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H2020 NanoDome Project: A Multiscale Approach to Gas Phase Nanoparticle Synthesis

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# NANODOME H2020 PROJECT: NANOMATERIALS VIA GAS PHASE SYNTHESIS

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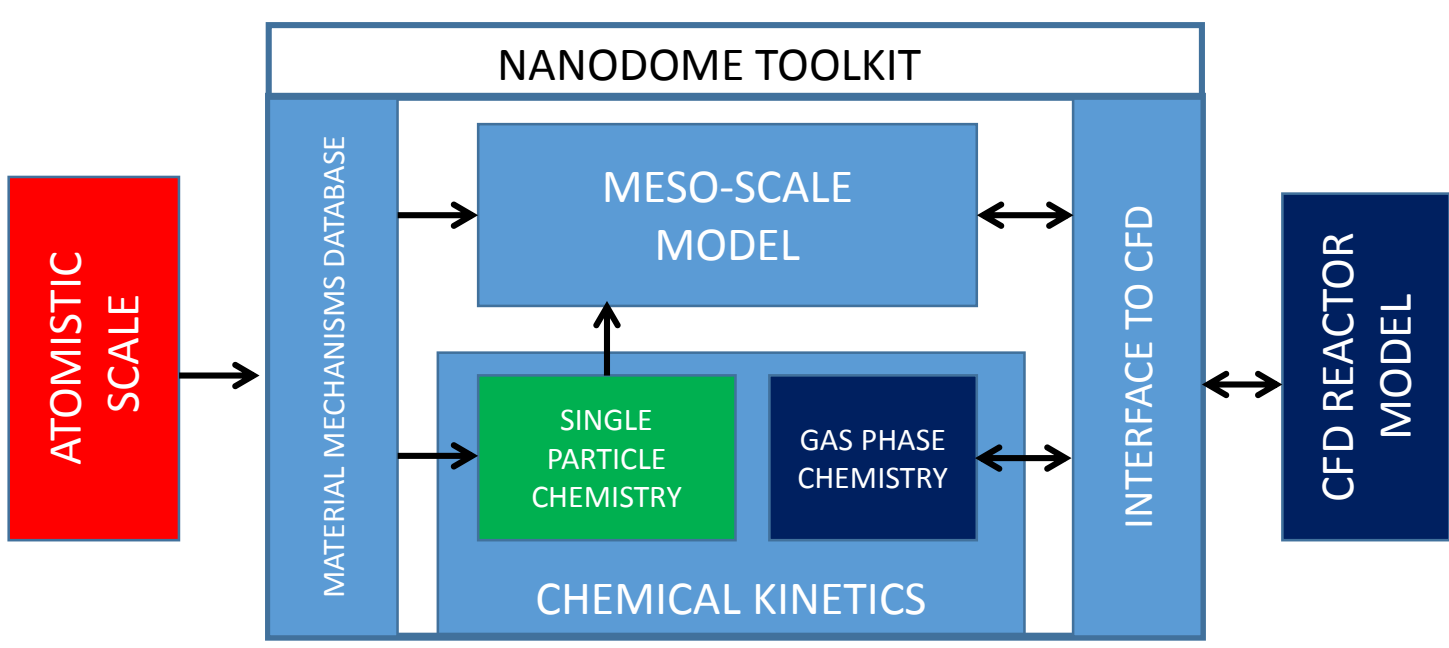
## ★ THE PROJECT

**THE MAIN OBJECTIVE**  
The main objective of the **H2020 NanoDome** project is to develop a **robust model-based design and engineering toolkit** for the detailed prediction of **complex nanomaterial structures** to:

- improve the control of the nanomaterial production and the **industrially-scalable gas phase synthesis processes** for more accurate final product properties.
- provide potential end-users (e.g. nanomaterial producers, research lab) with a **validated modeling tool** based on scientific principles that enables predictive design of novel gas phase production routes and novel nanomaterials thereby shortening their development process.

