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

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(Article begins on next page)

NANODOME H2020 PROJECT: NANOMATERIALS VIA GAS PHASE SYNTHESIS

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COMPUTATIONAL MODELLING CAMBRIDGE LIMITED (UK), UNIVERSITY OF CAMBRIDGE (UK)
CONSIGLIO NAZIONALE DELLE RICERCHE (Italy)



★ THE PROJECT

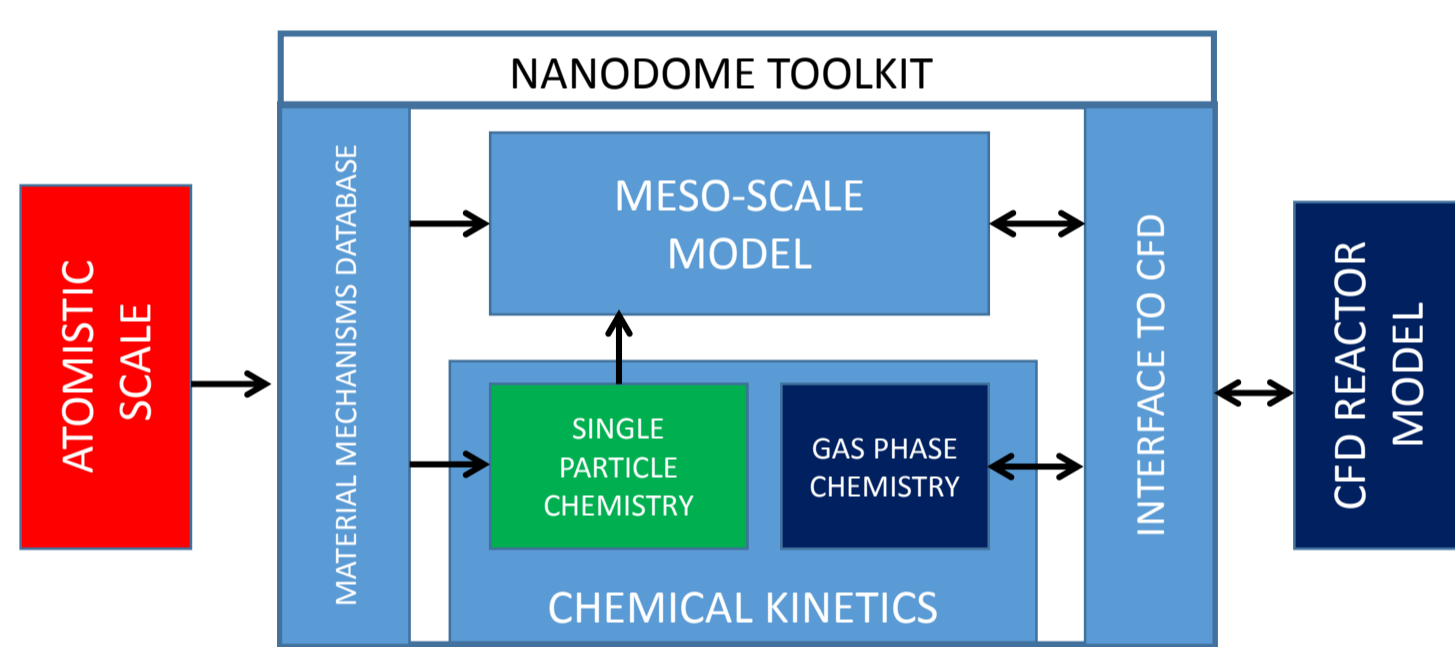
THE MAIN OBJECTIVE

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.

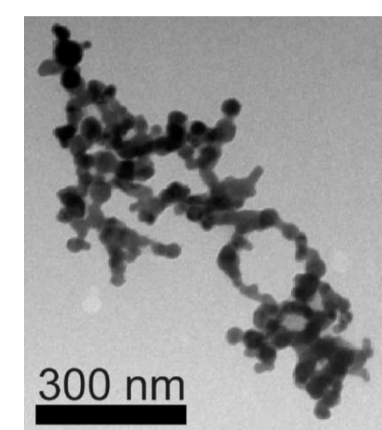
KEY OBJECTIVES

- 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.

