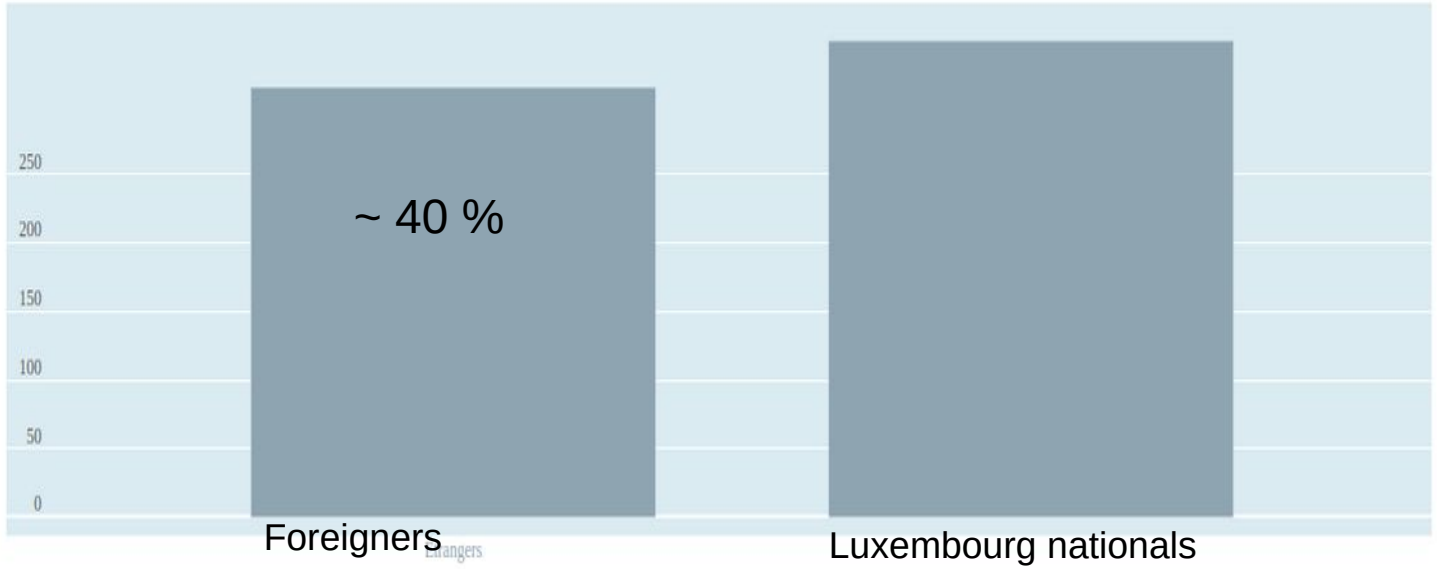


EU map

LUXEMBOURG

645 397
Population

Fréquence: Annuelle • *Période:* 2023



© Population par sexe et par nationalité au 1er janvier (x 1 000) STATEC

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Facts & Figures April 2023

THE UNIVERSITY

2003 Foundation

3 Faculties

3 Campuses

3 Interdisciplinary Centres

RANKINGS

#25 in the THE (Times Higher Education) Young University Rankings 2022

among the top #250 best universities worldwide according to the THE World University Rankings 2023

#4 worldwide for its international outlook according to the THE World University Rankings 2023

PEOPLE

3,000 Bachelor Students	2,400 Staff
2,000 Master Students	300 Professors
1,000 Doctoral candidates	1,500 Academic Staff
14.000+ Alumni (since 2003) thereof 1.500+ doctor's degrees	130 Nationalities

OUR VISION A University for Luxembourg and the World

OUR MISSION To be a world-class research university focusing on:

- Cutting-edge Research
- High-quality Education
- Contribution to the social, cultural and economic development of the country

OUR APPROACH

INTERNATIONAL	INTERDISCIPLINARY
MULTILINGUAL	RESEARCH ORIENTED

CLOSE TO EUROPEAN INSTITUTIONS, FINANCIAL INSTITUTIONS AND LEADING INDUSTRY PLAYERS

RESEARCH

2,438 Publications in 2022

1,000+ Ongoing Projects

172 Horizon projects accepted for H2020 and HEU[1]

EU funding

22m€ For EU funding awarded in 2022

138 FNR projects accepted in 2022

National fun

44m€ For FNR[2] funding awarded in 2022

camp

Determination of Reaction Rate Parameters in Heterogeneous Particulate Systems

Dr. Alvaro A. ESTUPINAN DONOSO

FACULTY OF SCIENCE, TECHNOLOGY AND MEDICINE

UNIVERSITÉ DU LUXEMBOURG

Who also is behind this contribution?

- **Mónica Arenas**
- **Maitsetseg Borchuluun**
- **Léopold Hillah**
- Dr. Xavier Besseron
- Dr. Alban Rousset
- Prof Bernhard Peters
- Prof Andreas Michels

- The HPC cluster of the University of Luxembourg
- The NanoMag group
- The LuXDEM research centre
- Beamline ID16b from the European Synchrotron Radiation Facility (ESRF)
- Ceratizit Luxembourg sarl

Content

- **Introduction**
  - Granular materials
  - Reactions in heterogeneous particulate systems
  - Numerical representations of reacting particulate systems
    - Lumped, continuous and discrete modeling approaches
- Discrete Element Methods (DEM)
  - DEM motivation and history
  - Thermochemical DEM simulations
    - What simulation parameters are employed in thermochemical DEM simulations
    - A difference between large-scale and small-scale experimentation
- Finding kinetic parameters for heterogeneous reaction systems
  - A chemical optimization problem
  - A grain growth proposed problem
- Takeaways

Granular materials

“Granular matter is a system composed of many discrete macroscopic particles”

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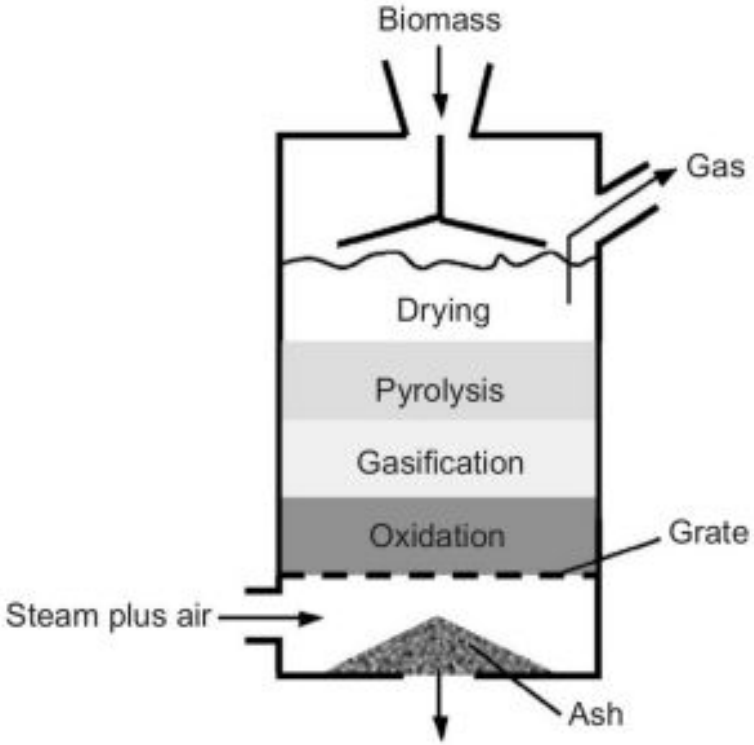
Reactions in heterogeneous particulate systems

Energy from biomass (E.g., Combustion, Gasification)



Biomass Gasifier/Combustor

$$\dot{w}_{H_2O} = \begin{cases} \frac{(T - Tevap)\rho\, c_p}{H_{evap}\, \delta t} & \text{if} \quad T \geq T_{evap} \\ 0 & \text{if} \quad T \leq T_{evap} \end{cases}$$

$$\begin{aligned} Wood &\rightarrow Char \\ Wood &\rightarrow Tar \\ Wood &\rightarrow \nu_{CO}\, CO + \nu_{CO_2}\, CO_2 \\ &\quad + \nu_{H_2O}\, H_2O + \nu_{H_2}\, H_2 + \nu_{CH_4}\, CH_4 \end{aligned}$$

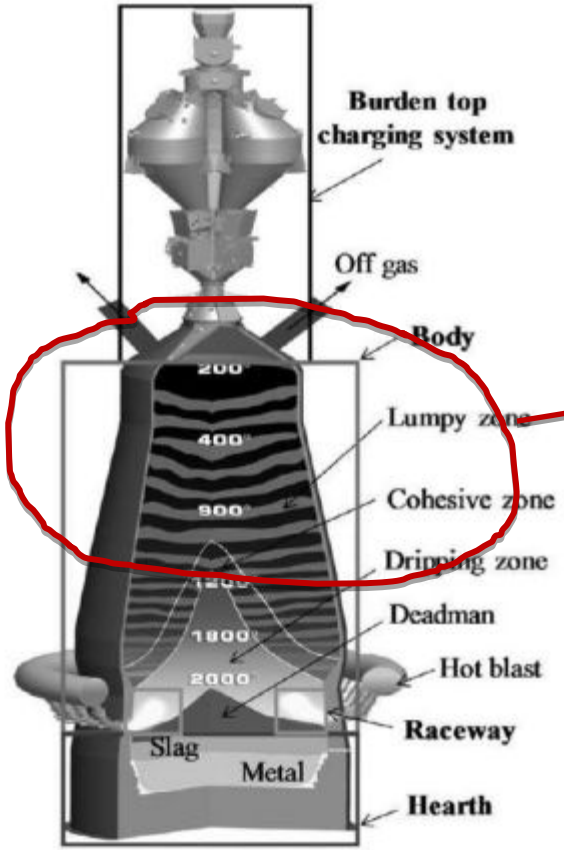
$$\begin{aligned} Tar \rightarrow \gamma_t\, Tar_{inert} &+ \gamma_{CO}\, CO + \gamma_{CO_2}\, CO_2 \\ &+ \gamma_{H_2}\, H_2 + \gamma_{CH_4}\, CH_4 \end{aligned}$$

Example of reaction rate model

$$\dot{w}_{wood} = k_0 e^{\frac{-E_a}{RT}}\, \rho_{wood}$$

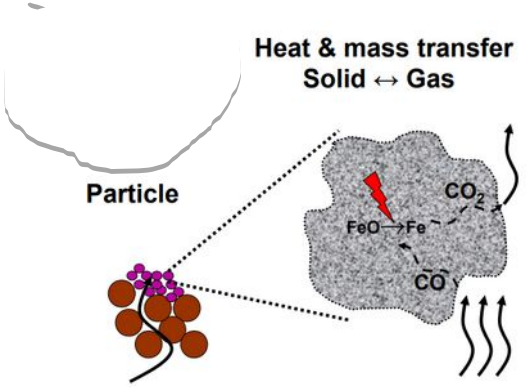
Reactions in heterogeneous particulate systems

Blast furnaces



Blast Furnace

Iron Oxide reduction



$$3Fe_2O_3 + CO \rightarrow 2Fe_3O_4 + CO_2$$
$$Fe_3O_4 + CO \rightarrow 3FeO + CO_2$$
$$FeO + CO \rightarrow Fe + CO_2$$

$$C_{(coke)} + CO_2 \rightarrow 2CO$$

$$2C_{(coke)} + O_2 \rightarrow 2CO$$

Example of reaction rate model

$$\frac{dc_k}{dt} = (\nu_k'' - \nu_k') \cdot k_f(T) \cdot \left(\prod_{i=1}^{N} c_{R_i}^{\nu_i'} - \frac{1}{K_{eq,c}(T)} \prod_{j=1}^{M} c_{P_j}^{\nu_j''} \right)$$

Numerical representations of reacting particulate systems

Example of **lumped** model for metal-oxide reduction (WO_3 reduction)

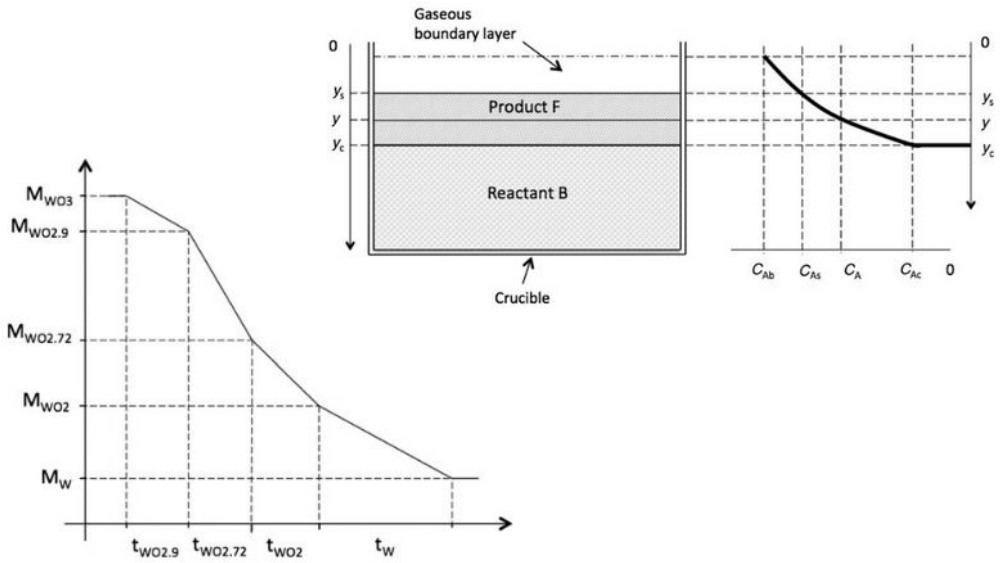


Fig. 18—Reduction scheme for modeling.