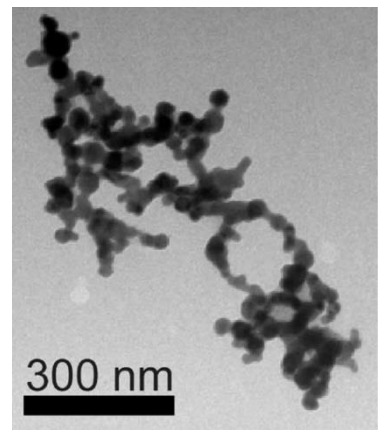
### KEY OBJECTIVES

- Formulation of a full **physical-mathematical model** for the description at mesoscale of the nanoparticle evolution.
- Extend existing mesoscopic nanomaterial synthesis modelling approaches (Lagrangian and stochastic) in a single discrete mesoscopic model and **integrate it with continuum reactor models** to provide a fully integrated model suite.
- Predict the detailed description of **nanoparticle composition** and internal **structure**.
- Provide **validation** means for the model from the research and industrial partners.
- Build a robust framework to ensure sustainability, commercialization and exploitation of the modelling, design and analysis toolkit.

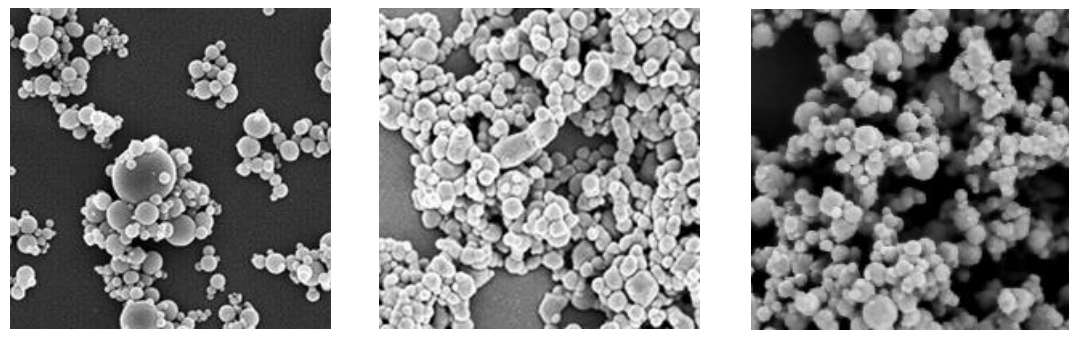


## ★ NANOPARTICLE SYNTHESIS PROCESSES

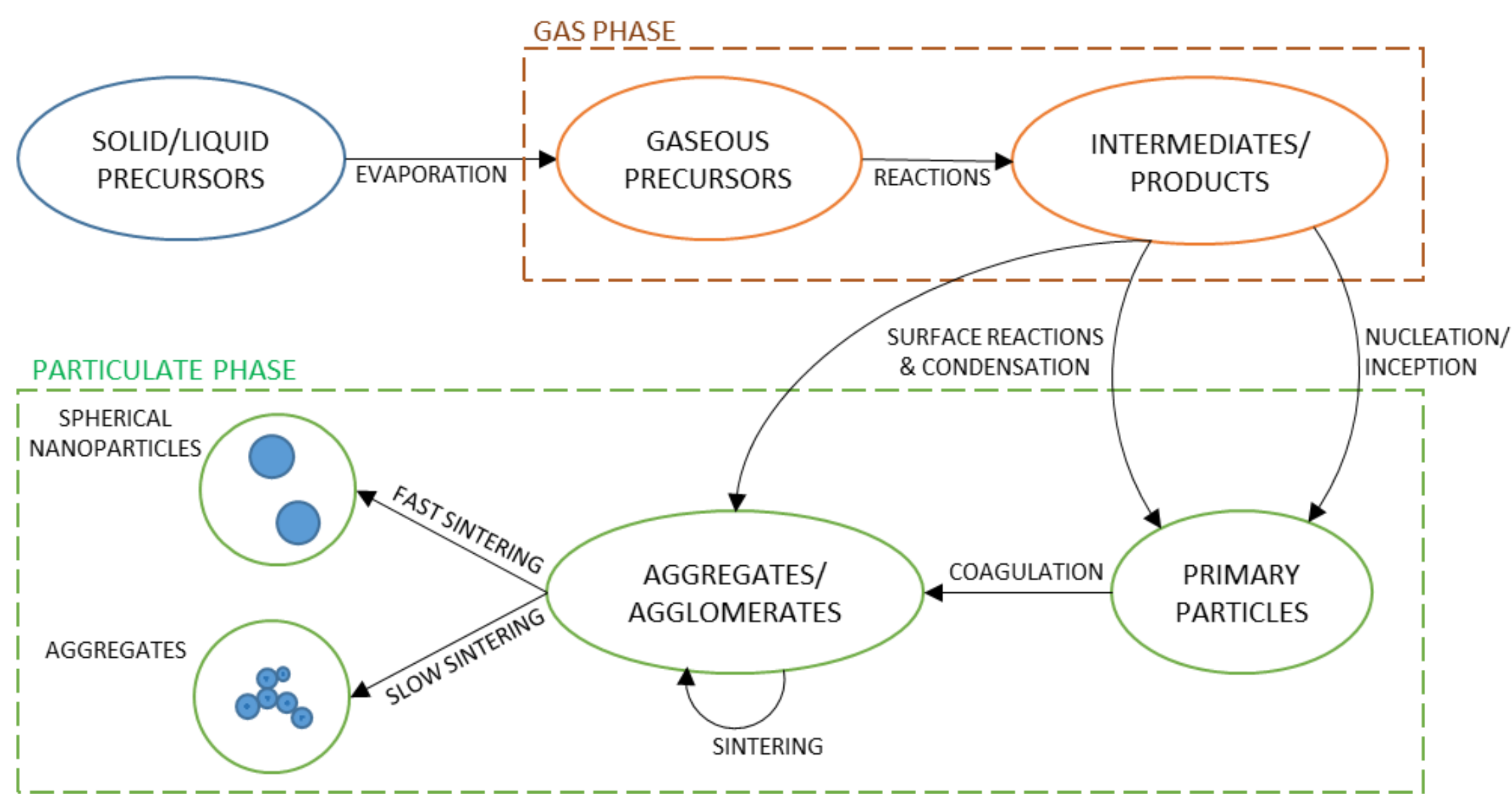
- The **NanoDome** model framework is designed for a generic **Gas Phase Condensation** synthesis process, to increase its usability in several existing commercial processes.
- NanoDome** project focuses on:
  - Plasma Synthesis Reactors**
  - Flame Combustion Processes**
  - Hot-Wall Reactors**



