Manuscript submitted to
AIMS' Journals
Volume **X**, Number **0X**, XX **200X**

Website: http://AIMsciences.org
pp. **X–XX**

HOMOGENIZATION-BASED NUMERICAL MATHODS

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(Communicated by the associate editor name)

Abstract. This note recalls what are "Homogenization-Based Numerical Methods". Then it introduces the papers of this Special Issue. In a third section it advocates for building a project in order to build "Homogenization-Based Software for Simulation of Multi-Scale Complex Systems".

1. **Introduction.** Since the previous opus : "Special Issue on Numerical Methods based on Homogenization and Two-Scale Convergence" of DCDS-S (Volume 8, Number 1, February 2015, [37], [36], [5], [50] [48] [1], [4], [12], [16], [41] and [30]), the advance on the topic has been important. It was time to take stock. This is the purpose of this new Special Issue "Homogenization-Based Numerical Methods" of DCDS-S.

A Homogenization-Based Numerical Method is a numerical method that incorporates in its conception concepts coming from Homogenization Theory. Doing this gives to the built method the capability to tackle efficiently heterogeneities or oscillations. This approach can be applied to problems occurring in a heterogeneous medium, that have oscillating boundary conditions or that are constrained to oscillate by an external action (for instance a magnetic field on a charged particle cloud).

Those methods are not only mathematically beautiful (in fact, they provide for all the oscillations and heterogeneities that could occur and embed ways to compute their mean actions and to reconstruct them without computing them via direct computation). Yet, they can play a crucial role in comprehending and harnessing complex systems subjected to oscillations and heterogeneities by developing new simulation methods for them.

In the main part of this paper, I advocate for building a project in order to build "Homogenization-Based Software for Simulation of Multi-Scale Complex Systems".

2. **On this Special Issue.** This Special Issue on "Homogenization-Based Numerical Methods" of DCDS-S gathers 3 types of papers. A first series introduces numerical methods that are genuine "Homogenization-Based Numerical Methods". The second series gathers papers that introduce homogenization problems that can directly generate "Homogenization-Based Numerical Methods". This Special Issue ends with a review paper questioning on the mathematical or physical nature of homogenization.

3. **Towards Homogenization-Based Software for Simulation of Multi-Scale Complex Systems.**

2000 *Mathematics Subject Classification.* Primary: 65L99, 65M99, 65N99.

Key words and phrases. Homogenization-Based Numerical Mathods; Homogenization; Asymptotic Analysis; Asymptotic Expansion; Numerical Simulation.

3.1. **Introducing a possible project.** In this section, I advocate for building a project in order to build "Homogenization-Based Software for Simulation of Multi-Scale Complex Systems" based on "Homogenization-Based Numerical Methods" that are already built or that will be built. This project is now described and detailed.
This project will pave the way to play a crucial role in comprehending and harnessing complex systems subjected to oscillations and heterogeneities by developing new simulation methods for them. Those simulation methods are based on "Homogenization-Based Numerical Methods". The project will demonstrate - thanks to operational software tools - how those simulation methods are relevant to solve models of the most complex systems subjected to oscillations and heterogeneities based on their fundamental equations (essentially PDE).

Four complex systems, which are of great scientific or technological importance, are planed to be used for this proof of concept: (i) magnetic fusion plasma, (ii) supernova neutrino transport, (iii) sediment transport in tidal coastal zones and (iv) town and country planning policy.

First, the project plans to expand the emerging breakthroughs in "Homogenization-Based Numerical Methods" in the field of Tokamak and Stellarator plasma into a simulation method embedded within a High Performance Computing environment. In the wake, acquired experience will be used in order to develop the new simulation methods for three other complex systems: one with oscillations (sediment transport in tidal coastal zones) and two with heterogeneities (supernova neutrino transport and town and country planning policy).

3.2. **The project scientific breakthrough.** The project will make a determinant step towards the simulation of complex systems subjected to oscillations and/or heterogeneities. For this, the project will set out new "Homogenization-Based Numerical Methods" to solution models of the systems based on their fundamental equations, which are generally partial differential equations (PDE). The project will implement those simulation methods within operational software tools.
For proof of concept, the project will focus on complex systems in the fields of:

- Magnetic fusion plasma physics, done in Tokamaks or Stellarators (where high frequency oscillations, are given to particles by a strong magnetic field),
- Supernova neutrino transport (which occures in a heterogeneous matter distribution),
- Sediment transport in tidal coastal ocean waters and its implications on the morphodynamics of beds and coasts (which typical evolution time is large compared to the tide period),
- Town and country planning and related public policy (which are made of nested entities, which involve several scales and which need to be observed at various time and space scales).

