



ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

ARCHIVIO ISTITUZIONALE DELLA RICERCA

Alma Mater Studiorum Università di Bologna Archivio istituzionale della ricerca

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

This is the submitted version (pre peer-review, preprint) of the following publication:

Published Version:

Availability:

This version is available at: <https://hdl.handle.net/11585/600251> since: 2019-04-26

Published:

DOI: <http://doi.org/>

Terms of use:

Some rights reserved. The terms and conditions for the reuse of this version of the manuscript are specified in the publishing policy. For all terms of use and more information see the publisher's website.

This item was downloaded from IRIS Università di Bologna (<https://cris.unibo.it/>).
When citing, please refer to the published version.

(Article begins on next page)

NANODOME H2020 PROJECT: NANOMATERIALS VIA GAS PHASE SYNTHESIS

UNIVERSITY OF BOLOGNA (Italy), UMICORE NV (BE), UNIVERSITÄT DUISBURG-ESSEN (DE)
COMPUTATIONAL MODELLING CAMBRIDGE LIMITED (UK), UNIVERSITY OF CAMBRIDGE (UK)
CONSIGLIO NAZIONALE DELLE RICERCHE (Italy)



★ THE PROJECT

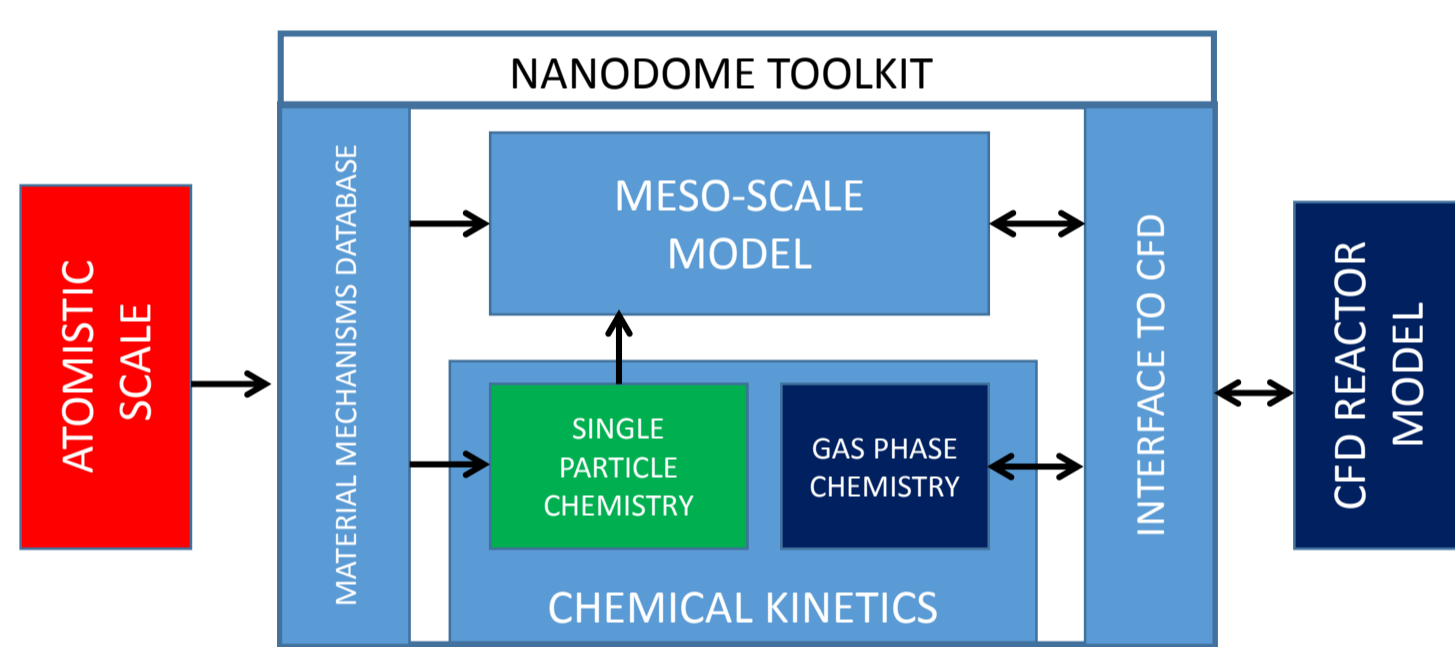
THE MAIN OBJECTIVE

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.