Bismuth nanoparticles by vapor condensation  
(K. Wegner et al., Chem. Eng. Sci. 57 (2002) 1753–1762)



Si, Ni and Cu nanoparticles by plasma synthesis  
(source Tekna Plasma Systems, [www.tekna.com](http://www.tekna.com))

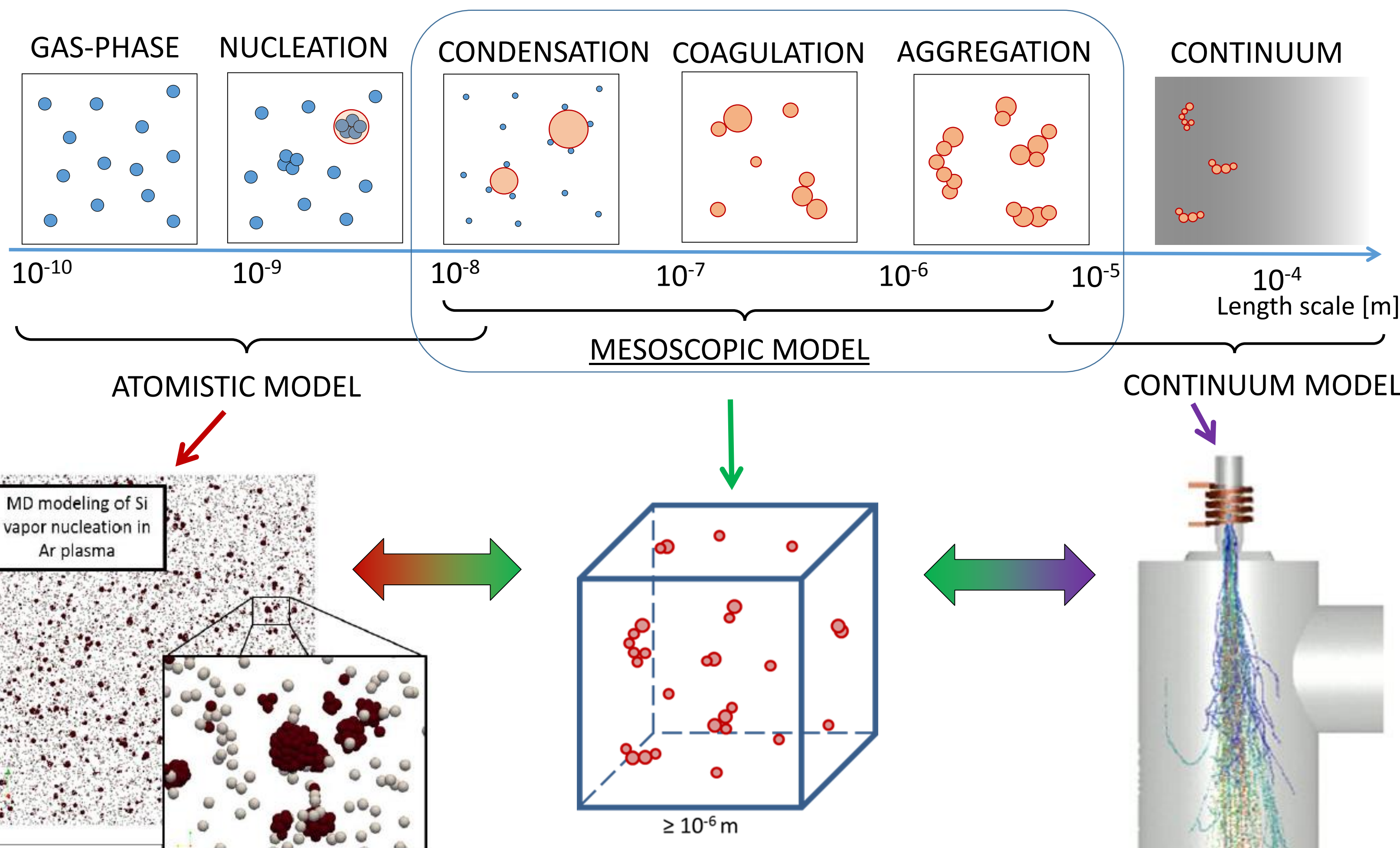


## ★ MULTISCALE APPROACH

The mesoscopic model is expected to describe the lifecycle of the **nanoparticles ensemble**, which ranges over a time up to **10 ms** inside a control volume of **1-10 µm** of side length, bridging the gap between the atomic and the continuum parts of the reactor model.

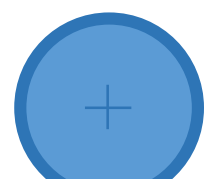