$$M_{WO_2} = 0.9310 M_0 \quad [21]$$

$$M_W = 0.7930 M_0 \quad [22]$$

The different times (min) can be expressed as follows:

$$t_{WO_{2.9}} = \frac{0.69}{3.68002 * P_{H_2}} \quad [23]$$

$$t_{WO_{2.72}} = \frac{M_0 * 0.0124}{22.093 * S_A * P_{H_2}} \quad [24]$$

$$t_{WO_2} = \frac{M_0 * 0.0497}{22.433 * S_A * P_{H_2}} \quad [25]$$

$$t_W = \frac{M_0 * 0.138}{6.5635 * S_A * P_{H_2}} \quad [26]$$

Table 1
Kinetic models and equations

Reaction model	g(α)
Diffusion	
One-dimensional	α^2
Two-dimensional	$\alpha+(1-\alpha)\ln(1-\alpha)$
Three-dimensional	
Jander equation	$[1-(1-\alpha)^{1/3}]^2$
Ginstling–Brounshtein equation	$[1-(2/3)\alpha]-(1-\alpha)^{2/3}$
Phase boundary reaction	
Two-dimensional	$1-(1-\alpha)^{1/2}$
Three-dimensional	$1-(1-\alpha)^{1/3}$
Random nucleation	
First order equation	$-\ln(1-\alpha)$
Avrami equation	$[-\ln(1-\alpha)]^{1/2}$
Erofeev equation	$[-\ln(1-\alpha)]^{1/3}$

SRC: Haboury et al. , *Metallurgical and Materials Transactions B*, 2014
Fouad, *Journal of Analytical and Applied Pyrolysis*, 1997

Numerical representations of reacting particulate systems

Example of continuous model for heat transfer in packed beds

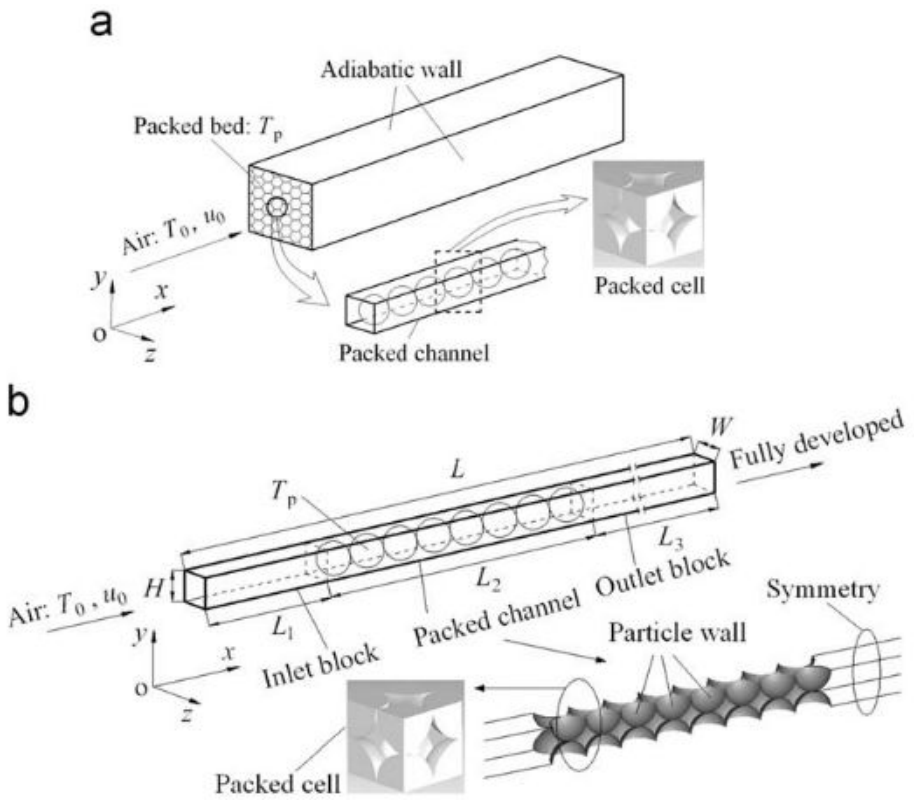
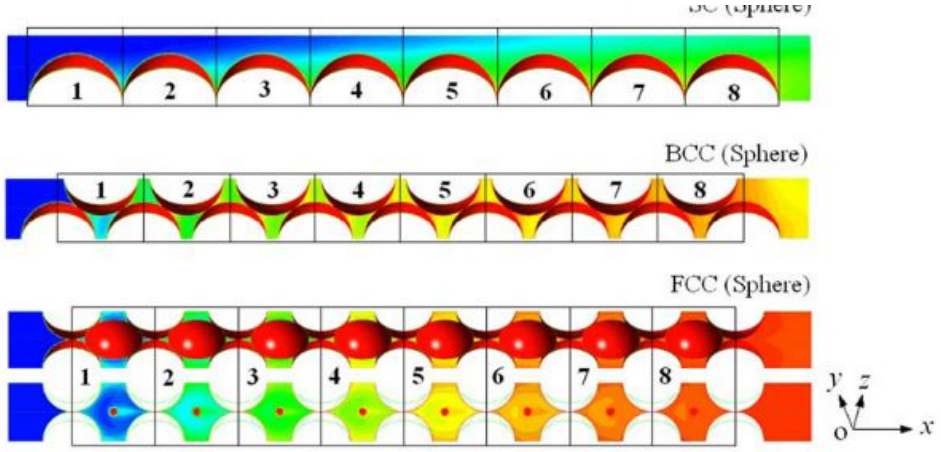


Fig. 1. Physical model: (a) structured packed bed and (b) representative computational domain.



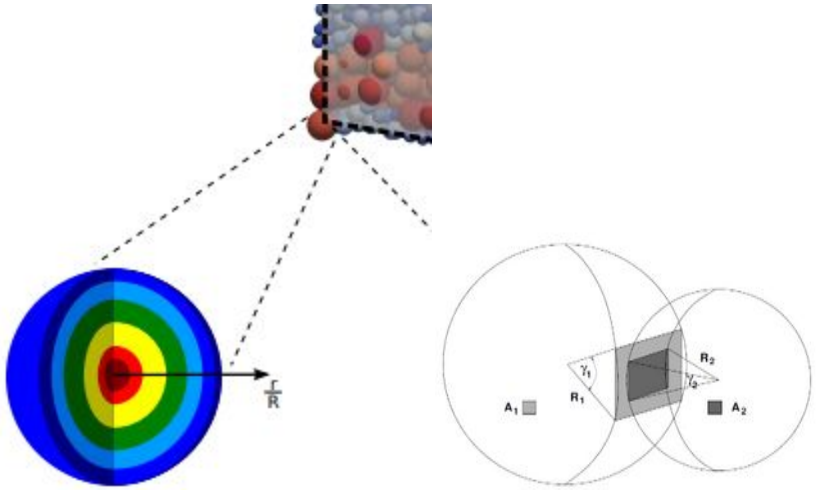
$$Nu_{sf} = \frac{h_{sf} \cdot d_P}{k_f} = a_1 + a_2 Pr^{1/3} \cdot Re^n \cdot \left(\frac{d_P}{d_h}\phi\right)^n$$

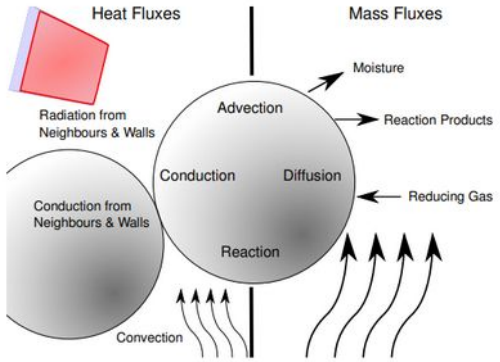
Packing model	ϕ	d_h (mm)	d_p (mm)	a_1	a_2	n
BCC (uniform sphere)	0.340	4.12	12.00	1.80	0.40	0.63
BCC-1 (non-uniform sphere)	0.293	3.00	10.64	1.80	0.49	0.63
Random (Wakao and Kaguei, 1982)	–	–	–	2.00	1.10	0.60

SRC: Yang, Jian et al. , *Chemical Engineering Science*, 2010

Numerical representations of reacting particulate systems

Example of continuous model for heat transfer in packed beds





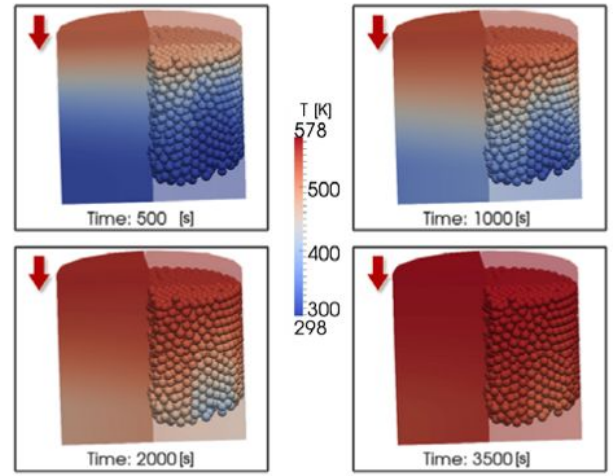


Fig. 8. XDEM fluid and particle temperature predictions at different time steps. Slate, heating-up case.

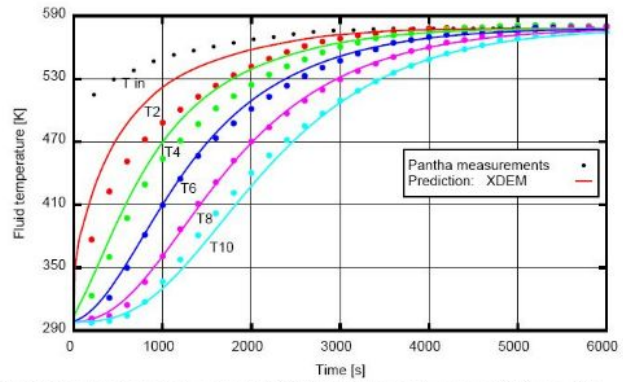
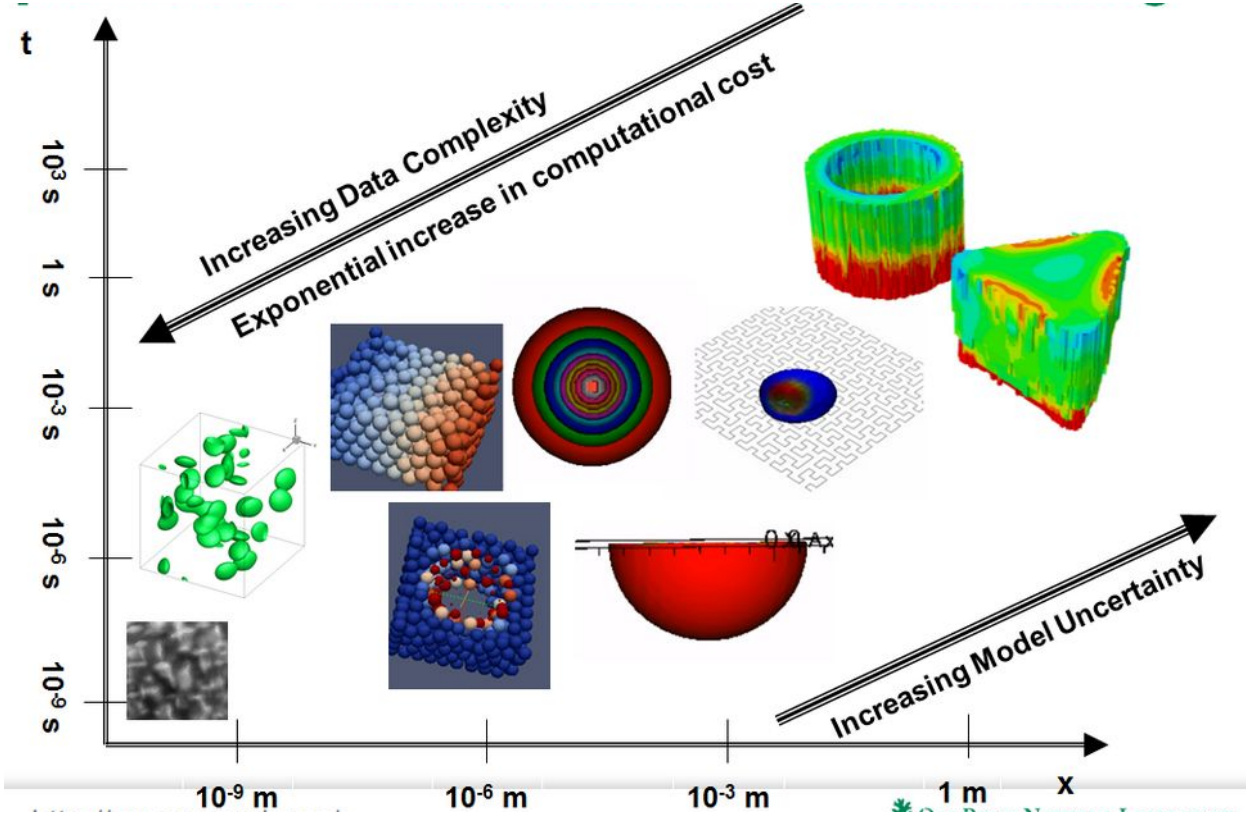