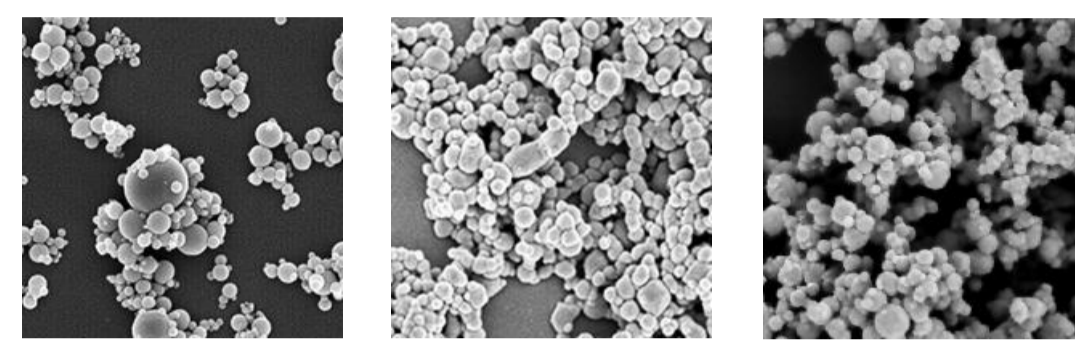


★ NANOPARTICLE SYNTHESIS PROCESSES

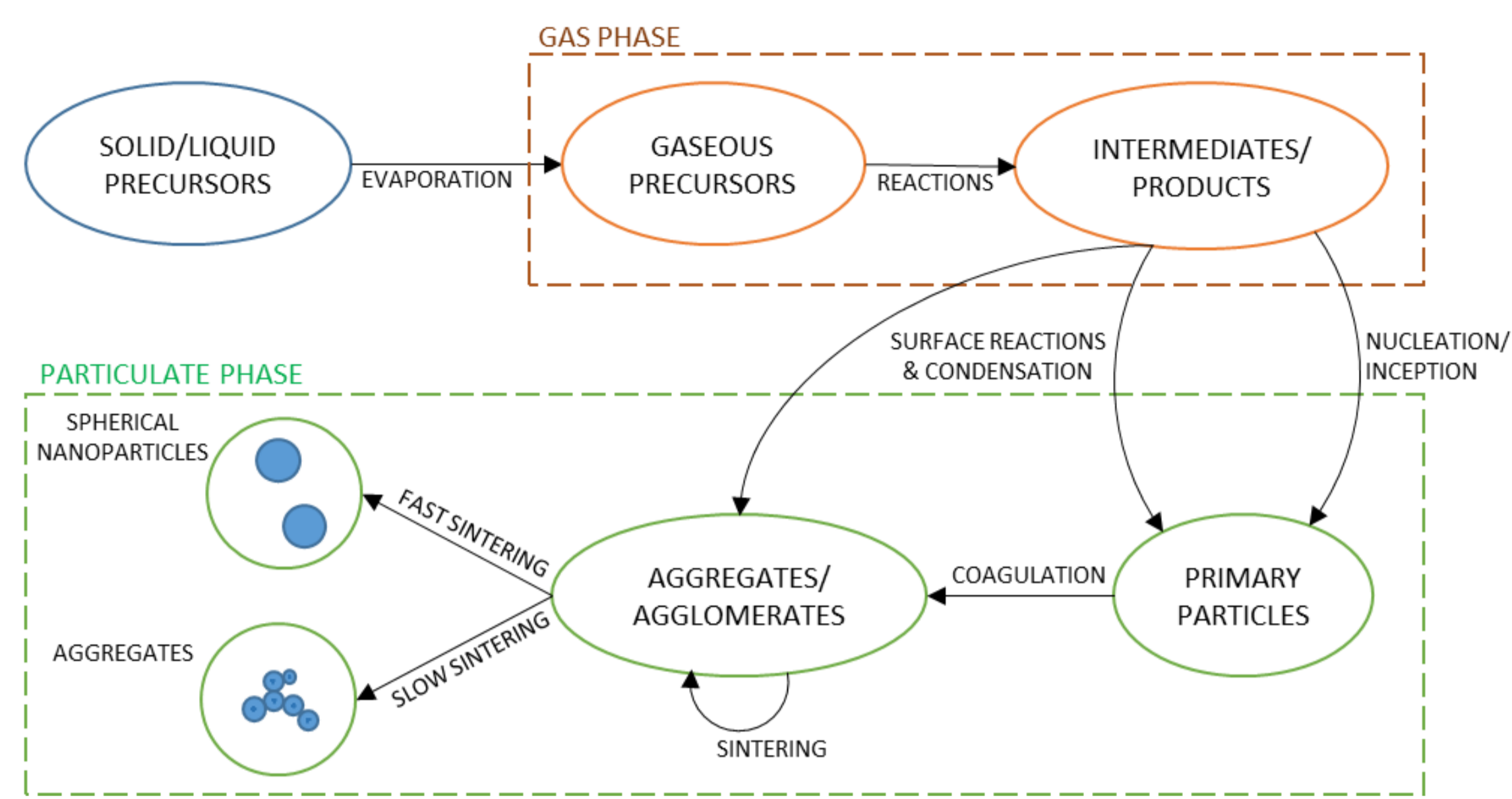
- The NanoDome model framework is designed for a generic **Gas Phase Condensation** synthesis process, to increase its usability in several existing commercial processes.
- NanoDome project focuses on:
 - Plasma Synthesis Reactors
 - Flame Combustion Processes
 - Hot-Wall Reactors