The mesoscopic model predicts **homogeneous and heterogeneous nucleation, coagulation, aggregation and morphology** of nanoparticles.

The mesoscopic model takes into account also the **composition and chemical kinetics** of each nanoparticle.



## ★ THE MESOSCOPIC MODEL CONCEPTS

### PARTICLE



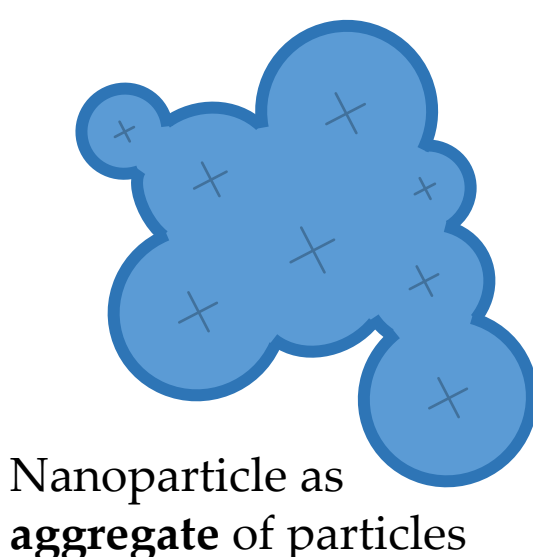
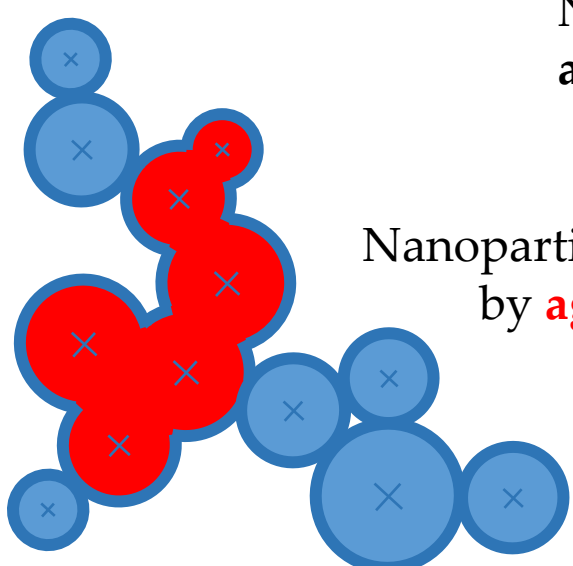
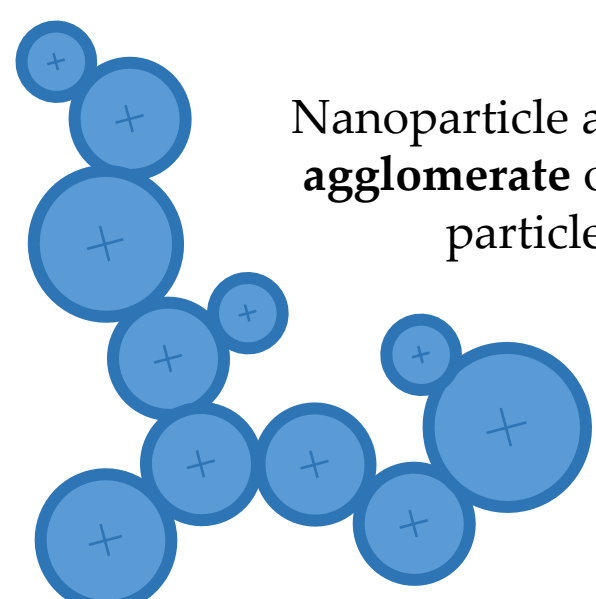
- Basic discrete physical object of the mesoscopic model
- Defined as the **minimum stable cluster** of molecules (i.e. primary particle)
- Particles are assumed to be of **spherical shape**
- Particles grow in size by **homogeneous condensation and coalescence**