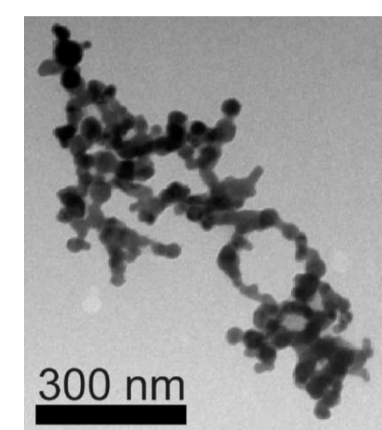
KEY OBJECTIVES

- 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.

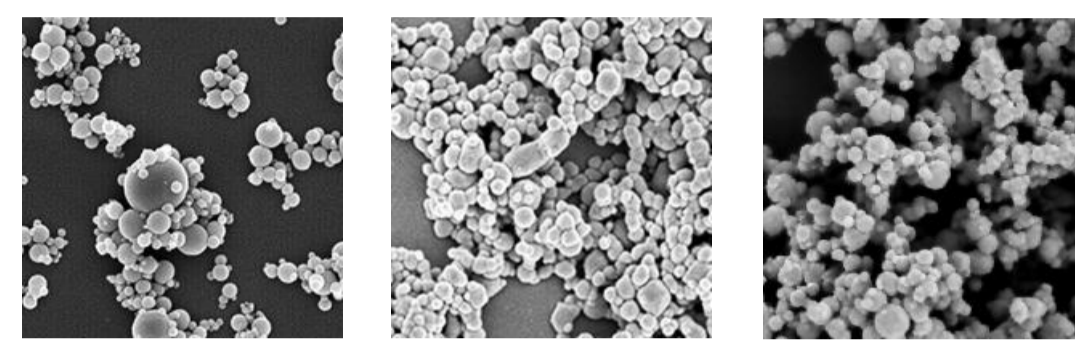


★ NANOPARTICLE SYNTHESIS PROCESSES

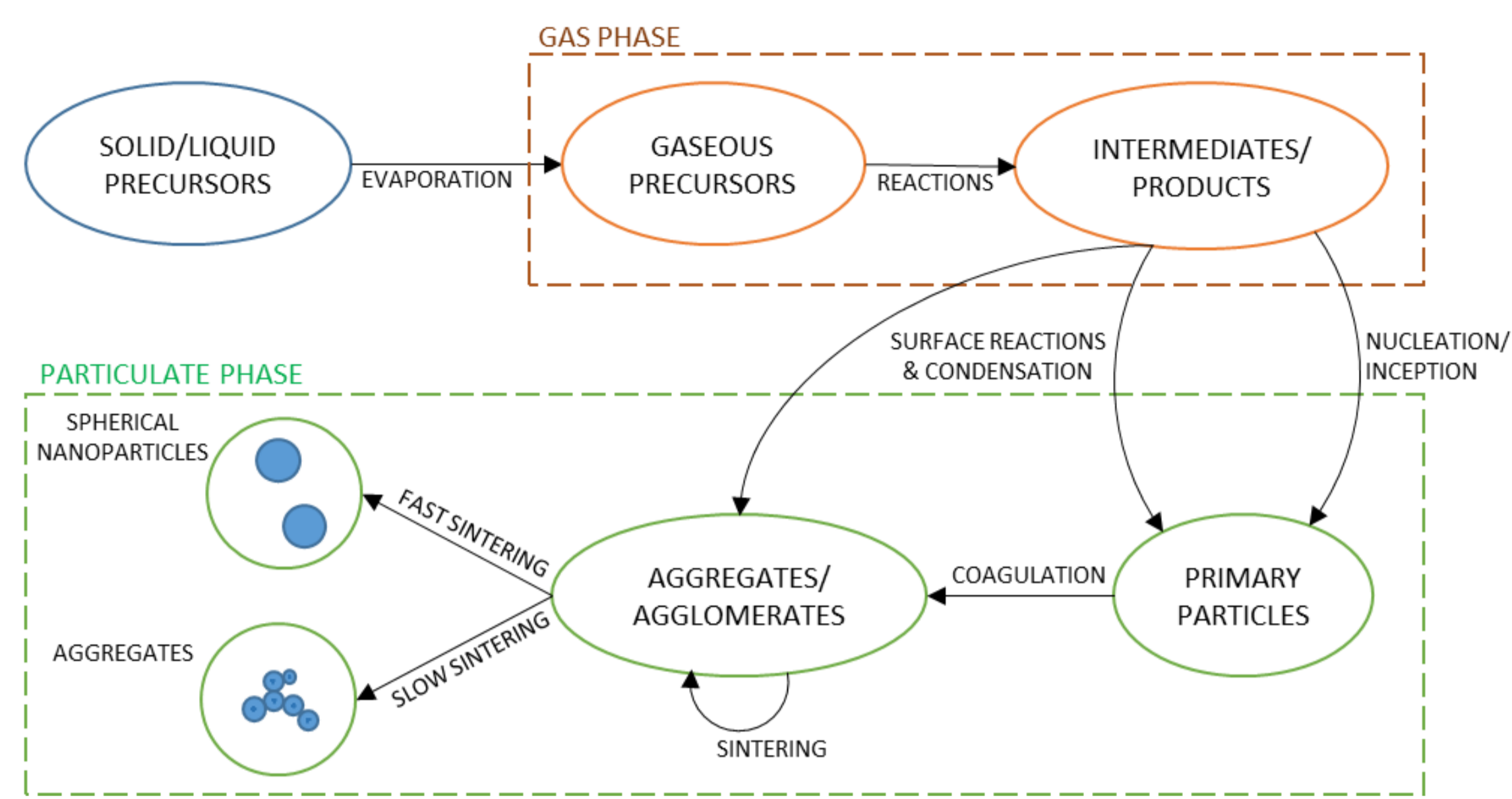
- The NanoDome model framework is designed for a generic **Gas Phase Condensation** synthesis process, to increase its usability in several existing commercial processes.
- NanoDome project focuses on:
 - Plasma Synthesis Reactors
 - Flame Combustion Processes
 - Hot-Wall Reactors



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)

