NanoDome H2020 Project: Nanomaterials via Gas-Phase Synthesis

Published:

DOI: http://doi.org/

NANODOME H2020 PROJECT: NANOMATERIALS VIA GAS PHASE SYNTHESIS

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NanoDome
www.nanodome.eu

THE PROJECT

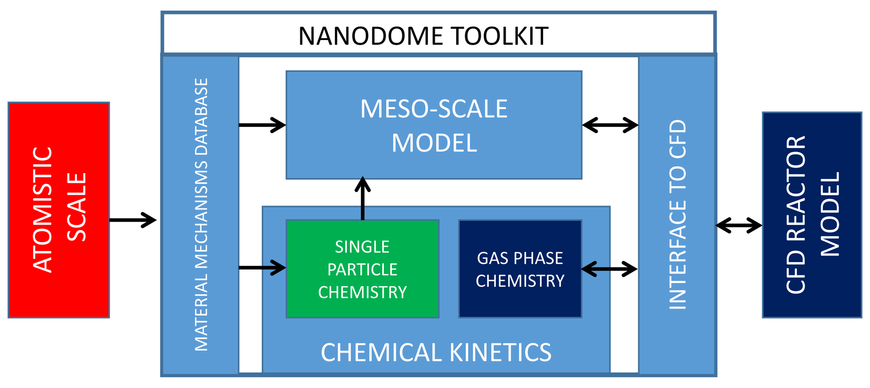
THE MAIN OBJECTIVE

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.

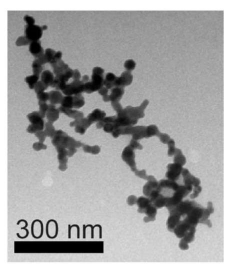
KEY OBJECTIVES

- 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.

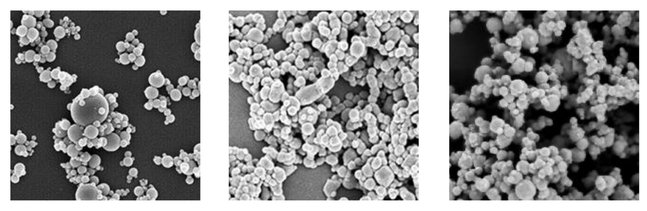


NANOPARTICLE SYNTHESIS PROCESSES

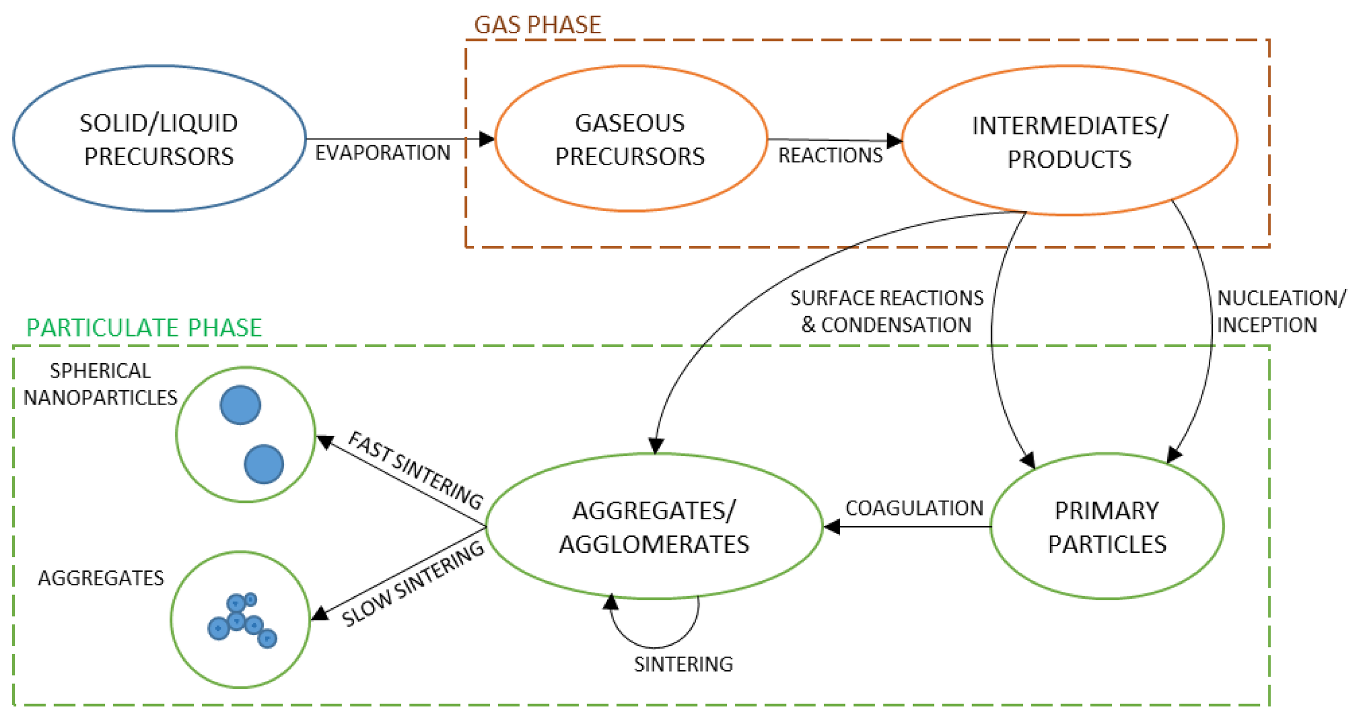
- The **NanoDome** model framework is designed for a generic Gas Phase Condensation synthesis process, to increase its usability in several existing commercial processes.
- **NanoDome** project focuses on:
  - **Plasma Synthesis Reactors**
  - **Flame Combustion Processes**
  - **Hot-Wall Reactors**



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)

