Final Report

Project: Modeling Mesoscale Processes of Scalable Synthesis

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CM4 and its goals

The "Collaboratory on Mathematics for Mesoscopic Modeling of Materials" (CM4) is a multi-institution DOE-funded project whose aim is to conduct basic and applied research in the emerging field of mesoscopic modeling of materials. The mesoscopic modeling of materials has grown out of the dual realization that the microscopic simulation of realistic materials in not feasible and that the use of purely macroscopic models is inadequate to describe all the interesting features of materials. The modeling of materials involves a vast range of scales and thus there is fertile ground for the development of multi scale methods to address the mesoscales which bridge the gap between the microscopic and the macroscopic. CM4 is a concerted effort combining the expertise of a diverse array of scientists to attack the problem of modeling materials in all its aspects. In particular, we envision the collaboratory to produce advances in several fields ranging from novel reduced models to commercially available software for large scale applications.

Contribution of the Minnesota research activity

The research activity in Minnesota focused on two related and equally important subjects: i) mesh refinement and ii) model reduction. Mesh refinement is important since for many problems we may not have enough computational power for a uniform resolution in the computational domain. Thus, one needs a judicious allocation of the available resources focusing on the areas that are more important dynamically. Model reduction is important since there are many problems where even the use of mesh refinement is not enough and one can quickly run out of resolution. In such cases, one would like to have access to accurate reduced models which can keep the salient features of the original problem. In my work I have sought to combine the two strands of research. In particular, I have advanced the idea that successful model reduction and mesh refinement rely on the same principle: the accurate estimation of the transfer of activity from the resolved to the unresolved variables. This opens the road to use accurate reduced models (if one has them) to construct mesh refinement algorithms. Also, it allows for the development of new reduced models which can operate in parameter regimes where traditional model reduction approaches could fail. The results obtained in both fronts during the first two years of CM4 were very encouraging. After relocating from Minnesota to the Pacific Northwest National Laboratory (PNNL) I have continued pursuing these themes and the results will be presented in more detail in the final report at the conclusion of the CM4 project. The advances made during my time in Minnesota and PNNL are in accordance with the goals and objectives outlined at the beginning of the CM4 project.

1 Review of Year 1 research activity in Minnesota

During the first year of the project I have investigated the following topics: i) a Markovian reformulation of the Mori-Zwanzig (MZ) formalism to deal with cases of finite memory, ii) application of this reformulation to the problem of reduced models for uncertainty quantification (UQ), iii) use of reduced models to construct mesh refinement schemes in *probability* space, iv) the scaling law behavior of renormalized coefficients for MZ reduced models and v) the rigorous proof of convergence of the solution a special case of renormalized MZ models (called the t-model) to singular solutions of partial differential equations. All the subjects investigated fall within the general theme of understanding better the MZ formalism and utilizing its structure to obtain meaningful reduced models and/or reliable tools for mesh refinement.

1.1 Markovian reformulation of the MZ formalism

Suppose that we are given a system of ordinary differential equations to solve (this covers also the case of partial differential equations after a suitable discretization). Many of the systems encountered in real life applications are too large for our present or foreseeable computational capacity. In addition, even if we are able to simulate a system on a computer we may need a reduced description for reasons of efficiency. Thus, out of necessity and/or efficiency we would like to have a formalism that allows a systematic construction of reduced models. The MZ formalism is such a formalism since it leads to an exact reformulation of the original system of equations [3, 4]. Then, one can use this reformulation to construct reduced models of various degrees of sophistication.

The problem inherent in MZ, as well as *any* other model reduction formalism, is that the effort required for the construction of an accurate reduced model can be quite substantial. In particular, the most expensive part of the construction of a reduced model is the representation of the memory term. The memory term involves an evolution operator (the orthogonal dynamics operator). This operator obeys an equation whose solution is prohibitively expensive except for very special cases. The purpose of the proposed Markovian reformulation of the MZ formalism in [11, 12] is to bypass the need for an exact solution of the orthogonal dynamics equation. It is based on the replacement of the calculation of the memory term by a hierarchy of ordinary differential equations. In principle, this hierarchy is infinite dimensional. However, under certain assumptions it can be safely truncated. In [11, 12] I have examined how the Markovian reformulation can be used in the case when the memory has only finite, but not necessarily short, length. The Markovian reformulation has been used so far in the construction of reduced models for uncertainty quantification (please see next section).