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)

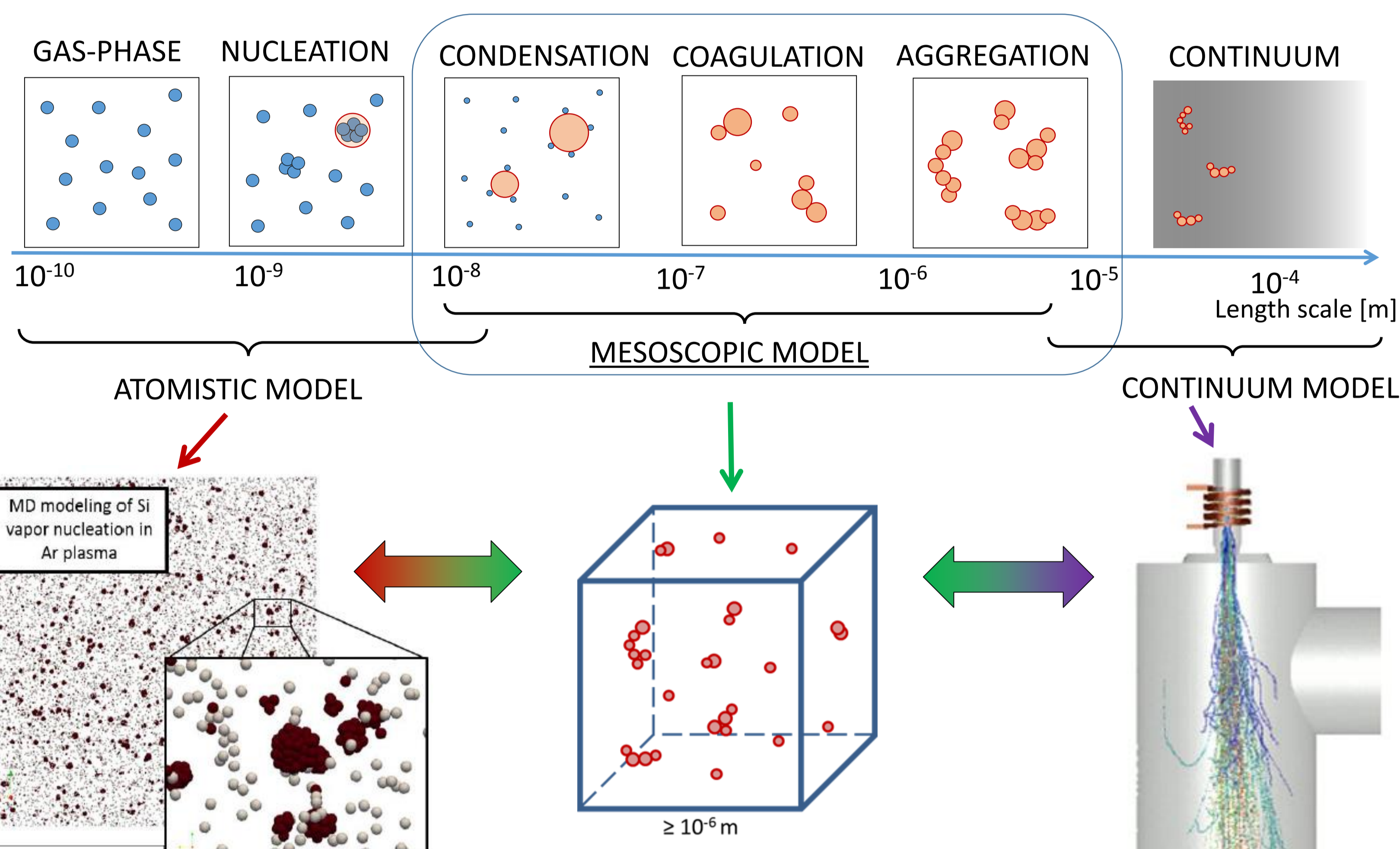


☐ MULTISCALE APPROACH

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.

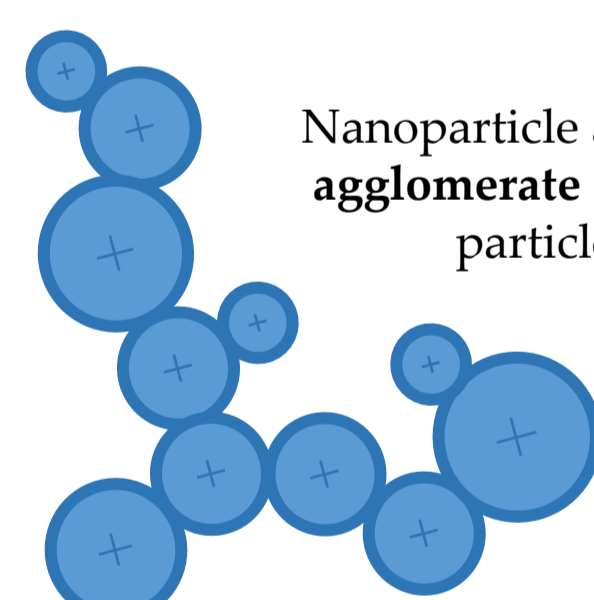