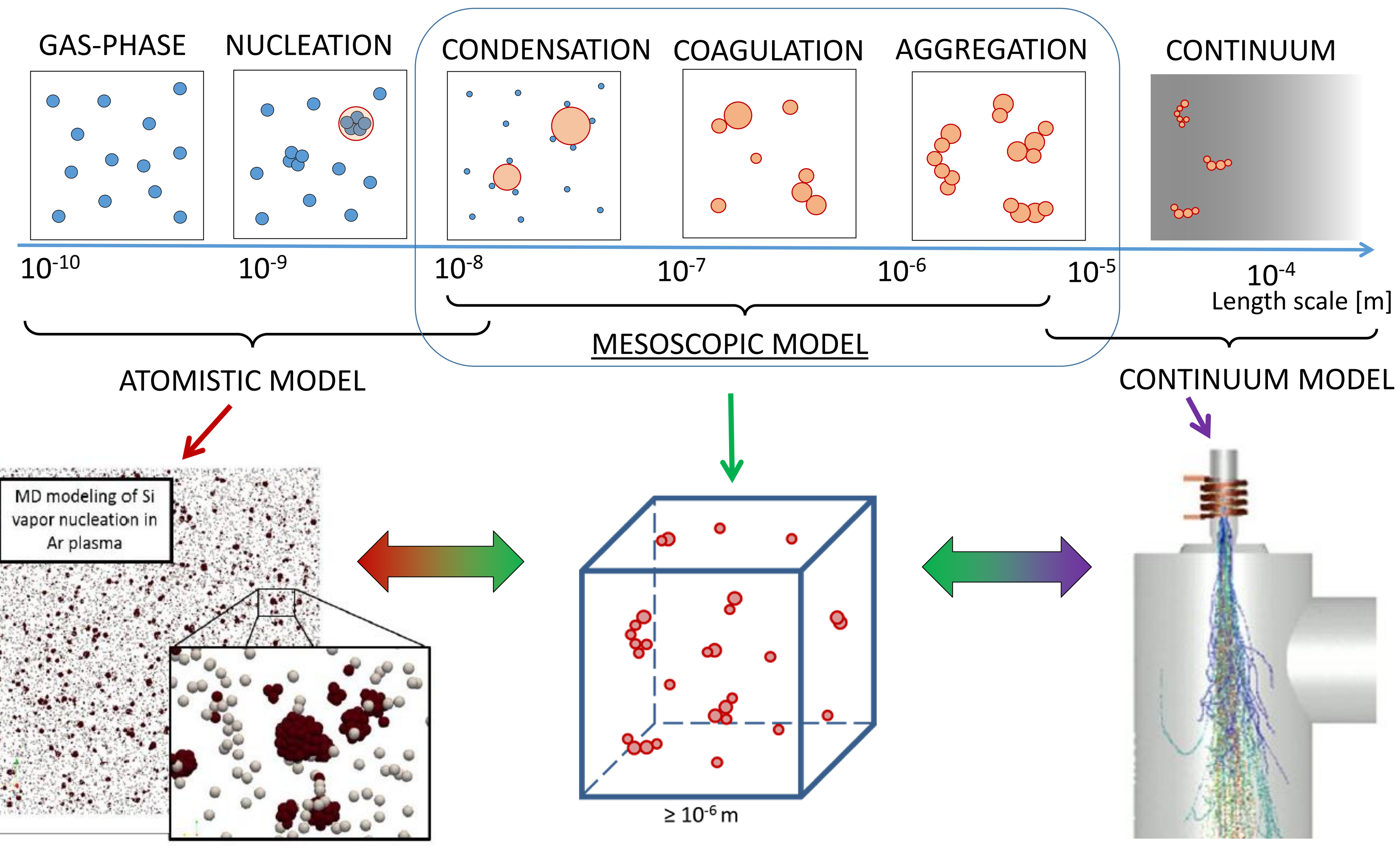


MULTISCALE APPROACH

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.

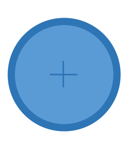
The mesoscopic model predicts **homogeneous** and **heterogeneous nucleation**, **coagulation**, **aggregation** and **morphology** of nanoparticles.

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



THE MESOSCOPIC MODEL CONCEPTS

PARTICLE



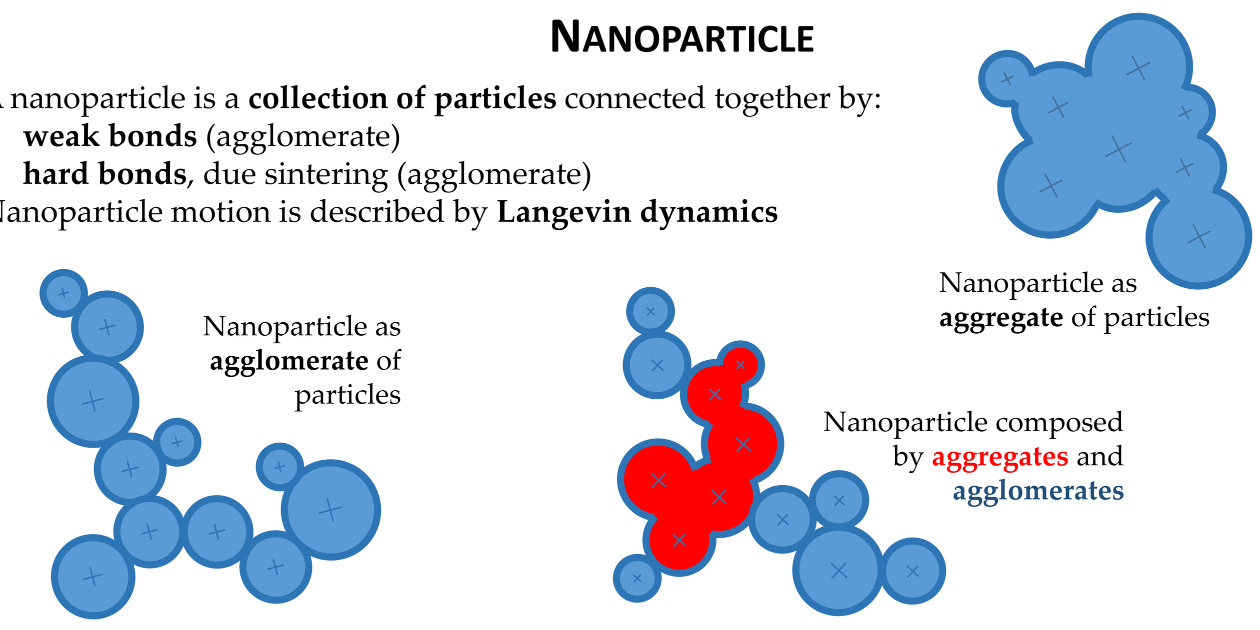
- **Basic discrete physical object** of the mesoscopic model
- Defined as **the minimum stable cluster** of molecules (i.e. primary particle)
- Particles are assumed to be of **spherical shape**
- Particles grow in size by **homogeneous condensation** and **coalescence**