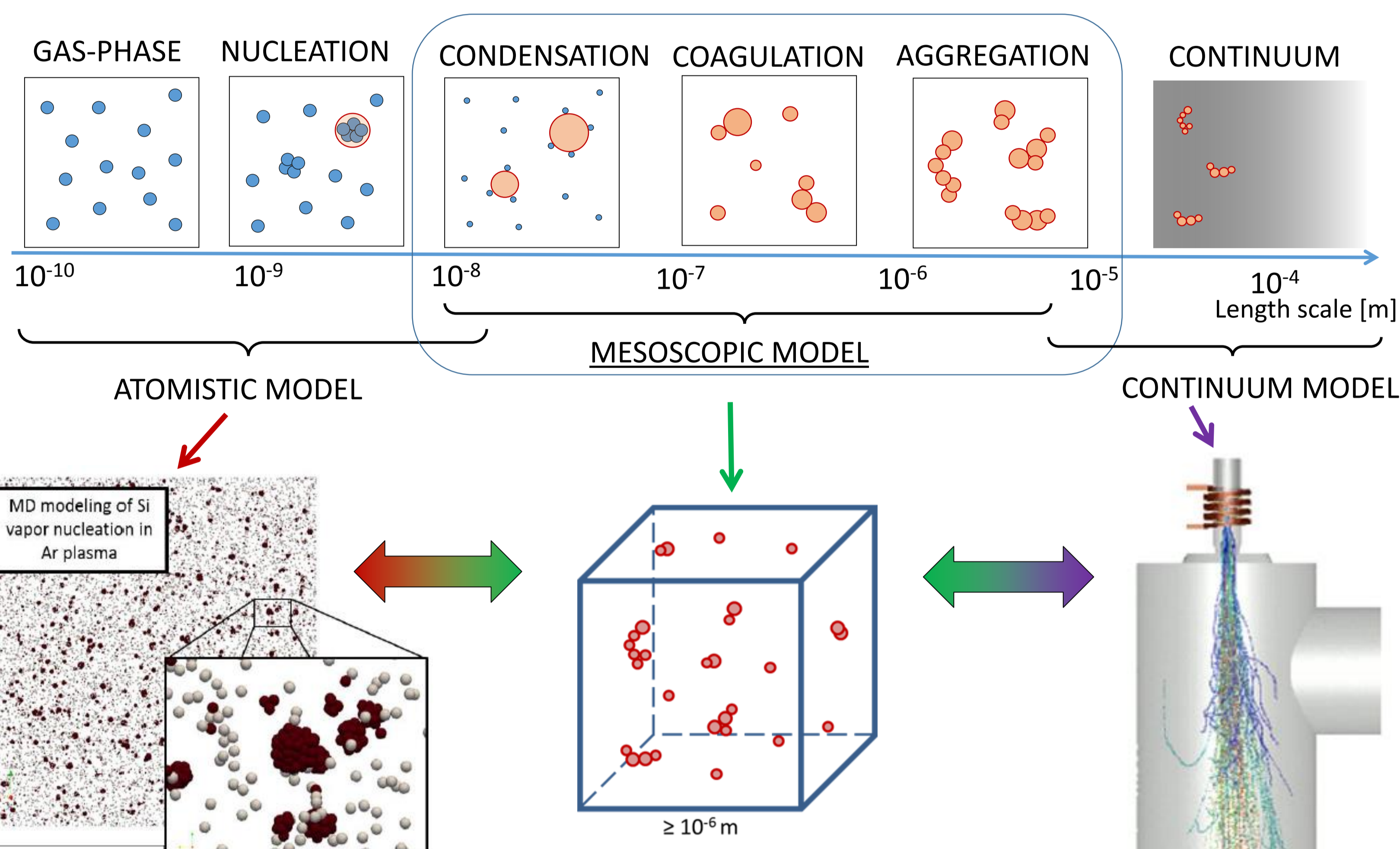


☐ MULTISCALE APPROACH

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.