Fig. 9. Comparison between XDEM fluid temperature predictions with the heating-up experiment measurements [27]. Slate, heating-up case

SRC: Estupinan Donoso et al. , *International Review of Mechanical Engineering*, 2013

Numerical representations of reacting particulate systems



Increase uncertainty

Lumped modelling
One (or One set) of equations
with analytical solution

Continuous modelling
One set of equations (e.g. Navier–Stokes)
numerically solved

Discrete modelling
N set of equations (e.g. Navier–Stokes),
boundary conditions and sources numerically solved

Continuous + Discrete modelling

Increase computational costs

Content

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- **Discrete Element Methods (DEM)**
  - DEM motivation and history
  - Thermochemical DEM simulations
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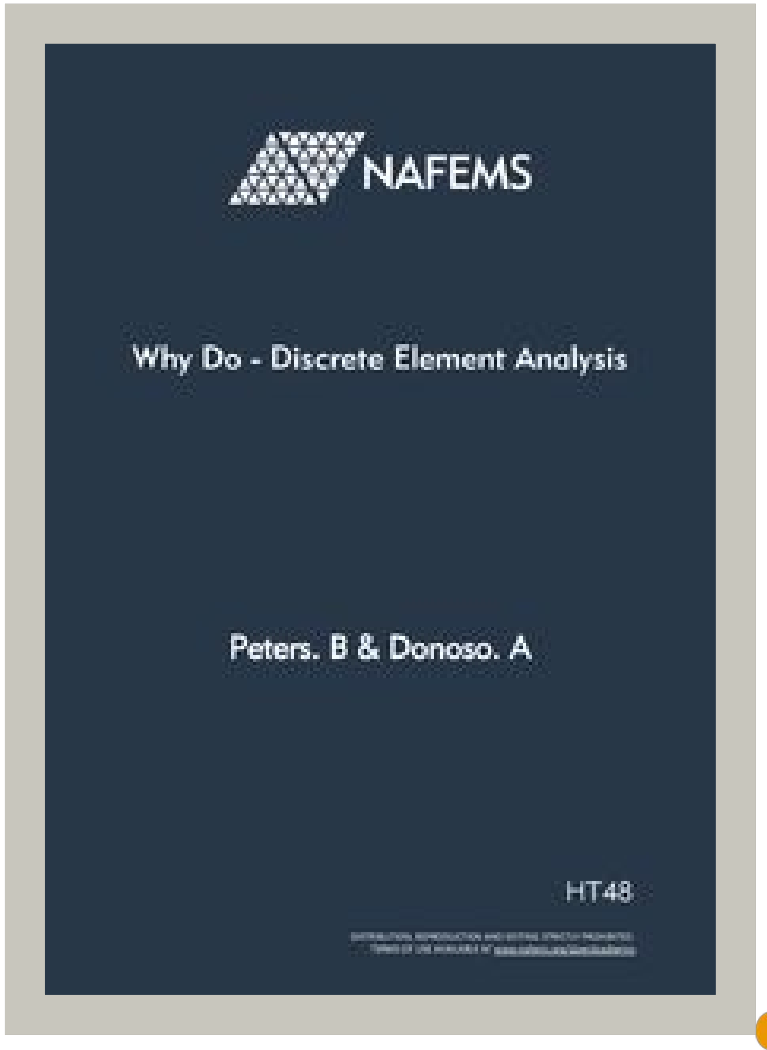
Discrete Element Method (DEM)

DEM motivation and history

- The Discrete Element Method (DEM) is a discrete approach that **enables accurate numerical calculation of finite particle displacements and rotations**, as well as automated contact detection for a group of particles.

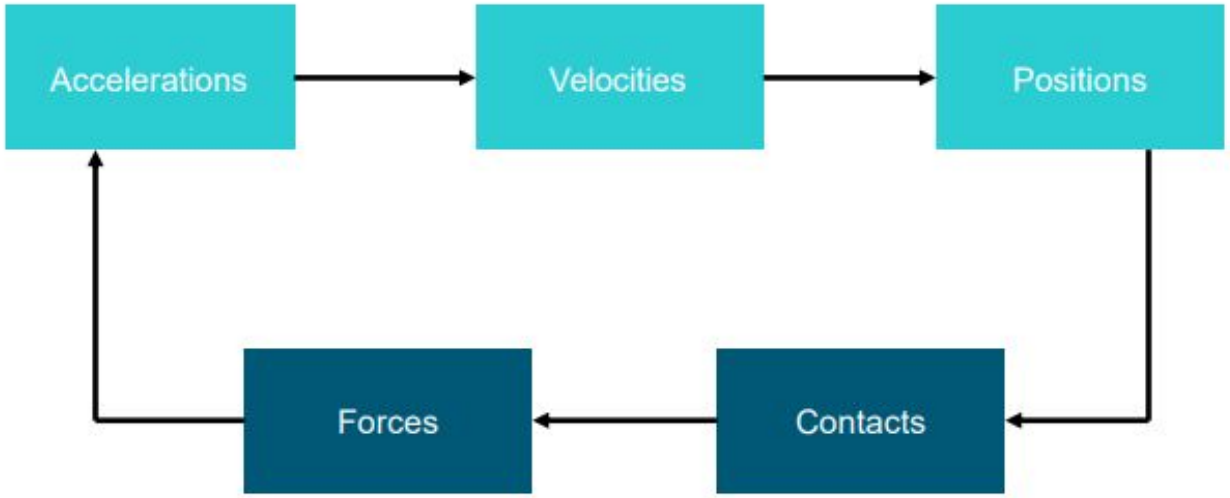
- The method was first **proposed in 1956 by Alder and Wainwright for molecular dynamics studies**. The method was **later developed by Cundall and Strack in the 1970s**, and since then, the principles of the discrete element method, also known as the distinct element method, have been widely used for simulating the behavior of granular materials and other discrete systems.

- Due to its discrete approach**, DEM is particularly well-suited for modeling the bulk behavior of materials.** Its ability to simulate discontinuous media can also **provide valuable insights into various processes, potentially reducing the number of physical experiments required to understand them**.



Discrete Element Method

How does it work ?



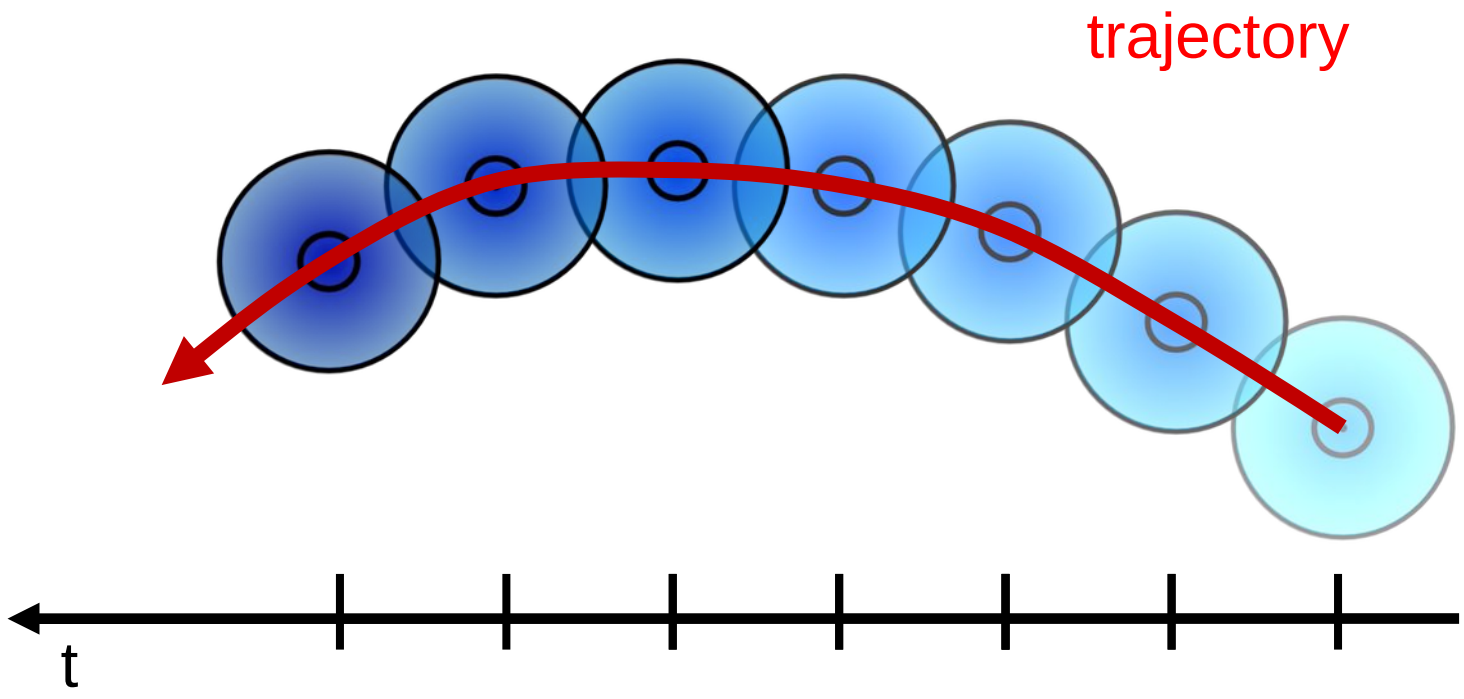
Newton Laws

Contact Mechanics

DEM software utilizes contact detection algorithms and appropriate contact models to calculate the forces acting on particles. By applying Newton's laws of motion and numerical integration, the software can then compute the accelerations, velocities, and positions of the particles.

SRC: ALTAIR

How can we calculate the trajectory of a particle ?



Discrete Element Method

How does it work ?