The mesoscopic model takes into account also the **composition and chemical kinetics** of each nanoparticle.



∫ f(x)dx 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**

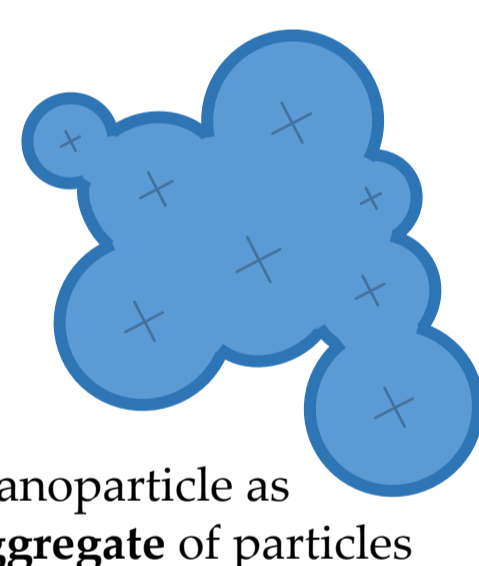
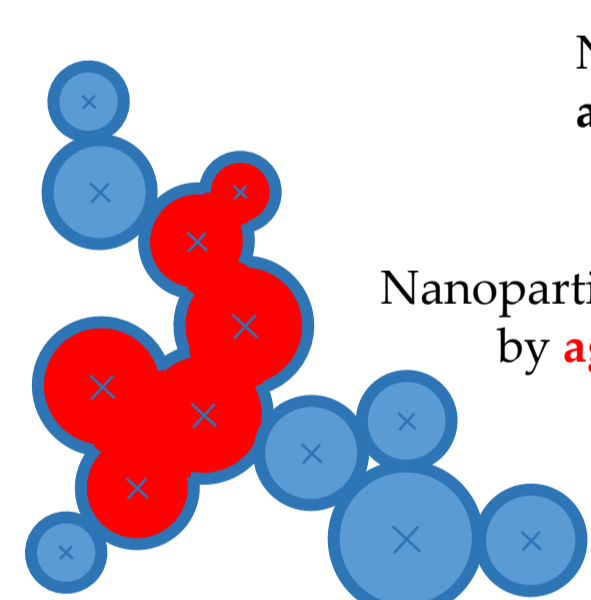