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

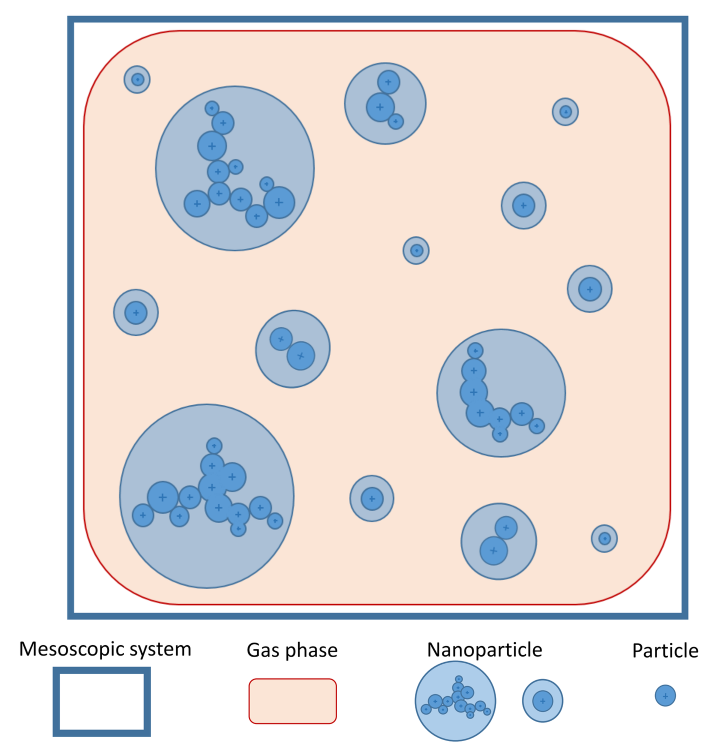
Gas phase is composed by all atoms and **molecules below the mesoscopic model scale**.

The gas phase state is defined by:

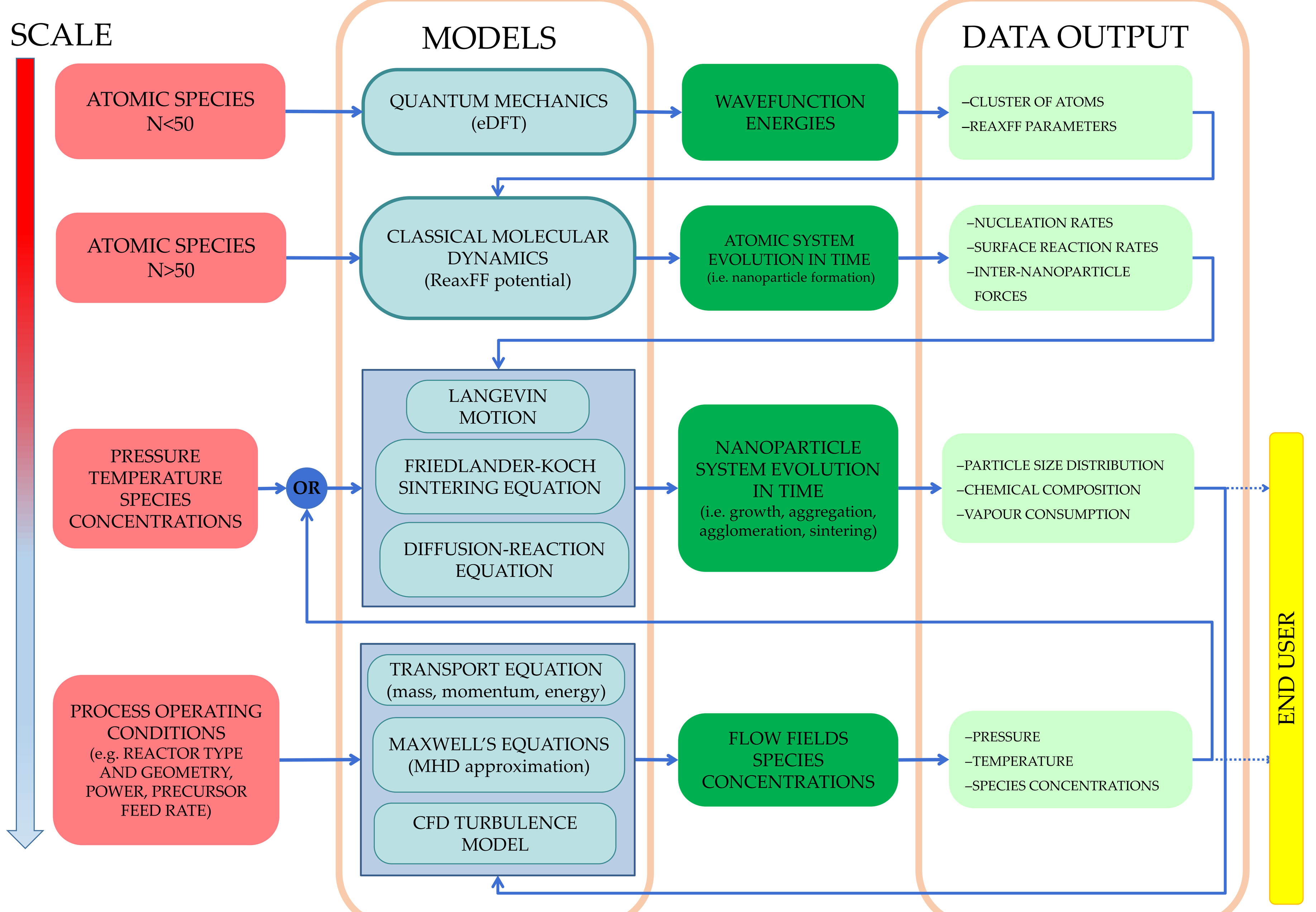
- pressure
- temperature
- species concentration

The gas phase state can be defined by **user** (XML based time dependend 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

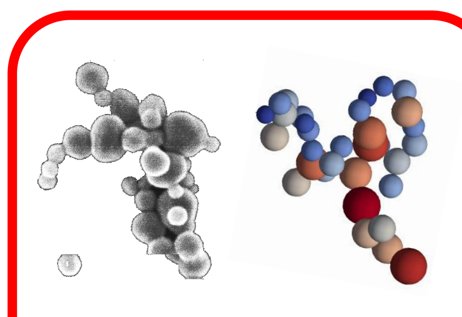


THE SOFTWARE

- **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 simultions, computed by the state-of-the-art QM or MD suites (Quantum Espresso, LAMPS, etc..).

Nanoparticles dynamics computed with Lagrangian and stochastic algorithms.