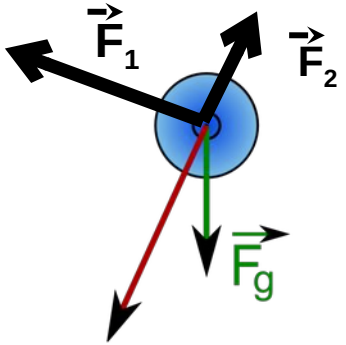
$$\vec{F} = m \cdot \vec{a} \qquad \text{Newton's 2nd law of motion}$$

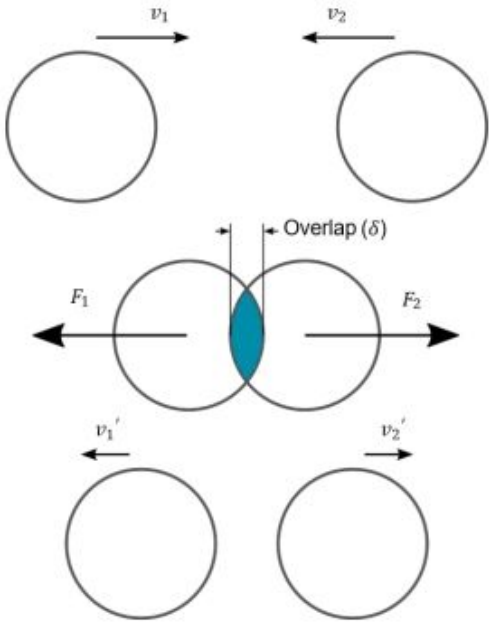
$$\vec{F} = m \cdot \vec{a}(t)$$

$$\vec{a}(t) = \frac{\sum \vec{F}}{m}$$

$$\xrightarrow{\int_{t_0}^{t_1}(\ldots)\,dt} \vec{x}(t_1) = \vec{v}(t_1) = \vec{v}_0 + \frac{\sum \vec{F}}{m} \cdot (t_1 - t_0)$$

$$\xrightarrow{\int_{t_0}^{t_1}(\ldots)\,dt} \vec{x}(t_1) = \vec{x}_0 + \vec{v}_0 \cdot (t_1 - t_0) + \tfrac{1}{2} \cdot \frac{\sum \vec{F}}{m} \cdot (t_1 - t_0)^2$$

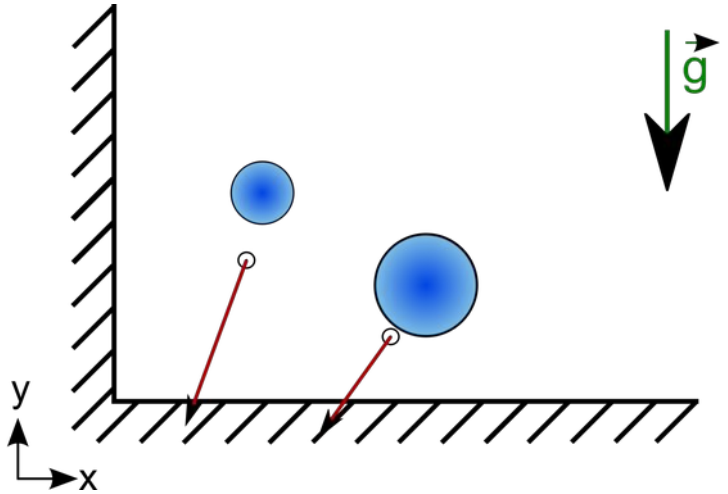


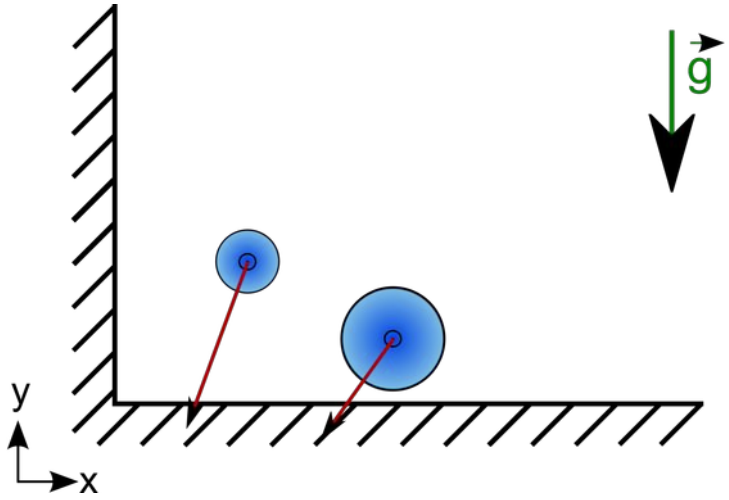


Discrete Element Method

How does it work ?

- Single Particle Contact





SRC: Yade - Open Source Discrete Element Method https://yade-dem.org/

Discrete Element Method

A dam break example

Setup

- 2.35M particles
- 10M CFD cells in the fine grid
- 500k CFD cells in the coarse grid
- Co-located partitions + Dual Grid
- Non-uniform distribution

SRC: XDEM software, https://luxdem.uni.lu/

Discrete Element Method

How does it work ?

Models for Various Material Behavior

In DEM, different types of material behavior can be simulated by a range of well-established models.

SRC: ALTAIR

Dry granular material

This type of material can be simulated in DEM by a variety of linear or nonlinear models. The most common ones include Linear Spring or Hertz-Mindlin (no slip), which is a default contact model in EDEM.

Bonding

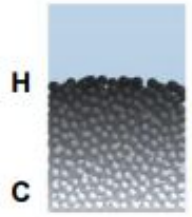
Particles in DEM can be bonded together to resist tangential and normal movement up to a maximum value (defined by the user) at which the bond breaks. This model is particularly useful in modelling concrete and rock structures.

Electrostatics

Longer-range electrostatic interactions can also be modelled in DEM. Particles are assigned a charge and experience forces based on the Coulomb's law. Applications like laser printer behavior can be simulated with such a module.

Cohesion

The cohesion models in DEM can simulate the influence of Van der Waals forces within the contact zones and allow the user to model strongly adhesive systems, such as dry powders or wet materials.



Heat transfer

For dense particulate systems, contacts between particles are substantial and heat conduction can be of significant importance. DEM simulations allow for modelling this inter-particle heat transfer and provide insight into variety of applications ranging from multi-phase reactors to kilns and calciners.

[Applications at LuXDEM]

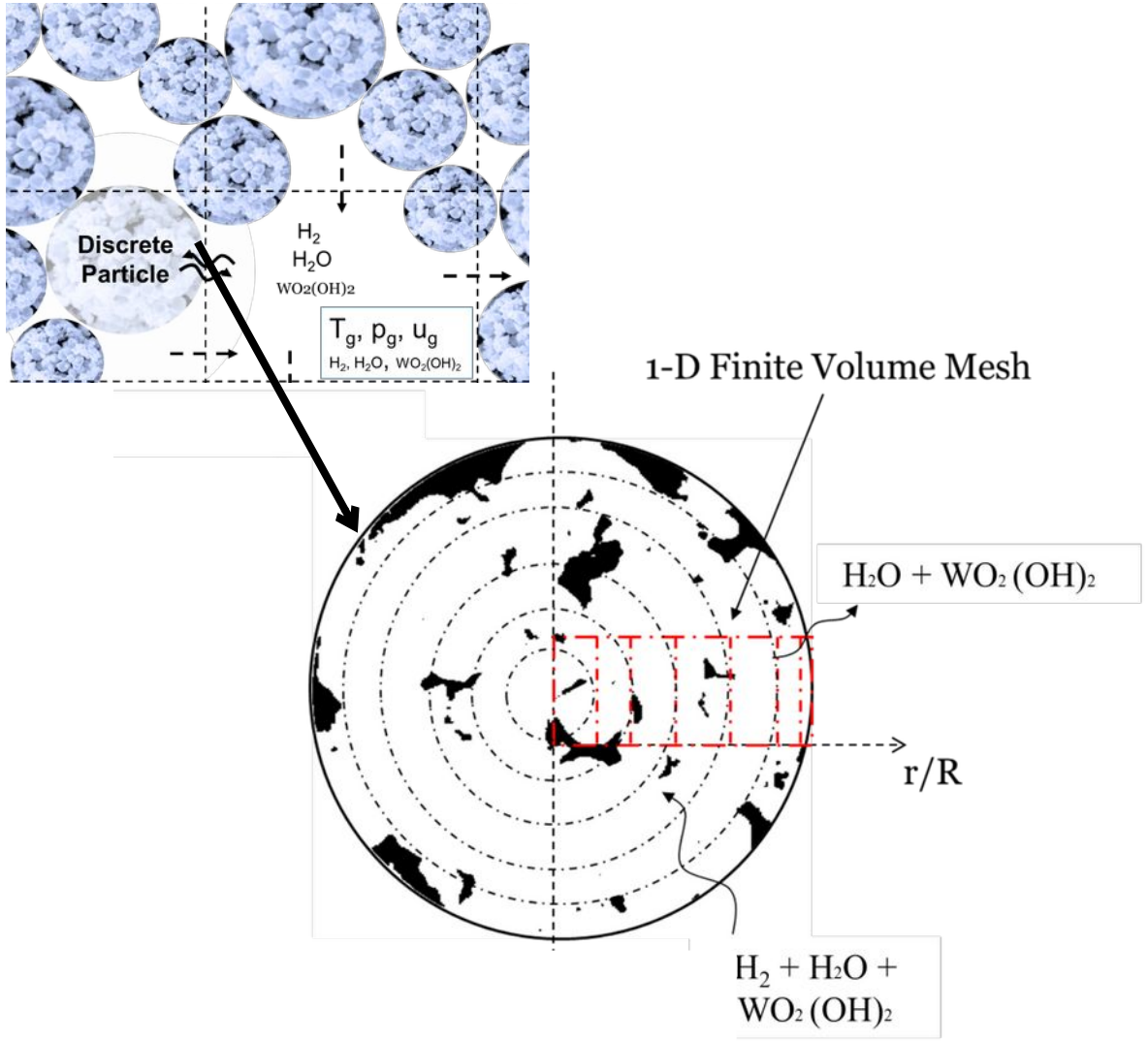
Thermochemical DEM simulations

The eXtended Discrete Element Method (XDEM)

Wikipedia: is a numerical technique that extends the dynamics of granular material or particles as described through the classical discrete element method (DEM) (Cundall [1] and Allen [2]) by additional properties such as the thermodynamic state, stress/strain or electro-magnetic field for each particle. Contrary to a continuum mechanics concept, the XDEM aims at resolving the particulate phase with its various processes attached to the particles. While the discrete element method predicts position and orientation in space and time for each particle, the extended discrete element method additionally estimates properties such as internal temperature and/or species distribution or mechanical impact with structures.

Thermochemical DEM simulations

The eXtended Discrete Element Method (XDEM)



Inner-particle processes predictions by PDEs for conservation:

Mass $\langle \rho_g \rangle^g = \sum_i \langle \rho_{i,g} \rangle^g$

Gas Species *g*

$$\frac{\partial(\epsilon_p \langle \rho_{i,g} \rangle^g)}{\partial t} + \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \langle \rho_{i,g} \rangle^g \langle u_g \rangle\right) = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n D_i \epsilon_p \frac{\partial}{\partial r}\langle \rho_{i,g} \rangle^g\right) + \epsilon_p \sum_k \dot{\omega}_{k,i,g}$$

Energy $\frac{\partial \langle \rho c_p T \rangle}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \lambda_{\text{eff}} \frac{\partial \langle T \rangle}{\partial r}\right) + \sum_{k=1}^{l} \dot{\omega}_k H_k$

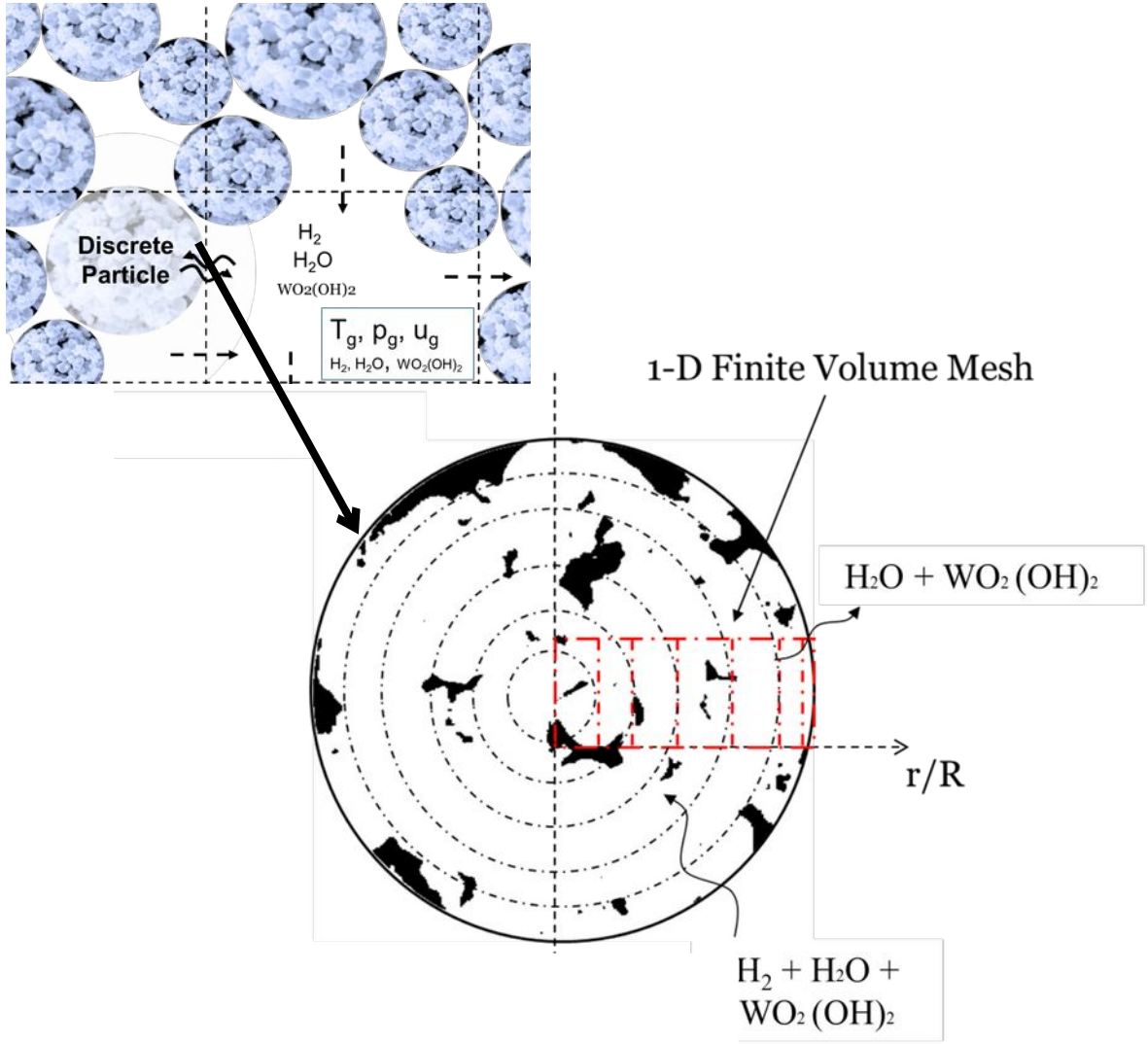
\+ Chemical conversion

Solid Species *k*. E.g., Equilibrium reaction

$$\frac{dc_k}{dt} = k_f(T) \cdot \left(\nu'_k \cdot \prod_{i=1}^{N} c_{R_i}^{\nu'_i} - \frac{\nu''_k}{K_{\text{eq,c}}(T)} \cdot \prod_{j=1}^{M} c_{P_j}^{\nu''_j} \right)$$