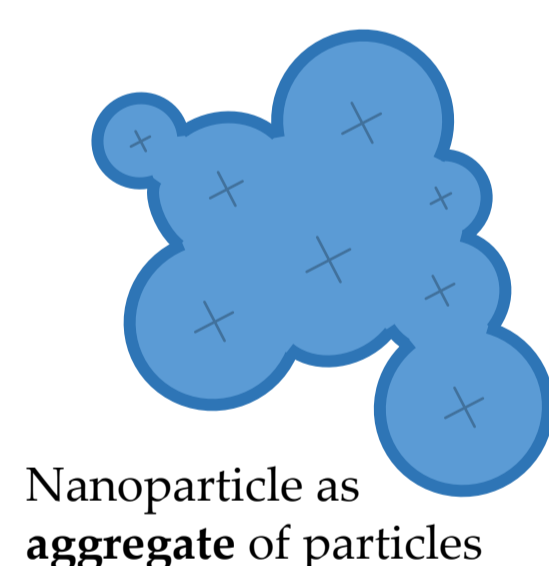
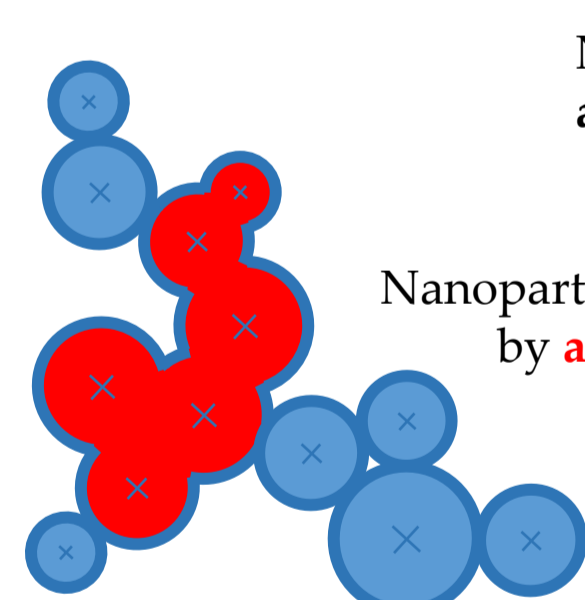
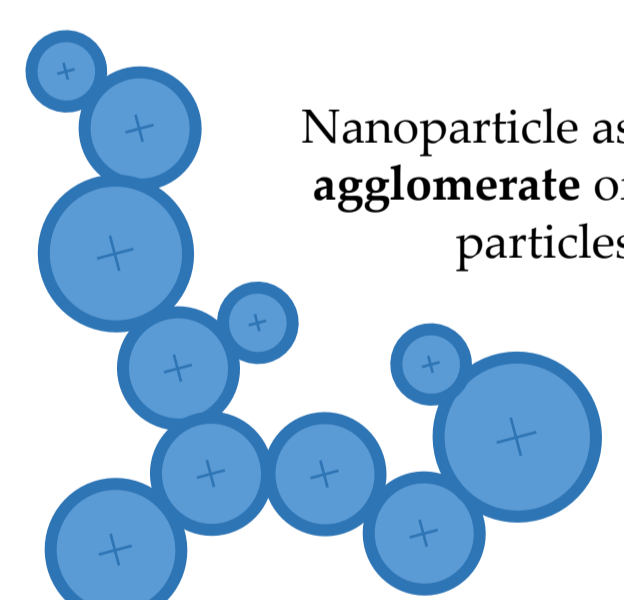