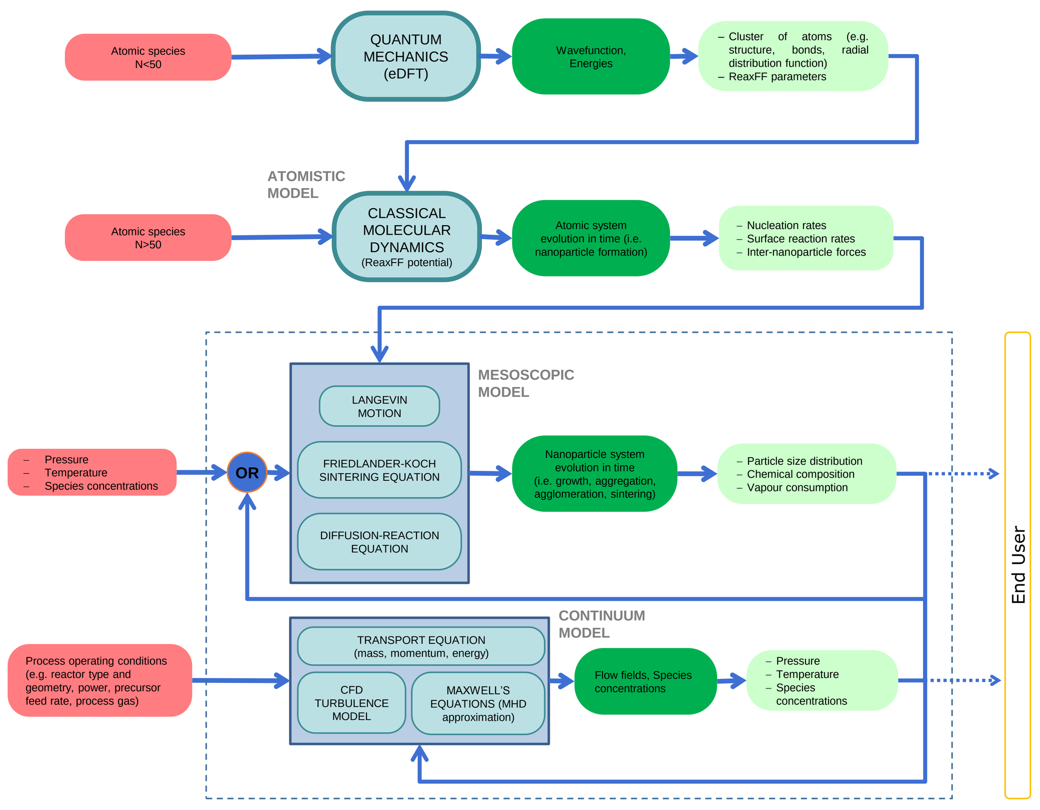
TEM image of a nanoparticle J. Guo et al., Plasma Sci. Tech. 12 2 (2010), 188-199

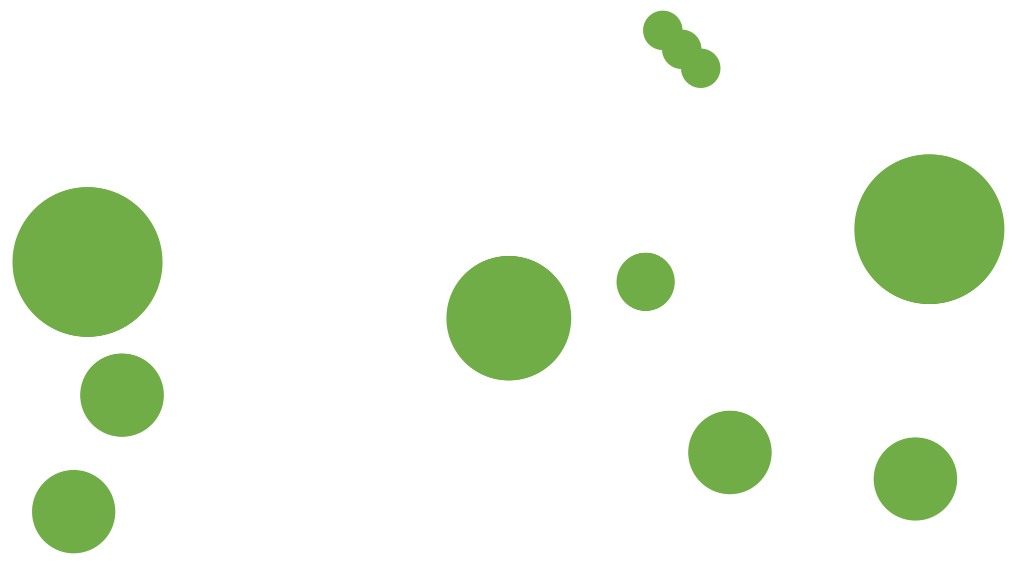
Nanoparticle computed by Nanodome

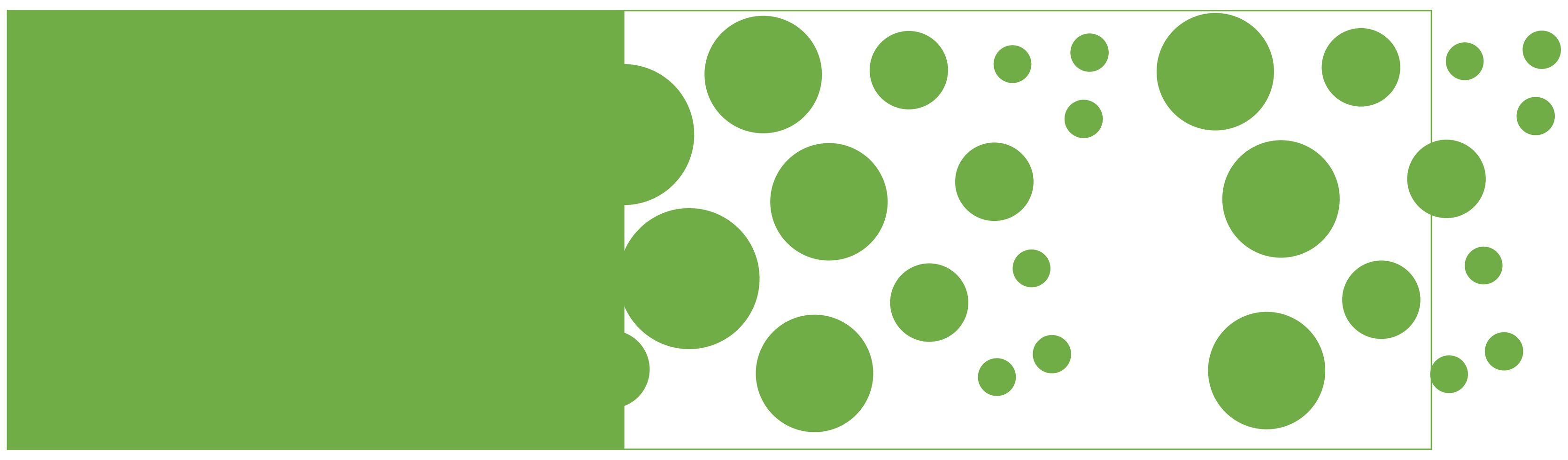
Linking/coupling with CFD simulation environments (ANSYS FLUENT™, OpenFOAM).