NANOPARTICLE

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

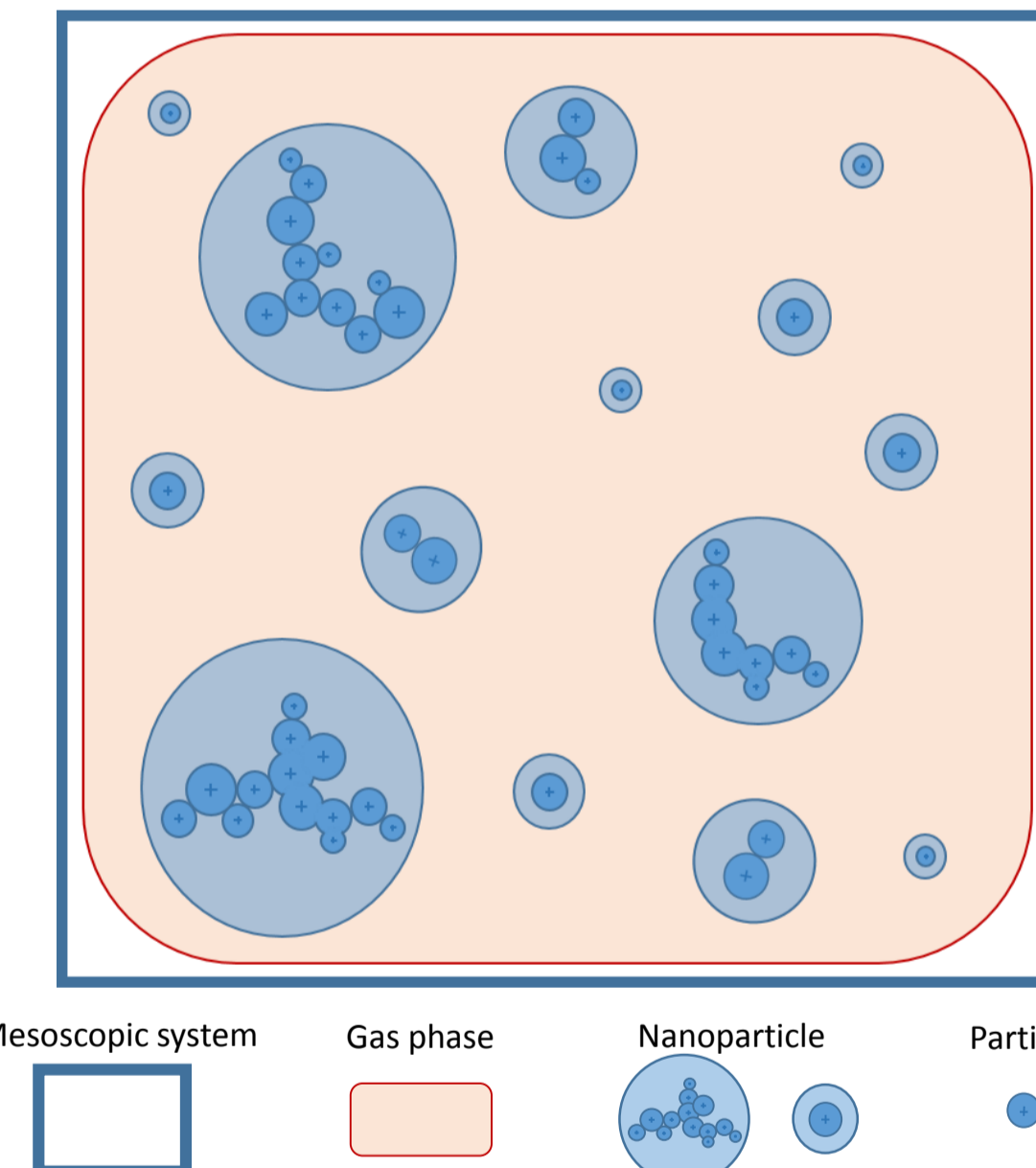
Gas phase is composed by all atoms and molecules **below the mesoscopic model scale**.