Thermochemical DEM simulations

The eXtended Discrete Element Method (XDEM)



Boundary Conditions and sources

$$
\begin{aligned}
-\lambda_{\text{eff}} \frac{\partial \langle T \rangle}{\partial r}\bigg|_{r=0} &= 0 \\
-\lambda_{\text{eff}} \frac{\partial \langle T \rangle}{\partial r}\bigg|_{r=R} &= \alpha(T_R - T_\infty) + \dot{q}''_{\text{rad}} + \dot{q}''_{\text{cond}} \\
-D_{\text{i,eff}} \frac{\partial \langle \rho_i \rangle}{\partial r}\bigg|_{r=R} &= \beta_i(\rho_{i,R} - \rho_{i,\infty})
\end{aligned}
$$

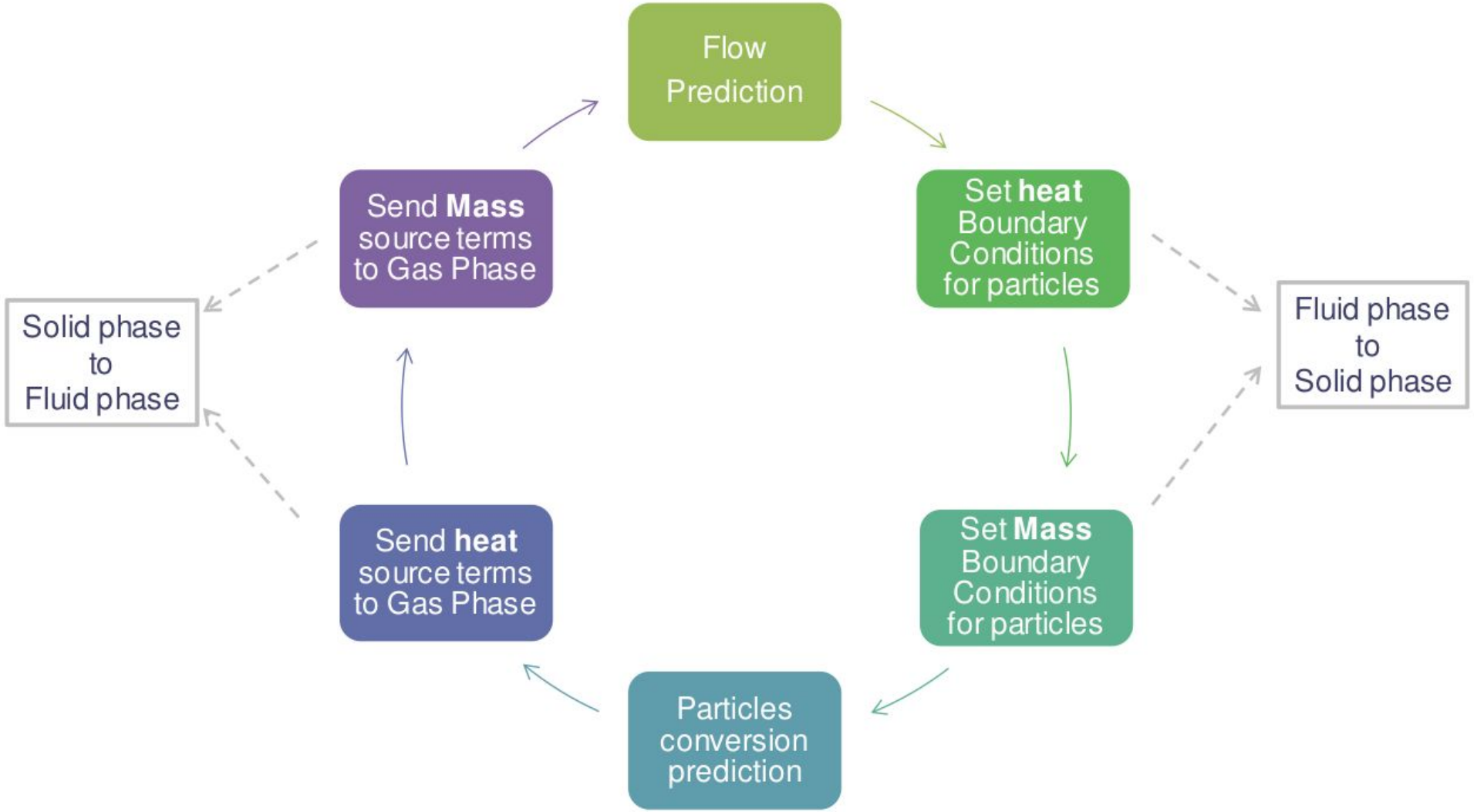
E.g., melting

$$
m' = \begin{cases} \frac{(h-h_m)}{h_{sl}\Delta t} & h \geq h_m \\ 0 & h \leq h_m \end{cases}
$$

Thermochemical DEM simulations

The eXtended Discrete Element Method (XDEM)

Continuous and discrete phases 4-way coupling for mass and energy



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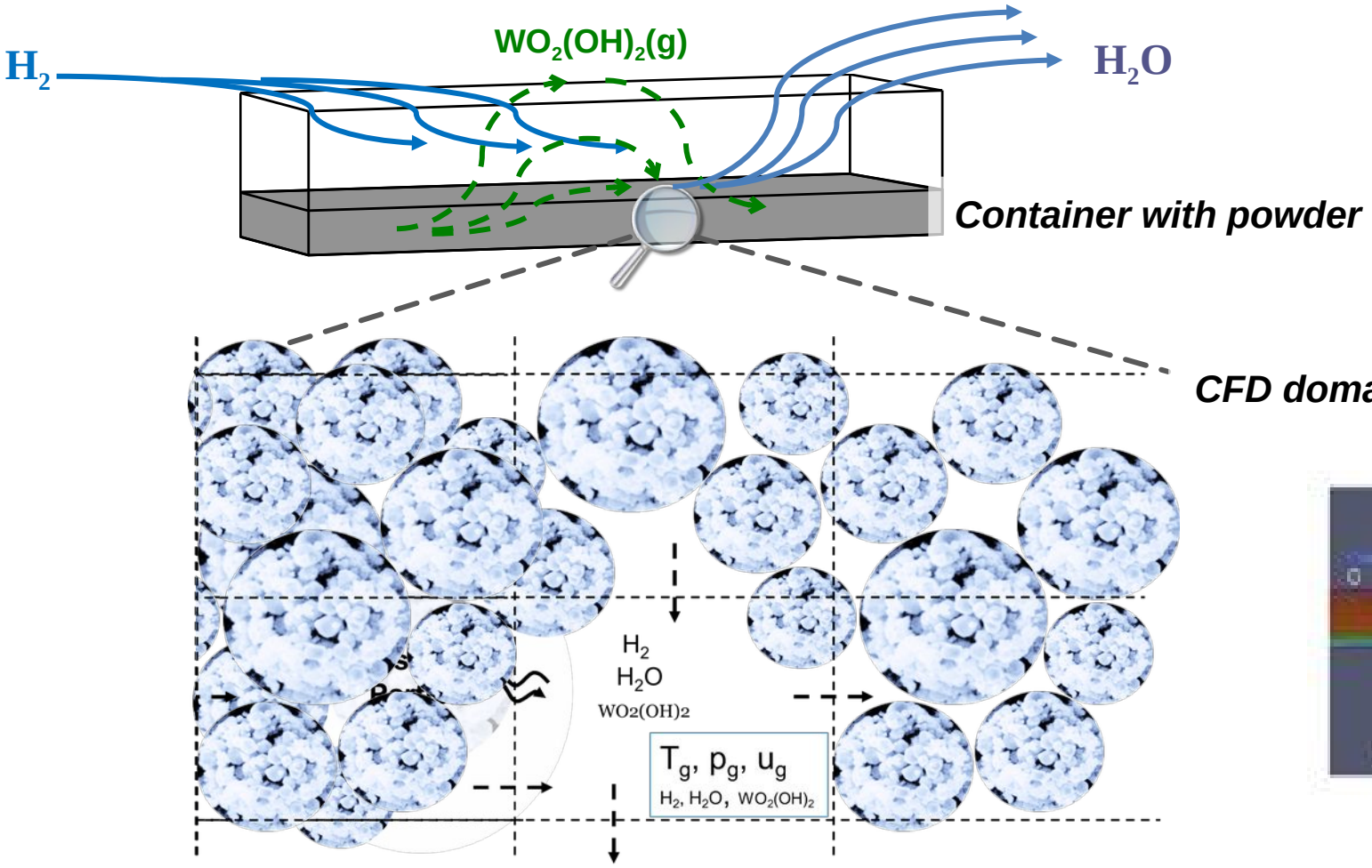
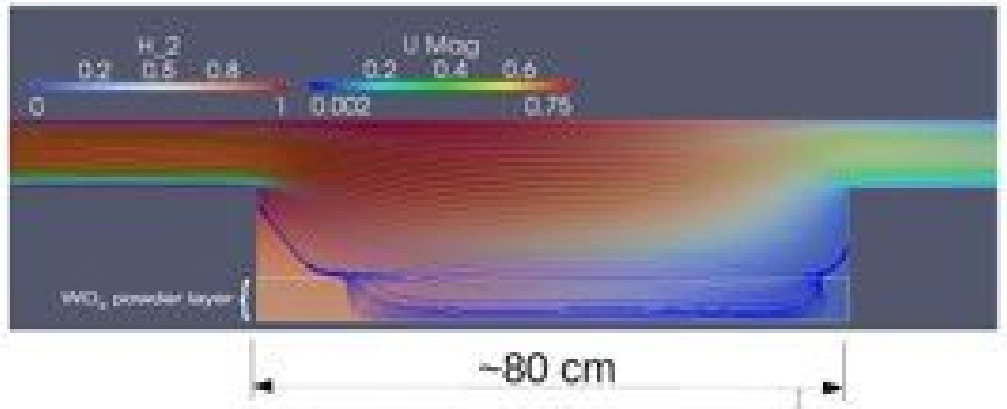
WHY?

Finding kinetic parameters for heterogeneous reaction systems

A chemical optimization problem





Finding kinetic parameters for heterogeneous reaction systems

A chemical optimization problem

SRC: Mónica Arenas, Maitsetseg Borchuluun, Léopold Hillah, 2020

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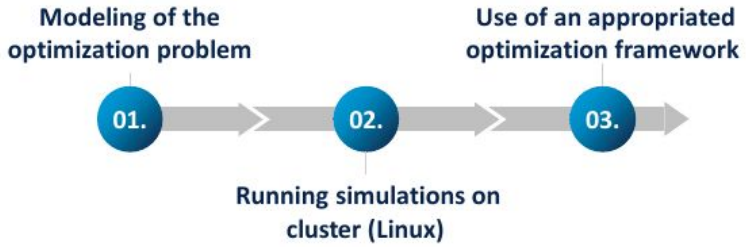
Introduction

One of the most important aspects of heterogeneous reactions is to understand and quantify the **evolution of the different transformations**. For instance, during metal-oxides reduction processes, it is of high importance to quantify the rate at which the pure metal is formed.

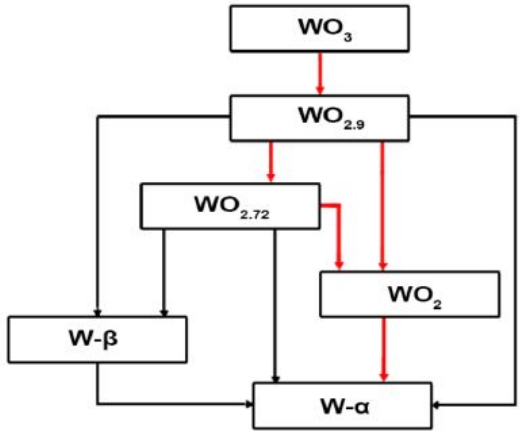
It is almost impossible to separately observe, accurately quantify and gain insight into these nonlinear physical and chemical processes by experimental means only. Thus, **XDEM** have become indispensable for studying complex systems without the need of costly experimental practices.