1.2 Dimensional reduction for uncertainty quantification

In many time-dependent problems of practical interest the parameters, the initial and/or the boundary conditions exhibit uncertainty. One way to address the problem of how this uncertainty impacts the solution is to expand the solution using polynomial chaos expansions and obtain a system of differential equations for the evolution of the expansion coefficients. In [11, 12] I have presented an application of the MZ formalism to the problem of constructing reduced models of such systems of differential equations. In particular, I have constructed reduced models for a subset of the polynomial chaos expansion coefficients that are needed for a full description of the uncertainty caused by uncertain parameters or uncertain initial conditions.

The construction of the reduced models was based on the Markovian reformulation presented in Section 1.1. In some cases [11], the unknown parameters that appear in the reformulation can be computed *without* having to solve the full system, while in others [12], I present a way of computing the necessary parameters on the fly.

1.3 Use of reduced models for probabilistic mesh refinement

There are situations in uncertainty quantification where the expansion of the solution in polynomial chaos expansions is not enough. The reason is that one needs more terms in the expansion than our present computational capacity will allow. However, the need for many terms in the expansion may be the result of the sensitivity of the solution to only a few values of the uncertain parameter e.g. specific values of the initial conditions. In such cases, it is advantageous to have a way of dividing the mesh of values for the uncertain parameters in pieces and then refining the mesh only where needed [17]. This can allow us to keep the order of the polynomial chaos expansions low within each piece at the cost of having to solve a larger number of such easier problems.

In previous work [10] I have found that reduced models can be used not only to effect a reduction of the dimensionality of a given system but also to decide when it is time to refine the mesh in physical space. Thus, I have applied this same reasoning to the construction of an adaptive mesh refinement scheme for probabilistic meshes. The advantage of the proposed probabilistic mesh refinement method is that it provides a physically sound refinement criterion which can also be automated. I have already applied the method, with very good results, to the mesh refinement of the uncertainty parameter range for the 1D Kraichnan-Orszag (KO) problem. The KO problem is a system of three ordinary differential equations whose limiting behavior changes from a fixed point to a limit cycle depending on the value of the initial condition. Thus, as shown in [17], a naive polynomial chaos expansion is not adequate for long time uncertainty quantification unless a tremendous amount of terms are kept. On the other hand, the probabilistic mesh refinement scheme allows accurate quantification of the uncertainty for long time integration. In current and future work with the DOE-funded postdoc Dr. Jing Li, we are investigating the application of the method to more challenging situations of uncertainty quantification.

1.4 Scaling laws and renormalization of MZ models

The construction of reduced models of a system of equations through the MZ (and any other) formalism, assumes that we have access to solutions of the full system. However, for several practical applications (from material science to fluid mechanics) this is not true. The reason is that the full system involves many orders of magnitude more degrees of freedom than we can hope to simulate in the foreseeable future. The construction of reduced models for such systems highlights the fact that the present reduction formalisms need to be improved. In mathematical terms, we need to find a way to account for the information that we cannot provide through direct numerical simulation. In [13], I have presented a way to address this problem in the context of the MZ formalism. The approach, which I have termed renormalized MZ (rMZ), is inspired by the Effective Field Theory approach pioneered in high energy physics [6].

In particular, we begin by embedding the reduced model we have at hand in a larger family of reduced models that involve terms of the same functional form but with arbitrary coefficients. These coefficients need to be estimated. We know that the largest system of equations that we can simulate will become under-resolved after some time. However, before this system becomes under-resolved we can use it to estimate (on the fly) the coefficients that appear in front of the reduced model terms. In essence, we renormalize the coefficients, hence the name, so that the reduced model reproduces certain features of the original system while the latter is still well-resolved. I have applied this approach successfully in the construction of reduced models for the inviscid 1D Burgers equation and the 3D Euler equations of incompressible flow. Based on dimensional analysis arguments I had expected the renormalized coefficients to follow scaling laws. While the calculations have proven rather delicate I have evidence that the renormalized coefficients depend on the ratio of the highest active Fourier mode in the initial condition to the highest Fourier mode allowed by the reduced model. This dependence does indeed take the form of a scaling law. In current, as well as future work, this dependence will be investigated further to establish its robustness and if possible deduce its mathematical origin.