∫ f(x)dx THE MESOSCOPIC MODEL CONCEPTS

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**



Nanoparticle composed by aggregates and agglomerates

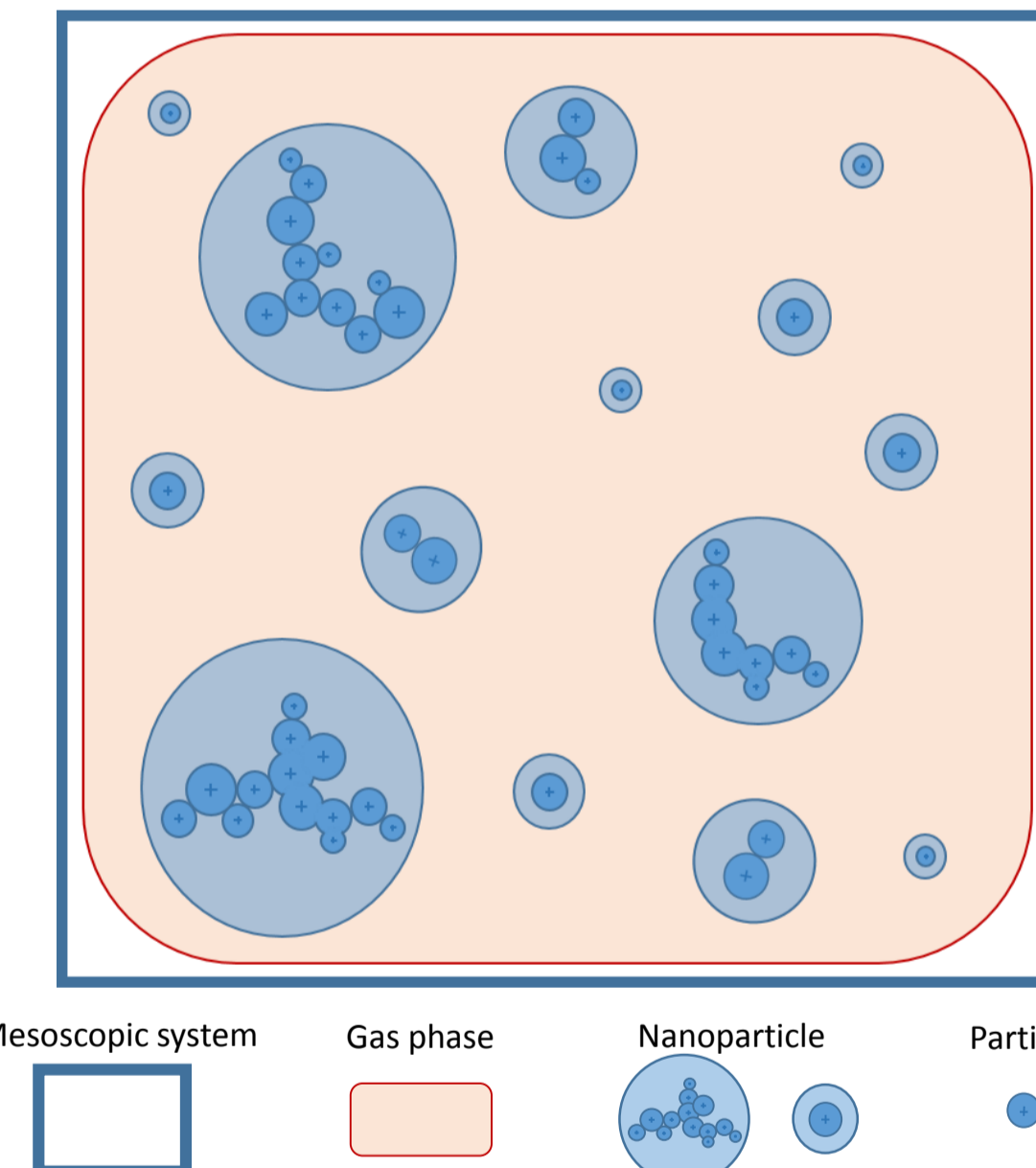