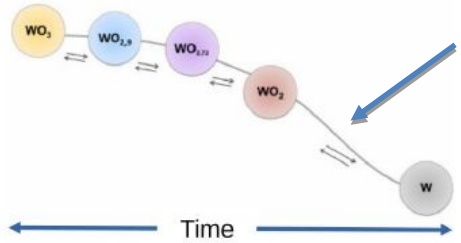
This tool is more efficient when implemented with optimization algorithms that help the finding of the **best optimal parameters**.



Goals

- Determine the **optimal parameters (E_a and k_r)** of each of the reduction steps involved in the dry-hydrogen reduction of tungsten trioxide.
- **Minimize the error** of XDEM simulations versus experimental data.





Objective Function

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Why DAKOTA?

- One flexible simulation interface, a wide array of algorithms
- Advanced modeling and simulation, support for engineering transformation
- Scalable parallel computing from desktop to HPC

DAKOTA Calibration Approach

- Simulation-based Optimization
- Objective : Adjust model parameters x to maximize agreement with a set of experimental data
- Minimize $f(x) = \sum_{i=1}^{n} (s_i(x) - d_i)^2$

  $s_i(x)$: simulation output that depends on x

  d_i: given data
- 3 Options:
  - Model returns simulation output to Dakota
  - Model returns residuals to Dakota
  - Model returns objective function value

Some methods:

- Tailored gradient-based
- Use any optimizer
- Bayesian inference

DAKOTA Optimization Approach

- Simulation-based Optimization
- Objective: Determine parameter values that yield extreme values (max/min) of objectives, while satisfying constraints
- Minimize / Maximize objective function
- 1 Option:
  - Model returns objective function value

Methods:

- Gradient-based local;
- Derivative-free local;
- Derivative-free global one can find Evolutionary Algorithms (EA), etc.;
- Global/heuristics
- Surrogate-based, multi-fidelity.

Any **Dakota optimization algorithm** can be applied to **calibration problems** arising in parameter estimation, system identification, and test/analysis reconciliation.

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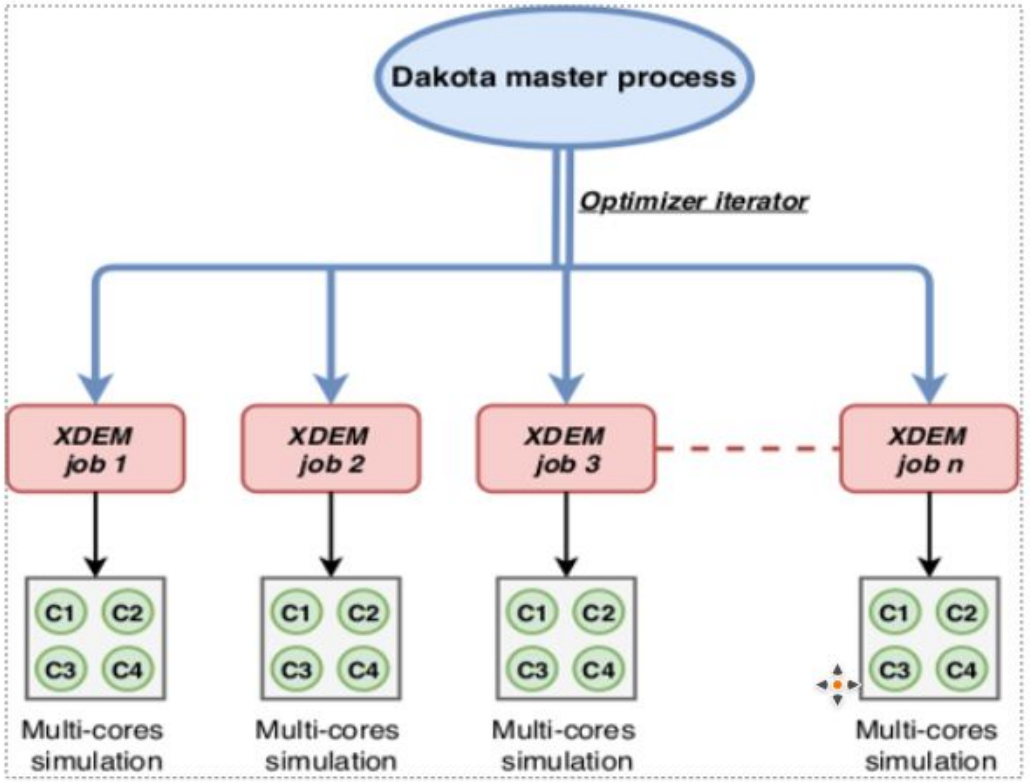
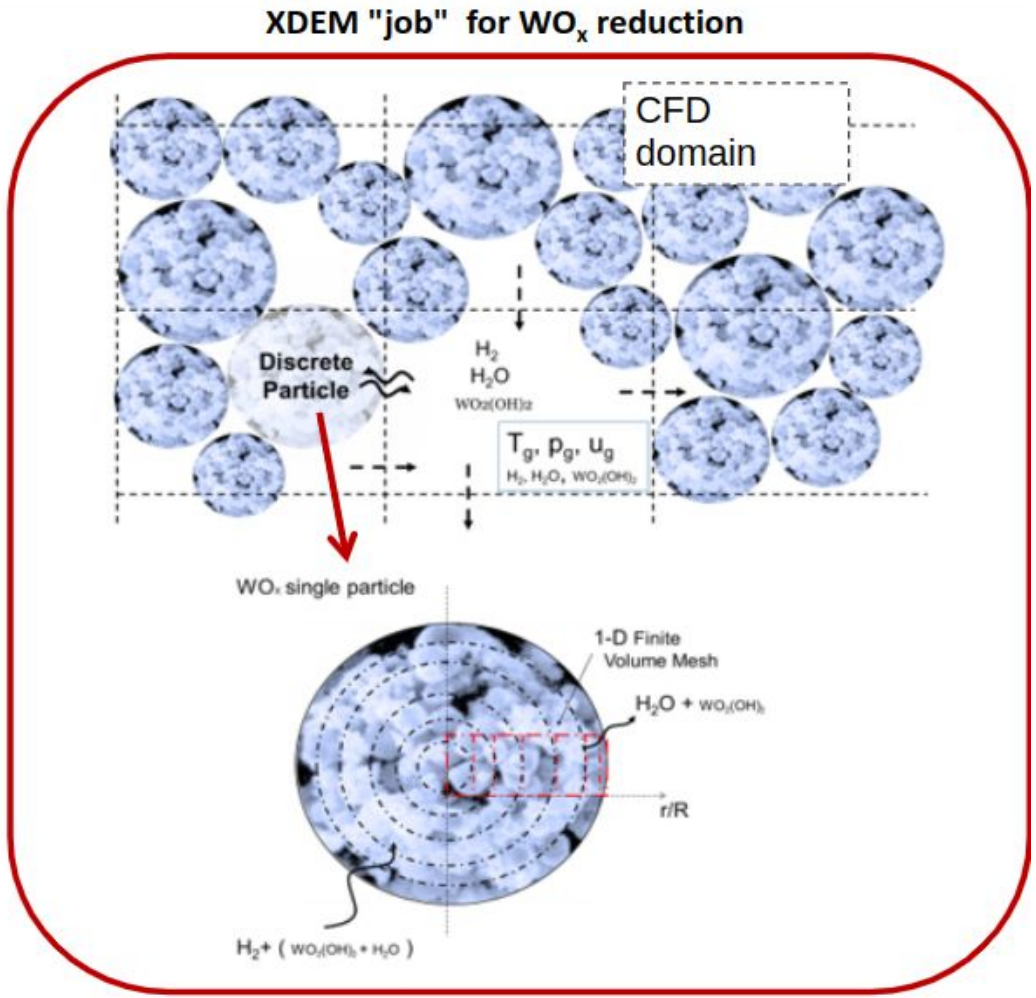
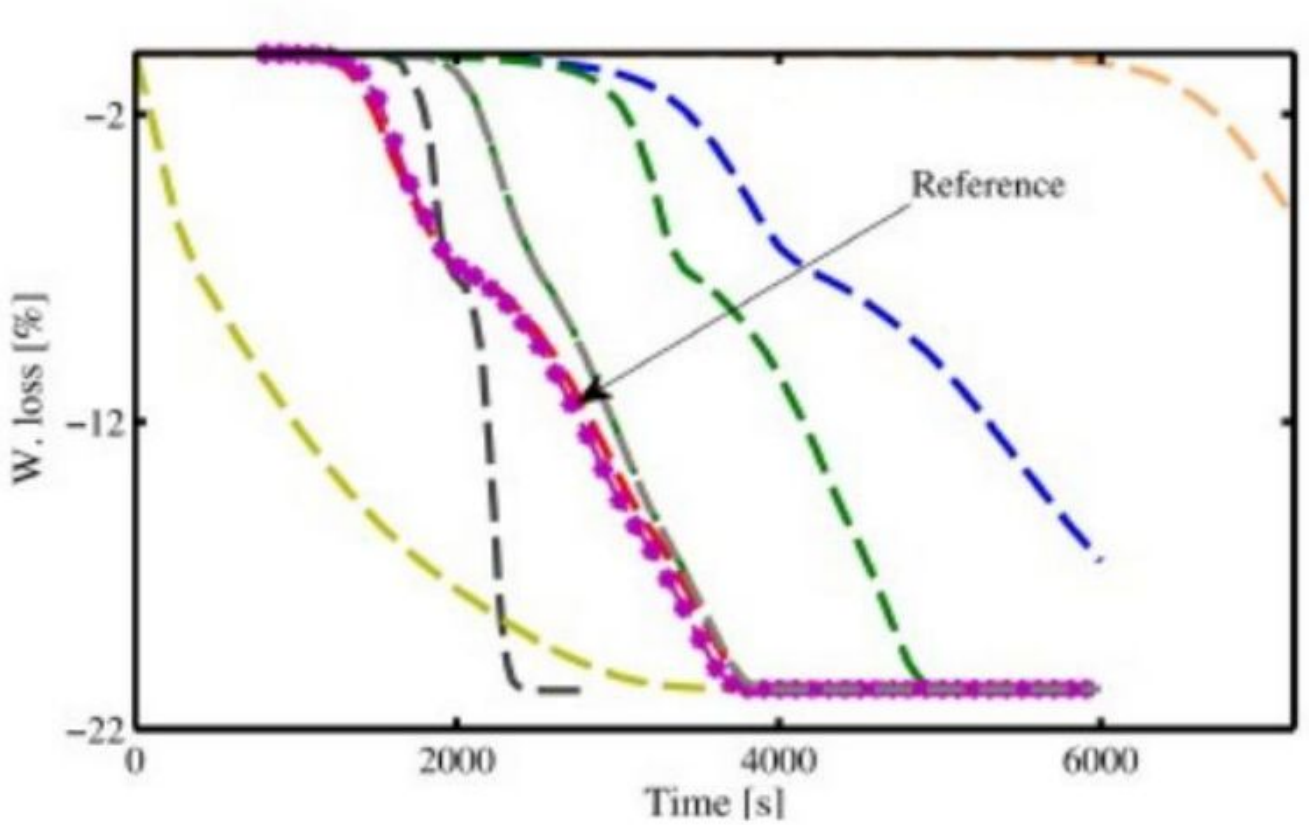
A chemical optimization problem



Source: Dr. A. Rousset, FNR grant *Grant 2018-2/13318107-VP4HPC*



A chemical optimization problem



Example of several "testing parameter" executions compared to the reference solution for the reduction of tungsten trioxide under dry atmospheres