### NANOPARTICLE

A nanoparticle is a **collection of particles** connected together by:

- weak bonds** (agglomerate)
- hard bonds**, due sintering (agglomerate)

Nanoparticle motion is described by **Langevin dynamics**



### GAS PHASE

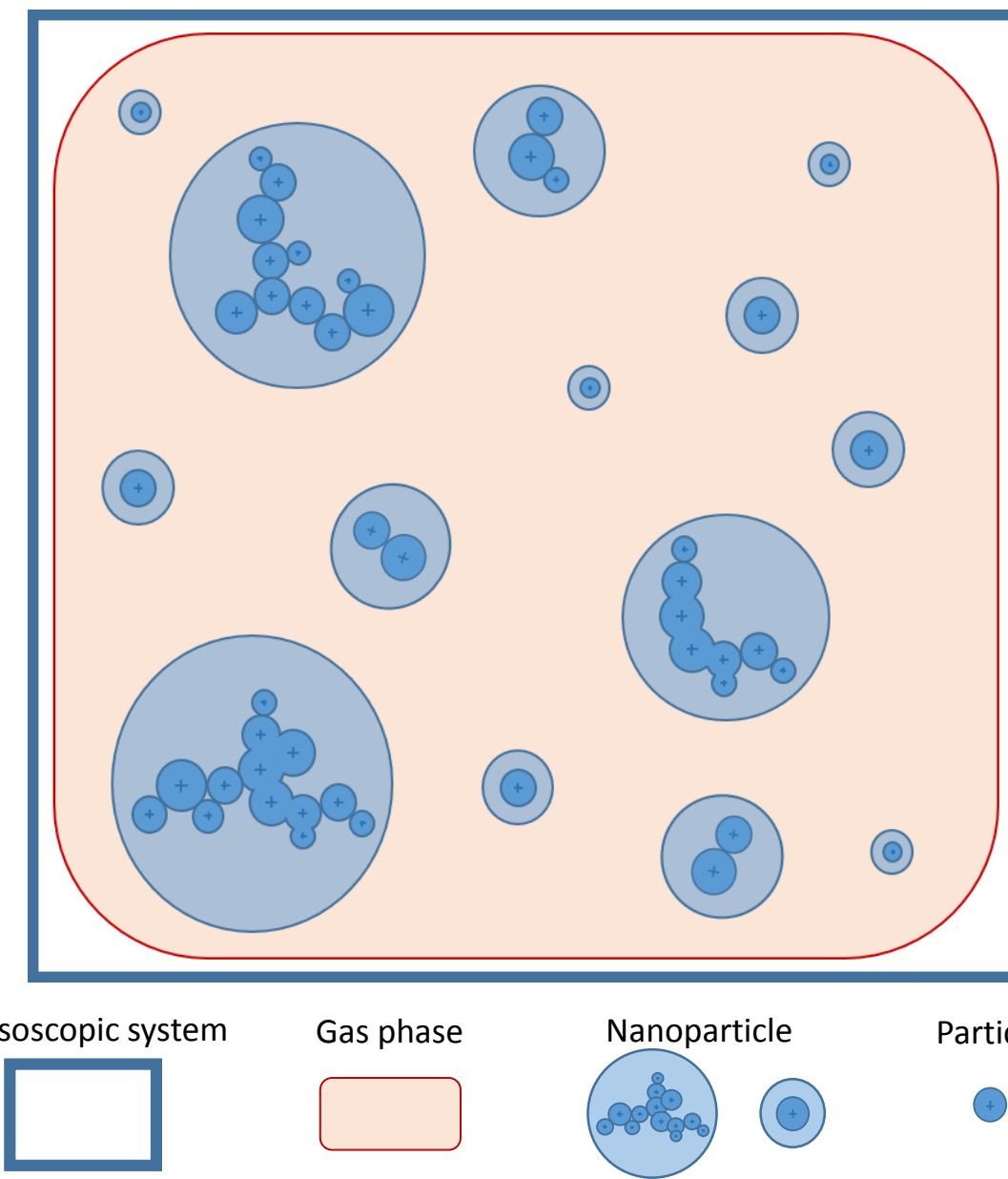
Gas phase is composed by all atoms and **molecules below the mesoscopic model scale**.