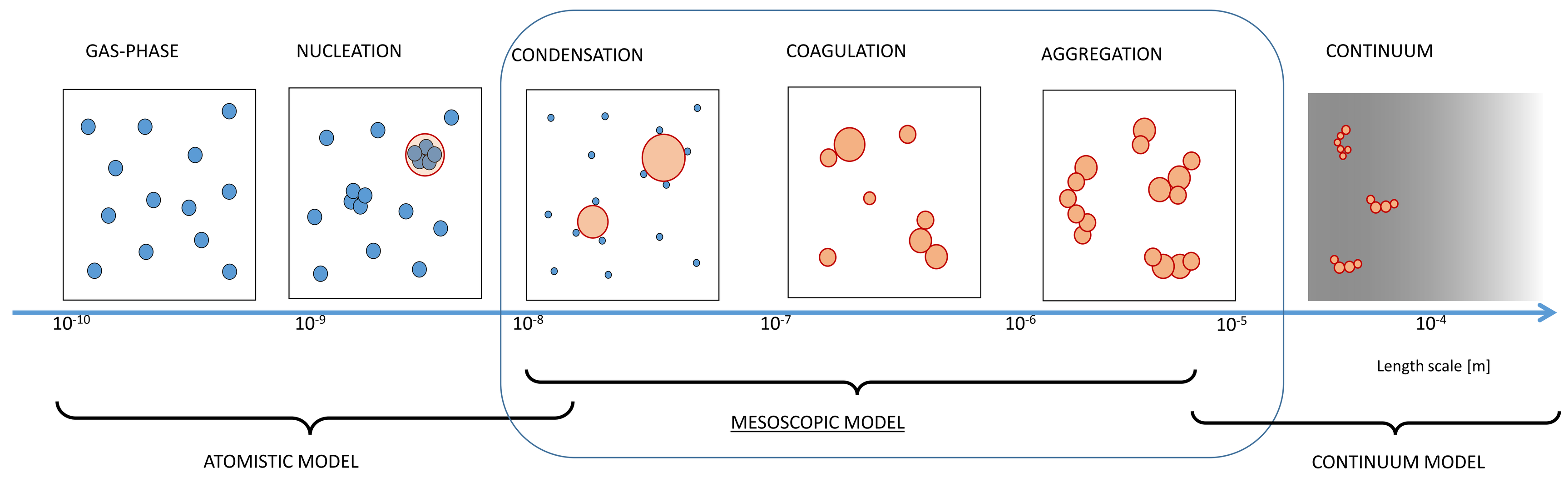
The NanoDome software can cooperate with chemical kinetics softwares (like KINETICS™ by CMCL).

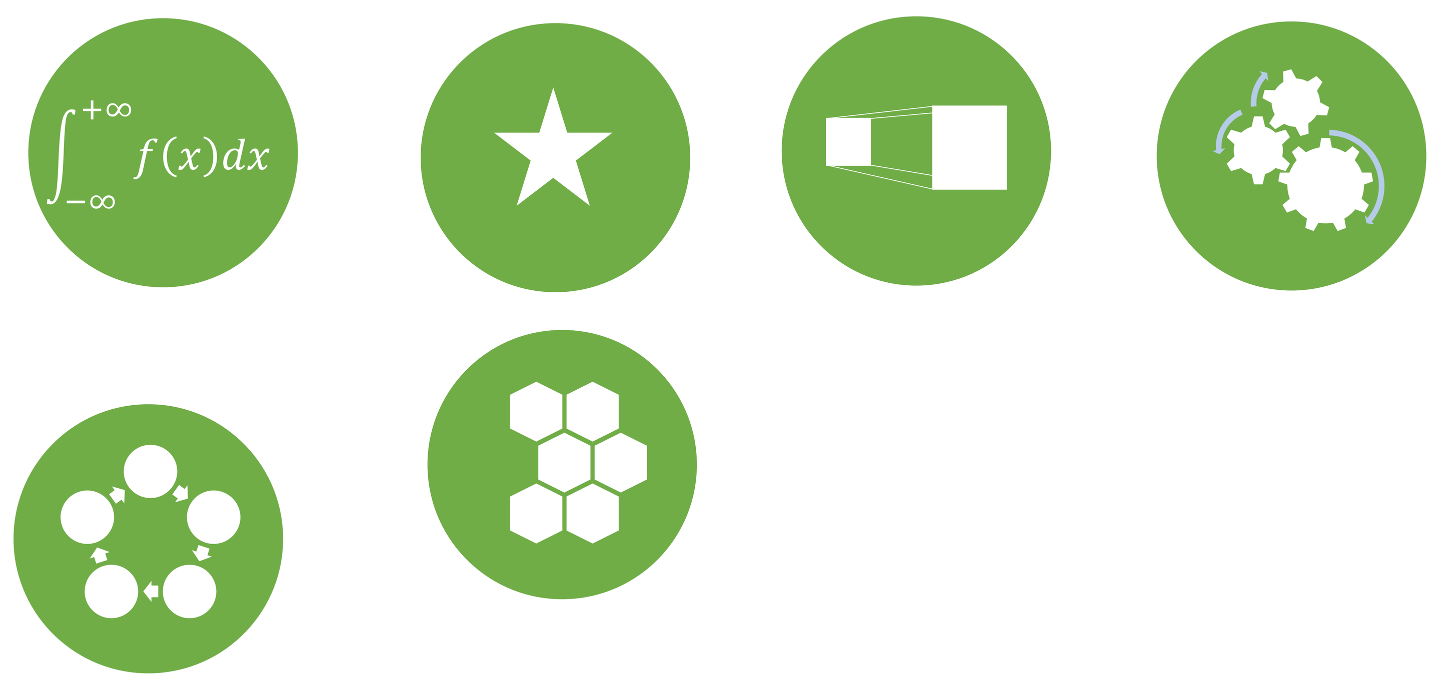
NanoDome project has received funding from the European Union's Horizon 202 Research and innovation Programme, under Grant Agreement n°646121.