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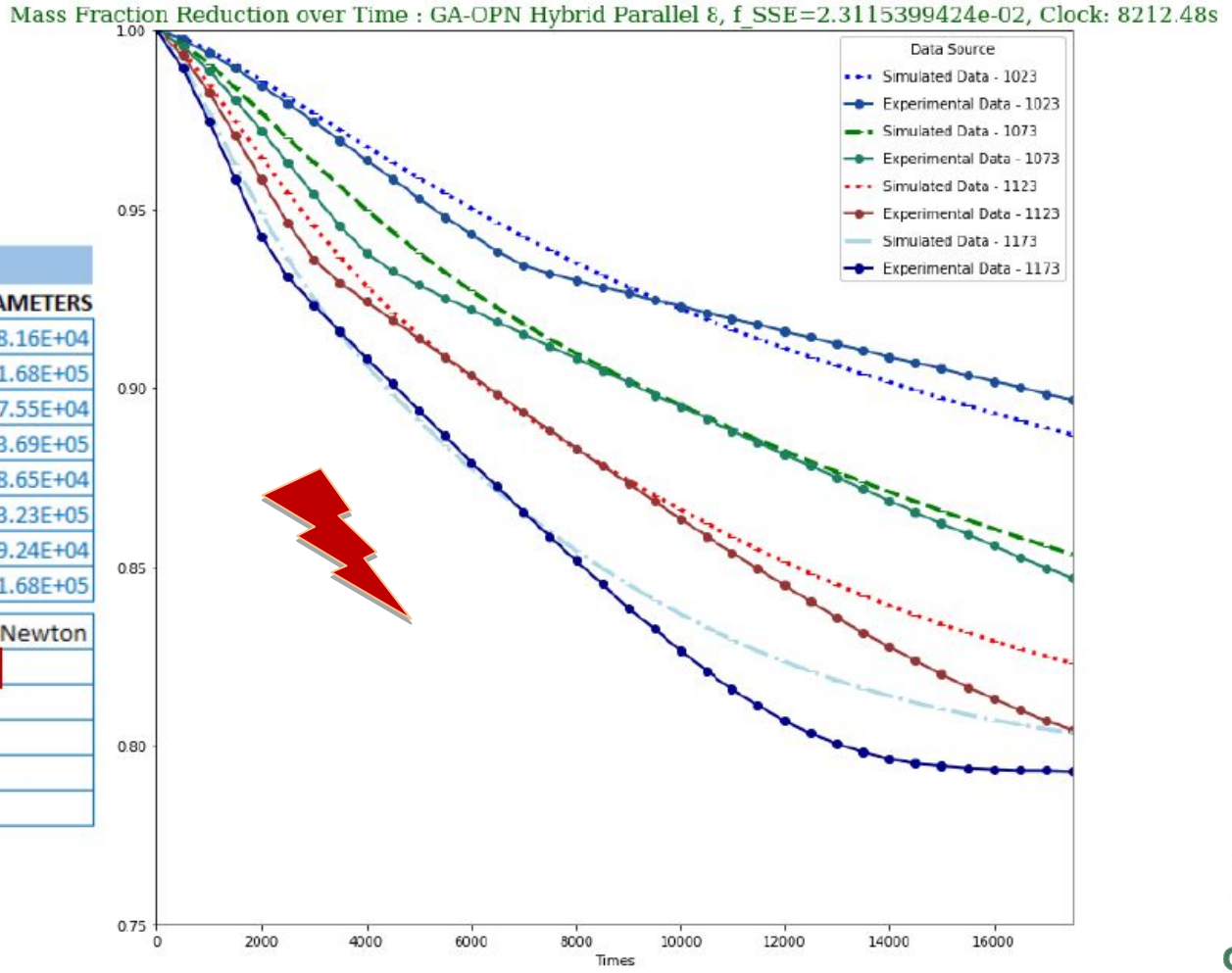
- Hybrid approach

  coliny_ea + optpp_newton

  - **Impact of Variable Range Values on Convergence**

	CASE 1			CASE 2		
PARAMETERS	**MIN**	**MAX**	**BEST PARAMETERS**	**MIN**	**MAX**	**BEST PARAMETERS**
ea1	1.00E-03	1.00E+06	1.74E+05	5.00E+04	1.00E+05	8.16E+04
kr1	1.00E-03	1.00E+10	7.28E+09	1.50E+05	2.50E+05	1.68E+05
ea2	1.00E-03	1.00E+06	8.47E+03	5.00E+04	1.00E+05	7.55E+04
kr2	1.00E-03	1.00E+10	3.64E+09	3.00E+05	5.00E+05	3.69E+05
ea3	1.00E-03	1.00E+06	1.68E+05	5.00E+04	1.00E+05	8.65E+04
kr3	1.00E-03	1.00E+10	4.27E+09	3.00E+05	6.00E+05	3.23E+05
ea4	1.00E-03	1.00E+06	6.30E+05	5.00E+04	1.00E+05	9.24E+04
kr4	1.00E-03	1.00E+10	4.60E+09	9.00E+04	2.00E+05	1.68E+05

Optimization Type	Hybrid Genetic Algorithm - Gauss Newton	Hybrid Genetic Algorithm - Gauss Newton
Best Objective Function	1.92E-01	2.31E-02
Function Evaluations	1071	1071
XDEM Runs	4284	4284
Total CPU (seconds)	3.94729	3.29619
Total Wall Clock (seconds)	9579.55	13351.1



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XDEM jobs: parallel performance

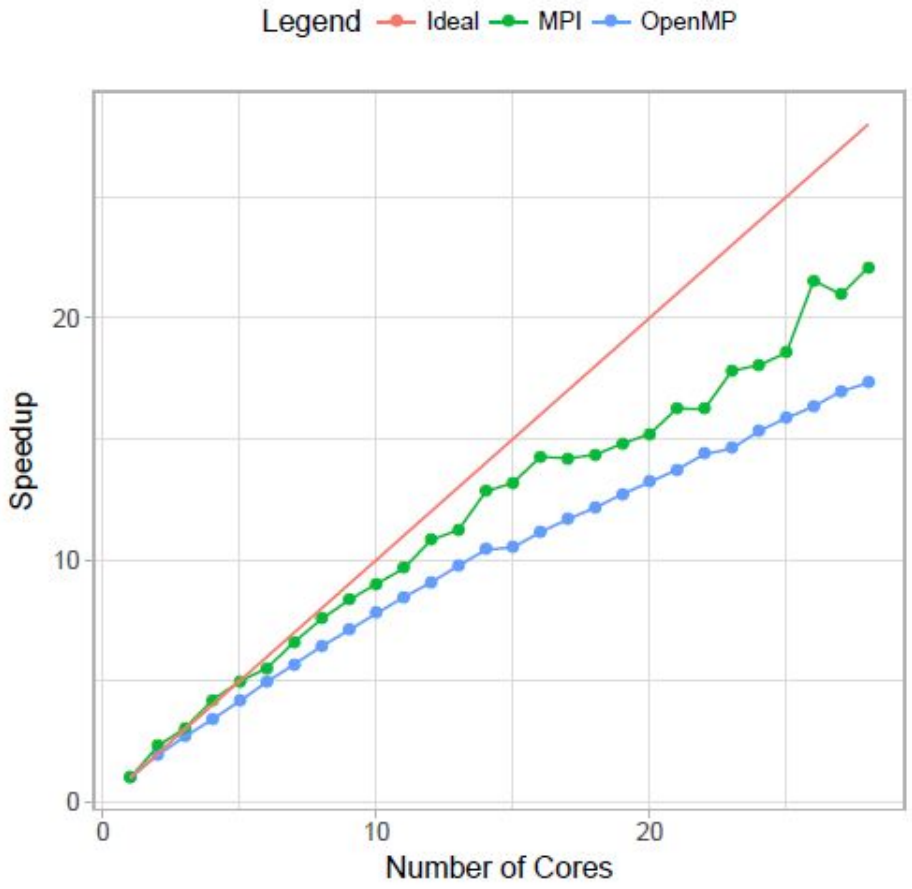


FIGURE 6.5: SpeedUp of MPI and OpenMP versions on one node *i.e.* up to 28 cores.

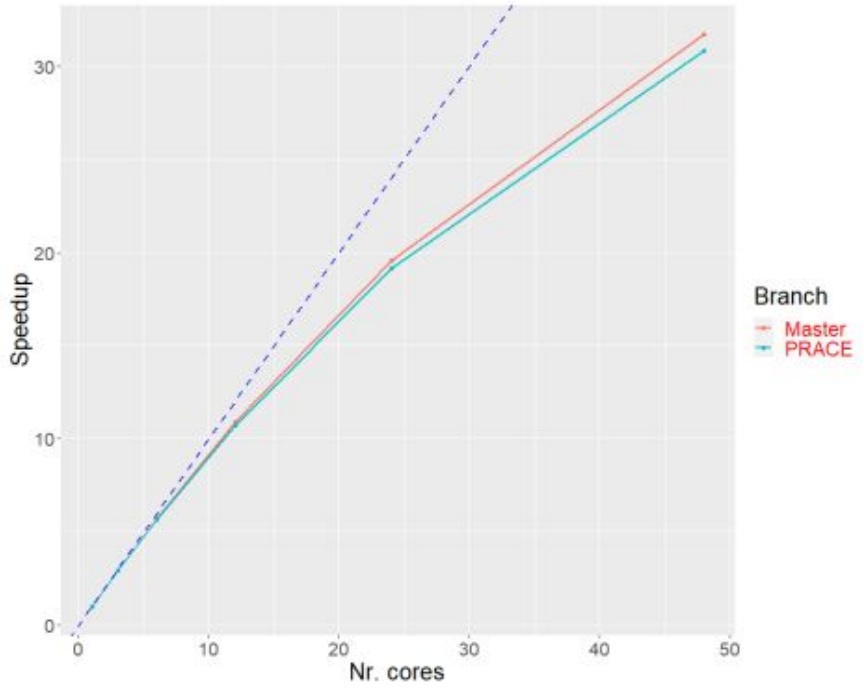
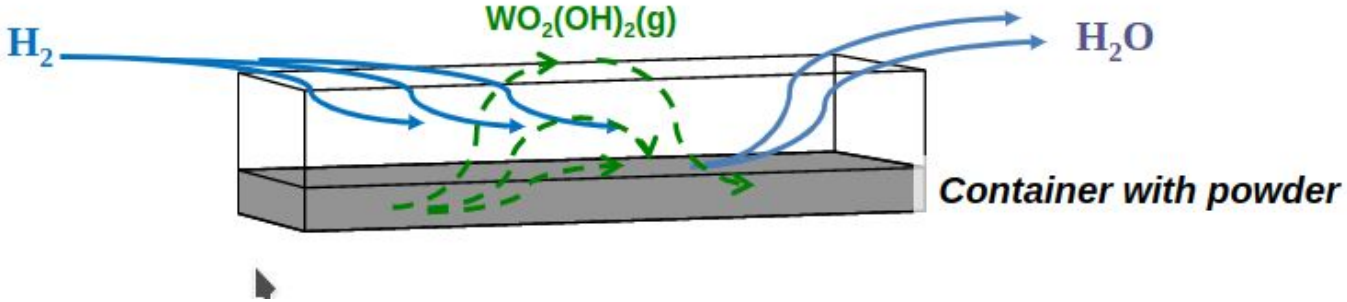


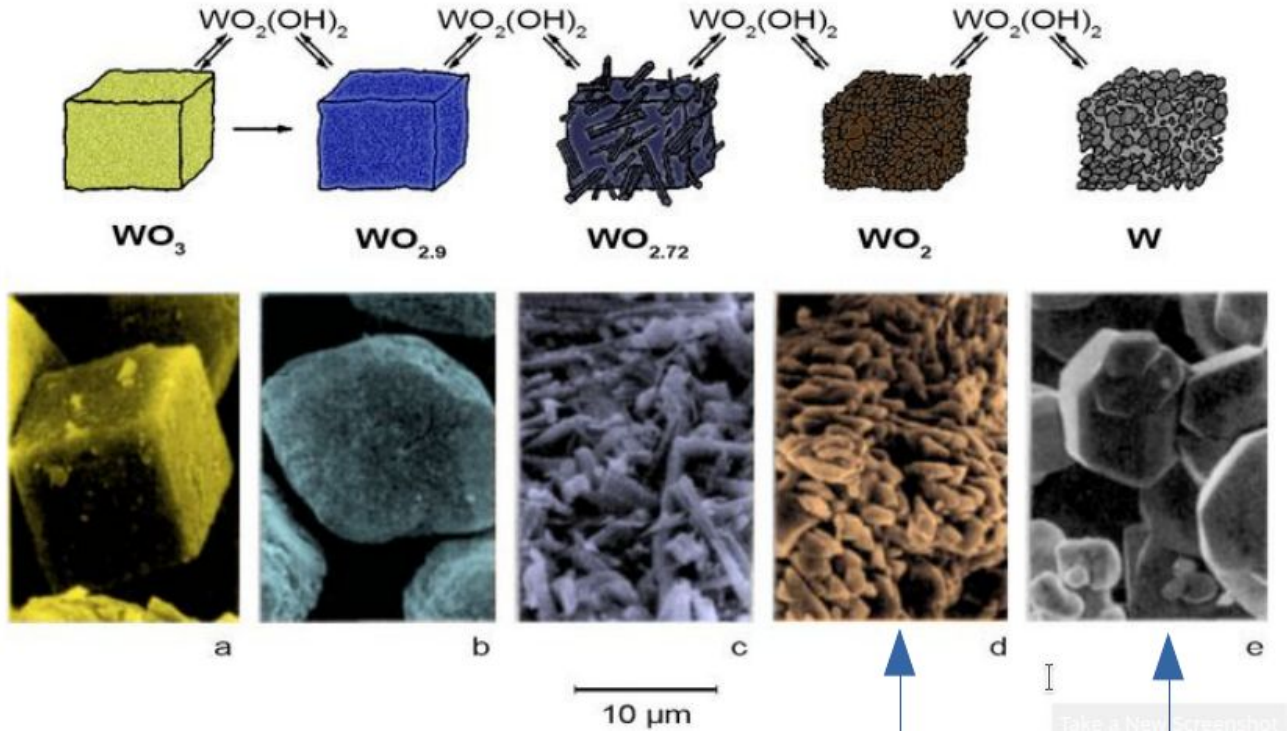
Figure 7. Speedup for the Conversion module as a function of the number of cores. Perfect scaling behaviour is shown with dashed-blue line.