The gas phase state is defined by:

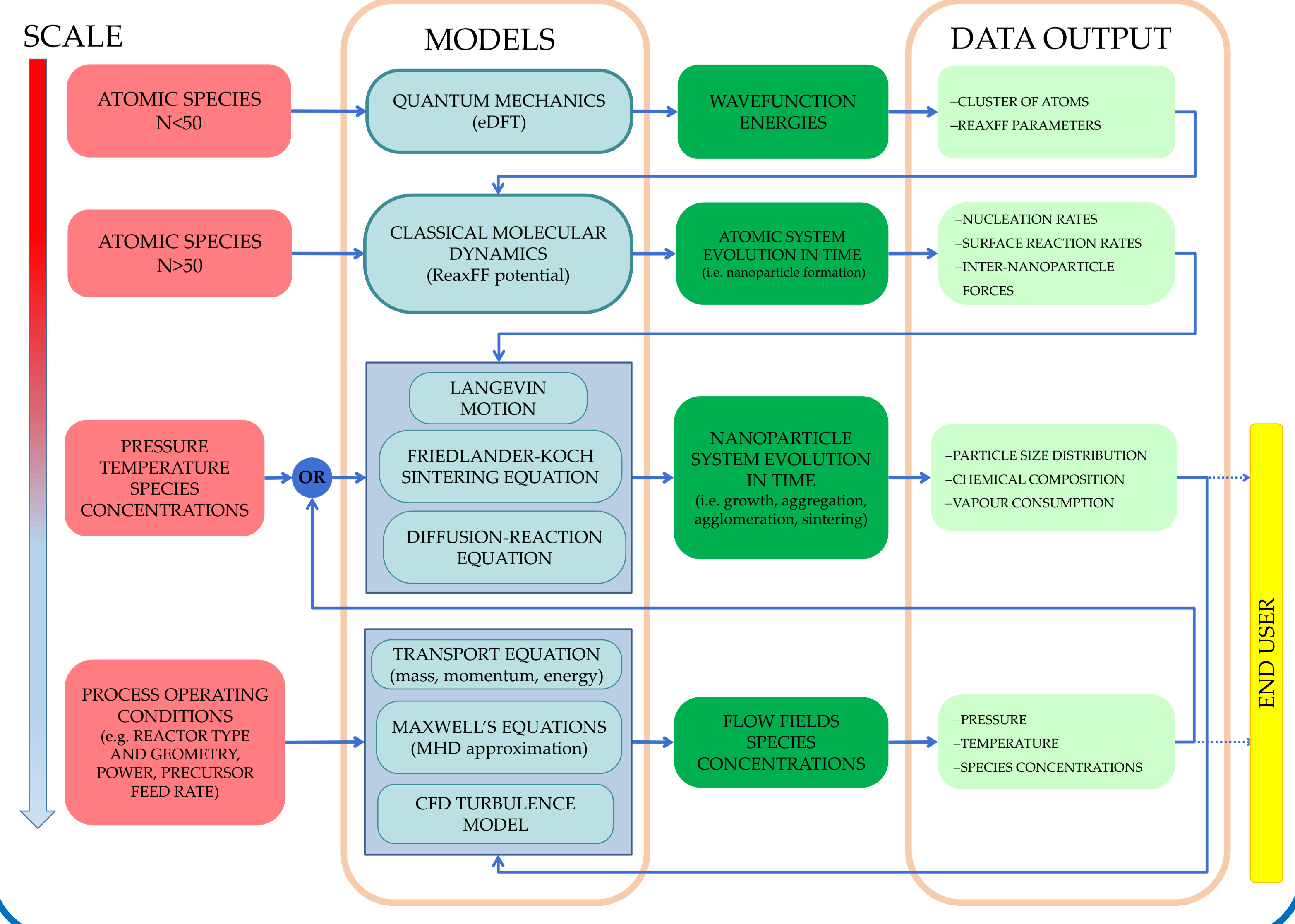
- pressure
- temperature
- species concentration

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.

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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