GAS PHASE

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

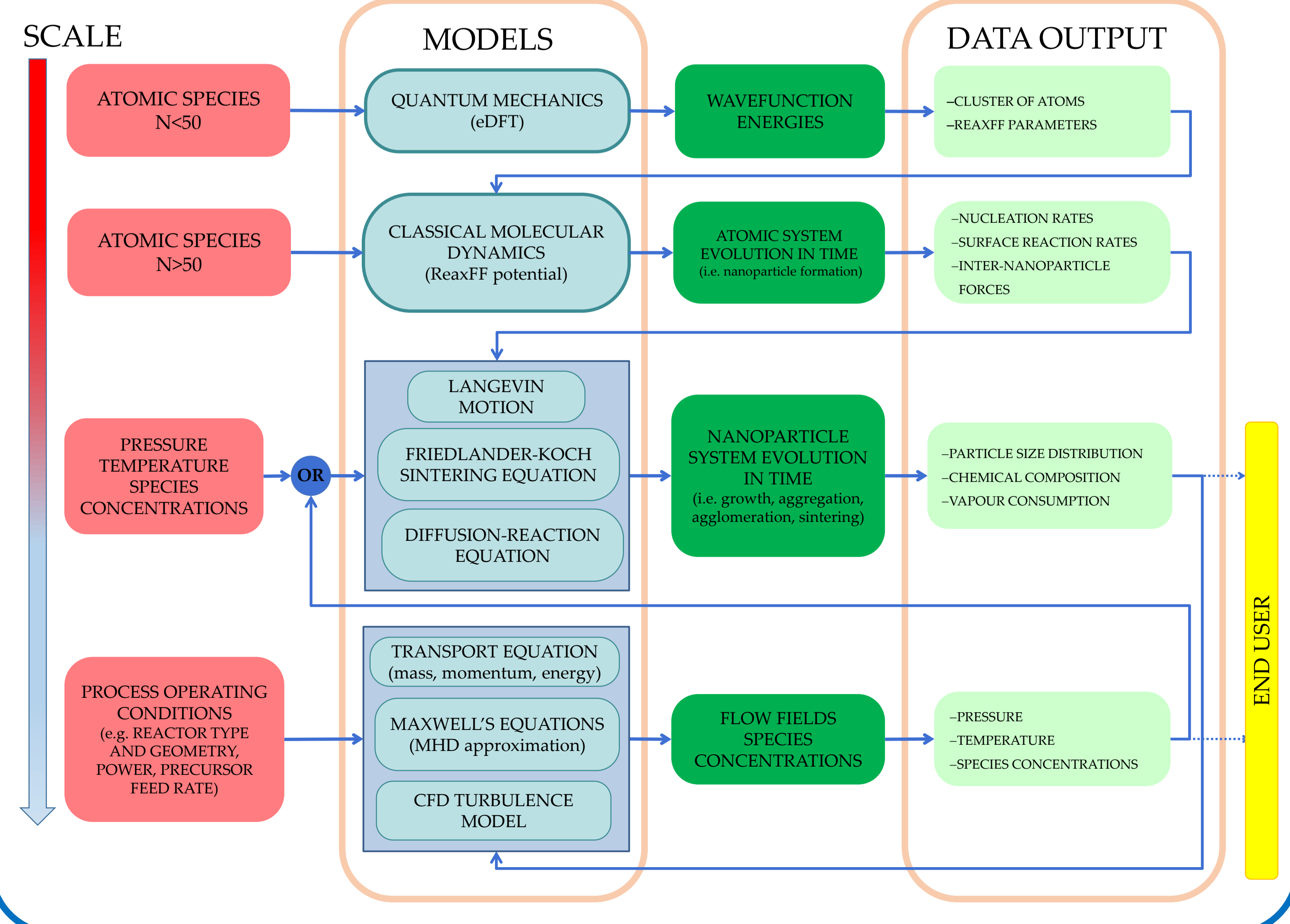
The gas phase state is defined by:
 • pressure
 • temperature
 • species concentration