SRC: Mainassara Chekaraou, A.W., *Large Scale Parallel Simulation For Extended Discrete Element Method*, Doctoral Thesis, 2020

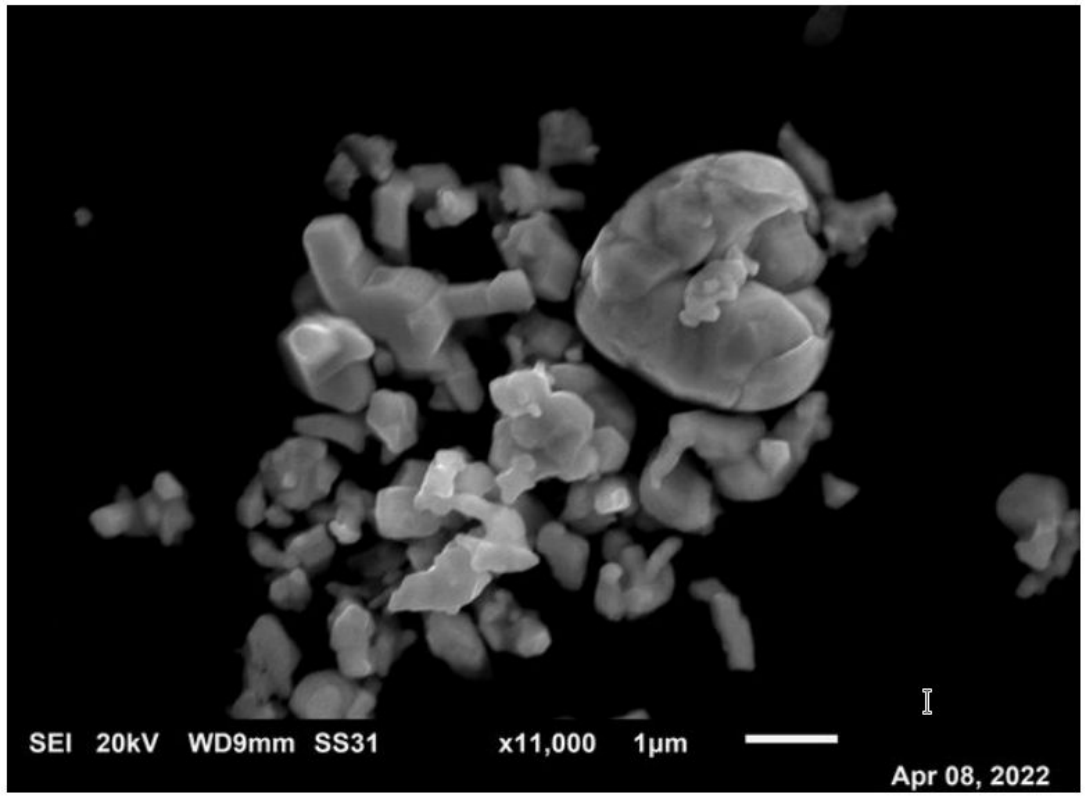
Rousset, A., *OpenMP optimisation of the eXtended Discrete Element Method (XDEM)*, Scientific Report, 2021

A grain growth proposed problem

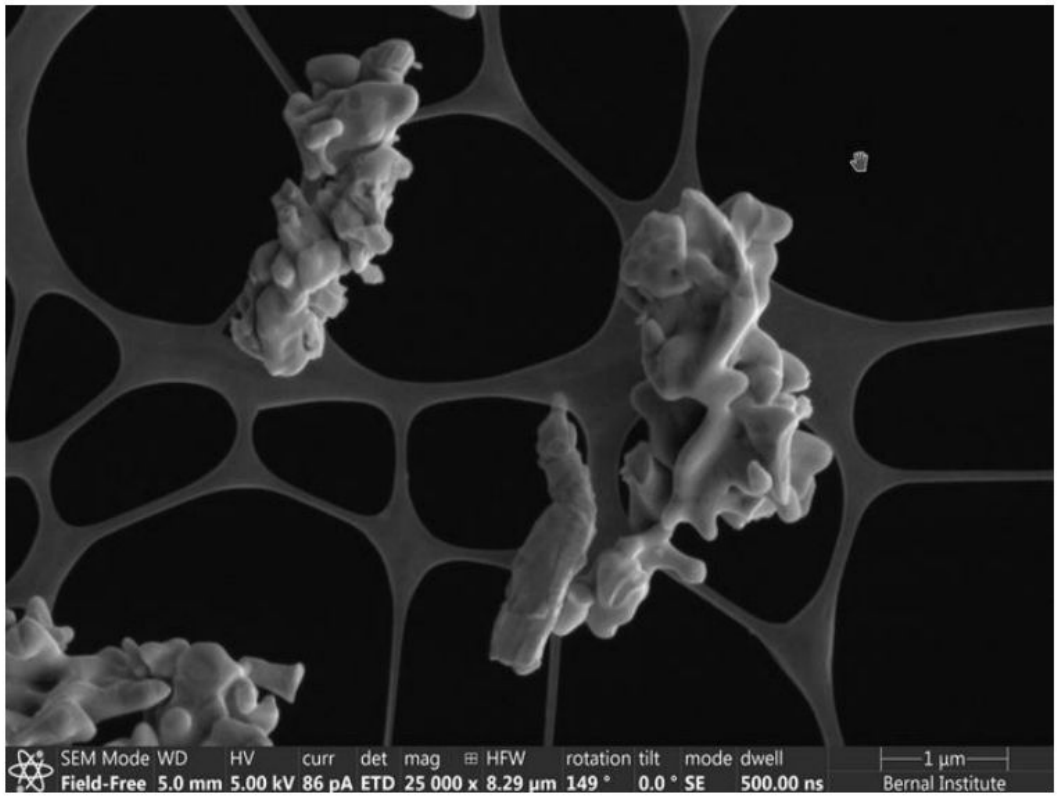




A grain growth proposed problem



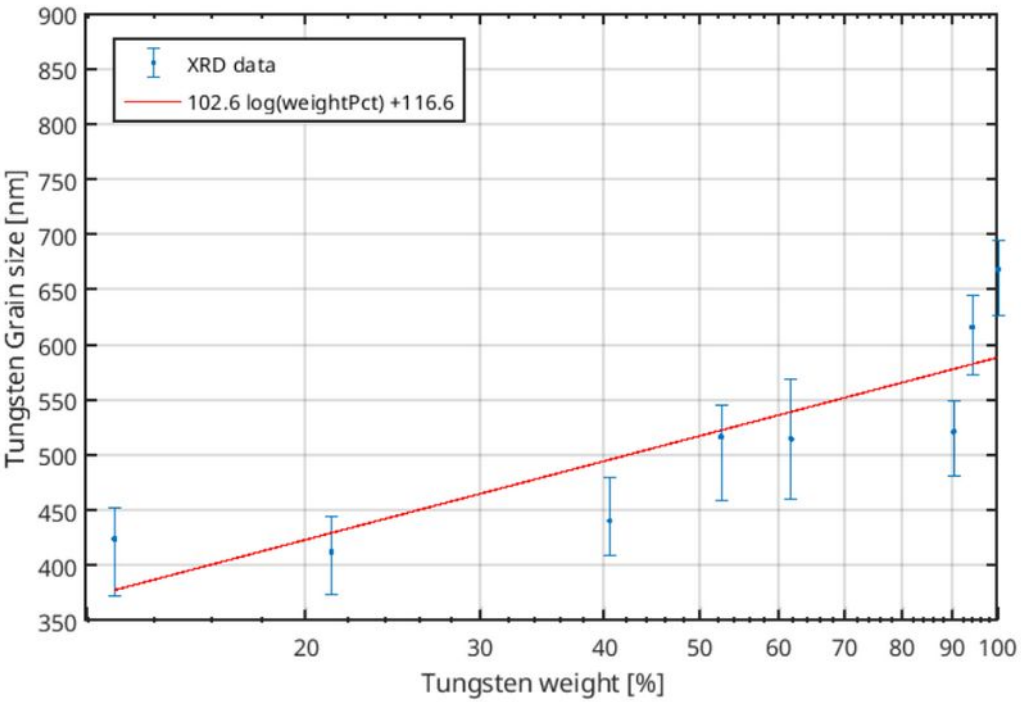
SEM image of WOx particles undergoing H2 reduction



TEM image of WOx particles undergoing H2 reduction

A grain growth proposed (optimization) problem

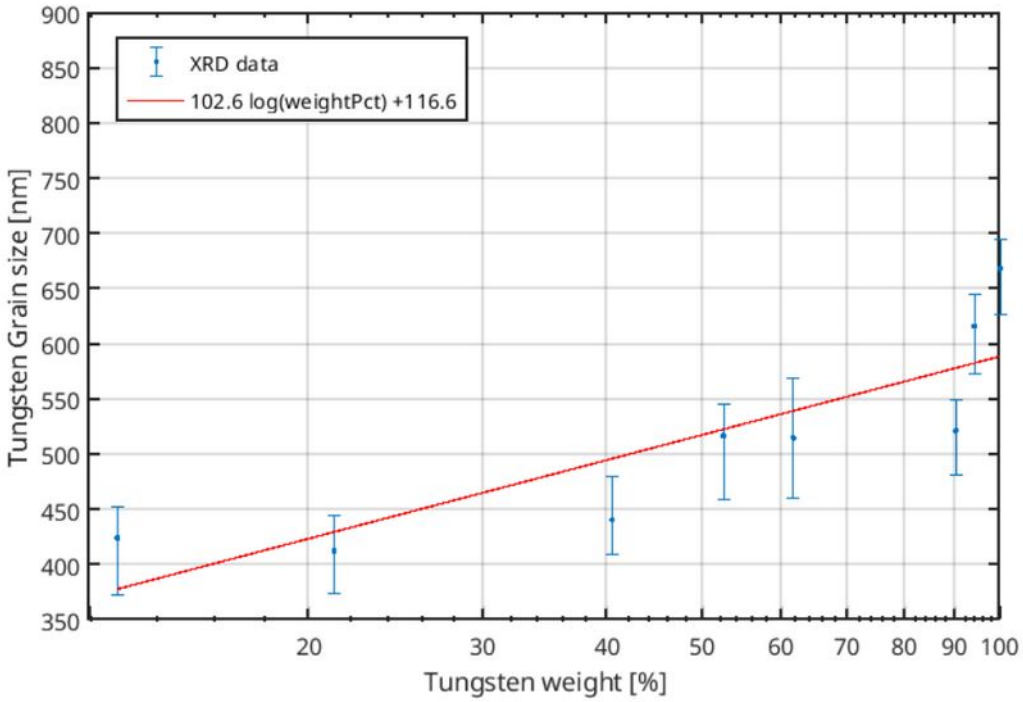
Objective Function



Synchrotron measurements: Volume reconstruction of Nano-holotomography.
Particle characteristic size L = 25 um. ESRF (Grenoble-Fr).

A grain growth proposed (optimization) problem

Objective Function



XDEM simulations

Vs

Nucleation + grain growth parameters


TO BE
CONTINUED...

Content

- Introduction
  - Granular materials
  - Reactions in heterogeneous particulate systems
  - Numerical representations of reacting particulate systems
    - Lumped, continuous and discrete modeling approaches
- Discrete Element Methods (DEM)
  - DEM motivation and history
  - Thermochemical DEM simulations
    - What simulation parameters are employed in thermochemical DEM simulations
    - A difference between large-scale and small-scale experimentation
- Finding kinetic parameters for heterogeneous reaction systems
  - A chemical optimization problem
  - A grain growth proposed problem
- **Takeaways**

Takeaways

- HPC has enabled an **accurate solution** of particulate systems undergoing physical/chemical transformations
- Different modeling approaches for particulate systems
- Extended discrete element methods are the closest numerical representation for particulate systems at "macro" scale
- In a real world, particulate matter interacts with a continuous medium. This interaction it is of pivotal interest and needs to be accounted for
- Warning: Reaction / diffusion parameters change with the dimension of the problem (except resolved methods)
- Synergy between computer-sc, phyms and engineering for a successful large-scale simulation. *"Zapatero a sus zapatos"*
- However, as a scientist, a good knowledge of both worlds is imperative for achieving meaningful results

Thank you!

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- For a virtual tour:
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Determination of Reaction Rate Parameters in Heterogeneous Particulate Systems

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