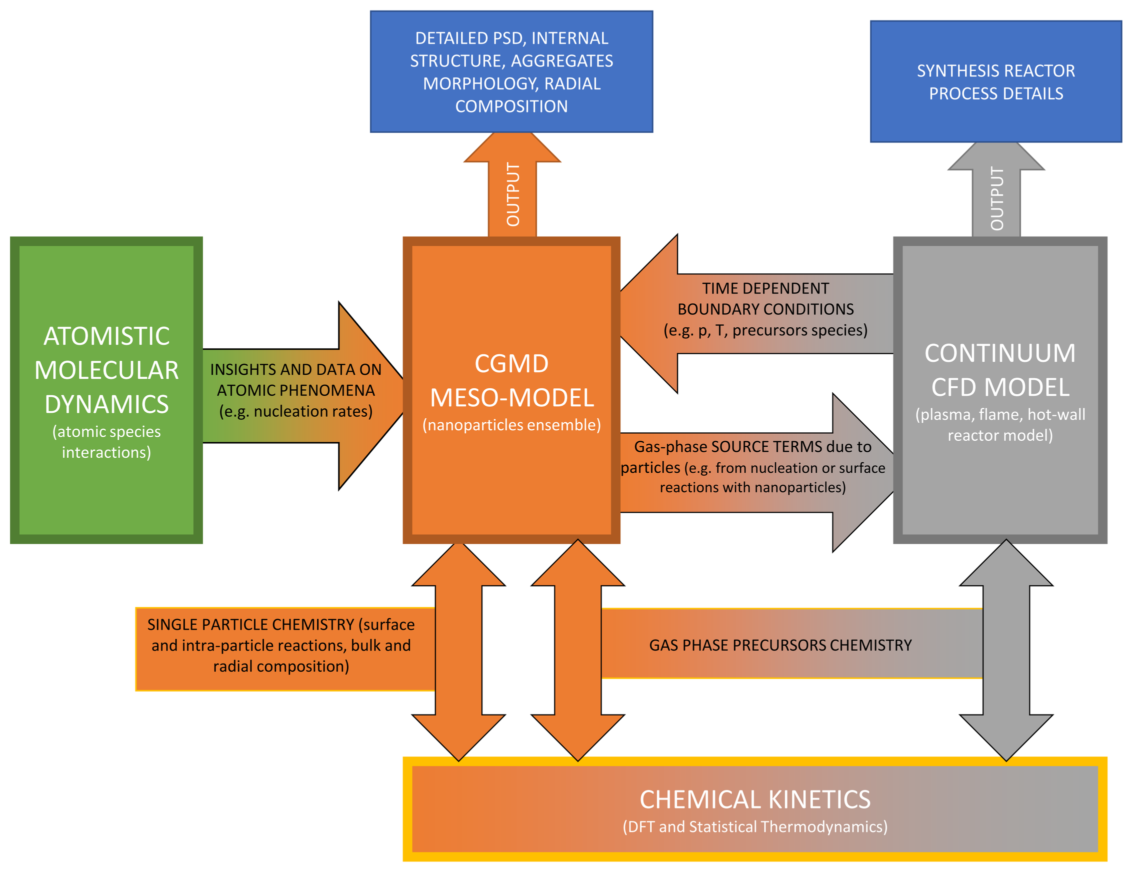


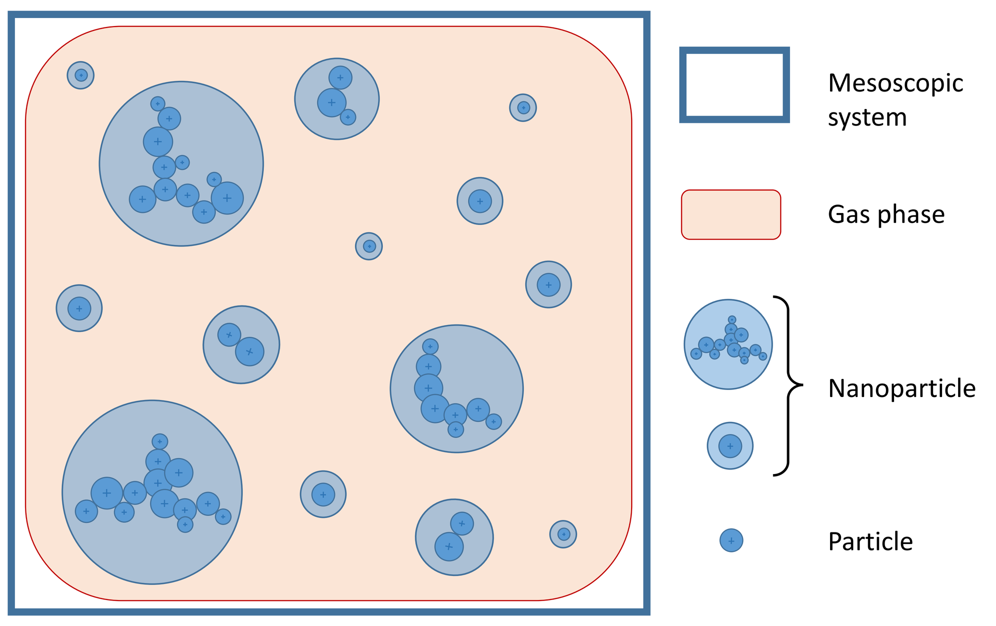


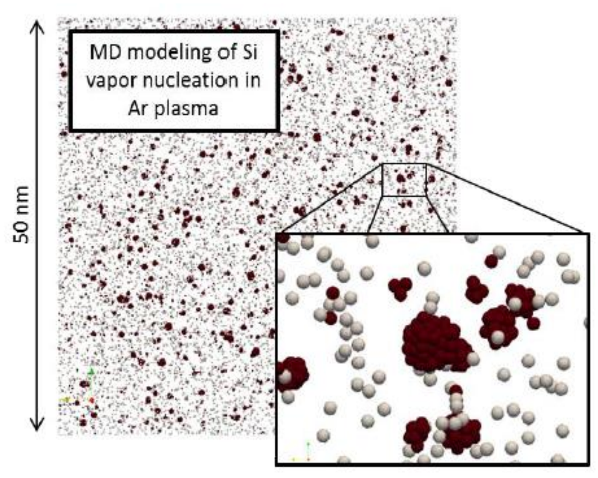


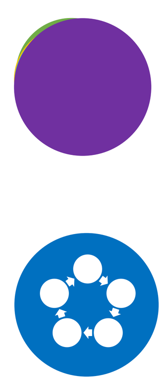

GAS-PHASE
NUCLEATION
CONDENSATION
COAGULATION
AGGREGATION
CONTINUUM
Length scale [m]
ATOMISTIC MODEL
MESOSCOPIC MODEL
CONTINUUM MODEL