1.5 Convergence proof of the renormalized t-model

The renormalized t-model is the simplest of the renormalized MZ models presented in [13]. Based on previous work [7] it can be shown that the renormalized t-model solution converges to the solution of the inviscid Burgers and 3D Euler equations as long as these solutions remain smooth. However, it was not known if the renormalized t-model converges to the unique entropy solution of inviscid Burgers after a shock has formed. In recent work I have undertaken the task of proving this fact using the method of compensated compactness [9, 15]. The proof is divided into two steps: i) proof that the solution of the renormalized t-model converges to a weak solution of Burgers and ii) proof that the solution it converges to is the unique entropy solution. In future work, I will investigate what an analogous proof (if it exists) could mean for the, as yet unresolved, problem of formation of singularities for the 3D Euler equations.

2 Review of Year 2 research activity in Minnesota

During the second year of the project I have investigated the following topics: i) mesh refinement schemes inspired by model reduction, ii) the scaling law behavior of renormalized coefficients for Mori-Zwanzig (MZ) reduced models and iii) the choice of "proper" coarse-grained variables. All the subjects investigated continue work that was started during Year 1 of CM4. The underlying theme is to obtain a suite of techniques/algorithms which will facilitate the tracking of the evolution of complex systems.

2.1 Mesh refinement schemes inspired by model reduction

At first sight putting together the concepts of mesh refinement and model reduction may appear counterintuitive. On the one hand, mesh refinement is concerned with the judicious allocation of computational power to allow focusing on the important characteristics of a solution. On the other hand, model reduction is concerned with the best way to approximate the effect of the unresolved scales of a simulation to the resolved ones. The element that connects these two subjects is the observation set forth in [10] that successful mesh refinement relies on the accurate monitoring of transfer of activity to the unresolved scales which is exactly the objective a good reduced model. Thus, if one possesses a good reduced model, it can be utilized to decide when and where to perform mesh refinement.

In my previous work [10] a reduced model was used to refine a mesh in physical space. In work that originated during Year 1 of CM4, Dr. J. Li and I have applied this idea to the construction of an adaptive mesh refinement scheme for probabilistic meshes [8]. The associated question is whether the proposed approach has a sound mathematical basis, i.e. whether it can be proved rigorously that it constitutes a safe way of controlling the transfer of activity to smaller scales. In [8] we provide such a proof in the case of *probabilistic* mesh refinement, while in [14] we provide a similar proof for *physical* mesh refinement.

What is needed to define a mesh refinement algorithm is a criterion to determine whether it is time to perform mesh refinement. In [10], this criterion was based on monitoring the rate of change of the L_2 norm of the solution at the resolved scales as computed by the reduced model (note that the L_2 norm corresponds to the mass or energy in many physical contexts). When this rate of change exceeds a prescribed tolerance the algorithm performs mesh refinement. In [8, 14] we show rigorously that this is a good refinement criterion. In particular, we show that the expression for the rate of change of the L_2 norm for the resolved scales has the same functional form as the expression for the rate of change of the L_2 error of the reduced model. Thus, by keeping, through mesh refinement, the rate of change of the L_2 norm for the resolved scales under a prescribed tolerance, we can keep the error of the calculation under control.

Although the construction of mesh refinement schemes that utilize reduced models was shown to be theoretically sound, it hinges on the existence of an accurate reduced model. For real world problems this is not always the case. Even though an accurate reduced model can be constructed in principle (e.g. through the MZ formalism), writing down the reduced model and computing all the necessary parameters may be very expensive. Motivated by this, we have found a way to implement the main idea of mesh refinement presented in [8, 14] *without* the need to write down the reduced model explicitly. In particular, we have found a way to monitor *indirectly* the rate of transfer of activity to the unresolved scales. This has allowed us to keep the good features of our mesh refinement scheme while making it much more generally applicable. We have applied the modified version to problems of mesh refinement in *physical* and *probability* space with excellent results. The fact that we are able to unify the physical and probability space mesh refinement in a common framework (which is also non-intrusive), is very helpful because it allows the simultaneous approach to the problem of uncertainty quantification and interface tracking. This unifies two of the subtasks that PI Stinis is involved with.

2.2 Scaling laws and renormalization of MZ models

During Year 1 of CM4, I investigated the application of ideas from renormalization and effective field theory to the problem of model reduction [13]. The rationale behind such an approach is similar to the one in high-energy and condensed matter physics where these concepts were initially developed. We are faced with systems whose size is far larger than anything we will be able to simulate in the foreseeable future. This highlights the need to improve on current model reduction formalisms. In other words, current formalisms assume that one has access to the simulation of the system one tries to reduce. If that is not possible, then there is information missing which is needed in the construction of the model. In physics such information is provided by laboratory experiments which allow the determination of the unknown parameters of the model [6]. In my work I opted for a situation which is slightly different. While the true system of interest is too expensive for a brute force simulation, I begin with the largest affordable system. Of course, the predictions of this system will become unreliable after some time. But, until this happens, the evolution of this system can provide us with meaningful information for the dynamics. This information can be used to estimate the parameters of a reduced model for a subsystem. The situation I have opted for is actually very informative. In particular, I have realized that the magnitude of the (renormalized) coefficients for the reduced model follow scaling laws. These scaling laws are delicate to determine but they point towards a new understanding of the coarse-graining process.