3.3. **Long-term vision.** The long term perspective is to allow to make essential contributions in all strategic issues where complex systems involving oscillations are present. in particular it will:

- contribute to grasp the simulation of the emergence and development of plasma turbulence in Tokamaks and Stellarators. Since plasma turbulence is the main obstruction to fusion mastering, this will be a determinant step towards the use of the fusion as a safe and clean energy source.
- Improve understanding of core-collapse supernova.
- Improve natural coastal zone management to contribute to a development in harmony with our environment.
- Improve territory development strategy building, accounting for their multi-scale natures, to help public authorities or governments to provide needs of their populations, respecting the overall balances.

In those fields, numerical simulation comes up against oscillations or heterogeneities: approaches using direct simulation of the fundamental equations requires too small discretization steps to make simulations over scales of interest and approximated models in used are close to their limits.

3.4. **The project : an essential step towards the goals.** To open the way towards the goals given above, clear answers are needed about the capability of "Homogenization-Based Numerical Methods" to tackle the models with their full complexity and all their oscillations and heterogeneities, to be implemented within operational software environments and to scale on parallel computers. For some complex systems chosen for proof of concept, "Homogenization-Based Numerical Methods" need to be improved or completed. For others, lacks in the description by PDE exist; they need to be filled in. The planed project will make those necessary tasks and will build the well adapted new simulation methods and provide them for the fields which the chosen complex systems belong to via Homogenization-Based Software.

3.5. **Objectives.** Plasma simulation by the kinetic approach consists of the solution of the 6-dimensional Vlasov-Maxwell or Vlasov-Poisson system by Particle-In-Cell (PIC) or Semi-Lagrangian methods.
The project will set out the confinement-dedicated-Two-Scale PIC and Two-Scale Semi-Lagrangian Methods - which are specific "Homogenization-Based Numerical Methods" - and implement them in software environments involving parallelism up to the dimension 4.

Neutrino transport simulation requires to solution the parametrized 5-dimensional Boltzmann equation by numerical methods close to the ones used for fusion plasmas (PIC, Semi-Lagrangian or Finite-Volumes). Homogenization-Bases versions of them integrating matter heterogeneity will be built, implemented and tested.
With regard to sediment transport in tidal coastal ocean waters, we will build a "Homogenization-Based Numerical Methods" coupling a Two-Scale and a Finite-Element approach within a software tool.

For town and country planning, models involving partial differential equations, at the finest possible scale (prescribed by available public data) will be built. From them, Aggregated and Homogenized ones will be deduced. "Homogenization-Based Numerical Methods" will be set out and Homogenization-Based Software developped.

3.6. **Novelty of Homogenization-Based Software.** The novelty in Homogenization-Based Software of is to offer the possibility to simulate complex systems accounting for all their oscillations and heterogeneities on the basis of computing solutions of their fundamental equations - and not only simplified ones - via "Homogenization-Based Numerical Method".

Simulating the fundamental equations describing complex systems with oscillations or heterogenities by software tools based on "Homogenization-Based Numerical Methods" challenges the viewpoint that to simulate such systems, the only way is refinement... which is an impossible tracking because of the limited computer capacities.

Beside this, for magnetic fusion, the project will offer alternative methods to the Gyro-Kinetic approach (which is not completely satisfactory) and to the direct simulation of the Vlasov-Poisson or Vlasov-Maxwell by PIC-methods (for which satisfactory accuracy cannot be reached for fusion experiments).

For neutrino transport simulation, the project will offer an alternative approach to the one based on the Isotropic Diffusion Source Approximation (IDSA).

For the time being they are no other ways than making CPU-costly simulations, on very restricted areas, with very small (with respect to the time span of interest) time steps of the Exner equation for sediment transport in tidal coastal ocean waters.

For town and country planning, the project will offer alternative approaches to existing software tools which are essentially, discrete-model-based expert-systems incorporating decision-makers knowledge and usual protocols.