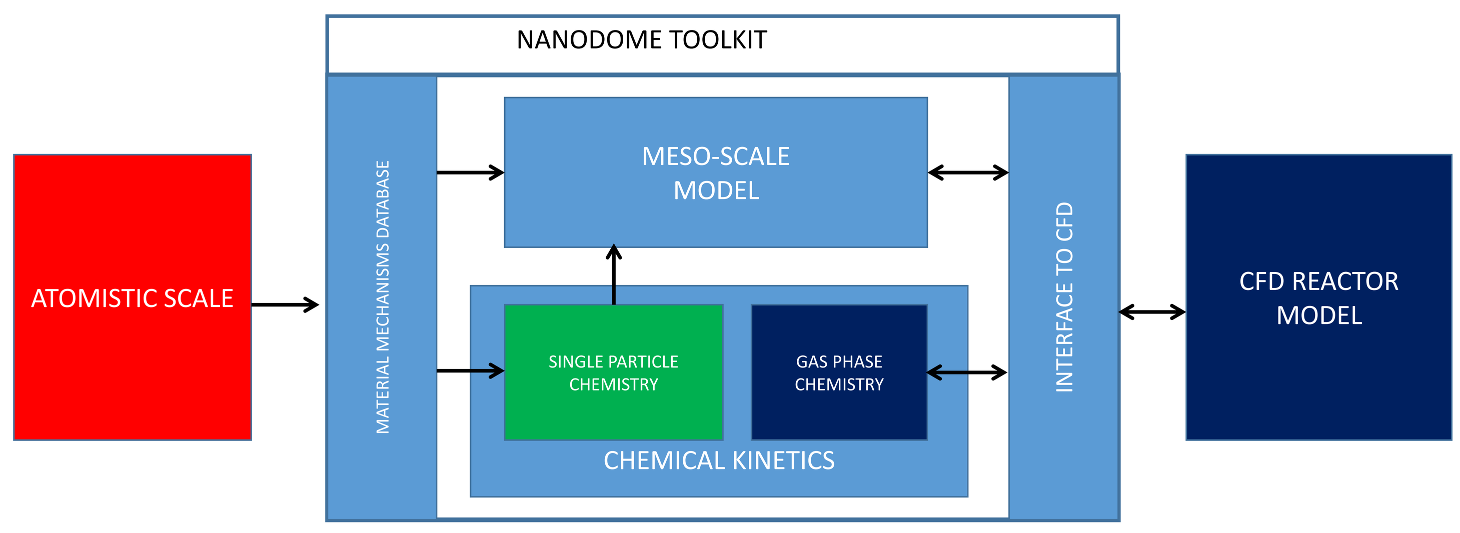


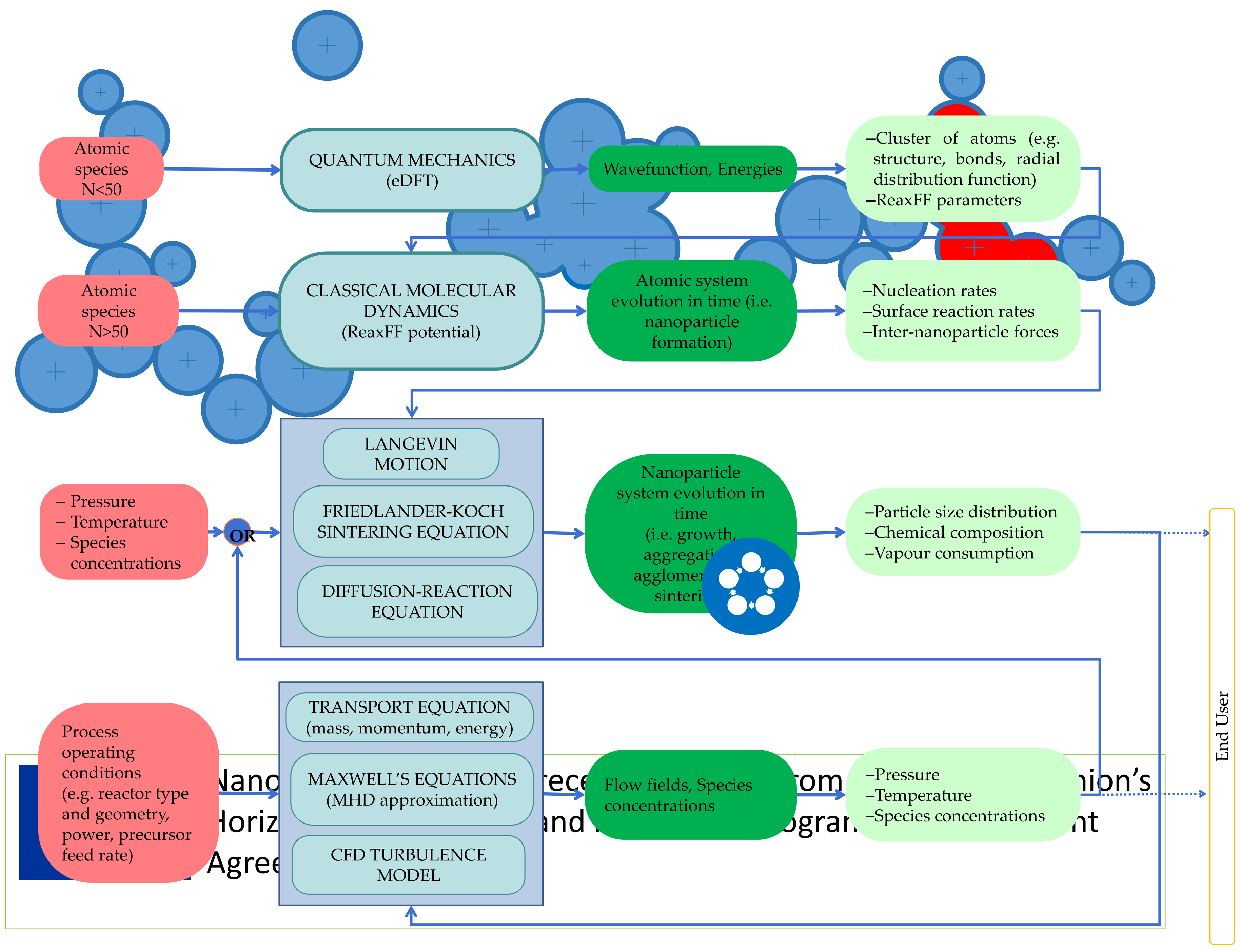

DETAILED PSD, INTERNAL STRUCTURE, AGGREGATES MORPHOLOGY, RADIAL COMPOSITION
SYNTHESIS REACTOR PROCESS DETAILS
ATOMISTIC MOLECULAR DYNAMICS
(atomic species interactions)
INSIGHTS AND DATA ON ATOMIC PHENOMENA (e.g. nucleation rates)
CGMD MESO-MODEL
(nanoparticles ensemble)
TIME DEPENDENT BOUNDARY CONDITIONS (e.g. p, T, precursors species)
Gas-phase SOURCE TERMS due to particles (e.g. from nucleation or surface reactions with nanoparticles)
CONTINUUM CFD MODEL
(plasma, flame, hot-wall reactor model)
SINGLE PARTICLE CHEMISTRY (surface and intra-particle reactions, bulk and radial composition)
GAS PHASE PRECURSORS CHEMISTRY
CHEMICAL KINETICS
(DFT and Statistical Thermodynamics)
OUTPUT