During Year 2, I have looked more closely at the origin of these scaling laws. My first attempt was to apply the technique of perturbative renormalization [5] to see if the scaling laws can be determined order by order. The idea behind perturbative renormalization is that although one needs extra information in order to make a predictive model, this information can be encoded in the coefficients in a succinct form. In particular, the coefficients can all be expressed as integer powers of a small quantity which appears naturally in the problem. Moreover, the determination of the coefficients can be obtained order by order in the expansion in terms of the small quantity. In the problems I examined there was a naturally occurring small quantity which is related to the smoothness of the initial condition. It turns out that, at least for the problems that I examined, the determination of the renormalized coefficients *cannot* be obtained order by order. Also, the exponents of the scaling laws are not integers. Instead, the exponents need to be determined all at once by using the dynamics of the system. This is reminiscent of problems exhibiting *self-similarity of the second kind* [1]. This situation refers to problems exhibiting self-similar behavior (expressed through scaling laws) which however cannot be determined by simple dimensional analysis arguments. The subject will be investigated further during Year 3.

2.3 "Proper" coarse-grained variables

The work reported in Section 2.2 has implications for another subtask that PI Stinis is involved with, namely that of determining "proper" variables for which to perform reduction. The adjective "proper" refers to the choice of variables that can facilitate the construction of reduced models and also make their implementation more efficient (e.g. by having shorter memory). As mentioned above, the small parameter that plays a crucial role in the renormalization of the MZ models is related to the smoothness of the initial condition. In particular, to the number of active modes (e.g. Fourier modes) compared to the number of variables in the reduced model. The smoother the initial condition, the fewer the significant terms in the renormalized expansion. This insight can be exploited in conjunction with methods for sparse representation or basis adaptation [2, 16]. Such methods allow to identify a good set of variables for which the initial condition would have a sparse representation and exhibit smoothness. Then, we can rotate the initial vector of variables and apply the ideas from Section 2.2. So, we approach the problem of "proper" coarse-grained variables as one of deciding the variables that will result in fewer significant terms in the renormalized expansion. This is a first step in building a renormalization theory for general complex systems outside of the realm of high-energy and condensed matter physics.

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3 Publications related to CM4 - Year 1

1. P. Stinis, Renormalized reduced models for singular PDEs, Comm. App. Math. Comp. Sci. Vol. 8 (2013), No. 1, pp. 39-66.
2. P. Stinis, Mori-Zwanzig reduced models for uncertainty quantification I: Parametric uncertainty, (2012), arXiv:1211.4285v1.
3. P. Stinis, Mori-Zwanzig reduced models for uncertainty quantification II: Initial condition uncertainty (2012), arXiv:1212.6360v1.

4 Presentations related to CM4 - Year 1

1. "Scaling and renormalization in model reduction", University of Chicago, Scientific and Statistical Computing Seminar, March 14 2013
2. "Scaling and renormalization in model reduction", Brown University, PDE and Scientific Computing Seminar, March 29 2013

3. ”Scaling and renormalization in model reduction”, PNNL, Scientific Computing Seminar, May 24 2013

5 Publications related to CM4 - Year 2

1. J. Li, P. Stinis, Mesh refinement for uncertainty quantification through model reduction, Journal of Computational Physics, 280 (2015), pp. 164-183.

2. P.Stinis, Renormalized Mori-Zwanzig reduced models for systems without scale separation, Proceedings of the Royal Society A Vol. 471 (2015) No. 2176, DOI: 10.1098/rspa.2014.0446.

3. P. Stinis, Model reduction and mesh refinement (2014), arXiv:1402.6402v1.

6 Presentations related to CM4 - Year 2

1. ”Scaling and renormalization in model reduction”, University of California Berkeley, Applied Mathematics Seminar, November 2013

2. ”Scale dependence and renormalization in model reduction”, Stanford University, Applied Mathematics Seminar, April 2014

3. ”Scale dependence and renormalization in model reduction”, SIAM Annual Meeting, July 2014