The gas phase state is defined by:

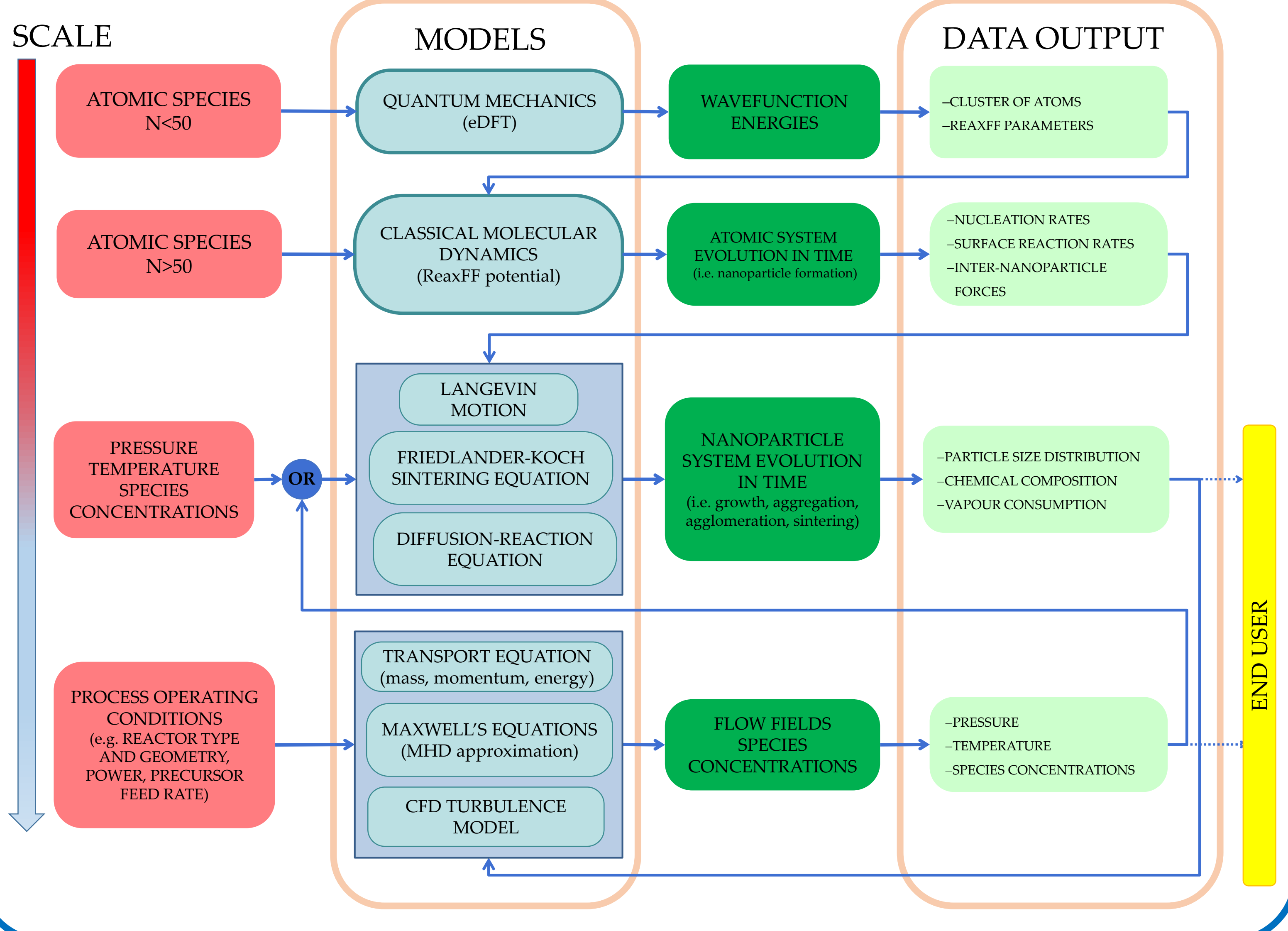
- pressure
- temperature
- species concentration