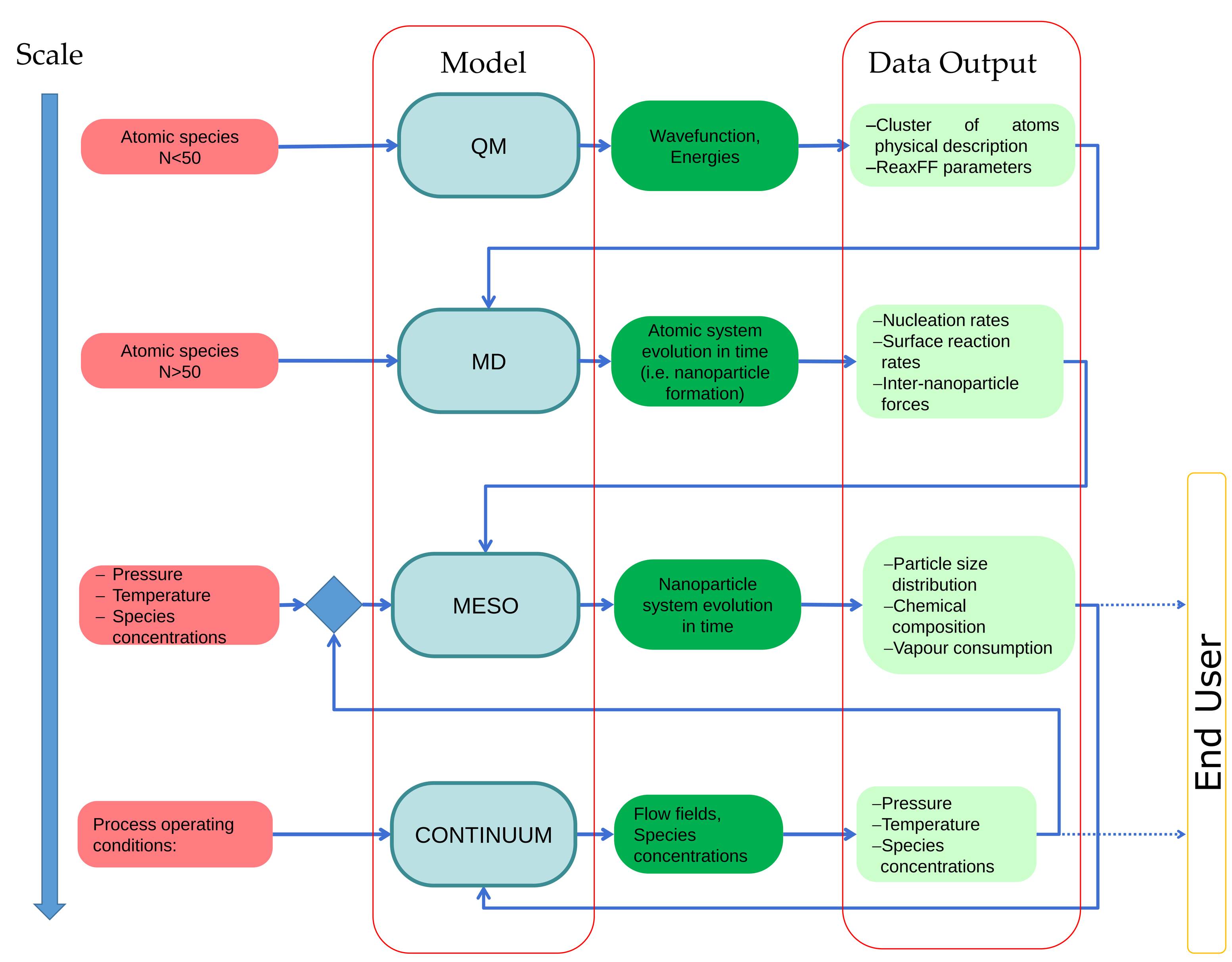

Mesoscopic system
Gas phase
Nanoparticle
Particle


MD modeling of Si vapor nucleation in Ar plasma
50 nm




NANODOME TOOLKIT
ATOMISTIC SCALE
MATERIAL MECHANISMS DATABASE
MESO-SCALE MODEL
SINGLE PARTICLE CHEMISTRY
GAS PHASE CHEMISTRY
CHEMICAL KINETICS
INTERFACE TO CFD
CFD REACTOR MODEL


Atomic species N<50
QUANTUM MECHANICS (eDFT)
Wavefunction, Energies
–Cluster of atoms (e.g. structure, bonds, radial distribution function)
–ReaxFF parameters
Atomic species N>50
CLASSICAL MOLECULAR DYNAMICS (ReaxFF potential)
Atomic system evolution in time (i.e. nanoparticle formation)
–Nucleation rates
–Surface reaction rates
–Inter-nanoparticle forces
– Pressure
– Temperature
– Species concentrations
OR
LANGEVIN MOTION
FRIEDLANDER-KOCH SINTERING EQUATION
DIFFUSION-REACTION EQUATION
Nanoparticle system evolution in time (i.e. growth, aggregation, agglomeration, sintering)
–Particle size distribution
–Chemical composition
–Vapour consumption
End User
Process operating conditions (e.g. reactor type and geometry, power, precursor feed rate)
TRANSPORT EQUATION (mass, momentum, energy)
MAXWELL'S EQUATIONS (MHD approximation)
CFD TURBULENCE MODEL
Flow fields, Species concentrations
–Pressure
–Temperature
–Species concentrations


Scale
Model
Data Output
Atomic species N<50
QM
Wavefunction, Energies
–Cluster of atoms physical description
–ReaxFF parameters
Atomic species N>50
MD
Atomic system evolution in time (i.e. nanoparticle formation)
–Nucleation rates
–Surface reaction rates
–Inter-nanoparticle forces
– Pressure
– Temperature
– Species concentrations
MESO
Nanoparticle system evolution in time
–Particle size distribution
–Chemical composition
–Vapour consumption
Process operating conditions:
CONTINUUM
Flow fields, Species concentrations
–Pressure
–Temperature
–Species concentrations
End User