3.7. **State-of-the-art.** **Homogenization theory** gathers methods from Mathematical Modeling, Analysis, Asymptotic Analysis and Numerical Analysis in order to remove - mathematically rigorously - from equations the explicit presence of oscillations or heterogeneities keeping their averaged effect with precision. Moreover, a good approximation of the oscillations or heterogeneities is gotten by applying an oscillating operator to the solution of the homogenized equation. In Economics world, homogenization models are called **microeconomics-based-macro-models**.
From those mathematical methods, "Homogenization-Based Numerical Methods" can be built. They have the capability to solution numerically the equations, with a good accuracy, at a scale larger than the one of the oscillations or heterogeneities they contain, without entering intimately their resolution. Moreover, good approximation of the oscillations or heterogeneities may also be computed.
Two-Scale Numerical Methods (see for instance [3], [2], [20], [21], [17], [29] and [8]), which are "Homogenization-Based Numerical Methods", on bi-dimensional kinetic models showed nice behaviors. They seem to describe correctly the evolution of a seabed dune which is already shaped.
In **Tokamaks or Stellarators**, plasma is confined using a strong magnetic field to reach the fusion. The strong magnetic field generates particle oscillations. As a non-linear result of those oscillations, over a few milliseconds, plasma turbulence emerges and opposes to a correct confinement. Hence, perceiving with more accuracy plasma turbulence aspects is important. This will be certainly achieved, if accurate simulations of magnetic fusion plasma can be done with a six-dimensional kinetic model, over about 10 milliseconds.
Up to now, actual Tokamak plasma kinetic simulation is based on the Gyro-Kinetic approximation (see [35], [24], [43], [44], [38, 39, 40] [34], [7], [10], [22], [27], [28], [45, 46, 47], [25, 26], [18, 19]) that is a five-dimensional approximated model of the Vlasov-Poisson system. Simulations of about one millisecond of a Tokamak working are possible.

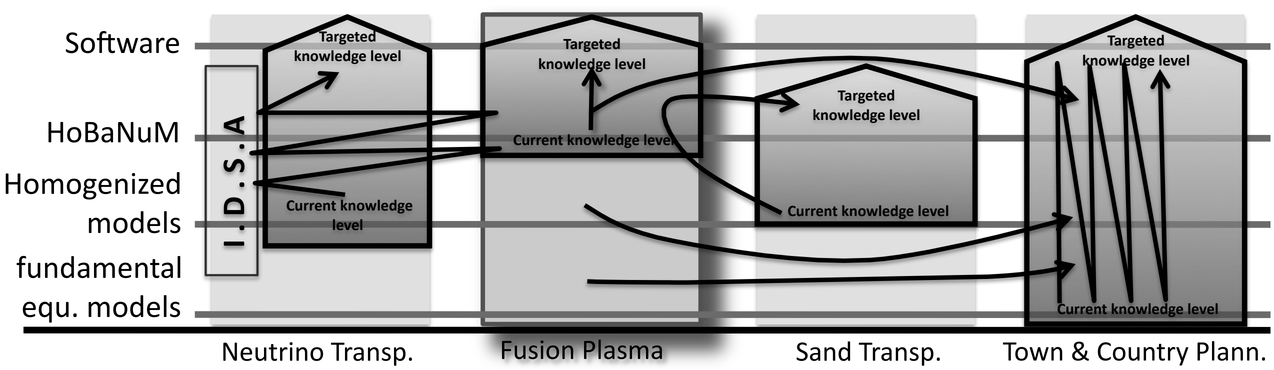

FIGURE 1. Starting points, the project targeted points and solution pathways, for the target applications. (HoBaNuM is for "Homogenization-Based Numerical Methods".)

In **supernovae**, more than 99% of the released gravitational binding energy is carried away by neutrinos. Hence, simulating neutrino transport is crucial for the understanding of supernova explosion. Moreover, supernova explosion seems to be related to spherical symmetry breaking. Hence, it is necessary to go towards simulations accounting for the full spatial matter distribution that leads to the solution of the parametrized 5-dimensional Boltzmann equation.
Since for the time being this system cannot be solved, a way currently explored consists in using an

approximated system of equations: the IDSA.

Evolution of seabed in coastal ocean waters is an important topic related to waterway or erosion issues. In areas submitted to tide, at every tide, a large amount of sand comes and goes, with a small resulting effect. Consequently, significant evolution of seabed occurs over time spans of tens of years, and seabeds may appear in a dynamical equilibrium while they are slowly evolving. Moreover, direct simulations based on the Exner equation cannot give results over the time spans of interest. Hence, offering the possibility to simulate seabed in tidal coastal ocean waters over time periods of several tens of years, based on the Exner equation, will be of great help for coastal zone management (see [49] , [42], [6], [31], [9], [32], [33], [14], [23]).
On this subject a first step was done in [11] and [13].