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

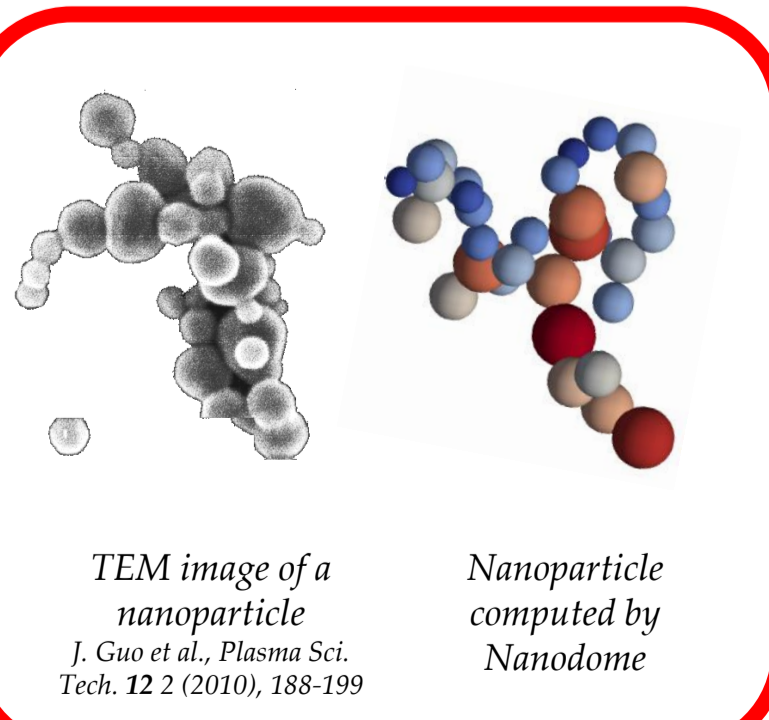
- The objective is to provide a **functional, flexible and open source software library, integrable with third party applications focused on the design of nanomaterials.**
- Object Oriented Design (OO).**
- Implemented in C++.**

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).



NanoDome project has received funding from the European Union's Horizon 2020 Research and innovation Programme, under Grant Agreement n°646121.