The gas phase state can be defined by **user** (XML based time dependent data), by a **coupled continuum reactor model** (linking library) or treated as a **self consistent 0D reactor**.

**Chemical kinetics** of particles precursors is included in the model



## ★ MULTISCALE APPROACH FLOWCHART

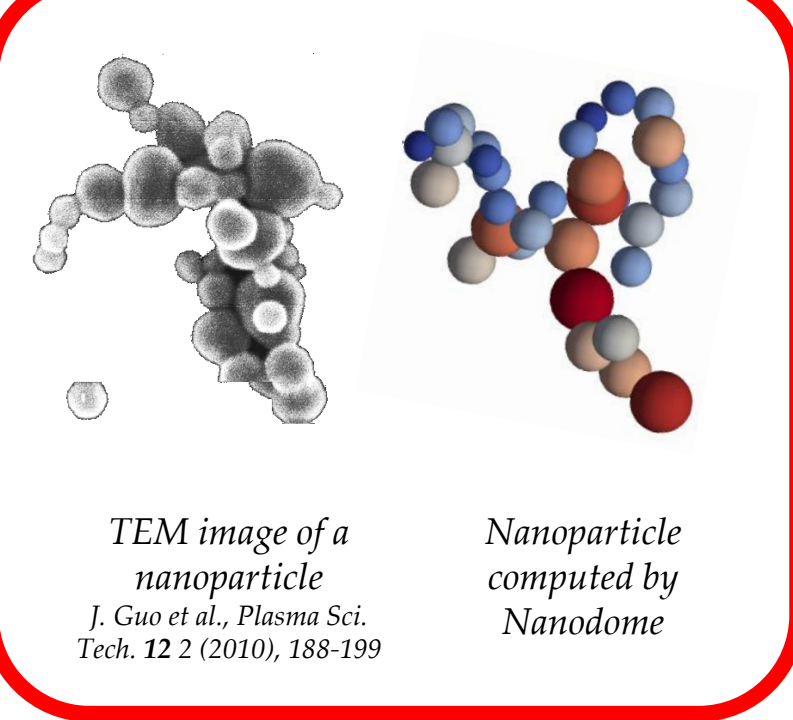


## ★ THE SOFTWARE

- The objective is to provide a **functional, flexible and open source software library**, integrable with third party applications focused on the **design of nanomaterials**.
- Object Oriented Design (OO)**.
- Implemented in C++**.

Collects Material Mechanism Data (e.g. Nucleation Rate, Interparticle Interactions, etc...) from atomistic scale simulations, computed by the state-of-the-art QM or MD suites (Quantum Espresso, LAMPS, etc.).

Nanoparticles dynamics computed with Lagrangian and stochastic algorithms.



TEM image of a nanoparticle  
J. Guo et al., Plasma Sci. Tech. 12 2 (2010), 188–199

Linking/coupling with CFD simulation environments (ANSYS FLUENT™, OpenFOAM).

The NanoDome software can cooperate with chemical kinetics softwares (like KINETICS™ by CMCL).



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