Territories are made of nested entities, affected by many factors and involve several time and space scales. They are managed by authorities and governments that, by nature, act at various time and space scales. Providing software tools that have the capability to analyze territories incorporating their multi-scale and multi-factorial nature and allowing observation of them at various scales will be welcome.
In view of the data available nowadays and in the near future, using mathematical modeling routines and econometric methods, it seems possible (see [15]) to build territory models involving density functions that are defined at several scales. Those models can then be observed at various scales by building homogenization-based approaches.

3.8. **Scientific and technological approach.** As represented in Fig. 1 we will start from current knowledge level - which are not the same for all the considered complex systems - and go gradually towards the full models incorporating the full complexity, learning at each step from experience and always programing with a high level of genericity to make reusable software tools.
As emphasized by Fig. 1, the development of the simulation methods and Homogenization-Based Software for the complex system of magnetic fusion plasma will have a motor role and will nurture the three others. For it, the methodology will be step-by-step to go from our present knowledge level (solution of a toy-model by Two-Scale PIC Method) to the targeted level (solution of 4D kinetic equations by Two-Scale PIC and Semi-Lagrangian Methods in an operational Homogenization-Based Software). At each step, attention will be paid to behaviors in front of complexity (testing on numerous examples) and scalability with respect to parallelism. The methods will be made more robust using geometrical principles. This will yield a succession of work packages as symbolized by Fig. 2.
For the complex system of sand transport the methodology will be less straightforward: Two-Scale Numerical Method building needs to be completed, using experience of fusion plasma, and coupled with a Finite-Element Method.
For neutrino transport, as the IDSA approach is under development, the methodology will make ideas of the fusion plasma part to interact with IDSA ones. "Homogenization-Based Numerical Methods" will be built, implemented and compared with IDSA-based ones.
Since models need to be built and used for "Homogenization-Based Numerical Methods" immediately, for town and country planning the methodology will follow cycles (see Fig. 1 and 2) over the following stages. In stage 1, we will build, implement and test on several territory examples an explicative model, based on socio-economics principles and adjusted by econometrical methods, valid at the finest possible scale (prescribed by existing public data granularity). In stage 2, we will embed financial status of public entities and study mutual influences of finance steering and territory steering. In stage 3, we will incorporate environmental factors and recent advances in modeling of population well-being. In stage 4, Aggregated Models will be deduced and their validity domain carefully studied. On their bases, captors and indicators for territory steering will be set out. In

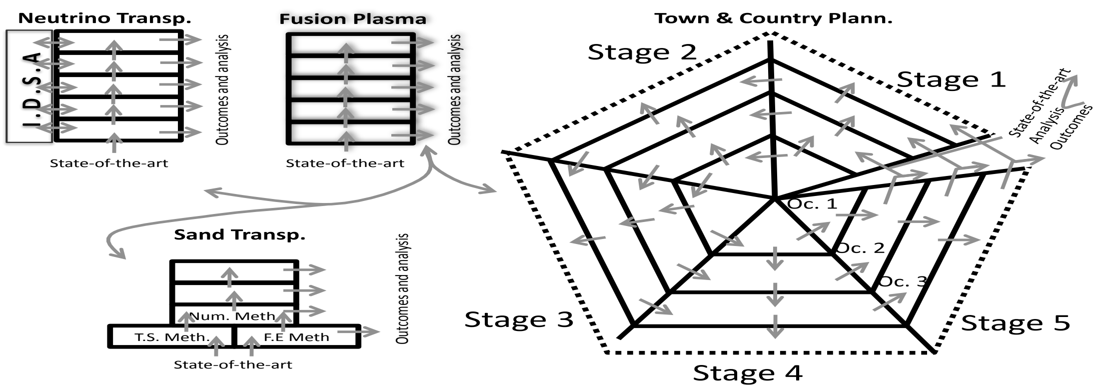

FIGURE 2. Possible project Work Package organization.

stage 5, Homogenized Models and "Homogenization-Based Numerical Methods" will be built, implemented, tested and used to describe trends or large scale dynamics. In the first cycle occurrence, we will do the five stages with a simplified model. In the second one, we will explore a model adjusted on some well-chosen territories.

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